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Discontinuous Galerkin methods for the second-order Boltzmann-based hydrodynamic models

By

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Last words are a poem by famous Persian poet, Ferdowsi¹,

نحجم زنده کردم بدین پارسی عجم زنده کردم بدین پارسی

که تخم سخن را پراکنده ام حکیم ابوالقاسم فردوسی

بسی رنج بردم در این سال سی نمیرم از این پس که من زنده ام

¹ The epic of kings, Ferdowsi, written 1010 A.C.E.

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ABSTRACT

Discontinuous Galerkin methods for the second-order Boltzmannbased hydrodynamic models

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Moments of the Boltzmann kinetic equation can be obtained by multiplying the classical Boltzmann equation with the microscopic quantity and integrating the product over all velocity space. In the thermal equilibrium state, the first five moments of the Boltzmann equation reduce to the closed nonlinear hyperbolic system, called as compressible Euler system in which collisional terms and all of the high-order terms vanish due to Maxwell distribution function and collisional invariants.

In this study, discontinuous Galerkin (DG) methods were first employed for solving the Euler system in order to obtain the solution of the one- and twodimensional Riemann problems. The basic structure of this hyperbolic system, such as contact discontinuity, shock wave, and rarefaction wave, was studied numerically. Various limiters and numerical flux functions were examined to capture the discontinuities sharply in steady and unsteady conditions. Although modern DG method has been successfully applied for solving the Euler equation, the validity of the Euler equation is restricted to equilibrium state and it is not valid for non-equilibrium flows.

In order to investigate non-equilibrium gas flows, a new set of DG methods based on mixed DG-framework are developed for solving the classical Navier-Stokes-Fourier (NSF) and second-order Boltzmann-based equations. The final judgment on the accuracy of the computational models is obtained through a rigorous study of verification and validation (V&V). The NSF and second-order

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Boltzmann-based models are compared with solution of DSMC and experiments by considering various problems. DG methods are comprehensively verified and validated for steady-state and unsteady transient flow problems as well as smooth and stiff solutions of the conservation laws. The analytical exact solutions of NSF in the shock wave structure are considered as a verification study on conservative, primitive, and non-conservative variables. The error norm analysis is extensively used to examine the performance of various limiters, including a new differentiable slope limiter, and numerical fluxes in DG framework.

The accuracy of finite volume method and DG method in capturing flow structure is also examined. A self-contained summary of numerical implementation of various limiters, numerical flux functions, and boundary conditions is provided for pedagogical purpose. Further, influence of curved boundaries on the accuracy of the Euler and NSF solutions is investigated at various Reynolds numbers. It is shown that, as the Reynolds number decreases, the numerical artifacts produced by linear mapping of curved boundaries decreases. In addition, the three-dimensional Maxwell slip boundary conditions are provided for arbitrary geometries. Efficient numerical methods for solving non-linear implicit algebraic equations arising from the second-order Boltzmann-based constitutive relations are described, and the solutions of the constitutive relations are analyzed in detail.

The computational cost of the first-order Boltzmann-based model (NSF) and nonlinear coupled constitutive relation (NCCR) solvers is investigated in the serial and parallel frameworks. It was shown that the computational cost of the NCCR solver behaves nonlinearly with respect to the number of elements, due to the dependence of the number of iterations of the NCCR solver on the flow structure and the degree of thermal non-equilibrium. Finally, a super-parallel performance of a mixed explicit discontinuous Galerkin method is reported for the second-order Boltzmann-based nonlinear coupled constitutive models of rarefied and microscale gases.

초록 (Abstract in Korean)

2차 볼츠만 기반 Hydrodynamic 모델에 관한 Discontinuous Galerkin 기법

아볼파즈 카르차니 경상대학교 공과대학 기계항공공학과 항공우주 전공 지도교수 : 명 노 신

볼츠만 방정식의 모우멘트는 볼츠만 방정식에 미시변수를 곱한 다음 모든 속도 공간에 대 해 적분하여 유도된다. 유동이 열평형 상태의 경우, 볼츠만 방정식의 처음 다섯 개의 운동량은 압축성 오일러 시스템으로 불리는 닫힌 비선형 쌍곡선 시스템을 이루게 된다. 오일러 시스템 에서는 물리학적 보존법칙 및 평형상태에 의해서 충돌 적분항이 없어진다.

본 연구에서는 먼저 오일러 시스템의 1차원, 2차원 Riemann 문제의 해를 구하기 위해 DG 기법을 연구하였다. 접촉 불연속, 충격파, 팽창파 등의 쌍곡선 시스템의 기본 구조를 수치적으 로 분석하였다. 정상 및 비정상 상태에서 불연속면을 정확하게 계산하기 위해 다양한 Limiter 와 Numerical Flux 기능을 비교하였다. 최신 DG 기법이 오일러 방정식을 해석하는 데는 성공 했지만, 오일러 방정식의 타당성은 평형 상태로 제한되어 있으며 비평성 유동에는 유효하지 않 다.

비평형 기체 유동을 해석하기 위해 고전 Navier-Stokes-Fourier (NSF) 및 2차 볼츠만 기 반 방정식에 적용할 수 있는 Mixed DG 구조를 기반으로 하는 일련의 신규 DG 기법을 개발하 였다. 전산 모델의 정확성에 대한 최종적인 판단은 엄격한 Verification 및 Validation (V&V) 과 정을 통하여 얻을 수 있다. 1차 및 2차 볼츠만 기반 모델을 다양한 문제에 적용한 다음, 그 결 과를 DSMC 예측결과 및 실험 데이터와 비교하였다. 개발된 DG 기법은 정상 상태 및 비정상 Transient 유동 문제와 함께 보존법칙의 Smooth 및 Stiff 해를 고려하여 심층적으로 검증하였 다. 충격파 내부구조에 대한 NSF의 해석해를 이용하여 보존, 원시, 비보존 변수에 대한 검증 연구를 수행하였다. 그리고 신규 미분가능 기울기 Limiter를 포함한 각종 Limiter와 Numerical Flux의 성능을 Error Norm 분석 기법을 사용하여 심층적으로 분석하였다.

유한체적과 DG 기법의 정확성을 분석한 다음, 다양한 Limiter, Numerical Flux 함수, 경계 조건을 실제 적용하는 방법에 대해 정리하였다. 다양한 레이놀즈 수에서의 오일러, NSF 방정 식의 해에 대한 곡선 경계의 영향을 분석하였다. 레이놀스 수가 감소함에 따라 곡선 경계의 선 형 Mapping에 의해 생성되는 수치적인 오류가 감소하는 것으로 나타났다. 또한 임의의 기하 학적 형상에도 적용할 수 있는 3차원 맥스웰 Slip 경계 조건을 제시하였다. 2차 볼츠만 기반 구 성 관계식에서 유도된 비선형 음함수 대수 방정식을 효율적으로 해석하는 수치기법을 묘사한 다음 해당 해들을 물리적으로 상세히 분석하였다.

1차 볼츠만 모델 (NSF) 과 비선형 결합 구성 관계식 (NCCR) Solver의 계산 비용을 직렬 및 병렬 코드 경우에 대해 분석하였다. NCCR Solver의 계산 비용은 NCCR 계산의 반복 횟수 가 유동 구조 및 열적 비평형의 정도에 의존하기 때문에 계산의 수에 비선형 거동하는 것으로 나타난다. 마지막으로 희박 및 마이크로 기체에 관한 2차 볼츠만 기반 비선형 결합 구성 모델 에 대해 개발된 Mixed Explicit DG 기법의 초 병렬 성능을 묘사하였다.

CHAPTER 1. Introduction

Francis Bacon (1561-1628):

"I found that I was fitted for nothing so well as the study of Truth; as having a nimble mind and versatile enough to catch the resemblance of things (which is the chief point), and at the same time steady enough to fix and distinguish their subtle differences..."

1.1 Objectives

As flow deviates from equilibrium state, classical continuum description of fluid may not provide an accurate information about the flow. Hence, application of kinetic theory, Boltzmann kinetic equation, or methods based on simplified kinetic theory are necessary to describe the flow with an acceptable level of accuracy. This work was motivated to elaborate the gas flows at equilibrium and not-far-from-equilibrium states using classical and non-classical constitutive relations derived from the Boltzmann equation, so-called Boltzmann-based models. The Boltzmann-based models considered in the present study are derived from Eu's hydrodynamics equations [1-3]. The resulting highly non-linear partial differential equations are solved using advanced mathematical and computational methods.

Along with the aforementioned objective, an attempt is made to describe the computational schemes used for solving Boltzmann-based models in deep level. Accordingly, detailed information in the development of a modal DG method for one-, two-, and three- dimensional systems, and application of various numerical flux functions, spurious Gibbs controllers, and boundary conditions are provided. As the DG method is still under development and most of the available books on this topic focus on the mathematical aspect, I aim to provide a self-contained material with comprehensive explanation on both numerical and mathematical aspect of the DG methods to help the researchers in the development of advanced high-order numerical schemes.

1.2 Outlines

The remaining part of the thesis is organized in eight chapters. Chapter 2 addresses the basics of the kinetic theory. In Section 2.1, the definition of the equilibrium and non-equilibrium processes is explained, and gas flows are categorized based on the level of non-equilibrium. The physical constraints and limitations of continuum theory and kinetic theory are discussed in Section 2.2. Approximation of mean free path, the definition of microscopic and macroscopic properties based on phase density distribution, and description of the Boltzmann kinetic equation are discussed in following sections of Chapter 2.

Chapter 3 is split into three parts; derivation of Boltzmann-based models, the numerical methods for solving algebraic constitutive relations, and explanation of the physics of the Boltzmann-based constitutive models. In Chapter 4, the development of a modal discontinuous Galerkin method for one-, and multi-dimensional system is presented. The presentation starts with introducing basics of numerical analysis and moves to reviewing first-order, and high-order numerical schemes. Afterwards, categories of spectral methods and difference of continuous and discontinuous Galerkin methods are reviewed. Later, the efficient discretization of a problem in space and time based on discontinuous Galerkin formulation is discussed in detail.

In Chapter 5, special attention is paid to verification of DG methods using stiff and smooth solution of Euler, and Navier-stokes-Fourier (NSF) equations. A summary of the trouble-cell-indicators, spurious limiter functions, and positivity preserving schemes are provided. A detail explanation on the discretization of the viscous and inviscid flux functions and a performance analysis on the order of accuracy of DG method using several viscous and inviscid flux functions is provided. In the end of Chapter 5, the importance of curvature boundaries for Euler and NSF equations is discussed, and general information on conventional boundary conditions for studying rarefied gas flows is provided.

Chapter 6 deals with verification and validation of DG methods for one-, and multidimensional problems. Various benchmark problems were solved and then their numerical results are compared with experiments, DSMC, and other numerical solutions. In Chapter 7, the new modal DG solver is employed for solving rarefied and microscale gas flow problems and results of Boltzmann-based models are compared with DSMC method. Chapter 8 provides detailed information of parallelization of DG methods using SPMD method and the computational cost of Boltzmann-based models using serial and parallel solvers. Finally, in Chapter 9, outlook on further development in the line of the present study is discussed.

CHAPTER 2. Kinetic theory of gases

Albert Einstein (1879-1955): "If the facts don't fit the theory, change the facts."

2.1 Classification of flow regimes

2.1.1 Traditional flow classification

Knudsen number is a dimensionless parameter, defined as the ratio of the molecular mean free path, λ , and a characteristic length, traditionally used to classify gas flow regimes. The value of Knudsen number was commonly served as the primary parameter to determine the degree of rarefaction and the degree of validity of Boltzmann-based models.



Figure 2-1 Traditional classification of the gas flow based on Knudsen number

As it is shown in Figure 2-1, the flow is commonly labeled as continuum (hydrodynamics), slip, transition, and free molecular regimes [1, 4]. Although this classification has been used widely in the high-speed rarefied community, it may not be suitable for categorizing flow regimes in general form. According to Buckingham's π -theorem [5] and Bridgman's principle [6], there are at least two parameters required for describing a simple monatomic gas flow in continuum fluid mechanics. Due to this fact in fluid mechanics, flow is usually classified based on the Reynolds number and velocity of the flow, as it is shown in Figure 2-2 [7, 8]. In order to elaborate the gas flows in all flow regimes from equilibrium to highly non-equilibrium states, it may be necessary to re-categorize the flow regimes based on the level of deviation from the equilibrium state [9, 10].



Figure 2-2 Approximate spectrum of Reynolds number versus velocity of objects or fluids for various systems²

To classify gas flows based the distance from the equilibrium state, it is important to know the physical meaning of the equilibrium, local equilibrium, and far from equilibrium state. In this section, the difference between the equilibrium and nonequilibrium conditions are provided in detail to proceed the section and introducing a classification of the flow regimes based on the dimensionless variables.

2.1.2 Equilibrium condition

A macroscopic system preserves some 'memory' of their recent history. Nonetheless, the memory eventually fades out and the system likes to descend to very simple state which is independent of its specific history. In some systems, the evaluation toward the simple state takes very short time, while for other systems it can be very slow. Although the evaluation time may be different for different systems, in all systems, there is an inclination to progress toward states in which the macroscopic properties are determined by intrinsic parameters and not by formerly applied external forces [11]. These simple terminal states are called equilibrium states, and thermodynamics aids to describe a system from this static 'equilibrium' states to which the systems eventually evolve.

² Adapted based on Lissaman 1983, and Glazner 2014.

A system is indeed in an equilibrium state when its potential is located in the minimum level and no change in the intensive parameters be observed, and when it is isolated from its surroundings. Note that, changes in a system may become time independent after a transient period and this condition is called steady state; however, it does not guarantee that the system is in the thermodynamics equilibrium state.

A system is considered to be in a thermodynamic equilibrium state when it is in thermal-, mechanical-, electrical-, and chemical equilibrium. The number of parameters required to characterize a thermodynamic equilibrium state may increase based on the level of the complexity of the interested closed system. The mechanical equilibrium means that all forces in the interior of a closed system or between a system and its surroundings are equally distributed and balanced. The chemical equilibrium states that there is no spontaneous change in chemical components of a system. The thermal equilibrium means that all modes of the energy including translational, rotational, vibrational, and electrical modes are equal and all energy in a system is equally distributed between all the modes [11-15].

In general, there are two kinds of thermodynamic equilibrium, namely global and local thermodynamic equilibrium in which energy, force, and a number of moles exchanges between systems are controlled by intensive parameters. In global (absolute) thermodynamic equilibrium, all interested intensive parameters are homogeneous in every part of a system and all the macroscopic intensive quantities have ceased to change during time evolution. On the other hand, in local thermodynamic equilibrium, the intensive quantities are varying locally and slowly such that the process occurs in times long compared to relaxation time $t_{evalution} \gg \tau$ for any point in space and time. Therefore, the system being allowed to come into a new equilibrium state at each step and one can assume a thermodynamic equilibrium in some neighborhood about that point. The whole system does not require to be stationary when it is placed in local thermodynamic equilibrium. Instead of having a constant temperature throughout the system, each location of the whole system may have a specific temperature. Nonetheless, the diversity of temperature should be such that temperature at each small locality of system changes slowly enough to essentially sustain its local Maxwell-Boltzmann distribution of molecular velocities.

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2.1.3 Non-equilibrium condition

Non-equilibrium process is an inhomogeneous and time-dependent process that occurs: in open systems, in the irreversible transformations, and in the transition between equilibrium states. A proper description of these processes necessitates values of the properties at all locations in the system. The detailed description of nonequilibrium processes is more complex than the description of quasi-static processes. A non-equilibrium process is an irreversible process that connects two or more homogeneous equilibrium states. When the intensive parameters are varying sufficiently fast and the process occurs in times short compared to relaxation time $t_{evalution} \ll \tau$ the system is not in an equilibrium state. The state of the system is placed in between of two equilibrium states while it is deviating from them considerably. When a system that is in a non-equilibrium state, discrepancies and inconsistencies come into the formalism and predicted results are at difference with experimental observations [11, 16]. This failure of the classical theories is utilized by the experimentalist as an inductive criterion for the detection of non-equilibrium states. In this situation, a more incisive quantum statistical theory and microscopic analysis of process usually deliver valid reasons for the failure of the system to attain equilibrium [11].

2.1.4 Near-equilibrium condition

A class of non-equilibrium processes deals with systems that are only very slightly deviated from equilibrium states are called the near-equilibrium state processes. In a system at near-equilibrium state, the intensive parameters change slowly, but not sufficiently to molecular velocity distributions be described with Maxwell-Boltzmann distribution. A time required for evaluation of a near-equilibrium process is in the same order of magnitude of the relaxation time $t_{evalution} \approx \tau$. At near-equilibrium state, the response of the system can be explained based on the classical linear theory by assuming that deviation from equilibrium state is negligible or at least it is very small [17].

2.1.5 Flow classification based on degree of non-equilibrium

When the variation of the intensive parameters in a system is considerably large, the assumptions based on the definition of the intensive parameters in a system breaks down, and the system will not be in global or local equilibrium state.

Introducing a general criterion to indicate the level of deviation from equilibrium is very challenging, and it is an open business in kinetic theory[10]. In the present section, it is tried to summarize the breakdown parameters very briefly by considering different prospective of the breakdown parameters based on thermodynamics, continuum theory, and kinetic theory.

According to the statistical thermodynamics, the process deviates from equilibrium state $\tau/t_{evaluation} \gg 1$, when the evaluation time $t_{evaluation}$ is not sufficiently larger than the relaxation time t. The first way comes to mind for measuring the degree of nonequilibrium is to measure the ratio of variation of these two time scales. From kinetic theory, it is known that the relaxation time is equivalent to mean collision time $\tau = \lambda/c_{thermal}$. The mean collision time can be defined as a function of free stream mean free path and mean thermal speed of the particles $c_{thermal} = \sqrt{8k_BT/\pi m}$. However, in contrast to relaxation time, characterizing the evaluation time is not easy. The relaxation time is in the order of the time required for the rarefaction to propagate across a system. whereas, the evaluation time required for reaching to an equilibrium state depends on several parameters including; the initial deviation from the equilibrium state, the geometry, and material [16]. For instance, change of heat or temperature at boundary of a system has diffusive nature and it diffuses slowly in the system, therefore, evaluation time is so slow for this phenomena. On the other hand, the propagation of the pressure change occurred at boundary of a system is very fast since pressure waves transfer information into the system with speed of sound. In addition, it is not possible to exactly determine the evaluation time for a non-equilibrium process in which intensive properties change so fast and there is no time for the system to reach equilibrium state during the process. Now the question is how to measure the level of non-equilibrium in an aero-thermodynamic process?

One way to estimate the level of departure from equilibrium is to approximate the value of the evaluation time, and relaxation time based on either microscopic or macroscopic properties. The simplest (and the most general) criterion for measuring the

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level of non-equilibrium is to calculate Knudsen number. The *Knudsen number is the ratio of the relaxation time to the evaluation time* in which the evaluation time is approximated by assuming that the intensive parameters inside a system with characteristics length of *L* changes with the rate of the average thermal particle speed. Smaller Knudsen number means slower thermodynamic process, and larger Knudsen number shows larger deviation from equilibrium state as the evaluation time is much smaller than the relaxation time.

$$Kn = \frac{\lambda}{L} \approx \frac{\tau}{t_{evaluation}},$$
 2-1

where the relaxation time is equal to $\tau = 1/n\overline{\sigma_{total}c_r} = \lambda/c$, the mean distance traveled by a particle between collisions is $\lambda = c/n\overline{\sigma_{total}c_r}$, and the evaluation time is $t_{evaluation} = L/c$. It is obvious that this approximation may not be quite appropriate and sufficient to measure the level of non-equilibrium for the process with time evaluation with rate solver than thermal velocity.

There are two commonly used parameters in rarefied gas flow, namely Knudsen number, and speed ratio $S = \mathbf{u}/c$. These parameters can be related to fluid dynamic dimensionless parameters due to the relationship between the molecular transport properties and mean collision time. For instance, the first coefficient of viscosity, defined as $\mu = \tau \rho c^2/2 \approx p\tau$, is a function of the mean collision time of the system which shows high potential for detecting the degree of non-equilibrium [10]. There are numerous ways to approximate the value of these two time scales; however, a few of them which has been often used in the literatures are studied in here.

Bird [4, 18] introduces a breakdown parameter based on new length scale definition. Therefore, the evaluation time is approximated based on the gradients of the intensive parameters rather than the magnitude of those intensive parameters. This breakdown parameter $Kn_B = \lambda / \left(\frac{p}{m_B} \right)$ considers the flow in local equilibrium condition when $Kn_B \leq 0.1$.

By combining the Bird's breakdown parameter with Damkohler number of chemically reaction flows, a rarefaction parameter defined as the average number of collisions per molecule during the time flow passes the body, can be represented as

$$\frac{\tau}{t_{evaluation}} \approx \frac{\tau}{t_{flow}} = \frac{M^2}{\text{Re}} \cong Kn.M$$
2-2

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Tsein's parameter, suggested in 1946 as a non-equilibrium criterion [9], was established by replacing the characteristics length scale *L* of the system with the thickness of boundary layer of the body $\delta_L \approx \alpha L/\sqrt{\text{Re}_L}$. In this breakdown parameter, the evaluation time is approximated by $t_{evaluation} = \sqrt{25L/2u_{ref}}$. The Tsein's parameter is related to Mach number and Reynolds number by $M/\sqrt{\text{Re}}$. The Bigger value of Tsein's parameter indicates a higher degree of rarefaction and larger distance from an equilibrium state as it is shown in Figure 2-3. This parameter can predict the degree of non-equilibrium fairly for high-speed flow problems. However, the disadvantage of this parameter is revealed when Reynolds number is very low and $M/\sqrt{\text{Re}} \ge 1$. It has been shown that this parameter reduces into classical Knudsen parameter (Eq. 2-1) for very low Reynolds number values[10].



Figure 2-3 A classification of the flow regime based on Tsein parameter ³

Alternatively, it is possible to show that the rarefaction parameter is *shear stress/pressure* and it is related to the square of the Tsein's parameter [10]. A

³ Adapted based on Tsein 1946, and Macrossan 2006.

dimensionless parameter called N_{δ} is defined to link hydrostatic pressure and viscous forces as

$$N_{\delta} = \frac{\gamma M^2}{\text{Re}}.$$
 2-3

Classification of the flow regimes based on this parameter is shown in Figure 2-4. It is very similar to the Cheng's parameter [19] whereas the correction factor in Cheng's parameter is not equal to specific heat ratio, and it is function of the collision cross section and molecular transport properties as

$$\xi = \frac{\mu_r T}{\mu T_r} \frac{M^2}{\text{Re}}.$$
 2-4

where the reference parameters are chosen based on the configuration of the system.



Figure 2-4 A classification of the flow regime based on N_{δ} parameter In the following chapters, the degree of rarefaction and non-equilibrium are measured based on (Eq. 2-3).

2.2 Physical constraints of kinetic theory

2.2.1 Level of flow description

A gas flow can be described at both macroscopic and microscopic levels depending on the detail of gas and the level of departure from equilibrium state. A macroscopic explanation of fluid considers flow as continuum material and tries to describe the behavior of that in terms of the spatial and temporal variation of the intensive parameters and macroscopic properties in a system. In this kind of description, the spatial coordinates and time are the only independent variables. The conventional mathematical model for describing the flow behavior is Euler and Navier-Stokes-Fourier equations. In contrast to macroscopic methods, the molecular approach studies the fluid at microscopic level. The flow is recognized by the particulate structure in phase space and the necessary information for analyzing gas flow are obtained from the position, velocity, and state of the internal modes of the molecules. Therefore, there are several independent variables on which the state of the system is defined. Liouville and Boltzmann equations are the models utilized for describing flows at microscopic level.



Figure 2-5 Levels of flow descriptions based on various theories

2.2.2 Assumptions in continuum mechanics

Figure 2-5 illustrates the level of description of physics of fluid based on the application of the mathematical models. In case that the number of molecules within the fluid element are sufficiently large, the thermodynamic process evolves so slowly, the flow can be considered as continuum material. So the classical continuum flow

theory can be served for describing the solution, although the continuum description of gas flows may breakdown when the inter-particle collisions are not sufficiently high [20]. In this condition, the gradient of the macroscopic flow properties becomes so big that their scale is of the same order of the distance traveled by the molecules between collisions (λ). Therefore, application of kinetic theory or quantum mechanics becomes essential for describing the flow behaviors.

2.2.3 Assumptions in kinetic theory

There are some physical constraints that should be satisfied by a system in order to describe it using classical physics rather employing complicated and advanced quantum mechanics theory.

2.2.3.1 Heisenberg constraint

The Heisenberg uncertainty principle, the first constraint for describing gas flows using kinetic theory, can be interpreted as

 $m\delta \mathbf{\bar{c}} \gg h$. 2-5 According to Heisenberg uncertainty principle [21], the product of the uncertainty in position $|\Delta \mathbf{r}|$ and momentum of the molecules $|\Delta m\mathbf{c}|$ is of the order of the Planck's constant $h = 6.62607004 \times 10^{-34} (m^2 kg/s)$. Hence, in order to describe the molecular position and momentum of fluid based on classical physics, the mean molecular spacing δ should be so much bigger than the uncertainties in position $|\Delta \mathbf{r}|$, and the mean molecular momentum of the system must be considerably smaller than the momentum of the molecules $|\Delta m\mathbf{c}|$ [22].

2.2.3.2 Molecular diameter constraint

Satisfying the Heisenberg uncertainty principle necessitates that mean molecular spacing be so much larger than the mean de-Broglie Wavelength of the molecules

$$\delta \gg d \gg \frac{h}{mc}.$$
 2-6

This constraint (Eq. 2-6) is implicitly related to the dilute gas condition, and it means that the effective molecular diameter must sufficiently be larger than de-Broglie wavelength in order to employ classical physics for describing gas molecules.

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2.2.3.3 Molecular velocity constraint

Molecular velocity similar to molecular diameter should be large enough to satisfy Heisenberg uncertainty principle (Eq. 2-5). It is possible to characterize the molecular speed constraint by,

$$\frac{\delta \mathrm{mc}'_{s}}{h} \gg 1$$
 2-7

From kinetic theory relation, it is known that the mean square of molecular speed C'_s in the equilibrium state is a function of the temperature and molecular mass, and can be defined as

$$\mathbf{c}'_s = \sqrt{\overline{c^2}} = \sqrt{\frac{3k_B T}{m}} \quad . \tag{2-8}$$

where $\overline{c'^2}$ is mean square molecular speed. Combining (Eq.2-7) with definition of the mean of the molecular speed (Eq. 2-8), and replacing the mean molecular spacing with inverse of cube root of the number density of gas flow $\delta = n^{-1/3}$, the molecular velocity constraint is defined as

$$\frac{\sqrt{3k_B mT}}{n^{1/3}h} \gg 1$$
2-9

The molecular velocity constraint holds for standard flow condition [22].

2.2.3.4 Dilute gas constraint

The number of molecules in one mole of a gas is always a constant value, called Avogadro's number which states that the volume occupied by a mole of the gas at standard temperature and pressure is equivalent for all gases. In classical physics, it is always assumed that a molecule is surrounded by a force field which rules the dynamics of the inter-molecular collisions. This field is assumed to be spherically and symmetric, in most of the cases, and the general amount of the force between two neutral molecules is assumed to be an inverse function of the distance between the nuclei r_{nuclei} and the cross section of the collision σ_{total} .

If a small portion of the space of a system (V) is occupied by the gas molecules, it is valid to assume that molecular spacing $\delta = n^{-1/3}$ is sufficiently large compared with the effective molecular diameter *d*. Therefore, only very small proportion of the space is occupied by the molecules and each molecule is practically outside of the range of influence the other molecules force field. As a result of that, most of the inter-particle

$$V^{1/3} \gg \delta \gg d \quad . \tag{2-10}$$

2.2.3.5 Molecular degree of freedom constraint

The final constraint for the validity of the classical physics and kinetic theory is that the number of available quantum states should be larger than the number of available molecules in the system. The standard number of available translational states to the molecules is of the order of unity. Therefore, classical physics is applicable to the translational motions which contributes three degrees of freedom to the gas. It also holds true for diatomic and polyatomic gases when rotational, vibrational and electrical quantum states are taken into account.

In summary, application of classical physics and kinetic theory holds if a system satisfy the Heisenberg constraints (Eq. 2-5), dilute gas constraint (Eq. 2-10), and it is in standard flow condition with a mean molecular diameter larger than the de-Broglie wavelength (Eq. 2-6). In the preceding chapters, it is implicitly assumed that the molecules are described by classical physics [22] and kinetic theory is applicable for studying gas behaviors. It is also assumed that a molecule does not change its identities before/after an inter-molecular collision.

2.3 Boltzmann kinetic equation

2.3.1 Estimation of mean free path

Consider a frame in phase space in which a class of molecules moves with a relative velocity of c_r while the other classes are assumed to be stationary. If look at a molecule in this class over a time interval smaller than the relaxation time of the system Δt , they may collide to any molecule which its nuclei is located inside a cylinder with volume of $c_r \Delta t \sigma_{total}$. Therefore, the chance of a successful collision between target molecule with a molecule of the same class is given by $\Delta n \sigma_{total} c_r \Delta t$. In dilute gas flows where only small portion of the molecular trajectory is affected by a collision, it is valid to remove time step restriction and re-write the probability of a collision as $\Delta n \sigma_{total} c_r$, and the mean collision time can be estimated by summing all class of molecules and their relative velocities as

$$\tau = \frac{1}{n \sum \frac{\Delta n \sigma_{total} C_r}{n}} \cdot 2-11$$

As number density ration inside the summation denotes the fraction of molecules with total cross section of σ_{total} and relative velocity of c_r , total number of binary collisions per unit of time and volume is $N_{collision} = n\tau/2 = n^2 \overline{\sigma_{total} c_r}/2$, and the mean collision time (relaxation time) is defined as

$$\tau = \frac{1}{n\overline{\sigma_{total}c_r}} \quad .$$

Since the mean distance traveled by a molecule between collisions is function of mean collision time of a system, it is possible to define it in general framework as

$$\lambda = c\tau = \frac{c}{n\overline{\sigma_{total}c_r}} \quad .$$
 2-13

where the mean magnitude of the relative velocity of the colliding molecules molecular is related to mean thermal velocity $_c$. Considering the relation between thermal velocity and mean magnitude of the relative velocity (Eq. 2-32), and assuming the total cross sections for the molecules is constant and equal to $\sigma_{total} = \pi d^2$, the mean free path relation for hard-sphere gas is defined as

$$\lambda^{HS} = \frac{1}{\sqrt{2}n\pi d^2} = \frac{16}{5} \frac{\mu}{\rho} \sqrt{\frac{m}{2\pi k_B T}} = \frac{\mu}{\rho \sqrt{RT}} \sqrt{\frac{\pi}{2}} . \qquad 2-14$$

Note that, the realistic mean free path value may not be equal to (Eq. 2-14) if the temperature variance is very high in a system or diameter of a molecule is changing due to a special condition in the system. For this conditions, it is better to estimate the value of total cross section using more advanced inter-molecular model. For instance, the mean free path value for variable hard-sphere (VHS) model is equal to

$$\lambda^{\text{VHS}} = \frac{1}{\sqrt{2}n\pi d^2 \left(\frac{T}{T_{ref}}\right)^{\omega - \frac{1}{2}}} .$$
 2-15

where the power index of temperature ratio $\omega = (\eta + 3)/(2\eta - 2)$ is a function of the power index of inverse power law model η . In this dissertation, for simplicity and clarity, the hard-sphere definition of the mean free path is used for all cases.

2.3.2 Microscopic properties

2.3.2.1 Basic molecular parameters

A monatomic molecule can be described based on three basic molecular parameters; m mass of molecules, d effective diameter of molecular, and molecular velocity v where can be written as a summation of stream velocity \mathbf{u} and \mathbf{c} peculiar velocity. A Molecule has several quantum energy states ζ which can be described based on the relation between the internal degrees of freedoms of the molecule. The linear Momentum (mv) is determined by the molecular parameters while the energy of a molecule ($mv^2/2$) can be split into internal ($m(c^2+2uc)/2$), kinetic ($mu^2/2$) and potential energies.

Total energy of system can be described by

$$E_{total} = E_{Kinetic} + E_{potential} + E_{internal}, \qquad 2-16$$

and the specific energy defined as the energy density per unit mass is given by

$$\varepsilon_{total} = \varepsilon_{Kinetic} + \varepsilon_{potential} + \varepsilon_{internal} \,. \tag{2-17}$$

Specific energy and total energy are related through below relation

$$E_{total} = \int_{V} \rho \varepsilon_{total} dV \,. \tag{2-18}$$

The potential energy is the energy generated due to external forces acting on a unit mass; it is realistic to assume that potential energies are conservative and they are negligible since the external forces were usually neglected. On the other hand, the internal energy is generated due to the inter-molecular interaction of the substance, and it can be split into the lower level of energy states; translational, rotational, vibrational, electrical energy states. The internal energy modes are defined as a summation of various internal states;

$$\zeta_{internal} = \zeta_{tr} + \zeta_{inter-atomic} \approx \zeta_{tr} + \zeta_{rot} + \zeta_{vib} + \zeta_{electerical} , \qquad 2-19$$

The translational states of internal energy are given by

$$E_{tr} = \frac{m}{2}c^{2} = \frac{\zeta_{tr}}{2}\rho RT_{tr}$$
 2-20

where translation degree of freedom of any molecule is equal to $\zeta_{tr} = 3$. The rest of the internal state of internal energy can be written as

$$E_{inter-atomic} = \frac{m}{2} \zeta_{inter-atomic} \varepsilon_{inter-atomic} = \frac{\zeta_{inter-atomic}}{2} RT_{inter-atomic} , \qquad 2-21$$

where the value of $\zeta_{inter-atomic}$ depends on the temperature of the gas compared to the characteristics temperatures Θ required for exciting the inter-atomic states of quantum

16

energy levels. For instance, $E_{inter-atomic}$ is equal to the rotational internal energy state when the gas temperature is larger than the characteristics temperature of rotation Θ_{m} and there is no other additional inter-atomic energy state. Rotational energy is usually excited for most of the diatomic gases in room temperature as the characteristics temperature for excitement of rotational energy is of the order of 10 Kelvin.

Note that the rotational degree of freedom leads to the generation of the angular momentum ($I\omega$) and angular energy of molecules ($I\omega^2/2$); however, they can be neglected for monatomic molecules, and for diatomic molecules about the internuclear axis. It is due to fact that monatomic molecules have only one atom and most of the diatomic gases are symmetrical respect to the internuclear axis, therefore, the moment of inertia *I* about the inter-nuclear axis is so small. A symmetric diatomic molecule owns two degrees of freedom associated with the inter-atomic axis normal to the internuclear axis. While the rotational degree of freedom for anti-symmetric diatomic molecules, triatomic and polyatomic molecules is varying between two and three.

2.3.2.2 Gas properties

The specific heat ratio of a gas molecule is related to the number of the excited internal degrees of freedoms, and it must be considered as variable in case that temperature is in order of $\Theta_{_{vib}}$. The specific heat ratio, mass of unit molecule, and ordinary gas constant can be defined as

$$m = M / N_{A}, \qquad 2-22$$

$$\gamma = (\zeta_{atomic} + 5) / (\zeta_{atomic} + 3), \qquad 2-23$$

$$R = k_{\rm p} / m, \qquad 2-24$$

and Prandtl number can be approximated using Eucken's formulation as

$$\Pr = \frac{4\gamma}{9\gamma - 5}.$$
 2-25

Here N_A denotes Avogadro's number and M represents the molecular weight of the gas.

The transport properties of a gas can be defined based the model used for describing inter-molecular potential forces. In case of power-law (Lenard-Jones 12-0) model which is a short range repulsive inter-molecular model, the first coefficient of viscosity and can be defined as

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{ref} \left(\frac{T}{T_{ref}} \right)^{\boldsymbol{\omega}}, \quad \boldsymbol{\kappa} = \boldsymbol{\kappa}_{ref} \left(\frac{T}{T_{ref}} \right)^{\boldsymbol{\omega}+1}.$$
where
$$\boldsymbol{\mu}_{ref} = \frac{15\sqrt{mk_B T_{ref}}}{2d_{ref}^2 \sqrt{\pi}(5-2\boldsymbol{\omega})(7-2\boldsymbol{\omega})}, \quad \boldsymbol{\kappa}_{ref} = \frac{\boldsymbol{\mu}_{ref} C_p}{Pr}.$$
2-26

2.3.3 Phase density distribution

In order to describe the microscopic properties in terms of macroscopic quantities, it is necessary to establish a formal relation between microscopic and macroscopic quantities. This can be achieved by studying the behavior of the gas molecules in statistical viewpoint.

The behavior of gases can be illustrated by listing the basic molecular parameters (i.e., position, velocity, and internal energy state) of all molecules at given time. However, the number of molecules in a system is usually very high so that it is not possible to trace each and every particle individually. Instead, it could be resort information into a statistical description in terms of either single particle probability distribution function $f(\mathbf{x}, \mathbf{v}, t)$ or velocity distribution function $\mathbf{f}(\mathbf{v})$. These two density functions are commonly being used in the kinetic theory textbooks; Bird [4] and Kennard [23] used velocity distribution functions. These two distribution functions related by

$$n\mathbf{f}(\mathbf{v}) = f(\mathbf{x}, \mathbf{v}, t) \,. \tag{2-27}$$

The velocity distribution function is normalized probability distribution function (PDF) since its integral in velocity space is unity $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\mathbf{v}) d\mathbf{v} = 1$. However, the single particle distribution function is not normalized PDF, and its integration in phase space is equal to a number of molecules in the physical space, $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} d\mathbf{x} = N$. Although these distribution functions have unique statistical characteristics, both of them characterize the behavior of the molecules in velocity and phases space, respectively. They cannot be negative or unbounded functions in whole space. They both tends to zero value when the molecular velocity approach to infinity.

In order to measure the macroscopic properties at each point in the system, it is necessary to find a relationship between the probability distribution functions and the average of the molecular quantities ψ at that point in physical space. This can happen by establishing of the moments of the distribution function. It is equivalent to the ensemble averaging over the molecular velocities of the molecules in an infinitesimal control volume in physical space $d\mathbf{x}$ at instantaneous time step dt which is served in particle-based method to obtain the macroscopic quantities.

The first moment of a probability distribution function provides the mean average of quantity $\overline{\psi}$ in macroscopic world;

$$\overline{\psi} = \langle \psi f \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = N \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi f(\mathbf{v}) d\mathbf{v} .$$
 2-28

2.3.3.1 Some useful expressions

Before starting derivation of more complicated kinetic theory relations, let's define several useful expressions which are commonly used in context of derivation of the conservation laws based on the fact that the molecular velocity $_{v}$ can be written as function of stream velocity u and thermal velocity c;

 $\mathbf{v} = \mathbf{u} + c$, 2-29 and mean thermal velocity and mean magnitude of the relative velocity of the colliding molecules can be related by

$$\bar{c} = \sqrt{\frac{8k_BT}{m}}, \quad 2-30$$

$$\overline{c_r} = \sqrt{\frac{16k_BT}{m}},$$
2-31

$$\overline{c_r} = \sqrt{2c} . \qquad 2-32$$

As the mean square thermal velocity is function of density and pressure properties, it can be also defined as

$$\overline{c^2} = \frac{3p}{\rho} = \frac{3k_BT}{m} , \qquad 2-33$$

where the root mean square of velocity is $c'_s = \sqrt{\overline{c^2}}$. The other important molecular velocities relations are given as follows;

$$\left\langle v_i f \right\rangle = u_i \tag{2-34}$$

$$\langle cf \rangle = \langle v_i f \rangle - u_i = u_i - u_i = 0$$
 2-35

$$v_i v_k = (u_i + c_i)(u_k + c_k) = u_i u_k + u_k c_i + u_i c_k + c_i c_k$$
2-36

$$c_i = v_i - u_i, \qquad 2-37$$

$$c^2 = \left(v_i - u_i\right)^2 \tag{2-38}$$
$$\left\langle c^{2}f\right\rangle = \overline{c^{2}} = \left\langle \left(v_{i} - u_{i}\right)^{2}f\right\rangle = \left\langle \left(v_{i}^{2} - 2v_{i}u_{i} + u_{i}^{2}\right)f\right\rangle = \left\langle v_{i}^{2}f\right\rangle - u_{i}^{2}$$
2-39

20

where $\overline{\alpha} \equiv \langle \alpha f \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \alpha f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = N \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \alpha f(\mathbf{v}) d\mathbf{v}$ denotes the statistical average of a

microscopic quantity α , in three-dimensional velocity space.

2.3.4 Macroscopic properties

For simplicity, clarity, and the sake of readers, several important and commonly used definitions in the content of this dissertation are defined in this section.

2.3.4.1 Density

The first macroscopic is density which expresses in terms of the number of molecules in unit volume n, and mass of the individual molecule m as

$$\rho = nm = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} mf(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m\mathbf{f}(\mathbf{v}) d\mathbf{v} .$$
 2-40

2.3.4.2 Temperature

Temperature is an intensive property of a system which can be defined only if a system is in global (or local) equilibrium condition. In the equilibrium state, the amount of energy distributed between excited modes of the internal energy states is identical, and all internal energy states contribute the same amount of energy to the system. The temperature defined for each state of energy is equal, hence, it is possible to define a unique temperature for the system. This temperature is called *thermodynamic temperature* [4] and it can be defined based on an equation of the states for an ideal gas (Eq.2-41) or (Eq.2-43) as

$$T = \frac{p}{\rho R} = \frac{2}{3} \frac{e_{tr}}{R},$$
 2-41

where p is hydrostatic pressure and ρ is density of gas; e_{tr} denotes translational energy density. Temperature can be written in terms of probability distribution function as

$$T = \frac{2}{3\rho R} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{mc^2}{2} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = \frac{2}{3R} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{c^2}{2} \mathbf{f}(\mathbf{v}) d\mathbf{v}., \qquad 2-42$$

In non-equilibrium condition, for diatomic and polyatomic gases, it is possible to measure temperature quantity for each state of the energy level as

$$T_{tr} = \frac{2}{\zeta_{tr}} \frac{m}{k_B} e_{tr} = \frac{m}{k_B} \frac{\overline{c^2}}{\zeta_{tr}} = T^{\text{thermodynamics}},$$
 2-43

$$T_{rot} = \frac{2}{\zeta_{rot}} \frac{m}{k_B} e_{rot},$$
 2-44

$$T_{vib} = \frac{2}{\zeta_{vib}} \frac{m}{k_B} e_{vib},$$
 2-45

$$T_{electerical} = \frac{2}{\zeta_{electerical}} \frac{m}{k_B} e_{electerical}.$$
 2-46

The overall temperature value in non-equilibrium condition [4] can be calculated based on weight averaging formulation as

$$T_{overall} = \frac{\zeta_{tr} T_{tr} + \zeta_{rot} T_{rot} + \zeta_{vib} T_{vib} + \zeta_{electerical} T_{electerical}}{\zeta_{tr} + \zeta_{rot} + \zeta_{vib} + \zeta_{electerical}}$$
2-47

2.3.4.3 Energy

The macroscopic internal energy, total energy, and enthalpy, for ideal gases, can also be defined in (local) thermodynamic equilibrium condition as

$$E_{internal} = \rho e_{internal} = C_V \rho T, \qquad 2-48$$

$$E_{total} = E_{kinetic} + E_{internal} + E_{potential} = \rho \frac{\|\mathbf{u}\|}{2} + \rho e_{internal},$$

$$2-49$$

$$E_{total} = C_V \rho T + \rho \frac{\|\mathbf{u}\|^2}{2} + \rho g H_{height}$$
$$H_{total} = E_{total} + \frac{p}{\rho} = C_V T + \frac{\|\mathbf{u}\|^2}{2} + \frac{p}{\rho}$$
2-50

The total energy can be determined using the first moment of the probability distribution function as

ρ

$$E_{total} = \left\langle \frac{m\mathbf{v}^2}{2} f \right\rangle,$$

$$E_{total} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{m\mathbf{v}^2}{2} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{m\mathbf{v}^2}{2} \mathbf{f}(\mathbf{v}) d\mathbf{v},$$
real energy states can also be presented based ensemble every and the

Internal energy states can also be presented based ensemble averaging and the first moment of single particle probability distribution function as

$$E_{internal} = \left\langle \left(\frac{m\mathbf{c}^2}{2} + E_{inter-atomic} \right) f \right\rangle, \qquad 2-52$$

$$E_{internal} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{m\mathbf{c}^2}{2} + E_{inter-atomic} \right) f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$
$$E_{internal} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{m\mathbf{c}^2}{2} + E_{inter-atomic} \right) \mathbf{f}(\mathbf{v}).$$

Here, $E_{inter-atomic}$ denotes the inter-atomic energy generated by internal quantum energy states. The inter-atomic energy and its energy density value are zero for monatomic gases, therefore, internal energy for monatomic gases can be defined as

$$E_{internal} = \left\langle \frac{m\mathbf{c}^2}{2} f \right\rangle,$$

$$E_{internal} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{m\mathbf{c}^2}{2} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{m\mathbf{c}^2}{2} \mathbf{f}(\mathbf{v}).$$
2-53

2.3.4.4 Stream velocity

Stream velocity (i.e., barycentric, or mass velocity), momentum density and the mean peculiar velocity are given by

$$\mathbf{u} = \langle \mathbf{v}f \rangle = \frac{1}{n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{v}f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{v}f(\mathbf{v}) d\mathbf{v}, \qquad 2-54$$

$$\rho \mathbf{u} = \langle m \mathbf{v} f \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \mathbf{v} \mathbf{f}(\mathbf{v}) d\mathbf{v}, \qquad 2-55$$

$$\langle mcf \rangle = \frac{1}{n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m(\mathbf{v} - \mathbf{u}) f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m(\mathbf{v} - \mathbf{u}) \mathbf{f}(\mathbf{v}) d\mathbf{v} = 0,$$
 2-56

2.3.4.5 Pressure tensor

Pressure tensor is a flux tensor which expresses the transport of momentum by the motion of thermal (peculiar) velocity. As the momentum of thermal velocity is a vector quantity, the pressure tensor is a second rank tensor given by

$$\mathbf{P} = \langle m\mathbf{c}\mathbf{c}f \rangle = \langle mc_i c_j f \rangle$$

$$\mathbf{P} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} mc_i c_j f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} mc_i c_j \mathbf{f}(\mathbf{v}) d\mathbf{v}.$$
2-57

Pressure tensor can be written as a sum of symmetric and anti-symmetric parts

$$\mathbf{P} = \mathbf{P}^{symmetric} + \mathbf{P}^{anti-symmetric}, \qquad 2-58$$

where anti-symmetric part diminishes when flow is assumed to be homogenous. The symmetric part of pressure tensor can be written as the following form

$$\mathbf{P}^{symmetric} = \mathbf{P}^{\text{Deviatoric}}_{symmetric} + \mathbf{P}^{\text{Isotripoic}}_{symmetric} 2-59$$

where deviatoric symmetry part is equivalent to traceless part of the symmetric pressure tensor, and isotropic part of the symmetric pressure tensor (Eq. 2-592-61) give scalar pressure (hydrostatic pressure) quantity;

$$\mathbf{P}^{\frac{\text{Deviatoric}}{\text{symmetric}}} = \mathbf{P}^{\frac{\text{trace-free}}{\text{symmetric}}} = \mathbf{\Pi},$$
2-60

$$\mathbf{P}^{\text{Isotripoic}} = \overline{p}\mathbf{I}.$$
 2-61

2.3.4.6 Viscous stress tensor

Viscous stress tensor can be defined as the traceless part of the symmetric pressure tensor. It can be defined based on moment of distribution functions as

$$\mathbf{\Pi} = \left\langle m \left[c_i c_j \right]^{(2)} f \right\rangle,$$

$$\Pi_{ij} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \left[c_i c_j \right]^{(2)} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \left[c_i c_j \right]^{(2)} \mathbf{f}(\mathbf{v}) d\mathbf{v}.$$
2-62

Here, $\begin{bmatrix} \end{bmatrix}^{(2)}$ denotes the traceless part of the thermal velocity production tensor $\begin{bmatrix} c_i c_j \end{bmatrix}$, and it is equal to

$$\left[c_{i}c_{j}\right]^{(2)} = \frac{1}{2}\left(c_{i}c_{j} + c_{j}c_{i}\right) - \frac{1}{3}c_{k}c_{k}\delta_{ij}.$$
 2-63

2.3.4.7 Thermodynamic & Mechanical pressure

The thermodynamic (scalar) pressure can be defined according to equation of state of ideal gases as

$$p = \rho R T_{tr}.$$
 2-64

Mechanical pressure is derived from isotropic part of symmetric pressure tensor;

$$\overline{p} = \frac{1}{3} P_{ii}^{\text{trace-free}} = \frac{1}{3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} mc_k c_k f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = \frac{n}{3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} mc_k c_k \mathbf{f}(\mathbf{v}) d\mathbf{v}.$$
 2-65

The mechanical pressure is average normal stress on the fluid element which can be written based on fluids kinematic as sum up thermodynamic pressure and pressure of sound absorption and attenuation.

$$\frac{1}{p} = \frac{\left(\Pi_{11} + \Pi_{22} + \Pi_{33}\right)}{3} = \rho RT_{tr} + \rho RT_{inter-atomic} \approx p - \left(\lambda + \frac{2}{3}\mu\right) \nabla \mathbf{.u} . \qquad 2-66$$

When gas is in an equilibrium state, the mechanical pressure is equal to hydrostatic pressure [26], and it is equal to any normal component of the stress tensor. However, it may not be equivalent to thermodynamic pressure for diatomic, polyatomic gases. Although the difference between thermodynamic pressure and mechanical pressure is

not significant in most of the gas flows, the exact meaning of mechanical pressure is still challenging issue [26]. In this dissertation, as gases are considered to be monatomic, the mechanical pressure and hydrostatic pressure are identical.

2.3.4.8 Heat flux vector

Heat flux vector is a flux vector which expresses the transport of energy of all states of the molecules by the motion of thermal (peculiar) velocity.

$$\mathbf{Q} = \left\langle E_{internal} \mathbf{c} f \right\rangle = \left\langle \left(\frac{mc^2}{2} + E_{inter-atomic} \right) c_j f \right\rangle$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{mc_r c_r}{2} + E_{inter-atomic} \right) c_j f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}$$
$$= n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{mc_r c_r}{2} + E_{inter-atomic} \right) c_j \mathbf{f}(\mathbf{v}) d\mathbf{v}.$$

where inter-atomic energy diminishes for monatomic gases, and then heat flux vector reads as

$$\mathbf{Q} = \left\langle E_{internal} \mathbf{c} f \right\rangle = \left\langle \frac{mc_r c_r}{2} c_j f \right\rangle$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{mc_r c_r}{2} c_j f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{mc_r c_r}{2} c_j \mathbf{f}(\mathbf{v}) d\mathbf{v}.$$
2-68

2.3.5 Classical Boltzmann kinetic equation

Boltzmann considered the dynamics of the inter-molecular binary collisions within the framework of the classical physics (deterministic) and combining it with a molecular chaos (statistical) assumption which is not coming from the mechanical origin and obviously cannot be derived from classical physics' principles alone. He obtained the time irreversible evolution equations for single particle distribution function in the concept of kinetic theory.

A single particle distribution function suffices for describing a molecule's state in phase space and for determining the macroscopic properties of the gas in the system, if the gas is sufficiently dilute, and the inter-molecular correlations are not significant. Let $f(\mathbf{x}, \mathbf{v}, t)$ denotes the single particle distribution, and $\mathbf{v}, \mathbf{x}, t$ represent the particle velocity, position and time, respectively.

The single particle distribution provides the probability of finding a particle in the class of range of $\mathbf{v} \sim \mathbf{v} + d\mathbf{v}$ and $\mathbf{x} + d\mathbf{x}$ at time *t*. A change in the particle probability

distribution in a small control volume $d\mathbf{v}d\mathbf{x}$ located at phase space at infinitesimally

$$\left(\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i^{external} \frac{\partial f}{\partial v_i}\right) d\mathbf{v} d\mathbf{x} dt .$$
 2-69

small time interval dt can be written in the form of

where high-order terms of order of $O(\Delta t^2)$ are truncated. Here $F_i^{external}$ is the vector of external forces on unit mass. This expression accounts for a *change in probability density function* due to the *streaming motion of the particles* in the phase space. When there is no collision between molecules, the changes in the single particle distribution $f(\mathbf{x}, \mathbf{v}, t)$ can be interpreted by a single particle Liouville equation called the collisionless Boltzmann equation,

$$\left(\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i^{external} \frac{\partial f}{\partial v_i}\right) = 0 \quad .$$
 2-70

Single particle Liouville equation does not contract the information of the system. It preserves the information of the system, and it describes the evolution of an incompressible probability fluid [23]. Nonetheless, in reality, the molecules collide each other and the probability density function will change inside the control volume of the phase space due to the inter-molecular collisions. Therefore, it is necessary to find a relation between the pre-collision $f(\mathbf{x}, \mathbf{v}, t)$, and post-collision $\hat{f}(\mathbf{x}, \mathbf{v}, t)$ probability density functions.

The collision operator $\Re(f, \hat{f})$ is the Boltzmann's lasting contribution to the kinetic theory which is not the invariant to the time reversal. It connects the dynamics of the inter-molecular collisions, the pre-collision-, and post-collision probability density functions such that the evaluation of the particle density function in time and phase space can be written as

$$\left(\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i^{external} \frac{\partial f}{\partial v_i}\right) = \Re\left(f, \hat{f}\right).$$
 2-71

The collision operator \Re depends on the way of approximating the collisional effects, and the statistical assumptions were made regarding the correlations of the particles in a binary collision. Boltzmann derived a classical form for \Re using his Stosszahl ansatz where the final form of this expression is given by

$$\Re(f,\hat{f}) = \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} \mathbf{c}_r (\hat{f}f_2 - ff_2) d\mathbf{v} d\varepsilon b db .$$
 2-72

Here *b*, is the first impact parameter, represents the distance of closest approach of the undisturbed trajectories in the center of mass reference frame; ε , is the second impact parameter, denotes the azimuthal angle of scattering. It illustrates the angle between collision plane and a reference plane. The pre-collision velocities of the two collision partners in a binary collision are defined by **V** and **V**₂ while the post-collision properties are denoted by a caret. The relative velocity **C**_{*r*} between two collision pair is defined by

$$\mathbf{c}_r = \mathbf{v} - \mathbf{v}_2 \,. \tag{2-73}$$

The relative velocity is unchanged during inter-molecular collision due to the conservation of the linear momentum and energy during the collision process. On substitution of Boltzmann collision integral (Eq. 2-72) into (Eq. 2-71), the classical Boltzmann kinetic equation is obtained;

$$\left(\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i^{\text{external}} \frac{\partial f}{\partial v_i}\right) = \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} \mathbf{c}_r \left(\hat{f}_2 - f_2\right) d\mathbf{v} \, d\varepsilon b db \quad .$$
 2-74

The Boltzmann kinetic equation is a well-known in kinetic theory. It has been considered as a proper nonlinear equation for studying rarefied gas flows. It can interpret the inter-molecular collisions and can describe the statistical behavior of molecules [27, 28]. However, solving the Boltzmann kinetic equation directly is not an easy task and usually, the analytical solution is limited to simple geometries due to the presence of the large number of independent variables in the equation, and the complexity and non-linearity of the collisional term [29].

As it is shown in Figure 2-6, there are several methods for approximation of the collisional integral such as BGK, ES-NGK, Shakhov, Fokker-Planck, and so on. The Boltzmann kinetic equation is commonly solved either by simplification and linearization of the collisional integral or direct physical simulation of the whole process. The other way to approximate the solution of the Boltzmann kinetic equations near the equilibrium condition is to derive moments of the Boltzmann equations and then approximate the shape of the probability distribution function.



Figure 2-6 Available methods for solving Boltzmann kinetic equation

2.4 Direct simulation of Boltzmann equation

2.4.1 DSMC method

Monte Carlo (MC) method was initially served around sixty years ago in order to study statistical mechanics and to integrate highly nonlinear integrals statistically. Despite the fact that MC is a very powerful method, it cannot demonstrate the evaluation of a system. An alternative for studying the microscopic behavior of materials is to use the molecular dynamic (MD) method which is a deterministic approach [30, 31]. However, it is a very costly and it is usually being used for simulating very small scale problems such as nano-materials, nano-tubes, and microsystems. Bird tried to overcome the difficulties in MD method by employing MC method inappropriate way [32]. As a result of that, the direct simulation Monte Carlo (DSMC) was introduced to study the molecular behavior of the rarefied and non-equilibrium flow [33].

DSMC is inherently a probabilistic method in which a large number of real particles are represented by one simulated particle. The cost of DSMC simulation is considerably less than molecular dynamic method [4]. The capability and the simplicity of the DSMC method persuade many researchers to utilize it as the standard solver for studying noncontinuum gas flows. It has being used to study various applications, such as micro gas flows, material processing, acoustics, high-speed gas flows, and gas mixing [34-40].

The conventional DSMC algorithms consider gases as a group of finite number of particle and describe the phase of the system by calculating the position and velocity of the particles. The continuous motion and collision of the gas particles are discretized within a small time step, Δt , and they are described in two consecutive and decoupled steps: movement and collision. These stages are equivalent to the advection and the collision term of the Boltzmann kinetic equation, respectively. In each time step Δt , the particles moves based on their own velocities throughout the gas flow without considering the interaction with other particles. Subsequently, if any particle reaches to a boundary, the proper action according to the type of boundary condition are taken into account and the particle positions are updated. Afterwards, the collision step is simulated by utilizing a *Markov process* in the collision cell during a given time interval. Therefore, the collision pairs are chosen randomly from particles within the same collision cell and the *collision probability* is calculated based on kinetic theory. Successful collisions are identified using *acceptance-rejection* method and finally, the post-collision properties are calculated in regard to the employed inter-particle potential model.

Generally, the movement phase is deterministic and does not involve any noticeable difficulties, while the collision phase is a probabilistic process. Collision process is composed of three important steps; counting the number of collisions, pair collision selection, and calculating the post-collision properties using inter-particle potential. In order to obtain an acceptable efficiency and accuracy in collision process, four features should be considered simultaneously: the computational efficiency, physical accuracy, reliability and implementing the collision step in the easiest way. Therefore, numbers of assumptions and simplifications should be taken into account. These assumptions or simplifications led to set up some requirements for physical parameters. For instance, time step should be selected small enough so that a particle just travels a fraction of collision cell length within a time step. The number of particles during a given interval more accurately. Finally, in order to minimize the statistical uncertainty and estimate the mean value of the estimators, the probability sampling process is added to the DSMC process [41, 42].

In fact, DSMC can be considered as a statistical solution of the Boltzmann equation in the case that the infinite number of particles are used and time step and grid size tending to zero [43]. However, Boltzmann kinetic equation cannot elaborate all aspects of DSMC approach [44]. The ability of the simulating the internal energy modes, chemical reactions and thermal radiations make DSMC more interesting for researchers. The statistical behavior of DSMC brings the ability to model the real hydrodynamic fluctuations [45, 46] in high-density conditions, although it can be considered as a drawback of the method due to produce undesirable statistical fluctuation in low-speed flow regimes. The biggest issue with DSMC method is that it is very expensive when the degree of non-equilibrium is low. This encouraged researcher to use moment-based methods for simulation of low speed or slightly deviated flows from equilibrium conditions.

2.4.2 Convergence of DSMC method

As Wagner [43] theoretically proved, the DSMC solution will converge to the solution of Boltzmann equation of a gas undergoing binary collisions between gas particles, if the value of time-step (Δ t), cell-size (Δ x), and the number of particles (N) parameters are chosen properly (and when no wall surface boundary condition is involved in the simulation) [41, 42, 47].

Bird [4] presented two conditions that the time-step value must be a fraction of the mean collision rate and the cell size value should be smaller than the mean free path. He suggested that the number of particles per cell should be greater than 20. Later, Meiburg [48] showed that these parameters need to be examined more carefully in order to yield accurate results. Many studies have been conducted to investigate the effects of computational parameters on either decomposition error or statistical error, and to quantify the amount of error associated with them [49-55]. Recently, a new verification method based on the exact physical laws of conservation—mass, linear momentum, and total energy—was introduced by the author to overcome the shortcomings of the previous researches and to investigate the behavior of various errors presented in a DSMC simulation [41, 42].



Figure 2-7 The percentage of absolute (a), and relative (b) errors for four different time steps

As it is shown in Figure 2-7, and Figure 2-8, our study confirmed that the error level of the DSMC method is negligible when the critical computational parameters—timestep, cell size, the number of particles—selected in the simulation, are well within the asymptotic range. This finding agrees with the results obtained theoretically by Wagner [12]. It was shown that the magnitude of error in DSMC simulation is not tangible if the number of particles in a cell are greater than 100, the time step is less than $10^{-1} \tau$ and cell size are in order of 10^{-1} of mean free path. Hence, in all of our DSMC simulations presented in this dissertation, the numbers of particles, and the values of time-step and cell-size is set such that above conditions hold.



Figure 2-8 The percentage of relative errors for (a) different cell length sizes; (b) different number of particles per cell.

2.5 The moments of Boltzmann kinetic equation

2.5.1 The equation of transfer

The classical Boltzmann kinetic equation (Eq. 2-74) can be written in the Cartesian coordinates $(\mathbf{x}, \mathbf{v}, t)$ as

$$\left(\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i^{\text{external}} \frac{\partial f}{\partial v_i}\right) = \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\frac{\pi}{2}} \left(\hat{f} \hat{f}_2 - f \hat{f}_2\right) \mathbf{c}_r \sigma \sin \chi d\chi d\varepsilon d\mathbf{v}, \qquad 2-75$$

where F_i^{external} is an external force, f denotes pre-collision, \hat{f} presents after collision distribution functions; σ , χ , and ε stand for collision cross section, deflection angle, the azimuthal angle of collisions, respectively.

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The equation of transfer can be obtained by multiplying ψ into classical Boltzmann kinetic equation (Eq. 2-75) and integration overall velocity speeds as

$$\frac{\partial \overline{\psi}}{\partial t} + \frac{\partial \langle \psi v_k f \rangle}{\partial x_k} - \left\langle F_k^{\text{external}} \frac{d\psi}{dv_k} f \right\rangle - \left\langle v_k \frac{\partial \psi}{\partial x_k} f \right\rangle - \left\langle \frac{\partial \psi}{\partial t} f \right\rangle = \Delta[\psi].$$
 2-76

As it is assumed that the external forces are independent of molecular velocity v, the (Eq. 2-76) can be simplified further as

$$\frac{\partial \rho \overline{\psi}}{\partial t} + \frac{\partial \langle \psi v_k f \rangle}{\partial x_k} - F_k^{external} \left\langle \frac{d\psi}{dv_k} f \right\rangle - \left\langle v_k \frac{\partial \psi}{\partial x_k} f \right\rangle - \left\langle \frac{\partial \psi}{\partial t} f \right\rangle = \Delta [\psi].$$
 2-77

Here the dissipation term $\Delta[\psi]$ is defined as

$$\Delta[\psi] = \int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{2\pi} \int_{0}^{\frac{\pi}{2}} \psi\left(\hat{f}_{2} - f_{2}\right) c_{r} \sigma \sin \chi d\chi d\varepsilon d\mathbf{v} \, d\mathbf{v}_{2}.$$
 2-78

The collisional term can be written in various alternative forms due to two characteristics of the collisional term; the collisional inverse and symmetries associated with the dynamic of the binary collision $(\mathbf{v}, \mathbf{v}_2 \rightleftharpoons \hat{\mathbf{v}}, \hat{\mathbf{v}}_2)$. For example, the collisional term can be written as following forms for further applications in next chapters,

$$\Delta[\psi] = \int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{4\pi} \psi_2 \left(\hat{f} \, \hat{f}_2 - f \, f_2 \right) c_r \sigma d\sigma d\mathbf{v} \, d\mathbf{v}_2, \qquad 2-79$$

$$\Delta[\psi] = -\int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{4\pi} \hat{\psi}_2 \left(\hat{f} \, \hat{f}_2 - f \, f_2 \right) c_r \sigma d\sigma d\mathbf{v} \, d\mathbf{v}_2, \qquad 2-80$$

$$\Delta[\psi] = -\int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{4\pi} \hat{\psi} \left(\hat{f} \hat{f}_2 - f f_2 \right) c_r \sigma d\sigma d\mathbf{v} d\mathbf{v}_2, \qquad 2-81$$

$$\Delta[\psi] = -\frac{1}{4} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{4\pi} (\psi + \psi_2 - \hat{\psi} - \hat{\psi}_2) (\hat{f} \hat{f}_2 - f f_2) c_r \sigma d\sigma d\mathbf{v} d\mathbf{v}_2, \qquad 2-82$$

$$\Delta[\boldsymbol{\psi}] = -\frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{4\pi} f f_2 \left(\boldsymbol{\psi} + \boldsymbol{\psi}_2 - \hat{\boldsymbol{\psi}} - \hat{\boldsymbol{\psi}}_2 \right) c_r \sigma d\sigma d\mathbf{v} d\mathbf{v}_2, \qquad 2-83$$

$$\Delta[\psi] = \frac{1}{2} n^2 \overline{\sigma_{total} c_r}.$$
 2-84

2.5.2 Collisional invariants

There are physical properties hidden in the definition of the collisional term that can be revealed based on the application of a different form of the collisional relation. For example, $(\psi + \psi_2 - \hat{\psi} - \hat{\psi}_2)$ reveals that the amount of change of a microscopic property ψ during a collision between two class of molecules v, v_2 . If any quantity ψ satisfies $\psi + \psi_2 - \hat{\psi} - \hat{\psi}_2 = 0$, the collisional integral vanishes from Boltzmann transfer equation and ψ is called collisional invariant. According to the classical physics, few molecular properties (mass *m*, momentum *mv*, and energy $mv^2/2$) are conserved during the molecular interaction, therefore, the collisional term and $\psi + \psi_2 - \hat{\psi} - \hat{\psi}_2$ vanish for these three molecular quantities and any linear combination of them. They are the only collisional invariant of the collisional integral.

2.5.3 Conservation laws

As collisional integral vanishes for mass, momentum, and energy of a molecule, it is possible to derive the conservation of laws based on Boltzmann transfer equation. Defining the macroscopic quantity equal to $\psi = [m, mv_i, mv^2/2]$, and multiply it into (Eq. 2-75) and integrating over velocity space. Then simplifying the equations by considering that ψ depends only on the particle position and time (**x**, *t*), lead to the differential form of the conservation of mass, momentum, energy (see appendix C):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0, \qquad 2-85$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_k}{\partial x_k} + \frac{\partial \Pi_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_k} - \rho F_k = 0, \qquad 2-86$$

$$\frac{\partial \rho e_{total}}{\partial t} + \frac{\partial \rho e_{total} u_k}{\partial x_k} + \frac{\partial Q_k}{\partial x_k} + \frac{\partial (\Pi_{ik} + p\delta_{ik}) u_i}{\partial x_k} - \rho F_k u_k = 0.$$
 2-87

or

$$\frac{D\rho}{Dt} + \rho \nabla \mathbf{.u} = 0, \qquad 2-88$$

$$\frac{D\rho \mathbf{u}}{Dt} + \nabla .\mathbf{\Pi} + \nabla p + \rho \mathbf{u} \nabla .\mathbf{u} - \rho \mathbf{F} = 0, \qquad 2-89$$

$$\frac{D\rho e_{total}}{Dt} + (\rho e_{total} + p)\nabla .\mathbf{u} + \nabla .\mathbf{Q} + \mathbf{\Pi} . \nabla .\mathbf{u} - \rho \mathbf{F} .\mathbf{u} = 0, \qquad 2-90$$

where total energy is equal to (Eq. 2-49); Π and Q are viscous stress tensor, and heat flux vectors, which are not defined yet. It must be emphasized that these physical conservation laws are the exact consequence of the Boltzmann kinetic equation, and they are valid for all degrees of non-equilibrium. Only after some approximations in the derivation of Π and Q quantities, they become approximate. In next chapter, nonconservative variables and the way to obtain an approximate constitutive relation for these variables are discussed in detail.

CHAPTER 3. Boltzmann-based hydrodynamic models

Albert Einstein (1879-1955):

"Imagination is more important than knowledge. Knowledge is limited. Imagination encircles the world."

As it was defined in the previous Chapter, the average of an extensive macroscopic quantity $\langle \psi f \rangle$ can be obtained by taking the first moment of a distribution function times the microscopic quantity $\psi(\mathbf{v})$. It was shown that the conservation laws can be obtained from the moment of Boltzmann equation without extra efforts for solving collision integral. However, the conservation laws remain open until some expressions for non-conserved variables are defined. In this chapter, it is assumed that the external forces are negligible and gas is consist of non-reacting monatomic molecules. The moment methods are applied to Boltzmann kinetic equation, and the extended hydrodynamic equations for non-conserved variables are derived. Afterwards, this exact but open equations are approximated based on Eu's closure, and Myong's balanced closure and then Boltzmann-based models are obtained.

3.1 Extended hydrodynamic equations based on the moment method

Let's define $\psi(\mathbf{v}) = \psi^{(n)}$ to denote the molecular expression for the nth *non-conserved* macroscopic variable $\overline{\psi}^{(n)}$ such that,

$$\overline{\boldsymbol{\Psi}}^{(n)} = \left\langle \boldsymbol{\Psi}^{(n)} f \right\rangle.$$
 3-1

Thus, the moment equations can be obtained by differentiating the $\Psi^{(n)}$ with respect to time and substituting df/dt from Boltzmann Kinetic equation (Eq. 2-71) as

$$\frac{\partial}{\partial t} \left\langle \boldsymbol{\Psi}^{(n)} f \right\rangle = \left\langle \boldsymbol{\Psi}^{(n)} \frac{\partial f}{\partial t} \right\rangle + \left\langle f \frac{\partial}{\partial t} \boldsymbol{\Psi}^{(n)} \right\rangle$$
$$= \left\langle \boldsymbol{\Psi}^{(n)} \left(\Re \left(f, \hat{f} \right) - \mathbf{v} \cdot \nabla f - F_i^{external} \nabla_v f \right) \right\rangle + \left\langle f \frac{\partial}{\partial t} \boldsymbol{\Psi}^{(n)} \right\rangle \qquad 3-2$$
$$= \left\langle \boldsymbol{\Psi}^{(n)} \Re \left(f, \hat{f} \right) \right\rangle - \left\langle \boldsymbol{\Psi}^{(n)} \mathbf{v} \cdot \nabla f \right\rangle - \mathbf{F}^{external} \left\langle \boldsymbol{\Psi}^{(n)} \nabla_v f \right\rangle + \left\langle f \frac{\partial}{\partial t} \boldsymbol{\Psi}^{(n)} \right\rangle$$

34

The external forces are assumed to be negligible, and the collisional term is symbolized by $\Delta \left[\psi^{(n)} \right] = \left\langle \psi^{(n)} \Re (f, \hat{f}) \right\rangle$, so above expression is reformed into

$$\frac{\partial}{\partial t} \left\langle \boldsymbol{\psi}^{(n)} f \right\rangle = \Delta \left[\boldsymbol{\psi}^{(n)} \right] - \left\langle \boldsymbol{\psi}^{(n)} \mathbf{v} \cdot \nabla f \right\rangle + \left\langle f \frac{\partial}{\partial t} \boldsymbol{\psi}^{(n)} \right\rangle.$$
 3-3

Considering the relation between microscopic, thermal, and stream velocities $(\mathbf{v} = \mathbf{c} + \mathbf{u})$, the above expression reads as

$$\frac{\partial}{\partial t}\overline{\mathbf{\psi}}^{(n)} = -\nabla \cdot \left(\mathbf{u}\left\langle\psi^{(n)}f\right\rangle\right) - \nabla \cdot \left\langle\mathbf{c}\psi^{(n)}f\right\rangle + \left\langle\mathbf{c}\cdot\nabla\psi^{(n)}f\right\rangle + \left\langle\left(\frac{\partial}{\partial t}+\mathbf{u}\cdot\nabla\right)\psi^{(n)}f\right\rangle + \Delta\left[\psi^{(n)}f\right].$$

If the high-order moment term is denoted as $\overline{\psi}^{\prime(n+1)} = \langle \boldsymbol{c} \psi^{(n)} f \rangle$, the (Eq. 3-4) reads as

$$\frac{\partial}{\partial t}\overline{\psi}^{(n)} = -\nabla \cdot \overline{\psi}^{\prime(n+1)} - \nabla \cdot \left(\mathbf{u}\left\langle\psi^{(n)}f\right\rangle\right) + \left\langle\mathbf{c}\cdot\nabla\psi^{(n)}f\right\rangle + \left\langle\left(\frac{\partial}{\partial t}+\mathbf{u}\cdot\nabla\right)\psi^{(n)}f\right\rangle + \Delta\left[\psi^{(n)}f\right]\right]^{-3}$$

$$3-5$$

As we are interested in derivation of first few leading high-order moment equations, let's set the molecular expression to be equal to the definition of viscous stress tensor (Eq. 2-62) and heat flux vector (Eq. 2-67), such that

$$\psi^{(1)} = m[\mathbf{c}_i \mathbf{c}_j]^{(2)},$$

$$\psi^{(2)} = \left[\frac{1}{2}m\mathbf{c}_k \mathbf{c}_k + E_{inter-atomic}\right]\mathbf{c}_j.$$
3-6

The equation of moment for viscous stress tensor $\overline{\Psi}_{ij}^{(1)} = \Pi_{ij}$ and heat flux vector $\overline{\Psi}_{i}^{(2)} = Q_{ij}$ read as:

$$\frac{d\Pi_{ij}}{dt} = -\nabla \cdot \overline{\psi}^{\prime(2)} - \nabla \cdot \left(\mathbf{u} \left\langle \psi^{(1)} f \right\rangle \right) + \left\langle f \frac{d}{dt} \psi^{(1)} \right\rangle + \left\langle \mathbf{c} f \cdot \nabla \psi^{(1)} \right\rangle + \Delta \left[\psi^{(1)} \right], \qquad 3-7$$

$$\frac{dQ_i}{dt} = -\nabla \cdot \overline{\psi}^{\prime(3)} - \nabla \cdot \left(\mathbf{u} \left\langle \psi^{(2)} f \right\rangle \right) + \left\langle f \frac{d}{dt} \psi^{(2)} \right\rangle + \left\langle \mathbf{c} f \cdot \nabla \psi^{(2)} \right\rangle + \Delta \left[\psi^{(2)} \right], \qquad 3-8$$

After massaging (Eq. 3-7) and (Eq. 3-8) and using the mass and momentum balance equation, and considering the macroscopic definition of conserved and non-conserved

variables defined in Section 2.3.4, the final form of stress and heat flux moment equations is obtained (see Appendix D);

$$\rho \frac{d\left(\frac{\mathbf{\Pi}}{\rho}\right)}{dt} = -\nabla \cdot \overline{\psi}^{\prime(2)} - 2p \left[\nabla \mathbf{u}\right]^{(2)} - 2\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)} + \Delta \left[\psi^{(1)}\right],$$

$$\rho \frac{d\left(\frac{\mathbf{Q}}{\rho}\right)}{dt} = -\nabla \cdot \overline{\psi}^{\prime(3)} - \overline{\psi}^{\prime\prime(3)} : \nabla \mathbf{u} + \frac{\mathbf{\Pi}}{\rho} \nabla \cdot (\mathbf{\Pi} + p\mathbf{I}) -$$
3-10

$$c_p \nabla T.(\mathbf{\Pi} + p\mathbf{I}) - \mathbf{Q}.\nabla \mathbf{u} + \Delta [\mathbf{Q}].$$

The conservation laws introduced in Section 2.5.3, together with extended hydrodynamics equations can be written in complete and compact form as;

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho \mathbf{e}_{total} \end{bmatrix} + \nabla \cdot \begin{bmatrix} -\mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ \rho \mathbf{e}_{total} \mathbf{u} + p \mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \mathbf{\Pi} \\ \mathbf{\Pi} \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\rho \frac{d \left(\frac{\mathbf{\Pi}}{\rho} \right)}{dt} = -\nabla \cdot \overline{\psi}^{\prime(2)} - 2p \left[\nabla \mathbf{u} \right]^{(2)} - 2 \left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} + \Delta \left[\psi^{(1)} \right], \qquad 3-11$$

$$\rho \frac{d \left(\frac{\mathbf{Q}}{\rho} \right)}{dt} = -\nabla \cdot \overline{\psi}^{\prime(3)} - \overline{\psi}^{\prime\prime(3)} : \nabla \mathbf{u} + \frac{\mathbf{\Pi}}{\rho} \nabla \cdot (\mathbf{\Pi} + p \mathbf{I}) - c_{p} \nabla T \cdot (\mathbf{\Pi} + p \mathbf{I}) - \mathbf{Q} \cdot \nabla \mathbf{u} + \Delta \left[\mathbf{Q} \right].$$

Here $\nabla \cdot \overline{\psi}^{\prime(2)}$ is $\nabla \cdot \langle m \boldsymbol{c}_k [\boldsymbol{c}_i \boldsymbol{c}_j]^{(2)} f \rangle$ in which the power of thermal velocity is three, and $\nabla \cdot \overline{\psi}^{\prime(3)} = \nabla \cdot \left(\left\langle \left[\frac{1}{2} m \boldsymbol{c}_k \boldsymbol{c}_k + E_{inter-atomic} \right] \boldsymbol{c}_l \boldsymbol{c}_m f \right\rangle - c_p T(p \mathbf{I} + \mathbf{\Pi}) \right)$ is a fourth-order function

with respect to thermal velocity, see 2.3.4. The second high-order moment term, $\bar{\psi}^{\prime\prime(3)} = \langle m \mathbf{ccc} f \rangle$, appeared in heat flux vector moment equation is also a cubic function of the thermal velocity of molecules.

It is clear that the higher-order moment terms and the integro-differential collisional term are not yet defined properly, therefore, the extended moment equations contain are still open. While there are several ways to close this system, we are going to use Eu's closure for closing this system of equations.

3.2 Eu's generalized hydrodynamic equations

3.2.1 Chapman-Enskog method

In 1912, Hilbert applied the Hilbert-Schmidt theory to Boltzmann equation, and expand phase distribution function in a power series of α . The resulting distribution function was the lowest-order solution of the Boltzmann kinetic equation which describes the local equilibrium states of gases. Application of this distribution function into (Eq. 3-9) and (Eq. 3-10), provides zero values of stress tensor and heat flux vector. Accordingly, the conservation laws will reduce into Euler hydrodynamic equations, *zero-order Boltzmann-based model*.

In 1917, Enskog[56] motivated by Hilbert theory, solved Boltzmann equation systematically, by increasing the power of expansion series of α , while Chapman [57] was working independently on the similar distribution function using Maxwell equations. They assumed that the phase distribution function is perturbed by a small amount from the equilibrium Maxwell distribution function, and derived the first-order approximation of Boltzmann equation (called Navier-Stokes-Fourier equations). In their approach, the distribution function *f* is expanded in powers of a smallness parameter α as follows;

 $f = f^{(0)} (1 + \alpha f^{(1)} + \alpha^2 f^{(2)} +)$. 3-12 where, $f^{(0)}$, $f^{(1)}$, and $f^{(2)}$ denote the first, second and third order approximation to the distribution function, respectively; the parameter α is defined based on Knudsen number.

Chapman-Enskog expansions for the stress tensor and for heat flux vector are defined as a linear expression of velocity and temperature gradients, respectively:

$$\Pi_{ij} = \Pi_{ij}^{\langle 0 \rangle} + \alpha \Pi_{ij}^{\langle 1 \rangle} + \alpha^2 \Pi_{ij}^{\langle 2 \rangle} + \dots$$

$$Q_i = Q_i^{\langle 0 \rangle} + \alpha Q_i^{\langle 1 \rangle} + \alpha^2 Q_i^{\langle 2 \rangle} + \dots,$$
3-13

where, $\mathbf{\Pi}^{\langle \alpha \rangle} = \langle m[\mathbf{cc}]^{(2)} f^{(\alpha)} \rangle, Q^{\langle \alpha \rangle} = \frac{1}{2} \langle mc^2 \mathbf{c} f^{(\alpha)} \rangle$. The coefficient of the gradients, known

as the familiar coefficient of viscosity and thermal conductivity, are obtained as series of Sonine polynomials. Although their approach is very valuable and helpful for extending continuum based methods, most of the high-order Chapman-Enskog models are unstable and violate the second law of thermodynamics.

3.2.2 Grad's 13-moment equations

An open set of high-order moment equations from the moment of Boltzmann equation was derived by Harold Grad in 1949 [58, 59]. Grad was motivated by work of Maxwell on transfer Boltzmann equation and tried to employ distribution function only when it is required. In grad moment equation, distribution function does not appear apparently in most of the terms of the moment equations; however, it has been served for evaluation of statistical formula $\langle mc...cf \rangle$ and the collisional (dissipation) term. Grad [58] expanded the distribution functions in Hermite polynomials for thermal velocity such that the coefficients of which are linear combinations of the moments as

$$f^{c} = f^{(0)} \left[1 + \mathbf{A}^{(1)} \cdot \mathbf{c} + \mathbf{A}^{(2)} : \left[m \mathbf{c} \mathbf{c} \right]^{(2)} + \mathbf{A}^{(3)} \cdot \left(\frac{1}{2} m \mathbf{c}^{2} - \frac{5}{2} k_{B} T \right) \mathbf{c} + \dots \right].$$
 3-14

Here $f^{(0)} = n \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left[-\frac{m\mathbf{c}^2}{2k_B T}\right]$ is Maxwell-Boltzmann distribution function,

$$\mathbf{A}^{(1)} = \frac{\langle m\mathbf{c}f \rangle}{p}, \ \mathbf{A}^{(2)} = \frac{1}{2} \frac{\mathbf{\Pi}}{p}, \ \text{and} \ \mathbf{A}^{(3)} = \left(\frac{2m^2}{5(k_B T)^3}\right) \frac{\mathbf{Q}}{\rho} - \frac{5}{2} \left(\frac{k_B T}{m}\right) \frac{\langle m\mathbf{c}f \rangle}{\rho}. \ \text{Considering the}$$

fact that $\langle mcf \rangle = 0$ for single species gases, defining $\beta = (m/2k_BT)^{1/2}$, and substituting $\mathbf{A}^{(i)}$ into (Eq. 3-14), the Grad distribution function reads as

$$f^{c} = f^{(0)} \left[1 + \frac{\Pi}{\rho} : \left[\beta \beta \right]^{(2)} + \frac{8}{5} \beta^{4} \mathbf{Q} (\beta^{2} - \frac{5}{2}) + \cdots \right], \qquad 3-15$$

where Π and Q are evaluated from non-conserved moment equations. Grad's distribution function indirectly influences the solution of the moment method by evolving the solution of non-conserved variables. Truncating this expansion up to fourth leading element terms and substituting the truncated expansion into collisional term of non-conserved moment equations, we can obtain Grad's dissipation function as a quadratic function,

$$\Delta\left[\psi^{(1)}\right] = \sum_{j=1}^{r} \left[R_{ij}^{(pp)} \mathbf{\Pi} + R_{ij}^{(pp)} \mathbf{\Pi} \cdot \mathbf{\Pi} + R_{ij}^{(qq)} \mathbf{Q} \mathbf{Q} \right],$$
 3-16

$$\Delta \left[\boldsymbol{\psi}^{(2)} \right] = \sum_{j=1}^{r} \left[R_{ij}^{(qq)} \mathbf{Q} + R_{ij}^{(qp)} \mathbf{Q} \cdot \mathbf{\Pi} + R_{ij}^{(pq)} \mathbf{\Pi} \cdot \mathbf{Q} \right].$$
 3-17

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Although Grad's moment method is basically different from Chapmann-Enskog theory, it shares the idea of functional hypothesis with Chapmann-Enskog method. As Eu's monograph [1] explained, the coefficients $R_{ij}^{(pp)}$, $R_{ij}^{(pq)}$, and $R_{ij}^{(qp)}$ are related to second-order Chapmann-Enskog approximation, and the distribution function evolves as a function of macroscopic conserved and non-conserved variables. The idea of Grad was great and promising; however, unfortunately, Grad distribution function, similarly to Chapmann-Enskog distribution function may or may not satisfy the laws of thermodynamics [1, 13]. It is proven that Grad's moment method fails in resolving of highly non-equilibrium phenomena [13, 60], and its entropy production, similar to Burnett equations, is inconsistence with second law of thermodynamics [1, 61, 62], Hence, employing an alternative closure for closing system of (Eq. 3-11) is demanding.

3.2.3 Eu's moment equations⁴

In Eu's theory [1], the kinetic theory of fluids is strictly connected to irreversible thermodynamics. The second law of thermodynamics is employed as a guiding principle for studying the fluid motion, and in particular, in high thermal non-equilibrium state. The beginning point of Eu's method is the balance equation for the calortropy $\hat{\Psi}$,

$$\rho \,\hat{\Psi}(\mathbf{x},t) = -k_B \left\langle \left[\ln f^c(\mathbf{v},\mathbf{x},t) - 1 \right] f(\mathbf{v},\mathbf{x},t) \right\rangle, \qquad 3-18$$

where $\hat{\Psi}$ is basically different from the Boltzmann *H-theorem*. Here the nonequilibrium canonical distribution function f^c represents the thermodynamic branch of the solution of the Boltzmann kinetic distribution function f. Applying moment method described in Section 3.1 and differentiating the local calortropy density $\hat{\Psi}$ with time, we obtain;

$$\rho \frac{d\hat{\Psi}}{dt} + \nabla \cdot \left(-k_B \left\langle \mathbf{c}(\ln f^c - 1)f \right\rangle \right) + k_B \left\langle f\left(\frac{d}{dt} + \mathbf{c} \cdot \nabla\right) \ln f^c \right\rangle = \sigma_c, \qquad 3-19$$
where $\sigma_c = \Delta \left[\ln f^c \right] = -k_c \left\langle \ln f^c \right\rangle \otimes \left(f(f(\hat{f})) \right\rangle$

where $\sigma_c \equiv \Delta \left[\ln f^c \right] = -k_B \left\langle \ln f^c \Re (f, \hat{f}) \right\rangle.$

In calculating the dissipation term, the distribution function f is written as sum up of the canonical distribution function and the fluctuations of the distribution function $f = f^c + \delta f$. If $\delta f = f - f^c$ is neglected, the absolutely positive calortropy production

⁴ More elaborative description can be found in Eu's 'kinetic theory and irreversible thermodynamics' book and Myong's paper on shock structure singularity.

function σ_c on the right-hand side of (Eq. 3-19) can further be expressed as relative velocity between collision pair particles \mathbf{c}_r using the govern collisional inverse and symmetries relations associated with dynamic of binary collision, and employing the collisional terms presented in (Eq. 2-82);

$$\sigma_{c} = \frac{1}{4} k_{B} \int_{-\infty}^{\infty} d\mathbf{v} \int_{-\infty}^{\infty} d\mathbf{v}_{2} \int_{0}^{4\pi} d\varepsilon \int_{0}^{\infty} \ln(\hat{f}^{c} \hat{f}_{2}^{c} / f^{c} f_{2}^{c}) (\hat{f}^{c} \hat{f}_{2}^{c} - f^{c} f_{2}^{c}) db \ b\mathbf{c}_{r} \ge 0.$$
 3-20

In case that the calortropy production σ_c is calculated before calculation of the dissipation term $\Delta[\psi^{(n)}]$, a thermodynamically consistent form of $\Delta[\psi^{(n)}]$ and a clear relation between σ_c and collisional (dissipation) term can be obtained. It is possible to write the distribution function f^c in the exponential form, rather than in form of quadratic polynomials function (Eq. 3-15), if the logarithmic form of the calortropy production $\ln f^c$ defined in (Eq. 3-19) is employed such that

$$f^{c} = \exp\left[-\beta'\left(\frac{1}{2}m\mathbf{c}^{2} + \sum_{n=1}^{\infty}\overline{X}^{(n)}\psi^{(n)} - A_{0}\right)\right],$$

$$\exp(-\beta'A_{0}) = \frac{1}{n}\left\langle \exp\left[-\beta\left(\frac{1}{2}m\mathbf{c}^{2} + \sum_{n=1}^{\infty}\overline{X}^{(n)}\psi^{(n)}\right)\right]\right\rangle, \ \beta' \equiv \frac{2}{mc_{mps}^{2}}.$$

$$3-21$$

In this expression $c_{mps} = \sqrt{2k_BT/m}$ is most probable molecular thermal speed, *n* is the number density, and $\bar{X}^{(n)}$, unknown macroscopic quantities, are the conjugate variables to the molecular expressions for moment $\psi^{(n)}$, and A_0 is constant which may be eliminated through the normalization condition $\int_{-\infty}^{\infty} f^c d\mathbf{v} = 1$. This requires that

$$\int_{-\infty}^{\infty} \exp\left[-\beta'\left(\frac{1}{2}m\mathbf{c}^{2} + \sum_{n=1}^{\infty}\bar{X}^{(n)}\psi^{(n)} - A_{0}\right)\right]d\mathbf{v} = 1.$$
3-22

In the mathematical sense, this distribution function is desirable as it *guarantees the non-negativity of the distribution function regardless of the level of approximations*. In the physical sense, this exponential form is the only form that satisfies the *additive property of the calortropy and calortropy production*, all of which are in the logarithmic form. It must also be noted that the number of moments in (Eq. 3-21) goes to infinity and there is no finite approximation for moments there. This is in contrast with a common practice in considering only the first 13th moments from the outset in the formulation of the theory.

Let's drop the superscripts c in the distribution function f^c for simplicity and use a short notation for the exponent. Therefore, the distribution function can be rewritten as

$$f = f^{(0)} \exp(-x)$$
 where $x \equiv \beta' \left(\sum_{n=1}^{\infty} \bar{X}^{(n)} \psi^{(n)} - A_0 \right).$ 3-23

With further introduction of notations and dimensionless variables

$$x_{12} = x_1 + x_2, \ y_{12} = y_1 + y_2 = \hat{x}_{12}, \ \overline{\sigma}_c = \frac{\sigma_c}{k_B/g}, \ g \equiv \frac{1}{n^2 d^2} \sqrt{\frac{m}{2k_B T}}, \ \overline{b} = \frac{b}{d},$$

$$\mathbf{w} = \mathbf{c} \sqrt{\frac{m}{k_B T}}, \ \omega(\mathbf{w}) \equiv \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{1}{2}\mathbf{w}^2\right),$$

$$\overline{g}_{12} = \mathbf{c}_{\mathbf{r}} \sqrt{\frac{m}{2k_B T}}, \ \omega_{12}(\mathbf{w}, \mathbf{w}_1) \equiv \frac{1}{(2\pi)^3} \exp\left(-\frac{1}{2}w^2 - \frac{1}{2}w_1^2\right),$$

$$\langle A \rangle_c \equiv \int d\hat{\Gamma}_{12} \omega_{12}(\mathbf{w}, \mathbf{w}_1) A(\mathbf{w}, \mathbf{w}_1),$$

$$\int d\hat{\Gamma}_{12} \cdots \equiv \int_{-\infty}^{\infty} d\mathbf{w} \int_{-\infty}^{\infty} d\mathbf{w}_2 \int_0^{2\pi} d\varepsilon \int_0^{\infty} \overline{b} \ d\overline{b} \ \overline{\mathbf{c}}_{\mathbf{r}} \cdots,$$

$$\int d\Gamma_{12} \cdots \equiv \int_{-\infty}^{\infty} d\mathbf{v} \int_{-\infty}^{\infty} d\mathbf{v}_2 \int_0^{2\pi} d\varepsilon \int_0^{\infty} \mathbf{c}_r b \ db \ \cdots,$$

(3-24)

the calortropy production can be expressed as

$$\sigma_{c} = -k_{B} \left\langle \ln f \ \mathcal{H}[f, f_{2}] \right\rangle = \frac{1}{T} \left\langle \left(\frac{1}{2} m \mathbf{c}^{2} + \sum_{n=1}^{\infty} \overline{X}^{(n)} : \psi^{(n)} - A_{0} \right) \mathcal{H}[f^{(0)} \exp(-x), f_{2}^{(0)} \exp(-x_{2})] \right\rangle$$

$$= \frac{1}{4} k_{B} \int d\mathbf{v} \int d\mathbf{v}_{2} \int_{0}^{2\pi} d\varepsilon \int_{0}^{\infty} db \ b \mathbf{c}_{\mathbf{r}} f^{(0)} f_{2}^{(0)} \left(x_{12} - y_{12} \right) \left[\exp(-y_{12}) - \exp(-x_{12}) \right]$$

$$= \frac{1}{4T} \int d\Gamma_{12} f^{(0)} f_{2}^{(0)} \left(x_{12} - y_{12} \right) \left[\exp(-y_{12}) - \exp(-x_{12}) \right].$$
Or simply

Or simply

$$\bar{\sigma}_{c} = \frac{1}{4} \left\langle \left(x_{12} - y_{12} \right) \left[\exp(-y_{12}) - \exp(-x_{12}) \right] \right\rangle_{c}.$$
3-26

This form of mathematical equation is suitable for so-called cumulant expansion, and it can be written in form of

$$\overline{\sigma}_{c} = \kappa_{1}^{2} q(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots) \text{ where } \kappa_{1} \equiv \frac{1}{2} \left\{ \left\langle \left(x_{12} - y_{12} \right)^{2} \right\rangle_{c} \right\}^{1/2}, \\ q(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots) \equiv \frac{1}{2\kappa_{1}} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^{l}}{l!} \kappa_{l}^{(+)} \right] - \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^{l}}{l!} \kappa_{l}^{(-)} \right] \right\}.$$

$$3-27$$

The positivity of the calortropy production regardless of the level of approximations is guaranteed using this expansion form [13]. The collisional term $\Delta \left[\psi^{(n)}\right]$ can be found as a function of calotropy function by inserting the distribution function (Eq. 3-21) into (Eq. 3-26) as

$$\sigma_{c} = -k_{B} \left\langle \ln f \ \mathcal{R}[f, f_{1}] \right\rangle = -k_{B} \left\langle -\beta' \sum_{n=1}^{\infty} \bar{X}^{(n)} \psi^{(n)} \mathcal{R}[f, f_{2}] \right\rangle$$

$$= \frac{1}{T} \sum_{n=1}^{\infty} \bar{X}^{(n)} \left\langle \psi^{(n)} \mathcal{R}[f, f_{1}] \right\rangle = \frac{1}{T} \sum_{n=1}^{\infty} \bar{X}^{(n)} \Delta \left[\psi^{(n)} \right].$$
3-28

The explicit form of the dissipation term $\Delta \left[\psi^{(n)}\right]$ can be derived from (Eq. 3-27) and (Eq. 3-28) by computing the first reduced collision integral κ_1 in terms of $\bar{X}^{(n)}$ as xperforming in κ_1 consists of a sum of several moments, $x \equiv \beta' \left(\sum_{n=1}^{\infty} \bar{X}^{(n)} \psi^{(n)} - A_0 \right)$, with the definition $SU^{(n)} = \omega^{(n)} - \hat{C}^{(n)}$ etc. ω^2 may be expressed as a quadratic form of \bar{X}

the definition $\delta h^{(n)} = \psi^{(n)} - \hat{\psi}^{(n)}$, etc., κ_1^2 may be expressed as a quadratic form of \overline{X} and \overline{X}_2 ,

$$\kappa_1^2 = \frac{1}{4} \sum_{n,l=1}^{\infty} \left\langle \left(\bar{X}^{(n)} \delta h^{(n)} + \bar{X}_2^{(n)} \delta h_2^{(n)} \right) \left(\bar{X}^{(l)} \delta h^{(l)} + \bar{X}_2^{(l)} \delta h_2^{(l)} \right) \right\rangle_c.$$
 3-29

On rearrangement of the terms, it may become as

$$\kappa_1^2 = \sum_{n,l=1}^{\infty} \bar{X}^{(n)} R_{12}^{(nl)} \bar{X}_2^{(l)}, \qquad 3-30$$

where $_{R_{12}^{(n)}}$ are scalar coefficients made up of collision bracket integrals of $_{\psi^{(n)}}$, and $_{\psi_{2}^{(l)}}$ for an isotropic system of dilute gases. After comparing (Eq. 3-27), (Eq. 3-28), (Eq. 3-30),

$$\overline{\sigma}_{c} = \kappa_{1}^{2} q(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots) = \beta' g \sum_{n=1}^{\infty} \overline{X}^{(n)} \Delta \left[\psi^{(n)} \right] = \sum_{n,l=1}^{\infty} \overline{X}^{(n)} R_{12}^{(nl)} \overline{X}_{2}^{(l)} q(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots),$$
3-31

the following dissipation term can be derived;

$$\Delta \left[\psi^{(n)} \right] = \frac{1}{\beta' g} \sum_{l=1}^{\infty} R_{12}^{(nl)} \overline{X}_{2}^{(l)} q(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots).$$
 3-32

The unknown macroscopic variables $\bar{X}^{(n)}$ can be defined in different ways. Eu [1] developed a way based on the equilibrium Gibbs ensemble theory to non-equilibrium processes and it can be summarized as

$$\frac{\left\langle \psi^{(n)} f \right\rangle}{\rho} = -k_B T \left(\frac{\partial}{\partial \bar{X}^{(n)}} \ln \bar{Z} \right)$$
3-33

where

$$\overline{Z} = \frac{1}{n} \left\langle \exp\left[-\frac{1}{k_B T} \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} \overline{X}^{(n)} \psi^{(n)}\right)\right] \right\rangle$$
3-34

Therefore, the $\bar{X}^{(n)}$ can be determined in terms of the macroscopic flux $\bar{\psi}^{(n)} = \langle \psi^{(n)} f \rangle$ by solving (Eq. 3-33). The leading approximate solutions terms of $\bar{X}^{(n)}$ are known to be

$$\bar{X}^{(1)} = -\frac{\Pi}{2p}, \ \bar{X}^{(2)} = -\frac{Q}{pC_pT}.$$
 3-35

As $\overline{\Psi}^{(n)}$ is an extensive physical property of the system, it is dependent on the size of the system or the amount of gases in the system. It is possible to write macroscopic properties in term of bulk (i.e. intensive) properties (i.e., $\overline{\Psi}^{(n)}/\rho$), and finally, re-write the viscous stress moment equations by replacing collisional (dissipation) term with (Eq. 3-32) as

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \nabla \cdot \overline{\mathbf{\psi}}^{\prime(2)} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \frac{\sqrt{2k_B^3 T^3}}{n^2 d^2 \sqrt{m}} \sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots).$$

$$\rho \frac{d}{dt} \left(\frac{\mathbf{Q}}{\rho}\right) + \nabla \cdot \overline{\mathbf{\psi}}^{\prime(3)} + \overline{\mathbf{\psi}}^{\prime\prime(3)} : \nabla \mathbf{u} - \nabla \cdot \left(p\mathbf{I} + \mathbf{\Pi}\right) \cdot \frac{\mathbf{\Pi}}{\rho} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot c_p \nabla T + pc_p \nabla T = \frac{\sqrt{2k_B^3 T^3}}{n^2 d^2 \sqrt{m}} \sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots).$$

$$3-37$$

where $\bar{\psi}^{\prime(3)} = \left\langle \frac{1}{2}mc^2 \mathbf{cc}f \right\rangle - c_p T(p\mathbf{I} + \mathbf{\Pi})$. Note that this still exact to the original Boltzmann equation since the number of terms in expanded dissipation series goes to infinity, and the kinematic high-order term is not yet approximated. Nevertheless, (Eq. 3-49) is in suitable shape for balanced treatment in approximating the kinematic high-order term in the left-hand side, and the dissipation term on the right-hand side.

3.3 Boltzmann-based constitutive models via the balanced closure

3.3.1 Zero-order Boltzmann-based model

As explained in Section 3.2.1, the zero-order Boltzmann-based model (Euler constitutive relations) is a direct consequence of assuming flow in an equilibrium state, and considering the density distribution to be a Maxwellian equilibrium distribution function. The statistical formulation of viscous stress tensor and heat flux vector using Maxwellian distribution function has simple, exact solution;

$$\mathbf{\Pi} = \overline{\mathbf{\Psi}}^{(1)} = \left\langle \psi^{(1)} f^{(0)} \right\rangle \equiv \int_{-\infty}^{\infty} nm \left(\frac{m}{2\pi k_{_B} T} \right)^{_{3/2}} [c_i c_j]^{(2)} \exp \left[-\frac{m\mathbf{c}^2}{2k_{_B} T} \right] d\mathbf{c} = 0,$$

$$\mathbf{Q} = \overline{\mathbf{\Psi}}^{(2)} = \left\langle \psi^{(2)} f^{(0)} \right\rangle \equiv \int_{-\infty}^{\infty} \frac{n}{2} \left(\frac{m}{2\pi k_{_B} T} \right)^{_{3/2}} [mc_k c_k + E_{inter-atomic}] c_j \exp \left[-\frac{m\mathbf{c}^2}{2k_{_B} T} \right] d\mathbf{c} = 0.$$
3-38

3.3.2 First-order Boltzmann-based model

The left-hand side of Boltzmann kinetic equation which demonstrates the change of particles due to the collisionless (transport) motion of the particles, changes with a time scale of the order of $nm/2k_{B}TL$. On the other hand, the right-hand side of Boltzmann kinetic equation demonstrates the net change in the number of gas molecules due to inter-molecule collisions. It is basically described by gain minus loss (exp^(nonequilibrium)) exp^(-nonequilibrium)), has the time scale of $n\sigma m/2k_{B}T$. Eu showed that the time scale of conserved variables and non-conserved variables are not similar. He estimates that the relaxation time of non-conserved variable is in the order of 10^{-10} seconds, and it is much shorter than conserved variables. Therefore evaluation of non-conserved variables near equilibrium state becomes linear and cumulant expansion of collisional term recovers the first-order Chapmann-Enskog approximation. It is possible to approximate the entropy production and consequently non-conserved evolution equations, such that the viscous stress tensor-, and heat flux vector moment equations are linearized by truncating collisional term — considering the first term of cumulant expansion $\frac{\sqrt{2k_{B}T^{3}}{n^{2}d^{2}\sqrt{m}}R_{12}^{(21)}X_{2}^{(1)}q(\kappa_{1}^{(\pm)})$ — and approximating transport process. The approximate

collisional (dissipation) terms can be written as following

$$\Delta \left[\psi^{(1)} \right] = -\frac{p}{\mu} \Pi q_{1st-order}(\kappa_1), \qquad 3-39$$

$$\Delta \left[\Psi^{(2)} \right] = -\Pr \mathbf{Q} \frac{p}{\mu} q_{1st-order} (\kappa_1) \equiv -\mathbf{Q} \frac{pc_p}{k} q_{1st-order} (\kappa_1).$$
3-40

where $q_{1st-order}(\kappa_1) = 1$, μ and k are the first coefficient of viscosity and thermal conductivity derived from Chapmann-Enskog transport analysis. In addition, Eu [1] showed that linearization of non-conserved moment equation implies exponentially decaying of the non-conserved variables as the time passes, although the conserved variables remain approximately unchanged [1]. It means that non-conserved variables change considerably faster than conserved variables, and they reach to steady state

condition much earlier than the conserved variables. It is valid to simplify the nonconserved equation by omitting the substantial time derivative from the equations;

$$\nabla \cdot \overline{\boldsymbol{\psi}}^{\prime(2)} + 2 \left[\boldsymbol{\Pi} \cdot \nabla \boldsymbol{u} \right]^{(2)} + 2 p \left[\nabla \boldsymbol{u} \right]^{(2)} = - \boldsymbol{\Pi} \frac{p}{\mu} \boldsymbol{q}_{1 \text{st-order}} (\boldsymbol{\kappa}_{1}), \qquad 3-41$$

$$\nabla \cdot \overline{\psi}^{\prime(3)} + \overline{\psi}^{\prime\prime(3)} : \nabla \mathbf{u} - \nabla \cdot \left(p\mathbf{I} + \mathbf{\Pi} \right) \cdot \frac{\mathbf{\Pi}}{\rho} + \mathbf{Q} \cdot \nabla \mathbf{u} - c_p \mathbf{\Pi} \cdot \nabla T + c_p p \nabla T$$

$$= -\mathbf{Q} \frac{c_p p}{k} q_{_{1st-order}} (\kappa_1).$$

3-42

To close the system of equations, the high-order moments appearing on the left-hand side of below equations must be known. According to balanced treatment introduced by Myong [13], the first-order approximation of collisional term requires the same order of approximation on the left-hand side of non-conserved moment equations. Therefore, not only $\nabla \cdot \overline{\psi}^{\prime(2)}$, $\nabla \cdot \overline{\psi}^{\prime(3)}, \overline{\psi}^{\prime\prime(3)} : \nabla \mathbf{u}$ will be removed from the first-order constitutive relations, but also $2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)}$ and $\nabla \cdot (p\mathbf{I} + \mathbf{\Pi}) \cdot \frac{\mathbf{\Pi}}{\rho} + \mathbf{Q} \cdot \nabla \mathbf{u} - c_p \mathbf{\Pi} \cdot \nabla T$ are needed to be eliminated for first-order approximation since thermal velocity appeared in their statistical formulations is of the order of two or more which can destroy the balance of the equations. As a result of that, first-order linear Boltzmann-based model (i.e., Navier-Stokes-Fourier constitute relations) are given by

$$\mathbf{\Pi} = -2\mu \left[\nabla \mathbf{u}\right]^{(2)}, \qquad 3-43$$

$$\mathbf{Q} = -k\nabla T. \tag{3-44}$$

3.3.3 Second-order Boltzmann-based model

A system far from equilibrium state has nonlinear behaviors which are preferable to retain in a higher approximation of the moment methods. Similarly to first-order Boltzmann-based approximation, it is possible to reduce non-conserved evaluation moment equations into the second-order model by applying adiabatic assumption and treating the high-order moments based on the balanced treatment [13]. The resulting equation can be expressed as

$$2\left[\boldsymbol{\Pi}\cdot\nabla\boldsymbol{\mathsf{u}}\right]^{(2)}+2p\left[\nabla\boldsymbol{\mathsf{u}}\right]^{(2)}=-\boldsymbol{\Pi}\frac{p}{\mu}q_{2nd-order}(\boldsymbol{\kappa}_{1}),$$
3-45

$$-\nabla \cdot \left(p\mathbf{I} + \mathbf{\Pi}\right) \cdot \frac{\mathbf{\Pi}}{\rho} + \mathbf{Q} \cdot \nabla \mathbf{u} - c_p \mathbf{\Pi} \cdot \nabla T + c_p p \nabla T = -\mathbf{Q} \frac{c_p p}{k} q_{2nd-order}(\kappa_1), \quad 3-46$$

where the first-order cumulant expansion $q_{2nd-order}(\kappa_1) = \sinh \kappa_1 / \kappa_1$, takes a form of hyperbolic sine function whose κ_1 argument is basically given in terms of a Rayleigh dissipation function [1, 13, 63];

$$\kappa_{1} \equiv \frac{(mk_{B})^{1/4}}{\sqrt{2}d} \frac{T^{1/4}}{p} \left(\frac{\Pi : \Pi}{\mu} + \frac{\mathbf{Q} \cdot \mathbf{Q} / T}{k}\right)^{1/2}.$$
 3-47

These algebraic second-order Boltzmann-based relations, so-called nonlinear coupled constitutive relations (NCCR), can be solved using an appropriate numerical method while the conserved variables are held constant during the evaluation process. The only remaining task is to solve these equations besides the conservation of laws using appropriate numerical methods.

Zero order Boltzmann-based model (Euler constitutive relations) $\mu, \kappa \to 0,$ $\mathbf{\Pi} = 0, \mathbf{Q} = 0.$ **First order Boltzmann-based model (Navier-Stokes-Fourier constitutive relations)** $\mu, \kappa \to f(T, \mathbf{p})$ $\mathbf{\Pi} = -2\mu [\nabla \mathbf{u}]^{(2)},$ $\mathbf{Q} = -\kappa \nabla \mathbf{T}.$ **Second order Boltzmann-based model (Nonlinear coupled constitutive relations)** $\mu, \kappa \to f(T, \mathbf{p})$ $2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p [\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu} \mathbf{\Pi} \frac{\sinh \kappa_1}{\kappa_1},$ $-\nabla \cdot (p\mathbf{I} + \mathbf{\Pi}) \cdot \frac{\mathbf{\Pi}}{\rho} + \mathbf{Q} \cdot \nabla \mathbf{u} - c_p \mathbf{\Pi} \cdot \nabla T + c_p p \nabla T = -\frac{c_p p}{k} \mathbf{Q} \frac{\sinh \kappa_1}{\kappa_1}.$

Figure 3-1 A set of Boltzmann-based constitutive models up to second-order

3.4 Governing equations for numerical simulation

The conservation laws represent a system of five differential equations, in three dimensions. However, the number of unknown field variables is thirteen, namely: ρ , ρu_i , ρe_{Total} , p, T, Π_{ij} , and Q_i . The non-conservative variables (symmetric stress tensor Π , and heat flux vector \mathbf{Q}) read from Boltzmann-based constitutive relations introduced as shown in Figure 3-1. Volume (or density), pressure and temperature are thermodynamic state variables, therefore, one can be obtained by the others using equation of states. In dilute gas conditions, where mean molecular spacing ($\delta = n^{-\frac{1}{3}}$) is

much bigger than molecular diameter *d*, it is fine to assume that the gas is a calorically perfect gas and behaves ideally;

$$p = nk_B T = (\gamma - 1)\rho \left\{ e_{total} - \frac{u_k u_k}{2} \right\}$$

$$3-48$$

where $k_{_B}$ is Boltzmann's constant, is *n* number density of the gas, defined in (Eq.2-40) and $\gamma = c_p/c_v$ is specific heat ratio (Eq.2-23). In addition to thirteen field unknown variables, there are few more unknowns related to microscopic properties of gas, called transport coefficients; the first coefficient of viscosity (or dynamic viscosity) μ , the first coefficient of thermal conductivity κ and the second coefficient of viscosity λ . They can be obtained from either inter-molecular force relations or Chapmann-Enskog relations.

3.4.1 Conservative form of the conservation laws

The \mathcal{D} -dimensional conservation laws conservation laws for monatomic gas can be represented in differential from by

$$\frac{\partial w_k}{\partial t} + \frac{\partial \mathbf{F}_k^{\text{inviscid}}}{\partial x_x} + \frac{\partial \mathbf{F}_k^{\text{viscous}}}{\partial x_x} = s_k \quad \text{in} \left[(t, \Omega) \middle| t \in (0, \infty), \Omega \subset \mathbb{R} \right],$$

$$\mathbf{w}(\mathbf{x}, 0) = \mathbf{w}_0(\mathbf{x}) \quad \text{in } \Omega,$$

$$3-49$$

where $\mathbf{F}^{inviscid} \in \mathbb{R}^{(\mathfrak{D}+2)\times\mathfrak{D}}$ and $\mathbf{F}^{viscous} \in \mathbb{R}^{(\mathfrak{D}+2)\times\mathfrak{D}}$ are flux functions. The former is related to convective transport of macroscopic quantities in the fluid. It is usually called vector of convective fluxes. The latter flux tensor named as a vector of viscous fluxes, and it contains the viscous stresses as well as heat diffusion terms. The source term $\mathbf{s} \in \mathbb{R}^{(\mathfrak{D}+2)}$ comprises all sources including body forces, electrical forces, and volumetric heating. Ω is a bounded computational domain, and $\mathbf{W} \in \mathbb{R}^{(\mathfrak{D}+2)}$ is a vector of conservative variables — Mass per unit volume, momentum vector, and energy — which are continuously differentiable in the domain.

$$w_{k} = \begin{bmatrix} \rho & \rho u_{k} & \rho e_{total} \end{bmatrix}^{T},$$

$$\mathbf{F}_{k}^{inviscid} = \begin{bmatrix} \rho u_{k} & \rho u_{k} u_{i} + p \delta_{ik} & (\rho e_{total} + p) u_{k} \end{bmatrix}^{T},$$

$$\mathbf{F}_{k}^{viscous} = \begin{bmatrix} 0 & \Pi_{ik} & (\Pi_{ik} u_{k} + Q_{k}) \end{bmatrix}^{T},$$

$$s_{k} = \begin{bmatrix} 0 & \rho F_{k} & (\rho F_{k} u_{k} + \dot{Q}_{k}) \end{bmatrix}^{T},$$

with $i, j, k = 1 \cdots \mathfrak{D}.$

3.4.2 Dimensionless form of the governing equations

In general, any dimensional homogeneous system of equation can be written in an entirely equivalent non-dimensional form which is more compact, and simpler to give a quick insight into the physical relationship. In order to derive the dimensionless form of the conservation laws, it is necessary to define relevant dimensionless variables, denoting them by an asterisk as

$$t^{*} = \frac{t}{t_{ref}}, \quad \mathbf{x}^{*} = \frac{\mathbf{x}}{L}, \quad \mathbf{u}^{*} = \frac{\mathbf{u}}{u_{ref}}, \quad T^{*} = \frac{T}{T_{ref}}, \quad \rho^{*} = \frac{\rho}{\rho_{ref}}, \quad p^{*} = \frac{p}{p_{ref}}, \\ \mathbf{\Pi}^{*} = \frac{\mathbf{\Pi}}{\Pi_{ref}}, \quad E^{*} = \frac{E}{E_{ref}}, \quad \mathbf{Q}^{*} = \frac{\mathbf{Q}}{q_{ref}}, \quad \mu^{*} = \frac{\mu}{\mu_{ref}}, \quad \kappa^{*} = \frac{\kappa}{\kappa_{ref}}, \\ c_{p}^{*} = \frac{c_{p}}{c_{p_{ref}}}, \quad c_{v}^{*} = \frac{c_{v}}{c_{v_{ref}}}, \quad \nabla^{*} = L\nabla.$$

Here, reference parameters, denoted by subscript ref, are defined using four base quantities (mass, length, time, and temperature) in (MLT) unit system as

$$t_{ref} = \frac{L}{u_{ref}}, \quad E_{ref} = u_{ref}^2, \quad \Pi_{ref} = \frac{\mu_{ref} u_{ref}}{L}, \quad q_{ref} = \frac{k_{ref} \Delta T_{ref}}{L}.$$
 3-51

Substitute the dimensionless variables from (Eq.3-50) into equations (Eq. 3-49) and divide it through by the leading dimensional coefficient resulting dimensionless form of the governing equation as

$$\frac{\partial \mathbf{w}^*}{\partial t} + \nabla^* \mathbf{F}^{*inviscid} + \nabla^* \mathbf{F}^{*viscous} = \mathbf{s}^*, \qquad 3-52$$

where the non-dimensional conservative variables \mathbf{w}^* are given by

$$\mathbf{w}^* = \begin{bmatrix} \rho^* & \rho^* \mathbf{u}^* & \rho^* e_{total}^* \end{bmatrix}^T.$$
 3-53

The dimensionless form of the inviscid and viscous flux vectors can be defined as,

$$\mathbf{F}^{*inviscid} = \begin{bmatrix} \rho^* \mathbf{u}^* & \rho^* \mathbf{u}^* \mathbf{u}^* + \frac{1}{N_{\delta} \operatorname{Re}} p^* \mathbf{I} & (\rho^* e_{total}^* + \frac{1}{N_{\delta} \operatorname{Re}} p^*) \mathbf{u}^* \end{bmatrix}^T,$$

$$\mathbf{F}^{*viscous} = \begin{bmatrix} 0 & \frac{1}{\operatorname{Re}} \mathbf{\Pi}^* & (\frac{1}{\operatorname{Re}} \mathbf{\Pi}^* \cdot \mathbf{u}^* + \frac{1}{\operatorname{Pe} Ec} \mathbf{q}^*) \end{bmatrix}^T,$$
3-54

where fluid dynamics dimensionless parameters – Mach *M*, Reynolds *Re*, Prandtl *Pr*, Knudsen *Kn*, composite number N_{δ} , specific heat ratio γ , Eckert *Ec*, and Pecklet number *Pe* – are defined as

$$M = \frac{u_{ref}}{a_{ref}}, Re = \frac{\rho u_{ref} L}{\mu_{ref}}, Pr = \frac{\mu_{ref} C_{p_{ref}}}{\kappa_{ref}}, Ec = (\gamma - 1)M^2,$$
 3-55

$$Kn = \frac{\lambda_{ref}}{L}, N_{\delta} = \frac{\mu_{ref}u_{ref}}{p_{ref}L}, \varepsilon = \frac{\Delta T_{ref}}{T_{ref}Ec \operatorname{Pr}},$$

Pe = Re Pr, $\frac{1}{\operatorname{Re}\operatorname{Pr}Ec} = \frac{1}{\operatorname{Pe}}\frac{T_{ref}C_{p_{ref}}}{u_{ref}^{2}}, \frac{1}{N_{\delta}\operatorname{Re}} = \frac{p_{ref}}{\rho_{ref}u_{ref}^{2}}$

The dimensionless form of the transport equations based on inverse power-law intermolecular model read as,

$$\mu^* = T^{*s}, \quad \kappa^* = T^{*s}.$$
 3-56

The dimensionless form of dissipation factor κ^* can be defined as

$$\kappa_{1}^{*} = \frac{\left(mk_{B}T_{ref}\right)^{1/4}}{\sqrt{\mu_{ref}}d_{ref}} \frac{T^{*1/4}}{2p^{*}d^{*}\sqrt{\mu^{*}}} N_{\delta} \left[\Pi^{*}:\Pi^{*} + 2\varepsilon \frac{\mathbf{q}^{*}.\mathbf{q}^{*}}{T^{*}}\right]^{1/2}.$$
 3-57

This equation can be written in compact form as the inverse power-law inter-molecular model is used in present work and $C_{N_{\delta}}$ is defined as

$$c_{N_{\delta}} = \frac{\left(mk_{B}T_{ref}\right)^{1/4}}{2\sqrt{\mu_{ref}}d_{ref}},$$
 3-58

$$\boldsymbol{\kappa}_{1}^{*} = \frac{c_{N_{\delta}}N_{\delta}}{p^{*}} \left[\boldsymbol{\Pi}^{*}: \boldsymbol{\Pi}^{*} + 2\varepsilon \, \frac{\boldsymbol{q}^{*} \cdot \boldsymbol{q}^{*}}{T^{*}} \right]^{1/2}$$
3-59

The dimensionless form the constitutive relations can be obtained based on proposed dimensionless variables, as shown in Figure 3-2.

Zero order Boltzmann-based model (Euler constitutive relations)

$$\mu^{*}, \kappa^{*} \rightarrow 0,$$

$$\Pi^{*} = 0, \mathbf{Q}^{*} = 0.$$
First order Boltzmann-based model (Navier-Stokes-Fourier constitutive relations)

$$\mu^{*}, \kappa^{*} \rightarrow f(T^{*})$$

$$\Pi^{*} = -2\mu^{*} \left[\nabla^{*} \mathbf{u}^{*} \right]^{(2)},$$

$$\mathbf{Q}^{*} = -\kappa^{*} \nabla^{*} T^{*}.$$
Second order Boltzmann-based model (Nonlinear coupled constitutive relations)

$$\mu^{*}, \kappa^{*} \rightarrow f(T^{*})$$

$$2 \left[\Pi^{*} \cdot \nabla^{*} \mathbf{u}^{*} \right]^{(2)} + \frac{2p^{*}}{N_{\delta}} \left[\nabla^{*} \mathbf{u}^{*} \right]^{(2)} = -\frac{1}{N_{\delta}} \frac{p^{*}}{\mu^{*}} \Pi^{*} \frac{\sinh \kappa_{1}}{\kappa_{1}},$$

$$-Ec \Pr \nabla \cdot \left(\frac{1}{N_{\delta} \operatorname{Re}} p^{*} \mathbf{I} + \frac{1}{\operatorname{Re}} \Pi^{*} \right) \cdot \frac{\Pi^{*}}{\rho^{*}} + \mathbf{Q}^{*} \cdot \nabla^{*} \mathbf{u}^{*} - \Pr \Pi^{*} \cdot \nabla^{*} T^{*} + \frac{\Pr}{N_{\delta}} p^{*} \nabla^{*} T^{*} = -\frac{\Pr}{N_{\delta}} \frac{p^{*}}{k^{*}} \mathbf{Q}^{*} \frac{\sinh \kappa_{1}}{\kappa_{1}},$$

Figure 3-2 A set of dimensionless Boltzmann-based constitutive models

In the rest part of present work, the non-dimensional equations are utilized, and the asterisk symbol is omitted in order to condense the notations. To solve (Eq. 3-52) using

advanced numerical methods. A numerical method for solving algebraic constitutive relations is provided in the remaining of this chapters; however, an explanation about available numerical methods for solving the partial differential equation of conservation laws is postponed to the next chapters.

3.5 An analysis on the Boltzmann-based constitutive models

As shown in Figure 3-2, the second-order constitutive relationships are a nonlinear and implicit function of pressure, velocity, velocity gradients, temperature, and temperature gradients; therefore, solving these relations numerically requires special attention. It is possible to recast these relations in reduced form by expressing them in terms of nonlinear coupled algebraic relations:

$$\hat{\boldsymbol{\Pi}}_{2nd-order} \boldsymbol{q}_{2nd-order} (\boldsymbol{c}_{N_{\delta}} \hat{\boldsymbol{R}}) = \hat{\boldsymbol{\Pi}}_{1st-order} + \left[\hat{\boldsymbol{\Pi}}_{2nd-order} \cdot \nabla \hat{\boldsymbol{u}} \right]^{(2)},$$

$$\hat{\boldsymbol{Q}}_{2nd-order} \boldsymbol{q}_{2nd-order} (\boldsymbol{c}_{N_{\delta}} \hat{\boldsymbol{R}}) = \hat{\boldsymbol{Q}}_{1st-order} + \hat{\boldsymbol{\Pi}}_{2nd-order} \cdot \hat{\boldsymbol{Q}}_{1st-order}.$$
3-60

Here the caret (^) over the symbol represents the quantities with the dimension of the ratio of the stress to the pressure which are defined as

$$\hat{\mathbf{\Pi}} = \frac{N_{\delta}}{p} \mathbf{\Pi}, \, \hat{\mathbf{Q}} = \frac{N_{\delta}}{p} \frac{\mathbf{Q}}{\sqrt{T/(2\varepsilon)}}, \, \nabla \hat{\mathbf{u}} = -2\mu \frac{N_{\delta}}{p} \nabla \mathbf{u}, \, \nabla \hat{T} = -k \frac{N_{\delta}}{p} \frac{\nabla T}{\sqrt{T/(2\varepsilon)}}.$$
3-61

 $\hat{\Pi}_{_{1st-order}}$ and $\hat{Q}_{_{1st-order}}$ values are reduced form of the first-order Boltzmann-based relations which are defined as

$$\hat{\boldsymbol{\Pi}}_{1st-order} = \left[\nabla \hat{\boldsymbol{u}}\right]^{(2)}, \qquad 3-62$$

$$\hat{\boldsymbol{Q}}_{_{1st-order}} = \nabla \hat{T}.$$
3-63

The nonlinear coupling factor $q(c\hat{R})$ and dimensionless form of the dissipation function \hat{R} derived from the Rayleigh–Onsager dissipation function [1] are given by

$$q_{2nd-order}(c_{N_{\delta}}\hat{R}) = \frac{\sinh\left(c_{N_{\delta}}\hat{R}\right)}{c_{N_{\delta}}\hat{R}},$$

$$\hat{R}^{2} \equiv \hat{\Pi} : \hat{\Pi} + \hat{Q} \cdot \hat{Q} .$$
3-64

3.5.1 One-dimensional compression-expansion constitutive relation

Considering the 1-D shock structure problem in which flow only evolves in x_1 direction, the viscous stress and heat flux constitutive relations (Eq. 3-60) can be written as

$$\begin{aligned} \hat{\Pi}_{1_{1_{zero-order}}} &= 0, \ \hat{Q}_{1_{zero-order}} = 0, \\ \hat{\Pi}_{1_{1_{first-order}}} &= \frac{2}{3} \frac{\partial \hat{u}_{1}}{\partial x_{1}}, \ \hat{Q}_{1_{1st-order}} = \frac{\partial \hat{T}_{1}}{\partial x_{1}}, \\ \begin{cases} \hat{\Pi}_{1_{1_{second-order}}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) = \hat{\Pi}_{1_{1_{second-order}}} (1 + \hat{\Pi}_{1_{1_{first-order}}}), \\ \hat{Q}_{1_{second-order}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) = (1 + \hat{\Pi}_{1_{1_{second-order}}}) \hat{Q}_{1_{1st-order}} + \frac{3}{4 \operatorname{Pr}} \hat{Q}_{1_{second-order}} \hat{\Pi}_{1_{1_{first-order}}}. \end{aligned}$$

where dissipation function reads as

$$\hat{R} = \sqrt{\frac{3}{2}\hat{\Pi}_{11_{second-order}}^2 + \hat{Q}_{1_{second-order}}^2},$$
3-66

and normal stress in y and z directions are defined as $\hat{\Pi}_{33} = \hat{\Pi}_{22} = -\frac{1}{2}\hat{\Pi}_{11}$ due to the traceless property of viscous stress tensor.

To obtain a general sense on the constitutive relations, the constitutive relation of Grad, and Burnett, and Boltzmann-based models are compared in Figure 3-3. It is shown that there exists a shock singularity in the constitutive profile of grad's model; however, the Boltzmann-based models are not influenced by an increment of compression force and there is no singularity in their solutions. They are well-posed (existence, uniqueness, and continuous dependence on the data) for all inputs, and they remove the high Mach number shock structure singularity completely [13, 64]. The solutions also show the free-molecular asymptotic behavior with increasing degree of expansion and velocity-shear, satisfying $\Pi_{11} \rightarrow -1$ or $\Pi_{11} + p \rightarrow 0$. This is due to the consistency of Eu's hydrodynamic equations with second laws of thermodynamics.



Figure 3-3 Comparison of Boltzmann-based constitutive models for shock-structure problem

3.5.2 One-dimensional shear-velocity constitutive relation

Considering the 1-D shear dominant flow problem in which flow only evolves in x_1 direction, while temperature gradients are negligible and velocity components are zero in x_2 and x_3 directions. The reduced form of viscous stress and heat flux constitutive relations can be derived from (Eq. 3-60) as

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$$\begin{aligned} \hat{\Pi}_{1_{1_{zero-order}}} &= 0, \ \hat{\Pi}_{1_{2_{zero-order}}} &= 0, \ \hat{Q}_{1_{zero-order}} &= 0, \\ \hat{\Pi}_{1_{1_{first-order}}} &= 0, \ \hat{\Pi}_{1_{2_{first-order}}} &= \frac{1}{2} \frac{\partial \hat{u}_{2}}{\partial x_{1}}, \ \hat{Q}_{1_{first-order}} &= 0, \\ \\ \begin{cases} \hat{\Pi}_{1_{second-order}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) &= -\frac{2}{3} \hat{\Pi}_{1_{2_{second-order}}} \hat{\Pi}_{1_{2_{first-order}}}, \\ \hat{\Pi}_{2_{2_{second-order}}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) &= \frac{4}{3} \hat{\Pi}_{1_{2_{second-order}}} \hat{\Pi}_{1_{2_{first-order}}}, \\ \hat{\Pi}_{1_{2_{second-order}}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) &= \left(\hat{\Pi}_{1_{second-order}} + 1 \right) \hat{\Pi}_{1_{2_{first-order}}}, \\ \hat{Q}_{1_{second-order}} &= 0. \end{aligned}$$

where dissipation function reads as

$$\hat{R} = \sqrt{3\hat{\Pi}_{11_{second-order}} (\hat{\Pi}_{11_{second-order}} - 1)}$$
, 3-68

and normal stress in y and z directions are defined as $\hat{\Pi}_{33} = \hat{\Pi}_{22} = -2\hat{\Pi}_{11}$ due to the traceless property of viscous stress tensor.

Note that the second-order constitutive relations are implicitly coupled to each other, therefore, they can be solved using the method of iterations. The general properties of the second-order constitutive relations for a monatomic gas are shown in Figure 3-4. It is obvious that the shear stress predicted by second-order model becomes very small compared to the first-order approximation since the large tangential velocity gradients are damped out due to sinus hyperbolic function in the second-order model. Such an asymptotic behavior indicates that the velocity slip phenomenon caused by the non-Newtonian effect can be explained in a very simple way. The ultimate origin of this behavior can be traced to the kinematic term – specifically, the constraint on the normal $(\hat{\Pi}_{22})$ and shear $(\hat{\Pi}_{12})$ stresses.



Figure 3-4 Comparison of Boltzmann-based constitutive models for 1-D shear-velocity problem

3.5.3 Two-dimensional decomposed constitutive relation

The full form of second-order constitutive relation in reduced form are given by

$$\hat{\mathbf{\Pi}}_{second-order} q_{2nd-order} (c_{N_{\delta}} \hat{R}) = \left[\nabla \hat{u} \right]^{(2)} + \left[\hat{\mathbf{\Pi}}_{second-order} \cdot \nabla \hat{u} \right]^{(2)},$$

$$\hat{\mathbf{Q}}_{second-order} q_{2nd-order} (c_{N_{\delta}} \hat{R}) = \hat{\mathbf{Q}}_{first-order} + \hat{\mathbf{\Pi}}_{second-order} \cdot \hat{\mathbf{Q}}_{first-order} + \frac{1}{2 \operatorname{Pr}} \hat{\mathbf{Q}}_{second-order} \cdot \nabla \hat{u}.$$

$$3-69$$

It is possible to rewrite these relations in expanded form as

$$\begin{split} \hat{\Pi}_{l_{1_{scont-order}}} q_{2nd-order}(c_{N_{s}}\hat{R}) &= \left[\frac{2}{3}\frac{\partial\hat{u}_{1}}{\partial x_{1}} - \frac{1}{3}\frac{\partial\hat{u}_{2}}{\partial x_{2}}\right] + \left[\hat{\Pi}_{l_{1_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{2}}\right] & 3-70 \\ \\ -\frac{1}{3}\left(\hat{\Pi}_{l_{1_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{2}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{2}}\right], & 3-70 \\ \\ \hat{\Pi}_{2_{2_{scont-order}}}q_{2nd-order}(c_{N_{s}}\hat{R}) &= \left[\frac{2}{3}\frac{\partial\hat{u}_{2}}{\partial x_{2}} - \frac{1}{3}\frac{\partial\hat{u}_{1}}{\partial x_{1}}\right] + \left[\hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{2_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{2}}\right], & 3-71 \\ \\ -\frac{1}{3}\left(\hat{\Pi}_{l_{1_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{2}}\right], & 3-71 \\ \\ -\frac{1}{3}\left(\hat{\Pi}_{l_{1_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{2}}\right], & 3-71 \\ \\ \hat{\Pi}_{l_{2_{scont-order}}}q_{2nd-order}(c_{N_{s}}\hat{R}) &= \frac{1}{2}\left[\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{2}}}{\partial x_{1}}\right] & 3-72 \\ \\ +\frac{1}{2}\left[\hat{\Pi}_{l_{1_{scont-order}}}\frac{\partial\hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\frac{\partial\hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{l_{2_{scont-order}}}\hat{\rho}_{1_{scont-order}}\frac{\partial\hat{u}_{1}}{\partial x_{2}}\right], & 3-72 \\ \\ \hat{Q}_{l_{scont-order}}q_{2nd-order}(c_{N_{s}}\hat{R}) &= \hat{Q}_{1}\left(+\left(\hat{\Pi}_{l_{1_{scont-order}}}\hat{\rho}_{1_{scont-order}}\frac{\partial\hat{u}_{2}}{\partial x_{2}} + \hat{\Pi}_{2_{2_{scont-order}}}\frac{\partial\hat{u}_{1}}}{\partial x_{2}}\right], & 3-72 \\ \\ \hat{Q}_{l_{scont-order}}q_{2nd-order}(c_{N_{s}}\hat{R}) &= \hat{Q}_{1}\left(+\left(\hat{\Pi}_{l_{1_{scont-order}}}\hat{\rho}_{1_{scont-order}}\frac{\partial\hat{u}_{2}}{\partial x_{2}} + \hat{\Pi}_{2_{2_{scont-order}}}\frac{\partial\hat{u}_{1}}}{\partial x_{2}}\right], & 3-73 \\ \\ \hat{Q}_{1_{scont-order}}q_{2nd-order}(c_{N_{s}}\hat{R}) &= \hat{Q}_{1}\left(+\left(\hat{\Pi}_{1_{scont-order}}\hat{\rho}_{1_{scont-order}\frac{\partial\hat{u}_{2}}{\partial x_{2}} + \hat{\Pi}_{2_{2_{scont-order}\frac{\partial\hat{u}_{2}}{\partial x_{2}}}\right), & 3-73 \\ \end{array}$$

$$\hat{Q}_{2_{second-order}} q_{2nd-order} (c_{N_{\delta}} \hat{R}) = \hat{Q}_{2_{first-order}} + \left(\hat{\Pi}_{12_{second-order}} \hat{Q}_{1_{first-order}} + \hat{\Pi}_{22_{second-order}} \hat{Q}_{2_{first-order}}\right) + \frac{1}{2 \operatorname{Pr}} \left(\hat{Q}_{1_{second-order}} \frac{\partial \hat{u}_{2}}{\partial x_{1}} + \hat{Q}_{2_{second-order}} \frac{\partial \hat{u}_{2}}{\partial x_{2}} \right),$$

$$3-74$$

with

$$\hat{R}^{2} = \hat{\Pi}_{second-order} : \hat{\Pi}_{second-order} + \hat{\mathbf{Q}}_{second-order} \cdot \hat{\mathbf{Q}}_{second-order}$$
$$= \hat{\Pi}_{11_{second-order}}^{2} + \hat{\Pi}_{22_{second-order}}^{2} + 2\hat{\Pi}_{12_{second-order}}^{2} + \hat{Q}_{1_{second-order}}^{2} + \hat{Q}_{2_{second-order}}^{2}.$$

$$3-75$$

In order to study the natural behavior of the Boltzmann-based constitutive models for a range of flow variations, the non-conserved variables obtained by first-order and second-order Boltzmann-based model are compared for a monatomic gas in Figure 3-5. It is obvious that the response of the first-order constitutive model to the applied stressand thermal forces are linear whereas the second-order model behaves nonlinearly.

The viscous stress tensor is not a function of the thermal force for the first-order linear model. The stress values are found to be symmetry with respect to the adiabatic line, and they are not influenced by the thermal forces. For the second-order model, the viscous stress tensor is a function of the shear forces and the thermal forces due to strong coupling between non-conserved variables through the Rayleigh-Onsager dissipation function. The stress values are influenced more by the stress forces than the thermal forces. Similarly to the first-order model, the monotonicity of the solution is preserved and the solution is symmetrical with respect to the adiabatic line while the solution is changing nonlinearly respect to the forces.



Figure 3-5 Comparison of the non-conservative stress variable determined by first-order and second-order Boltzmann-based constitutive models.

The response of heat flux vector to the thermal- and stress forces is shown in Figure 3-6. In the first-order constitutive model, the heat flux shows a linear and monotone behavior respect to thermal force. On the other hand, the second-order heat flux constitutive relations are influenced nonlinearly with respect to the both forces.



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Figure 3-6 Comparison of the non-conservative heat flux variable determined by first-order and second-order Boltzmann-based constitutive models.

Figure 3-7 illustrates a comparison between computed Rayleigh-Onsager dissipation parameter \hat{R} , using first-order and second-order constitutive models. As is known, \hat{R} implicitly represents the degree of thermal nonequilibrium for a process. In first-order models, the dissipation parameter has a circular shape which presents a uniform distribution of thermal nonequilibrium along the thermal stress and stress forces in all directions. On the other hand, in the second-order Boltzmann-based model, the deviation from equilibrium is not equally distributed state. It is shown that the weight of the stress forces on deviation from equilibrium state is more, and the thermal forces are considered as a secondary parameter which can influence the flow.



Figure 3-7 Comparison of the dimensionless dissipation parameter K_1 computed by first-order and second-order Boltzmann-based constitutive models.

3.5.4 Three-dimensional constitutive relation

The final and complete form of the constitutive relations in three-dimensional coordinates is given by

$$\begin{aligned} \hat{\mathbf{\Pi}}_{zero-order} &= 0, \ \hat{\mathbf{Q}}_{zero-order} = 0, \\ \hat{\mathbf{\Pi}}_{first-order} &= \left[\nabla \hat{\mathbf{u}}\right]^{trace-less}, \ \hat{\mathbf{Q}}_{first-order} = \nabla \hat{T}, \\ \hat{\mathbf{\Pi}}_{second-order} \mathbf{q}_{2nd-order} (c_{N_{\delta}} \hat{R}) &= \left[\nabla \hat{\mathbf{u}}\right]^{trace-less} + \left[\hat{\mathbf{\Pi}}_{second-order} \cdot \nabla \hat{\mathbf{u}}\right]^{trace-less}, \\ \hat{\mathbf{Q}}_{second-order} \quad \mathbf{q}_{2nd-order} (c_{N_{\delta}} \hat{R}) &= \hat{\mathbf{Q}}_{1st-order} + \hat{\mathbf{\Pi}}_{second-order} \cdot \hat{\mathbf{Q}}_{1st-order} + \frac{1}{2 \operatorname{Pr}} \hat{\mathbf{Q}}_{second-order} \cdot \nabla \hat{\mathbf{u}}. \end{aligned}$$

It can be written in index notation form as

$$\begin{split} \hat{\mathbf{\Pi}}_{\mathbf{1}_{1_{accont-outler}}} \mathbf{q}_{2nd-conder}(\mathbf{c}_{N_{s}}\hat{\mathbf{R}}) &= \begin{bmatrix} \frac{2}{3} \frac{\partial \hat{u}_{1}}{\partial x_{1}} - \frac{1}{3} \left(\frac{\partial \hat{u}_{2}}{\partial x_{2}} + \frac{\partial \hat{u}_{3}}{\partial x_{3}} \right) \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \frac{\partial \hat{u}_{1}}{\partial x_{1}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \frac{\partial \hat{u}_{1}}{\partial x_{2}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \frac{\partial \hat{u}_{1}}{\partial x_{3}} \end{bmatrix} - \alpha, \qquad 3-77 \\ \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \mathbf{q}_{2nd-conder}(\mathbf{c}_{N_{s}}\hat{\mathbf{R}}) = \begin{bmatrix} \frac{2}{3} \frac{\partial \hat{u}_{2}}{\partial x_{2}} - \frac{1}{3} \left(\frac{\partial \hat{u}_{1}}{\partial x_{1}} + \frac{\partial \hat{u}_{3}}{\partial x_{3}} \right) \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \frac{\partial \hat{u}_{2}}{\partial x_{2}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{2}_{accont-outler}} \frac{\partial \hat{u}_{2}}{\partial x_{2}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{2}_{accont-outler}} \frac{\partial \hat{u}_{2}}{\partial x_{3}} \end{bmatrix} - \alpha, \qquad 3-78 \\ \hat{\mathbf{\Pi}}_{\mathbf{3}_{accont-outler}} \mathbf{q}_{\mathbf{2}nd-conder}(\mathbf{c}_{N_{s}}\hat{\mathbf{R}}) = \begin{bmatrix} \frac{2}{3} \frac{\partial \hat{u}_{3}}{\partial x_{3}} - \frac{1}{3} \left(\frac{\partial \hat{u}_{1}}{\partial x_{1}} + \frac{\partial \hat{u}_{2}}{\partial x_{2}} \right) \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{\Pi}}_{\mathbf{1}_{accont-outler}} \frac{\partial \hat{u}_{2}}{\partial x_{2}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{2}_{accont-outler}} \frac{\partial \hat{u}_{3}}{\partial x_{1}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{2}_{accont-outler}} \frac{\partial \hat{u}_{3}}{\partial x_{1}} + \\ \hat{\mathbf{\Pi}}_{\mathbf{3}_{accont-outler}} \frac{\partial \hat{u}_{3}}{\partial x_{3}} \end{bmatrix} - \alpha, \qquad 3-79 \\ \hat{\mathbf{\Pi}}_{\mathbf{3}_{accont-outler}} \mathbf{q}_{\mathbf{3}$$
$$\begin{split} \hat{\Pi}_{3_{anvalued}} q_{2nd-order}(c_{N_s}\hat{R}) &= \frac{1}{2} \left[\frac{\partial \hat{u}_1}{\partial x_3} + \frac{\partial \hat{u}_3}{\partial x_1} \right] + \frac{1}{2} \left[\begin{array}{c} \hat{\Pi}_{1_{anvalued}} \frac{\partial \hat{u}_1}{\partial x_2} + \hat{\Pi}_{1_{3_{anvalued}}} \frac{\partial \hat{u}_1}{\partial x_3} + \hat{\Pi}_{1_{3_{anvalued}}} \frac{\partial \hat{u}_1}{\partial x_2} + 1 \right] \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{3_{anvalued}}} \frac{\partial \hat{u}_1}{\partial x_3} + 1 \\ \hat{\Pi}_{3_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_3} + \hat{\Pi}_{3_{3_{anvalued}}} \frac{\partial \hat{u}_1}{\partial x_3} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_1} + \hat{\Pi}_{3_{anvalued}} \frac{\partial \hat{u}_1}{\partial x_3} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{3_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_1} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + \hat{\Pi}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_2} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_2} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_3} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_3} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_3} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_2}{\partial x_3} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_3}{\partial x_3} + 1 \\ \hat{\Omega}_{2_{anvalued}} \frac{\partial \hat{u}_4}{\partial x_4} + 1 \\ \hat{\Omega}_{2_{anvalued}$$

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where

$$\alpha = \frac{1}{3} \begin{pmatrix} \hat{\Pi}_{1_{1_{second-order}}} & \frac{\partial \hat{u}_{1}}{\partial x_{1}} + \hat{\Pi}_{1_{2_{second-order}}} & \frac{\partial \hat{u}_{2}}{\partial x_{1}} + \hat{\Pi}_{1_{3_{second-order}}} & \frac{\partial \hat{u}_{3}}{\partial x_{1}} + \\ \hat{\Pi}_{1_{2_{second-order}}} & \frac{\partial \hat{u}_{1}}{\partial x_{2}} + \hat{\Pi}_{2_{2_{second-order}}} & \frac{\partial \hat{u}_{2}}{\partial x_{2}} + \hat{\Pi}_{2_{3_{second-order}}} & \frac{\partial \hat{u}_{3}}{\partial x_{2}} + \\ \hat{\Pi}_{1_{3_{second-order}}} & \frac{\partial \hat{u}_{1}}{\partial x_{3}} + \hat{\Pi}_{2_{3_{second-order}}} & \frac{\partial \hat{u}_{2}}{\partial x_{3}} + \hat{\Pi}_{3_{3_{second-order}}} & \frac{\partial \hat{u}_{3}}{\partial x_{3}} + \\ \hat{\Pi}_{3_{3_{second-order}}} & \frac{\partial \hat{u}_{1}}{\partial x_{3}} + \hat{\Pi}_{2_{3_{second-order}}} & \frac{\partial \hat{u}_{2}}{\partial x_{3}} + \hat{\Pi}_{3_{3_{second-order}}} & \frac{\partial \hat{u}_{3}}{\partial x_{3}} \end{pmatrix}, \quad 3-85$$
and
$$\hat{R} = \sqrt{\hat{\Pi}_{second-order}} : \hat{\Pi}_{second-order} + \hat{Q}_{second-order} \cdot \hat{Q}_{second-order}}. \quad \text{Knowing that}$$

$$\hat{\Pi}_{3_{3_{second-order}}}} = -\left(\hat{\Pi}_{1_{1_{second-order}}}} + \hat{\Pi}_{2_{2_{second-order}}}}\right) \text{ due to the traceless property of the stress tensor,}$$

 \hat{R} can be written in more compact form as

$$\hat{R} = \sqrt{\frac{2\left(\hat{\Pi}_{11_{second-order}}^{2} + \hat{\Pi}_{22_{second-order}}^{2} + \hat{\Pi}_{11_{second-order}}^{2} \hat{\Pi}_{22_{second-order}}^{2}\right) + 2\left(\hat{\Pi}_{12_{second-order}}^{2} + \hat{\Pi}_{13_{second-order}}^{2} + \hat{\Pi}_{23_{second-order}}^{2}\right) + .$$

$$\hat{Q}_{1_{second-order}}^{2} + \hat{Q}_{2_{second-order}}^{2} + \hat{Q}_{3_{second-order}}^{2} + \hat{Q}_{3_{second-order}}^{2}$$

$$3-86$$



the stress acts on a plane normal to the *x*-axis, in the *z*-direction.



the stress acts on a plane normal to the y-axis, in the z-direction.

Figure 3-8 Comparison of the stress tensor for first-order and second-order constitutive models in 3-D phase space.

Figure 3-8 depicts a quantitative comparison of stress tensor between first-order (NSF) and second-order (NCCR) constitutive models in three-dimensional space. The 3-D NCCR relations are solved directly using a coupled solver based on Brydon's method, while first-order models are computed explicitly. The first-order model shows a linear behavior of the stress tensor; however, nonlinear behavior of NCCR model in the computation of the stress tensor is tangible. The magnitude of stress value computed by the second-order model is considerably less than of that determined by the first-order model. In the first-order model, the variation of stress tensor in *xz*-direction is not observed, whilst this variation is not negligible for the second-order model.

Figure 3-9 shows the response of Boltzmann-based models to the thermal-, and stress forces implied in the z-direction. It is shown that the first-order model does not predict any heat flux in x and y directions since thermal forces in these directions are zero. In contrary, the second-order model predicts the considerable amount of heat flux in those directions due to the coupling of the thermal- and stress forces through Rayleigh-Onsager dissipation parameter.



Heat flux value in *z*-direction

Figure 3-9 Comparison of the heat flux for first-order (NSF) and second-order (NCCR) constitutive models in 3-D Space.

3.6 Numerical solvers for solving nonlinear coupled constitutive relations

3.6.1 Iterative method

The second-order Boltzmann-based model consists of nine nonlinear implicit algebraic equations of the non-conserved variables $(\hat{\Pi}_{11}, \hat{\Pi}_{12}, \hat{\Pi}_{13}, \hat{\Pi}_{22}, \hat{\Pi}_{23}, \hat{\Pi}_{33}, \hat{Q}_1, \hat{Q}_2, \hat{Q}_3)$ for the eleven known variables $(p, T, \nabla u, \nabla T)$. Owing to the highly nonlinear terms (e.g., $q_{2nd}(c\hat{R})$ function), developing a proper numerical method for solving the nonlinear system appears to be a daunting task. Nevertheless, it was shown that this task can be done by serving the *method of iterations* [14, 64, 65].

In the case of the three-dimensional problems, the viscous stress and heat flux components $\hat{\Pi}_{11}$, $\hat{\Pi}_{12}$, $\hat{\Pi}_{13}$, \hat{Q}_1 on a line in the physical plane induced by thermodynamic forces (velocity and temperature gradients, $\partial u_1 / \partial x_1$, $\partial u_2 / \partial x_1$, $\partial u_3 / \partial x_1$, $\partial T / \partial x_1$) can be approximated as the sum of three solvers; a solver on $(\partial u_1 / \partial x_1, 0, 0, \partial T / \partial x_1)$ and solvers on $(0, \partial u_2 / \partial x_1, 0, 0)$ and $(0, 0, \partial u_3 / \partial x_1, 0)$.

Hence, the shear stress $(\Pi_{xx}, \Pi_{xy}, \Pi_{xz}, Q_x)$ in the case of x-direction can be decomposed as function of (u_x, v_x, w_x, T_x) ;

$$f(u_x, \mathbf{v}_x, \mathbf{w}_x, \mathbf{T}_x) = f_1(u_x, 0, 0, \mathbf{T}_x) + f_2(0, \mathbf{v}_x, 0, 0) + f_3(0, 0, \mathbf{w}_x, 0).$$

The iteration procedures can be designed for these solvers, individually. In the first solver which represents the compression and expansion of a monatomic gas, the positive shear stress $\hat{\Pi}_x$ and heat flux \hat{Q}_x values are determined based on

$$\hat{R}_{n+1} = \frac{1}{c_{N_{\delta}}} \sinh^{-1} \left[c_{N_{\delta}} \left(\hat{\Pi}_{xx_{n}} + 1 \right) \hat{R}_{0} \right],$$

$$\frac{\hat{Q}_{x_{n+1}}}{\hat{\Pi}_{xx_{n+1}}} = \frac{\hat{Q}_{x_{n}}}{\hat{\Pi}_{xx_{n}}} = \frac{\hat{Q}_{x_{0}}}{\hat{\Pi}_{xx_{0}}},$$
3-87

and negative value of $\hat{\Pi}_{x}$ and \hat{q}_{x} are calculated by

$$\hat{\Pi}_{xx_{n+1}} = \frac{\Pi_{xx_0}}{q_{2nd-order}(c_{N_{\delta}}\hat{R}_n) - \hat{\Pi}_{xx_0}},$$

$$\hat{Q}_{x_{n+1}} = \frac{(\hat{\Pi}_{xx_n} + 1)}{q_{2nd-order}(c_{N_{\delta}}\hat{R}_n)}\hat{Q}_{x_0}.$$
3-88

In the second, and the third solver of the shear flow, the $\hat{\Pi}_{xx}$ can be obtained for a given $\hat{\Pi}_{xy_0}$, $\hat{\Pi}_{xz_0}$ through the iterative relation

$$\hat{\Pi}_{xx_{n+1}} = \frac{\hat{\Pi}_{xy_0}^2}{3q_{2nd-order}^2(c_{N_\delta}\hat{R}_n)/2 + \hat{\Pi}_{xy_0}}, \ \hat{\Pi}_{xy_{n+1}} = \operatorname{sign}(\hat{\Pi}_{xy_0}) \left[-\frac{3}{2}(\hat{\Pi}_{xx_{n+1}} + 1)\hat{\Pi}_{xx_{n+1}} \right]^{1/2}.$$
(2.15)

Here $\hat{\Pi}_{xx_1}$ and \hat{Q}_{x_1} denote the initial guesses of the solution. The summary of these solvers and their outcomes are shown in below;

$$\begin{array}{c|c} f_1(u_x,0,0,\mathrm{T}_x) & f_2(0,\mathrm{v}_x,0,0) & f_3(0,0,\mathrm{w}_x,0) \\ \hline \hat{\Pi}_{xx-1x}, \hat{\Pi}_{yy-1x} = -\frac{1}{2}\hat{\Pi}_{xx-1x}, & \hat{\Pi}_{xx-2x}, \hat{\Pi}_{xy-2x}, & \hat{\Pi}_{xx-3x}, \hat{\Pi}_{xz-3x}, \\ \widehat{\Pi}_{xy-1x} = 0, \hat{\Pi}_{xz-1x} = 0, & \hat{\Pi}_{xz-2x} = 0, \hat{\Pi}_{yz-2x} = 0, \\ \widehat{\Pi}_{yy-2x} = -2\hat{\Pi}_{xx-2x}, & \hat{\Pi}_{yy-3x} = 0, \hat{\Pi}_{yz-3x} = 0, \\ \widehat{\Pi}_{yy-3x} = \hat{\Pi}_{xx-3x}, & \hat{\Pi}_{zz-3x}, \\ \widehat{\Pi}_{zz-2x} = \hat{\Pi}_{xx-2x}, & \hat{\Pi}_{zz-3x} = -2\hat{\Pi}_{xx-3x}, \\ \widehat{\Pi}_{zz-3x} = -2\hat{\Pi}_{xx-3x}, & \hat{\Pi}_{zz-3x} = -2\hat{\Pi}_{xx-3x}, \\ \widehat{\Pi}_{zz-3x} = 0, & \hat{\Pi}_{zz-3x} = 0. \end{array}$$

Similarly, it is possible to find the value of stress and heat flux in two other primary directions. In the case of y-direction, the shear stress $\hat{\Pi}_{yx}$, $\hat{\Pi}_{yy}$, $\hat{\Pi}_{yz}$, \hat{Q}_y on a line in the physical plane induced by thermodynamic forces (velocity and temperature gradients, $\partial u_1 / \partial x_2$, $\partial u_2 / \partial x_2$, $\partial u_3 / \partial x_2$, $\partial T / \partial x_2$) can be approximated as the sum of three solvers;

$$f(u_{y}, \mathbf{v}_{y}, \mathbf{w}_{y}, \mathbf{T}_{y}) = f_{1}(0, \mathbf{v}_{y}, 0, \mathbf{T}_{y}) + f_{2}(u_{y}, 0, 0, 0) + f_{3}(0, 0, \mathbf{w}_{y}, 0)$$

where

$$\begin{array}{ccc} f_1(0,\mathbf{v}_y,0,\mathbf{T}_y) & f_2(u_y,0,0,0) & f_3(0,0,\mathbf{w}_y,0) \\ \hat{\Pi}_{yy-1y},\hat{\Pi}_{xx-1y} = -\frac{1}{2}\hat{\Pi}_{yy-1y}, & \hat{\Pi}_{xy-2y},\hat{\Pi}_{yy-2y}, & \hat{\Pi}_{yy-3y},\hat{\Pi}_{yz-3y}, \\ \hat{\Pi}_{xy-1y} = 0,\hat{\Pi}_{xz-1y} = 0, & \hat{\Pi}_{xz-2y} = 0, \hat{\Pi}_{yz-2y} = 0 & \hat{\Pi}_{xy-2y} = 0, \\ \hat{\Pi}_{xx-2y} = -2\hat{\Pi}_{yy-2y}, & \hat{\Pi}_{xx-3y} = 0, \\ \hat{\Pi}_{xx-2y} = -2\hat{\Pi}_{yy-2y}, & \hat{\Pi}_{xz-3y} = \hat{\Pi}_{yy-3y}, \\ \hat{Q}_y = \hat{Q}_{1y}, & \hat{Q}_{2y} = 0, & \hat{Q}_{3y} = 0. \end{array}$$

In the case of *z*-direction, the shear stress $\Pi_{zx}, \Pi_{zy}, \Pi_{zz}, q_z$ are decomposed into three functions;

$$f(u_z, v_z, w_z, T_z) = f_1(0, 0, w_z, T_z) + f_2(u_z, 0, 0, 0) + f_3(0, v_z, 0, 0)$$

such that

$$\begin{array}{c|c} f_1(0,0,\mathbf{w}_z,\mathbf{T}_z) & f_2(u_z,0,0,0) & f_3(0,\mathbf{v}_z,0,0) \\ \hline \hat{\Pi}_{zz^{-1z}}, \hat{\Pi}_{xx^{-1z}} = -\frac{1}{2}\hat{\Pi}_{zz^{-1z}}, & \hat{\Pi}_{xz^{-2z}}, \hat{\Pi}_{zz^{-2z}}, & \hat{\Pi}_{zz^{-2z}}, \\ \hat{\Pi}_{xy^{-2z}} = 0, \hat{\Pi}_{yz^{-2z}} = 0, \\ \hat{\Pi}_{xz^{-2z}} = 0, \hat{\Pi}_{yz^{-2z}} = 0, \\ \hat{\Pi}_{xz^{-2z}} = -2\hat{\Pi}_{zz^{-2z}}, & \hat{\Pi}_{xx^{-3z}} = 0, \\ \hat{\Pi}_{xx^{-3z}} = \hat{\Pi}_{zz^{-3z}}, \\ \hat{\Pi}_{yy^{-2z}} = \hat{\Pi}_{zz^{-2z}}, & \hat{\Pi}_{yy^{-3z}} = -2\hat{\Pi}_{zz^{-3z}}, \\ \hat{\Pi}_{yy^{-3z}} = -2\hat{\Pi}_{zz^{-3z}}, & \hat{\Pi}_{yy^{-3z}} = -2\hat{\Pi}_{zz^{-3z}}, \\ \hat{Q}_{zz} = \hat{Q}_{1z}, & \hat{Q}_{2z} = 0, & \hat{Q}_{3z} = 0. \end{array}$$

Finally, we have

$$\begin{split} \hat{\Pi}_{xx} &= \hat{\Pi}_{xx-1x} + \hat{\Pi}_{xx-2x} + \hat{\Pi}_{xx-3x} - \left(\frac{\hat{\Pi}_{yy-1y}}{2} + \frac{\hat{\Pi}_{zz-1z}}{2}\right) - 2\left(\hat{\Pi}_{yy-2y} + \hat{\Pi}_{zz-2z}\right) + \hat{\Pi}_{yy-3y} + \hat{\Pi}_{zz-3x}, \\ \hat{\Pi}_{yy} &= \hat{\Pi}_{yy-1y} + \hat{\Pi}_{yy-2y} + \hat{\Pi}_{yy-3y} - \left(\frac{\hat{\Pi}_{xx-1x}}{2} + \frac{\hat{\Pi}_{zz-1z}}{2}\right) - 2\left(\hat{\Pi}_{xx-2x} + \hat{\Pi}_{zz-3z}\right) + \hat{\Pi}_{zz-2z} + \hat{\Pi}_{xx-3x}, \\ \hat{\Pi}_{zz} &= \hat{\Pi}_{zz-1z} + \hat{\Pi}_{zz-2z} + \hat{\Pi}_{zz-3z} - \left(\frac{\hat{\Pi}_{xx-1x}}{2} + \frac{\hat{\Pi}_{yy-1y}}{2}\right) - 2\left(\hat{\Pi}_{xx-3x} + \hat{\Pi}_{yy-3y}\right) + \hat{\Pi}_{xx-2x} + \hat{\Pi}_{yy-2y}, \\ \hat{\Pi}_{xy} &= \hat{\Pi}_{xz-2x} + \hat{\Pi}_{xz-2y}, \quad \hat{\Pi}_{xz} = \hat{\Pi}_{xz-3y} + \hat{\Pi}_{xz-2z}, \quad \hat{\Pi}_{yz} = \hat{\Pi}_{yz-3y} + \hat{\Pi}_{yz-3z}, \\ \hat{Q}_{x} &= \hat{Q}_{1x}, \quad \hat{Q}_{y} = \hat{Q}_{1y}, \quad \hat{Q}_{z} = \hat{Q}_{1z}, \quad \hat{\Pi}_{xx} + \hat{\Pi}_{yy} + \hat{\Pi}_{zz} = 0. \end{split}$$

After convergence, the converged values are implemented back into dimensionless space as

$$\mathbf{\Pi} = \frac{p}{N_{\delta}} \hat{\mathbf{\Pi}}, \mathbf{Q} = \hat{\mathbf{Q}} \frac{p}{N_{\delta}} \sqrt{T/(2\varepsilon)}, \quad \nabla \mathbf{u} = -\nabla \hat{\mathbf{u}} \frac{p}{2\mu N_{\delta}}, \quad \nabla T = -\nabla \hat{T} \frac{p\sqrt{T/(2\varepsilon)}}{kN_{\delta}}.$$
 3-89

3.6.2 Broyden method

Broyden's method is a quasi-Newton method which is used for finding roots of a nonlinear system of equations. In Newton's method, the exact Jacobian matrix is required for solving a nonlinear system f(x) = 0 at each iteration. However, computing this Jacobian is a difficult and expensive operation for most of the nonlinear systems. Broyden's method computes the whole Jacobian only at the first iteration and updates it at the other iterations.

To solve nonlinear system of constitutive equations based on Broyden method, first it is necessary to bring all terms on left-hand side and makes a list of functions and unknown variables $\mathbf{x} = [\hat{\Pi}_{11}, \hat{\Pi}_{12}, \hat{\Pi}_{13}, \hat{\Pi}_{22}, \hat{\Omega}_{2}, \hat{Q}_{1}, \hat{Q}_{2}, \hat{Q}_{3}],$

62

$$f(\mathbf{x}) = \begin{cases} \hat{\mathbf{\Pi}}_{second-order} q_{2nd-order} (c_{N_{j}} \hat{R}) - [\nabla \hat{\mathbf{u}}]^{(2)} - [\hat{\mathbf{\Pi}}_{second-order} \cdot \nabla \hat{\mathbf{u}}]^{(2)} = 0 & \text{for } x_{i} = [x_{i} \dots x_{s}], \\ \hat{\boldsymbol{\mathcal{Q}}}_{second-order} q_{2nd-order} (c_{N_{j}} \hat{R}) - \hat{\boldsymbol{\mathcal{Q}}}_{1st-order} - \hat{\mathbf{\Pi}}_{second-order} \cdot \hat{\boldsymbol{\mathcal{Q}}}_{1st-order} - \frac{1}{2 \operatorname{Pr}} \hat{\boldsymbol{\mathcal{Q}}}_{second-order} \cdot \nabla \hat{\mathbf{u}} = 0 & \text{for } x_{i} = [x_{i}, x_{j}, x_{s}], \end{cases}$$

Then, the Jacobian matrix is determined iteratively based on a secant equation as

$$\mathbf{J}^{n} \approx \mathbf{J}^{n-1} + \frac{f(\mathbf{x}^{n}) - f(\mathbf{x}^{n-1}) - \mathbf{J}^{n}(\mathbf{x}^{n} - \mathbf{x}^{n-1})}{\|\mathbf{x}^{n} - \mathbf{x}^{n-1}\|^{2}} \left[\mathbf{x}^{n} - \mathbf{x}^{n-1}\right]^{T}.$$
3-90

where n denotes the iteration index. The inverse of Jacobian matrix can be updated using Sherman-Morrison formulation to obtain well behavior Broyden scheme,

$$\mathbf{J}^{n \text{ inverse}} \approx \mathbf{J}^{n-1 \text{ inverse}} + \frac{(\mathbf{x}^{n} - \mathbf{x}^{n-1}) - \mathbf{J}^{n-1 \text{ inverse}} \left(f(\mathbf{x}^{n}) - f(\mathbf{x}^{n-1}) \right)}{\left[\mathbf{x}^{n+1} - \mathbf{x}^{n} \right]^{T} \mathbf{J}^{n-1 \text{ inverse}} \left(f(\mathbf{x}^{n}) - f(\mathbf{x}^{n-1}) \right)} \left[\mathbf{x}^{n+1} - \mathbf{x}^{n} \right]^{T} \mathbf{J}^{n-1 \text{ inverse}}}.$$
 3-91

Finally, the unknowns are updating in Newton direction as

$$\mathbf{x}^{n+1} \approx \mathbf{x}^n - \mathbf{J}^{n \text{ inverse}} f(\mathbf{x}^n), \qquad 3-92$$

and the process is repeated until the solver converges.

CHAPTER 4. Discontinuous Galerkin method: Foundations

Percy W. Bridgman (1882-1961):

"...what a man means by a term is to be found by observing what he does with it, not by what he says about it."

4.1 **Basic of numerical analysis**

The initial step of a numerical analysis is to employ or develop an appropriate mathematical model for describing the physics of a given problem. The model must be able to explain the physics in an acceptable level of accuracy, and must be as simple as possible. This branch of fluid dynamics has been under development from two centuries ago[1, 13, 14, 28, 58, 66-70]. As a result of the mathematical modeling, a set of the nonlinear partial differential equation is obtained and solved by the aid of the legitimate numerical method.

Several compromises need to be involved in design process of a numerical method, as clarified in Figure 4-1. It is well known that there is no perfect numerical method. Every method has its drawbacks.



Figure 4-1 Required steps to develop a reliable and accurate numerical model

Accuracy of a numerical method for solving the convective-diffusive system depends on two factors; the way of domain decomposition (i.e., triangulation), and the properties of the employed discretization techniques. It can be shown that there exists at least one weak solution for a system of equations, if the numerical flux functions are Lipschitz continuous [71, 72]. The convective-dominant flows are commonly highly nonlinear, and the vigorous entropy violation commonly presents in the vicinity of the steep and sharp gradients like strong discontinuities, boundary layers, and stagnation points [73]. Thus, finding an appropriate way to direct the numerical solution into the entropy solution is more emphasized.

Considering the weak form the hyperbolic system of partial differential equations, and applying the method of line (MOL) to decouple the time and spatial coordinates, the decoupled system in time and space achieves in which time and space are discretized independently. As a consequence of sequence arrangement of the numerical efforts, a system of algebraic equation can be obtained

$$\frac{\partial \mathbf{w}}{\partial t} + \nabla \mathbf{F}^{inviscid}(\mathbf{w}) + \nabla \mathbf{F}^{viscous}(\mathbf{w}, \nabla \mathbf{w}) = \mathbf{s} \quad \rightarrow \quad \mathbf{Aw} = \mathbf{B}$$

$$4-1$$

where the coefficient of the matrix \mathbf{A} , and \mathbf{B} are tied-up to both the applied discretization method and the way of the numerical interpolation.

The properties of the matrix \mathbf{A} and the discrete operators involved in the assembly of the right-hand side \mathbf{B} may make or break the entire numerical simulation. It is necessary to define certain physical and numerical criteria [74] that guarantee the wellposedness and robustness of the designed numerical method with an acceptable level of accuracy for a wide range of the applications.

To guarantee the well-posedness of the numerical method, at least few constraints must be satisfied. According to Lax-Richtmyer theorem, the linear stability and consistency are necessary and sufficient conditions for convergence of the initial boundary value problems (IBV) to a solution [75]. However, the satisfaction of these constraints does not guarantee that the obtained weak solution is the entropy solution.

It is needed to enforce a set of constraints — conservation, Boundedness, and positivity — at the discrete level in order to converge the conservation laws into the entropy solution [71, 76]. The obligation of the physical and numerical constraints^{5,6} to the numerical method, results in a physical numerical solution for conservation laws, only if the time step and cell size *h* have been chosen sufficiently small.

As defining 'the sufficiently small' value is highly problem dependent, the final judgment on the accuracy of the mathematical, and numerical models should be postponed until the validation and verification (V&V) are fulfilled [77]. The importance of these constraints and their effect on the accuracy of the approximate solution are investigated in the development of the present Modal DG methods.

⁵ Kruzkov's theorem said that there exist the unique weak solution of the conservation laws, on the condition that numerical solution satisfies the cell entropy inequality

⁶ Lax-Wendroff states that any *bounded*, *consistent*, *and conservative* method converges to the weak solution (i.e., *entropy solution*) of the nonlinear conservation law.

4.2 First-order numerical methods

In the early 20th century, many researches were established to design the robust and efficient numerical methods [78-80]. Most of the studies were directed to solve either the scalar model equations (i.e., burger and viscous burgers) or Euler gas dynamics equations [80]. The extension of the numerical models for solving Navier-stokes-Fourier (NSF) equations started from the end of the twentieth century and continues until today.



Figure 4-2 Taxonomy of first-order numerical methods

There are numerous first-order methods in which the exact solution is approximated by a piecewise constant polynomial, as shown in Figure 4-2. The first-order methods are not accurate enough to be served solely for studying nonlinear hyperbolic systems where any compression wave will turn into a discontinuity regardless to matter that how much initial condition is smooth. In estimated solution by first order methods, the discontinuities are smeared and a substantial amount of artificial diffusion are generated in a numerical process due to the dissipative properties of these methods. Thus, they are commonly considered as a building block for development of the high-order methods and are served to obtain a very crude approximation of the true solution.

4.3 High-order numerical methods

Higher-order methods are beneficial and advantageous in sense of computational costs and accuracy, even though, they are very sensitive to the initial conditions and highly motivated to generate spurious oscillations near discontinuities [81].

Many researches have been conducted for the development of the high-order methods during the past 50 years [76, 82-92]; however, there are few available detailed summaries on high-order methods in the books. As one of the motivations of the present work is to provide a self-contained summary of the numerical methods, a taxonomy of high-order methods is depicted in Figure 4-3. As it is obvious, there are several ways for obtaining high-order solutions such as; expanding a Taylor series; reconstructing a high-order flux function at interface of the control volumes; correcting the numerical flux functions using anti-diffusion treatment; reconstruction high-order solution based on nonlinear stencils; employing the spectral methods.

Among all high-order methods, there is a class of numerical schemes, called the spectral *hp* methods which are particularly efficient for the high-order approximation of the CFD applications. According to the terminology defined in [93, 94], spectral methods are those in which the numerical solution is fitted by series of functions and the accuracy of the approximate solution improves with increasing the number of modal functions. Based on the definition of the polynomial space (ansatz) function, spectral *hp* methods can be classified into several categories.

4.4 Spectral categories

The choice of test functions distinguishes the number of standard formulations for the spectral methods, such as *collocation*, *Petrov-Galerkin*, *Galerkin* methods. Although Galerkin method provides the most robust FEM formulation and it is recommended for most of the problems, it may not a bad idea to address the features of the other methods very briefly.

In collocation method, the test functions are defined as delta functions at discretely chosen points, so-called collocation points. In this method, the differential equations are needed to be satisfied exactly at the collocation points. However, in Galerkin and Petrov-Galerkin methods, the differential equations are solved using the method of weighted residual (MWR) requiring that the integral of the residual of the FEM formulation becomes zero inside the computational domain. In Galerkin method, test

functions are chosen to be the same as the basis function. They are selected to be infinitely smooth functions in order to satisfy some or all of the boundary conditions. However, in Petrov-Galerkin formulation, the basis functions are different from the test functions, and none of the test functions need to satisfy the boundary conditions. Thus, an additional set of equations is considered for enforcing the boundary conditions [95].



Figure 4-3 Taxonomy of high-order numerical schemes

4.5 Spectral *hp* methods

In spectral hp methods, the computational domain is divided into a number of local elements with a size of h and the solution in each local element is approximated using a polynomial expansion of degree p. In these methods, attaining a high-order solution by increasing the degree of p can be computationally more expensive than reducing the size of h by the same factor [94, 96, 97]. However, the accuracy gain obtained with p enhancement is normally greater than the gain obtained with the h refinement [93].

The choice of the polynomial space function is the main feature that distinguishes high-order methods from finite difference and finite volume methods. Spectral *hp* methods can be classified based on the definition of the polynomial space (ansatz) function into several categories including; discontinuous Galerkin (DG), spectral difference (SD), spectral volume (SV) and correction procedure via reconstruction (CPR) methods.

4.6 Discontinuous Galerkin (DG) versus continuous Galerkin (CG)

Finite element Galerkin method is divided into two branches: continuous Galerkin (CG) and discontinuous Galerkin (DG) methods. The difference between DG and CG polynomial space functions is depicted in Figure 4-4.



Figure 4-4 Discontinuous Galerkin solution versus continuous Galerkin solution

In CG methods, the global solution is discretized using the finite dimensional functions which are locally continuous in character with finite regularities that attempt to represent the shape of the true solution. Therefore, they may not always produce the true solution at some flow conditions like high-speed conditions [95]. A Hilbert space $H^1(\Omega)$ is used to approximate the finite polynomial space function. It means that, if

function f(x) belongs to Hilbert space $H^{1}(\Omega)$, it has to be continuous across the elements and satisfy

$$\int_{\Omega} \left(f\left(x\right)^2 + \nabla f(x) \cdot \nabla f(x) \right) d\Omega \le \infty.$$
4-2

On the other hand, the DG spectral methods consider globally smooth functions as the test functions and allow more freedom to define polynomial space function which provides enough capability to study the high-speed problems. They use a least-square space function $L^2(\Omega)$ for approximating the polynomial space function, therefore, the space function needs to be continuous inside the element space but not over the elemental interfaces

$$\int_{\Omega} f(x)^2 d\mathbf{\Omega} \le \infty. \tag{4-3}$$

In DG method, the degree of freedoms (DOFs) are overlapped on the elemental edges and vertices. Therefore, the computational cost of DG method for inverting the mass matrix is higher than that of CG method. Nonetheless, DG may not always be more expensive than CG method since the application of additional DOFs in DG method yields more accurate solutions than CG method on the same mesh. In addition, owing to the discontinuous polynomial space function and usage of an upwind monotone numerical flux function at the interface of the elements [98], DG method is often considered the best choice for numerically solving convective-dominated problems.

4.7 Discontinuous Galerkin method

4.7.1 History of DG methods

The first mathematical analysis on DG method was investigated by Le-Saint and Raviart [99]. They reported the order of accuracy of 2p+1 for original DG method when polynomials up to degree p are used. In 1986, Johnson and Pitkaranta [100] employed the original DG method to study a linear scalar hyperbolic problem with a smooth solution. They proved the rate of convergence of p+1/2 for general triangulations discretization.

Next, Richter [101] proposed the extension of the original DG method to linear scalar convection-diffusion equation, and showed that the order of convergence of the

original DG method is p+1/2 when the viscosity coefficient is in the same order of the mesh size, and convection is dominant. Cockburn and Shu [92, 98, 102] matured the original DG method and introduced the explicit Runge-Kutta discontinuous Galerkin method (RK-DG). Bassi and Rebay [103], and Cockburn and Shu [104] studied the hyperbolic systems with very smooth solutions using the RK-DG method. They reported the order of convergence of p+1 for very smooth solutions of DG method.

Later, many other researchers study the convergence behavior of DG methods on both Cartesian and unstructured grids and reports mostly the order of p+1/2 for DG methods [105, 106]. Although there are numerous available convergence analyses for DG method, they have a common point. All reported convergence analysis assumed that the solution of the interested problem is sufficiently smooth and there is no shock in the domain. As the best knowledge of the author, there is no reported convergence analysis of DG methods for viscous shock problem in the literature.

As a part of this dissertation, it is decided to conduct a performance analysis on DG method at presence of the strong and stiff flow conditions. Thus, in the following chapters, the order of accuracy of DG method for both very smooth and very stiff solutions are examined and reported [107, 108].

4.7.2 Modal DG method versus nodal DG method

In Galerkin framework, there are two general approaches to characterize the polynomial approximate solutions w_h : nodal and modal approaches. Modal DG methods are generalization of the nodal DG methods. The modal solutions can be converted into the nodal solutions using Vandermonde transformation tensor. However, it is not possible to obtain modal solutions from nodal solutions.

Modal DG methods are more advantageous than nodal DGs for nonlinear problems [93]. They had been widely used in the development of the RK-DG method and had been employed for solving hyperbolic systems, and gas dynamics equations [98, 102, 103, 109-112]. In present work, the modal DG approach is desired and used; nevertheless, a very brief explanation about nodal DGs is presented in below.

In nodal approach, elemental space are represented by multiple nodes and local polynomial functions are determined based on nodal deformation as

$$\mathbf{w}(\mathbf{x},t) \approx \mathbf{w}_{h}(\mathbf{x},t) = \sum_{j=1}^{N_{p}} \hat{w}_{j}(\mathbf{x},t) l_{j}(\mathbf{x}), \qquad 4-4$$

where $\hat{w}_j(\mathbf{x},t)$ represents the nodal degree of freedoms and $l_j(\mathbf{x}_i) = \delta_{ij}$ is a Lagrange polynomial function. The advantage of nodal basis function is that enforcement of the boundary conditions at nodal point on the boundaries are relatively simple, and allowing use of less expensive smoothers/preconditioners. The nodal coefficients $\hat{w}_j(\mathbf{x},t)$ are a function of space and time, and they are equal to zero on everywhere in the element except at a particular node [95].

In modal DG method, p adaptation is simple and straightforward since the existing basis functions do not need to change with the increase of the order of polynomial approximation in the element. The solution is represented by sum of modal coefficients (local degree of freedoms) multiplied by a set of smooth polynomial functions as

$$\mathbf{w}(\mathbf{x},t) \approx \mathbf{w}_{h}(\mathbf{x},t) = \sum_{j=1}^{N_{p}} \hat{\mathbf{w}}_{j}(t) \boldsymbol{\varphi}_{j}(\mathbf{x}), \qquad 4-5$$

where Modal coefficients $\hat{w}_j(t)$ are only a function of time, and they are usually nonzero on the entire element. $\varphi_j(\mathbf{x})$ symbolizes the modal basis functions and they can be any orthogonal polynomials Eigenfunctions of singular Sturm-Liouville problems.

4.7.3 Modal Discontinuous Galerkin features

Discontinuous Galerkin (DG) method is known as one of the most conducive and robust high-order methods. It has recently found its way into the mainstream of CFD as an alternative to finite volume method. DG method combines essential features of the finite volume and finite element methods and has been employed to solve many scientific and industrial problems. It is not only very compact method; also it is a conserved, stable and robust method with strong mathematical supports.

Furthermore, it is suitable for unstructured triangulation, parallelization, and *hp*-adaptivity. It requires very simple treatment at the boundaries, and achieves the uniform high-order of accuracy throughout the domain, at least for smooth problems. Nevertheless, there are certain challenging issues [105] in development of the DG methods that are necessary to be addressed; a) how to efficiently discretize the diffusion terms required for the Navier-Stokes equations; b) how to control spurious oscillations effectively in the presence of strong discontinuities; c) how to treat with curved boundary; d) how to overcome the computational cost of DG methods efficiently.

4.7.4 Problem definition in DG framework

In order to construct a DG discretized system for \mathfrak{D} -dimensional conservation laws (Eq. 3-52), let's consider a bounded domain $\Omega \in \mathbb{R}^{\mathfrak{D}}$ with boundary of Γ which is decomposed into a region of Dirichlet boundary conditions Γ_p and a region of Neumann boundary conditions Γ_{N} ;

$$\frac{\partial \mathbf{w}}{\partial t} + \nabla \mathbf{F}^{inviscid} \left(\mathbf{w} \right) + \nabla \mathbf{F}^{viscous} \left(\mathbf{w}, \nabla \mathbf{w} \right) = \mathbf{s} \left(\mathbf{w}, \nabla \mathbf{w} \right),$$

$$\mathbf{w} \left(\mathbf{x} \right) = \mathbf{w}_{0}, \quad \text{at } t = t_{0},$$

$$\mathbf{w} \left(\mathbf{x} \right) = g_{D} \left(\mathbf{w} \right), \quad \text{for all } \mathbf{x} \in \Gamma_{D},$$

$$\mathbf{w} \left(\mathbf{x} \right) = g_{N} \left(\nabla \mathbf{w} \right), \quad \text{for all } \mathbf{x} \in \Gamma_{N},$$

$$4-6$$

where $g_D(\mathbf{w})$ and $g_N(\nabla \mathbf{w})$ are boundary operators derived from the boundary conditions. These operators can be a function of information either at one side or both sides of the boundary interfaces.

As determination of the viscous flux vector which contains second-order derivatives of the conservative variables requires additional efforts, a set of auxiliary variables $\Theta \in \mathbb{R}^{(\mathfrak{D}+2)\times\mathfrak{D}}$, are defined to recast the second-order partial differential form of the conservation laws (Eq. 4-6) into two first-order differential systems as

 $\Theta - \nabla \mathbf{u} = 0.$ 4-7 Substituting (Eq. 4-7) into equation (Eq. 4-6) gives the mixed formulation of the conservation laws in global domain framework as

$$\begin{cases} \frac{\partial \mathbf{w}}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \mathbf{F}_{k}^{inviscid}(\mathbf{w}) + \frac{\partial}{\partial \mathbf{x}} \mathbf{F}_{k}^{viscous}(\mathbf{w}, \mathbf{\Theta}) = \mathbf{s}(\mathbf{w}, \mathbf{\Theta}), \\ \Theta_{i} - \frac{\partial \mathbf{w}}{\partial \mathbf{x}} = 0. \end{cases}$$

$$4-8$$

Notice that introduction of an extra set of equations for the auxiliary variables is the main drawback of the mixed-DG formulations since the appearance of the auxiliary variables leads to additional computational cost.

In FEM-based methods, auxiliary variables are only utilized as an intermediate step in the derivation of the discretized system. Later, they will eliminate it by reforming the equations from the flux formulation to the primal formulation. Nonetheless, unfortunately, it is not possible to eliminate the auxiliary system for solving high-order Boltzmann-based models in which viscous fluxes are a nonlinear and implicit function of the conservative variables and their derivatives. Thus, in present work, instead of reformulating the governing equations in primal (bilinear) form, the mixed-DG formulation are utilized and auxiliary equations are solved besides the primary equations.

4.7.5 Spatial discretization of the problem

To discretize the conservation laws in global framework (Eq. 4-8), the global spatial domain Ω can be approximated by Ω_h such that $\Omega_h \to \Omega$ as $h \to 0$. Accordingly, the approximate domain Ω_h is tessellated in space $\mathcal{T}_h = {\Omega_e}$, and it is paved by the N_e number of the non-overlapping bounded elementary control volumes (e.g., triangles, quadrilaterals, tetrahedrons) $\Omega_e \in \mathcal{T}_h$.

The boundaries of every element $\partial \Omega_e$ are divided into two parts: interfaces Γ_F^e and boundaries Γ_B^e . Note that, the interfaces are those which are shared with the neighboring elements and the boundaries are the others. The j^{th} face of the local element Ω_e is symboled by $\Gamma_{F_i}^e$, and the adjacent elements associated with the j^{th} face of the element Ω_e is denoted by Ω_{NEei} .

The global set of the interfaces and the boundary faces of the tessellated domain T_h are denoted by I_h and \mathcal{B}_h , and are given by

$$I_{h} = \{ \Gamma_{F_{j}}^{e} \},$$

$$\downarrow_{j \in \Omega_{e}} \qquad 4-9$$

$$\forall_{e \in T_{h}}$$

$$\mathcal{B}_{h} = \{ \Gamma_{B_{j}}^{e} \},$$

$$\downarrow_{j \in \Omega_{e}} \qquad 4-10$$

$$\forall_{j \in \Omega_{e}} \qquad 4-10$$

If the space of the polynomial functions are defined appropriately in a standard region (master element region), the numerical solution in local element Ω_e can be expressed in terms of a polynomial field that accumulates the multiplication of local degree of freedoms (or modal moments, i.e., $\mathbf{u}_{h^e}^l, \Theta_{h^e}^l$) with corresponding smooth polynomial functions of degree p as

$$\mathbf{w}_{h^{e}}(\xi,t) = \sum_{l=1}^{N_{p}} \mathbf{w}_{h^{e}}^{l}(t)\phi_{l}(\xi), \quad \Theta_{h^{e}}(\xi,t) = \sum_{l=1}^{N_{p}} \Theta_{h^{e}}^{l}(t)\phi_{l}(\xi).$$

$$4-11$$

Here N_p denotes the number of basis (ansatz) functions required for approximating the smooth and continuous solution inside the space of the polynomial functions.

The exact solution of the global variables and their derivatives can be approximated by the numerical solution obtained in every element as follows

$$\mathbf{w}(\mathbf{x},t) \approx \mathbf{w}_{h} = \bigoplus_{e=1}^{N_{e}} \mathbf{w}_{h}^{e}(\mathbf{x},t) \equiv \left\{\mathbf{w}_{h}^{1} + \ldots + \mathbf{w}_{h}^{N_{e}}\right\},$$

$$\mathbf{\Theta}(\mathbf{x},t) \approx \mathbf{\Theta}_{h} = \bigoplus_{e=1}^{N_{e}} \mathbf{\Theta}_{h}^{e}(\mathbf{x},t) \equiv \left\{\mathbf{\Theta}_{h}^{1} + \ldots + \mathbf{\Theta}_{h}^{N_{e}}\right\}.$$

$$4-12$$

 $\mathcal{P}^{p}(\Omega_{e})$ and $\mathcal{M}^{p}(\Omega_{e})$ are defined to denote the space of polynomial functions of degree at most p in the element Ω_{e} such that,

$$\mathbf{V}_{h} \coloneqq \left\{ \boldsymbol{\upsilon} \in \left[L^{2}(\Omega_{h}) \right]^{\mathfrak{D}+2} : \boldsymbol{\upsilon} \mid_{\Omega_{e}} \in \left[\mathcal{P}^{p}(\Omega_{e}) \right]^{\mathfrak{D}+2} \,\forall \Omega_{e} \in \mathcal{T}_{h} \right\},$$

$$4-13$$

$$\boldsymbol{\mathcal{Y}}_{h} \coloneqq \left\{ \boldsymbol{\Phi} \in \left[L^{2}(\boldsymbol{\Omega}_{h}) \right]^{(\mathfrak{D}+2)\times\mathfrak{D}} : \boldsymbol{\Phi} \mid_{\boldsymbol{\Omega}_{e}} \in \left[\mathcal{M}^{p}(\boldsymbol{\Omega}_{e}) \right]^{(\mathfrak{D}+2)\times\mathfrak{D}} \,\forall \boldsymbol{\Omega}_{e} \in \boldsymbol{\mathcal{T}}_{h} \right\},$$
 4-14

the vector-valued \mathbf{V}_h and tensor-value $\boldsymbol{\mathcal{Y}}_h$ spaces denote the least-square discrete finite element spaces of the discontinuous polynomial function of degree p on a local element.

4.7.5.1 Standard elements and basis (ansatz) functions

4.7.5.1.1 One-dimensional problems

In case of 1-D problems ($\mathcal{D}=1$), the local elements Ω_e are equally spaced $\Delta x = x_R - x_L$, and the space coordinates x in element Ω_e is linked to local spatial coordinates $\xi \in \mathbb{R}^{\mathcal{D}=1}$ in a master element $\Omega_e^{\mathcal{D}=1} \in [-1,1]$ through a sub-parametric mapping (transformation) function of $f_{x \to \xi}^{\mathcal{D}=1}$;

$$\Omega_e: \Omega_0^{\mathcal{D}=1} \to f_{x \to \xi}^{\mathcal{D}=1}(x) = 2 \frac{x - x_L}{x_R - x_L} - 1 \qquad \forall x \in \Omega_e,$$

$$4-15$$

$$\Omega_0^{\mathcal{D}=1}:\Omega_e \to f_{\xi \to x}^{\mathcal{D}=1}(\xi) = \frac{1-\xi}{2} x_L + \frac{1+\xi}{2} x_R \quad \forall \xi \in \Omega_0^{\mathcal{D}=1}.$$
4-16

As it is shown in Figure 4-5, the local master element is defined in range of $-1 \le \xi \le 1$;

$$\Omega_0^{\mathcal{D}=1} = \left\{ \xi \left| -1 \le \xi \le 1 \right\}.$$

$$4-17$$

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The polynomial space function is set to be orthogonal scaled Legendre functions $\mathcal{P}^{P}(\Omega_{e}) = \mathcal{L}_{p'}(\xi)$, and it can be defined as

$$\mathcal{L}_{p'}(\xi) = \left\{ \frac{2^{p'}(p'!)^2}{(2p')!} L^{p'}(\xi); 0 \le p' \le p; \xi \in \Omega_0 \right\},$$

$$\upsilon_i(\xi_1, \xi_2) = \mathcal{L}_{p'}(\xi), \qquad 1 \le i \le (p+1).$$

$$4-18$$

Figure 4-6 depicts a set of the basic functions for an order of p = 5 in master element. As it is obvious, the ansatz functions of v and Φ are adopted to lie in this polynomial space function.



Figure 4-5 Linear mapping from local element to 1-D master element



Figure 4-6 Complete scaled Legendre polynomial space for one-dimensional element up to the order of p=5

4.7.5.1.2 Two-dimensional problems

In the case of 2-D problems ($\mathcal{D} = 2$), the space coordinates x in the local element Ω_{e} are related to local spatial coordinates $\xi \in \mathbb{R}^{2^{2}}$ in a master element $\Omega_{0}^{2^{2}}$ through a mapping process.

Quadrilateral elements

For quadrilateral elements, the space coordinates \mathbf{x} in local element Ω_{e} are linked to local spatial coordinates $\boldsymbol{\xi} \in \mathbb{R}^{\mathcal{D}=2}$ in a local master element $\Omega_{0}^{\mathcal{D}=2} \in [-1,1]^{2}$ based on a bilinear mapping (transformation) function $f_{\boldsymbol{\xi} \to \mathbf{x}}^{\mathcal{D}=2}$;

$$\begin{split} \Omega_{0}^{\mathcal{D}=2} : \Omega_{e} &\to f_{\xi \to \mathbf{x}}^{\mathcal{D}=2}(\xi) = \mathbf{x}_{A_{e}} \, \frac{1 - \xi_{1}}{2} \frac{1 - \xi_{2}}{2} + \mathbf{x}_{B_{e}} \frac{1 + \xi_{1}}{2} \frac{1 - \xi_{2}}{2} + \\ \mathbf{x}_{C_{e}} \, \frac{1 + \xi_{1}}{2} \frac{1 + \xi_{2}}{2} + \mathbf{x}_{D_{e}} \frac{1 - \xi_{1}}{2} \frac{1 + \xi_{2}}{2}. \end{split}$$

$$\begin{aligned} 4-19 \\ \end{split}$$

Figure 4-7 illustrates the process of mapping for quadrilateral elements with the master rectangular element of

$$\Omega_0^{\mathcal{D}=2,\operatorname{Rectangular}} = \left\{ \left(\xi_1, \xi_2\right) \middle| -1 \le \xi_1, \xi_2 \le 1 \right\}.$$
4-20

This parametric mapping function is the simplest mapping for transforming an arbitrary shaped straight side quadrilateral element into the master element. It has been reported that DG methods are very sensitive to the shape of the geometry [111], therefore, it may be better to use an iso-parametric mapping function to handle curved side quadrilateral elements.



Figure 4-7 Linear mapping from a quadrilateral element to rectangular master element

In order to develop a set of multi-dimensional basis functions using full-tensorial (or serendipity) expansion of the orthogonal basis functions inside $L^2(\Omega)$ space, it is

desirable to use the product of two $f(\xi_1), f(\xi_2)$ unidirectional orthogonal polynomial functions [93, 113].

According to Pascal's triangle, the polynomial function of order p is defined, $\mathcal{P}^{P}(\Omega_{e}) = \mathcal{Q}_{p',q'}(\xi_{1},\xi_{2})$, such that $\upsilon_{j}(\xi_{1},\xi_{2}) = \phi_{p'q'}(\xi_{1},\xi_{2})$ lies in the polynomial space defined inside the master element as

$$\mathcal{Q}_{p',q'}(\xi_1,\xi_2) \coloneqq \left\{ L^{p'}(\xi_1) L^{q'}(\xi_2); 0 \le p', q' \le p; (\xi_1,\xi_2) \in \Omega_0^{\mathcal{D}=2} \right\},
\upsilon_i(\xi_1,\xi_2) = \mathcal{Q}_{p',q'}(\xi_1,\xi_2), \qquad 1 \le i \le (p+1)^2.$$
4-21

were p' and q' are the modes of $L^{p'}(\xi_1), L^{q'}(\xi_2)$ two Legendre functions.



Figure 4-8 Complete polynomial space, based on Pascal's triangle, for *full* quadrilateral expansion up to order of p=6

Figure 4-8 depicts the modes of the quadrilateral basis functions inside the local master element of $\Omega_0^{\mathfrak{D}=2} \in [-1,1]^2$. Note that, for convenient, the multi-dimensional basis functions are sorted such that by a single index *j* all *p*'-*q*' modes can be addressed. The full tensorial quadrilateral basis functions up to order of p=2 can be defined as

$$\begin{split} \upsilon_{1}(\xi_{1},\xi_{2}) &= \mathcal{Q}_{0,0}(\xi_{1},\xi_{2}) = 1, \quad \upsilon_{5}(\xi_{1},\xi_{2}) = \mathcal{Q}_{0,2}(\xi_{1},\xi_{2}) = \frac{1}{2} \Big(3\xi_{2}^{2} - 1 \Big), \\ \upsilon_{2}(\xi_{1},\xi_{2}) &= \mathcal{Q}_{0,1}(\xi_{1},\xi_{2}) = \xi_{2}, \quad \upsilon_{6}(\xi_{1},\xi_{2}) = \mathcal{Q}_{1,2}(\xi_{1},\xi_{2}) = \frac{1}{2} \Big(3\xi_{2}^{2} - 1 \Big) \xi_{1}, \\ \upsilon_{3}(\xi_{1},\xi_{2}) &= \mathcal{Q}_{1,1}(\xi_{1},\xi_{2}) = \xi_{1}\xi_{2}, \quad \upsilon_{7}(\xi_{1},\xi_{2}) = \mathcal{Q}_{2,2}(\xi_{1},\xi_{2}) = \frac{1}{4} \Big(3\xi_{2}^{2} - 1 \Big) \Big(3\xi_{1}^{2} - 1 \Big), \\ u_{4}(\xi_{1},\xi_{2}) &= \mathcal{Q}_{1,0}(\xi_{1},\xi_{2}) = \xi_{1}, \quad \upsilon_{8}(\xi_{1},\xi_{2}) = \mathcal{Q}_{2,1}(\xi_{1},\xi_{2}) = \frac{1}{2} \Big(3\xi_{1}^{2} - 1 \Big) \xi_{2}, \\ \upsilon_{9}(\xi_{1},\xi_{2}) &= \mathcal{Q}_{2,0}(\xi_{1},\xi_{2}) = \frac{1}{2} \Big(3\xi_{1}^{2} - 1 \Big). \end{split}$$

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As it is obvious in Figure 4-9, the mass matrix of quadrilateral basis functions is not diagonal due to bilinear mapping transformation, and computational cost of quadrilateral elements is higher than triangle elements.



Figure 4-9 Plot of the mass matrix for complete polynomial space up to order p=6 for full quadrilateral expansion.

Triangular elements

The special coordinate mapping, named as collapsed coordinate transformation, in conjugation with an orthogonal set of basis functions can be utilized to benefiting a diagonal mass matrix in the triangular domain [93, 114].

In collapsed coordinate transformation; the master triangular and rectangular elements are defined as

$$\Omega_{0\Delta}^{\mathcal{D}=2,\text{Triangualr}} = \left\{ \left(\eta_1, \eta_2\right) \middle| -1 \le \eta_1, \eta_2; \eta_1 + \eta_2 \le 0 \right\},$$

$$4-23$$

$$\Omega_{0\square}^{\mathcal{D}=2,\text{Rectangular}} = \left\{ \left(\xi_1, \xi_2\right) \middle| -1 \le \xi_1, \xi_2 \le 1 \right\}.$$
4-24

The space coordinates \mathbf{x} is linked to local spatial coordinates $\boldsymbol{\xi} \in \mathbb{R}^{\mathcal{D}=2}$ through a twosteps parametric mapping (transformation) function $f_{\mathbf{x}\to\boldsymbol{\xi}}^{\mathcal{D}=2} = f_{\mathbf{x}\to\boldsymbol{\eta}}^{\mathcal{D}=2} + f_{\boldsymbol{\eta}\to\boldsymbol{\xi}}^{\mathcal{D}=2}$;

$$\Omega_{0\Box}^{\mathcal{D}=2}:\Omega_{e} \rightarrow \begin{cases} f_{\eta \to \mathbf{x}}^{\mathcal{D}=2}(\eta) = -\mathbf{x}_{A_{e}} \frac{\eta_{1} + \eta_{2}}{2} + \mathbf{x}_{B_{e}} \frac{1 + \eta_{1}}{2} + \mathbf{x}_{C_{e}} \frac{1 + \eta_{2}}{2}, \\ f_{\xi \to \eta}^{\mathcal{D}=2}(\xi) = \left(\frac{(1 + \xi_{1})(1 - \xi_{2})}{2} - 1, \xi_{2}\right). \end{cases}$$

$$4-25$$

To understand this two-step transformation process, the transformation from physical coordinate system to collapsed coordinate system is depicted in Figure 4-10. As it is obvious, two vertices are collapsing into one as the quadrilateral becomes a triangle. This is the main reason for calling this two-step transformation as collapsed coordinate transformation.



Figure 4-10 Special mapping from a triangular element to rectangular master element

The collapsed coordinate transformation is very practical and it is utilized by several researchers; however, an extra work is required to be done for transformation a singular point from rectangular master element to triangular master element [114]. Due to appearance of a singular point in mapping function, it is necessary to re-define the mapping transformation at singular point such that

$$f_{\xi \to \eta}^{\mathcal{D}=2}(\xi) = (-1,1), \forall \xi_2 = -1.$$
4-26

The inverse mapping from collapse coordinate system into the master triangle, and then transformation from master triangle coordinate system to physical coordinate system can be defined as

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$$\Omega_{e}: \Omega_{0\Delta}^{\mathcal{D}=2} \to f_{\mathbf{x} \to \mathbf{\eta}}^{\mathcal{D}=2}(\mathbf{x}) = \begin{pmatrix} \frac{2x_{1}(x_{2}^{C} - x_{2}^{A}) - 2x_{2}(x_{1}^{C} - x_{1}^{A})}{4|J|_{\mathbf{x} \to \mathbf{\eta}}} + \\ \frac{(x_{1}^{C} - x_{1}^{A})(x_{2}^{C} + x_{2}^{B}) - (x_{2}^{C} - x_{2}^{A})(x_{1}^{C} + x_{1}^{B})}{4|J|_{\mathbf{x} \to \mathbf{\eta}}} , \\ \frac{2x_{1}(x_{2}^{B} - x_{2}^{A}) - 2x_{2}(x_{1}^{B} - x_{1}^{A})}{4|J|_{\mathbf{x} \to \mathbf{\eta}}} + \\ \frac{(x_{1}^{B} - x_{1}^{A})(x_{2}^{C} + x_{2}^{B}) - (x_{2}^{B} - x_{2}^{A})(x_{1}^{C} + x_{1}^{B})}{4|J|_{\mathbf{x} \to \mathbf{\eta}}} , \\ \end{pmatrix}$$

$$\Omega_{0\Delta}^{\mathcal{D}=2}:\Omega_{0\Box}^{\mathcal{D}=2} \to f_{\eta \to \xi}^{\mathcal{D}=2}(\mathbf{x}) = \left(2\frac{\left(1+\eta_{1}\right)}{\left(1-\eta_{2}\right)}-1,\eta_{2}\right).$$
4-28

Here determinants of the Jacobian of transformations are given by

$$\left|J\right|_{\mathbf{x}\to\mathbf{\eta}} = \left|\frac{\partial \mathbf{x}}{\partial \mathbf{\eta}}\right| = \begin{vmatrix} x_{1_{\eta_{1}}} & x_{1_{\eta_{2}}} \\ x_{2_{\eta_{1}}} & x_{2_{\eta_{2}}} \end{vmatrix} = x_{1_{\eta_{1}}} x_{2_{\eta_{2}}} - x_{1_{\eta_{2}}} x_{2_{\eta_{1}}} = \frac{\Omega_{\Delta}}{2},$$

$$4-29$$

$$|J|_{\eta \to \xi} = \left| \frac{\partial \eta}{\partial \xi} \right| = \left| \begin{matrix} \eta_{1_{\eta_{1}}} & \eta_{1_{\eta_{2}}} \\ \eta_{2_{\eta_{1}}} & \eta_{2_{\eta_{2}}} \end{matrix} \right| = \det \left(\begin{matrix} \frac{1 - \xi_{2}}{2} & -\frac{1 + \xi_{1}}{2} \\ 0 & 1 \end{matrix} \right) = \frac{1 - \xi_{2}}{2}, \qquad 4-30$$

where Ω_{A} denotes the area of the original triangle in the physical coordinate system.

In collapsed coordinates, the eigenfunctions of a particular Sturm-Liouville problem, PKD (Proriol, Koornwinder, and Dubiner) polynomials [115-117], are commonly employed as orthogonal basis functions. The orthogonal PKD basis functions are built using a simple product of two unidimensional polynomials —two Jacobi polynomials with certain weights— in $L^2(\Omega)$ space.

According to Pascal's triangle, a complete polynomial space function of order p can be defined in rectangular reference by defining $\mathcal{P}^{P}(\Omega_{e}) = \mathcal{T}_{p',q'}(\xi_{1},\xi_{2})$ such that

$$\mathcal{T}_{p',q'}(\xi_1,\xi_2) \coloneqq \left\{ P_{p'}^{0,0}(\xi_1)(1-\xi_2)^{p'} P_{q'}^{2p'+1,0}(\xi_2); 0 \le p'+q' \le p; (\xi_1,\xi_2) \in \Omega_{0\square}^{\mathcal{D}=2} \right\}, \\ \upsilon_i(\xi_1,\xi_2) = \mathcal{T}_{p',q'}(\xi_1,\xi_2), \qquad 1 \le i \le \frac{1}{2} (p+1)(p+2).$$

$$4-31$$

Here, two indices (*p* ' and *q* ') are used to address specific basis functions in polynomial space function $\mathcal{P}^{P}(\Omega_{e})$.

The mass matrix of PKD basis functions is a diagonal matrix, as shown in Figure 4 13, therefore, application of this basis functions for non-quadrilateral elements is computationally more efficient than orthogonal Legendre polynomials.



Figure 4-11 Plot of mass matrix for complete polynomial space up to order p=6 for full triangle expansion

The complete polynomial space in terms of Pascal's triangle is depicted for PKD basis functions in Figure 4-12. It is shown that the multi-dimensional PDK basis functions, similar to quadrilateral basis functions, are sorted such that all p'-q' modes are addressed by a single index *j*.



Figure 4-12 Complete polynomial space, based on Pascal's triangle, for *full* triangular expansion up to order of p=6

The PKD basis functions up to order of p = 3 are listed below and

$$\begin{split} \upsilon_{1}(\xi_{1},\xi_{2}) &= \mathcal{T}_{0,0}(\xi_{1},\xi_{2}) = 1, \\ \upsilon_{2}(\xi_{1},\xi_{2}) &= \mathcal{T}_{0,1}(\xi_{1},\xi_{2}) = \frac{1}{2}(3\xi_{2}+1), \\ \upsilon_{3}(\xi_{1},\xi_{2}) &= \mathcal{T}_{1,0}(\xi_{1},\xi_{2}) = \frac{1}{2}(\xi_{2}-1)\xi_{1}, \\ \upsilon_{4}(\xi_{1},\xi_{2}) &= \mathcal{T}_{0,2}(\xi_{1},\xi_{2}) = \xi_{2} + \frac{5\xi_{2}^{2}}{2} - \frac{1}{2}, \\ \upsilon_{5}(\xi_{1},\xi_{2}) &= \mathcal{T}_{1,1}(\xi_{1},\xi_{2}) = \frac{1}{4}(1-\xi_{2})(3+5\xi_{2})\xi_{1}, \\ \upsilon_{6}(\xi_{1},\xi_{2}) &= \mathcal{T}_{2,0}(\xi_{1},\xi_{2}) = \frac{1}{8}(\xi_{2}-1)^{2}(3\xi_{1}^{2}-1), \\ \upsilon_{7}(\xi_{1},\xi_{2}) &= \mathcal{T}_{0,3}(\xi_{1},\xi_{2}) = \frac{1}{8}(1-\xi_{2})(1+3\xi_{2}(6+7\xi_{2}))\xi_{1}, \\ \upsilon_{9}(\xi_{1},\xi_{2}) &= \mathcal{T}_{1,2}(\xi_{1},\xi_{2}) = \frac{1}{8}(1-\xi_{2})(1+3\xi_{2}(6+7\xi_{2}))\xi_{1}, \\ \upsilon_{9}(\xi_{1},\xi_{2}) &= \mathcal{T}_{2,1}(\xi_{1},\xi_{2}) = \frac{1}{16}(\xi_{2}-1)^{2}(5\xi_{1}^{2}-3)\xi_{1}. \end{split}$$

4.7.5.1.3 Three-dimensional problems

In case of 3-D problems ($\mathcal{D}=3$), the space coordinates \mathbf{x} in tetrahedron element Ω_e is linked to local spatial coordinates $\boldsymbol{\xi} \in \mathbb{R}^{\mathcal{D}=3}$ in a canonical master element $\Omega_0^{\mathcal{D}=3}$ based on a linear mapping (transformation) function $f_{\boldsymbol{\xi} \to \mathbf{x}}^{\mathcal{D}=3}$ as



Figure 4-13 Linear mapping from a tetrahedron element to canonical master element

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The canonical master element can be defined as

$$\Omega_0^{\mathcal{D}=3,\text{Tetrahedron}} = \left\{ \left(\xi_1, \xi_2, \xi_3\right) 0 \le \xi_1 \le 1; \ 0 \le \xi_2 \le 1 - \xi_1; \ 0 \le \xi_3 \le 1 - \xi_1 - \xi_2 \right\}, \qquad 4-34$$

and a linear mapping is used for transformation of a tetrahedron element into the canonical master element, as illustrated in Figure 4-13. It is possible to obtain an inverse mapping relation $f_{x \to \xi}^{\mathcal{D}=3}$ using crammer rule such that

$$\Omega_{e}: \Omega_{0}^{\mathcal{D}=3} \to f_{\xi \to \mathbf{x}}^{\mathcal{D}=3}(\mathbf{x}) = \frac{1}{|J|_{\mathbf{x} \to \xi}} \begin{cases} \left| \begin{array}{c} x_{1} - x_{1A_{e}} & x_{1C_{e}} - x_{1A_{e}} & x_{1D_{e}} - x_{1A_{e}} \\ x_{2} - x_{2A_{e}} & x_{2C_{e}} - x_{2A_{e}} & x_{2D_{e}} - x_{2A_{e}} \\ x_{3} - x_{3A_{e}} & x_{3C_{e}} - x_{3A_{e}} & x_{3D_{e}} - x_{3A_{e}} \\ x_{2B_{e}} - x_{1A_{e}} & x_{1} - x_{1A_{e}} & x_{1D_{e}} - x_{1A_{e}} \\ x_{2B_{e}} - x_{2A_{e}} & x_{2} - x_{2A_{e}} & x_{2D_{e}} - x_{2A_{e}} \\ x_{3B_{e}} - x_{3A_{e}} & x_{3} - x_{3A_{e}} & x_{3D_{e}} - x_{3A_{e}} \\ x_{2B_{e}} - x_{2A_{e}} & x_{2C_{e}} - x_{2A_{e}} & x_{2D_{e}} - x_{2A_{e}} \\ x_{2B_{e}} - x_{2A_{e}} & x_{2C_{e}} - x_{2A_{e}} & x_{2D_{e}} - x_{2A_{e}} \\ x_{2B_{e}} - x_{2A_{e}} & x_{2C_{e}} - x_{2A_{e}} & x_{2D_{e}} - x_{2A_{e}} \\ x_{2B_{e}} - x_{2A_{e}} & x_{2C_{e}} - x_{2A_{e}} & x_{2} - x_{2A_{e}} \\ x_{3B_{e}} - x_{3A_{e}} & x_{3C_{e}} - x_{3A_{e}} & x_{3} - x_{3A_{e}} \\ \end{array} \right|,$$

$$4-35$$

Here determinant of the Jacobean of the transformation $|J|_{x \to \xi}$ is given by

$$\left|J\right|_{\mathbf{x}\to\xi} = \left|\frac{\partial \mathbf{x}}{\partial \xi}\right| = \left|\frac{\partial x_1}{\partial \xi_1} - \frac{\partial x_1}{\partial \xi_2} - \frac{\partial x_1}{\partial \xi_3}\right| = 6\Omega_{tet}, \qquad 4-36$$

$$\left|\frac{\partial x_2}{\partial \xi_1} - \frac{\partial x_2}{\partial \xi_2} - \frac{\partial x_3}{\partial \xi_2} - \frac{\partial x_3}{\partial \xi_3}\right| = 6\Omega_{tet}, \qquad 4-36$$

where Ω_{tet} is the volume of real tetrahedral in x coordinate system.

In order to develop a set of multi-dimensional orthogonal basis functions inside $L^2(\Omega)$ space, three polynomial functions are defined in terms of *Jacobi polynomials* function $P_n^{\alpha,\beta}(x)$ in three independent directions, and then the product of these unidirectional orthogonal polynomial functions are adopted as multi-dimensional basis functions.

A complete polynomial space function of order p can be defined inside the canonical tetrahedron system by defining $\mathcal{P}^{p}(\Omega_{e}) = \mathcal{J}_{p',q',r'}(\xi_{1},\xi_{2},\xi_{3})$ such that

$$\mathcal{J}_{p',q',r'}(\xi_1,\xi_2,\xi_3) \coloneqq \begin{cases} \psi_{p'}^1 \left(\frac{2\xi_3}{1-\xi_1-\xi_2} - 1 \right) \psi_{p',q'}^2 \left(\frac{2\xi_1}{1-\xi_2} - 1 \right) \psi_{p',q',r'}^3 \left(2\xi_2 - 1 \right); \\ 0 \le p' + q' + r' \le p; (\xi_1,\xi_2,\xi_3) \in \Omega_0^{\mathcal{D}=3} \end{cases}$$

$$4-37$$

Here three principle functions are

$$\psi_{p',q'}^{1}(\mathbf{x}) = P_{p'}^{0,0}(\mathbf{x}),$$

$$\psi_{p',q'}^{2}(\mathbf{x}) = \left(\frac{1-\mathbf{x}}{2}\right)^{p'} P_{q'}^{2p'+1,0}(\mathbf{x}),$$

$$\Psi_{p',q',r'}^{3}(\mathbf{x}) = \left(\frac{1-\mathbf{x}}{2}\right)^{p'+q'} P_{r'}^{2p'+2q'+2,0}(\mathbf{x}),$$

$$4-38$$

and the Jacobi polynomial functions defined in the interval of $\left[-1,1\right]$ are expressed as

$$P_{n}^{\alpha,\beta}(\mathbf{x}) = \frac{(-1)^{n}}{2^{n}n!} (1+\mathbf{x})^{\alpha} (1+\mathbf{x})^{-\beta} \frac{d^{n}}{dx^{n}} \left\{ (1-\mathbf{x})^{\alpha+n} (1-\mathbf{x})^{\beta+n} \right\}, \quad \alpha,\beta > -1.$$
 4-39

Similar to two-dimensional basis functions, three-dimensional basis functions are sorted such that all p'-q'-r' modes can be addressed by a single index *j*.

$$\upsilon_{i}(\xi_{1},\xi_{2},\xi_{3}) = \mathcal{J}_{p',q',r'}(\xi_{1},\xi_{2},\xi_{3}), \qquad 1 \le i \le \frac{1}{3!} (p+1)(p+2)(p+3).$$
 4-40

The 3-D *orthogonal hierarchical* basis functions up to order of p = 2 can be written as

$$\begin{split} \nu_{1}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,0,0}(\xi_{1},\xi_{2},\xi_{3}) = 1, \\ \nu_{2}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{1,0,0}(\xi_{1},\xi_{2},\xi_{3}) = 2\xi_{1} + \xi_{2} + \xi_{3} - 1, \\ \nu_{3}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,1,0}(\xi_{1},\xi_{2},\xi_{3}) = 3\xi_{2} + \xi_{3} - 1, \\ \nu_{4}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,0,1}(\xi_{1},\xi_{2},\xi_{3}) = 4\xi_{3} - 1, \\ \nu_{5}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{2,0,0}(\xi_{1},\xi_{2},\xi_{3}) = 6(\xi_{1}^{2} + \xi_{1}) + (\xi_{2} + \xi_{3} - 1) + (\xi_{2} + \xi_{3} - 1)^{2}, \\ \nu_{6}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{1,1,0}(\xi_{1},\xi_{2},\xi_{3}) = (2\xi_{1} + \xi_{2} + \xi_{3} - 1)(6\xi_{3} - 1), \\ \nu_{7}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{1,0,1}(\xi_{1},\xi_{2},\xi_{3}) = 10\xi_{2}^{2} + 8\xi_{2}(\xi_{3} - 1) + (\xi_{3} - 1)^{2}, \\ \nu_{8}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,2,0}(\xi_{1},\xi_{2},\xi_{3}) = (6\xi_{3} - 1)(3\xi_{2} + \xi_{3} - 1), \\ \nu_{9}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,1,1}(\xi_{1},\xi_{2},\xi_{3}) = 1 + 5\xi_{3}(3\xi_{3} - 2), \\ \nu_{10}(\xi_{1},\xi_{2},\xi_{3}) &= \mathcal{J}_{0,0,2}(\xi_{1},\xi_{2},\xi_{3}) = 20\xi_{1}^{3} + (\xi_{2} + \xi_{3} - 1) \{ 30\xi_{1}^{2} + 12\xi_{1}(\xi_{2} + \xi_{3} - 1) + (\xi_{2} + \xi_{3} - 1) + (\xi_{2} + \xi_{3} - 1) \} \\ \end{split}$$

The mass matrix is diagonal matrix due to the orthogonality of 3-D basis functions inside the canonical tetrahedron master element, as shown in Figure 4-14.



Figure 4-14 Plot of mass matrix for complete polynomial space up to order p=3 for full tetrahedron expansion

4.7.5.2 Elemental formulation

Taking the product of the conservation laws with vector $\mathbf{v} = [v_i]$ and the product of the auxiliary equations (Eq. 4-8) with tensor $\mathbf{\Phi} = [\Phi_{ik}] = [\varphi_k]$, and then integrating by parts over the solution domain results in

$$\begin{cases} \int_{\mathbb{R}^{D}} \upsilon \frac{\partial \mathbf{w}}{\partial t} d\Omega + \int_{\mathbb{R}^{D}} \upsilon \nabla \mathbf{F}^{inviscid}(\mathbf{w}) d\Omega + \int_{\mathbb{R}^{D}} \upsilon \nabla \mathbf{F}^{viscous}(\mathbf{w}, \mathbf{\Theta}) d\Omega = \int_{\mathbb{R}^{D}} \upsilon \mathbf{s}(\mathbf{w}, \mathbf{\Theta}) d\Omega, \\ \int_{\mathbb{R}^{D}} \mathbf{\Phi} \mathbf{\Theta} d\Omega - \int_{\mathbb{R}^{D}} \mathbf{\Phi} \nabla \mathbf{w} d\Omega = 0. \end{cases}$$

$$4-42$$

where it can be written in component form as

$$\begin{cases} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \frac{\partial w_{i}}{\partial t} d\Omega + \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \left(\frac{\partial \mathbf{F}_{ik}^{inviscid}(\mathbf{w})}{\partial x_{k}} + \frac{\partial \mathbf{F}_{ik}^{viscous}(\mathbf{w}, \mathbf{\Theta})}{\partial x_{k}} \right) d\Omega = \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} s_{i}(\mathbf{w}, \mathbf{\Theta}) d\Omega, \\ \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Theta_{ik} d\Omega - \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \frac{\partial w_{i}}{\partial x_{k}} d\Omega = 0. \end{cases}$$

$$4-43$$

with $i = 1 \dots \mathcal{D} + 2$.

Splitting the volume integral over Ω_h into sum of the integrals over the local elements Ω_e and application of divergence theorem to (Eq. 4-47) leads to elemental formulation of the governing equations as

$$\begin{cases} \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \frac{\partial w_{h_{i}^{e}}}{\partial t} d\Omega_{e} \\ + \sum_{e \in T_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \left(\mathbf{F}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) + \mathbf{F}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{+} \right) \right) n_{k}^{-} d\Gamma_{e} \\ - \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \frac{\partial \upsilon_{i}}{\partial x_{k}} \left(\mathbf{F}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}} \right) + \mathbf{F}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}, \mathbf{\Theta}_{h^{e}} \right) \right) d\Omega_{e} = \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} s_{i} \left(\mathbf{w}_{h^{e}}, \mathbf{\Theta}_{h^{e}} \right) d\Omega_{e}, \\ \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Theta_{ik} d\Omega_{e} - \sum_{e \in T_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \mathbf{F}_{ik}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) n_{k}^{-} d\Gamma_{e} \\ + \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} w_{h^{e_{i}}} \frac{\partial \Phi_{ik}}{\partial x_{k}} d\Omega_{e} = 0. \end{cases}$$

Here $d\Gamma_e$ denotes the boundaries of the local element, and **n** is the outward unit normal vector.

The system of equations introduced in (Eq. 4-44) is not solvable since the degree of freedom belonging to every element is not linked to the degree of freedoms in other elements of Ω_{h} . Thus, establishing a weak inter-element connection via introducing an appropriate monotone numerical fluxes at interfaces and boundaries of elements Ω_{e} is essential to obtain an approximate spectral solution.

4.7.5.3 Weak and strong formulation

Replacing the discontinuous fluxes $-\mathbf{F}_{i}^{inviscid}, \mathbf{F}_{i}^{viscous}$, and $\mathbf{F}_{ik}^{auxiliary}$ – at the border of local elements with numerical flux functions $-\mathbf{\tilde{F}}_{i}^{inviscid}, \mathbf{\tilde{F}}_{i}^{viscous}$, and $\mathbf{\tilde{F}}_{ik}^{auxiliary}$ – leads to a weak formulation of DG method on local elements Ω_{e} . The weak formulation can be expressed as

$$\begin{cases} \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \frac{\partial W_{h^{e_{i}}}}{\partial t} d\Omega_{e} \\ + \sum_{e \in \mathcal{T}_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \left(\tilde{\mathbf{F}}_{ik}^{inviscid} (\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}) + \tilde{\mathbf{F}}_{ik}^{viscous} (\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{+}) \right) n_{k}^{-} d\Gamma_{e} \\ - \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \frac{\partial \upsilon_{i}}{\partial x_{k}} \left(\mathbf{F}_{ik}^{inviscid} (\mathbf{w}_{h^{e}}) + \mathbf{F}_{ik}^{viscous} (\mathbf{w}_{h^{e}}, \mathbf{\Theta}_{h^{e}}) \right) d\Omega_{e} = \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} s_{i} (\mathbf{w}_{h^{e}}, \mathbf{\Theta}_{h^{e}}) d\Omega_{e}, \\ \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Theta_{ik} d\Omega_{e} - \sum_{e \in \mathcal{T}_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \tilde{\mathbf{F}}_{ik}^{auxiliary} (\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}) n_{k}^{-} d\Gamma_{e} \\ + \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} w_{h^{e_{i}}} \frac{\partial \Phi_{ik}}{\partial x_{k}} d\Omega_{e} = 0. \end{cases}$$

The weak formulation not only leads to the unique solution at the interface between two elements, but also it leads to prescribing the boundary conditions in the weak sense

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$$\begin{aligned} &\sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{P}}} \upsilon_{i} \frac{\partial w_{h_{i}^{e}}}{\partial t} d\Omega_{e} \\ &+ \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{P}}} \upsilon_{i} \left(\nabla \cdot \mathbf{F}_{i}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-} \right) + \nabla \cdot \mathbf{F}_{i}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-} \right) \right) d\Omega_{e} \\ &= \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{P}}} \upsilon_{i} S_{i} \left(\mathbf{w}_{h^{e}}, \mathbf{\Theta}_{h^{e}} \right) d\Omega_{e} \\ &+ \sum_{e \in \mathcal{T}_{h}} \oint_{\mathbb{R}^{\mathcal{P}}} \upsilon_{i} \left(\mathbf{F}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-} \right) - \tilde{\mathbf{F}}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) \right) \eta_{k}^{-} d\Gamma_{e} \\ &+ \sum_{e \in \mathcal{T}_{h}} \oint_{\mathbb{R}^{\mathcal{P}}} \upsilon_{i} \left(\mathbf{F}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-} \right) - \tilde{\mathbf{F}}_{ik}^{iviscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{+} \right) \right) \eta_{k}^{-} d\Gamma_{e}, \end{aligned}$$

$$4-46$$

$$\sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{P}}} \Phi_{ik} \Theta_{ik} d\Omega_{e} - \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{P}}} \Phi_{ik} \nabla \mathbf{w}_{h^{e}}^{-} d\Omega_{e} = \\ - \sum_{e \in \mathcal{T}_{h}} \oint_{\mathbb{R}^{\mathcal{P}}} \Phi_{ik} \left(w_{h^{e}_{i}}^{-} - \tilde{\mathbf{F}}_{ik}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) \right) \eta_{k}^{-} d\Gamma_{e}.$$

The resulting formulation is called a two-steps mixed-DG method in which the test functions, accordingly to Galerkin method [118], are chosen to be equal to the basis (ansatz) functions defined in Section 0. In mixed DG method, the auxiliary equations are initially solved at the beginning of every time step, and the gradients of primary variables $\boldsymbol{\Theta}_{h^e}$ are updated based on the global solutions \mathbf{W}_{h^e} at current time step. Afterwards, the primary system is solved, using the values of $\boldsymbol{\Theta}_{h^e}$ obtained from step one.

4.7.6 Time discretization of the problem

Considering the weak formulation and applying the method of line (MOL) for decoupling time and spatial coordinates, the decoupled system of equations in time and space achieves in which time and space are discretized independently.

Figure 4-15, there are several implicit, and explicit single level or multi-level timestepping schemes. The choice of the scheme for integration of the time depends on several items; the desired accuracy for transition state, the robustness of the scheme, and more importantly the stability and computational cost of the scheme.

The explicit methods required smaller time steps compared to implicit methods; however, they are accurate and easy to parallelize for studying unsteady problems. In explicit schemes, it is well known that the grid spacing Δx and the time step size Δt must be chosen such that the Courant–Friedrichs–Lewy (CFL) criterion is satisfied.



Figure 4-15 Time integration schemes

Chavent and Salzano [119] developed an explicit version of DG method and utilized it for solving one-dimensional scalar conservation laws. They discretized time utilizing the simple forward Euler method. According to their von-Neumann analysis, DG method is stable if $\Delta t/\Delta x$ is in order of $\sqrt{\Delta x}$, and it is unconditionally unstable when $\Delta t/\Delta x$ is held to be constant. Although their conclusion was for a linear scalar hyperbolic equation, it might hold for a non-linear system of equations.

Cockburn and Shu [92] proposed an approximation of the CFL number as

$$CFL \approx \left| \lambda_{\max} \right| \frac{\Delta t}{\Delta x} \le \frac{1}{2p+1}.$$
 4-47

This CFL condition was proved to be exact for the case of $p \le 1$ [120]. Cockburn and Shu reported that CFL number for a numerical analysis should be around 5% less than above CFL condition when order of the polynomial is greater than two $p \ge 2$ [92]. Therefore, in all of the simulation in present work, CFL number is determined using

$$CFL \approx \left| \lambda_{\max} \right| \frac{\Delta t}{\Delta x} \le \frac{0.95}{2p+1}.$$
 4-48

Although obtaining an appropriate range of CFL number is essential, but it is not sufficient. It is proven that the forward Euler method applied to semi-discrete systems is unconditionally unstable in the case that the degree of approximate solution, p, is greater than 2 when Courant number is constant [120, 121].

In finite volume methods, classical-Runge-Kutta schemes are commonly used. However, they may not be a good choice for high-order DG methods. There is a chance to have non-monotone results during time marching process by application of these time-stepping schemes[122]. Strong-stability-preserving (SSP) method are basically designed to improve the capability of the explicit multi-level time-stepping schemes.

The first SSP scheme was introduced by Cockburn and Shu in 1988[123]. In this scheme, the temporal operator itself does not increase the total variation of the solution due to the *total variation diminishing* (TVD) feature of the scheme [122, 124]. In this scheme, time-stepping is enforced to be formulated as a convex combination of forward

Euler steps with time step size of $\frac{\beta_{il}}{\alpha_{il}} \Delta t$,

$$\frac{d\mathbf{u}_{h}^{n+1}}{dt} = L(\mathbf{u}_{h}^{n}) \rightarrow \begin{cases} \mathbf{u}_{h}^{(0)} = \mathbf{u}_{h}^{n} \\ \mathbf{u}_{h}^{(i)} = \sum_{l=0}^{i-1} \boldsymbol{\alpha}_{il} \left\{ \frac{\boldsymbol{\beta}_{il}}{\boldsymbol{\alpha}_{il}} \Delta t \ L(\mathbf{u}_{h}^{(l)}) + \mathbf{u}_{h}^{(l)} \right\}, \quad i=1,\dots,t.$$

$$4-49$$

Many researches have been conducted to improve the traditional SSP scheme by choosing efficient values for α , β . Nevertheless, the 3rd order-3rd stages Strong-stability-preserving (SSP 3-3) method is widely used for the solution of the advection-diffusion equations, gas dynamics, and electromagnetics applications since it is low-storage, compact, simple to code, optimal, and stable for all order of accuracy in spatial space. I also used (SSP 3-3) scheme,

$$U^{(1)} = U^{n} + \Delta t \ L(U^{n})$$

$$U^{(2)} = \frac{3}{4}U^{n} + \frac{1}{4}\left(U^{(1)} + \Delta t \ L(U^{(1)})\right)$$

$$U^{n+1} = \frac{1}{3}U^{n} + \frac{2}{3}\left(U^{(2)} + \Delta t \ L(U^{(2)})\right)$$
4-50

to integrate time space in present work.

4.7.6.1 Time step calculation

The time step value Δt for non-linear system of differential equations can be predicted by

$$\Delta t_I = CFL \frac{\Omega_I}{\left(\hat{\Lambda}_c^x + \hat{\Lambda}_c^y + \hat{\Lambda}_c^z\right)_I + C\left(\hat{\Lambda}_v^x + \hat{\Lambda}_v^y + \hat{\Lambda}_v^z\right)_I} \cdot 4-51$$

Here, the convective spectral radii are defined as

$$\hat{\Lambda}_{c}^{x} = (|u|+c)\Delta\hat{S}^{x}, \ \hat{\Lambda}_{c}^{y} = (|v|+c)\Delta\hat{S}^{y}, \ \hat{\Lambda}_{c}^{z} = (|w|+c)\Delta\hat{S}^{z},$$
4-52

and the viscous spectral radii are given by

$$\hat{\Lambda}_{\nu}^{x} = \max\left(\frac{4}{3\rho}, \frac{\gamma}{\rho}\right) \left(\frac{\mu}{\Pr}\right) \frac{\left(\Delta S^{x}\right)^{2}}{\Omega},$$

$$\hat{\Lambda}_{\nu}^{y} = \max\left(\frac{4}{3\rho}, \frac{\gamma}{\rho}\right) \left(\frac{\mu}{\Pr}\right) \frac{\left(\Delta S^{y}\right)^{2}}{\Omega},$$

$$\hat{\Lambda}_{\nu}^{z} = \max\left(\frac{4}{3\rho}, \frac{\gamma}{\rho}\right) \left(\frac{\mu}{\Pr}\right) \frac{\left(\Delta S^{z}\right)^{2}}{\Omega}.$$

$$4-53$$

Note that C is a constant parameter which is set; zero for zero-order Boltzmann-based model; 2 for first-order Boltzmann-based model; 4 for second-order Boltzmann-based model. $\Delta \hat{S}^x$, $\Delta \hat{S}^y$, $\Delta \hat{S}^z$ are the projections of the control volume on the *y*-*z*, *x*-*z* and *x*-*y* planes, respectively. They can be defined as

$$\Delta \hat{S}^{x} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{x}|_{J}, \Delta \hat{S}^{y} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{y}|_{J}, \Delta \hat{S}^{z} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{z}|_{J}.$$
4-54

where S_x, S_y, S_z denote the *x*-,*y*- and the *z*-component of the face vector $\vec{S} = \mathbf{n} \cdot \Delta S$.

4.7.7 Rules of the numerical integration

In weak formulation (Eq. 4-45), the volume and surface integrals are needed to be approximated as a weighted summation of function evaluation at a number of points. The choice of quadrature rule limits the order of DG method, therefore, choosing an appropriate numerical integration method is essential to obtain highly accurate DG solutions.

In case of one-dimensional problems, a volume integral can be determined numerically on the master element region $\Omega_0 \in [-1,1]$ as

$$\int_{\mathbb{R}^{\mathcal{D}}} f(x) dx = \int_{-1}^{1} f(\xi) |J|_{x \to \xi} d\xi \approx \frac{\Delta x}{2} \sum_{i=1}^{N_{GP}} \omega_i f(\xi_i)$$

$$4-55$$

where N_{GP} is the number of required quadrature points and $\mathbf{0}_i$ is the weight coefficient value of those and ξ_i is the corresponding Gauss point locations. In this dissertation, the Gaussian Legendre quadrature rule is employed for solving integrals inside the element, and over the element interfaces which necessitates the application of the exact polynomials of degree 2p and 2p+1 for the numerical integrations inside elements and over the faces, respectively[110].


Figure 4-16 Number of required quadrature points for integrating inside and over faces of a 1-D and 2-D element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials

In two-dimensional cases, performing integration on the master elements is a trivial since the master elements are rectangular shapes with perpendicular edges. The integrals can be determined using the tensor product of two uni-dimensional quadrature rules [125, 126]. Figure 4-16 shows the distribution of the Gauss-Legendre quadrature points inside and over the master element for 1-D and 2-D elements.

In case of three-dimensional DG method, the numerical integration of the boundaries and volumes are performed using a symmetrical integration rule. The surface Integrals are approximated by the following formulation

$$\int_{\mathbb{R}^{\mathcal{D}}} f\left(x_{1}, x_{2}\right) d\Gamma_{e} = \int_{0}^{1} \int_{0}^{1-r} f\left(\xi_{1}, \xi_{2}\right) \left|J\right|_{\mathbf{x} \to \mathbf{\eta}} d\boldsymbol{\xi} \approx \left|\mathbf{A}_{\Omega_{0}}\right| \sum_{i=1}^{N_{p}} \omega_{i} f\left(\xi_{1}, \xi_{2}\right),$$

$$4-56$$

where $|A_{\Omega_0}|$ is the surface area of the standard (reference) triangle element and ω_i is the associated weight with the quadrature points. The volume integrals are estimated by

$$\int_{\mathbb{R}^{\mathcal{D}}} f(x_1, x_2, x_3) d\Omega_e = \int_{0}^{1} \int_{0}^{1-r} \int_{0}^{1-r-s} f(\xi_1, \xi_2, \xi_3) |J|_{\mathbf{x} \to \mathbf{\eta}} d\boldsymbol{\xi} \approx |\Omega_0| \sum_{i=1}^{N_p} \omega_i f(\xi_1, \xi_2, \xi_3)$$

$$4-57$$

where $|\Omega_0|$ denotes the volume of master tetrahedral element.



Figure 4-17 Number of required quadrature points for numerical integration in a tetrahedron element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials

4.7.8 Pseudo-algorithm of a modal DG solver

Figure 4-18 demonstrates the pseudo flowchart of a multi-dimensional discontinuous Galerkin solver for compressible Navier-Stokes equations.



Figure 4-18 The pseudo flow chart of a 2-D DG solver.

CHAPTER 5. Discontinuous Galerkin method: Special topics

Albert Einstein (1879-1955):

"... all knowledge starts from experience and ends in it. Propositions arrived at by purely logical means are completely empty as regards reality."

In this Chapter, an analytical solution of the Navier-Stokes-Fourier (NSF) equation is provided for viscous shock structure problem. Various limiter and numerical flux functions are reviewed and analyzed in detail. The performance of limiters and flux functions are reported for stiff and smooth solutions of NSF and Euler equations. The sensitivity of the modal DG method to the linear mapping of the curved boundaries is examined for Euler and NSF equations.

5.1 Stiff but continuous benchmark problem

Majority of the challenging engineering problems are irreversible and contain a process with a rapid change of the field properties. NSF is the most well-known model which is commonly used for studying the engineering fluid dynamics problems, although its application in far-from-equilibrium conditions is questionable [57]. It is expected that the solution of NSF equation is only being qualitatively in agreement with experimental results in case that solution departs considerably from equilibrium state. Nonetheless, computational study of NSF model in any thermodynamic condition can pave the way for designing a robust and an accurate numerical method.

One of the complicated and cumbersome type of thermal non-equilibrium appears in compression and expansion shock waves where a rapid change of flow properties occurs within a very thin region [13, 107]. In almost all of the high-speed flows, there is a front shock wave with a thickness of order of few mean free path length that significantly influences the flow behavior in another region of the flow field. This frontal shock wave is usually analogous to the one-dimensional viscous shock structure problem, as shown in Figure 5-1.

In viscous shock wave, the flow speed is higher than sound-speed since the speed of moving gas particles is much higher than the gas particle's peculiar velocity. Thus, in

macroscopic sense, the convective terms of momentum conservation laws tend to create a discontinuous jump alongside the shock wave whilst the thermal and viscous dissipations — originating the lack of enough number of particle collisions in shock region— try to decay and fade the level of the flow stiffness by converting the translational energy into the internal energy. Thus, viscous shock wave solution is mathematically continuous and smooth, but it is extremely stiff and strong enough to arouse the numerical wiggles near shock waves.

Analyzing the viscous shock wave and studying the physics of shock wave structures for varying Mach numbers — such as shock thickness, separation distance, and asymmetry — have been the center of attention of the physicists from the past century [13, 70, 127-130]. The numerical difficulties associated with the stiffness of the shock structure has also been studied by many mathematicians [65, 112, 131, 132].



Figure 5-1 The appearance of the shock structure in multi-dimensional problems. The zoomed region illustrates the location of front shock structure. The lower and upper figures display the shock profiles and the variation of the shock density thickness versus Mach numbers for different gas molecules, respectively.

There are two different approaches for solving viscous shock wave problem; recasting the equations into ordinary differential form and then solving them numerically using dynamical systems; solving the partial differential equations by aid of CFD [41, 70, 108, 127, 133, 134]. The physicists prefer the former so as to avoid the numerical difficulties (artifacts) in solving a partial differential equation.

It was found that the numerical results of the shock structure are very sensitive to the extent of the computational domain, the imposed downstream boundary conditions, the level of intrinsic physical and artificial viscosity and thermal conductivity, and the employed time integration schemes [14, 65, 131, 135-137]. Therefore, it may be useful to solve this problem using advanced high-order methods in order to examine the performance of the methods for this stiff but continuous solution of the NSF equations.

In the following of this chapter, this benchmark problem is extensively used to measure the performance of the limiters, flux functions, and to compare the capability of the finite volume methods with DG method in capturing shock waves.

5.1.1 Analytical analysis of viscous shock-wave

The viscous shock wave problem was initially solved analytically for the case that viscosity and thermal conductivity were constant and independent from temperature variations [133]. However, the effects of temperature variation are significant and not negligible for shock wave problem. So, the analytical solution of the viscous shock wave, considering the variation of the transport coefficients due to temperature variation, had been demanding until the general closed form of the analytical solution of the viscous shock was derived by Myong in 2014 [127].

The full derivation of the analytical solution of the viscous shock wave for Maxwellian and the hard-sphere gas molecules was described in [127]. Therefore, only the exact analytical solution of the flow properties is provided here. To the interested readers, it is recommended to study [107, 127] for further information about the derivation of the exact viscous shock wave problem.

5.1.1.1 Density function of Maxwellian molecule

The analytic solution of the density profile for the Maxwellian molecule [127] is defined as

$$3\theta_{1}M\left(\frac{\gamma\pi}{2}\right)^{1/2}(\overline{x}-x_{r_{a}}) = \frac{1}{r_{a}}\left(\frac{5}{4}+\frac{1}{2r_{a}}\right) - \frac{1}{r}\left(\frac{5}{4}+\frac{1}{2r}\right) + \frac{4}{\beta}\ln\frac{\left[(r_{1}^{-1}-r_{-}^{-1})/(r_{1}^{-1}-r_{a}^{-1})\right]^{(2\alpha-r_{1}^{-2})/r_{1}}}{\left[(r^{-1}-r_{2}^{-1})/(r_{a}^{-1}-r_{2}^{-1})\right]^{(2\alpha-r_{2}^{-2})/r_{2}}}.$$
5-1

where the subscripted 1 denotes the upstream, and the subscripted 2 stands for the downstream conditions; $r_a = 5/4\alpha$ is the integration constant value and r is density

variable in reduced form; x_{r_a} is the location where local density becomes equal to the arithmetic average of the upstream and downstream density. The constant parameters of α and β are defined by

$$\alpha = \frac{\gamma^2 M^2 \left[2 + (\gamma - 1)M^2 \right]}{2(\gamma - 1)(1 + \gamma M^2)^2},$$
5-2

$$\beta = \sqrt{25 - 32\alpha}.$$

5.1.1.2 Density function of hard-sphere molecule

Analytical solution of the hard-sphere gas molecule reads as

$$\begin{split} M\left(\frac{9\gamma\pi\theta_{1}}{10}\right)^{1/2}(\bar{x}-x_{r_{a}}) &= \\ (2\alpha-r^{-2})^{1/2}-(2\alpha-r_{a}^{-2})^{1/2}+\\ &\frac{5}{4}\left(\tan^{-1}(2\alpha r_{a}^{2}-1)^{-1/2}-\tan^{-1}(2\alpha r^{2}-1)^{-1/2}\right)+\\ &\frac{4}{\beta}r_{1}^{-1}(2\alpha-r_{1}^{-2})^{1/2}\left(\tanh^{-1}\frac{(2\alpha-r_{1}^{-2})^{1/2}(2\alpha-r_{a}^{-2})^{1/2}}{2\alpha-r_{1}^{-1}r_{a}^{-1}}\right)-\\ &-\tanh^{-1}\frac{(2\alpha-r_{1}^{-2})^{1/2}(2\alpha-r^{-2})^{1/2}}{2\alpha-r_{1}^{-1}r^{-1}}\right)-\\ &\frac{4}{\beta}r_{2}^{-1}(2\alpha-r_{2}^{-2})^{1/2}\left(\tanh^{-1}\frac{(2\alpha-r_{2}^{-2})^{1/2}(2\alpha-r_{a}^{-2})^{1/2}}{2\alpha-r_{2}^{-1}r_{a}^{-1}}\right)-\\ &-\tanh^{-1}\frac{(2\alpha-r_{2}^{-2})^{1/2}(2\alpha-r_{2}^{-2})^{1/2}}{2\alpha-r_{2}^{-1}r_{a}^{-1}}\right). \end{split}$$

5.1.1.3 Solution of other variables

Density solution is obtained by solving equation (Eq. 5-1) or (Eq. 5-4) using bisection method. The solution of the other variables is dependent to the density solution, and they can be easily calculated using the following relations:

$$\upsilon = r^{-1}, \theta = \frac{2\alpha - r^{-2}}{5}, \ \phi = \frac{2\alpha - r^{-2}}{5r^{-1}},$$

$$\sigma = \frac{-4r^{-2} + 5r^{-1} - 2\alpha}{5r^{-1}}, \ \varphi = \frac{4r^{-2} - 5r^{-1} + 2\alpha}{5\alpha},$$

$$5-5$$

where r, υ , θ , σ , ϕ are density, velocity, temperature, normal stress, and heat flux variables in reduced form.

5.1.2 Verification of numerical methods

The DG method has been mostly verified based on examination of the global conserved solution, although the most important variables are generally those quantities of engineering interest – e.g. non-equilibrium non-conserved variables, lift, drag, shock density thickness, and so on. In this section, the numerical results of the not only global quantities but also the non-conserved variables are compared with the exact analytical solution of NSF equations for hard-sphere and Maxwellian gas molecules.

5.1.2.1 Finite volume method vs. discontinuous Galerkin method

The analytical solution of the hard-sphere molecule is compared with finite volume and DG approximate solutions at three different Mach numbers. The computational domain was tessellated with the same number of the element for both numerical methods. All numerical solutions are shown at sub-cell level rather than cell average resolution to observe more detail of the solution and to compare the methods fairly.

The normalized solution of the density profile is depicted for coarse and fine resolutions in Figure 5-2. Results illustrate that the piecewise constant solution is the most diffusive solution. It is obvious that the location of X_{r_a} is not captured accurately when piecewise constant DG method or second order FVM method using coarse grid is employed. FVM method using coarse grid under-predicts the density profile compared to the analytical solution. This discrepancy becomes more tangible when Mach number increases. On the other hand, it is obvious that the difference between analytical solution and DG approximate solution becomes negligible by increase of the degree of the polynomial. Almost for all cases, DG high-order approximate solutions are closer to the analytical solution compare to solutions obtained by the same order FVM method.



Figure 5-2 Comparative analysis of the normalized shock density profile between finite volume methods, DG spectral method, and exact analytical solution at three different Mach numbers. (left) Coarse spatial resolution solution Ne=20, and (right) fine spatial resolution solution Ne=100.

For the case that DG quadratic or linear piecewise polynomials are utilized, the location of shock-wave is estimated accurately even if 20 computational elements are used. Nevertheless, the piecewise linear approximation, obtained using 20

computational elements, is deviated from the exact solution in rapid changing region of the upstream side. This discrepancy becomes more obvious when Mach number increases; however, it disappears when the number of computational elements is sufficiently large.



Mach=15, Ne=100

Figure 5-3 Comparing the normalized shock profiles of the DG polynomial approximated solution with exact analytical solution of hard-sphere gas (left), and Maxwellian gas molecule (right) at three different Mach numbers.

This comparison shows that the finite volume methods — both MUSCL and piecewise linear reconstruction schemes— are more diffusive than DG methods if the same grid resolution and order of accuracy is being used for the simulation. The results also demonstrated that as Mach number increases, either more computational elements or higher-order polynomial solutions are required to capture the shock position and its profiles.

5.1.2.2 Profile verification

In Figure 5-3, the profiles of the conservative and primitive (density, velocity, and temperature) variables are displayed for the hard-sphere and Maxwellian molecules at three different Mach numbers. The black solid line indicates the analytical solutions while the gray solid and scatter lines correspond to the numerical solutions with the polynomial order of zero, one, and two.

Figure 5-3, illustrates that the DG approximate solution becomes closer to the analytical solution by increase of the degree of polynomial. The results illustrate that larger computational domain is required for simulation of Maxwellian gas molecule in compared to hard-sphere gas type. This is because that the shock profile of hard-sphere gas becomes more tightly packed and compressed by increasing the Mach number, whilst the shock profile of Maxwellian gas becomes more diffusive and disperse.

It is also shown that the lower-order DG approximate solution of Maxwellian gas molecule displays better qualitatively matches with analytical solution compare with hard-sphere gas molecule. This is because that the Maxwellian molecule has the biggest viscosity power-index among all kind of the gas molecules which causes the increase of the viscosity in the shock region, and generation of the most diffused and smoothest shock profiles among all type of the gas molecules.

Figure 5-4 depicts the profiles of the non-conservative variables – normal stress and heat flux– for the hard-sphere and Maxwellian gases at three different Mach numbers. A noticeable physical feature is that the shock transition regime extends further to upstream as the molecule deviates from the hard-sphere type. It is shown that the piecewise constant solution smears the stress and heat flux profiles more than high-order DG solutions since the level of the numerical diffusion is the highest for first-order solution approximation, and the second-order derivatives are not resolved accurately in low-order approximation.

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Hard-Sphere Molecule

Maxwell Molecule



Mach=15, Ne=100

Figure 5-4 Comparing the normalized stress and heat flux profiles of the DG polynomial approximated solution with exact analytical solution of hard-sphere gas (left), and Maxwellian gas molecule (right) at three different Mach numbers.

It is also obvious that the prediction of shock properties for hard-sphere molecule using piecewise constant solution is erroneously as the Mach number increases. This is reverse in the case of Maxwellian gas molecule that low-order solution becomes closer to the analytical solution by increasing the upstream Mach number due to the fact that the shock wave becomes thicker and smoother by increasing the upstream Mach number. The results also reveal that the stress profile is analogous to heat flux profile and it becomes more compressed by increasing the upstream Mach number. In the case of hard-sphere gas molecule, the maximum normal stress and minimum heat flux values are located at same position although this does not hold for Maxwellian gas molecule where the distance between stress and heat flux extrema increases by increasing the upstream Mach number.

5.2 Spurious oscillations

5.2.1 Gibbs phenomena

DG method similar to other high-order methods suffers from the existence of the spurious oscillations at near the discontinuities due to Gibbs phenomena. A taxonomy of the spurious oscillation controllers is depicted in Figure 5-5. There are three general approaches to eliminate wiggles from the numerical solution: artificial viscosity, digital filters, and limiters. Among those, limiters may take more attention since they can be used not only to control wiggles but also to enforce the nonlinear stability in the numerical scheme.

The choice of limiter functions distinguishes three different limiter categories for high-order methods; slope limiters, spectral limiters, and non-oscillatory limiters. Slope limiters were initially developed for finite volume method and later they are served in spectral *hp* methods. One way to group the slope limiters is to label them base on the behavior of their limiter functions $\phi(r)$ in Harten's TVD region[84] (or in Spekreijse Monotonicity region [91]). According to this classification, total variation diminishing (*TVD*), total variation bounded (*TVB*), local extremum diminishing (LED), essentially local extremum diminishing (ELED), monotonicity preserving (MP) and multidimensional limiters can be distinguished from each other.

In spite of the slope limiters that have been designed for finite volume method, the spectral limiters were designed originally for high-order spectral methods. High-order sub-cell limiter, moment limiter, and the modified moment limiter belong to this class of limiters.

Final class of limiters is the non-oscillatory limiters which can also be considered as a high-order reconstruction scheme. Harten [89] was the first person who employed nonlinear reconstruction stencils at interface of the control volumes and introduced ENO high-order reconstruction scheme. Later, this scheme has been developed more, and many novel non-oscillatory schemes are introduced such as weighted essentially non-oscillatory (WENO)[86], monotonicity preserving weighted essentially non-oscillatory (MPWENO)[138], Hermite weighted essentially non-oscillatory (HWENO) [139-141], and so on.



Figure 5-5 Taxonomy of spurious oscillations controllers

Although there are many choices for limiters, the numerical experiments reveal that most of them does not have privilege to the others [142]. Some of the limiters perform better at some specific problems, and the others are better in other problems. Even though there is no rigorous guideline for selecting a proper limiter for certain problem, a systematic analysis on the limiters is essential to find out their overall performance. The application of the limiters eliminates unphysical oscillations and preserves the nonlinear stability of the numerical method, but preservation of the global order of accuracy is still questionable. In most of the time, application of the limiters degrades the solution accuracy such that the order of accuracy reduces to first-order near stiff regions. In the other words, the obtained accuracy using limiters is usually far less than expected global order of accuracy.

In this section, some of the limiters which are noticed more in DG community – total variation diminishing (*TVD*)[80], total variation bounded (*TVB*)[109], generalized moment (GM), simple monotonicity preserving (SMP), positivity preserving (PP)[143-145], Hermite WENO (HWENO)[139-141], and differentiable and monotonicity preserving (DAMP) limiters– are selected for studying the performance of limiters for viscous shock wave problem.

In previous studies on performance of the limiters, the accuracy of limiters was investigated by either qualitatively comparison of the limited solution profile with exact solution of the Euler equation or studying a very smooth solution of the scalar model-, inviscid Euler-, or NSF equations. The error norm analysis was only provided for the case that shock waves do not exist in the domain, and the point-to-point profiles comparison between the limited solutions and exact solution was preferred for measuring the performance of limiters in the case that a stiff region exists in the computational domain [142].

Nonetheless, in order to indicate the real order of the accuracy of DG methods in conjugation with oscillation controllers, it is essential to analyze the convergence rate when a strong but continuous gradient exists in the computational domain. Hence, viscous shock problems can be considered as a unique benchmark problem for studying the performance of limiters, since the solution is smooth enough to measure error norms and convection terms are strong enough to induce unphysical oscillations.

5.2.2 Trouble cell indicator

Shock indicators have been commonly used, besides limiters, to minimize the numerical diffusion of the limiters, to avoid use of limiters in smooth flow regions, and to reduce the computational cost of the limiting process.

Let's assume the limited solution at right and left side of the local element in a general form of

$$\mathbf{w}_{h^{e}}\Big|_{x_{i+1/2}} = \mathbf{w}_{i}^{0} + \tilde{\mathbf{w}}_{i}, \ \mathbf{w}_{h^{e}}\Big|_{x_{i-1/2}} = \mathbf{w}_{i}^{0} + \tilde{\tilde{\mathbf{w}}}_{i},$$
 5-6

where \mathbf{w}_i^0 presents the average of the solution in the local element; $\tilde{\mathbf{w}}_i$, $\tilde{\tilde{\mathbf{w}}}_i$ are the limited projection of the high-order terms at right and left side of the local element defined as

 $\tilde{\mathbf{w}}_{i} = \sum_{l=1}^{N_{p}} \widehat{\mathbf{w}}_{h^{e}}^{l}(t) \phi_{n}(\xi_{i+1/2}), \quad \tilde{\tilde{\mathbf{w}}}_{i} = \sum_{l=1}^{N_{p}} \widehat{\mathbf{w}}_{h^{e}}^{l}(t) \phi_{n}(\xi_{i-1/2}) \text{ in which the limited moment (local degree of freedom) of the approximate polynomial solution in the limited element are denoted by <math>\widehat{\mathbf{w}}_{h^{e}}^{l}$.

If the limited moment value is not equal to original moment value $\mathbf{w}_{h^e} \neq \mathbf{w}_{h^e}^{t}$, a limiter is activated and the high-order moments in the troubled element are replaced with limited moment values. This approach is the simplest way for deciding whether limiting the moments of the DG solution in the local elements is needed or not. However, it is very diffusive and may not be applicable to use accompanied by several kinds of the limiters.

Application of more advanced shock-detectors as the initial stage of limiting process is more fruitful. There are several shock-detector methods that can be utilized for finding the troubled cells; nonetheless, KXRCF has shown a decent performance for several applications compared with the others [146]. In present work, KXRCF shock detector in cooperation with several limiters — including *TVB*, GM, SMP, HWENO, and DAMP limiters— is employed in order to examine the performance of the limiters in the application of viscous shock wave problem.

The KXRCF shock-detection technique was introduced by Krivodonova et al. [147]. It works based on the super-convergence property of discontinuous Galerkin (DG) method at the outflow boundaries of an element in the smooth regions. Krivodonova et al. [147] demonstrated that the smooth solutions of DG method exhibit a strong superconvergence phenomena at outflow boundaries such that

$$\frac{1}{\left|\partial\Omega_{e}^{+}\right|} \oint_{\partial\Omega_{e}^{+}} \left(\varepsilon_{h_{e_{j}}} - \varepsilon_{h_{neigh_{j}}}\right) d\Gamma_{e} = O(h^{2p+1}), \qquad 5-7$$

where $\varepsilon_{h_{e_j}}$ and $\varepsilon_{h_{neigh_j}}$ are the arbitrary quantity derived from a solution component on the adjacent interfaces between the element and its neighboring element on the side of $\partial \Omega_e^+$. *h* indicates the radius of the circumscribed circle in the element Ω_e , and is equivalent to cell size Δx in one-dimensional problem. $\left|\partial \Omega_e^+\right|$ indicates the length of $\partial \Omega_{e}^{+}$, For a given linear or nonlinear differential system, the boundaries of an element $\partial \Omega_{e}^{-}$ can be divided into two parts: the inflow boundary $\partial \Omega_{e}^{-}$ where the flow comes into the element (**v.n** < 0), and the outflow boundary $\partial \Omega_{e}^{+}$ where the flow goes out of the element (**v.n** > 0). In case of one-dimensional problem; $\partial \Omega_{e}^{+}$ drops out from (Eq. 5-7) since it consists of only one point; the right face is considered as an inflow boundary if the velocity is negative at the right interface, otherwise, it is known as an outflow boundary.

The KXRCF detector can be defined more specifically employing above information, and setting a specific value for Λ_e (for example 1.0) as a trigger value in order to label the cell as the troubled cell;

$$\Lambda_{e} = \frac{\left| \oint_{\partial \Omega_{e}^{-}} \left(\varepsilon_{h_{e_{j}}} - \varepsilon_{h_{neigh_{j}}} \right) d\sigma \right|}{h^{(p+1)/2} \left| \partial \Omega_{e}^{-} \right| \left\| \varepsilon_{h_{e}} \right\|}.$$
5-8

Here $\|\varepsilon_{h_e}\|$ is the maximum norm based on the local solution maxima at quadrature points, and is equivalent to the element average for one-dimension problems.

5.2.3 Conventional limiter functions

5.2.3.1 Total variation diminishing (TVD) limiter

The first implementation of limiters in DG framework was done by Chavent and Cockburn in 1989 [121]. They implemented Van Leer [83] total variation diminishing (*TVD*) slope limiter for improving the stability of the DG method. In completion of their work, Cockburn et. al. [105] showed that the slope limiter must be applied not only in stiff regions but also in some part of the smooth regions where is affected by spurious oscillations.

Application of TVD limiters yield to solution of at most first-order of accuracy in non-smooth regions due to strictly enforcement of the monotonicity condition. It is not possible to design any high-order schemes with the *TVD* property which maintains the high-order solution uniformly throughout the computational domain [148]. Nonetheless, it is still important to know the performance of this commonly used limiter for DG framework, without employing the shock trouble indicator, in presence of viscous shock wave.

A non-differentiable Minmod function returns the smallest argument if all arguments are positive, or the largest argument when all arguments are negative, and zero otherwise. The general form of the Minmod function with *n* arguments is given by

$$m(a_1, a_2, \dots, a_n) = s \cdot \min\{|a_1|, |a_2|, \dots, |a_n|\},$$
5-9

where

$$s = \frac{1}{2} [sign(a_1) + sign(a_2)].$$

$$\left(\left| \frac{1}{2} [sign(a_1) + sign(a_3)] \cdots \frac{1}{2} [sign(a_1) + sign(a_n)] \right| \right).$$
5-10

Accordingly, the TVD-Minmod slope limiter can be defined as

$$\widehat{\mathbf{w}}_{h^{e}}^{l} = \mathbf{m}(\widehat{\mathbf{w}}_{h^{e}}^{l}, \Delta_{+} \overline{\widehat{\mathbf{w}}}_{h^{e}}, \Delta_{-} \overline{\widehat{\mathbf{w}}}_{h^{e}}), \qquad 5-11$$

where $\Delta_{+}\overline{\mathbf{w}}_{i} = \overline{\mathbf{w}}_{h^{e+1}} - \overline{\mathbf{w}}_{h^{e}}, \ \Delta_{-}\overline{\mathbf{w}}_{i} = \overline{\mathbf{w}}_{h^{e}} - \overline{\mathbf{w}}_{h^{e-1}}.$

5.2.3.2 Total variation bounded (TVB) limiter

Cockburn and Shu [109] designed *TVB* slope limiters by replacing the *TVD*-*Minmod* function with a modified Minmod function in which a user input adjusting parameter is needed to tune the critical threshold value for maintaining the formal accuracy of the scheme at extrema. A *TVB* limiter may maintain the high-order accuracy of the solution, but it does not satisfy the strict maximum principle condition. It may also not possible to prove the existence of high-order solution with *TVD* property in multidimensional problems.

In general, a TVB limiter function can be defined as

$$\widehat{\mathbf{w}}_{h^{e}}^{l} = \widehat{\mathbf{m}}(\mathbf{w}_{h^{e}}^{l}, \Delta_{+} \overline{\mathbf{w}}_{h^{e}}, \Delta_{-} \overline{\mathbf{w}}_{h^{e}}), \qquad 5-12$$

where

$$\hat{\mathbf{m}}(a_1, a_2, a_3) = \begin{cases} a_1 & \text{if } |a_1| > Mh^2, \\ m(a_1, a_2, a_3) & \text{otherwise.} \end{cases}$$
5-13

Here \hat{m} is the non-differentiable modified Minmod function and *M* is a constant positive threshold value. Cockburn and Shu [109] showed that the *M* parameter is related to second-order derivatives of the local solution components for scalar problems. Nonetheless, estimating *M* value for the system of equations is more difficult, and it should be defined by user input.

In fact, the critical threshold parameter M is a shock detector criterion, and the value of M indicates the resolution of the solution at near the shock waves. If M is chosen to be a small value, unnecessary elements will be identified as troubled elements, in consequence of that the computational cost increases and accuracy reduces to be maximum first-order at marked elements. On the other hand, if M is chosen to be a large value, wiggles and oscillations may not be controlled properly and appear in the solution.

In this study, the performance of *TVB* limiter is studied while it was employed in conjugation with KXRCF indicator to eliminate the ambiguity in choice of M parameters.

5.2.3.3 Monotonicity preserving (MP) limiter

The monotonicity-preserving (MP) limiter was initially designed by Suresh in 1997 [90]. MP limiter was designed to enforce monotonicity strictly at near the extrema regions. In this limiter, high-order local degree of freedoms of the solution were neglected in the troubled element, and the solution was reconstructed linearly in such way that monotonicity is preserved. However, it was highly possible that the order of accuracy reduces miserably, and density becomes negative due to imposing the strict monotonicity constraint.

The simplified version of MP limiter with fewer restriction on enforcement of the monotonicity condition was introduced by Ride and Margolin [149]. The simple monotonicity preserving (SMP) is placed in the category of the slope limiters. Various limiters — including sign-preserving limiter [149], positivity preserving [139, 143], DAMP limiter, multi-dimensional Barth Jespersen [150] and MLP-u limiters [151]— were designed based on the concept introduced in this limiter.

In SMP, the solution is initially reconstructed at interfaces using piecewise linear interpolation, and then the gradients of the solution at interfaces are multiplied with a scalar limiter function ϕ as

$$\mathbf{w}_{i}^{h} = \mathbf{w}_{i}^{0} + \varphi_{i} \nabla \overline{\mathbf{w}}^{h}.$$
 5-14

The performance of the various derivations of this limiter is highly related to the definition of the scalar function φ_i , and the stencil used in limiting process. The classical definition of this non-differentiable function is defined such that the limited reconstructed solution is locally bounded;

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$$\varphi_{i} = \min\left\{1, \frac{\Delta \bar{\mathbf{w}}_{i}^{\max}}{\Delta_{\max} \bar{\mathbf{w}}_{i}^{h}}, \frac{\Delta \bar{\mathbf{w}}_{i}^{\min}}{\Delta_{\min} \bar{\mathbf{w}}_{i}^{h}}\right\},$$
5-15

where

$$\Delta \bar{\mathbf{w}}_i^{\max} = \bar{\mathbf{w}}_i^{\max} - \bar{\mathbf{w}}_i, \qquad 5-16$$

$$\Delta \overline{\mathbf{w}}_i^{\min} = \overline{\mathbf{w}}_i^{\min} - \overline{\mathbf{w}}_i, \qquad 5-17$$

$$\Delta_{\max} \overline{\mathbf{w}}_{i}^{h} = \max_{x \in \Omega_{e}} \mathbf{w}_{h^{e}}(\boldsymbol{\xi}) - \overline{\mathbf{w}}_{i}, \qquad 5-18$$

$$\Delta_{\min} \overline{\mathbf{w}}_{i}^{h} = \min_{x \in \Omega_{e}} \mathbf{w}_{h^{e}}(\boldsymbol{\xi}) - \overline{\mathbf{w}}_{i}.$$
5-19

Here $\overline{\mathbf{w}}_i^{\max}$ and $\overline{\mathbf{w}}_i^{\min}$ are the maximum and minimum value of the \mathbf{w}_h in all the elements adjacent to the troubled element, respectively. $\Delta_{\max} \overline{\mathbf{w}}_i^h$ is the maximum value of the DG solution throughout Gauss quadrature points inside the troubled element.

5.2.3.4 Generalized moment (GM) limiter

There are very few existing limiters that were originally designed for DG method. Biswas et al. [152] introduced first generalized moment slope limiter in 1994. This slope limiter have two distinct features; it can be used for employing *hp*-adaptivity in DG; it can detect the local critical points without any need for user input parameters.

In generalized moment (GM) limiter, the non-differentiable Minmod function is employed as a base function, and hierarchical limiting process deliberate to limit only necessary moments. The highest moment of the solution is limited first; then lowermoments will be limited consecutively if the higher moments have been changed in the limiting process.

The GM limiter function can be expressed as

$$\widehat{\mathbf{w}}_{h^e}^{l} = \frac{1}{2l-1} \operatorname{m}\left((2l-1) \mathbf{w}_{h^e}^{l}, \Delta_{+} \mathbf{w}_{h^e}^{l}, \Delta_{-} \mathbf{w}_{h^e}^{l}\right), \quad 1 \le l \le N_p,$$
5-20

where the second and third terms in (Eq. 5-20) are defined as $\Delta_+ \hat{\mathbf{w}}_{h^e}^{l} = \hat{\mathbf{w}}_{h^{e+1}}^{l-1} - \hat{\mathbf{w}}_{h^e}^{l-1}$ and

$$\Delta_\hat{\mathbf{w}}_{\scriptscriptstyle h^e}^{\scriptscriptstyle l} = \hat{\mathbf{w}}_{\scriptscriptstyle h^e}^{\scriptscriptstyle l-1} - \hat{\mathbf{w}}_{\scriptscriptstyle h^{e-1}}^{\scriptscriptstyle l-1}.$$

Burbeau et al. [153] revised GM limiter and introduced the modified generalized moment (MGM) limiter. MGM is very similar to the original one; however, an additional process is considered to improve the accuracy of the original generalized moment limiter. The limited moments are first calculated using (Eq. 5-20). Next, they are modified by employing a Maxmod function as

$$\widehat{\mathbf{w}}_{h^e}^{l} = \widehat{\mathbf{M}}(\mathbf{w}_i^{l,Max}, \widehat{\mathbf{w}}_{h^e}^{l,(GM)}), \qquad 5-21$$

where maximum mode variable $\mathbf{w}_{i}^{l,Max}$ is given by

$$\mathbf{w}_{i}^{l,Max} = \frac{1}{2l-1} m((2l-1)\mathbf{w}_{i}^{(l)}, \ \mathbf{w}_{i+\frac{1}{2}}^{(l-1)+} - \mathbf{w}_{i}^{(l-1)}, \ \mathbf{w}_{i}^{(l-1)} - \mathbf{w}_{i+\frac{1}{2}}^{(l-1)-}), \ 1 \le l \le N_{p}, \qquad 5-22$$

$$\mathbf{w}_{i+\frac{1}{2}}^{(l-1)+} = \mathbf{w}_{i+1}^{(l-1)} - (2l-1)\mathbf{w}_{i+1}^{(l)},$$
5-23

$$\mathbf{w}_{i-\frac{1}{2}}^{(l-1)-} = \mathbf{w}_{i-1}^{(l-1)} - (2l-1)\mathbf{w}_{i-1}^{(l)} .$$
 5-24

and Maxmod function \hat{M} is defined as

$$\widehat{M}(a_1, a_2) = \begin{cases} \max\{a_1, a_2\} & \text{if } sign(a_1) = sign(a_2) > 0, \\ \min\{|a_1|, |a_2|\} & \text{if } sign(a_1) = sign(a_2) < 0, \\ 0 & \text{otherwise.} \end{cases}$$
5-25

5.2.3.5 Positivity-preserving limiter

Positivity preservation of the physical properties — density and pressure — is the obligatory condition for enforcing the monotonicity principle. If the density or pressure becomes negative, the system of (Eq. 4-8) will be ill-posed and unsolvable. Nevertheless, preservation of positivity of physical parameters does not guarantee the boundedness of the solution; it will only keep density and pressure away from negative values.

Most of the high-order limiters do not satisfy the positivity property automatically [143]. Although there are some researches [143, 145, 154] showing that the application of positivity preserving schemes are sufficient for studying some applications, it is better to always employ a positivity preserving scheme in conjugation with a high-order limiter to guarantee the boundedness of the solution.

The first positivity preserving (PP) limiter for DG method was introduced by Zhang and Shu [143]. The PP limiter does not satisfy the strict monotonicity constraint; instead, it preserves the positivity of the density and pressure by multiplication of the moments of the solution with a simple scaling factor. The PP limiter is a non-differentiable slope limiter that is computationally very cheap and easy to implement in structured and unstructured grids.

PP limiter can be considered as a simplified version of SMP limiter in which the scaling function performs such that density and pressure solutions become positive [149]. In PP limiter, it is tried to relax the monotonicity principal constraint in order to enforce the positivity condition without destroying the accuracy of the high-order solution [143]. It is reported that PP limiter maintains the global order of accuracy in

smooth regions [155]; however, the performance of this limiter for more cumbersome condition (like shock region) is still questionable.

Implementation of the PP limiter starts with defining a small number ε based on the average value of density and pressure in the target cell $\varepsilon = \min\{\overline{\rho}, \overline{p}, 10^{-13}\}$. Afterwards, the positivity of density is surveyed by finding the minimum value of destiny ρ_{min} looping over the quadrature points in the local elements. Next, positivity of density maintains by multiplying Θ_1 to all higher-order moments of the density solution. As a result, the modified and positive solution of density is obtained;

$$\theta_{1} = \min\left\{1, \frac{\varepsilon - \overline{\rho}}{\rho_{\min} - \overline{\rho}}\right\},$$
5-26

$$\left|\rho\right|_{h} = \rho_{h} + \theta_{1}(\rho_{h}^{n} - \rho_{h}).$$
5-27

Next, the solution of density in evaluating time step is replaced by the modified polynomial solution $|\rho|_{h}$ in the troubled elements.

Second step of PP limiting process is intended to preserve the positivity of the pressure. This requires the scaling of all high-order moments with θ_2 for all conservative variables as

$$\mathbf{w}_h = \mathbf{w}_h + \mathbf{\theta}_2(\mathbf{w}_h^n - \mathbf{w}_h), \qquad 5-28$$

where evaluating the value of θ_2 requires solving of

$$p\left[(1-t)\overline{\mathbf{w}}_{i}-t\mathbf{w}_{i}^{n}\right]=\varepsilon,$$
5-29

for t and setting θ_2 as the minimum value of t among all quadrature points.

5.2.3.6 Differentiable and monotonicity preserving limiter

It is well-known that non-differentiability of the limiter functions tends to cause severe convergence problems at steady-state [156]. Differentiable and monotonicity preserving limiter (DAMP) is inspired by the work of Michalak and Gooch [156]. Nevertheless, it is distinguished from their work, as it is a vertex based slope limiter with a differentiable limiter function designed for spectral *hp* methods.

A differentiability of the limiter function requires that φ_i to be continuous and conservative for all input data. Thus, φ_i should always be positive and should be retained under the non-differentiable Minmod function profile such that the limited value of the modal moment coefficients does not exceed the unlimited values of those.

As it is shown in Figure 5-6, it is obvious that most of the differentiable limiters are violating above conditions after some specific value of r. DAMP limiter function is designed such that above constraints and requirements are strictly satisfied;

$$\varphi(r) = 0, \quad \frac{\partial \varphi(r)}{\partial r} = 0, \quad \text{at } r \le 0,$$

$$\varphi(r) = 1, \quad \frac{\partial \varphi(r)}{\partial r} = 0, \quad \text{at } r \ge 1,$$

$$\lim_{r \to \infty} \varphi(r) = 1.$$

5-30



Figure 5-6 Comparison of the several differentiable slope limiter based on $\phi(r)$.

The preservation of high-order solution on uniform grid requires that the difference between unlimited solution and limited solution becomes less than $O(\Delta x^p)$. DAMP considers a threshold parameter ε to define the level of desirable numerical diffusion in the limiting process and to minimize the loss of the accuracy during limiting process. Figure 5-7 shows the behavior of its limiter function for different value of ε . It is obvious that smaller ε value yields to less numerical diffusion in the limiting process; however, very small value of ε can affect the stability of the numerical method. The choice of ε parameter is trade of between preservation of the accuracy on non-uniform grids and maintenance of the good convergence behavior of the DG method in steady state solution.

DAMP limits each degree of freedom individually using the differentiable limiter function obtained by employing a coplanar fitting technique, as shown in Figure 5-7.

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In DAMP limiter, the solution is initially split into three major parts: cell average, linear, and nonlinear reconstructed parts of the solution;

$$\mathbf{w}_{i}^{h} = \mathbf{w}_{i}^{0} + \mathbf{w}_{i}^{linear} + \sum_{l=2}^{N_{p}} \mathbf{w}_{i}^{nonlinear,l}, \qquad 5-31$$

where the *i*th projection of the solution in the target element is denoted by Π_h^i and the linear and nonlinear contributions are given by $\mathbf{w}_i^{linear} = \Pi_h^1 \mathbf{w}_i^h - \mathbf{w}_i^0$, $\mathbf{w}_i^{nonlinear,l} = \Pi_h^l \mathbf{w}_i^h - \Pi_h^{l-1} \mathbf{w}_i^h$.

Coplanar fitting technique



Figure 5-7 Differentiable slope function of DAMP limiter

The linear and nonlinear parts of the unlimited solution are multiplied with an individual scalar differentiable limiter functions φ and ϕ to control spurious oscillations generated in a high-order solution;

$$\mathbf{w}_{i}^{h} = \mathbf{w}_{i}^{0} + \varphi_{i} \mathbf{w}_{i}^{linear} + \sum_{l=2}^{N_{p}} \phi_{i}^{l} \mathbf{w}_{i}^{nonlinear,l}.$$
5-32

 φ_i enforces the monotonicity of the solution at interfaces of the local elements, and ϕ_i^l controls spurious oscillations contributed by high-order moments. Assuming that the ϕ_i^l function is identical to φ_i , the linear differentiable limiter function φ_i can be defined as

$$\varphi(x) = \begin{cases} x & x \le \varepsilon_a \\ \sqrt{r^2 - (x - x_r)^2} + y_r & \varepsilon_a \le x \le \varepsilon_b, \\ 1 & x \ge \varepsilon_b \end{cases}$$

$$\varepsilon_a = \frac{2 - \sqrt{2}\varepsilon}{2}, \ \varepsilon_b = 1 + \varepsilon,$$

$$r = \varepsilon \tan(\frac{\alpha}{2}), x_r = 1 + \frac{r}{\tan(\frac{\alpha}{2})}, \ y_r = 1 - r.$$
5-34

where the differentiability parameter \mathcal{E} is set to be 1/5 and $\alpha = 3\pi/4$. The input value of the limiter function *x* is given by

$$x = \begin{cases} \frac{\overline{\mathbf{w}}_{i}^{\min} - \mathbf{w}_{i}^{0}}{\mathbf{w}_{i}^{h} - \mathbf{w}_{i}^{0}} & \mathbf{w}_{i}^{h} - \mathbf{w}_{i}^{0} < 0, \\ \frac{\overline{\mathbf{w}}_{i}^{\max} - \mathbf{w}_{i}^{0}}{\mathbf{w}_{i}^{h} - \mathbf{w}_{i}^{0}} & \mathbf{w}_{i}^{h} - \mathbf{w}_{i}^{0} > 0, \\ 1 & \text{otherwise,} \end{cases}$$
5-35

where $\overline{\mathbf{w}}_i^{\text{max}}$ and $\overline{\mathbf{w}}_i^{\text{min}}$ are the maximum and minimum values of the global solution inside the adjacent element of the troubled element vertexes.

5.2.3.7 Non-oscillatory limiters

Although, Godunov's barriers theorem [81] discouraged CFD developers to find any high-order methods with order of accuracy higher than one, Harten [89] showed that this theorem holds true only when linear reconstruction scheme is used for obtaining the solution at interfaces. He took the advantages of nonlinear reconstruction stencils and introduced ENO high-order reconstruction scheme.

In general, non-oscillatory schemes are considered as a high-order reconstruction methods that can also be employed as high-order limiters in spectral *hp* methods. Even though non-oscillatory limiters are providing very promising results, but they do not necessarily maintain the TVD properties of the solution. Hence, they cannot satisfy the maximum principles strictly. Furthermore, they need to use very broad stencils for reconstructions of the solution in the troubled element which makes them difficult to use for unstructured grid and parallel processing.

Hermite weighted essentially non-oscillatory (HWENO) schemes are known as the compact non-oscillatory reconstruction schemes. The compactness in those is achieved by evolving the function used in the reconstruction of HWENO scheme and its first derivatives in time.

Hermite WENO reconstruction, as a limiter, reconstructs the high-order moments of the troubled element using the derivatives of that element and its adjacent neighboring, while the first moment of the solution (i.e., element-average) does not change. This means that regardless of the order of accuracy of DG discretization, the troubled cells accuracy will reduce to the HWENO order of accuracy which is a major improvement compared to the other limiters in which the order of accuracy of the troubled cells is uncertain. Nonetheless, defining the value of nonlinear weights, evaluation of smoothness function, and application of characteristics field in the progress of reconstruction is very important and essential. The interested readers are referred to [86, 141] for further information.

5.2.4 Performance of limiters for modal DG method

In this section, a one-dimensional modal mixed DG method is employed to solve scalar hyperbolic-, Euler-, and Navier-Stokes-Fourier equations. DG solution in conjugation with various limiters are compared with analytical solutions in profile level. The viscous shock structure problem is solved using various limiters, and the least square error norm is calculated for this stiff flow problem. Accordingly, performance of several well-known limiters based on variety of important physical parameters is investigated.

5.2.4.1 Performance of limiters based on profile analysis

There are several exact solutions for the scalar hyperbolic equation and inviscid Euler equation that can be considered as the benchmark problems to examine the level of accuracy of the limiters[118].

A scalar hyperbolic equation with the initial sinusoidal distribution is considered as the first benchmark problem,

$$\partial_t u + \partial_x u = 0, \quad 0 \le x \le 1, t \ge 0,$$

$$u(x, 0) = \sin(2\pi x),$$

$$u(x_t, t) = u(x_t, t).$$

5-36

The periodic boundary condition is applied to the both sides of the computational domain, and the length of the computational domain is chosen to be one wavelength ($0 \le x \le 1$). The exact solution of this *linear* problem is very smooth. Therefore, employing limiters are not basically necessary. This problem is an appropriate case to measure the loss of accuracy inflicted by the limiters in smooth regions.

Figure 5-8 shows the distribution of the solutions throughout the 200 elements at time=4 seconds. It can be observed that the first-order approximation is very diffusive even for this smooth problem. The initial sinusoidal wave is significantly damped by time evolving. However, the higher-order unlimited approximations yield very accurate results. It is obvious that the accuracy of the unlimited high-order solutions is not compromised and the high-order solutions remain very smooth. Figure 5-8 displays that there is no spurious oscillations and wiggles within the distributed solution. This is not surprising because there are no stiff regions in the computational domain and application of limiters is not necessary.



Figure 5-8 The smooth solutions of the linear advection problem at t=4 seconds

Various limiters are applied in the smooth regions for the purpose of examining the performance and effect of the limiters in the smooth regions. The MP and HWENO limiters do not degrade the solution accuracy significantly even if these limiters are used without a trouble cell indicator. However, the small discrepancy between exact solution and HWENO limited solution may be observed near both ends of the domain.

On the other hand, application of TVD and GM limiters leads to a significant deviation

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from the exact solution. They cannot provide accurate results in smooth regions; therefore, application of a trouble cell indicator for detecting target elements is essential.

Scalar hyperbolic equation with the initial square jump distribution is considered as the next benchmark problem. This problem can be considered as the simplified version of the shock wave problem whereas the shock structure is a stationary problem. There are two stiff jumps within the solution distribution. This problem is a good benchmark problem for investigating on the capability of the limiters for damping oscillations in the scalar hyperbolic equation.

Figure 5-9 shows the distribution of the unlimited, limited, and exact solutions all over the computational domain. It is obvious that the spurious oscillations are not very severe and only appears on both sides of the square jump with small amplitude. Hermite WENO limiter shows a decent level of precision when the order of p is sufficiently big, and the number of elements is adequate. Maximum principle limiter provides very accurate result for all degrees of p due to fact that the threshold quantities for judging whether limiting process should start or not is based on the maximum and minimum value of the initial condition, therefore, as it was expected that the maximum principle limiter performs better than the others for this linear hyperbolic problem where the maximum and minimum of the domain do not change by evaluation of the time. Results also illustrate that generalized moment limiter damps the discontinuity although the limited solution is still being symmetrical. TVD limiter performs relatively better on the left side of the discontinuity, although the solution is considerably damped throughout the domain.



Figure 5-9 Solution distribution of the linear advection problem with initial square jump condition at t=1 second.

Inviscid Burger problem is considered as the next studied benchmark problem to investigate the total variation of the solution and its coefficients in smooth flow regions when different limiters functions have been served. The periodic boundary condition and smooth sinusoidal initial distribution are used for this *nonlinear* scalar time evaluating problems.

The problem setup is given by,

$$\partial_{t}u + u\partial_{x}u = 0, \quad -1 \le x \le 1, t \ge 0,$$

$$u(x,0) = \frac{1 + \sin(\pi x)}{2}, \qquad 5-37$$

$$u(x_{L},t) = u(x_{R},t).$$



Figure 5-10 Distribution of solution of the inviscid Burger's problem with sinusoidal initial distribution using 50 elements at t=0.7 seconds.

Figure 5-10 depicts that Hermite WENO limiter can successfully preserve the accuracy of the solution. However, more number of the elements are required to capture the exact solution employing this limiter. The maximum principle limiter is performing fairly although it damps the oscillations insufficiently at an inflection point for the case of the piecewise linear approximation. Generalize moment limiter and TVD limiter provide almost identical results with the same order of deviation from the exact solution.



Figure 5-11 The solutions of the stationary contact discontinuity problem at t=0.012 seconds.

In order to check the performance of limiters for a system of equations, the present modal RKDG method was applied for solving the Euler system. One-dimensional Riemann problem with an initial stationary contact discontinuity located at x=0.8 is considered as a benchmark problem. Computational domain is discretized into 200 equal-sized elements and the simulation is run until the time reaches to t=0.012 seconds.

Figure 5-11 shows the unlimited and limited numerical solutions. It can be seen that the unlimited solutions of the piecewise linear, quadratic, and cubic polynomial approximations are contaminated with a considerable amount of oscillations. The HWENO and MP limiters which performed well in the case of the linear and nonlinear advection problems turns out not to be able to eliminate all spurious oscillations from the high-order solutions. Interestingly, the TVD and GM limiters, which performed poorly in the case of the linear and non-linear scalar hyperbolic problems, show better performance than the MP and WENO limiter for degree of $p \le 2$ in the Euler system.

As the next benchmark problem, Sod's shock tube flow that contains a left-running expansion wave, a contact discontinuity, and a right-running shock wave is considered. In this problem, the computational domain is discretized with 200 elements and the simulation is run until the time reaches to t=0.2 seconds. Figure 5-12 shows the density profiles of the Sod's shock tube problem.

As can be seen, the TVD limiter degrades the solution considerably. In particular, the TVD limiter for piecewise quadratic and cubic solutions (p=2, 3) yields unsatisfactory results. Similarly, the GM limiter suffers non-negligible wiggles in case of the piecewise quadratic and cubic solutions. Interestingly, it gives non-oscillatory density profile in case of the piecewise linear solution. On the other hand, the MP limiter, which is free from user inputs, provides an accurate approximation in the better level than HWENO limited solution. Nonetheless, it must be mentioned that obtaining an accurate solution using the MP limiter requires an accurate specification of the global maximum and minimum of the solution.



No limiter



Figure 5-12 The solutions of the Sod's shock tube problem with 200 elements at t=0.2 seconds.

Two rarefaction wave propagation near vacuum [157] is the another studied problem. For this particular problem, the negative density and pressure may appear in the process of simulation. As a result, linearized Riemann solvers can fail by returning negative pressures or densities in one or more of the intermediate states for very strong rarefactions. Therefore, the positivity preserving limiter is expected to play a critical role in the problem. Density profile solution of this problem is shown in Figure 5-13. It is shown that the TVD and GM limiters degrade the accuracy of DG solution significantly. However, the MP and HWENO limiters in conjunction with positivity preserving feature can preserve the solution accuracy within an acceptable level.



Figure 5-13 The solutions of Einfeldt's strong rarefaction problem with 200 elements at t=0.15 seconds.

5.2.4.2 Performance of limiters based on error norm analysis

5.2.4.2.1 Performance of limiters based on conservative variables

The first analysis on the performance of the limiter is investigated thereby examining the error of the density and linear momentum solutions which are the global solution of the DG approximation.



Figure 5-14 The Euclidean norm of *density* solution of hard-sphere gas molecule for several limiters
The Euclidean norm of the density and linear momentum solutions are depicted for several limiters in Figure 5-14 and Figure 5-15, respectively.



Figure 5-15 The Euclidean norm of *momentum* solution of hard-sphere gas molecule for several limiters

Results illustrate that TVD limiter degrades the order of accuracy considerably, and the maximum order of accuracy achieved using this limiter is less than one. Generalized

moment limiter without application of any trouble cell indicator acts very poorly. However, the performance of this limiter improves noticeably when KXRCF trouble indicator is employed. Among all limiters, HWENO shows the best performance calculated based on the error norm of the conservative variables. DAMP and SMP limiters in conjugation with KXRCF trouble cell indicator are the next limiters which provide acceptable performance, respectively.



Figure 5-16 The Euclidean norm of *temperature* solution of hard-sphere gas molecule for several limiters

5.2.4.2.2 Performance of limiters based on primitive variables

Temperature is a primitive variable obtained from mass, momentum, and energy relations. It may be useful to report the order of accuracy of DG method based on temperature error norm for viscous shock problem.

Figure 5-16 shows the calculated energy norm of temperature variable for several limiters. It demonstrates that the order of accuracy obtained by temperature error norm analysis is roughly higher than the order of accuracy which was obtained by conservative analysis.

5.2.4.2.3 Performance of limiters based on non-conservative variables

Non-conservative variables – normal stress and heat flux – are another parameters in studying of shock waves [13]. The developed numerical methods for solving the non-equilibrium phenomena are very sensitive to the precision of the estimated non-conservative variables. Knowing the order of accuracy of the DG method based on non-conservative variables is very important and useful for gas dynamic applications [112].

Figure 5-17 and Figure 5-18 provide the energy norm of normal stress and heat flux for various limiters. The results show that the slope of stress and heat flux error norms do not differ much from the error norms obtained for conservative and primitive variable. In case that TVD limiter was applied the order of accuracy is degraded significantly since all high order terms are truncated in troubled cell to satisfy the monotonicity condition strictly. GM limiter without using KXRCF indicator does not provide likely results, and, similar to TVD limiter, the calculated order of accuracy is mostly less than one. However, this limiter performs much better when it (GM-KXRCF) is applied only in the troubled elements. The error norm analysis of stress and heat flux variables for GM- KXRCF limiter illustrate that the order of accuracy obtained based on heat flux is slightly higher than that for normal stress. The convergence rate of heat flux is still higher than that for normal stress.

All in all, the convergence rate is mostly higher than p for mostly all limiters – GM-KXRCF, positivity preserving, SMP-KXRCF, DAMP, and HWENO-KXRCF – and magnitude of error calculated for heat flux and normal stress not is satisfactory for all limiters except, TVD and GM limiters.



Figure 5-17 The Euclidean norm of *normal stress* solution of hard-sphere gas molecule for several limiters



Figure 5-18 The Euclidean norm of *heat flux* solution of hard-sphere gas molecule for several limiters

5.3 Discretization of numerical fluxes

In second-order FVM schemes like MUSCL and piecewise linear reconstruction (PLR) schemes, the physical quantities are reconstructed based on a piecewise linear

polynomial, and the gradients of the physical quantities are sought to be constant inside every local element. Therefore, the evaluation of viscous terms is at most first-order of accurate which is not adequate for studying viscous dominant flows (e.g., boundary shear layer, rarefied gas flows, viscous shock wave, etc.) unless very fine grid is used [107].

In spite of finite volume method, application of the DG method brings the possibility to compute the viscous fluxes in the same order of accuracy as inviscid fluxes. Nevertheless, the local approximation of the viscous flux will be discontinuous at the interface of two elements due to the absence of a direct enforcement of the elemental continuity through the polynomial space. Thus, employing stable and continuous numerical flux functions on the boundary of the elements is crucial for prescribing the viscous fluxes. The estimation and evaluation of viscous flux function are still evolving; however, the numerical treatment for determining the inviscid fluxes is borrowed from finite volume method and it is matured.

There are numerous articles that rigorously speak about the mathematical aspects of discretization of the viscous fluxes [113, 158-160], though the numerical implementation of the viscous flux functions is rarely explained in the literature. In following, several numerical flux functions are explained in detail. The physical concepts behind the inviscid and viscous numerical flux functions are illustrated; the technical information for implementation of the viscous numerical flux functions — which are barely explained in the literature— is taken into account. Various viscous and inviscid numerical flux functions and theirs combination are analyzed for nonlinear Euler equation with smooth solution, scalar heat equation, and viscous shock structure problem

5.3.1 Feasible numerical flux function

As mentioned in previous chapter, the lack of existence of the unique solution at interface of the local elements can be resolved by employing feasible numerical flux functions $(\tilde{\mathbf{F}}^{inviscid}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+), \tilde{\mathbf{F}}^{viscous}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+, \mathbf{\Theta}_{h^e}^-, \mathbf{\Theta}_{h^e}^+)$, and $\tilde{\mathbf{F}}^{auxiliary}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+))$ at interior interfaces and boundary faces.

Three important conditions should be satisfied by any numerical flux functions in order that the numerical solution converges to the physical (entropy) solution;



Figure 5-19 Taxonomy of monotone numerical flux functions for discretization of the inviscid and viscous fluxes.

a) Consistency condition $\tilde{\mathbf{F}}(\phi_1, \phi_1) = \tilde{\mathbf{F}}(\phi_1)$; b) Continuity condition $\tilde{\mathbf{F}}(\phi_1, \phi_2) = \tilde{\mathbf{F}}(\phi_2, \phi_1)$ where $\tilde{\mathbf{F}}$ is restricted to be a Lipschitz continuous function for ϕ_1 and ϕ_2 ; c) Monotonicity condition that enforces \tilde{F} to be a non-decreasing function of ϕ_1 and nonincreasing function of ϕ_2 . There are several numerical flux functions that satisfy these conditions, as is shown in Figure 5-19; however, few of them has been often used in DG methods.

5.3.2 Inviscid numerical flux functions

The inviscid numerical flux introduces a coupling between the conservative variables of the element and its adjacent neighboring element at the common edge of j. In general, any monotone, consistent and continuous numerical flux function can be used as inviscid numerical fluxes. As it is depicted in Figure 5-19 there are several schemes for discretization of the inviscid flux functions that can satisfy above mentioned conditions.

Among all choices, the numerical flux function obtained based on flux-difference splitting approach can be considered as an appropriate choice for discretizing the inviscid flux function. Here, the evaluation of inviscid numerical flux functions using flux-difference splitting approach is explained briefly. Nonetheless, further information about inviscid numerical flux functions can be found in [80].

The goal of a numerical flux is to approximate the physical flux function at interfaces with a minimum amount of error. Flux difference splitting schemes consider the eigenvalues and eigenvectors of the transformation matrix to evaluate the numerical flux function. They describe all properties according to the Riemann invariants (or characteristics variables) of the Riemann problem solved at interfaces of the elements. Considering the advection part of the conservation laws (Eq. 4-6), a hyperbolic differential system can be defined as

$$\frac{\partial \mathbf{w}}{\partial t} + \nabla \mathbf{F}^{inviscid} \left(\mathbf{w} \right) = 0, \qquad 5-38$$

where it can be reformulated in quasilinear form as

$$\frac{\partial \mathbf{w}}{\partial t} + \frac{\partial \mathbf{F}^{inviscid}\left(\mathbf{w}\right)}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{x}} = 0.$$
5-39

Introducing a Jacobian matrix of transformation $\mathbf{A}^{inviscid}(\mathbf{w}) \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}}$, the system

(Eq. 5-39) reads as

$$\frac{\partial \mathbf{w}}{\partial t} + \mathbf{A}^{inviscid} \left(\mathbf{w} \right) \frac{\partial \mathbf{w}}{\partial \mathbf{x}} = 0.$$
 5-40

Considering the fact that \mathbf{W}_{h^e} varies *smoothly normal to the interface* of the elements, it is only needed to find a one-dimensional flux function normal to the elemental interfaces.

Following Beam -Warming and Hyett scheme [161] and defining a general matrix of Jacobian as a linear combination of $\mathbf{A}^{inviscid}(\mathbf{w})$ and normal vector components

$$\hat{\mathbf{A}}_{i}^{inviscid}\left(\mathbf{w},\mathbf{n}\right) \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}} : \ \hat{\mathbf{A}}_{i}^{inviscid}\left(\mathbf{w},\mathbf{n}\right) = A_{ik}^{inviscid}\left(\mathbf{w}\right)n_{k},$$
5-41

the one-dimensional system can be defined as

$$\frac{\partial \mathbf{w}}{\partial t} + \hat{\mathbf{A}}^{inviscid} \left(\mathbf{w}, \mathbf{n} \right) \frac{\partial \mathbf{w}}{\partial \mathbf{n}} = 0.$$
5-42

Knowing the fact that $\mathbf{A}_{i}^{inviscid}$ is diagonalizable tenor, and Jacobian matrix of $\mathbf{A}_{i}^{inviscid}$ has real eigenvalues with a complete set of eigenvectors, it is possible to write this system in characteristics form as

$$\hat{\mathbf{A}}^{inviscid} (\mathbf{w}, \mathbf{n}) = \mathbf{R} \mathbf{\Lambda} \mathbf{R}^{-1},$$

$$\left| \hat{\mathbf{A}}^{inviscid} (\mathbf{w}, \mathbf{n}) \right| = \mathbf{R} |\mathbf{\Lambda}| \mathbf{R}^{-1},$$
5-43

where the columns of $\mathbf{R} \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}}$ and $\mathbf{R}^{-1} \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}}$ contain the right and left eigenvectors, respectively; $\Lambda \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}}$ is a diagonal matrix of the eigenvalues of the transformation matrix $\Lambda = \lambda \mathbf{I}$.

Taking the product of (Eq. 5-42) with tensor of left eigenvectors \mathbf{R}^{-1} and setting $\mathbf{R}^{-1}\mathbf{w} = \mathbf{Q}$ gives

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{\Lambda} \frac{\partial \mathbf{Q}}{\partial \mathbf{n}} = 0.$$
 5-44

where \mathbf{Q} is the Riemann invariant vector. This is a decoupled system of equations where coupling between equations remains only through the eigenvalues of the system. Each scalar invariant Q_i is advected at the speed λ_i . The speed is inward to the normal direction of the interface when $\lambda_i > 0$ and the speed is opposite to the normal direction if $\lambda_i < 0$. According to the theory of characteristics, the solution of this system for an initially discontinuous state is

$$Q_i = Q_i^+ \quad \text{if } \lambda_i > 0,$$

$$Q_i = Q_i^- \quad \text{if } \lambda_i < 0.$$
5-45

Suppose that $\tilde{\mathbf{F}}^{inviscid}(\mathbf{w}_{h^e}, \mathbf{w}_{h^e}^+)$ is the solution of a Riemann problem at an elemental interface, the flux function in normal direction to the interface can be expressed by

$$\mathbf{F}^{inviscid}(\mathbf{w}_{h^e}).\mathbf{n} = \tilde{\mathbf{F}}^{inviscid}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+).\mathbf{n},$$
5-46

and the general form of the upwinding numerical flux can be obtained after some manipulations on (Eq. 5-44) and (Eq. 5-46) [80, 162].

In case of linear flux functions, a linearization of the inviscid flux $\hat{A}^{inviscid} w \approx F^{inviscid} (w).n$ can be used to define the numerical inviscid function as

$$\tilde{\mathbf{F}}^{inviscid}(\mathbf{w}_{h^e}^{-}, \mathbf{w}_{h^e}^{+}).\mathbf{n} = \left\langle \hat{\mathbf{A}}^{inviscid} \mathbf{w}_{h^e}^{-} \right\rangle + \frac{1}{2} \left| \hat{\mathbf{A}}^{inviscid} \right| [[\mathbf{w}_{h^e}]], \qquad 5-47$$

where $\hat{\mathbf{A}}^{inviscid}$ is constant tensor; $\langle \mathbf{w}_{h^e} \rangle$ and $[[\mathbf{w}_{h^e}]]$ are the average and jump of \mathbf{w}_{h^e} at interface. The *linear numerical flux function* can be further simplified as $\hat{\mathbf{A}}^{inviscid}$ is not function of neither $\mathbf{w}_{h^e}^-$ nor $\mathbf{w}_{h^e}^+$, therefore, we have

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-},\mathbf{w}_{h^{e}}^{+}\right).\mathbf{n}=\widehat{\mathbf{A}}^{inviscid}\left[\mathbf{w}_{h^{e}}^{-}+\widehat{\mathbf{A}}^{inviscid}\mathbf{w}_{h^{e}}^{+}\right].$$
5-48

In case of *nonlinear flux vectors*, the nonlinearity of the inviscid flux function yields to a consistent numerical flux as

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-},\mathbf{w}_{h^{e}}^{+}\right)\cdot\mathbf{n} = \left\langle \mathbf{F}^{inviscid}\left(\mathbf{w}\right)\right\rangle\cdot\mathbf{n}^{-} + \frac{1}{2}\left|\widehat{\mathbf{A}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-},\mathbf{w}_{h^{e}}^{+},\mathbf{n}\right)\right|\left[\left[\mathbf{w}_{h^{e}}^{-}\right]\right], \qquad 5-49$$

where $\hat{\mathbf{A}}^{inviscid}$ is a function of $\mathbf{w}_{h^e}^{\pm}$ and outward normal vector \mathbf{n} , therefore, more efforts are required for estimation of the $\hat{\mathbf{A}}^{inviscid}$. There are two possible choices for calculation of $\hat{\mathbf{A}}_{i}^{inviscid}$ [163],

$$\left| \hat{\mathbf{A}}_{\text{inv}_{i}} \right| = \left| \hat{\mathbf{A}}_{\text{inv}_{ik}} \left(\left\langle \mathbf{w}_{h_{i}^{e}} \right\rangle \right) \right| n_{k},$$
5-50

$$\left| \hat{\mathbf{A}}_{inv_{i}} \right| = \left| \left\langle \hat{\mathbf{A}}_{inv_{ik}} \left(\mathbf{w}_{h_{i}^{e}} \right) \right\rangle \right| n_{k}.$$
 5-51

For case that equation (Eq. 5-51) is chosen, extra efforts is needed to be considered to ensure that $|\hat{\mathbf{A}}_{inv_i}|$ has real eigenvalues [80, 163]. Note that, the definition of $|\hat{\mathbf{A}}_{inv_i}|$ distinguishes several approximate Riemann solvers from each other.

Application of the exact solution of Riemann problem at the interface of the every element gives the original Godunov method. It provides the smallest numerical viscosity, but it is very costly and delicate. As it is shown in Figure 5-19, there are several alternative approximate flux functions such as Rusanov (LLF), Roe, Harten-Lax-Van Leer (HLL) and HLLC flux functions that consider some (or all) of the characteristics waves in the process of the evaluation of inviscid flux function [163]. The conceptual definition of the these flux functions is given as follows,

$$\left| \hat{\mathbf{A}}_{inv} \right| = \begin{cases} \mathbf{R} \left| \lambda \right| \mathbf{R}^{-1} & \text{Roe, all but linearized waves} \\ \frac{(1-\alpha)\lambda^{+}\lambda^{-} + \alpha(\lambda^{-}\mathbf{w}^{+} + \lambda^{+}\mathbf{w}^{-})}{\lambda^{+} - \lambda^{-}} - \frac{1}{2} \frac{\lambda^{+} + \lambda^{-}}{\lambda^{+} - \lambda^{-}} \mathbf{A}^{inviscid} (\mathbf{w}) & \text{HLLC, three waves} \\ \frac{\lambda^{+}\lambda^{-}}{\lambda^{+} - \lambda^{-}} - \frac{1}{2} \frac{\lambda^{+} + \lambda^{-}}{\lambda^{+} - \lambda^{-}} \mathbf{A}^{inviscid} (\mathbf{w}) & \text{HLL, two waves} \\ \frac{\lambda_{max} \left| \mathbf{I} \right|}{\lambda_{max} \left| \mathbf{I} \right|} & \text{Rusanov (LLF), one wave} \\ \frac{\Delta x}{\Delta t} \mathbf{I} & \text{Lax-Friedrichs, zero wave} \end{cases}$$

Here $\mathbf{I} \in \mathbb{R}^{\mathcal{D} \times \mathcal{D}}$ is the identity matrix.



Figure 5-20 Approximation of convective characteristics wave using numerical flux functions.

Although there are available several more numerical inviscid functions, three of well-used inviscid flux functions —Rusanov (LLF), Roe, and HLL — are considered in this study to examine the performance of the inviscid flux functions in combination with viscous flux functions.

Rusanov flux function — sometimes called as local-Lax-Friedrichs (LLF) — is commonly used in DG method due to its simplicity and efficiency in cost, even though this monotone numerical flux function is the most diffusive numerical flux function and smears discontinuities considerably. In Rusanov flux function, only one wave is considered, and considerable amount of the numerical dissipation is added to stabilize this wave. It is defined as

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-},\mathbf{w}_{h^{e}}^{+}\right)\cdot\mathbf{n} = \left\langle \mathbf{F}^{inviscid}\left(\mathbf{w}\right)\right\rangle\cdot\mathbf{n}^{-} + \frac{1}{2}\left|\lambda_{\max}\right|\mathbf{I}[[\mathbf{w}_{h^{e}}]],$$
5-53

where λ_{max} is the largest eigenvalue of the convective flux function on the interface of the element.

Roe flux function linearizes the Jacobian of inviscid flux and considers all linearized characteristics waves in the calculation of numerical flux function. The linearization is applied in such a way that the nonlinear physical jumps like a shocks and contact discontinuities are recognized correctly. The method turns to the exact solution of the linear hyperbolic systems; however, it may face difficulties for nonlinear systems when very strong discontinuity, shock diffraction, or nonlinear instability (i.e., carbuncle) exist in the computational domain.

Harten-Lax-Van Leer (HLL) flux function is a symmetric flux with either nonlinear or linear numerical dissipation function. It considers two characteristics waves and divides the *x*-*t* phase space into three separate sub-regions while individual actions are considered for handling each of the sub-region. The method is accurate when contact discontinuities exist in the computational domain, whilst it turns to exact solution only for systems with two equations like one-dimensional shallow water system. The modified version of HLL method was introduced by Toro et al. [164] to overcome the short comes of the HLL scheme. However, in case of viscous shock wave where the role of velocity-shear phenomena is negligible, application of HLL flux function instead of more complicated fluxes like HLLC may end to the same conclusion.

5.3.3 Viscous numerical flux functions

In general, there are two different viewpoints that mirror the primal and flux formulation of the governing equations. The primal formulation is the viewpoint of the finite element researcher, and the flux formulation is the preferred notation of the traditional finite volume supporters. The followers of finite element method try to write system of equations in global compact form rather than elemental form to enhance the efficiency of their schemes by the elimination of the auxiliary variables. However, finite volume followers prefers elemental formulations, and try to enforce the continuity and stability of the solution through novel implementation of the numerical viscous flux function in elemental formulation [165].

Arnold et al. [166] showed that both approaches are conceptually similar when the primal formulation is converted to the flux formulation or backwards. They provided [159] a unified analysis of discontinuous Galerkin methods for the 1-D elliptic problem by transforming the flux formulation into the primal formulation and proving several properties of the schemes including convergence behavior of the schemes, and so on. As it is shown in Figure 5-19, there are various choices for discretization of the viscous flux, including Baumann–Oden method, Bassi-Rebay first scheme (BR1), local discontinuous Galerkin (LDG), compact discontinuous Galerkin (CDG), Bassi-Rebay second scheme (BR2), interior penalty (SIP), and recovery based discontinuous Galerkin (RDG), and so on.

For hyperbolic equations, it is shown that these numerical flux functions behave differently in terms of efficiency, stability, and accuracy [167]. According to the efficiency of the schemes, local DG, and compact DG methods similar to BR1 method

require an extra set of variables (i.e., auxiliary variables) for evaluating higher-order derivatives. It means that more memory and computational cost are required for BR1, LDG, and CDG in compared to the other method.

In contrast to above schemes, SIP and BR2 schemes do not need to solve any extra set of equations for evaluation of the second-order derivatives. In these methods, data from the adjacent neighbors is only required for calculation of the viscous term, hence, they are more efficient than BR1, LDG and CDG methods in the sense of computational cost. However, the numerical implementation of these schemes is more complicated and requires an understanding of the rigorous mathematical formulation used in the derivation of these schemes.

Comparing the SIP method to the second method of Bassi and Rebay, the SIP method is more efficient regarding the computational effort. However, an extension of the SIP method to the Navier-Stokes-Fourier equations yields undesirable convergence rate for the even polynomial degree of p [168]. Moreover, SIP is developed based on primal formulation which cannot be utilized for discretizing nonlinear physical viscous flux functions since the Jacobean transformation matrix is not an explicit function of the velocity gradients [112, 169].

In the following, the generalized formulation of viscous flux function is initially introduced. Later, mathematical derivation, numerical implementation of the viscous flux functions— BR1, LDG, and BR2— are briefly explained to ease computational coding.

5.3.3.1 Jump and average operators

To proceed the evaluation of viscous and auxiliary fluxes, it is necessary to define the average $\langle \cdot \rangle$ and jump [[.]] operators for a function of g on the face of I_h and \mathcal{B}_h . Average operator can be defined as

$$\left\langle g \right\rangle = \begin{cases} \frac{g^{-} + g^{+}}{2} & \text{on } I_{h} \\ g^{boundary} & \text{on } \mathcal{B}_{h} \end{cases}$$
 5-54

and jump operator is given by

$$[[g]] = g^{-}\mathbf{n}^{-} + g^{+}\mathbf{n}^{+}.$$
 5-55

As normal unit vector on both sides of an interface are related by $\mathbf{n}^+ = -\mathbf{n}^-$, jump operator which can be written as

$$[[g]] = \begin{cases} \left(g^{-} - g^{+}\right)\mathbf{n}^{-} & \text{on } \mathbf{I}_{h} \\ g^{boundary}\mathbf{n}^{-} & \text{on } \mathcal{B}_{h} \end{cases}.$$
 5-56

The jump vector in index notation can be written as

$$[[g]]_k = g^- n_k^- + g^+ n_k^+.$$
 5-57

Noting that the jumps and average operators are only needed to be calculated at interior (left), and exterior (right) trace of the function g at an interface. Considering the multiplication of vector a and tensor A, the identity relation can be defined such that jump operator satisfies the following product rule at interfaces

$$[[a_j \mathbf{A}_{jk}]] = \langle \mathbf{A}_{jk} \rangle [[a_j]]_k + \langle a_j \rangle [[\mathbf{A}_{jk}]]_k.$$
5-58

This identity relation can be verified by substitution of (Eq. 5-54) and (Eq. 5-55) in (Eq. 5-58). By application of (Eq. 5-58) in the integrals over the elements and using divergence theorem, we have

$$\int_{\Omega_h} \nabla .(\boldsymbol{a}\mathbf{A})_h d\Omega = \sum_{e \in \mathbf{I}_h} \int_{\mathbb{R}^{\mathcal{D}}} (\langle \boldsymbol{a} \rangle [[\mathbf{A}]] + [[\boldsymbol{a}]] \langle \mathbf{A} \rangle) d\Gamma_e + \sum_{e \in \mathcal{B}_h} \int_{\mathbb{R}^{\mathcal{D}}} \boldsymbol{a}\mathbf{A}.\mathbf{n}^- d\Gamma_e.$$
 5-59

Considering equation (Eq. 5-58) and (Eq. 5-59)

$$\sum_{e \in \mathcal{I}_h} \int_{\Omega_e} \nabla . (\boldsymbol{a} \mathbf{A})_h d\Omega = \sum_{e \in \mathbf{I}_h} \int_{\mathbb{R}^{\mathcal{D}}} (\langle \boldsymbol{a} \rangle [[\mathbf{A}]] + [[\boldsymbol{a}]] \langle \mathbf{A} \rangle) d\Gamma_F^e + \sum_{e \in \mathcal{B}_h} \int_{\mathbb{R}^{\mathcal{D}}} \boldsymbol{a} \mathbf{A} . \mathbf{n}^- d\Gamma_B^e, \quad 5-60$$

$$\sum_{e \in \mathcal{T}_h} \int_{\mathbb{R}^{\mathcal{D}}} (\boldsymbol{a}_j \mathbf{A}_{jk})_{h^e} \mathbf{n}_k^- d\Gamma_e = \sum_{e \in \mathbf{I}_h} \int_{\mathbb{R}^{\mathcal{D}}} [[\boldsymbol{a}_j \mathbf{A}_{jk}]]_k d\Gamma_F^e + \sum_{e \in \mathcal{B}_h} \int_{\mathbb{R}^{\mathcal{D}}} \boldsymbol{a}_j \mathbf{A}_{jk} \mathbf{n}_k^- d\Gamma_B^e.$$
 5-61

Note that in the sum over *all boundary integrals*, the *internal faces are counted twice*. Thus, jump operator appeared to count the contributions of the left and the right states.

5.3.3.2 Generalized numerical flux formulation

Although we are interested in the discretization of the numerical viscous flux of NSF equation, it can be useful to initially present the general discretization form of the viscous flux for a simpler problem.

Arnold et al. [159] and Castillo et al.[170] introduced the general form of the flux formulation for the scalar equation. The flux formula was obtained from a stability analysis of a linear elliptic model problem. Although this formulation was originally derived for scalar equation [159], it is preferred to write it in vector form to easily extend it for multidimensional problem;

$$\hat{\boldsymbol{\Theta}} = \langle \boldsymbol{\Theta}_h \rangle - C_{11}[[\boldsymbol{w}_h]] + C_{12}[[\boldsymbol{\Theta}_h]], \qquad 5-62$$

$$\hat{\mathbf{w}} = \langle \mathbf{w}_h \rangle - \mathbf{C}_{12}[[\mathbf{w}_h]] - C_{22}[[\mathbf{\Theta}_h]].$$

where $\hat{\Theta}$ is analogous to the viscous numerical flux and $\hat{\mathbf{w}}$ is comparable to the auxiliary flux function of conservation laws. Various numerical schemes for elliptic problems can be derived by choosing the value of C_{11} , C_{12} and C_{22} parameters.

Castillo et al. [37] proved that stabilizing parameters $(C_{11} > 0, C_{22} \ge 0)$ should be positive to obtain a unique and stable approximate solution. Although stabilizing parameters can be any positive value, the majority of schemes takes $C_{22} = 0$ to decouple the solution of \mathbf{W}_h and $\mathbf{\Theta}_h$, and solve viscous variables independently from auxiliary variables. In the following, it is assumed that the second stabilizing parameter is zero $C_{22} = 0$.

5.3.3.3 Bassi-Rebay first method (BR1)

Bassi and Rebay [103] introduced mixed-DG formulation and recast system of equations into two first-order systems. Bassi-Rebay's first method (BR1) can be derived from the generalized numerical flux function if C_{11} , C_{12} and C_{22} parameters are chosen to be zero. In original work of Bassi-Rebay [103], an arithmetic mean average function is served for discretization of the diffusion and auxiliary flux functions such that

$$\widetilde{\mathbf{F}}^{viscous}(\mathbf{w}_{h^e}^{-}, \mathbf{w}_{h^e}^{+}, \mathbf{\Theta}_{h^e}^{-}, \mathbf{\Theta}_{h^e}^{+}) = \frac{1}{2} \Big(\mathbf{F}^{viscous}(\mathbf{\Theta}_{h^e}^{-}, \mathbf{w}_{h^e}^{-}) + \mathbf{F}^{viscous}(\mathbf{\Theta}_{h^e}^{+}, \mathbf{w}_{h^e}^{+}) \Big)$$

$$-0 \times [[\mathbf{w}_{h}]] + 0 \times [[\mathbf{\Theta}_{h}]],$$

$$5-63$$

$$\tilde{\mathbf{F}}^{auxiliary}(\mathbf{w}_{h^e}^{-},\mathbf{w}_{h^e}^{+}) = \frac{1}{2}(\mathbf{w}_{h}^{-}+\mathbf{w}_{h}^{+}) - 0 \times [[\mathbf{w}_{h}]] - 0 \times [[\mathbf{\Theta}_{h}]].$$
5-64

This choice of the numerical flux seems to be a very natural choice as diffusion does not prefer any direction. This flux has been employed in several studies [103, 112, 169, 171, 172] since it is simple to implement in the developed numerical solvers. It provides the moderate performance for several applications. However, further investigations reveal that BR1 has some limitations when applied to study; viscous dominants flows, pure elliptic problems, high transition, and free molecular rarefied flows.

Unfortunately, BR1 similar to Baumann-Oden method is weakly unstable [104, 159, 173] due to lack of existence of stabilizer term in viscous flux function. The stability of the BR1 method may become grid dependence, which is clearly undesirable, due to fact

that the viscous contribution to the Jacobian of viscous flux may be singular on some meshes [174, 175].

Furthermore, it does not optimally converge to design order of accuracy even for the case of the simple scalar equation. It achieves a convergence rate of $O(h^{p})$ for p odd while the convergence rate of the method is of the order of $O(h^{p+1})$ when p is even [92, 158].

5.3.3.4 Local discontinuous Galerkin (LDG)

LDG method was introduced by Cockburn and Shu [104] as an extension of BR1 method in order to generalized DG methods for any convective-diffusion problem. Local DG method can be considered as a stabilized mixed-DG method [173]. It is a general scheme which can be employed for solving systems with higher derivatives [176]. In case of linear problems, it is known that LDG achieves uniform convergence rate for any order of p, whereas the convergence rate of BR1 method depends on p being even or odd.

The local DG method is a non-compact and inefficient scheme when it is employed with cooperation of an implicit time integration method due to dealing with the second neighbors of the elemental faces in the evaluation of the viscous fluxes. On the other hand, LDG is compact and optimal for using in explicit time stepping schemes [177].

In explicit methods, the auxiliary equations are solved at the beginning of each time step, and then the auxiliary variables are stored as the extra degree of freedoms. Subsequently, the primary system of differential equations are solved by employing a strong stability preserving (SSP) method. The process is repeated at every time step until DG method converges to desired solution. The only disadvantage of LDG for explicit time marching condition is that the extra memory is required for storing the Θ_{h} .

A local discontinuous Galerkin method can be derived from the generalized formulation of the viscous fluxes (Eq. 5-62) if the stabilizing parameters are defined as

$$C_{11} = \beta,$$

 $C_{12} = \tilde{C}_{12} \frac{\mathbf{n}^{\dagger}}{2},$ 5-65
 $C_{22} = 0.$

LDG fluxes on the boundary of the elements are given by

$$\hat{\Theta}_{ik} = \Theta_{h_{ik}}^{-} - \beta(w_{h_i} - w_{h_i^{e_i}}^{boundary})n_k^{-}, \qquad 5-66$$

$$\hat{w}_i = w_i^{boundary}, \qquad 5-67$$

where exterior boundary state $\mathbf{w}_{h^e}^{boundary}$ is a function of the interior state and known boundary data.

By this definition of the stabilizing parameters, the viscous flux is penalized by β times of the jumps in \mathbf{W}_h and $\mathbf{n}_k^{\pm}/2$ times the jump in $\boldsymbol{\Theta}_h$, and auxiliary flux is penalized by $\mathbf{n}_k^{\pm}/2$ times the jump in \mathbf{W}_h . Any arbitrary value can be chosen as \mathbf{C}_{12} , for example, it can be chosen to be a function of normal vectors (n^+, n^-) . However, LDG becomes unstable when β is set to be zero and \mathbf{C}_{12} is not defined correspondingly.

A larger value of β on the boundary faces means more strictly enforcement of the boundary conditions which means that the boundary conditions are enforced in a strong sense in the limit of $\beta \rightarrow \infty$ [95]. In practice, penalty term β is defined as

$$\beta = \frac{\eta_{LDG}}{h},$$
 5-68

where η_{LDG} is the stabilization constant. *h* indicates the radius of the circumscribed circle in the elementis, and it is equivalent to cell size Δx in one-dimensional problem.

The minimal dissipation LDG formulation — which sometimes called as 'upwinding in two opposite directions', 'alternating-flux', or 'upwind-downwind' scheme — can be derived if C_{11} is set to be zero and the direction of C_{12} is restricted to be non-parallel to the normal vectors of the elemental faces;

$$\hat{\Theta}_{ik} = \frac{1 + \tilde{C}_{12}}{2} \Theta_{h_{ik}}^{+} + \frac{1 - \tilde{C}_{12}}{2} \Theta_{h_{ik}}^{-} - C_{11}[[w_{h_i}]]_k, \qquad 5-69$$

$$\hat{w}_{i} = \frac{1 - \tilde{C}_{12}}{2} w_{h_{i}}^{+} + \frac{\tilde{C}_{12} - 1}{2} w_{h_{i}}^{-}.$$
5-70

where $\tilde{C}_{12} \in \{-1,1\}$ gives the flip-flop nature of the scheme.

Considering highlights of minimal dissipation LDG and setting \tilde{C}_{12} equal to -1/2, a class of LDG method can be obtained for *Navier-Stokes-Fourier* as

$$\widetilde{\mathbf{F}}^{viscous}(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{+}) = \mathbf{F}^{viscous}(\mathbf{\Theta}_{h^{e}}^{-}, \mathbf{u}_{h^{e}}^{-}),$$

$$\widetilde{\mathbf{F}}^{auxiliary}(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}) = \mathbf{w}_{h}^{+} + 0 \times [[\mathbf{w}_{h}^{-}]].$$
5-71

Note that utilizing this scheme at boundary interfaces requires that viscous flux function at the boundary faces takes the shape of

$$\widetilde{\mathbf{F}}^{viscous}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+, \mathbf{\Theta}_{h^e}^-, \mathbf{\Theta}_{h^e}^+) = \mathbf{F}^{viscous}(\mathbf{\Theta}_{h^e}^- - C_{11}(\mathbf{w}_h - \mathbf{w}_{h^e}^{boundary})\mathbf{n}^-, \mathbf{w}_{h^e}^-),$$

$$\widetilde{\mathbf{F}}^{auxiliary}(\mathbf{w}_{h^e}^-, \mathbf{w}_{h^e}^+) = \mathbf{w}_h^+.$$

5-72

5.3.3.5 Bassi-Rebay second method (BR2)

Application of the implicit time stepping schemes in DG method for simulating advection–diffusion problems (e.g., turbulent flows) motivates Bassi et al. to introduce Bassi-Rebay's second method (BR2) method.

BR2 method has been employed in several studies due to the compactness of the scheme and optimal convergence rates for odd and even polynomial degrees in solving viscous dominant problems[178, 179]. In the original paper [158], the mathematical derivation of the BR2 scheme for model elliptic equation — instead of Navier-Stokes-Fourier — was interpreted rigorously while the detail of the numerical implementation of the scheme, and the process for evaluation of the lifting operators were not addressed.

In this section, the mathematical derivation and numerical implementation of the BR2 method for Navier-Stokes-Fourier system are illustrated; evaluation of the global and local lifting operators are described; the numerical process for discretization of viscous flux functions is summarized.

The weak formulation (Eq. 4-45) can be reformulated into the global form by replacing the surfaces integrals with the sum over all elemental interfaces and boundaries as

$$\begin{cases} \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \frac{\partial w_{h_{e}^{e}}}{\partial t} d\Omega_{e} \\ + \sum_{e \in I_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} [[\upsilon_{i}]]_{k} \left(\tilde{\mathbf{F}}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) + \tilde{\mathbf{F}}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}, \Theta_{h^{e}}^{-}, \Theta_{h^{e}}^{+} \right) \right) d\Gamma_{F}^{e} \\ + \sum_{e \in B_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} \left(\tilde{\mathbf{F}}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{-} \right) + \tilde{\mathbf{F}}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{-} \right) \right) d\Gamma_{F}^{e} \\ - \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \frac{\partial \upsilon_{i}}{\partial x_{k}} \left(\mathbf{F}_{ik}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-} \right) + \mathbf{F}_{ik}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{-} \right) \right) d\Omega_{e} \\ = \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \upsilon_{i} S_{i} \left(\mathbf{w}_{h^{e}}^{-}, \Theta_{h^{e}}^{-} \right) d\Omega_{e}, \qquad 5-73 \end{cases}$$

$$\sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Theta_{ik} d\Omega_{e} - \sum_{e \in I_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \left[\left[\Phi_{ik} \right] \right]_{k} \tilde{\mathbf{F}}_{ik}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+} \right) d\Gamma_{F}^{e} \\ - \sum_{e \in B_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \tilde{\mathbf{F}}_{ik}^{nuviliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{-boundary} \right) n_{k}^{-} d\Gamma_{B}^{e} + \sum_{e \in T_{h}} \int_{\mathbb{R}^{\mathcal{D}}} w_{h^{e}_{i}}^{-} \frac{\partial \Phi_{ik}}{\partial x_{k}} d\Omega_{e} = 0.$$

Note that the viscous numerical flux depends not only from the jump on the edge j but also from the jumps on all the edges belonging to the element Ω_{e} and neighboring elements sharing the edge j.

By the integration by part, and applying divergence theorem to the fourth integral term of the auxiliary equation, it reads as

$$\sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} w_{h_{i}^{e}} \frac{\partial \Phi_{ik}}{\partial x_{k}} d\Omega_{e} = \sum_{e \in \mathcal{B}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} w_{h_{i}^{e}}^{-} n_{k}^{-} d\Gamma_{B}^{e} + \sum_{e \in I_{h}} \int_{\mathbb{R}^{\mathcal{D}}} [[\Phi_{ik} w_{h_{i}^{e}}^{-}]]_{k} d\Gamma_{F}^{e} - \sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \frac{\partial w_{h_{i}^{e}}}{\partial x_{k}} d\Omega_{e} .$$

$$5-74$$

The auxiliary system can be re-formulated, substituting (Eq. 5-74) in auxiliary equation (Eq. 5-73) as

$$\sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Theta_{ik} d\Omega_{e} - \sum_{e \in I_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} [[\Phi_{ik}]]_{k} \tilde{\mathbf{F}}_{ik}^{auxiliary} (\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{+}) d\Gamma_{F}^{e}$$
$$- \sum_{e \in \mathcal{B}_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \tilde{\mathbf{F}}_{ik}^{auxiliary} (\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}) n_{k}^{-} d\Gamma_{B}^{e} + \sum_{e \in \mathcal{B}_{h}} \int_{\Gamma_{B}^{e}} \Phi_{ik} w_{h^{e}_{i}}^{-} n_{k}^{-} d\Gamma_{B}^{e}$$
$$+ \sum_{e \in I_{h}} \int_{\Gamma_{F}^{e}} [[\Phi_{ik} w_{h^{e}_{i}}]]_{k} d\Gamma_{F}^{e} - \sum_{e \in \mathcal{T}_{h}} \int_{\Omega_{e}} \Phi_{ik} \frac{\partial w_{h^{e}_{i}}}{\partial x_{k}} d\Omega = 0.$$

Discretizing auxiliary flux function as

$$\widetilde{\mathbf{F}}_{ik}^{auxiliary} = \begin{cases} \left\langle \mathbf{w}_{h^e} \right\rangle & \text{on } \mathbf{I}_h \\ \mathbf{w}_{h^e}^{boundary} & \text{on } \mathcal{B}_h \end{cases},$$
5-76

and replacing $[[\Phi_{ik} w_{h_i^e}]]_k$ with equivalent equation introduced in (Eq. 5-58) yields

$$\sum_{e \in \mathcal{I}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \left(\Theta_{ik} - \frac{\partial w_{h_{i}^{e}}}{\partial x_{k}} \right) d\Omega_{e} + \sum_{e \in \mathcal{B}_{h}} \oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} (w_{h_{i}^{e}}^{-} - w_{h_{i}^{e}}^{boundary}) n_{k}^{-} d\Gamma_{B}^{e} + \sum_{e \in I_{h}} \int_{\Gamma_{F}^{e}} [[w_{h_{i}^{e}}^{-}]]_{k} \langle \Phi_{ik} \rangle d\Gamma_{F}^{e} = 0.$$

5-77

In order to obtain the explicit expression for the auxiliary variables, it is essential to define a global lifting operator $\mathfrak{R}_h \in \mathbb{R}^{(\mathfrak{D}+2)\times \mathfrak{D}}$ as

$$\Re_{h_{ik}} = \left(\Theta_{ik} - \frac{\partial W_{h_i^e}}{\partial x_k}\right).$$
 5-78

Substituting (Eq. 5-78) in (Eq. 5-77) results in the weak formulation of global lifting operator as

$$\sum_{e \in \mathcal{T}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \Re_{h_{ik}} d\Omega_{e} = -\sum_{e \in \mathcal{I}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \left\langle \Phi_{ik} \right\rangle [[w_{h_{i}^{e}}]]_{k} d\Gamma_{F}^{e} - \sum_{e \in \mathcal{B}_{h}} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik}^{-} (w_{h_{i}^{e}}^{-} - w_{h_{i}^{e}}^{boundary}) n_{k}^{-} d\Gamma_{B}^{e}.$$
5-79

According to (Eq. 5-78) and (Eq. 5-79), the auxiliary variable Θ_{ik} can be expressed as a sum of the solution gradient $\frac{\partial w_{h_i^*}}{\partial x_k}$ and correction factor (i.e., global lifting operator) which is taken into account due to the jumps in $w_{h_i^*}$ at interfaces and jump between the value of $w_{h_i^*}$ and $w_{h_i^{e}}^{boundary}$ at elemental boundaries. This means that the global lifting operator \Re_h is to penalize the jumps at the faces, although it is equal to zero in smooth regions.

Replacing the surface integral in auxiliary equation (Eq. 5-73) with volume integral using (Eq. 5-79) and summing over all the local elements Ω_e , the global lifting operator function over all elements of Ω_h can be expressed as

$$\int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \mathfrak{R}_{h_{ik}} d\Omega = \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} \left(\Theta_{ik} - \frac{\partial W_{h_i^e}}{\partial x_k} \right) d\Omega .$$
 5-80

In order to eliminate the non-compactness of the scheme, it is possible to replace the auxiliary variable with weak definition as

$$\int_{\Omega_h} \Phi_{ik} \Theta_{h_{ik}} d\Omega = \int_{\Omega_h} \Phi_{ik} \left(\nabla_k w_{h_i} + \Re_{h_{ik}} \right) d\Omega \,.$$
 5-81

This definition of auxiliary variables could be employed to derive the primal formulation of conservation laws, although we are only interested in the flux formulation of the scheme.

The process of the determination of the global lifting operator was not addressed in [158]. We can compute the global lifting operator directly by considering (Eq. 5-81) and (Eq. 5-79) and defining the Φ_{h^e} using defined polynomial expansions in Section 0. If we express the global lifting operator by polynomial expansion as

$$\Re_{h_{ik}}(\xi,t) = \sum_{l=1}^{N_p} \hat{\Re}_{h_{ik}}(t) \phi_l(\xi),$$
5-82

The coefficient of global lifting operator can be obtained by solving

$$\int_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{-}(\xi) \mathfrak{R}_{h_{k}}(t) d\Omega_{e} = -\frac{1}{2} \oint_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{-}(\xi) [[w_{h_{i}^{e}}]]_{k} d\Gamma_{e} - \oint_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{-}(\xi) (w_{h_{i}^{e}}^{-} - w_{h_{i}^{e}}^{boundary}) n_{k}^{-} d\Gamma_{e}.$$
5-83

Nevertheless, it is shown [158] that using the global lifting operator, can lead to unsatisfactory convergence rate for polynomial approximations of odd order. Moreover, application of global lifting operator may lead to wide stencil which is obviously undesirable [158, 175]. These issue is resolved by introducing a local lifting operator $\mathbf{r}_h^j \in \mathbb{R}^{(\mathcal{D}+2)\times\mathcal{D}}$ as an approximation of the global lifting operator \mathfrak{R}_{h_i} ,

$$\mathfrak{R}_{h_{ik}} = \sum_{e \in I_h} \mathbf{r}_{h_{ik}}^{\Gamma_{Fj}} + \sum_{e \in B_h} \mathbf{r}_{h_{ik}}^{\Gamma_{Bj}} .$$
5-84

In order to employ local lifting operator in the process of the viscous flux discretization, it is necessary to find \mathbf{r}_h^j for every interface and boundary edge of the element such that

$$\sum_{e \in \mathcal{I}_h} \int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} r_{h_{ik}}^j d\Omega_e = \begin{cases} -\oint_{\mathbb{R}^{\mathcal{D}}} \langle \Phi_{ik} \rangle [[w_{h_i^e}]]_k d\Gamma_F^e & \text{on } \Gamma_F^e \in I_h \\ -\oint_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik}^- (w_{h_i^e}^- - w_{h_i^e}^{boundary}) \mathbf{n}_x^- d\Gamma_B^e & \text{on } \Gamma_B^e \in \mathcal{B}_h \end{cases}.$$
 5-85

Note that the local lifting operator can not be computed directly, although it can be represented by a linear polynomial expansion as

$$r_{h_i}^{j}(\xi,t) = \sum_{l=1}^{N_p} \hat{r}_{h_i^{e}}(t)\phi_l(\xi).$$
 5-86

where $\phi_l(\xi)$ belongs to $\mathcal{P}^p(\Omega_e)$ space. The linear system of (Eq. 5-86) must be solved in order to obtain the coefficients of lifting operators \hat{r}_{h^e} . According to (Eq. 5-85), the local lifting operators are only non-zero on the interfaces of the local elements. Therefore,

$$\int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} r_{h_{ik}}^{j} d\Omega_{e} + \int_{\Omega_{N_{e_{i,j}}}} \Phi_{ik} r_{h_{ik}}^{j} d\Omega = -\int_{\mathbb{R}^{\mathcal{D}}} \left\langle \Phi_{ik} \right\rangle [[w_{h_{i}}^{e}]]_{k} d\Gamma_{\Omega_{N_{e_{i,j}}}} .$$
5-87

As the value of lifting operator function is equal for the element Ω_e and neighboring elements sharing the edge *j*, and test function is an arbitrary polynomial function, equation (Eq. 5-87) reads as

$$\int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} r^{-j}_{h_{ik}} d\Omega_{e} = -\frac{1}{2} \int_{\mathbb{R}^{\mathcal{D}}} \Phi^{-}_{ik} [[w_{h_{i}^{e}}]]_{k} d\Gamma_{\Omega_{N_{i,j}}},$$
5-88

$$\int_{\mathbb{R}^{\mathcal{D}}} \Phi_{ik} r^{+j}_{h_{ik}} d\Omega_{\Omega_{N_{e_{i,j}}}} = -\frac{1}{2} \int_{\mathbb{R}^{\mathcal{D}}} \Phi^{+}_{ik} [[w_{h_{i}^{e}}]]_{k} d\Gamma_{\Omega_{N_{e_{i,j}}}}.$$
5-89

Replacing local lifting operator by approximate polynomial function and considering Φ_{*} to be equal to $\phi_{i}(\xi)$, according to Galerkin method, yields to

$$\int_{\mathbb{R}^{\mathcal{D}}} \hat{r}_{h_{ik}^{e}}^{-}(t)\phi_{j}(\xi)\phi_{l}(\xi)d\Omega_{e} = -\frac{1}{2}\int_{\mathbb{R}^{\mathcal{D}}}\phi_{j}^{-}(\xi)[[w_{h_{i}^{e}}]]_{k}d\Gamma_{\Omega_{Ne_{i,j}}},$$
5-90

$$\int_{\mathbb{R}^{\mathcal{D}}} \hat{r}_{h_{k}^{e}}^{+}(t)\phi_{j}(\xi)\phi_{l}(\xi)d\Omega_{e} = -\frac{1}{2}\int_{\mathbb{R}^{\mathcal{D}}}\phi_{j}^{+}(\xi)[[w_{h_{l}^{e}}]]_{k}d\Gamma_{\Omega_{N_{i},j}}.$$
5-91

Considering that $\int_{\mathbb{R}^{\mathcal{D}}} \phi_j(\xi) \phi_l(\xi) d\Omega_e$ is the elemental Mass matrix which can be inverted to the \mathbf{M}_{rj}^{-1} , and knowing that $\hat{r}_{h_i^e}^{-}(t)$ is only function of time, the expansion coefficients of the local lifting operator on face *j* of element Ω_e are given by

$$\hat{r}_{h_{k,r}}^{-}(t) = -\frac{1}{2} (\mathbf{M}_{rj}^{-1})^{-} \int_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{-}(\boldsymbol{\xi}) [[w_{h_{i}}^{e}]]_{k} d\Gamma_{\Omega_{N_{i,j}}}, \qquad 5-92$$

$$\hat{r}_{h_{k,r}}^{+}(t) = -\frac{1}{2} (\mathbf{M}_{rj}^{-1})^{+} \int_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{+}(\boldsymbol{\xi}) [[w_{h_{i}}^{-}]]_{k} d\Gamma_{\Omega_{N_{i,j}}}.$$
5-93

The local lifting coefficients of the boundary faces are determined analogously as

$$\hat{r}_{h_{ik,r^{e}}}(t) = -\frac{1}{2} (\mathbf{M}_{rj}^{-1})^{-} \int_{\mathbb{R}^{\mathcal{D}}} \phi_{j}^{-}(\boldsymbol{\xi}) (w_{h_{i}^{e}}^{-} - w_{h_{i}^{e}}^{boundary}) \mathbf{n}_{k}^{-} d\Gamma_{\Omega_{Ne_{i,j}}}.$$
5-94

Finally, the viscous numerical flux of BR2 method can be defined by considering an arithmetic mean average of the viscous fluxes while the auxiliary variables are approximated in weak sense as

$$\tilde{\mathbf{F}}^{viscous} = \begin{cases} \frac{1}{2} \left\{ \mathbf{F}^{viscous} \left(\nabla \mathbf{w}_{h}^{-} + \eta_{BR2}^{-} \mathbf{r}_{h}^{-}, \mathbf{w}_{h}^{e} \right) + \mathbf{F}^{viscous} \left(\nabla \mathbf{w}_{h}^{+} + \eta_{BR2}^{-} \mathbf{r}_{h}^{+}, \mathbf{w}_{h}^{e} \right) \right\} & \text{on } \mathbf{I}_{h} \\ \mathbf{F}^{viscous} \left(\nabla_{k} \mathbf{w}^{Boundary} + \eta_{BR2}^{-} \mathbf{r}_{h}^{j-}, \mathbf{w}_{h}^{Boundary} \right) & \text{on } \mathcal{B}_{h} \end{cases}, \quad 5-95$$

where η_{BR2} is stabilization constant which is required to be greater than the number of element faces in order to prove stability for the BR2 scheme [159].

Oliver [174] and Shahbazi [180] introduced an explicit formula for evaluation of this parameter. However, it has been shown in several researches [158, 165, 181, 182] that there is no serious stability issue when η_{BR2} is chosen to be less than stability criterion. Note that, the solution gradients ∇w_h used in the evaluation viscous flux function, are the real gradient of the global solution w_h and they can be evaluated using either differentiation matrices [93] or expanding a polynomial series on the gradients of basis functions.

The numerical evaluation of the viscous flux function using BR2 method is illustrated in following. First, the real gradient of the local solution is calculated based on polynomial expansion as

$$\nabla_k \mathbf{w} = \sum_{l=1}^{N_p} \mathbf{w}^l(t) \nabla_k \phi_l(\boldsymbol{\xi}), \qquad 5-96$$

where the moments of the gradient expansion can be explicitly calculated from the partial derivative of the local solution expansion (i.e., $\nabla_k \mathbf{w} = \frac{1}{|J|_{\mathbf{x}\to\xi}} \sum_{l=1}^{N_r} \hat{\mathbf{w}}_{h'}^{l}(t) \nabla_k \phi_l(\xi)$) using projection technique. For case of one-dimension problem, the gradient of local solution at the elemental interfaces is given by,

$$\left(\frac{\partial w_{h_l^e}}{\partial x_1}\right)^- = \frac{2}{\Delta x} \sum_{l=1}^{N_p} \mathbf{w}_{h^e}^l(t) \frac{\partial \phi_l^-(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}, \quad \left(\frac{\partial w_{h_l^e}}{\partial x_1}\right)^+ = \frac{2}{\Delta x} \sum_{l=1}^{N_p} \mathbf{w}_{h^e}^l(t) \frac{\partial \phi_l^+(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}.$$
 5-97

Next, the local lifting operators are calculated according to equation either (Eq. 5-92) or (Eq. 5-93) for every face of the local element Ω_e . Afterward, the global lifting operator is evaluated using

$$\Re_{h_i}(\xi,t) = \sum_{j=1}^{N_F} r_h^{\Gamma_{F_j}}(\xi,t) + \sum_{j=1}^{N_B} r_h^{\Gamma_{B_j}}(\xi,t),$$
5-98

where $N_{_F}$ and $N_{_B}$ denote the number of interfaces and boundary faces in the element $\Omega_{_e}$. Finally, the second derivatives of auxiliary variables are estimated using following relations,

$$\Theta_{h_{ik}}^{+}\Big|_{j} = \frac{\partial w_{h_{i}^{e}}}{\partial x_{k}}\Big|_{j}^{+} + \eta_{BR2}r_{h_{ik}}^{+}(t,\boldsymbol{\xi}_{j}), \qquad 5-99$$

$$\Theta_{h_{ik}}^{-}\Big|_{j} = \frac{\partial w_{h_{i}^{e}}}{\partial x_{k}}\Big|_{j}^{-} + \eta_{BR2} r_{h_{k}}^{-}(t, \xi_{j}), \qquad 5-100$$

$$\Theta_{h_{ik}}\Big|_{GP_i} = \frac{\partial w_{h_i^e}}{\partial x_k}\Big|_{GP_i} + \eta_{BR2} \Re_{h_{ik}}(t, \xi_{GP_i}), \qquad 5-101$$

where *j* index indicates the *j*th face of the element Ω_e and *GP*_i stands for *i*th quadrature points inside the element. The resulting solution of second-order derivatives can be used for evaluation of viscous flux function in (Eq. 5-95).

Considering the above-mentioned processes for evaluation of the viscous fluxes, an explicit formula for one-dimensional problem is obtained as

$$\tilde{\mathbf{F}}^{viscous} = \frac{1}{2} \begin{cases} \left(\frac{\partial w_{h_l^e}}{\partial x}\right)^- + \left(\frac{\partial w_{h_l^e}}{\partial x}\right)^+ \\ + \frac{\eta_{BR2}}{2} \left(\mathbf{w}_{h^e}^+ - \mathbf{w}_{h^e}^-\right) \sum_{l=1}^{N_p} \left((\mathbf{M}_{ll}^{-1})^+ \phi_l^- (\boldsymbol{\xi}) - (\mathbf{M}_{ll}^{-1})^- \phi_l^+ (\boldsymbol{\xi})\right) \end{cases}$$
5-102

5.3.4 Performance of flux functions

Arnold et al. [159] studied the performance of several viscous numerical fluxes for Laplace problem and found out that only a few numerical flux functions yields the optimal order of convergence for this simple scalar equation. Namely, the second method of Bassi and Rebay (BR2) [158], SIP scheme [183], and the local discontinuous Galerkin (LDG) scheme [104].

Qiu et al. [184] studied various monotone inviscid numerical flux functions for the couple of the benchmark problems. They showed that the Rusanov flux requires the least CPU time among all inviscid fluxes, whilst the level of numerical diffusion is the worst. They also showed that performance of inviscid flux function depends on the degree of the polynomial expansion.

Although, these analyses on the performance of numerical fluxes in DG framework are available, *there is no comprehensive verification analysis that examines the performance of viscous fluxes in combination with inviscid numerical fluxes for DG method.* In this section performance of various numerical flux functions based on Euclidean error norm is surveyed.

5.3.4.1 Performance of the inviscid fluxes for smooth problem

The Euler equation (i.e., zero-order Boltzmann model) with smooth initial condition is considered as a benchmark problem. The periodic boundary conditions are applied at both side of the domain and initial condition is set to be

$$\begin{cases} u(x,0) = 1, \\ \rho(x,0) = 1.0 + 0.2\sin(\pi x), \\ p(x,0) = 1. \end{cases}$$
 5-103

The exact solution of this problem is also given by

$$\begin{cases} u(x,t) = 1, \\ \rho(x,t) = 1.0 + 0.2\sin(\pi(x-t)), \\ p(x,t) = 1. \end{cases}$$
 5-104

In order to measure the order of accuracy of the DG method using various inviscid flux function, several inviscid flux functions are tested and the density distribution of the solution is shown for various degree of p in Figure 5-21.



Rusanov (LLF) flux function

Figure 5-21 Comparison of various inviscid flux discretization schemes for smooth solution of Euler equation; (left) profile comparison, (right) Euclidean norm of density

It is obvious that piecewise constant solution is very diffusive and far from exact solution; however, application of more advanced flux functions such as Roe's flux and HLL can improve the level of accuracy of piecewise constant solution. To judge more precisely about the performance of inviscid flux function, the numerical errors and the orders of accuracy is calculated based on the density solution. As it is shown in Figure 5-21, all numerical flux functions —Rusanov, HLL, and Roe— can achieve the expected order of accuracy of p+1. This observation is consistent with the result obtained by Qiu et al. [184].

5.3.4.2 Performance of the viscous fluxes for smooth problem

In order to measure the order of accuracy of viscous flux functions for the smooth problem and verify our numerical implementation of the viscous flux functions, a onedimensional parabolic (heat) equation which has been studied in several previous studies, is considered as a benchmark problem.

The differential equation of heat problem can be defined as

$$\frac{\partial w_t}{\partial t} + \frac{\partial^2 w}{\partial x^2} = 0,$$
 5-105

where the length of the computational domain is chosen to be equal to one wavelength $(0 \le x \le 2\pi)$ of the initial sinusoidal distribution with amplitude of 1.0. The periodic boundary conditions are applied at both side of the computational domain, and exact analytical solution is given by

$$w(x,t) = e^{-t} \sin(x).$$
 5-106

It was shown that the application of real gradient without correction term for discretizing the numerical flux leads to inaccurate approximation of the global solution [176]. To verify this issue, the heat equation is solved using central flux function while the real gradient of global solution has been employed for calculating the second-order derivative of W_h .

The discrepancy between exact solution and numerical approximated solution is obvious in Figure 5-22. It is due to fact that solution is discontinuous at interface of the elements, therefore, application of central numerical flux with real gradient of the global solution at inter-element boundaries yields inconsistent solution of the heat problem.



Figure 5-22 DG approximated solution of the heat equation without considering any correction on real gradient of the global solution.



Figure 5-23 Comparison of the heat equation solution for BR1, BR2, LDG schemes.

Figure 5-23 shows the solution of heat problem using BR1, BR2, and LDG schemes at time equal to 0.7 second. LDG scheme acts very good in capturing both the solutions of w_h , and its gradient ∇w_h . Nonetheless, considerable amount of jump in solution of w_h and ∇w_h is obvious in BR1 solution. This is due to fact that BR1 scheme does not use any stabilizer for minimizing the jumps of the global solution in inter-element connections.



Figure 5-24 Performance of BR1, BR2, LDG methods for one-dimensional heat equation based on the Euclidean norm of W_h .

The solution of heat equation obtained by BR2 scheme retains the accuracy at everywhere; however, the precision of the method in approximation of the gradients is one order less than the global solution.

Figure 5-24 depict the Euclidean norm of the global solution of heat problem for all schemes. It is obvious that BR1 method does not optimally converge for odd degree of p while the convergence rate of BR2 is in order of $O(h^{p+1})$ for case that p > 0, and LDG method shows uniform convergence rate for any order of p.

5.3.4.3 Performance of the inviscid and viscous fluxes for stiff problem

The distribution of the density, velocity, temperature, normal stress, and heat flux solutions along shock-wave are shown for two Mach numbers in Figure 5-25 to Figure 5-27. The upstream Mach number is set to be 2 and 5. Hard-sphere gas molecule is chosen as the working gas flow. Various numerical flux functions is served for discretizing the fluxes. In all profiles, the black solid line indicates the analytical solution while the gray thin solid and scatters lines correspond to the numerical solutions with polynomial order of zero, one, and two.

Results illustrate that the numerical solution becomes closer to the analytical solution by increasing the degree of the polynomial order, as is expected. The discrepancy between the exact and numerical approximate solutions are relatively less in profiles of the conservative and primitive variables compared with the non-conservative variables. It seems that the non-conservative variables are more sensitive than the conservative variables to the choice of the viscous numerical flux function, despite that all profiles are influenced similarly from choosing the inviscid numerical flux function.

The piecewise constant solution smears the conservative and non-conservative properties of gases more than any high-order DG solution. The piecewise constant profile predicted by use of Rusanov (LLF) flux function is the most diffusive and disperse solution compared with the others. However, the numerical diffusion generated by this flux function is negligible when the order of polynomial approximation is more than one. It is obvious that application of Roe and HLL flux functions lead to less numerical diffusion in piecewise constant approximation; whereas there is not significant numerical advantages in those for high-order DG solution. Indeed, the lower orders of polynomial approximate solution are more delicate to the choice of the inviscid numerical flux function than high-order degree of p.

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Figure 5-25 Comparing the normalized shock profiles of the DG polynomial approximated solution with exact analytical solution for hard-sphere gas at Mach=2.

Comparing the results predicted by BR1, BR2 and LDG methods in conjugation with various inviscid flux functions confirm that application of the different inviscid numerical flux function does not result to the instability of the numerical method even if Mach number is very high, at least for this particular problem. However, choosing different numerical schemes for discretizing viscous terms yields to significant change in the performance of the numerical solution.



Figure 5-26 Comparing the normalized stress and heat flux profiles of the DG polynomial approximated solution with exact analytical solution for hard-sphere gas at Mach=2.



Figure 5-27 Comparing the normalized shock profiles of the DG polynomial approximated solution with exact analytical solution for hard-sphere gas at Mach=5.

Figure 5-29 shows the profile of non-conservative variables for BR1, BR2, and LDG schemes at three different Mach number. It is shown that employing BR1 scheme yields the moderate approximation of the exact solution for low Mach case; however, it may not work properly for high Mach conditions. Actually, BR1 method can be employed

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for solving the high Mach number shock waves only if the numerical solver is equipped with a proper positivity preserving treatment [144]. Results illustrate that BR1 scheme becomes fully unstable when Mach number is greater than 5 even if the positivity preserving limiter is used.



Figure 5-28 Comparing the normalized stress and heat flux profiles of the DG polynomial approximated solution with exact analytical solution for hard-sphere gas at Mach=5.

Figure 5-29 also illustrates that obtained first-order solutions using BR2 scheme are undesirable and inaccurate since the $\partial \mathbf{w}_h / \partial x$ vanishes which causes that the second-

order derivatives do not participate in the calculation process of the non-conservative variables. Thus, piecewise constant solutions are equivalent to Euler solutions when BR2 scheme is used. Nevertheless, BR2 scheme can provide moderate high-order solutions at all three tested Mach numbers even though the amount of discrepancy between the approximated non-conservative variable and exact solution increases by increasing the Mach number value for the case of piecewise linear solution.



Figure 5-29 Comparing the accuracy of the normalized stress and heat flux profiles with exact analytical solution for hard-sphere gas; HLL is chosen as the inviscid numerical flux; 50 elements used for discretizing computational domain.

Local DG scheme presents a consistent performance at all three Mach numbers. It is always stable and the discrepancy between exact solution and numerical approximation is negligible in most of the cases. The solution has an acceptable level of accuracy for both case of conservative and non-conservative variables; however, the value of CFL number should be chosen more carefully compared to BR1 and BR2 schemes. I had tested LDG method even for higher Mach numbers (e.g. Mach =40), it works without any stability issue and could provide decent numerical solutions.

5.3.4.3.1 Performance of fluxes based on error norm analysis

Conservative variables

The numerical error and order of accuracy for density solution is depicted in Figure 5-30. Results illustrate that the performance of the inviscid flux functions depends on the degree of the polynomial order. It is obvious that DG method does not achieved the designed order of accuracy due to enabling limiter function. Nonetheless, it is still possible to have a fair comparison between various numerical flux functions since same limiter function is served for all simulations.

The comparison analysis reveals that BR2 and LDG method degrade solution more than BR1 whenever the order of the polynomial approximation is equal to p=2. While they perform better than BR1 when a proper inviscid flux function is used and $p \ge 3$.

Primitive variables

Figure 5-30 shows the energy norm of density and temperature for several combination of the viscous and inviscid flux functions. Results demonstrate that there is no significant difference between error norm computed by temperature for various inviscid flux function. It means that the computed order of accuracy based on temperature is less sensitive to the choose of inviscid flux function compared with density.

Non-conservative variables

Non-conservative variables are another important parameters in studying shock waves and gas dynamics problems [13]. Knowing the order of accuracy of the DG method based on non-conservative variables is very important [112]. A numerical method developed for studying rarefied gas flows should be very accurate in estimation of the non-conservative variables.

Figure 5-31 provides the energy norm of normal stress and heat flux variables for various combination of numerical flux functions. The results show that BR1 and BR2 schemes cannot provide an expected order of accuracy for piecewise linear

approximation (p=1). However, order of accuracy obtained by LDG is relatively higher than BR1 and BR2 schemes.



Figure 5-30 Comparing the order of accuracy of DG approximate solution based on the Euclidean norm of density and temperature solution of viscous shock wave problem for several combination of viscous and inviscid flux functions.


Figure 5-31 Comparing the order of accuracy of DG approximate solution based on the Euclidean norm of normal stress solution of viscous shock wave problem for several combination of viscous and inviscid flux functions.

In second-order finite volume method, a geometry with curved boundaries is usually represented by segments of straight side lines or planar facets. However, this simple representation of curved boundaries does not describe the geometry appropriately for high-order DG methods [103].

As Bassi and Rebay reported [111] that discontinuous Galerkin method requires more accurate treatment on the walls than that allowed by traditional finite volume methods. In DG method, it is essential to pay a significant attention to the curved boundaries. A curved boundary is a smooth physical surface, and it has to be handled as it is. Employing a linear sub-parametric mapping for high-order DG approximation ends to significant degradation of the solution at curved boundaries. It results in appearance of unphysical wakes and spurious oscillations in solution.

The importance of curved boundary treatment for DG method has been subject of several researches during last decade [103, 185-191]. There are two ways to solve this problem; approximation of the normal vectors at each Gauss quadrature point on surface[187], or using iso-/ super-parametric mapping [126, 192]. The first method is the simplest way in which the normal vector on quadrature points are approximated using either exact geometry information or approximated based on interpolation from neighboring faces. Application of this method is not straightforward for three-dimensional geometries, and it can be generally considered as a temporary cure for written codes rather than firm and strong treatment. The fundamental approach to model curved boundaries is to map them using high-order polynomial expansions. Interested readers are referred to [179] for further information.

In this section, the importance of curved solid boundaries in a DG simulation is investigated by simulating flow over a cylinder at Mach=0.4 using various order of polynomials for various Knudsen flow regimes. Figure 5-32 shows that mapping the curved boundaries using sub-parametric mapping does influence the accuracy of solution for Euler equation.

It is shown that refinement of grid on the curved boundaries does not improve the accuracy of the solution, instead, it magnifies the amplitude of unphysical wakes. As I experienced during this work, similar to many other researchers [193], it is highly possible that a numerical solver diverges due to negativity of density and pressure caused by spurious oscillations generated on the wall. Therefore, simulation of curved

boundary problems without appropriate treatment on curved boundaries will results in degradation of the solution accuracy and even instability of the numerical methods at low/high-speed flow conditions.



Piecewise constant solution



Piecewise linear solution



Piecewise quadratic solution

Figure 5-32 Mach contour solution of Euler equation over a cylinder for flow stream Mach of 0.4 on the grid with size of h=0.25.



Piecewise constant solution



Piecewise linear solution



Piecewise quadratic solution

Figure 5-33 Mach contour solution of Euler equation over a cylinder for flow stream Mach of 0.4 and Kn $\rightarrow \infty$ on the grid with size of *h*=0.025.

The influence of curved boundary on the solution accuracy is less important for Navier-Stokes-Fourier equations. It is shown in Figure 5-34 that mapped curved boundary using linear polynomial will results in tangible numerical artifact for flows at very low Knudsen regimes; however, in contrary to Euler equations, the streamline are not affected by low accuracy modeling of the physical curved boundary.



Piecewise constant solution



Piecewise linear solution



Piecewise quadratic solution

Figure 5-34 Mach contour solution of Navier-Stokes-Fourier equation over a cylinder for flow stream Mach of 0.4, and Kn= 10^{-8} on the grid with size of h=0.25.

It is shown in Figure 5-35 that the importance of true mapping of curved geometry reduces as Knudsen number increases. It is due to fact that the thickness of viscous shear layer on the wall increases, and it diffuses the numerical artifacts generated due to inaccurate mapping of the curved walls.



Piecewise constant solution



Piecewise linear solution



Piecewise quadratic solution

Figure 5-35 Mach contour solution of Navier-Stokes-Fourier equation over a cylinder for flow stream Mach of 0.4 and Kn= 10^{-1} on the grid with size of h=0.025.

The numerical implementation of the boundary conditions is tricky and it demands special attention. The accuracy of the simulation, rate of residual convergence, and stability of the numerical solver are strongly dependent on the implementation of the boundary conditions.

As discussed in CHAPTER 4, the present modal DG method imposes the boundary conditions in a weak manner through the prescribed boundary operators. So it is possible to construct any kind of boundary conditions — Dirichlet, Riemann, and Neumann — for DG method based on information at exterior and interior state of the boundary faces.

5.5.1 Far-field boundary

Two requirements must be satisfied in numerical implementation of the far-field boundary conditions [194]. First, the cutting of the physical domain should not have any considerable effect on the flow solution as compared to the unbounded domain. Inadequate truncation of the domain can lead to a severe slowdown of steady state convergence rate. This issue is more sensible in simulation of subsonic and transonic flow problems which are naturally elliptic and parabolic. Second, any outgoing noise should have no influence on the flow field.

Based on concept of characteristics variables, all information are transported into the computational domain along the characteristics waves when incoming flow is supersonic. Therefore, all eigenvalues have the similar sign, and boundary operator is solely defined based on conservative variables at boundary side as

$$\mathbf{w}_{h^e}^{boundary} = \begin{pmatrix} \rho_{\infty} & \mathbf{u}_{\infty} & \rho e_{\infty} \end{pmatrix}^T, \qquad 5-107$$

where the subscript ∞ denotes to the free-stream values. Accordingly, the numerical inviscid, viscous, and auxiliary flux functions can be approximated as

$$\widetilde{\mathbf{F}}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right),$$

$$\widetilde{\mathbf{F}}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{-} - C_{11} \left(\mathbf{w}_{h^{e}}^{-} - \mathbf{w}_{h^{e}}^{boundary} \right) \mathbf{n}^{-} \right),$$

$$\widetilde{\mathbf{F}}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right).$$
5-108

5.5.2 Outflow boundary

If the outgoing flow is a supersonic flow, the sign of all eigenvalues is same and all characteristics waves leave the computational domain[194]. Considering behavior of the characteristics waves, the boundary operator can be defined as

$$\mathbf{w}_{h^e}^{boundary} = \mathbf{w}_{h^e}^{-} = \left(\rho^{-} \quad \mathbf{u}^{-} \quad \rho^{-}e^{-}\right)^{T},$$

$$\mathbf{\Theta}_{h^e}^{boundary} = \mathbf{\Theta}_{h^e}^{-} - C_{11}(\mathbf{w}_{h^e} - \mathbf{w}_{h^e}^{boundary})\mathbf{n}^{-}.$$
5-109

The numerical inviscid, viscous, and auxiliary flux functions can also be approximated as

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{F}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-}\right),$$

$$\widetilde{\mathbf{F}}^{viscous}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{boundary}\right) = \mathbf{F}^{viscous}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}\right),$$

$$\widetilde{\mathbf{F}}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{F}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{-}\right).$$
5-110

5.5.3 Symmetry plane

Symmetry boundary condition should guarantee no flux across the boundary. To satisfy this condition; the velocity normal to the symmetry plane must be zero; the gradients of scalar quantities normal to the boundary, and the gradient of tangential velocity on the boundary must be zero. It is also necessary that the gradient of normal velocity along the boundary vanishes. The summary of these conditions can be written in form of mathematical relation as

$$\mathbf{n} \cdot \nabla \mathbf{w} = 0,$$

$$\mathbf{n} \cdot \nabla (\mathbf{u} \cdot \mathbf{l}) = \mathbf{n} \cdot \nabla (\mathbf{u} \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})) = 0,$$

$$\mathbf{t} \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = 0.$$

5-111

where, *t* denotes a vector tangential to the symmetry boundary and \otimes means dyadic vector product.

There are two treatments for implementation of symmetry boundary condition. First is based on finite volume approach in which the mathematical constraints, defined in (Eq. 5-111), are imposed by introducing the concept of reflected cell. It can be formulated as

$$\mathbf{w}_{h^e}^{boundary} = \mathbf{w}_{h^e}^- = \left(\rho^- \quad \mathbf{u}^- \quad \rho^- e^-\right)^T,$$

$$\mathbf{\Theta}_{h^e}^{boundary} = \mathbf{\Theta}_{h^e}^- - C_{11}(\mathbf{w}_{h^e} - \mathbf{w}_{h^e}^{boundary})\mathbf{n}^-,$$

5-112

where the normal gradient of the normal velocity in the exterior state equals to that in the interior state, but it has a reversed sign [194]. The numerical flux functions over boundary interface is defined as

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{F}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-}\right),$$

$$\widetilde{\mathbf{F}}^{viscous}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, -\mathbf{\Theta}_{h^{e}}^{-}\right),$$

$$\widetilde{\mathbf{F}}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{F}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{-}\right).$$
5-113

Alternative way to define symmetry boundary condition is to prescribe the derivatives of the global solution on the boundary side as follows,

$$\boldsymbol{\Theta}_{h^{e}}^{boundary} = \boldsymbol{\Theta}_{h^{e}}^{-} - \left(\mathbf{n}^{-} \cdot \boldsymbol{\Theta}_{h^{e}}^{boundary}\right) \mathbf{n}^{-}, \qquad 5-114$$

where $(\mathbf{n}^- \cdot \mathbf{\Theta}_{h^e}^{boundary})\mathbf{n}^-$ can be written in index notation form as $(n_i^- \cdot \mathbf{\Theta}_{h_a^e}^{boundary})n_k^-$. The symmetry constraints are prescribed such that below equations vanish on the symmetry plane

$$\mathbf{n} \cdot \nabla \left(\mathbf{u} \cdot \mathbf{t} \right) = \begin{bmatrix} (1 - n_1^2) \frac{\partial u_1}{\partial x_1} - n_1 n_2 \frac{\partial u_2}{\partial x_1} - n_2 n_3 \frac{\partial u_3}{\partial x_1} \\ -n_1 n_2 \frac{\partial u_1}{\partial x_2} + (1 - n_2^2) \frac{\partial u_2}{\partial x_2} - n_2 n_3 \frac{\partial u_3}{\partial x_2} \\ -n_1 n_2 \frac{\partial u_1}{\partial x_3} - n_2 n_3 \frac{\partial u_2}{\partial x_3} + (1 - n_3^2) \frac{\partial u_3}{\partial x_3} \end{bmatrix}, \qquad 5-115$$

$$\mathbf{t} \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = \begin{bmatrix} (1 - n_1^2)\alpha_1 - n_1n_2\alpha_2 - n_2n_3\alpha_3 \\ -n_1n_2\alpha_1 + (1 - n_2^2)\alpha_2 - n_2n_3\alpha_3 \\ -n_1n_2\alpha_1 - n_2n_3\alpha_2 + (1 - n_3^2)\alpha_3 \end{bmatrix}$$
5-116

where

$$\boldsymbol{\alpha}_{1} = n_{1} \frac{\partial u_{1}}{\partial x_{1}} + n_{2} \frac{\partial u_{2}}{\partial x_{1}} + n_{3} \frac{\partial u_{3}}{\partial x_{1}},$$
$$\boldsymbol{\alpha}_{2} = n_{1} \frac{\partial u_{1}}{\partial x_{2}} + n_{2} \frac{\partial u_{2}}{\partial x_{2}} + n_{3} \frac{\partial u_{3}}{\partial x_{2}},$$
$$\boldsymbol{\alpha}_{3} = n_{1} \frac{\partial u_{1}}{\partial x_{3}} + n_{2} \frac{\partial u_{2}}{\partial x_{3}} + n_{3} \frac{\partial u_{3}}{\partial x_{3}}.$$

The numerical flux functions are given by

$$\widetilde{\mathbf{F}}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right) = \mathbf{F}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-} \right),$$

$$\widetilde{\mathbf{F}}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{boundary} \right),$$

$$\widetilde{\mathbf{F}}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right) = \mathbf{F}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-} \right).$$

$$5-117$$

5.5.4 Inviscid wall boundary

In the case of inviscid flow [194], the velocity vector should be tangent to the surface and it is not zero as there is no friction force on the surface. The fluid slips over the surface while it does not penetrate into wall. To prescribe zero normal velocity on the surface, the inner cross product of velocity and outward unit normal vectors must vanishes as

 $\mathbf{u} \cdot \mathbf{n} = 0.$ 5-118 While the inviscid flux function is computed by adjusting the wall velocity to have zero normal component, the viscous and auxiliary flux functions are zero by default;

$$\mathbf{w}_{h^e}^{boundary} = \mathbf{w}_{h^e}^- = \left(\rho^- \quad \mathbf{u}^- - 2\left(\mathbf{u}^- \cdot \mathbf{n}^-\right)\mathbf{n}^- \quad \rho^- e^-\right)^T,$$

$$\mathbf{\Theta}_{h^e}^{boundary} = 0.$$

5-119

$$\widetilde{\mathbf{F}}^{inviscid} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right),$$

$$\widetilde{\mathbf{F}}^{viscous} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{boundary} \right) = 0,$$

$$\widetilde{\mathbf{F}}^{auxiliary} \left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary} \right) = 0.$$

$$5-120$$

5.5.5 No-slip viscous wall boundary

In no-slip wall, the relative velocity between solid wall and fluid attached to the surface is assumed to be zero. Therefore, the physical velocity on the solid should be defined such that

$$\mathbf{u}^{boundary} - \mathbf{u}^{solid} = \mathbf{0}.$$
 5-121

If the wall boundary maintains the temperature, solid temperature should be given explicitly; however, if heat flux vector is prescribed at wall, the normal heat flux on the wall should be defined as $\mathbf{q}^{solid} = \mathbf{n} \cdot \mathbf{q}^{boundary}$. For NSF equations, where Fourier law is employed for modeling heat flux vector, the normal gradient of temperature on the surface must be set zero for adiabatic wall boundary condition;

$$\mathbf{n}.\nabla T^{boundary} = n_i \frac{\partial T^-}{\partial x_i}, \qquad 5-122$$

Although prescribing the velocity and temperature is straightforward, defining pressure and density have been treated in a number of different ways in several researches [195-199].Prescribing noslip wall boundary condition in simplest way is preferred for most of the applications. Nevertheless, the stability of this approach is not the same as the characteristics based boundary condition.

The most straightforward method to define no-slip boundary condition is to use following relations [126] for adiabatic wall

$$\mathbf{w}_{h^{e}}^{boundary} = \begin{pmatrix} \rho^{-} & 0 & \rho^{-}e^{-} \end{pmatrix}^{T}, \\ \mathbf{\Theta}_{h^{e}}^{boundary} = \mathbf{\Theta}_{h^{e}}^{-} - C_{11}(\mathbf{w}_{h^{e}}^{-} - \mathbf{w}_{h^{e}}^{boundary})\mathbf{n}^{-}.$$
5-123

and

$$\widetilde{\mathbf{F}}^{inviscid}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) \approx \mathbf{F}^{inviscid}\left(\mathbf{w}_{h^{e}}^{boundary}\right),$$

$$\widetilde{\mathbf{F}}^{viscous}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{\Theta}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{boundary}\right) = \mathbf{F}^{viscous}\left(\mathbf{w}_{h^{e}}^{boundary}, \mathbf{\Theta}_{h^{e}}^{boundary}\right),$$

$$\widetilde{\mathbf{F}}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{-}, \mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{F}^{auxiliary}\left(\mathbf{w}_{h^{e}}^{boundary}\right) = \mathbf{w}_{h^{e}}^{boundary}.$$

$$5-124$$

In this approach, the gradient of temperature on the boundary state are defined according to (Eq. 5-122) as

$$\nabla_i T^{boundary} = \nabla_i T^- - n_i \frac{\partial T^-}{\partial x_i}.$$
5-125

Although this approach is useful but it is vulnerable to the numerical instability when the variation of the density near a wall is not small [196, 200]. These instabilities usually happens in the initial stages of a steady-state simulation, or in a simulation of an transient (unsteady) flows in which the temperature difference between wall and interior state is non-negligible and the speed of the fluid is considerably high.

An alternative approaches can be obtained by assist of finite volume method and defining boundary operator using one of below approaches

if first approach is picked. the numerical fluxes at wall can be obtained according to (Eq. 5-124). Whereas using the second approach leads to calculation of the numerical flux function based on interior and boundary state values.

5.5.5.1 Evaluation of the wall properties

Let's assume that the flow is laminar with no enforced body force and no significant gradients of pressure in the tangential direction over the wall. Assume also that the normal velocity on the wall vanishes and the velocity gradients in tangential direction are small compared to velocity gradients in the normal direction. We can express the continuity and the simplified momentum balance on the wall as

$$\frac{\partial \rho}{\partial t}\Big|_{wall} + \frac{\partial (\rho \mathbf{u} \cdot \mathbf{n})}{\partial n}\Big|_{wall} = 0.$$

$$\frac{\partial \mathbf{\Pi}_n}{\partial \mathbf{n}}\Big|_{wall} + \frac{\partial p}{\partial \mathbf{n}}\Big|_{wall} = 0.$$
5-127

where ρ^{wall} is wall density.

According to (Eq. 5-127), the pressure gradient in normal direction to the wall is mainly balanced by the normal gradient of viscous forces. The variations of the normal velocity and the pressure gradient in the normal direction can be ignored *if the variation*

of the density at the wall is negligible. Thus, a simple extrapolation from the interior state can be used for prescribing the wall pressure:

$$p^{wall} = \begin{cases} p^{-}, \text{ or} \\ \frac{1}{6} (5p^{-} + \overline{p}^{-}). \end{cases}$$
 5-128

and wall temperature, for case of isothermal wall, is defined by extrapolating from the interior state and specified wall temperature as

$$T^{wall} = \begin{cases} T^{solid}, \text{ or} \\ \frac{1}{6} (5T^{solid} + T^{-}), \text{ or} \\ \frac{1}{8} (6T^{solid} + T^{-} + \overline{T}^{-}), \text{ or} \\ (2T^{solid} - T^{-}). \end{cases}$$
5-129

The total energy and wall density is given by

$$\rho^{boundary} = \begin{cases} \rho^{-} \text{ for adiabatic wall,} \\ \frac{p^{wall}}{RT^{wall}} \text{ for isothermal wall,} \end{cases}$$
5-130

$$E^{wall} = \begin{cases} E^{-} \text{ or adiabatic wall,} \\ f\left(T^{solid}, p^{solid}, \rho^{solid}, \mathbf{u}^{solid}\right) \text{ isothermal wall.} \end{cases}$$
 5-131

If the variation of density is not small or the normal velocity gradient and the pressure gradient near the wall cannot be ignored [196], application of (Eq. 5-128) results in numerical instability because of the inconsistency between a zero-pressure gradient enforced at the wall and pressure gradient inside the local element. Therefore, it is essential to revisit definition of wall pressure at wall such that the continuity equation, momentum equation on the wall, and the given thermal conditions are integrated together in smart way. The wall density is first defined by evaluating continuity equation on the wall, and then pressure on the wall is calculated using updated density on the wall and given temperature on the wall. For case of adiabatic walls, normal gradient of temperature can be determined using $\partial (p/\rho)/\partial x_i n_i$ [198].

5.5.6 Langmuir slip wall boundary

It is necessary to introduce the velocity slip and temperature jump boundary conditions on the surface for studying the rarefied and microscale gas flows. Among various slip models [201-204], the Langmuir slip model [201, 205-208] which is based on the physical adsorption isotherm [14] can be utilized to model the slip effects.

Langmuir slip model takes the interfacial gas–surface molecular interaction into account and turns out to be qualitatively the same as the conventional Maxwell slip model in most cases. However, its numerical implementation is simpler than the first-order Maxwell boundary condition since it is Dirichlet-type boundary condition.

In Langmuir boundary condition, a coverage fraction α , defined as a function of wall pressure, is limited to be in the range of $0 \le \alpha \le 1$. For monatomic molecules, the coverage fraction can be expressed as

$$\alpha = \frac{\beta p}{1 + \beta p}$$
 5-132

where *p* is the dimensional surface pressure and β is defined by considering the gassurface molecular interaction process as a chemical reaction,

$$\beta = \frac{\lambda \sigma_g}{k_B T^{wall}} \exp\left(\frac{D_e}{R_{universal} T^{wall}}\right).$$
 5-133

Here heat of adsorption D_e depends on the gas-solid interaction specifications and $R_{universal}$ denotes the universal gas constant. λ denotes the freestream mean free path and σ_g represents the mean area of a site which can be approximated using hard-sphere total cross-sectional area,

$$\sigma_g = \pi d^2.$$
 5-134

The velocity slip and temperature jump boundary conditions in the Langmuir model are determined as

$$\mathbf{u}_{tagential}^{wall} = \alpha \mathbf{u}_{tagential}^{solid} + (1 - \alpha) \mathbf{u}_{\lambda},$$

$$T^{wall} = \alpha T^{solid} + (1 - \alpha) T_{\lambda},$$

5-135

where tangential velocity vector \mathbf{u}_{λ} and temperature of gas T_{λ} outside of the Knudsen layer can be approximated based on either free stream condition or the values in adjacent element to the wall boundary interface.

5.5.7 Maxwell slip wall boundary

5.5.7.1 The original Maxwell boundary condition

The original Maxwell slip boundary condition [202, 207, 209] was defined first in form of the stress tensor and heat flux vector along the wall direction as

$$\mathbf{u}_{tangential}^{wall} - \mathbf{u}_{tangential}^{solid} = -\left(\frac{2-\sigma_{v}}{\sigma_{v}}\right)\frac{\lambda}{\mu}\boldsymbol{\tau}_{tangential} - \frac{3}{4}\frac{\Pr(\gamma-1)}{\gamma p}\boldsymbol{q}_{tangential}, \qquad 5-136$$

where tangential stress and heat flux are defined using $S = (I - n \otimes n)$ tangential operator as

$$\boldsymbol{\tau}_{tangential} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S}, \qquad \mathbf{q}_{tangential} = \mathbf{q} \cdot \mathbf{S}.$$
 5-137

Here, \mathbf{n} is the outward normal vector and \mathbf{I} is the second-order unit tensor defined as

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
 5-138

This equation is valid for any three-dimensional arbitrary geometry problem and can be written in form of vector products as

$$\mathbf{u}_{tangential}^{wall} - \mathbf{u}_{tangential}^{solid} = -\left(\frac{2-\sigma_{v}}{\sigma_{v}}\right)\frac{\lambda}{\mu} (\mathbf{n} \cdot \mathbf{\Pi}) \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) - \frac{3}{4} \frac{\Pr(\gamma - 1)}{\gamma p} \mathbf{q} \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}).$$
 5-139

Later, it was simplified for one-dimensional NSF equation, and commonly used for solving multi-dimensional problems.

5.5.7.2 First-order Maxwell boundary condition

In case of NSF equations where the non-conservative variables are modeled using linear uncoupled constitutive relations (i.e. first-order Boltzmann-based model), the stress tensor and heat flux vector on the wall for monatomic gases are defined as

$$\Pi_{ij} = -\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}, \ q_i = -k \nabla_i T \ .$$
 5-140

Therefore, the original Maxwell boundary condition (Eq. 5-139) can be simplified using these first-order constitutive relations as

$$\mathbf{u}_{tangential}^{wall} - \mathbf{u}_{tangential}^{solid} = \left(\frac{2 - \sigma_{v}}{\sigma_{v}}\right) \lambda \mathbf{n} \cdot \left[\left(\nabla \mathbf{u}\right) + \left(\nabla \mathbf{u}\right)^{T} - \frac{2}{3}\mathbf{I}\left(\nabla \mathbf{u}\right)\right] \cdot \left(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}\right) + \frac{3}{4}\frac{\mu}{\rho T} \left(\nabla T\right) \cdot \left(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}\right),$$
5-141

5.5.7.3 Maxwell boundary condition for 1-D Couette flow

In order to obtain the simplified Maxwell boundary conditions for Couette flow problem, let's define the heat flux and shear stress values on the wall using classical linear relations

$$q_{1} = -k \frac{\partial T}{\partial x_{1}},$$

$$\Pi_{12} = -\mu \frac{\partial u_{1}}{\partial x_{2}}.$$
5-142

and define gas properties using caloric perfect gas relations for ideal gas flows $C_p = \gamma R / \gamma - 1$, $\Pr = C_p \mu / k$, $p = \rho RT$.

As Couette flow is purely one-dimensional flow the problem, thus it is possible to eliminate several terms from (Eq. 5-139) as

$$n_{1} = n_{3} = 0, \quad n_{2} \neq 0,$$

$$\Pi_{11} = \Pi_{22} = \Pi_{33} = 0, \\ \Pi_{13} = \Pi_{31} = \Pi_{23} = \Pi_{32} = 0, \quad \Pi_{12} \neq 0$$

$$q_{2} = q_{3} = 0, \quad q_{1} \neq 0$$

$$u_{2} = u_{3} = 0 \text{ at wall}$$

5-143

Applying above condition into (Eq. 5-139), the one-dimensional Maxwell Slip boundary condition for Couette flow problem reads as

$$u_{1}\Big|_{tangential}^{wall} - u_{1}\Big|_{tangential}^{solid} = \left(\frac{2 - \sigma_{v}}{\sigma_{v}}\right) \lambda \frac{\partial u_{1}}{\partial n} + \frac{3}{4} \frac{\mu}{\rho T} \frac{\partial T}{\partial x_{1}}.$$
 5-144

Although this model is derived for one-dimensional Couette flow problem, it is often used in multidimensional problems by considering it as the most simplified version of Maxwell boundary condition.

CHAPTER 6. Verification & validation of discontinuous Galerkin method

Albert Einstein (1879-1955):

"Not everything that counts can be counted, and not everything that can be counted counts."

Verification and validation become critical practical issues when laboratory level research of computational models is used in the mature, real world (application) problems. However, such study is often complicated and subtle since verification and validation of computational models depend on the properties considered, and in many cases, overall multi-faceted agreement is very difficult to achieve. DG has been successfully verified for various scalar equations and variety of hyperbolic/elliptic systems. There are numerous numerical and mathematical researches directed on the study of the accuracy of method for either Euler or Navier-Stokes-Fourier equations [98-100, 103, 111]. In this Chapter, various well-known benchmark problems are solved, in order to verify the accuracy of the modal DG method.

6.1 Scalar linear problem

Scalar hyperbolic equation with mixed initial condition consists of a combination of the Gaussians, a square pulse, a sharp triangle, half-ellipse profiles, is a well-known benchmark problem due to the appearance of several different smooth and stiff extreme together in the computational domain. This problem is considered to check performance of KXRCF troubled cell indicator and accuracy of present Modal DG solver.

As it is shown in Figure 6-1, the precision of DG approximation increases by increase of the polynomial expansion; however, the improvement in the solution accuracy is not tangible for p>2. Moreover, it is shown that KXRCF indicator detects troubled cells nicely; however, some cells in smooth regions near the local smooth extrema are labeled falsely.



Figure 6-1 Scalar hyperbolic equation with mixed initial condition (Right) Modal DG solutions, (b) Performance of KXRCF indicator in detecting troubled cells.

6.2 Two-dimensional Riemann problems

The one-dimensional centered waves are associated with gas dynamics equations consist of contact-discontinuities, shock-waves, and rarefaction-waves. Studying 1-D Riemann problems can pave the way for developing large class so-called upwinding methods [81, 210]. Contrasting to 1-D problems, there is no general exact Riemann solver available in the 2-D cases.

Generally, 2-D Riemann solvers are not considered as a building block for development of CFD schemes. A multi-dimensional upwinding scheme recasts into a one-dimensional Riemann problem at interface of a two-dimension control volume. As several researchers [211-214] predicted that there are at least 19 admissible types of 2-D Riemann problems which are genuinely different from each other, must be studied case by case.

Although 2-D Riemann problems has been analyzed by many researchers in last decades [79, 215-217], studying these problems using DG methods provides very useful information about capability of DG methods in handling with purely multi-dimensional problems. It can also provide valuable information about capability of positivity preserving DG schemes in dealing with strong and complicated gas dynamics problems.

In order to analyze performance of modal DG method for solving purely multidimensional problems, the solution of present modal DG method are compared to solution of high-order finite difference scheme for two cases (namely: case 4 and case 6) out of 17 distinguishable cases available in [217]. In a 2-D Riemann problem, computational domain is divided into four quadrant and the initial data in each quadrant are set to be constant initially such that one-dimensional expansion waves (rarefaction waves), one-dimensional compression waves (shock waves) and contact discontinuities (slip line) appears at interfaces between the quadrants.

In order to compare present method with results presented in [217], density lines are distributed with 29 levels (minimum level of 0.52 and maximum of 1.92), pressure variation is plotted by color contour and velocity is depicted by streamline. Figure 6-2 shows that DG and high-order finite difference methods resolve all discontinuities; two straight 1-D shocks splitting two constant states and the two curved shocks separating the bow shaped region of higher density. As it is obvious, the DG polynomial approximate solution with grid resolution of 200x200 predicts a thinner shock wave and resolves the discontinuities more clearly than high-order finite difference method.



Figure 6-2 Comparison between piecewise quadratic modal DG solution(right) and multiadaptive finite difference solution [217](left) for solving 2-D Riemann problem (Case 4).

Figure 6-3 shows a well agreement between present DG method and high-order finite difference method. It is obvious that a strong low-pressure region appears near to the origin of jump condition, and waves come out from the initial jump origin and propagate into the all four quadrants since their speed is faster than the speed of the main contact discontinuity. DG approximate solution obtained for 200x200 cells is almost equivalent to the solution of high-order finite difference method using 400x400 grids. It is obvious that solution estimated by DG method is more accurate than those of high order finite difference solution at the same grid size distribution.



Figure 6-3 Comparison between piecewise quadratic modal DG solution(right) and multiadaptive finite difference solution [217](left) for solving 2-D Riemann problem (Case 6).

6.3 Unsteady flow problems

Unsteady shock-dominated flows are strongly influenced from the uncertainties and exhibit highly non-linear responses to perturbations. In order to examine stability and accuracy of present DG method for solving Euler equation, three classical well-known benchmark problems in unsteady compressible fluid dynamics are studied; forward facing step, backward facing step, double Mach reflection.

6.3.1 Forward facing step flow

Consider the supersonic flow over a forward facing step in a channel, known as the classical Woodward-Colella problem [218]. The objective is to capture the position of the shock waves and Kelvin-Helmholtz instability near the top of the domain. The free-stream Mach number is 3, and domain compromises of an inlet section followed by a forward-facing step.

In this problem, as shown in Figure 6-4, a stable moving shock hits a rectangular step at a particular instant of time after the impulsive start of the channel. Then, a stable shock-wave pattern consists of standing Mach stem develops at top of the corner. Later, Kelvin-Helmholtz instability origins from this Mach-stem and floating in domain.

Several numerical schemes are failed in simulation of this problem due to existence of very sharp singularity (90-degree corner). They cannot capture the Kelvin-Helmholtz instability because of over-limiting of the solution at local extrema. At present work, it is simulated without use of any special entropy correction scheme for the corner region.

6.3.2 Backward-facing step flow

Diffraction of shock and detonation waves is one of the fundamental problems in gas dynamics [219]. The diffraction of a shock at a sudden (sharp) expansion of a planar channel is a special benchmark problem due to high chance of negativity of density at corner region. Note that, the viscous effects are unimportant in this problem, therefore, they can be neglected and Euler equation is used for this problem[220].

The results shown in Figure 6-5 verify that DG solution is in well agreement with experiments and numerical solution of the other research. It is shown in Figure 6-6 that the secondary shock wave appears near the 90-degree edge as the incident shock wave pass the diffraction edge. As there is a high pressure, low-velocity gas below the contact discontinuity stream and there is a low pressure, high velocity expanded gas above this stream, the secondary shock wave is generated to adjust flow between these two regions. Therefore, a lambda shock wave appears near diffraction edge due to flow separation forced by the increasing strength of the secondary shock wave.



Figure 6-4 Numerical Schlieren sequence of Woodward-Colella forward facing step problem.



Figure 6-5 Computed shock-wave diffraction density contour on a backward-facing step for M=1.5 (left) present DG solution, (right) Experimental data of [219]

6.3.3 Double Mach reflection problem

Let's consider a strong oblique shock incident on flat surface with angle of 60° to the direction of shock propagation. The moving shock with Mach of 10 is propagating in stationary domain where flow is at rest before facing with moving shock. This unsteady high-speed problem is so-called double Mach reflection, and it was studied in detail by Woodward and Colella [218] and later many other researchers. As the accuracy of capturing propagating and reflecting shocks in double Mach region is highly sensitive to the boundary condition and numerical scheme, this problem is always considered as important benchmark problem for verification of a numerical solver.

Figure 6-7 shows the DG approximate solution for four levels of mesh refinements, and Figure 6-8 shows that the zoomed secondary shock waves for this problem. It is obvious that all shocks and contact discontinuities are well captured when the global domain is decomposed into large number of elements and order of polynomial expansion is considerably high.

185



Figure 6-6 Grid study for shock-wave diffraction on a backward-facing step for M=1.5.



Figure 6-7 Case study of double shock-reflection problem with M=10.

6.4 Steady flow problems

Steady-state internal and external flows can be mostly influenced by the viscous boundary layer appearing near the wall. In order to examine the accuracy of present DG method for solving shock-dominant flow problems and shear-dominant flow problems, I studied two classical well-known benchmark problems using classical Navier-Stokes-Fourier model; flow around a cylinder, and compressible lid-driven cavity flow[221].



Figure 6-8 Double shock-reflection region for four level of mesh refinement.

6.4.1 Compressible lid driven cavity

Two-dimensional compressible lid-driven cavity problem is a laminar, viscousdominant, subsonic flow in which fluid is driven by steadily moving wall in x direction with constant velocity of 50m/s. In this problem, all walls (expect driven wall) are stationary with equal temperatures, while the Knudsen number can vary by changing flow conditions. The results of this problem are important as they can be used to investigate the effects of the Reynolds number and the Mach number on the flow structure and to study the accuracy of wall boundary condition.

Reynolds number is small and flow is derived due to viscous forces generated by driven wall, therefore, this problem can be considered as a benchmark problem to check ability of compressible modal DG method in handling very low-speed viscous dominant flows. As is shown in Figure 6-10, the present DG solution is comparable with result obtained from unified-gas kinetic scheme. It is obvious that the flow structure consists

of two separate co-rotating vortices contiguous to the moving walls. It is shown in Figure 6-9 that DG piecewise constant solution cannot resolve the vortexes generated at corners of the domain, while all high-order DG approximate solutions can predict these physical vortexes accurately and identically.



Piecewise constant solution





Piecewise linear solution



Piecewise quadratic solution

Piecewise cubic solution

Figure 6-9 Mach contour over a lid-driven cavity flow for cases for four level of refinement of degree of the polynomial expansion.



UGKS solution

Figure 6-10 Mach contour over a lid-driven cavity flow for Re=1000, driven wall velocity u=0.165 (left) present DG solution, (right) UGKS solution [112].

6.4.2.1 Flow at various Reynolds numbers

Flow over a cylinder at various Reynolds number is considered to verify the range of validity of present Modal DG solver. For all cases, a cylinder with radius of one is used and the outer boundary is set approximately 15 times of the diameter away from the cylinder surface in order to avoid interaction between the boundary conditions.



Piecewise constant solution



Piecewise linear solution

Piecewise quadratic solution

Figure 6-11 Steady creeping flow over a cylinder in Re=1 In creeping flow condition, streamlines are analogous to those of the solution of the potential equations and there is no separation or recirculation behind the cylinder. As is shown in Figure 6-11 and Figure 6-13, DG method can easily capture the flow structure of the low Reynolds number conditions with any order of polynomial considering piecewise constant approximation. It is shown that piecewise linear and piecewise quadratic solutions are providing qualitatively similar solutions, and there is no wake at behind of the cylinder as it is expected. Figure 6-11 also shows that there is no need of using very high-order numerical approximation for studying creeping steady state flow problems unless it is desired to use less grids.

In Reynolds number 40, flow is still laminar while two large stable wakes appears behind the moving cylinder. Figure 6-12 shows that first-order compressible DG solver cannot predict the essence of the flow properly, whereas the second-order and thirdorder numerical solutions predicts flow behavior correctly, as shown in Figure 6-14. It is obvious that the size and location of the wakes are predicted accurately compared with experimental results.



Piecewise constant solution



Piecewise linear solution

Piecewise quadratic solution

Figure 6-12 Steady laminar flow with two steady separated wakes behind a cylinder at, Re=40



Piecewise constant solution



Piecewise linear solution



Piecewise quadratic solution

Figure 6-13 Unsteady laminar flow with von-Karman vortex street over a cylinder at, Re=150.

When Reynolds number increases sufficiently, the wakes behind the cylinder becomes unstable and start moving, although flow is still laminar. Figure 6-13 shows that simulation of moderate Reynolds number flows requires application of high-order DG methods, particularly when there are some wakes or circulations inside the computational domain, and compressible form of the conservation laws are served. The von Karman vortex street does not appear in piecewise constant solution. This states that piecewise constant approximation of solution using DG is not sufficient for studying laminar flows with low Reynolds number values. Although the quality of piecewise constant solution may improve if million grids are used in a simulation, highorder DG methods can easily capture the von-Karman vortex streets even if the computational grids are coarse.



Modal DG Experiment Figure 6-14 Stream lines over a cylinder for M=0.1, Re=40 (left) present DG solution, (right) Experiment adapted from [222].

6.4.2.2 Verification and validation DG method for high-speed flows

As the main focus of present work is to study the physics of non-equilibrium flows, the level of accuracy of present solver for capturing physics in rarefied conditions is examined by comparing present Modal DG solution with second-order validated finite volume solution, and direct simulation Monte-Carlo method. As shown in Figure 6-15 and Figure 6-16, the results of modal DG are in well agreement with solution of the second-order finite volume method for Kn=0.05. It is shown that the thickness of shock wave and its location is predicted similarly for both methods.



Modal DGSecond-order finite volume methodFigure 6-15Density contour over a cylinder for M=5.48, Kn=0.05 (left) presentDG solution, (right) second-order vertex-based finite volume solution.

Second-order finite volume method



Modal DG

Figure 6-16 Comparison of flow field contours over a half of cylinder for M=5.48, Kn=0.05 (left) density contour, (upper side) pressure contour.

6.4.2.3 DG-P adaptability

The flow around a cylinder with free-stream Mach number of 5.48 is considered as the next benchmark problem in order to know which order of polynomial expansion is sufficient for simulation of steady-state high-speed flow in a moderate grid size. Figure 6-17 shows the solution of this problem using Modal DG method for three level of polynomial refinements. It is shown that in piecewise constant solution shock-wave smears considerably even if the considerable number of element is used.



Figure 6-17 Computed bow shock-wave Mach contour over a cylinder for cases with different order of polynomial expansion.

The results of present modal DG solver is also compared with direct solution of Boltzmann equation at low speed (M=0.1, Kn=0.1) and high-speed flow (M=5.48, Kn=0.05) stream conditions, in order to verify application of present DG solver in conjugation with second-order Boltzmann-based constitutive relations for studying rarefied gas flows. It is shown that application of present modal DG method for studying rarefied gas flows is valid, and results are, qualitatively and quantitatively, comparable with direct solution of Boltzmann equation.



Figure 6-18 Mach contour over a cylinder for M=0.1, Kn=0.1 (left) present DG solution, (right) DSMC solution [112].



Figure 6-19 Mach contour over a cylinder for M=5.48, Kn=0.5 (left) present DG solution, (right) DSMC solution [112].

To summarize this chapter, it has to mention that the DG methods developed for 1-D, 2-D, and 3-D is employed for solving various problems and the results were verified and validated with other numerical solutions, and experiments. These analysis give us enough trust and confidence to apply present DG method for studying the physics of rarefied flows over an arbitrary geometry in next chapter.

CHAPTER 7. Solution of the Boltzmann-based models for simple gas flows

Albert Einstein (1879-1955):

"If we knew what it was we were doing, it would not be called research, would it?"

In case that flow deviates from local thermal equilibrium state, application of the moment method into the classical Boltzmann equations leads to Boltzmann-based models where the non-conservative variables are being linearly or nonlinearly proportional to the gradient of the velocity (strain rate) and temperature (thermal strain rate) state variables. The objective of this chapter is to measure the level of accuracy of the Boltzmann-based models. Therefore, solutions of the Boltzmann-based models are compared with each other, the solution of the DSMC method, and experimental data.

One-dimensional shock structure is simulated using Boltzmann-based model and the results are compared with experiments and DSMC. Flow over a cylinder is also studied in detail. Then, a comparative analysis between different slip boundary conditions is provided using Navier-Stokes-Fourier (i.e., 1st order Boltzmann-based) equation. Finally, a flow over sphere is simulated using modal DG method.

7.1 Compression dominant flow problems: 1-D shock structure

The density solution of viscous shock structure for three different Mach stream conditions is shown in Figure 7-1. The zero-order solutions are way off from the experiment, whilst first-order and second-order Boltzmann-based models can predict the shock density profile moderately for all Mach flow conditions. It is also shown that the difference between first-order solution and experiments become noticeable for high Mach number flows, while second-order Boltzmann-based solution is very close to the experiments.



Figure 7-1 Density profile of shock structure problem for Argon gas at three different flow stream Mach numbers

The shock density thickness is known as one of the important parameters on accuracy of the models, therefore, the solution of Boltzmann-based models are compared with experimental data in Figure 7-2. It is obvious that second-order Boltzmann-based method can precisely capture the shock-density thickness for all Mach number regimes.



Figure 7-2 Computed shock density thickness of Argon gas

In case of the asymmetry of shock solution, as shown in Figure 7-3, the first-order and second-order Botlzmann-based models remain qualitatively the same, increases fo the asymmetry property Q with Mach number. In contrast, the quasi-linear generalized hydrodynamics model [223] shows a different behavior, reaching a maximum in Q and then decreasing with Mach number.



Figure 7-3 Computed shock asymmetry of Argon gas using Boltzmann-based models.

Another important parameter for analyzing shock structure problem is the distance between density and temperature profiles. Figure 7-4 demonstrates the temperaturedensity distance for Argon gas. It is shown that the second-order Boltzmann-based model provides very similar results in comparison with direct physical solution (DSMC) of Boltzmann equation.



Figure 7-4 Computed temperature-density distance of Argon gas using DSMC and Boltzmann-based models.

7.2 Multi-dimensional flow problems

In previous chapter, the present DG method was extensively verified and validated for studying flow over cylinder. It was shown that piecewise linear solution of DG method can provide very accurate results for steady-state low-speed and high-speed flows. Therefore, in the rest of the work, the piecewise linear solution of DG method will be used for studying rarefied gas flows.

7.2.1 Effects of Langmuir slip boundary condition

One of the challenging issues in simulation of rarefied flows using continuum method is to model slip effect accurately. Unfortunately, most of the explicit numerical solvers often suffer a numerical instability in case of Maxwell slip boundary condition, and therefore, development of an alternative slip model would be necessary.
In this work, Langmuir slip model is used for simulation of rarefied gas flows; therefore, special attention will be given to investigate the level of accuracy of this slip model.

The slip velocity and temperature jump values predicted by this model are highly dependent on the quantity of β and the potential D_e parameters. D_e can take various values based on the type of the molecular bonding between the gas molecules and the surface atoms. It motivates us to measure the influence of D_e parameter on slip magnitude. Figure 7-5 demonstrates the importance of D_e value on computation of slip properties, and it shows that smaller D_e value will result in bigger magnitude of slip. It also shows that the computed slip velocity using Langmuir slip boundary condition with smallest D_e value is still significantly far from DSMC solution.



Figure 7-5 Computed slip velocity profile over cylinder with flow stream of Mach 5.48, Kn=0.05 using first-order Boltzmann-based model in cooperation with Langmuir slip boundary condition for various values of De parameter.



Figure 7-6 Computed density contour over cylinder with flow stream of Mach 5.48, Kn=0.05 using first-order and second-order Boltzmann-based models in cooperation with Langmuir slip boundary condition for three different values of D_e .

Figure 7-6 presents the contour of density over cylinder with steam Mach number of 5.48. It is shown that application of slip velocity together with the first-order and second-order Boltzmann-based models results in different magnitude of slip value for these models, although the Knudsen number is not significantly high for this case. This discrepancy is due to fact that application of second-order model results in reduction of the viscous stress tensor and heat flux vector compared to first-order model, therefore, flow experiences less amount of resistance for the case of second-order Boltzmann-based model even for same value of D_e .

7.2.2 Effects of various slip boundary condition

In order to study the slip effects, it is necessary to make sure that the no-slip boundary condition is prescribed accurately. Flow over a flat plate at Mach of 4.38 and Knudsen of 0.0013 is considered as the next benchmark problem. Figure 7-7 shows that enforcing zero velocity strictly on the wall using modal DG method requires application of the high-order DG approximation. It also shows that the numerical artifacts degrade the high-order subcell solutions when inappropriate limiter function is served. Therefore, application of proper enough number of elements in the boundary layer, utilizing a proper limiter function (multi-dimensional limiters) is essential to obtain non-oscillatory world class solutions.



Figure 7-7 Computed no-slip velocity for viscous wall using modal DG method and various degree of *p* polynomial expansion.

In order to compare the effect of various slip conditions, two different set of wall boundary conditions are defined according to Section 5.5.5, and the level of accuracy of those are examined for simulation of rarefied gas flows. In the first set of wall boundary conditions, it is assumed that the normal gradient of pressure on the wall is negligible, and the normal velocity on the wall is zero. This is called the pressure-based wall boundary, whilst the density-based wall boundary, second boundary configuration, is developed based on (Eq. 5-127). In this case, first density is obtained and then the wall pressure is calculated based on updated density and temperature values.



Figure 7-8 A comparison between various slip models and viscous wall boundary conditions in computation of the slip velocity profile on the flat plate.

A comparison between DSMC slip results and modal DG solution shows that application of density-based viscous wall boundary condition provides better result than pressure-based wall boundary. Figure 7-8 also shows that the increase of the degree of polynomial expansion results in better resolution of the slip velocity on the wall. A comparison between the result generated by present modal DG using various slip condition and DSMC solution is conducted, as shown in Figure 7-12. It shows that the Karniadakis slip model [224] performs better than the other available models for this particular problem since it is a second-order slip boundary condition [203]. Next to the Karniadakis model, the generalized Maxwell, and Langmuir slip models stands

respectively. Nonetheless, all models provides a fairly accurate slip velocity prediction compared to DSMC solution.



Figure 7-9 Computed slip velocity profile on the flat plate using various slip models at M=4.38, Kn=0.0013.

The temperature predicted on the wall using Langmuir, Karniadakis, and Maxwell-Smoluchowski model are compared with DSMC, as shown in Figure 7-10. It is obvious that second-order Karniadakis model provides better result than the others; however, the Langmuir and Maxwell models provides almost similar solutions. It is reported in [203, 225] that replacing the Smoluchowski model with Paterson temperature jump model in Maxwell slip configuration may lead to better agreement with DSMC.



Figure 7-10 Computed temperature profile on the flat plate using various slip models at M=4.38, Kn=0.0013.

7.2.3 Flow over cylinder

7.2.3.1 Equilibrium state

Figure 7-11 shows the Mach contour over cylinder at M=5.48 for three Boltzmannbased solutions and direct physical solution of the Boltzmann equations. The solutions of all the Boltzmann-based models are very similar to the exact solution of the problem, due to the fact that the level on non-equilibrium for this problem is negligible. Thus the simplest Boltzmann-based model is sufficient for simulation of the bulk region, whilst application of higher-order (at least first-order) Boltzmann-based models for prediction of the boundary layer adjacent to wall is necessary. Note that, simulation of this problem using Boltzmann-based models requires only few hours, whereas DSMC method has significantly slow converge rate since it needs at least 50,000,000 representative molecules, and significantly small time step value to provide an accurate solution.



Figure 7-11 Computed Mach contour over cylinder with flow stream of Mach 5.48, Kn=0.0002

7.2.3.2 Near equilibrium state

In order to analyze performance of Boltzmann-based models near equilibrium state, flow over cylinder at Mach=5.48 and Knudsen number of 0.02 is simulated and results are shown in Figure 7-12. It is obvious that the shock thickness increases in comparison with the previous simulated case due to bigger viscous dissipation generated inside the

shock region. It is shown that the shock thickness predicted by second-order model is slightly thicker than this of the first-order model, other than that both models are performing similarly and they can provide almost similar solution compared with DSMC solution.



Figure 7-12 Computed Mach contour over cylinder with flow stream of Mach 5.48, Kn=0.02

7.2.3.3 Non-equilibrium state

In order to check the performance of Boltzmann-based models at a state considerably deviated from equilibrium state, flow over cylinder at M=5.48, Kn=0.2 is simulated. It is obvious that the increase of Knudsen parameter, will magnify the thickness of shock and boundary layer; however, it does not change the general shape of the solution formed by conservation laws. In Figure 7-13, the solution of DSMC is compared with zero-, first-, and second-order Boltzmann-based solution. It is shown that the second-order Boltzmann-based solution to the direct physical solution of Boltzmann. However, the shock thickness predicted with the Boltzmann-based models is not as thick as the predicted one by DSMC method.



Figure 7-13 Computed Mach contour over cylinder with flow stream of Mach 5.48, Kn=0.2

7.2.4 Flow over a sphere

7.2.4.1 Analytical solution of drag over sphere

The low Reynolds number isothermal gas flow past a sphere is the last problem studied. The understanding of this flow may become important when one tries to estimate the drag experienced by a microsphere subjected to unconfined low Reynolds number gas flow. Unlike the internal flows, pressure does not change significantly in external creeping flows, and density can be assumed to be constant. Thus the flow can be also described by using either the incompressible or compressible Navier–Stokes-Fourier equations with proper slip model. It is possible to extend the Stokes' analytical solution for creeping flow past a sphere [226-229] by considering the incompressible form of the conservation laws, and deriving the analytical solution of the problem based on desired slip model.

Let's consider the incompressible form of the Navier-Stokes-Fourier equations;

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{u}.$$
7-1

where μ is constant viscosity coefficient, **u** is the velocity vector, and *p* is pressure. Introducing the dimensionless variables,

$$\mathbf{u}^{*} = \frac{\mathbf{u}}{u_{ref}}, \ t^{*} = \frac{t}{L/u_{ref}}, \ \nabla^{*} = L\nabla, \ \nabla^{2*} = L^{2}\nabla^{2}, \ p^{*} = \frac{p}{\left(\mu u_{ref}/L\right)},$$
 7-2

and after removing asterisks, the dimensionless form of the equations can be written as

$$\nabla \cdot \mathbf{u} = 0,$$

Re $\frac{d\mathbf{u}}{dt} = -\nabla p + \mu \nabla^2 \mathbf{u}.$ 7-3

For small Reynolds number $(Re \ll 1)$, the inertia term on the left-hand side of the momentum equation can be neglected, therefore reduced equations, so-called Stoke's equation, are given by

$$\nabla \cdot \mathbf{u} = 0,$$

$$\nabla p = \mu \nabla^2 \mathbf{u}.$$
7-4

Now let us consider a stationary solid microsphere of radius R in an unbounded incompressible monatomic gas flow. The infinitely far from the sphere is of uniform flow with speed of U_{∞} . Owing to the symmetry in the flow direction, (Eq. 7-4) can be written in the spherical coordinates (r, ϕ) as,

$$\frac{\partial u_r}{\partial r} + \frac{1}{r} \left(\frac{\partial u_{\phi}}{\partial \phi} + 2u_r + u_{\phi} \cot \phi \right) = 0,$$

$$\frac{\partial p}{\partial r} = \mu \left(\nabla^2 u_r - \frac{2}{r^2} \frac{\partial u_{\phi}}{\partial \phi} - \frac{2u_r}{r^2} - \frac{u_{\phi} \cot \phi}{r^2} \right),$$

$$\frac{1}{r} \frac{\partial p}{\partial \phi} = \mu \left(\nabla^2 u_{\phi} + \frac{2}{r^2} \frac{\partial u_r}{\partial \phi} - \frac{u_{\phi} \cot \phi}{r^2 \sin^2 \phi} \right),$$

$$re \nabla^2 = \frac{\partial^2}{\partial \phi} + \frac{2}{r^2} \frac{\partial}{\partial \phi} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi} + \frac{\cot \phi}{r^2 \sin^2 \phi} = \ln \text{ these expression } r \phi \text{ denotes the radiu}$$

where, $\nabla^2 \equiv \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} + \frac{\cot \phi}{r^2} \frac{\partial}{\partial \phi}$. In these expression, r, ϕ denotes the radius

and cone angle in spherical coordinates. To account the analysis the slip effects near the sphere surface, the governing equation (Eq. 7-5) are solved in conjunction with slip velocity boundary condition:

$$u_{\phi} = u_{\phi_{slip}}, \text{ at } r = R, \quad 0 \le \phi \le \pi$$
 7-6

No flow should penetrate inside the wall and also flow at the far field boundary should be taken as the reference value, therefore,

$$u_r = 0$$
, at $r = R$, $0 \le \phi \le \pi$
 $u_r = U_\infty \cos \phi$, $u_\phi = -U_\infty \sin \phi$, $p = p_\infty$ at $r \to \infty$.
7-7

The only remaining task is to determine slip velocity on the wall. For Maxwell slip model, the slip velocity boundary condition can be written [206] as

$$u_{\phi_{slip}} = -\frac{\sigma}{\mu} \frac{Kn}{2R} \left[\Pi_{r\phi} \right]_{r=R},$$
7-8

where σ is the tangential momentum accommodation coefficient (TMAC). Therefore, the solution of governing (Eq. 7-5) can be obtained using the method of separation of variables and employing (Eq. 7-7) and (Eq. 7-8) such that

$$u_{r} = U_{\infty} \cos \phi \left[1 + k_{1} \left(\frac{R}{r} \right) + k_{2} \left(\frac{R}{r} \right)^{3} \right]$$

$$u_{\phi} = -U_{\infty} \sin \phi \left[1 + \frac{k_{1}}{2} \left(\frac{R}{r} \right) - \frac{k_{2}}{2} \left(\frac{R}{r} \right)^{3} \right],$$

$$p = p_{\infty} + \frac{1}{r} k_{1} \mu R U_{\infty} \cos \phi,$$
where $k_{1} = -\frac{3}{2} \frac{(1 + 4\sigma Kn)}{(1 + 6\sigma Kn)}, \quad k_{2} = \frac{1}{2(1 + 6\sigma Kn)}.$

$$7-9$$

As total drag on the microsphere is a combination of three components, namely, skin friction drag, normal stress drag and pressure drag

$$Drag_{total} = [Drag]_{skin-friction} + [Drag]_{normal-stress} + [Drag]_{presure}.$$
 7-10

The total drag can be expressed in terms of pressure and stress forces as

$$\operatorname{Drag}_{\operatorname{total}} = 2\pi R^2 \left[\int_{0}^{\pi} \prod_{r\phi} \Big|_{r=R} \sin^2 \phi d\phi + \int_{0}^{\pi} \left[-\prod_{rr} \right]_{r=R} \sin \phi \cos \phi d\phi + \int_{0}^{\pi} \left[-p \right]_{r=R} \sin \phi \cos \phi d\phi \right]$$
 7-11

where the shear stress and normal stress are given as

$$\Pi_{r\phi} = -\mu \left(\frac{1}{r} \frac{\partial u_r}{\partial \phi} - \frac{1}{r} u_{\phi} + \frac{\partial u_{\phi}}{\partial r} \right).$$

$$7-12$$

$$\Pi_{rr} = -2\mu \frac{\partial u_r}{\partial r}$$
7-13

Note that there is a contrinution in drag due to viscous normal stress. From the relations (Eq. 7-9) and (Eq. 7-11), a coefficient of the total drag obtained by Maxwell slip model can be derived as

$$\left[C_{D}\right]_{Maxwell} = \frac{24}{2\rho U_{\infty}R/\mu} \left(\frac{1+4\sigma Kn}{1+6\sigma Kn}\right)$$
7-14

The next available slip model is Langmuir slip model which describe the slip velocity on the wall [206] as

$$u_{\phi_{slip}} = \frac{u_{\phi}\left(r = eR\right)}{1 + \overline{\beta}},$$
7-15

where

$$\overline{\beta} = \frac{1}{4\omega Kn}, \quad \omega = \frac{\sqrt{32}\sigma_{N_{\delta}}^2}{\pi^{3/2}} \exp\left(-\frac{D_e}{k_B T_w}\right) \left(\frac{T_w}{T_r}\right)^{s+1/2}, \quad s = \frac{1}{2} + 2/(\upsilon - 1), \quad \sigma_{N_{\delta}} = \frac{\sqrt[4]{mk_B T_{ref}}}{2d\sqrt{\mu_{ref}}}, \quad \text{and}$$

 $1 < e < \infty$. Applying the method of separation of variables similar to Maxwell slip model, and using (Eq. 7-15) and (Eq. 7-16) the solution of governing (Eq. 7-5) differ only in the expression of the constants k_1 and k_2 which are given as

$$k_{1} = \frac{e^{-3} - 1 - 3\overline{\beta}}{2(\overline{\beta} + 1 - E)}, k_{2} = \frac{e^{-1} - 1 + \overline{\beta}}{2(\overline{\beta} + 1 - E)},$$
7-16

with $E = \frac{1}{2} (e^{-1} + e^{-3})$. Accordingly, the total drag coefficients using Langmuir slip model can be obtained as

$$\left[C_{D}\right]_{Langmuir} = \frac{24}{2\rho U_{\infty}R/\mu} \left(\frac{\overline{\beta} + \left(1 - e^{-3}\right)/3}{\overline{\beta} + 1 - E}\right).$$
7-17

In case of choosing free stream velocity as reference velocity of the Langmuir slip model or taking $e \rightarrow \infty$, then with $\overline{\beta} = \frac{1}{4\omega Kn}$, the drag coefficient reduces as

$$\left[C_{D}\right]_{Langmuir} = \frac{24}{2\rho U_{\infty}R/\mu} \left(\frac{1+4\omega Kn/3}{1+4\omega Kn}\right)$$
7-18

In case of choosing free stream velocity as reference velocity of the Langmuir slip model or taking $e \rightarrow \infty$, then with $\overline{\beta} = \frac{1}{4\omega Kn}$, the drag coefficient reduces as

$$\left[C_{D}\right]_{Langmuir} = \frac{24}{2\rho U_{\infty}R/\mu} \left(\frac{1+4\omega Kn/3}{1+4\omega Kn}\right) = \left[C_{D}\right]_{no-slip} \left(\frac{1+4\omega Kn/3}{1+4\omega Kn}\right),$$
7-19

where $[C_D]_{no-slip} = \frac{24}{2\rho U_{\infty}R/\mu}$.

7.2.4.2 Numerical simulation of flow over sphere

The results obtained for second-order Boltzmann-based model using the 3-D modal DG method are compared with direct physical solution of Boltzmann equation at Mach of 5.48 and Knudsen of 0.05. In this low Knudsen number flow condition, there is a recirculating region behind the sphere which is captured properly by present DG method, as shown in Figure 7-15. Next step, is to compare the results of Boltzmann-based models with DSMC solution at the same flow condition. It is shown in Figure 7-14 that application of Langmuir slip boundary condition with proper

adjustment of D_e value in cooperation with second-order Boltzmann-based constitutive model may lead to acceptable resolution of the flow field compared with DSMC.





Direct simulation of Boltzmann

Figure 7-14 Computed density and Mach contours over a sphere with flow stream of Mach 5.48, Kn=0.05 using second-order Boltzmann-based model in cooperation with Langmuir slip boundary condition and direct simulation of Monte Carlo (DSMC).



Figure 7-15 Flow behind a sphere at M=5.48, Kn=0.05



Density contour Mach contour First-order Boltzmann-based model



Density contour Mach contour Second-order Boltzmann-based model



Figure 7-16 shows the density and Mach contour distribution for solution of the firstorder and second-order Boltzmann-based constitutive relations at M=5.48. There is no significant difference between solutions of these two models since the degree of nonequilibrium is negligible. It is shown that the degree of non-equilibrium for threedimensional problems, is much smaller than two-dimensional flows due to extra spatial coordinate and extra degree of freedom given to flow for movement in the flow field. Nevertheless, it is obvious in Figure 7-18 that once flow becomes so much rarefied the difference between first-order and second-order Boltzmann-based constitutive relations becomes sensible. In order to investigate the performance of second-order Boltzmannbased models in higher Knudsen number, it is necessary to improve the slip boundary condition, employ very small time steps, and reduce the computational cost using paralleled DG code which is the future work of the present study.



Density contour Mach contour First-order Boltzmann-based model



Density contour Mach contour Second-order Boltzmann-based model

Figure 7-17 Computed density and Mach contours over a sphere with flow stream of Mach 0.1, Kn=0.04 using first-, and second-order Boltzmann-based model in cooperation with Langmuir slip boundary condition.



Density contour Mach contour First-order Boltzmann-based model



Second-order Boltzmann-based model

Figure 7-18 Computed density and Mach contours over a sphere with flow stream of Mach 0.1, Kn=0.4 using first-, and second-order Boltzmann-based model in cooperation with Langmuir slip boundary condition.

CHAPTER 8. Parallelization

Jalaluddin Rumi (1207-1273):

"Stop acting so small. You are the universe in ecstatic motion."

One of the challenging issues in the discontinuous Galerkin (DG) methods is the higher computational cost compared with the traditional finite volume method (FVM) for a given set of grids. In the present chapter, the focus is on the computational cost of the modal DG method for solving the conservation laws in conjunction with the first-and second-order constitutive laws. The computational cost of the Navier-Stokes-Fourier (NSF) and second-order Boltzmann-based model is investigated in the serial and parallel frameworks.

In DG methods, an arbitrarily high-order approximate solution can be achieved by increasing the degree of polynomial expansion in least square finite element space. Due to this locality feature of DG method and compactness of the stencils, parallelization of DG method is very promising. As parallelization is one of DG most enticing features, a considerable amount of research has been directed to study parallelization techniques, implementations of parallel techniques, and measure the performance of paralleled DG method for hyperbolic conservation law [152, 165, 185, 230, 231]. Biswas et al. [152] applied a third-order quadrature-based DG method to solve a scalar wave equation which was one of the early works on DG parallelization. Bey et al. [230] implemented an effective parallel algorithm based on hp-adaptive discontinuous Galerkin approximation of linear, scalar, hyperbolic conservation laws on structured grids. They obtained nearly optimal speedup in case that the ratio of interior elements to subdomain interface elements is sufficiently large. Baggag et al. [231] applied a parallel implementation of the discontinuous Galerkin method for time-dependent simulations based on unstructured grids. Hong Luo [185] implemented a parallel, reconstructionbased discontinuous Galerkin method for the solution of the compressible Navier-Stokes equations on arbitrary grids using domain partitioning and single program multiple data (SPMD) parallel programming model. Recently, Landmann et al. [165] implemented an efficient parallel algorithm on high-order discontinuous Galerkin code

for laminar and turbulent flows. Nevertheless, a very few parallel DG researches is available in the study of rarefied gas flows [232]. In present work, a single program multiple data (SPMD) parallel model using a message-passing-interface (MPI) library was employed to parallelize the present mixed modal DG method for solving rarefied gas flow problems.

There are several sources for higher computational cost of a DG methods in comparison with the traditional FVM methods for a given set of grids. An obvious source of additional cost is the increase in degree of freedom associated with extra numerical calculation at every Gaussian quadrature point located inside of the elements. Application of mixed-DG formulation (for LDG, BR1 schemes) is another source, because the it requires extra sets of equations for every degree of freedom of the primary and auxiliary variables, resulting in a system of equations with more unknowns for an equal number of elements, compared to continuous Galerkin method or high-order finite volume method. Further, additional cost is incurred when solving the high-order constitutive models are solved with conservation laws, where the computational cost is a nonlinear function of the physics of the problem.

In the following, the parallelization of the DG method for the first-order model (NSF) is explained in detail. The speed-up and efficiency of the DG method for piecewise constant and higher-order polynomial approximate solutions are then reported. Finally, the computational cost of the second-order Boltzmann-based model is compared with that of the NSF model for both serial and parallel solvers.

8.1 Background

DG method is compact and highly parallelizable due to the local nature of the discretization. The solution is approximated independently in each element, where inter-element data sharing is only needed among the face neighbor elements (elements sharing a common face) to calculate numerical fluxes. Therefore, *inter-process communication* is only required between the corresponding neighboring processes for the computations at partition boundary faces (i.e., faces having their *left* and *right* elements with different processes). In this work, a single program multiple data (SPMD) parallel model using a message-passing-interface (MPI) library was employed to

parallelize the present mixed modal DG method. The MPI library guarantees the maximal flexibility of the parallel programming, portability, and scalability of the distributed memory parallel architectures [233]. A shell program was developed to unify all the parallel processing steps, as illustrated in Figure 8-1.



Figure 8-1 Illustration of unified shell program for parallel processes.

The software setup including MPICH (i.e., a high-performance and widely portable implementation of the MPI standard) and 64-bit compilers with double precision accuracy was used for all the floating point operations. Moreover, a Linux cluster sharable among multiple users was established using Intel Xenon processors with ten cores at each node. This cluster is equipped with eighty cores interconnected by dual port Gigabit Ethernet. The steps in the parallelization of the DG solver for rarefied gas flows including domain decomposition, communication process, merging of sub-domains and parallel performance measurements are described in the following subsections.

8.2 Domain decomposition

Mesh partitioning is the first step in the parallel programming, where the computational domain is decomposed into several sub-domains and then individual sub-domains are assigned to each processor. Decomposition of the domain into several sub-domains was done using open source software, ParMETIS [234]. ParMETIS is an MPI-based parallel library that implements a variety of algorithms for computing fill-reducing orderings of sparse matrices, and partitioning of the unstructured graphs. It decomposes the given mesh such that each processor has approximately the same number of elements, which balances the load for the processors and the number of links cut by the decomposition is minimized. This feature is crucial to minimizing communication among the processors [234]. After the decomposition of the domain, the partitioned results, including the node and element connectivity information, are

assigned to the processors. The sub-domains generated by ParMETIS for the case of flows around a cylinder and a sphere are shown in Figure 8-2.



Figure 8-2 Triangular mesh partition using ParMETIS.; different colors represent subdomains owned by different processors.

8.3 Communication process

The present parallel solver is based on a single program, multiple data (SPMD), which executes the same program in all processors with different data. The SPMD model can manage the processors to conditionally execute only certain parts of the program. Therefore, some of the processors may not necessarily need to execute the entire program. The parallelization was achieved without compromising the serial algorithm for the purpose of higher parallel performance. Moreover, the present parallel algorithm allows the MPI communications to completely overlap with the computations. This type of algorithm is usually referred to as hiding communication behind computation, which is easier to achieve in explicit time marching schemes [231] as summarized in Figure 8-3.

The point-to-point communication methodology of MPI was used such that the message passing operation may only occur between two different processors. While one processor is performing a *send* operation, the other processor performs a matching *receive* operation. There are various types of *send* and *receive* routines that are available in MPI point-to-point communication. Either blocking or non-blocking routines are often used in the SPMD model due to their flexibility and for the sake of implementation. Both communication methods use a buffer to avoid data loss and

confusion during the transmission of data from one processor to another. Hence, data will be copied to the buffer before it is received by the partner processor. A buffer is a region of memory storage designed to temporarily store data during the communication process.



Figure 8-3 Flow chart of DG parallel algorithm.

In the blocking *send* and *receive* routines, the *send* routine will only return (block) after the completion of communication. Hence, computations cannot be done by the respective processors involved in communication until the process is completed. On the contrary, non-blocking communication functions return immediately (i.e., do not block) even if the communication is not finished. While using non-blocking communications, care should be taken to use the proper *wait* comment, to see whether the communication has finished or not. Non-blocking communications are primarily used to overlap computation with communication and exploit possible performance gains.

The communication module of the DG solver starts working by sending data (adjacent to partition boundaries) to neighbor partitions and this is followed by

receiving data from a corresponding neighbor. These communications should be repeated for each of the Gaussian quadrature points on the element boundaries. However, the number of Gaussian quadrature points will increase with the increasing order of accuracy of the DG approximation. As a result, the amount of data communication will also increase as the DG order of accuracy increases, as shown in Figure 8-4.



Figure 8-4 Data communication through Gaussian quadrature points for (a) DG piecewise constant scheme, and (b) DG higher-order approximation (data package is the solution information.).

Non-blocking sending and receiving were used in the parallelization in order to save processor waiting time and avoid deadlock. Therefore, the application of MPI_CHECK and MPI_WAIT was essential to confirm the completion of communication without data loss. These operations were started by calling standard MPI routines, MPI_ISEND and MPI_IRECV. Furthermore, the MPI_WAITALL routine was used to ensure the completion of the communication process. Once communication was completed, the data received from the neighboring processors were used for further computations.

8.4 Merging of sub-domains

During the parallel computations, all the partitioned sub-domains execute the same DG solver with respective data inputs and solve the flow fields in their local domain. After the solution converges, each of the processors plots its solution for post-processing purposes. However, it is noticeable in Figure 8-5 that the results are visually not smooth at the boundaries of the sub-domains due to biased interpolation of the solution and as a result of not considering all vertex neighborhoods for interpolations. The merging subroutine is designed for better analysis and post-processing of the DG

paralleled solution. In this subroutine, all subdomain results were exported into a unified single domain for better visualization and there is no other purpose behind this subroutine. The DG approximate solutions are sought in the finite element space and then solution at any point inside the computation cell can be calculated by summing up the product of moment of the solution and basis function. Although each element contains their individual solutions, in order to post processing purpose the solution have to be interpolated to the node in commercial software like Tecplot.



Figure 8-5 Pressure contour of unmerged sub-domains.



Figure 8-6 Merging of the sub-domains for post-processing of the solutions; Pressure contour of unified merged domain.

So the biased interpolation, without considering all the neighbors of the node, results in poor numerical visualization. In order to avoid this discrepancy merging of subdomains is necessary. In order to avoid this discrepancy, the merging of subdomains was performed for post processing after terminating parallel processing, as demonstrated in Figure 8-6 Moreover, as the space polynomial function is defined in least square space and the solution in each DG element is calculated locally, the results are not depending on number of processors.

8.5 Parallel performance measurement

The measurement of parallel computation is essential for assessing the efficiency and applicability of the parallel solver. Generally, parallel performance is measured by relative speed-up, relative efficiency or scalability [235]. The definition of speed-up (S_p) was established by Amdahl's law [236]. According to this law, it is a metric for the relative improvement in performance when executing a task. However, speed-up can be used more generally to show the effect of any performance enhancement. The relative speed-up is given by

$$S_p = \frac{t_s}{t_p},$$
8-1

where S_p is speed-up, t_s and t_p denote the elapsed time taken by a *single* processor and p processors, respectively. Relative efficiency (*E*) is a metric of the utilization of the resources of the improved parallelized system read as

$$E = \frac{S_p}{p}.$$
 8-2

A performance analysis indicates the level of speed-up and efficiency of the parallel solver. Speed-up of the code varies with the increase in the number of processors for a fixed problem size. Linear speed-up usually remains less than p, and efficiency lies between 0 and 1. In ideal cases, elapsed time taken by p processors is equal to $t_p = t_1/p$, relative speed-up is equal to $S_p = p$, and relative efficiency is equal to E = 1.

8.6 Computational cost of Boltzmann-based models

Figure 8-7 shows the global computational cost of Boltzmann-based constitutive models measured empirically using serial modal DG solvers for various cases with different numbers of elements. It can be seen that the computational cost of 2nd order model does not change linearly with respect to the number of elements either for piecewise constant or piecewise linear polynomial approximations. In fact, the numerical experiment shows that the computational cost of the 2nd order Boltzmann-based model increases exponentially with the increasing number of elements, and it is higher than that of 1st order model for all cases. Moreover, the computational cost of the piecewise linear DG approximation is considerably higher than that of the piecewise constant approximation as expected. This is because, for higher-order DG

approximation, extra efforts are needed to obtain solution at added Gaussian quadrature points on the element interfaces, and inside the volume of the elements.



Figure 8-7 Computational cost of solving Boltzmann-based constitutive models.

8.7 Parallel performance of Boltzmann-based models

Figure 8-8 illustrates the speed-up of the piecewise constant and higher-order DG approximations for elements ranging from 4,000 to 200,000, and with a range of processors from 1 to 64. The plots indicate that the speed-up increases almost linearly as the number of processors increases, and the speed-up is enhanced in the case of higher-order approximations. Figure 8-9 shows the relative efficiency of the parallel code for piecewise constant and higher-order DG approximations, respectively. The communication overload increases as the number of processors increases, and, as a result, the required run-time for communication between processors becomes comparable to the computational time of the simulations, for cases with a smaller number of elements. Hence, the speed-up and parallel efficiency are higher for cases with larger numbers of elements (200,000) and processors (64). Moreover, the speedup of the higher-order scheme is substantially higher than that of the piecewise constant scheme due to the reduction in communication overload between processors in comparison with the numerical computation overload. Overall, the present results demonstrate that the higher-order DG schemes are highly parallelizable and a better choice for parallelization.



Figure 8-8 Parallel speed-up S_p for 1st order Boltzmann-based model: (left) DG piecewise constant scheme, and (right) DG higher-order scheme.



Figure 8-9 Parallel relative efficiency, *E*, for 1st order Boltzmann-based model: (left) DG piecewise constant scheme, and (right) DG higher-order scheme.

Figure 8-10 depicts the rate of cost reduction in the parallel Boltzmann-based models. In the ideal case, according to Amdahl's law, it is expected a linear reduction of computational cost for paralleled DG solver, which is barely never happens. For 1st order linear constitutive model, computational cost reduces linearly but not optimally which is compatible with the Amdahl's law [236]. For second-order model, however, the computational cost reduces with very fast rate, almost exponentially, as the number of processors increases. This super-parallel performance is due to the nonlinear behavior of the model, which demands less computational effort for *smaller* numbers of elements. Therefore, decomposing the domain into several sub-domains will boost the performance of 2nd order Boltzmann-based model.



Figure 8-10 Comparison analysis on parallel performance of modal DG solver for Boltzmann-based models: (left) rate of cost reduction (right) normalized computational cost.

Figure 8-10 also shows the normalized computational cost of the parallel Boltzmann-based models for different numbers of processors. It is reported that the cost of the 2nd order Boltzmann-based model reduces with a much higher rate than that of the 1st order model, for both the piecewise constant and higher-order approximations. In summary, because of the super-parallel performance associated with the nonlinear behavior of the cost, the second-order Boltzmann model has higher potential for parallelization than the 1st order Boltzmann-based model.

CHAPTER 9. Conclusion and Recommendations

Arnold Sommerfeld (1868-1951):

"Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you anymore."

9.1 Outlook

The application of Boltzmann-based constitutive models to the study of gas flows has been considered in this work. Starting from Eu's moment equations for monatomic gases derived in the framework of irreversible thermodynamics, the origin of the Boltzmann-based models, in particular, the second-order models based on the balanced closure, was described in detail. It was shown that application of these constitutive models in conjunction with the conservation laws provides valuable insight into the study of gas flows, while their computational cost may be considerably higher than conventional classical first-order linear constitutive relations. The complete set of the constitutive models for one-, two-, and three-dimensional flows were provided, and their characteristics were investigated for a wide range of the thermodynamic forces, viscous stress and heat flux. Interestingly, it has been shown that the computational cost of the second-order Boltzmann-based model can be significantly reduced by employing parallel algorithms, owing to a super-parallel performance of the NCCR solver of the second-order Boltzmann-based model.

Further, the discontinuous Galerkin method has been extensively studied as the basic numerical scheme for solving the Boltzmann-based models. It is shown that the DG method is suitable for solving the conservation laws together with the Boltzmann-based constitutive models. The mixed type DG methods were developed for solving onedimensional and multi-dimensional problems, and they were verified for both smooth and stiff flow problems. The solutions of DG method were compared with analytical and other numerical solutions, DSMC, and experimental data. The error norm analysis was conducted on global, conserved, and non-conserved variables, and the performance of various limiters and flux functions was comprehensively examined. A new differentiable limiter proposed for the DG method was also tested for several benchmark problems. It was observed that selection of proper limiter function and viscous numerical flux function plays a critical role in obtaining accurate DG solutions. It was also found that in case of highly rarefied gas flows, sub-parametric mapping for curved boundaries has little influence on the accuracy of solution and, consequently, a simple linear mapping may be used.

In case of high speed and low Reynolds flows, it was shown that the local DG method is preferred for discretizing viscous fluxes than other DG methods. The order of accuracy of the present DG method is proved to be p+1 for smooth flow problems, while the accuracy for stiff flow problems is shown to be highly sensitive to the choice of the limiters, and numerical flux functions, in particular, viscous flux functions. Several boundary value problems has also been studied using the DG method; forward facing step flow, backward facing step flow, double Mach reflection, one- and twodimensional Riemann problems, and external flow over sphere and cylinder. It was found that solutions of the second-order Boltzmann-based models are always in better agreement with DSMC data than the classical first-order linear model and appropriate slip/jump boundary conditions remain essential for studying rarefied and microscale gas flows.

Finally, a comprehensive review of the DG methods, including limiter functions, numerical flux functions, boundary conditions, and curved boundary effects, was given to explain various numerical aspects of the DG method.

9.2 Future works

After having developed a mixed explicit modal DG method for the conservation laws in conjunction with the first- and second-order Boltzmann-based constitutive relations, the following topics may be considered as future work.

No-slip/slip boundary treatment for high speed flows

As discussed in Chapter 5, implementation of no-slip wall boundary for compressible gas flows is not straight ward. There are still unsolved issues in the accurate treatment of conservative variables on solid wall. The next step in development of more accurate DG solver may be a study on improvement of slip/no-slip boundary conditions.

Curved boundary treatment

In order to provide a unified DG solver for all flow regimes, it is essential to prescribe the solid wall boundary of the geometry accurately. Therefore, extension of the present solver to curved boundary case may be considered as an important topic.

WENO limiter

Recently, a compact and highly accurate WENO limiter was introduced. It was known to perform better than other limiters for smooth and stiff flow problems. It is worth developing a new WENO-type limiter for multi-dimensional DG solvers.

Study on validity of the second-order Boltzmann-based model for various Mach and Knudsen numbers

To identify the range of application of the second-order Boltzmann-based models, comprehensive studies may be conducted for various Mach and Knudsen numbers from simple monatomic gas to diatomic gases. As the degree of non-equilibrium increases, the classical linear Boltzmann-based model breaks down. It is interesting to examine the range of validity of the second-order Boltzmann-based models.

Improvement of the robustness of numerical solver for studying viscousdominated problems using the second-order Boltzmann-based model

As the Mach number increases, the stability of numerical solver may be reduced due to appearance of spurious oscillations near boundaries and discontinuities. Moreover, in case of highly rarefied flows near vacuum condition, very small variation in pressure or density may violate the positivity-preserving property of numerical solver. Hence, it is necessary to further improve the stability of the DG solver for studying high nonequilibrium flows.

APPENDIX A. Vector and tensor calculus

Albert Einstein (1879-1955):

Anyone who has never made a mistake has never tried anything new

Unit vectors

Let's define unit vectors e and its derivatives as following,

$$\boldsymbol{e} = \left(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\right) = \left\{ \begin{bmatrix} 1\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\1\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1 \end{bmatrix} \right\}.$$
 A - 1

The Kronecker Delta function δ_{ij} can be defined as

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwaise} \end{cases}.$$
 A - 2

It also can be written in terms of unit vectors as

$$e_i \cdot e_j = \delta_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
 A - 3

The cross product of two unit vectors can be written as a permutation (Levi-Civita) tensor

$$e_i \times e_j = \varepsilon_{ijk} e_k = \begin{cases} 1 & \text{for even permuations} \\ -1 & \text{for odd permutations} \\ 0 & \text{for any repeated index} \end{cases}$$
 A - 4

Vector definition

Now, If **u** and **v** are vectors such as

$$\mathbf{u} = (u_1, u_2, u_3)^T, \qquad A - 5$$
$$\mathbf{v} = (v_1, v_2, v_3)^T.$$

The vector **u** can be defined in terms of unit vector as

$$\mathbf{u} = \sum_{i} u_{i} e_{i} = u_{1} e_{1} + u_{2} e_{2} + u_{3} e_{3} = u_{1} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + u_{2} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + u_{3} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$
 A - 6

Product operators

228

7

Inner product of two vector is defined as

$$\mathbf{u}.\mathbf{v} = u_i v_i = (u_1 v_1 + u_2 v_2 + u_3 v_3).$$

The cross product of two vectors can be written as

$$\mathbf{w} = \mathbf{u} \times \mathbf{v} = u_i e_i \times v_j e_j = u_i v_j \left(e_i \times e_j \right) = u_i v_j \varepsilon_{ijk} e_k.$$
 A - 8

The area covered by two vector can be obtained using norm of the cross product of two vectors

Area =
$$|\mathbf{u} \times \mathbf{v}| = \sqrt{(\mathbf{u}_2 \mathbf{v}_3 - \mathbf{u}_3 \mathbf{v}_2)^2 + (\mathbf{u}_3 \mathbf{v}_1 - \mathbf{u}_1 \mathbf{v}_3)^2 + (\mathbf{u}_1 \mathbf{v}_2 - \mathbf{u}_2 \mathbf{v}_1)^2}$$
. A - 9

The volume formed by three vectors can be calculated by

Volume = Area.w =
$$|\mathbf{u} \times \mathbf{v}|$$
.w = $|\mathbf{u} \times \mathbf{v}||\mathbf{w}|\cos\beta$. A - 10

Normal vector

Let's $\mathbf{n} = (n_1, n_2, n_3)$ denotes the normal vector on a surface, then it is possible to write dyadic product of two normal vectors $\mathbf{n} \otimes \mathbf{n}$ as

$$\mathbf{n} \otimes \mathbf{n} = \mathbf{n} \mathbf{n}^{T} = \begin{bmatrix} n_{1}n_{1} & n_{1}n_{2} & n_{1}n_{3} \\ n_{2}n_{1} & n_{2}n_{2} & n_{2}n_{3} \\ n_{3}n_{1} & n_{3}n_{2} & n_{3}n_{3} \end{bmatrix} = \begin{bmatrix} n_{1}^{2} & n_{1}n_{2} & n_{1}n_{3} \\ n_{2}n_{1} & n_{2}^{2} & n_{2}n_{3} \\ n_{3}n_{1} & n_{3}n_{2} & n_{3}^{2} \end{bmatrix}.$$
 A - 11

Tensor definition

A scalar value is a zero-order tensor, and a vector is first-order tensor. Nevertheless, the lowest-order tensor which generally describes a tensor characteristics is second-order tensor. A second-order tensor \mathbf{A}_{ij} has 9 components, a third order tensor \mathbf{A}_{ijk} has 27 quantities, and fourth-order tensor \mathbf{A}_{ijkl} has four indices with 81 components. The most useful tensor used in fluid and solid mechanics is the second-order stress tensor which is defined as

$$\mathbf{\Pi} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix}.$$
 A - 12

The tensor Π can be defined in terms of unit vector as

$$\mathbf{\Pi} = \sum_{j=1}^{3} \sum_{i=1}^{3} \mathbf{\Pi}_{ij} e_i \otimes e_j.$$
 A - 13

The addition of two tensor is a tensor of a the same rank

$$\mathbf{\Pi} + p\mathbf{I} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} + \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix} = \begin{bmatrix} \Pi_{11} + p & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} + p & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} + p \end{bmatrix}.$$
 A - 14

In index notation, we would write

$$\mathbf{\Pi} + p\mathbf{I} = \Pi_{ij} + p\delta_{ij}.$$
 A - 15

Product of a vector and a tensor

The product of a tensor Π and a vector **u** is a vector as

$$\mathbf{v} = \mathbf{\Pi} \cdot \mathbf{u} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} \Pi_{11}u_1 + \Pi_{12}u_2 + \Pi_{13}u_3 \\ \Pi_{21}u_1 + \Pi_{22}u_2 + \Pi_{23}u_3 \\ \Pi_{31}u_1 + \Pi_{32}u_2 + \Pi_{33}u_3 \end{bmatrix}, \quad \mathbf{A} - \mathbf{16}$$

or simply in index notation forms

$$v_i = \prod_{ij} u_j.$$
 A - 17

The product of $\Pi.\mathbf{u} \neq \mathbf{u}.\Pi$, therefore,

$$\mathbf{v} = \mathbf{u}.\mathbf{\Pi} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} = \begin{bmatrix} \Pi_{11}u_1 + \Pi_{21}u_2 + \Pi_{31}u_3 \\ \Pi_{12}u_1 + \Pi_{22}u_2 + \Pi_{32}u_3 \\ \Pi_{13}u_1 + \Pi_{23}u_2 + \Pi_{33}u_3 \end{bmatrix}.$$
 A - 18

Alternatively, using index notation

$$v_j = u_i \Pi_{ij}.$$
 A - 19

As a result, the traction of stress tensor on normal vector \mathbf{n} is defined as

$$\mathbf{t} = \mathbf{n} \cdot \mathbf{\Pi} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \cdot \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} = \begin{bmatrix} \Pi_{11}n_1 + \Pi_{12}n_2 + \Pi_{13}n_3 \\ \Pi_{21}n_1 + \Pi_{22}n_2 + \Pi_{23}n_3 \\ \Pi_{31}n_1 + \Pi_{32}n_2 + \Pi_{33}n_3 \end{bmatrix}.$$
 A - 20

Transpose of a tensor

The transpose of a tensor is defined so that

$$\mathbf{\Pi}^{Transpose} = \mathbf{\Pi}_{ji}, \qquad \qquad \mathbf{A} - 21$$

$$\mathbf{u}.\mathbf{\Pi}^{Transpose} = \mathbf{\Pi}.\mathbf{u}. \tag{A - 22}$$

It is obvious that the columns and rows of the tensor are switched by transpose operator. Using transpose operator it is possible to write $(\mathbf{\Pi}.\nabla \mathbf{u})^{Transpose} = \nabla \mathbf{u}^{Transpose} .\mathbf{\Pi}^{Transpose}$.

Dyadic operator

One way to construct a tensors is to use of the dyadic operator. The dyadic product of two vectors can be defined as following,

$$\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}^{T} = \begin{bmatrix} u_{1} \\ u_{2} \\ u_{3} \end{bmatrix} \begin{bmatrix} v_{1} & v_{2} & v_{3} \end{bmatrix} = \begin{bmatrix} u_{1}v_{1} & u_{1}v_{2} & u_{1}v_{3} \\ u_{2}v_{1} & u_{2}v_{2} & u_{2}v_{3} \\ u_{3}v_{1} & u_{3}v_{2} & u_{3}v_{3} \end{bmatrix}.$$
 A - 23

Note that the dyadic product of two vectors is shown by $\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}^T$. Nevertheless, many papers are showing it as $\mathbf{u}\mathbf{v}$ which is not mathematically correct!

A third/fourth-order tensor can be derived from a dyadic product of three/ four vectors as

$$\mathbf{A}_{ijk} = \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w} = u_i v_j w_k, \qquad \qquad \mathbf{A} - 24$$

$$\mathbf{A}_{ijkl} = \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w} \otimes \mathbf{y} = u_i v_j w_k y_l.$$
 A - 25

Gradient operator

A scalar has no directional dependence while it can be heterogeneous, which means that it can vary from point to point within a body. The gradient of scalar variable $(\nabla \phi)$ shows how a scalar value changes in physical space, and it is a vector quantity given by

grad
$$\phi = \frac{\partial \phi}{\partial x_i} e_i = \frac{\partial \phi}{\partial x_1} e_1 + \frac{\partial \phi}{\partial x_2} e_2 + \frac{\partial \phi}{\partial x_3} e_3.$$
 A - 26

The gradient of vector $(\nabla \cdot \mathbf{u})$ is a second rank tensor and is defined as

grad
$$\mathbf{u} = \nabla \otimes \mathbf{u} = \nabla_j u_i = \frac{\partial u_i}{\partial x_i} e_i \otimes e_j.$$
 A - 27

It can also be written as

$$\operatorname{grad} \mathbf{u} = \nabla \otimes \mathbf{u} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{bmatrix}^{\operatorname{in Cartesian coordinate}} \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}.$$
 A - 28

The divergence of a vector which physically measure the net flux of a quantity through a surface can be defined mathematically as

$$div \mathbf{u} = \nabla \mathbf{u} = \frac{\partial u_i}{\partial x_i} e_i \cdot e_j = \frac{\partial u_i}{\partial x_i} \delta_{ij} = \frac{\partial u_i}{\partial x_i}.$$
 A - 29

In general, the gradient operator creates a higher ranked tensor from the entities while the divergence creates a lower ranked tensor from the same entities. The gradient of a second-order tensor is defined as

grad
$$\mathbf{A} = \nabla \otimes \mathbf{A} = \nabla_k A_{ij} = \frac{\partial A_{ij}}{\partial x_k}$$
, A - 30

and the divergence of a second-order tensor gives a vector as

$$div \mathbf{A} = \nabla \cdot \mathbf{A} = \frac{\partial A_{ij}}{\partial x_j} e_i = \begin{pmatrix} \frac{\partial A_{11}}{\partial x_1} + \frac{\partial A_{12}}{\partial x_2} + \frac{\partial A_{13}}{\partial x_3}, \\ \frac{\partial A_{21}}{\partial x_1} + \frac{\partial A_{22}}{\partial x_2} + \frac{\partial A_{23}}{\partial x_3}, \\ \frac{\partial A_{31}}{\partial x_1} + \frac{\partial A_{32}}{\partial x_2} + \frac{\partial A_{33}}{\partial x_3} \end{pmatrix}.$$
 A - 31

Product of two tensors

The product of two tensors is a tensor of the same rank

$$\mathbf{B} = \mathbf{\Pi} \cdot \nabla \mathbf{u} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{bmatrix}.$$
 A - 32

It can be written in component form as

$$\begin{bmatrix} \Pi_{11} \frac{\partial u_1}{\partial x_1} + \Pi_{12} \frac{\partial u_2}{\partial x_1} + \Pi_{13} \frac{\partial u_3}{\partial x_1} & \Pi_{11} \frac{\partial u_1}{\partial x_2} + \Pi_{12} \frac{\partial u_2}{\partial x_2} + \Pi_{13} \frac{\partial u_3}{\partial x_2} & \Pi_{11} \frac{\partial u_1}{\partial x_3} + \Pi_{12} \frac{\partial u_2}{\partial x_3} + \Pi_{13} \frac{\partial u_3}{\partial x_3} \\ \Pi_{21} \frac{\partial u_1}{\partial x_1} + \Pi_{22} \frac{\partial u_2}{\partial x_1} + \Pi_{23} \frac{\partial u_3}{\partial x_1} & \Pi_{21} \frac{\partial u_1}{\partial x_2} + \Pi_{22} \frac{\partial u_2}{\partial x_2} + \Pi_{23} \frac{\partial u_3}{\partial x_2} & \Pi_{21} \frac{\partial u_1}{\partial x_3} + \Pi_{22} \frac{\partial u_2}{\partial x_3} + \Pi_{23} \frac{\partial u_3}{\partial x_3} \\ \Pi_{31} \frac{\partial u_1}{\partial x_1} + \Pi_{32} \frac{\partial u_2}{\partial x_1} + \Pi_{33} \frac{\partial u_3}{\partial x_1} & \Pi_{31} \frac{\partial u_1}{\partial x_2} + \Pi_{32} \frac{\partial u_2}{\partial x_2} + \Pi_{33} \frac{\partial u_3}{\partial x_2} & \Pi_{31} \frac{\partial u_1}{\partial x_2} + \Pi_{32} \frac{\partial u_2}{\partial x_3} + \Pi_{33} \frac{\partial u_3}{\partial x_3} \end{bmatrix}$$

The index notation of this product is

$$B_{ij} = \prod_{ik} \nabla_k u_j \,. \tag{A-33}$$

Note that tensor products are not commutative $\Pi . \nabla \mathbf{u} \neq \nabla \mathbf{u} . \Pi$.

Inner product of two tensors

The inner product (Contraction) of two tensor of second rank is a scalar quantity as

$$\mathbf{A} : \mathbf{B} \equiv A_{ii} : B_{ii} . \qquad \mathbf{A} - 34$$

The component form of the inner product of two second-order tensor is

$$\mathbf{A}:\mathbf{B} = \begin{pmatrix} A_{11}B_{11} + A_{12}B_{12} + A_{13}B_{13} + \\ A_{21}B_{21} + A_{22}B_{22} + A_{23}B_{23} + \\ A_{31}B_{31} + A_{32}B_{32} + A_{33}B_{33} \end{pmatrix}, \qquad A - 35$$

and the inner product of a tensor with identity tensor is defined as

$$\mathbf{A}:\mathbf{I}=A_{ii}.$$
 A - 36

Outer product of two tensors

The outer product of two second-order tensor is a scalar value

$$\mathbf{A}_{\circ}^{\circ}\mathbf{B} = \begin{pmatrix} A_{11}B_{11} + A_{21}B_{12} + A_{31}B_{13} + \\ A_{12}B_{21} + A_{22}B_{22} + A_{32}B_{23} + \\ A_{13}B_{31} + A_{23}B_{32} + A_{33}B_{33} \end{pmatrix}.$$
 A - 37

The invariant of a tensor

All individuals except scalar quantities will vary by changing the coordinate systems. Therefore, vectors and tensors are direction dependent. Nevertheless, the eigenvalues and invariants of a tensor are independent of direction and do not change by changing the coordinates. The invariant of the tensors usually having some physical meaning therefore, the eigenvalues and invariants of second-order tensors are given as

$$\mathbf{Inv}^{1st} \mathbf{\Pi} = \mathbf{\Pi}_{ii} = Trace(\mathbf{\Pi}) = \mathbf{\Pi}_{11} + \mathbf{\Pi}_{22} + \mathbf{\Pi}_{33}.$$
 A - 38
The second invariant of stress tensor is

$$\mathbf{Inv}^{2th} \mathbf{\Pi} = \frac{1}{2} \Big(\mathbf{\Pi}_{ii} \mathbf{\Pi}_{jj} - \mathbf{\Pi}_{ij} \mathbf{\Pi}_{ji} \Big), \qquad \mathbf{A} - 39$$

which can be written in opened form as

$$\mathbf{Inv}^{2th} \mathbf{\Pi} = \frac{1}{2} \begin{bmatrix} (\mathbf{\Pi}_{11}\mathbf{\Pi}_{22} - \mathbf{\Pi}_{21}\mathbf{\Pi}_{12}) + (\mathbf{\Pi}_{22}\mathbf{\Pi}_{11} - \mathbf{\Pi}_{12}\mathbf{\Pi}_{21}) + \\ (\mathbf{\Pi}_{11}\mathbf{\Pi}_{33} - \mathbf{\Pi}_{31}\mathbf{\Pi}_{13}) + (\mathbf{\Pi}_{33}\mathbf{\Pi}_{11} - \mathbf{\Pi}_{13}\mathbf{\Pi}_{31}) + \\ (\mathbf{\Pi}_{22}\mathbf{\Pi}_{33} - \mathbf{\Pi}_{32}\mathbf{\Pi}_{23}) + (\mathbf{\Pi}_{33}\mathbf{\Pi}_{22} - \mathbf{\Pi}_{23}\mathbf{\Pi}_{32}) \end{bmatrix}.$$
 A - 40

Due to conservation of angular momentum $\Pi_{ij} = \Pi_{ij}$ so that second invariant of stress tensor can be simplified as

$$\mathbf{Inv}^{2th} \ \mathbf{\Pi} = \left(\mathbf{\Pi}_{11}\mathbf{\Pi}_{22} - \mathbf{\Pi}_{12}^{2}\right) + \left(\mathbf{\Pi}_{11}\mathbf{\Pi}_{33} - \mathbf{\Pi}_{13}^{2}\right) + \left(\mathbf{\Pi}_{22}\mathbf{\Pi}_{33} - \mathbf{\Pi}_{23}^{2}\right).$$
 A - 41

The third invariant of stress tensor is defined as

$$\mathbf{Inv}^{3th} \mathbf{\Pi} = \det(\mathbf{\Pi}) = \varepsilon_{ijk} \mathbf{\Pi}_{1i} \mathbf{\Pi}_{2j} \mathbf{\Pi}_{3k}, \qquad \mathbf{A} - 42$$

which can be simplified by eliminating the zeros due to permutation tenors as

$$\mathbf{Inv}^{3th} \ \mathbf{\Pi} = \begin{pmatrix} \mathbf{\Pi}_{11} \mathbf{\Pi}_{22} \mathbf{\Pi}_{33} + \mathbf{\Pi}_{12} \mathbf{\Pi}_{23} \mathbf{\Pi}_{31} + \mathbf{\Pi}_{13} \mathbf{\Pi}_{21} \mathbf{\Pi}_{32} \\ -\mathbf{\Pi}_{11} \mathbf{\Pi}_{23} \mathbf{\Pi}_{32} - \mathbf{\Pi}_{12} \mathbf{\Pi}_{21} \mathbf{\Pi}_{33} - \mathbf{\Pi}_{13} \mathbf{\Pi}_{22} \mathbf{\Pi}_{31} \end{pmatrix}.$$
 A - 43

In index notation, this can be written as

$$\mathbf{Inv}^{3th} \mathbf{\Pi} = \frac{1}{6} \varepsilon_{ijk} \varepsilon_{lmn} \mathbf{\Pi}_{li} \mathbf{\Pi}_{mj} \mathbf{\Pi}_{nk} \,. \qquad \mathbf{A} - 44$$

Moreover, it may be useful to note that

$$\det(\mathbf{A}) = \det(\mathbf{A}^{Transpose}), \qquad \mathbf{A} - 45$$

$$det(\mathbf{A}.\mathbf{B}) = det(\mathbf{A}) det(\mathbf{B}), \qquad A - 46$$

The eigenvalues of the second-order tensor can be calculated by solving the following cubic equations

$$|\mathbf{A} - \lambda \mathbf{I}| = 0 \rightarrow \lambda^3 - \lambda^2 \mathbf{Inv}^{1st} \mathbf{A} + \lambda \mathbf{Inv}^{2nd} \mathbf{A} - \mathbf{Inv}^{3th} \mathbf{A} = 0.$$
 A - 47

The trace-free part of a symmetrical tensor

The trace-free part of a tensor is given by

$$\left[\mathbf{A}\right]^{(2)} = \frac{1}{2} \left[\mathbf{A} + \mathbf{A}^{T}\right] - \frac{1}{3} Trace(\mathbf{A})\mathbf{I}.$$
 A - 48

Consequently, the trace-free part of the velocity gradient tensor is defined as

$$\left[\nabla \mathbf{u}\right]^{(2)} = \frac{1}{2} \left[\nabla \mathbf{u} + \nabla \mathbf{u}^{T}\right] - \frac{1}{3} (\nabla \mathbf{u}) \mathbf{I}$$
 A - 49

Alternatively, the index notation is given by

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$$\left[\nabla \mathbf{u}\right]_{ij}^{(2)} = \frac{1}{2} \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{1}{3} \left(\frac{\partial u_k}{\partial x_k} \right) \delta_{ij}$$
 A - 50

The trace-free part of $\mathbf{\Pi} \cdot \nabla \mathbf{u}$ can also be defined as

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]_{ij}^{(2)} = \frac{1}{2} \left[\Pi_{ik} \frac{\partial u_j}{\partial x_k} + \Pi_{jk} \frac{\partial u_i}{\partial x_k} \right] - \frac{1}{3} \delta_{ij} \Pi_{lk} \frac{\partial u_l}{\partial x_k}, \qquad A - 51$$

Tensor relations on the surface

Therefore, traction vector on surface $\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$ is a second-order tensor which can be defined as

$$\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2^2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3^2 \end{bmatrix}, \quad \mathbf{A} - 52$$
$$\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) = \begin{bmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_2 n_1 & 1 - n_2^2 & -n_2 n_3 \\ -n_3 n_1 & -n_3 n_2 & 1 - n_3^2 \end{bmatrix}.$$

The gradient operator tangent to surface cane be defined as $\nabla_s = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla = \mathbf{S} \cdot \nabla$. Accordingly, calculation of field vectors and tensors variables on surface can be defined as follows, the gradient of temperature along the surface $\nabla_s T = \nabla T \cdot \mathbf{S}$ is given by

$$(\nabla T) \cdot \mathbf{S} = \begin{bmatrix} \frac{\partial T}{\partial x_1} \\ \frac{\partial T}{\partial x_2} \\ \frac{\partial T}{\partial x_3} \end{bmatrix} \begin{bmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_2 n_1 & 1 - n_2^2 & -n_2 n_3 \\ -n_3 n_1 & -n_2 n_3 & 1 - n_3^2 \end{bmatrix},$$
 A - 53

after multiplication and simplification, it reads as

$$(\nabla T) \cdot \mathbf{S} = \begin{bmatrix} \left(1 - n_1^2\right) \frac{\partial T}{\partial x_1} - n_1 n_2 \frac{\partial T}{\partial x_2} - n_1 n_3 \frac{\partial T}{\partial x_3} \\ -n_2 n_1 \frac{\partial T}{\partial x_1} + \left(1 - n_2^2\right) \frac{\partial T}{\partial x_2} - n_2 n_3 \frac{\partial T}{\partial x_3} \\ -n_3 n_1 \frac{\partial T}{\partial x_1} - n_2 n_3 \frac{\partial T}{\partial x_2} + \left(1 - n_3^2\right) \frac{\partial T}{\partial x_3} \end{bmatrix}.$$
 A - 54

Similarly, the tangent velocity on the surface $\mathbf{u}_t = \mathbf{u} \cdot \mathbf{S}$ can be defined as

$$\mathbf{u}_{t} = \mathbf{u} \cdot \mathbf{S} = \begin{bmatrix} (1 - n_{1}^{2})u_{1} - n_{1}n_{2}u_{2} - n_{1}n_{3}u_{3} \\ -n_{2}n_{1}u_{1} + (1 - n_{2}^{2})u_{2} - n_{2}n_{3}u_{3} \\ -n_{3}n_{1}u_{1} - n_{2}n_{3}u_{2} + (1 - n_{3}^{2})u_{3} \end{bmatrix}.$$
 A - 55

The tangent stress vector $\vec{\tau} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S}$ on the surface is given by

$$\vec{\boldsymbol{\tau}} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S} = \begin{bmatrix} \Pi_{11}n_1 + \Pi_{12}n_2 + \Pi_{13}n_3 \\ \Pi_{21}n_1 + \Pi_{22}n_2 + \Pi_{23}n_3 \\ \Pi_{31}n_1 + \Pi_{32}n_2 + \Pi_{33}n_3 \end{bmatrix} \begin{bmatrix} 1 - n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_2n_1 & 1 - n_2^2 & -n_2n_3 \\ -n_3n_1 & -n_3n_2 & 1 - n_3^2 \end{bmatrix}.$$
 A - 56

Alternatively, it can be written in more specific form as
$$\vec{\tau} = \begin{bmatrix} \left(1 - n_1^2\right)\theta_1 - n_1 n_2 \theta_2 - n_1 n_3 \theta_3 \\ -n_2 n_1 \theta_1 + \left(1 - n_2^2\right)\theta_2 - n_2 n_3 \theta_3 \\ -n_3 n_1 \theta_1 - n_3 n_2 \theta_2 + \left(1 - n_3^2\right)\theta_3 \end{bmatrix},$$
A - 57

where

or

$$\begin{aligned} \theta_1 &= \Pi_{11} n_1 + \Pi_{12} n_2 + \Pi_{13} n_3, \\ \theta_2 &= \Pi_{21} n_1 + \Pi_{22} n_2 + \Pi_{23} n_3, \\ \theta_3 &= \Pi_{31} n_1 + \Pi_{32} n_2 + \Pi_{33} n_3. \end{aligned}$$
 A - 58

The Π : **n** \otimes **n** is defined as

$$\mathbf{\Pi}: \mathbf{n} \otimes \mathbf{n} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} : \begin{bmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2^2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3^2 \end{bmatrix}, \qquad \mathbf{A} - 59$$

which can be written in more simplified form as

$$\mathbf{\Pi} : \mathbf{n} \otimes \mathbf{n} = \Pi_{11} n_1^2 + \Pi_{12} n_1 n_2 + \Pi_{13} n_1 n_3 + \Pi_{21} n_2 n_1 + \Pi_{22} n_2^2 + \mathbf{A} - 60$$
$$\Pi_{23} n_2 n_3 + \Pi_{31} n_3 n_1 + \Pi_{32} n_3 n_2 + \Pi_{33} n_3^2.$$

The normal $q_n = \mathbf{q} \cdot \mathbf{n}$ and tangential heat flux vector $\vec{\mathbf{q}}_t = \mathbf{q} \cdot \mathbf{S}$ on the surface also can be defined as

$$q_{n} = \mathbf{q} \cdot \mathbf{n} = q_{1}n_{1} + q_{2}n_{2} + q_{3}n_{3},$$

$$\vec{\mathbf{q}}_{t} = \mathbf{q} \cdot \mathbf{S} = \begin{bmatrix} q_{1} \\ q_{2} \\ q_{3} \end{bmatrix} \cdot \begin{bmatrix} 1 - n_{1}^{2} & -n_{1}n_{2} & -n_{1}n_{3} \\ -n_{2}n_{1} & 1 - n_{2}^{2} & -n_{2}n_{3} \\ -n_{3}n_{1} & -n_{3}n_{2} & 1 - n_{3}^{2} \end{bmatrix},$$

$$\mathbf{A} - 62$$
or simply $\vec{\mathbf{q}}_{t} = \left((1 - n_{1}^{2})q_{1} - n_{1}n_{2}q_{2} - n_{1}n_{3}q_{z} \right) \mathbf{e}_{1} + \left(-n_{2}n_{1}q_{1} + (1 - n_{2}^{2})q_{2} - n_{2}n_{3}q_{3} \right) \mathbf{e}_{2} + \left(-n_{3}n_{1}q_{1} - n_{3}n_{2}q_{2} + (1 - n_{3}^{2})q_{3} \right) \mathbf{e}_{3}.$

The normal gradient of velocity $\mathbf{n} \cdot \nabla \mathbf{u}$ on the surface is given by

$$\mathbf{n} \cdot \nabla \mathbf{u} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} n_x + \frac{\partial u_2}{\partial x_1} n_2 + \frac{\partial u_3}{\partial x_1} n_3 \\ \frac{\partial u_1}{\partial x_2} n_x + \frac{\partial u_2}{\partial x_2} n_2 + \frac{\partial u_3}{\partial x_2} n_3 \\ \frac{\partial u_1}{\partial x_3} n_x + \frac{\partial u_2}{\partial x_3} n_2 + \frac{\partial u_3}{\partial x_3} n_3 \end{bmatrix}, \quad \mathbf{A} - 63$$

and the normal of the transposed gradient of velocity $\mathbf{n} \cdot (\nabla \mathbf{u})^T$ is

$$\mathbf{n} \cdot \left(\nabla \mathbf{u}\right)^{T} = \begin{bmatrix} n_{1} \\ n_{2} \\ n_{3} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} & \frac{\partial u_{2}}{\partial x_{1}} & \frac{\partial u_{3}}{\partial x_{1}} \\ \frac{\partial u_{1}}{\partial x_{2}} & \frac{\partial u_{2}}{\partial x_{2}} & \frac{\partial u_{3}}{\partial x_{2}} \\ \frac{\partial u_{1}}{\partial x_{3}} & \frac{\partial u_{2}}{\partial x_{3}} & \frac{\partial u_{3}}{\partial x_{3}} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} n_{1} + \frac{\partial u_{1}}{\partial x_{2}} n_{2} + \frac{\partial u_{1}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{2}}{\partial x_{1}} n_{1} + \frac{\partial u_{2}}{\partial x_{2}} n_{2} + \frac{\partial u_{2}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{3}}{\partial x_{1}} n_{1} + \frac{\partial u_{3}}{\partial x_{2}} n_{2} + \frac{\partial u_{3}}{\partial x_{3}} n_{3} \end{bmatrix}.$$
 A - 64

The dilatation of velocity vector $\mathbf{I}ig(
abla\cdot\mathbf{u}ig)$ is defined as

$$\mathbf{I}(\nabla \cdot \mathbf{u}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right), \qquad \mathbf{A} - 65$$

and then $\mathbf{n} \cdot \mathbf{I} \big(\nabla \cdot \mathbf{u} \big)$ is defined as

$$\mathbf{n} \cdot \mathbf{I} \left(\nabla \cdot \mathbf{u} \right) = \begin{bmatrix} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_1 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_2 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_3 \end{bmatrix},$$
 A - 66

 $(\mathbf{n} \cdot \nabla \mathbf{u}) \cdot \mathbf{S}$ is defined as

$$\left(\mathbf{n}\cdot\nabla\mathbf{u}\right)\cdot\mathbf{S} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1}n_1 + \frac{\partial u_2}{\partial x_1}n_2 + \frac{\partial u_3}{\partial x_1}n_3\\ \frac{\partial u_1}{\partial x_2}n_1 + \frac{\partial u_2}{\partial x_2}n_2 + \frac{\partial u_3}{\partial x_2}n_3\\ \frac{\partial u_1}{\partial x_3}n_1 + \frac{\partial u_2}{\partial x_3}n_2 + \frac{\partial u_3}{\partial x_3}n_3 \end{bmatrix} \begin{bmatrix} 1-n_1^2 & -n_1n_2 & -n_1n_3\\ -n_2n_1 & 1-n_2^2 & -n_2n_3\\ -n_3n_1 & -n_3n_2 & 1-n_3^2 \end{bmatrix}, \qquad \mathbf{A} - \mathbf{67}$$

which can be written in full component form as

$$\begin{bmatrix} \left(1-n_1^2\right)\left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_1}n_2+\frac{\partial u_3}{\partial x_1}n_3\right)-n_1n_2\left(\frac{\partial u_1}{\partial x_2}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_2}n_3\right)-n_1n_3\left(\frac{\partial u_1}{\partial x_3}n_1+\frac{\partial u_2}{\partial x_3}n_2+\frac{\partial u_3}{\partial x_3}n_3\right)\\ -n_2n_1\left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_1}n_2+\frac{\partial u_3}{\partial x_1}n_3\right)+\left(1-n_2^2\right)\left(\frac{\partial u_1}{\partial x_2}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_2}n_3\right)-n_2n_3\left(\frac{\partial u_1}{\partial x_3}n_1+\frac{\partial u_2}{\partial x_3}n_2+\frac{\partial u_3}{\partial x_3}n_3\right)\\ -n_3n_1\left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_1}n_2+\frac{\partial u_3}{\partial x_1}n_3\right)-n_2n_3\left(\frac{\partial u_1}{\partial x_2}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_2}n_3\right)+\left(1-n_3^2\right)\left(\frac{\partial u_1}{\partial x_3}n_1+\frac{\partial u_2}{\partial x_3}n_2+\frac{\partial u_3}{\partial x_3}n_3\right)\end{bmatrix}$$

This equation is written in shorten hand form as

$$(\mathbf{n} \cdot \nabla \mathbf{u}) \cdot \mathbf{S} = \begin{bmatrix} (1 - n_1^2) \alpha_1 - n_1 n_2 \alpha_2 - n_1 n_3 \alpha_3 \\ -n_1 n_2 \alpha_1 + (1 - n_2^2) \alpha_2 - n_1 n_3 \alpha_3 \\ -n_1 n_3 \alpha_1 - n_2 n_3 \alpha_2 + (1 - n_3^2) \alpha_3 \end{bmatrix}, \quad \mathbf{A} - 68$$

where

$$\alpha_{1} = \left(\frac{\partial u_{1}}{\partial x_{1}}n_{1} + \frac{\partial u_{2}}{\partial x_{1}}n_{2} + \frac{\partial u_{3}}{\partial x_{1}}n_{3}\right),$$

$$\alpha_{2} = \left(\frac{\partial u_{1}}{\partial x_{2}}n_{1} + \frac{\partial u_{2}}{\partial x_{2}}n_{2} + \frac{\partial u_{3}}{\partial x_{2}}n_{3}\right),$$

$$\alpha_{3} = \left(\frac{\partial u_{1}}{\partial x_{3}}n_{1} + \frac{\partial u_{2}}{\partial x_{3}}n_{2} + \frac{\partial u_{3}}{\partial x_{3}}n_{3}\right).$$
A - 69

Finally, $(\mathbf{n} \cdot (\nabla \mathbf{u})^T) \cdot \mathbf{S}$ can be written as

$$\left(\mathbf{n} \cdot \left(\nabla \mathbf{u}\right)^{T}\right) \cdot \mathbf{S} = \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} n_{1} + \frac{\partial u_{1}}{\partial x_{2}} n_{2} + \frac{\partial u_{1}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{2}}{\partial x_{1}} n_{1} + \frac{\partial u_{2}}{\partial x_{2}} n_{2} + \frac{\partial u_{2}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{3}}{\partial x_{1}} n_{1} + \frac{\partial u_{3}}{\partial x_{2}} n_{2} + \frac{\partial u_{3}}{\partial x_{3}} n_{3} \end{bmatrix} \cdot \begin{bmatrix} 1 - n_{1}^{2} & -n_{1}n_{2} & -n_{1}n_{3} \\ -n_{2}n_{1} & 1 - n_{2}^{2} & -n_{2}n_{3} \\ -n_{3}n_{1} & -n_{3}n_{2} & 1 - n_{3}^{2} \end{bmatrix}, \quad \mathbf{A} - 70$$

which can be written in full component form as

$$\begin{bmatrix} \left(1-n_1^2\right) \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_1 n_2 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) - n_1 n_3 \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_2 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) + \left(1-n_2^2\right) \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_2}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_1}{\partial x_2}n_2+\frac{\partial u_1}{\partial x_3}n_3\right) - n_2 n_3 \left(\frac{\partial u_2}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) + \left(1-n_3^2\right) \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) - n_3 \left(\frac{\partial u_3}{\partial x_1}n_1+\frac{\partial u_3}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_2}n_2+\frac{\partial u_3}{\partial x_3}n_3\right) - n_3 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial x_3}n_3\right) \\ -n_3 n_1 \left(\frac{\partial u_1}{\partial x_1}n_1+\frac{\partial u_2}{\partial$$

and the shorten hand form of above equation is given by

$$\left(\mathbf{n} \cdot (\nabla \mathbf{u})^{T}\right) \cdot \mathbf{S} = \begin{bmatrix} (1 - n_{1}^{2})\beta_{1} - n_{1}n_{2}\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{2}\beta_{1} + (1 - n_{2}^{2})\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{3}\beta_{1} - n_{2}n_{3}\beta_{2} + (1 - n_{3}^{2})\beta_{3} \end{bmatrix}, \quad \mathbf{A} - 71$$

where

$$\beta_{1} = \left(\frac{\partial u_{1}}{\partial x_{1}}n_{1} + \frac{\partial u_{1}}{\partial x_{2}}n_{2} + \frac{\partial u_{1}}{\partial x_{3}}n_{3}\right),$$

$$\beta_{2} = \left(\frac{\partial u_{2}}{\partial x_{1}}n_{1} + \frac{\partial u_{2}}{\partial x_{2}}n_{2} + \frac{\partial u_{2}}{\partial x_{3}}n_{3}\right),$$

$$\beta_{3} = \left(\frac{\partial u_{3}}{\partial x_{1}}n_{1} + \frac{\partial u_{3}}{\partial x_{2}}n_{2} + \frac{\partial u_{3}}{\partial x_{3}}n_{3}\right).$$
A - 72

Calculation for ' $(\mathbf{n} \cdot \mathbf{I} \cdot (\nabla \cdot \mathbf{u})) \cdot \mathbf{S}$ '

$$\left(\mathbf{n}\cdot\mathbf{I}\cdot\left(\nabla\cdot\mathbf{u}\right)\right)\cdot\mathbf{S} = \begin{bmatrix} \left(\frac{\partial u_{1}}{\partial x_{1}}+\frac{\partial u_{2}}{\partial x_{2}}+\frac{\partial u_{3}}{\partial x_{3}}\right)n_{1}\\ \left(\frac{\partial u_{1}}{\partial x_{1}}+\frac{\partial u_{2}}{\partial x_{2}}+\frac{\partial u_{3}}{\partial x_{3}}\right)n_{2}\\ \left(\frac{\partial u_{1}}{\partial x_{1}}+\frac{\partial u_{2}}{\partial x_{2}}+\frac{\partial u_{3}}{\partial x_{3}}\right)n_{3}\\ \end{bmatrix} \cdot \begin{bmatrix} 1-n_{1}^{2}&-n_{1}n_{2}&-n_{1}n_{3}\\ -n_{2}n_{1}&1-n_{2}^{2}&-n_{2}n_{3}\\ -n_{3}n_{1}&-n_{3}n_{2}&1-n_{3}^{2} \end{bmatrix}.$$
 A - 73

which can be written in shorten hand form as

$$\left(\mathbf{n}\cdot\mathbf{I}\cdot\left(\nabla\cdot\mathbf{u}\right)\right)\cdot\mathbf{S} = \begin{bmatrix} n_1\left(1-n_1^2\right)\omega - n_1n_2^2\omega - n_1n_3^2\omega\\ -n_2n_1^2\omega + n_2\left(1-n_2^2\right)\omega - n_2n_3^2\omega\\ -n_3n_1^2\omega - n_3n_2^2\omega + n_3\left(1-n_3^2\right)\omega \end{bmatrix}.$$
 A - 74

where

$$\omega = \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right).$$
 A - 75

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APPENDIX B. Three-dimensional form of the Maxwell slip boundary condition on arbitrary geometry

The original Maxwell boundary condition

The opened form of the original Maxwell equation holds for any arbitrary geometry.

Can be defined by opening and simplify products appeared in (Eq. 5-139) as

$$\mathbf{u}_{tangential}^{wall} - \mathbf{u}_{tangential}^{solid} = -\left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \frac{\lambda}{\mu} \begin{bmatrix} \left(1-n_{1}^{2}\right)\theta_{1} - n_{1}n_{2}\theta_{2} - n_{1}n_{3}\theta_{3} \\ -n_{2}n_{1}\theta_{1} + \left(1-n_{2}^{2}\right)\theta_{2} - n_{2}n_{3}\theta_{3} \\ -n_{3}n_{1}\theta_{1} - n_{3}n_{2}\theta_{2} + \left(1-n_{3}^{2}\right)\theta_{3} \end{bmatrix}$$
B-1
$$-\frac{3}{4} \frac{\Pr(\gamma-1)}{\gamma p} \begin{bmatrix} \left(1-n_{1}^{2}\right)Q_{1} - n_{1}n_{2}Q_{2} - n_{1}n_{3}Q_{3} \\ -n_{y}n_{x}Q_{1} + \left(1-n_{2}^{2}\right)Q_{2} - n_{2}n_{3}Q_{3} \\ -n_{3}n_{1}Q_{1} - n_{3}n_{2}Q_{2} + \left(1-n_{3}^{2}\right)Q_{3} \end{bmatrix},$$

where

$$\begin{aligned} \theta_1 &= \Pi_{11} n_1 + \Pi_{12} n_2 + \Pi_{13} n_3, \\ \theta_2 &= \Pi_{21} n_1 + \Pi_{22} n_2 + \Pi_{23} n_3, \\ \theta_3 &= \Pi_{31} n_1 + \Pi_{32} n_2 + \Pi_{33} n_3. \end{aligned}$$
B-2

First-order Maxwell boundary condition

The opened form of first-order Maxwell boundary condition for an arbitrary geometry can be defined by calculating the value of $(\mathbf{n} \cdot \nabla \mathbf{u}) \cdot \mathbf{S}, (\mathbf{n} \cdot (\nabla \mathbf{u})^T) \cdot \mathbf{S}$,

 $(\mathbf{n} \cdot (\nabla \mathbf{u})^T) \cdot \mathbf{S}$, and $(\nabla T) \cdot \mathbf{S}$, and replacing them into (Eq.).

$$\begin{split} \mathbf{u}_{tangential}^{wall} &- \mathbf{u}_{tangential}^{solid} = \left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \lambda \begin{bmatrix} \left(1-n_{1}^{2}\right)\alpha_{1} - n_{1}n_{2}\alpha_{2} - n_{1}n_{3}\alpha_{3} \\ -n_{1}n_{2}\alpha_{1} + \left(1-n_{2}^{2}\right)\alpha_{2} - n_{1}n_{3}\alpha_{3} \\ -n_{1}n_{3}\alpha_{1} - n_{2}n_{3}\alpha_{2} + \left(1-n_{3}^{2}\right)\alpha_{3} \end{bmatrix} \\ &+ \left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \lambda \begin{bmatrix} \left(1-n_{1}^{2}\right)\beta_{1} - n_{1}n_{2}\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{2}\beta_{1} + \left(1-n_{2}^{2}\right)\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{3}\beta_{1} - n_{2}n_{3}\beta_{2} + \left(1-n_{3}^{2}\right)\beta_{3} \end{bmatrix} \\ &- \frac{2}{3} \left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \lambda \begin{bmatrix} n_{1}\left(1-n_{1}^{2}\right)\omega - n_{1}n_{2}^{2}\omega - n_{1}n_{3}^{2}\omega \\ -n_{2}n_{1}^{2}\omega + n_{2}\left(1-n_{2}^{2}\right)\omega - n_{2}n_{3}^{2}\omega \\ -n_{3}n_{1}^{2}\omega - n_{3}n_{2}^{2}\omega + n_{3}\left(1-n_{3}^{2}\right)\omega \end{bmatrix} \\ &+ \frac{3}{4}\frac{\mu}{\rho T} \begin{bmatrix} \left(1-n_{1}^{2}\right)\frac{\partial T}{\partial x_{1}} - n_{1}n_{2}\frac{\partial T}{\partial x_{2}} - n_{1}n_{3}\frac{\partial T}{\partial x_{3}} \\ -n_{2}n_{1}\frac{\partial T}{\partial x_{1}} + \left(1-n_{2}^{2}\right)\frac{\partial T}{\partial x_{2}} - n_{2}n_{3}\frac{\partial T}{\partial x_{3}} \end{bmatrix}, \end{split}$$

Where

$$\alpha_{1} = \left(\frac{\partial u_{1}}{\partial x_{1}}n_{1} + \frac{\partial u_{2}}{\partial x_{1}}n_{2} + \frac{\partial u_{3}}{\partial x_{1}}n_{3}\right), \quad \alpha_{2} = \left(\frac{\partial u_{1}}{\partial x_{2}}n_{1} + \frac{\partial u_{2}}{\partial x_{2}}n_{2} + \frac{\partial u_{3}}{\partial x_{2}}n_{3}\right),$$

$$\alpha_{3} = \left(\frac{\partial u_{1}}{\partial x_{3}}n_{1} + \frac{\partial u_{2}}{\partial x_{3}}n_{2} + \frac{\partial u_{3}}{\partial x_{3}}n_{3}\right).$$

$$\beta_{1} = \left(\frac{\partial u_{1}}{\partial x_{3}}n_{1} + \frac{\partial u_{1}}{\partial x_{2}}n_{2} + \frac{\partial u_{1}}{\partial x_{3}}n_{3}\right), \quad \beta_{2} = \left(\frac{\partial u_{2}}{\partial x_{3}}n_{1} + \frac{\partial u_{2}}{\partial x_{2}}n_{2} + \frac{\partial u_{2}}{\partial x_{3}}n_{3}\right),$$

$$B-4$$

$$\beta_{1} = \left(\frac{\partial u_{1}}{\partial x_{3}}n_{1} + \frac{\partial u_{1}}{\partial x_{3}}n_{2} + \frac{\partial u_{1}}{\partial x_{3}}n_{3}\right), \quad \beta_{2} = \left(\frac{\partial u_{2}}{\partial x_{3}}n_{1} + \frac{\partial u_{2}}{\partial x_{3}}n_{2} + \frac{\partial u_{2}}{\partial x_{3}}n_{3}\right),$$

$$\beta_{1} = \left(\frac{\partial u_{1}}{\partial x_{1}} + \frac{\partial u_{2}}{\partial x_{2}} + \frac{\partial u_{3}}{\partial x_{3}}n_{3}\right), \quad B-5$$

$$\beta_{3} = \left(\frac{\partial u_{1}}{\partial x_{1}} + \frac{\partial u_{2}}{\partial x_{2}} + \frac{\partial u_{3}}{\partial x_{3}}n_{3}\right), \quad B-6$$

APPENDIX C. Derivation of conservation laws from the Boltzmann kinetic equation (monatomic gas)

The Boltzmann kinetic equation for the monatomic gas particles without external body force can be read as

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f\left(\mathbf{v}, \mathbf{r}, t\right) = \mathcal{R}[f, f_1].$$
 C - 1

Let's define the few of the macroscopic quantities appearing in the balance equation once more based on the statistical mechanical formula as follows:

density :
$$\rho = \langle m f(\mathbf{v}, \mathbf{r}, t) \rangle$$
,
momentum : $\rho \mathbf{u} = \langle m \mathbf{v} f(\mathbf{v}, \mathbf{r}, t) \rangle$,
energy : $\rho E = \langle \frac{1}{2}mc^2 f(\mathbf{v}, \mathbf{r}, t) \rangle$,
stress tensor : $\mathbf{P} = \langle m cc f(\mathbf{v}, \mathbf{r}, t) \rangle$,
heat flux : $\mathbf{Q} = \langle \frac{1}{2}mc^2 f(\mathbf{v}, \mathbf{r}, t) \rangle$.

Here the thermal velocity is $\mathbf{c} = \mathbf{v}\cdot\mathbf{u}$. It is important to note that $(\mathbf{x}, \mathbf{v}, \text{ and } t)$ are independent variables, whereas thermal velocity is not independent from *space and time*. It is possible to re-write Boltzmann equation in form of thermal velocity as

$$\frac{df}{dt} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{x}} = \mathcal{R}[f, f_1], \qquad C - 3$$

where $d/dt = \partial/\partial t + \mathbf{v} \partial/\partial \mathbf{x}$.

Mass Conservation

Multiplication of Boltzmann equation with $\psi = m$ and then subsequent integration over velocity space yields

$$\left\langle m\frac{\partial f}{\partial t}\right\rangle + \left\langle m\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}}\right\rangle = \left\langle m\mathcal{R}[f,f_1]\right\rangle.$$
 C - 4

Due to conservation of mass collisional integral vanishes, then

$$\left\langle \frac{\partial mf}{\partial t} \right\rangle + \left\langle \frac{\partial m\mathbf{v}f}{\partial \mathbf{x}} \right\rangle - \left\langle mf \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right\rangle = 0, \qquad C - 5$$

which is equivalent to

$$\frac{\partial \rho}{\partial t} + \nabla . (\rho \mathbf{u}) = 0. \qquad C - 6$$

Momentum Conservation

Multiplication of Boltzmann equation with $\psi = m\mathbf{v}$ and subsequent integration over velocity space yields

$$\left\langle m\mathbf{v}\frac{\partial f}{\partial t}\right\rangle + \left\langle m\mathbf{v}\mathbf{v}\frac{\partial f}{\partial \mathbf{x}}\right\rangle = \left\langle m\mathbf{v}\mathcal{R}[f, f_1]\right\rangle,$$
 C - 7

where collisional term is zero due to conservation of momentum in collisions. Since we need to integrate over velocity, we have to convert molecular velocity into peculiar velocity and then bring it together with f as

$$\left\langle \frac{\partial m \mathbf{v} f}{\partial t} \right\rangle - \left\langle f \frac{\partial m \mathbf{v}}{\partial t} \right\rangle + \left\langle \frac{\partial m \mathbf{v} \mathbf{v} f}{\partial \mathbf{x}} \right\rangle - \left\langle f \frac{\partial m \mathbf{v} \mathbf{v}}{\partial \mathbf{x}} \right\rangle = 0.$$
 C - 8

Due to independence of molecular velocity from spatial and time coordinates, we have

$$\left\langle \frac{\partial mv_i f}{\partial t} \right\rangle - 0 + \left\langle \frac{\partial mv_i v_k f}{\partial x_k} \right\rangle - \left\langle mv_i f \frac{\partial v_k}{\partial x_k} \right\rangle - \left\langle mfv_k \frac{\partial v_i}{\partial x_k} \right\rangle = 0, \qquad C - 9$$

$$\left\langle \frac{\partial m v_i f}{\partial t} \right\rangle - 0 + \left\langle \frac{\partial m v_i v_k f}{\partial x_k} \right\rangle - 0 - 0 = 0, \qquad C - 10$$

$$\left\langle \frac{\partial mv_i f}{\partial t} \right\rangle + \left\langle \frac{\partial m(u_i + c_i)(u_k + c_k) f}{\partial x_k} \right\rangle = 0, \qquad C - 11$$

$$\left\langle \frac{\partial mv_i f}{\partial t} \right\rangle + \left\langle \frac{\partial mc_k c_i f}{\partial x_k} \right\rangle + \left\langle \frac{\partial mu_i u_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial mu_i c_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial mu_k c_i f}{\partial x_k} \right\rangle = 0, \quad C - 12$$

$$\left\langle \frac{\partial mv_i f}{\partial t} \right\rangle + \left\langle \frac{\partial mc_k c_i f}{\partial x_k} \right\rangle + \left\langle \frac{\partial mu_i u_k f}{\partial x_k} \right\rangle + 0 + 0 = 0.$$
 C - 13

Then splitting the thermal velocity tensor as

$$\left\langle \frac{\partial mv_i f}{\partial t} \right\rangle + \left\langle \frac{\partial mu_i u_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial \left[mc_k c_i \right]^{(2)} f}{\partial x_k} \right\rangle + \left\langle \frac{1}{3} \frac{\partial mc_l c_l f}{\partial x_k} \delta_{ik} \right\rangle = 0.$$
 C - 14

Using the macroscopic definition of the statistical formula, we have

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_k}{\partial x_k} + \frac{\partial \Pi_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_i} = 0, \qquad C - 15$$

Finally, we have

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla . \rho \mathbf{u} \mathbf{u} + \nabla . \mathbf{\Pi} + \nabla p = 0.$$
 C - 16

Energy Conservation

Multiplication of Boltzmann equation with $\psi = mv^2/2$ and subsequent integration over velocity space yields

$$\left\langle \frac{mv^2}{2} \frac{\partial f}{\partial t} \right\rangle + \left\langle \frac{mv^2}{2} \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} \right\rangle = \left\langle \frac{mv^2}{2} \mathcal{R}[f, f_1] \right\rangle, \qquad C - 17$$

where collisional term is zero due to conservation of total energy in collisions. Since we need to integrate over velocity, we have to convert molecular velocity into peculiar velocity and then take all terms beside f to find appropriate macroscopic variable as

$$\left\langle \frac{\partial mv^2/2 f}{\partial t} \right\rangle - \left\langle \frac{1}{2} mf \frac{\partial v^2}{\partial t} \right\rangle + \left\langle \frac{\partial mv^2/2 \mathbf{v} f}{\partial \mathbf{x}} \right\rangle - \left\langle mf \frac{\partial \mathbf{v} v^2/2}{\partial \mathbf{x}} \right\rangle = 0. \quad C - 18$$

Due to independence of molecular velocity from spatial and time coordinates, we have

$$\left\langle \frac{\partial mv^2/2f}{\partial t} \right\rangle - 0 + \left\langle \frac{\partial mv^2/2\mathbf{v}f}{\partial \mathbf{x}} \right\rangle - 0 = 0.$$
 C - 19

Now let's write the molecular velocity as summation of thermal velocity and stream velocity, the we have

$$\left\langle \frac{\partial m/2 \left(u^2 + c^2 + 2\mathbf{uc} \right) f}{\partial t} \right\rangle - 0 + \left\langle \frac{\partial m/2 \left(u^2 + c^2 + 2\mathbf{uc} \right) \mathbf{v} f}{\partial \mathbf{x}} \right\rangle - 0 = 0, \qquad C - 20$$

$$\left\langle \frac{\partial \left(mu^2/2 + mc^2/2 \right) f}{\partial t} \right\rangle + \left\langle \frac{\partial m/2 \left(u^2 + c^2 + 2u_i c_i \right) v_k f}{\partial x_k} \right\rangle = 0, \qquad C - 21$$

$$\left\langle \frac{\partial \left(mu^2/2 + mc^2/2 \right) f}{\partial t} \right\rangle + \left\langle \frac{\partial u^2 mv_k f/2}{\partial x_k} \right\rangle + \left\langle \frac{\partial mc^2 v_k f/2}{\partial x_k} \right\rangle + \left\langle \frac{\partial u_i mc_i v_k f}{\partial x_k} \right\rangle = 0, \quad C - 22$$

where

$$\left\langle \frac{\partial mc^2 \left(c_k + u_k \right) f / 2}{\partial x_k} \right\rangle = \left\langle \frac{\partial \frac{1}{2} mc^2 c_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial u_k \frac{1}{2} mc^2 f}{\partial x_k} \right\rangle, \quad C - 23$$

$$\left\langle \frac{\partial \frac{1}{2} mc^2 c_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial u_k \frac{1}{2} mc^2 f}{\partial x_k} \right\rangle = \frac{\partial Q_k}{\partial x_k} + \frac{\partial \rho u_k e_{\text{int}}}{\partial x_k}, \quad \text{C} - 24$$

and

$$\left\langle \frac{\partial u_i m c_i v_k f}{\partial x_k} \right\rangle = \left\langle \frac{\partial u_i m c_i c_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial u_i m c_i u_k f}{\partial x_k} \right\rangle, \quad C - 25$$

$$\left\langle \frac{\partial u_i m c_i c_k f}{\partial x_k} \right\rangle + \left\langle \frac{\partial u_i u_k m c_i f}{\partial x_k} \right\rangle = \left\langle \frac{\partial u_i \left[m c_i c_k \right]^{(2)} f}{\partial x_k} \right\rangle + \left\langle \frac{1}{3} \frac{\partial u_i m c_l c_l f}{\partial x_k} \delta_{ik} \right\rangle, \qquad C - 26$$

$$\left\langle \frac{\partial u_i \left[mc_i c_k \right]^{(2)} f}{\partial x_k} \right\rangle + \left\langle \frac{1}{3} \frac{\partial u_i mc_i c_l f}{\partial x_k} \delta_{ik} \right\rangle = \frac{\partial u_i \Pi_{ik}}{\partial x_k} + \frac{\partial u_k p}{\partial x_k} .$$
 C - 27

Putting all calculated terms together we have

$$\frac{\partial \left(\rho u^2/2 + \rho e_{\text{int}}\right)}{\partial t} + \frac{\partial u_k \rho u^2/2}{\partial x_k} + \frac{\partial u_k \rho e_{\text{int}}}{\partial x_k} + \frac{\partial Q_k}{\partial x_k} + \frac{\partial u_i \Pi_{ik}}{\partial x_k} + \frac{\partial u_k p}{\partial x_k} = 0, \qquad \text{C} - 28$$

and finally the conservation of total energy reads as

$$\frac{d(\rho u^2/2 + \rho e_{\text{int}})}{dt} + (\rho u^2/2 + \rho e_{\text{int}})\nabla \mathbf{.u} + p\nabla \mathbf{.u} + \nabla \mathbf{.Q} + (\nabla \mathbf{.\Pi}) \mathbf{.u} = 0.$$
 C - 29

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APPENDIX D. Derivation of constitutive equations from the Boltzmann kinetic equation (monatomic gas)

Stress balance equation

Multiplication of Boltzmann equation with $\psi = m [\mathbf{cc}]^{(2)}$ and subsequent integration over velocity space yields

$$\left\langle m \left[\mathbf{cc} \right]^{(2)} \frac{df}{dt} \right\rangle + \left\langle m \left[\mathbf{cc} \right]^{(2)} \mathbf{c} \frac{\partial f}{\partial \mathbf{x}} \right\rangle = \left\langle m \left[\mathbf{cc} \right]^{(2)} \mathcal{R} \left[f, f_1 \right] \right\rangle, \qquad D - 1$$

where the collisional term is not zero and denotes by $\Delta[\mathbf{\Pi}] = \langle \mathbf{m}[\mathbf{cc}]^{(2)} \mathcal{R}[\mathbf{f},\mathbf{f}_1] \rangle$. As we need to integrate over velocity, we have to convert the molecular velocity into peculiar velocity and then bring it together with f as

$$\left\langle \frac{dm [\mathbf{cc}]^{(2)} f}{dt} \right\rangle - \left\langle mf \frac{d [\mathbf{cc}]^{(2)}}{dt} \right\rangle + \left\langle \frac{\partial m [\mathbf{cc}]^{(2)} \mathbf{c}f}{\partial \mathbf{x}} \right\rangle - \left\langle mf \frac{\partial m [\mathbf{cc}]^{(2)} \mathbf{c}}{\partial \mathbf{x}} \right\rangle = \Delta [\mathbf{\Pi}]. \quad \mathbf{D} - 2$$

et's to write this equation in index notation form as

Let's to write this equation in index notation form as

$$\left\langle \frac{dm[c_i c_j]^{(2)} f}{dt} \right\rangle - \left\langle mf[\frac{dc_i}{dt} c_j]^{(2)} \right\rangle - \left\langle mf[c_i \frac{dc_j}{dt}]^{(2)} \right\rangle + \left\langle \frac{\partial m[c_i c_j]^{(2)} c_k f}{\partial x_k} \right\rangle - \left\langle mf \frac{\partial [c_i c_j]^{(2)} c_k}{\partial x_k} \right\rangle = \Delta[\Pi_{ij}].$$
D-3

Now, let's manipulate this equation as follows, by considering the independence of molecular velocity from spatial and time coordinates

$$\left\langle \frac{dm[c_i c_j]^{(2)} f}{dt} \right\rangle + \left\langle mf[\frac{du_i}{dt} c_j]^{(2)} \right\rangle + \left\langle mf[c_i \frac{du_j}{dt}]^{(2)} \right\rangle + \left\langle \frac{\partial m[c_i c_j]^{(2)} c_k f}{\partial x_k} \right\rangle$$

$$- \left\langle mf \frac{\partial [c_i c_j]^{(2)} c_k}{\partial x_k} \right\rangle = \Delta [\Pi_{ij}],$$

$$D - 4$$

$$\left\langle \frac{dm[c_ic_j]^{(2)}f}{dt} \right\rangle + \left\langle mf[\frac{du_i}{dt}c_j]^{(2)} \right\rangle + \left\langle mf[c_i\frac{du_j}{dt}]^{(2)} \right\rangle + \left\langle \frac{\partial m[c_ic_j]^{(2)}c_kf}{\partial x_k} \right\rangle +$$

$$\left\langle mf[\frac{\partial u_i}{\partial x_k}c_j]^{(2)}c_k \right\rangle + \left\langle mfc_k[c_i\frac{\partial u_j}{\partial x_k}]^{(2)} \right\rangle + \left\langle mf[c_ic_j]^{(2)} \right\rangle \frac{\partial u_k}{\partial x_k} = \Delta[\Pi_{ij}],$$

$$\left\langle \frac{dm[c_ic_j]^{(2)}f}{dt} \right\rangle + \left\langle mf[\frac{du_i}{dt}c_j]^{(2)} \right\rangle + \left\langle mf[c_i\frac{du_j}{dt}]^{(2)} \right\rangle + \left\langle \frac{\partial m[c_ic_j]^{(2)}c_kf}{\partial x_k} \right\rangle +$$

$$D - 5$$

$$D - 6$$

where

$$\left\langle mf\left[c_{i}\frac{du_{j}}{dt}\right]^{(2)}\right\rangle = \frac{1}{2} \left(\left\langle mfc_{i}\frac{du_{j}}{dt}\right\rangle + \left\langle mfc_{j}\frac{du_{i}}{dt}\right\rangle \right) - \frac{1}{3} \left\langle mfc_{k}\frac{du_{k}}{dt}\delta_{ij}\right\rangle = \frac{1}{2} \left(\left\langle mfc_{i}\right\rangle \frac{du_{j}}{dt} + \left\langle mfc_{j}\right\rangle \frac{du_{i}}{dt} \right) - \frac{1}{3} \left\langle mfc_{k}\right\rangle \frac{du_{k}}{dt}\delta_{ij} = D - 7 \frac{1}{2} \left(0\frac{du_{j}}{dt} + 0\frac{du_{i}}{dt} \right) - \frac{1}{3} 0\frac{du_{k}}{dt}\delta_{ij} = 0.$$

Therefore,

$$\left\langle mf[c_j \frac{du_i}{dt}]^{(2)} \right\rangle = \left\langle mf[c_i \frac{du_j}{dt}]^{(2)} \right\rangle = 0.$$
 D - 8

It is possible to simplified (D - 6) further;

$$2\left\langle mf\left[\frac{\partial u_i}{\partial x_k}c_j\right]^{(2)}c_k\right\rangle = \left\langle mfc_jc_k\frac{\partial u_i}{\partial x_k}\right\rangle + \left\langle mfc_ic_k\frac{\partial u_j}{\partial x_k}\right\rangle - \frac{2}{3}\left\langle mfc_rc_k\frac{\partial u_r}{\partial x_k}\delta_{ij}\right\rangle, \qquad \mathbf{D} - 9$$

$$\left\langle \frac{dm[c_ic_j]^{(2)}f}{dt} \right\rangle + \left\langle \frac{\partial m[c_ic_j]^{(2)}c_kf}{\partial x_k} \right\rangle + \left\langle mfc_jc_k \right\rangle \frac{\partial u_i}{\partial x_k} + \left\langle mfc_ic_k \right\rangle \frac{\partial u_j}{\partial x_k} - \frac{2}{3} \left\langle mfc_rc_k \right\rangle \frac{\partial u_r}{\partial x_k} \delta_{ij} + \left\langle mf[c_{ij}]^{(2)} \right\rangle \frac{\partial u_k}{\partial x_k} = \Delta[\Pi_{ij}].$$

Now, it is the time for opening the thermal velocity tensor and simplified stress transfer equation such that;

$$\left\langle \frac{dm[c_ic_j]^{(2)}f}{dt} \right\rangle + \left\langle \frac{\partial m[c_ic_j]^{(2)}c_kf}{\partial x_k} \right\rangle + \left\langle mf[c_jc_k]^{(2)} \right\rangle \frac{\partial u_i}{\partial x_k} + \frac{1}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_i}{\partial x_k} \delta_{jk} + \left\langle mf[c_ic_k]^{(2)} \right\rangle \frac{\partial u_j}{\partial x_k} + \frac{1}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_j}{\partial x_k} \delta_{ik} + \frac{1}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_i}{\partial x_k} \delta_{ik} + \frac{1}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_i}{\partial x_k} \delta_{ik} + \frac{1}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_i}{\partial x_k} \delta_{ik} + \frac{1}{3} \left\langle mf[c_ic_j]^{(2)} \right\rangle \frac{\partial u_i}{\partial x_k} \delta_{ij} - \frac{2}{3} \left\langle mfc_rc_r \right\rangle \frac{\partial u_r}{\partial x_r} \delta_{ij} + \left\langle mf[c_ic_j]^{(2)} \right\rangle \frac{\partial u_k}{\partial x_k} = \Delta[\Pi_{ij}].$$

Using the macroscopic definition of the statistical formula, we have

$$\frac{d\Pi_{ij}}{dt} + \left\langle \frac{\partial m[c_i c_j]^{(2)} c_k f}{\partial x_k} \right\rangle + \Pi_{jk} \frac{\partial u_i}{\partial x_k} + p \frac{\partial u_i}{\partial x_j} + \Pi_{ik} \frac{\partial u_j}{\partial x_k} + p \frac{\partial u_i}{\partial x_k} + \frac{\partial$$

From mass balance it is known that $\nabla \mathbf{u} = -\frac{1}{\rho} \frac{d\rho}{dt}$, therefore, stress balance equation

can be written as

$$\rho \frac{d\left(\frac{\mathbf{\Pi}}{\rho}\right)}{dt} + \left\langle \nabla \cdot \left(m[\mathbf{cc}]^{(2)}\mathbf{c}f\right) \right\rangle + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \Delta[\mathbf{\Pi}].$$
 D - 13

which is the same as one derived in [1, 13].

Heat flux balance equation

Multiplication of Boltzmann equation with $\Psi = \left(\frac{m}{2}c^2 + m\varepsilon_{\text{inter-atomic}}\right)\mathbf{c}$ and

subsequent integration over velocity space yields

$$\left\langle \left(\frac{m}{2}c^{2} + m\varepsilon_{\text{inter-atomic}}\right)\mathbf{c}\frac{df}{dt}\right\rangle + \left\langle \left(\frac{m}{2}c^{2} + m\varepsilon_{\text{inter-atomic}}\right)\mathbf{c}\mathbf{c}\frac{\partial f}{\partial \mathbf{x}}\right\rangle = \left\langle \left(\frac{m}{2}c^{2} + m\varepsilon_{\text{inter-atomic}}\right)\mathbf{c}\mathcal{R}[f, f_{1}]\right\rangle, \qquad D - 14$$

where the collisional term is equal to $\Delta[\mathbf{Q}] = \left\langle \left(\frac{m}{2}\mathbf{c}^2 + m\varepsilon_{inter-atomic}\right)\mathbf{c}\mathcal{R}[\mathbf{f},\mathbf{f}_1] \right\rangle$. Note

that the $\mathcal{ME}_{inter-atomic}$ is zero for monatomic gases.

As we need to integrate over velocity, we have to convert the molecular velocity into peculiar velocity and then bring it with f together as

$$\left\langle \frac{d \frac{m}{2} c^2 \mathbf{c} f}{dt} \right\rangle - \left\langle mf \frac{d \frac{c^2}{2} \mathbf{c}}{dt} \right\rangle + \left\langle \frac{\partial \frac{m}{2} c^2 \mathbf{c} \mathbf{c} f}{\partial \mathbf{x}} \right\rangle - \left\langle \frac{m}{2} f \frac{\partial c^2 \mathbf{c} \mathbf{c}}{\partial \mathbf{x}} \right\rangle = \Delta [\mathbf{Q}]. \quad \mathbf{D} - 15$$

Now, let's manipulate this equation as follows, by considering the independence of molecular velocity from spatial and time coordinates

$$\left\langle \frac{d \frac{m}{2} c^2 c_i f}{dt} \right\rangle - \left\langle mf \frac{d \frac{c^2}{2} c_i}{dt} \right\rangle + \left\langle \frac{\partial \frac{m}{2} c^2 c_k c_i f}{\partial x_k} \right\rangle - \left\langle \frac{m}{2} f \frac{\partial c^2 c_k c_i}{\partial x_k} \right\rangle = \Delta \left[Q_i \right] \quad \text{D-16}$$

such that

$$\left\langle \frac{d \frac{m}{2} c^{2} c_{i} f}{dt} \right\rangle + \left\langle \frac{\partial \frac{m}{2} c^{2} c_{k} c_{i} f}{\partial x_{k}} \right\rangle - \left\langle m f \frac{c_{r} c_{r}}{2} \frac{d c_{i}}{dt} \right\rangle - \left\langle m f c_{i} c_{r} \frac{d c_{r}}{dt} \right\rangle$$
$$- \left\langle \frac{m}{2} f c^{2} c_{k} \frac{\partial c_{i}}{\partial x_{k}} \right\rangle - \left\langle \frac{m}{2} f c^{2} c_{i} \frac{\partial c_{k}}{\partial x_{k}} \right\rangle - \left\langle m f c_{k} c_{i} c_{r} \frac{\partial c_{r}}{\partial x_{k}} \right\rangle = \Delta [Q_{i}].$$

Knowing that $\frac{dc}{dx} = -\frac{du}{dx}, \frac{dc}{dt} = -\frac{du}{dt}$, we have

$$\left\langle \frac{d \frac{m}{2} c^2 c_i f}{dt} \right\rangle + \left\langle \frac{\partial \frac{m}{2} c^2 c_k c_i f}{\partial x_k} \right\rangle + \left\langle mf c_k c_i c_r \right\rangle \frac{\partial u_r}{\partial x_k} + \left\langle mf \frac{c_r c_r}{2} \right\rangle \frac{du_i}{dt} + D - 18$$
$$\left\langle mf c_i c_r \right\rangle \frac{du_r}{dt} + \left\langle \frac{m}{2} f c^2 c_k \right\rangle \frac{\partial u_i}{\partial x_k} + \left\langle \frac{m}{2} f c^2 c_i \right\rangle \frac{\partial u_k}{\partial x_k} = \Delta [Q_i].$$

From momentum and mass balance we know that;

$$\frac{\partial \rho u_i}{\partial t} + u_k \frac{\partial \rho u_i}{\partial x_k} + \rho u_i \frac{\partial u_k}{\partial x_k} + \frac{\partial \Pi_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_i} = 0,$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0,$$

$$D - 19$$

such that

$$\frac{du_i}{dt} = -\frac{1}{\rho} \left(\frac{\partial \Pi_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_k} \delta_{ik} \right).$$
 D - 20

It is possible to simplified (D - 18) further by replacing $\frac{du_i}{dt}$ from (D - 20);

$$\frac{d\left\langle\frac{m}{2}c^{2}c_{i}f\right\rangle}{dt} + \frac{\partial\left\langle\frac{m}{2}c^{2}c_{k}c_{i}f\right\rangle}{\partial x_{k}} + \left\langle mfc_{k}c_{i}c_{r}\right\rangle\frac{\partial u_{r}}{\partial x_{k}} - e_{internal}\left(\frac{\partial\Pi_{ik}}{\partial x_{k}} + \frac{\partial p}{\partial x_{k}}\delta_{ik}\right) \qquad D - 21$$
$$-\frac{1}{\rho}\left(\Pi_{ir} + p\delta_{ir}\right)\left(\frac{\partial\Pi_{rk}}{\partial x_{k}} + \frac{\partial p}{\partial x_{k}}\delta_{rk}\right) + Q_{k}\frac{\partial u_{i}}{\partial x_{k}} + Q_{i}\frac{\partial u_{k}}{\partial x_{k}} = \Delta[Q_{i}],$$

or

$$\frac{dQ_{i}}{dt} + \frac{\partial \left\langle \frac{m}{2} c_{i} c^{2} c_{k} f \right\rangle}{\partial x_{k}} + \left\langle mfc_{k} c_{i} c_{r} \right\rangle \frac{\partial u_{r}}{\partial x_{k}} - \frac{\Pi_{ir}}{\rho} \left(\frac{\partial \Pi_{rk}}{\partial x_{k}} + \frac{\partial p}{\partial x_{r}} \right)$$

$$- \left(\frac{p}{\rho} + e_{internal} \right) \frac{\partial \Pi_{ik}}{\partial x_{k}} - \left(\frac{p}{\rho} + e_{internal} \right) \frac{\partial p}{\partial x_{i}} + Q_{k} \frac{\partial u_{i}}{\partial x_{k}} + Q_{i} \frac{\partial u_{k}}{\partial x_{k}} = \Delta [Q_{i}].$$

$$1 dQ = p$$

Knowing that $\nabla \mathbf{u} = -\frac{1}{\rho} \frac{d\rho}{dt}$ and $\frac{p}{\rho} + e_{internal} = c_p T$, we can write above equation as

$$\rho \frac{d\left(\frac{\mathbf{Q}}{\rho}\right)}{dt} + \nabla \cdot \left(\left\langle\frac{m}{2}c^{2}\mathbf{ccf}\right\rangle - c_{p}T(\mathbf{\Pi} + p\mathbf{I})\right) + \left\langle mf\mathbf{ccc}\right\rangle : \nabla \mathbf{u} - \frac{\mathbf{\Pi}}{\rho}\nabla \cdot \left(\mathbf{\Pi} + p\mathbf{I}\right) + c_{p}\nabla T \cdot (\mathbf{\Pi} + p\mathbf{I}) + \mathbf{Q} \cdot \nabla \mathbf{u} = \Delta[\mathbf{Q}].$$

which is the same as one derived in [1, 13].

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