A Thesis for the Degree of Doctor of Philosophy

Development of a 3D discontinuous Galerkin method for the second-order Boltzmann-Curtiss based hydrodynamic models of diatomic and polyatomic gases

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Last words are the Indian Mythology "Bhagavad Gita, Chapter II, Verse 47",

कर्मणये वाधिकारस्ते मां फलेषु कदाचन । मां कर्मफलहेतुर्भूः मांते संङगोस्त्वकर्मणि ।।

Dedication

In the memory of my loving mother Late Smt. Vidya Devi

Table of Contents

Acknowledgement	iii
Dedication	iv
Table of Contents	V
List of Figures	xii
Nomenclatures	xix
Abstract	xxiv
Abstract in Korean	xxvii
Chapter 1. Introduction	1
1.1 Objective	1
1.2 Contents of the thesis	2
Chapter 2. Basics of gas kinetic theory	4
2.1 Gas flow regimes classification	4
2.1.1 Flow regimes based on Knudsen number	4
2.1.2 Flow regimes based on Tsien's parameter	5
2.1.3 Estimation of mean free path	7
2.2 Thermal nonequilibrium phenomena and bulk viscosity	8
2.2.1 Thermal nonequilibrium phenomena	8
2.2.2 Bulk viscosity derivation from conventional theory	10
2.2.3 Physical interpretation of bulk viscosity	13
2.3 Microscopic properties	15
2.3.1 Basic molecular properties	15
2.3.2 Gas properties	17
2.3.3 Phase density distribution	19
2.4 Macroscopic properties	19
2.4.1 Density	19

2.4.2 Velocity	20
2.4.3 Temperature	20
2.4.4 Energy	21
2.4.5 Pressure tensor	22
2.4.6 Viscous stress tensor	22
2.4.7 Excess normal stress	22
2.4.8 Hydrostatic pressure	23
2.4.9 Heat flux vector	23
2.5 Classical Boltzmann kinetic equation	24
2.6 Classical Boltzmann-Curtiss kinetic equation	26
2.7 Direct Simulation Monte Carlo method	
2.8 Moments of Boltzmann-Curtiss kinetic equation	30
2.8.1 Collisional invariants	30
2.8.2 Conservation laws	31
Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33
Chapter 3. Boltzmann-Curtiss based hydrodynamic models	 33
Chapter 3. Boltzmann-Curtiss based hydrodynamic models 3.1 The moment method 3.2 Eu's generalized hydrodynamic equations	33
Chapter 3. Boltzmann-Curtiss based hydrodynamic models 3.1 The moment method 3.2 Eu's generalized hydrodynamic equations 3.3 Boltzmann-Curtiss based constitutive models via the balance closure	33
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 33 37 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 33 42 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 33 42 42 42 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 33 42 42 42 42 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models 3.1 The moment method 3.2 Eu's generalized hydrodynamic equations 3.3 Boltzmann-Curtiss based constitutive models via the balance closure 3.3.1 Zero-order Boltzmann-Curtiss based model 3.3.2 First-order Boltzmann-Curtiss based model 3.3 Second-order Boltzmann-Curtiss based model 3.4 Governing equations for numerical simulation 3.4.1 Conservative form of the conservation laws 	33 33 42 42 42 42 42 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 37 42 42 42 42 42 42 42 42 42 42 42 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	33 33 37 42
 Chapter 3. Boltzmann-Curtiss based hydrodynamic models	

3.5.2 One-dimensional shear-velocity constitutive relation	
3.6 Numerical Solver of the second-order Boltzmann-Curtiss based constitutiv	ve relations:
iterative method	
3.7 Breakdown parameters	
3.7.1 Bird's breakdown parameter	64
3.7.2 Boyd's breakdown parameter	65
3.7.3 Rayleigh-Onsagar's breakdown parameter	65
Chapter 4. Discontinuous Galerkin method	68
4.1 Numerical methods for modern CFD	
4.1.1 Finite difference method	
4.1.2 Finite element method	69
4.1.3 Finite volume method	
4.1.4 High order spectral method	71
4.2 Discontinuous Galerkin method	
4.3 Problem definition in DG framework	74
4.3.1 Discontinuous Galerkin spatial discretization	75
4.3.2 Elemental formulation	77
4.3.3 Weak DG formulation	
4.4 Elemental transformation to computational space	
4.4.1 One-dimensional elemental transformation	
4.4.2 Two-dimensional elemental transformation	
4.4.3 Three-dimensional elemental transformation	
4.5 Foundation of basis functions	
4.5.1 Number of required basis functions	
4.5.2 Basis functions for one-dimensional problem	
4.5.3 Basis functions for two-dimensional problem	
4.5.4 Basis functions for three-dimensional problem	95

4.5.5 Derivatives of basis functions	95
4.5.6 Evaluation of mass Matrix	96
4.6 Numerical integration in computational domain	97
4.6.1 Numerical integration in one-dimensional space	98
4.6.2 Numerical integration in two-dimensional space	99
4.6.3 Numerical integration in three-dimensional space	101
4.7 Initialization of DG solver	102
4.8 Time discretization of the problem	103
4.8.1 Time step calculation	103
4.9 Numerical flux functions	104
4.10 Numerical boundary conditions	106
4.10.1 Far-field boundary	106
4.10.2 Inviscid wall boundary	107
4.10.3 No-slip viscous wall boundary	108
4.10.4 Viscous slip wall boundary	108
4.10.5 Symmetry boundary	111
4.10.6 Outflow boundary	112
4.11 Implementation of limiters	112
4.11.1 Positivity preserving limiter	112
4.11.2 The Barth Jespersen limiter	113
Chapter 5. Solutions of zero and first-order Boltzmann-Curtiss bas	ed
hydrodynamic models	115
5.1 One-dimensional problems	116
5.1.1 One-dimensional Riemann problem	116
5.2 Two-dimensional problems	119
5.2.1 Two-dimensional double Mach reflection problem	119
5.2.2 Two-dimensional forward facing step problem	

5.2.3 Two-dimensional shock-vortex interaction problem	
5.2.4 Two-dimensional shock-bubble interaction problem	
5.3 Three-dimensional problems	127
5.3.1 Three-dimensional Sod shock tube problem	127
5.3.2 Three-dimensional 123 problem	131
5.3.3 Three-dimensional explosion problem	131
5.3.4 Three-dimensional double Mach reflection problem	133
5.3.5 Three-dimensional forward facing step problem	134
5.3.6 Three-dimensional transonic flow over a G400 aircraft	135
5.3.7 Three-dimensional subsonic viscous flow past a sphere	137
Chapter 6. Solution of second-order Boltzmann-Curtiss based	
hydrodynamic models: 1D and 2D problems	140
6.1 One-diemensional compression dominant problem: shock structure	140
6.2 Two-dimensional hypersonic flow past a cylinder	144
6.3 Two-dimensional hypersonic flow over a rectangular block	149
6.4 Shock-vortex interaction problem	151
6.4.1 Problem definition	153
6.4.2 Important physical quantities in SVI Problem	155
6.4.3 Grid refinement and validation of numerical solver	158
6.4.4 Effects of diatomic and polyatomic gases on SVI	
6.4.5 Characteristics of micro SVIs in diatomic and polyatomic gases	171
Chapter 7. Solution of second-order Boltzmann-Curtiss based	
hydrodynamic models: 3D problems	179
7.1 Hypersonic flow over a sphere: effect of slip boundary condition	179
7.2 Hypersonic flow over a sphere: second-order Boltzmann-Curtiss solutions.	
7.3 Three-dimensional supersonic flow over a flat plate	
7.4 Three-dimensional hypersonic gas flow past a re-entry vehicle	

Chapter 8. Parallelization of DG Solver	185
8.1 Background	185
8.2 Domain decomposition	186
8.3 Communication process	187
8.4 Merging of sub domains	
8.5 Parallel performance measurement	191
8.6 Computational cost of Boltzmann-Curtiss based models	192
8.7 Parallel performance of Boltzmann-Curtiss based models	193
Chapter 9. Conclusion and future works	197
9.1 Conclusion of present thesis	197
9.2 Scope of future works	
9.2.1 Study on various numerical solvers for viscous-dominant problems	
9.2.2 Vibrational nonequilibrium effects on gas flow problems	199
9.2.3 Study of rarefied gas flows between rotating concentric cylinders	199
9.2.4 Unsteady turbulent flow problems	200
Appendix A. Basics of vector and tensor theory	202
Appendix B. Derivation of conservation laws from Boltzmann-Curti	SS
kinetic equation	213
Appendix C. Derivation of constitutive equations from Boltzmann-C	Curtiss
kinetic equation	218
Appendix D. Three-dimensional form of second-order Boltzmann-C	urtiss
based constitutive equations	222
Appendix E. Quadrature points for numerical integration	227
Appendix F. Flow chart of development of 3D DG solver	230
Appendix G. Computational cost comparison between DG and FV	
methods	236

Appendix H. Basics of aerodynamics theory	241
Bibliography	248

List of Figures

Figure 2-1. Flow regime classification based on Knudsen number
Figure 2-2. Flow regime classification based on Tsien's parameter
Figure 2-3. Physical paramters of monatomic, diatomic and polyatomic gases14
Figure 3-1. A glance of Boltzmann-Curtiss based consitutive models up to second order 46
Figure 3-2. Comparison of stress tensor for first-order (top) and second-order (bottom)
Boltzmann-Curtiss constitutive models
Figure 3-3. Comparison of excess normal stress for first-order (top) and second-order (bottom)
Boltzmann-Curtiss constitutive models
Figure 3-4. Comparison of heat flux for first-order (top) and second-order (bottom) Boltzmann-
Curtiss constitutive models
Figure 3-5. Comparison of Rayleigh-Onsager dissipation parameter for first-order (top) and
second-order (bottom) Boltzmann-Curtiss constitutive models
Figure 3-6. Second-order model (diatomic and monatomic) relative to the first-order model in
the compression-expansion flow. The horizontal and vertical axes represent the
strain (force) term and the normal stress, respectively (Reproduced with
permission from Myong [39])
Figure 3-7. Second-order model (diatomic and monatomic) relative to the first-order model in
the shear flow. The horizontal and vertical axes represent the strain (force) term
and the shear and normal stress, respectively (Reproduced with permission from
Myong [39])
Figure 3-8. Comparison of the breakdown parameters in hypersonic rarefied gas flow with
M=5.48, Kn=0.5 [64]67
Figure 4-1. Transformation from physical line elment to computational standard element in
interval [-1,1]
Figure 4-2. Transformation from physical line elment to computational standard element in
interval [0,1]
Figure 4-3. Transformation from physical rectangular elment to computational standard
rectangular element in interval [-1,1]
Figure 4-4. Transformation from physical triangular element to computational triangular
element in interval [0,1]
Figure 4-5. Transformation from physical tetraherdral element to computational tetraherdral
element in interval [0,1]

Figure 4-6. Number of required basis (polynomial) functions up to 5 th order
Figure 4-7. Modes of one-dimensional Legendre basis functions up to 5 th order
Figure 4-8. Modes of one-dimensional scaled Legendre basis functions up to 5 th order 90
Figure 4-9. Complete scaled Legendre polynomial space, based on Pascal's triangle, for full
standard rectangular expansion up to 4 th order
Figure 4-10. Complete scaled Legendre polynomial space, based on Pascal's triangle, for full
standard triangular expansion up to 4 th order
Figure 4-11. A plot of the computed mass matrix for complete orthogonal polynomial space
up to 4 th order for full tetrahedral expansion
Figure 4-12. Number of required quadrature points for integrating inside and over one-
dimensional master element for (a) $p=0$, (b) $p=1$, and (c) $p=2$ order of space
polynomials
Figure 4-13. Number of required quadrature points for integrating inside and over the two-
dimensional master triangular element for (a) $p=0$, (b) $p=1$, and (c) $p=2$ order of
space polynomials
Figure 4-14. Number of required quadrature points for integrating inside and over the two-
dimensional master rectangular element for (a) $p=0$, (b) $p=1$, and (c) $p=2$ order of
space polynomials
Figure 4-15 Number of required quadrature points for numerical integration in a three-
dimensional tetrahedron element for (a) $p=0$, (b) $p=1$, and (c) $p=2$ order of space
polynomials
Figure 5-1. Initial conditions of various one-dimensional Riemann test cases 116
Figure 5-2. One-dimensional Riemann problem: Sod shock tube problem (left): the density,
pressure, velocity distribution contours at $t=0.25$, and Lax shock tube problem
(right): the density, pressure, velocity distribution contours at $t=0.14117$
Figure 5-3. One-dimensional Riemann problem: 123 problem (left): the density, pressure,
velocity distribution contours at $t=0.15$, and blast wave problem (right): the density,
pressure, velocity distribution contours at <i>t</i> =0.012
Figure 5-4. Two-dimensional double Mach refelction problem: computational domain and
intial configuration
Figure 5-5. Two-dimensional double Mach reflection problem: density distribution contours
at <i>t</i> =0.2120
Figure 5-6. Two-dimensional forward facing step problem: computational domain

Figure 5-7. Two-dimensional forward facing step problem: density contours at various time Figure 5-8. Two-dimensional shock-vortex interaction problem: computational domain... 124 Figure 5-9. Two-dimensional shock-vortex interaction problem: computed (a) vorticity and (b) density distribution contours with shock Mach =1.2, Vortex Mach =0.5 at t=2.5. Figure 5-10. Two-dimensional shock-vortex interaction problem: computed (a) vorticity and (b) density distribution contours with shock Mach = 1.5, Vortex Mach = 0.7 at t=2.5. Figure 5-11. Two-dimensional shock-bubble interaction (SBI) problem: schematic diagram of Figure 5-12. Two-dimensional shock-bubble interaction (SBI) problem: schlieren images for Figure 5-13. Three-dimensional Sod shock tube problem: schematic diagram and initial Figure 5-14. Three-dimensional Sod shock tube problem: produced different waves after broken diaphragm......128 Figure 5-15. Three-dimensional Sod shock tube problem: the computed density (left) and pressure (right) distributions in three-dimensional view (upper); two-dimensional view (middle) and one-dimensional profiles (bottom) at t=0.2...... 129 Figure 5-16. Three-dimensional Riemann 123 problem: the computed density (left) and pressure (right) distributions in three-dimensional view (upper); two-dimensional Figure 5-17. Three-dimensional explosion problem: initial configuration at t = 0 sec. 132 Figure 5-18. Three-dimensional explosion problem: the computed density contours at t = 0.2Figure 5-19. Three-dimensional double Mach reflection problem: computed density contours. Figure 5-20. Three-dimensional forward facing step problem: computed density contours. 135 Figure 5-21. Three-dimensional transonic flow over a G400 aircraft: computational domain Figure 5-22. Three-dimensional transonic flow over a G400 aircraft: computed C_p value.. 136 Figure 5-23. Three-dimensional transonic flow over a G400 aircraft: pressure contours on wing.

Figure 5-24. Three-dimensional transonic flow over a G400 aircraft: computed streamlines. Figure 5-25. Three-dimensional subsonic viscous flow past a sphere: computational domain with unstructured tetrahedral mesh with 98,000 elements and 25,344 grid points. Figure 5-26. Three-dimensional subsonic viscous flow past a sphere: computed streamlines of the flow field (left) and from experiment (right) at Mach =0.3, Re=118 and AoA=0 Figure 5-27. Three-dimensional subsonic viscous flow past a sphere: computed Mach contours Figure 6-1. One-dimensional shock structure problem: normalized density profile for argon Figure 6-2. One-dimensional shock structure problem: normalized density profile for nitrogen gas at four different flow stem Mach numbers......143 Figure 6-3. One-dimensional shock structure problem: computed inverse shock density thickness profile for (a) argon, and (b) nitrogen gas. 144 Figure 6-4. Validation of second-order Boltzmann-Curtiss based model (NCCR) with the DSMC in density distribution for (a) M = 5.48, Kn = 0.05, and (b) M = 0.1, Kn =Figure 6-5. Comparison of normalized density contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen numbers...... 146 Figure 6-6. Comparison of Mach contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen numbers......146 Figure 6-7. Comparison of the degree of non-equilibrium contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen Figure 6-8. Pressure coefficient distribution around a cylinder at various Knudsen numbers for (a) the first-order, and (b) the second-order Boltzmann-Curtiss models [137]. 148 Figure 6-9. Normalized wall shear stress distribution around a cylinder at various Knudsen numbers for (a) the first-order, and (b) the second-order Boltzmann-Curtiss models Figure 6-10. Mach contours (Left), normalized density contours (middle), and streamlines (right) over a rectangular block for the second-order Boltzmann-Curtiss based

model at Mach=5.48, AoA=30 degree with various Knudsen numbers. 150

Figure 6-11. Schematic diagram of the flow model for shock-vortex interaction problem. 153
Figure 6-12. Grid refinement study: density contours in macro SVI
Figure 6-13. Grid refinement study: density (upper) and pressure (below) profiles at center-
line of computational domain in macro SVI
Figure 6-14. First-order Botlzmann-Curtiss constitutive model (Navier-Fourier) validation:
circumferential distribution of the pressure amplitude in macro SVI (Air gas). 159
Figure 6-15. Second-order Boltzmann-Curtiss based constitutive model validation: time
evolution of area-weighted enstrophy in micro SVI (Argon gas) 160
Figure 6-16. Time evolution of sound pressure for macro SVI161
Figure 6-17. Time evolution of sound pressure for micro SVI
Figure 6-18. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom):
sound pressure contours
Figure 6-19. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom):
vorticity contours
Figure 6-20. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom):
degree of thermal non-equilibrium contours
Figure 6-21. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom):
time evolution of enstrophy169
Figure 6-22. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom):
time evolution of dissipation rate
Figure 6-23. Vortex deformation in micro SVI: sound pressure contours with $M_{\nu} = 1.0.$ 172
Figure 6-24. Vortex deformation in micro SVI: time evolution of (a) Enstrophy and, (b)
dissipation rate with $M_{y} = 1.0$
Figure 6-25. Vortex deformation in micro SVI: time evolution of (a) net vorticity, (b) net
dilatational vorticity, (c) net baroclinic vorticity and, (d) net viscous vorticity with
<i>M</i> _w =1.0
Figure 6-26 Comparison of first-order (upper) and second-order (bottom) constitutive models
on micro SVI: sound pressure contours with different incoming shock Mach
number and $M = 10$, $r = 10\lambda$ 176
Eigure 6.27 Comparison of first order and second order constitutive models for distance
(nitrogen) gas on micro SVI: time evolution of (a) enstronby and (b) discinction
(introgen) gas on micro S vi. time evolution of (a) ensurophy and, (b) dissipation rote with $M = 10$, $r = 10^{2}$
rate with $M_{\nu} = 1.0, r_1 = 10\lambda$.

Figure 6-28. Comparison of the classical first-order Navier-Stokes-Fourier, first-order Navier-
Fourier and second-order models for polyatomic (methane) gas on micro SVI:
degree of non-equilibrium contours with $M_s = 2.0$, $M_v = 0.8$, $r_1 = 10\lambda$
Figure 7-1. Hypersonic flow over sphere: slip boundary effects at $M = 5.48$, $Kn=0.0001180$
Figure 7-2. Computed Mach contours of hypersonic flow over sphere: a comparison between
first-order and second-order Boltzmann-Curtiss based constitutive models at
Mach=5.48, Kn = 0.1
Figure 7-3. Three-dimensional supersonic gas flows over a flat plate problem: computational
domain with unstructured tetrahedral elements
Figure 7-4. Three-dimensional supersonic gas flows over a flat plate problem: Mach contours
with M=4.36 and Re = 5.0×10^6
Figure 7-5. Three-dimensional hypersonic flow past a re-entry vehicle: computational domain
with unstructured tetrahedral meshes
Figure 7-6. Three-dimensional hypersonic flow past a re-entry vehicle: computed Mach
contours for first- and second-order Boltzmann-Curtiss based constitutive models
at Mach = 5.0 and Kn= 0.2 and AoA = 15 degree (upper) and AoA = 45 degree. 184
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
 at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184 Figure 8-1. Illustration of unified shell program for parallel processes. 186 Figure 8-2 Tetrahedral mesh partition using ParMETIS; different colors represent sub-domains owned by different processors. 187 Figure 8-3. Flow chart of DG parallel algorithm. 188 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). 189 Figure 8-5 Non-blocking communication pattern (Isend and Irecv block diagram). 189 Figure 8-6. Merging of the sub-domains for post-processing of the solutions: pressure contour of unified merged domain. 191 Figure 8-7 Computational cost of solving (a) the first-order Boltzmann-Curtiss constitutive relations, and (b) the second-order Boltzmann-Curtiss constitutive relations [137].
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184Figure 8-1. Illustration of unified shell program for parallel processes.186Figure 8-2 Tetrahedral mesh partition using ParMETIS; different colors represent sub-domains owned by different processors.187Figure 8-3. Flow chart of DG parallel algorithm.188Figure 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).189Figure 8-5 Non-blocking communication pattern (Isend and Irecv block diagram).189Figure 8-6. Merging of the sub-domains for post-processing of the solutions: pressure contour of unified merged domain.191Figure 8-7 Computational cost of solving (a) the first-order Boltzmann-Curtiss constitutive relations [137]. .193Figure 8-8 Parallel speed-up, S_p for the first-order Boltzmann-Curtiss constitutive model with
at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree. 184Figure 8-1. Illustration of unified shell program for parallel processes.186Figure 8-2 Tetrahedral mesh partition using ParMETIS; different colors represent sub-domains owned by different processors.187Figure 8-3. Flow chart of DG parallel algorithm.188Figure 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).189Figure 8-5 Non-blocking communication pattern (Isend and Irecv block diagram).191Figure 8-6. Merging of the sub-domains for post-processing of the solutions: pressure contour of unified merged domain.191Figure 8-7 Computational cost of solving (a) the first-order Boltzmann-Curtiss constitutive relations, and (b) the second-order Boltzmann-Curtiss constitutive relations [137].193Figure 8-8 Parallel speed-up, S_p for the first-order Boltzmann-Curtiss constitutive model with (a) DG piecewise constant, and (b) DG piecewise linear scheme [137].

model with (a) DG piecewise constant, and (b) DG piecewise linear scheme. 195

Nomenclatures

Greek

α	-	angle of attack
β	-	side-slip angle
γ	-	specific heat ratio
μ	-	first coefficient of dynamic (shear) viscosity
$\mu_{\scriptscriptstyle bulk}$	-	coefficient of bulk viscosity
λ	-	second coefficient of viscosity
ĸ	-	heat conduction coefficient
•	-	vector of auxiliary variable
	-	approximated auxiliary variable solution
$\mathbf{\Theta}_{h}^{L},\mathbf{\Theta}_{h}^{R}$		approximated auxiliary solution for left and right state
ξ,η,ζ	-	reference coordinates
ρ	-	density
λ_{mean}	-	mean free path
δ	-	boundary thickness layer of the body
$\pmb{\sigma}, \sigma_{_{ij}}$	-	stress tensor
τ, $τ_{ij}$, Π	-	viscous stress tensor
$\Pi_{xx}, \Pi_{yy}, \Pi_{zz}$	-	normal stress components
$\Pi_{xy}, \Pi_{xz}, \Pi_{yz}$	-	viscous stress components
Δ	-	excess normal stress
E, <i>E</i> _{ij}	-	symmetric or rate-of-strain tensor
ω, <i>ω</i> _{ij}	-	anti-symmetric tensor
$ abla \cdot \mathbf{u}$	-	dilatational term
ζ^{dof}	-	molecular internal degree of freedoms
$\zeta_{\rm internal}^{dof}$	-	internal energy modes
$\mathcal{E}_{ ext{kinetic}}$	-	specific kinetic energy per unit mass
$\mathcal{E}_{\text{internal}}$	-	specific internal energy per unit mass
$\mathcal{E}_{\text{potential}}$	-	specific potential energy per unit mass
ω	-	angular frequency
$\boldsymbol{\omega}_{\scriptscriptstyle B}$	-	vector of angular frequency
μ_{mass}	-	reduced mass of molecule
V	-	exponent of the inverse power law
Ψ	-	azimuth angle
$\mathbf{\Lambda}^{(n)}$	-	dissipation term
$\mathbf{\Psi}^{(n)}$	-	high-order moments

$\hat{\Psi}$	-	local calortropy density
$\sigma_{_c}$	-	calortropy production
$\mu_{_{Normalized}}$	-	normalized factor
\mathcal{D}	-	dimension of the space
∇_{v}	-	gradient with respect to velocity-space
Ω	-	bounded domain of the body
Ω_h	-	approximated domain
Ω_{e}	-	discretization element (local element)
$\partial \Omega$	-	boundary of the domain Ω
$\partial\Omega_{_D},\partial\Omega_{_N}$	-	region Dirichlet boundary, region of Neumann boundary
\mathbb{P}^k	-	space of polynomial functions of degree at most k
υ	-	test function
Ω_e^{st}	-	standard element
$J_{x \to \xi}$	-	jacobian of transformation
$P_n^{\alpha,\beta}$	-	orthogonal Jacobi polynomials
χ	-	flow properties
$\hat{\Lambda}^{x}_{inv}, \hat{\Lambda}^{y}_{inv}, \hat{\Lambda}^{z}_{inv}$	-	inviscid spectral radii
$\hat{\Lambda}_{vis}^{x}, \hat{\Lambda}_{vis}^{y}, \hat{\Lambda}_{vis}^{z}$	-	viscous spectral radii

Latin

L	-	charactertics length scale
Т	-	time
Kn	-	Knudsen number based on characteristics length scale
Kn_{δ}	-	Knudsen number based on boundary thickness layer
Kn _{GLL}	-	gradient length local based Knudsen number
N_{δ}	-	composite number
$B_{\rm max}$	-	Bird's breakdown parameter
Kn _{max}	-	Boyd's breakdown parameter
М	-	Mach number
Re	-	Reynolds number
Pr	-	Prandtl number
Ec	-	Eckert number
n	-	normal vector
r, x	-	position vector
V	-	particle velocity
u	-	bulk velocity vector
<i>u</i> , <i>v</i> , <i>w</i>	-	Cartesian components of velocity vector

J	-	Jacobian matrix
n	-	number density (molecule per unit volume)
d	-	molecular diameter
Т	-	overall temperature
$T_{_{W}}$	-	wall temperature
р	-	pressure
\overline{P}	-	mean pressure
K_{B}	-	Boltzmann constant
N_A	-	Avogadro number
R_{gas}	-	gas constant
C_{ijmn}	-	fourth-order viscosity coefficient tensor
$f_{\it bulk}$	-	ratio of bulk viscosity to shear viscosity
m	-	molecular mass
E_{total}	-	total energy
$E_{\rm kineic}$	-	kinetic energy
$E_{\rm internal}$	-	internal energy
$E_{\rm potential}$	-	potential energy
$E_{\mathrm{viberational}}$	-	vibrational energy
Ι	-	moment of inertia
j , <i>j</i>	-	angular momentum, magnitude of angular momentum
C_p	-	specific heat at constant pressure
C_{v}	-	specific heat at constant volume
S	-	viscosity index number
С	-	peculiar velocity
$H_{_{total}},h,\hat{h}$	-	total enthalpy, specific enthalpy, enthalpy density
Р	-	pressure tensor
Q	-	heat flux vector
Q_x, Q_y, Q_z	-	heat flux components
T_x, T_y, T_z	-	temperature components
Ι	-	unit tensor
H_{rot}	-	rotational Hamiltonian of the molecule
\overline{E}_{rot}	-	average rotational energy density
$f(\mathbf{v},\mathbf{r},t)$	-	single particle distribution
$f^{0}(\mathbf{v},\mathbf{r},t)$	-	equilibrium distribution function
f^{c}	-	nonequilibrium canonical distribution function
$\mathbf{F}^{external}$	-	vector of external forces
$C(f, f_2)$	-	collision operator

\mathbf{L}_r	-	internal Liouville operator
$h^{(n)}$	-	molecular expression for moments
$\mathbf{Z}^{(n)}$	-	kinematic term arising from hydrodynamic streaming effect
q_{1st}	-	first-order dissipation term
q_{2nd}	-	second-order dissipation term
k_1	-	first cumulant expansion
Ŕ	-	Rayleigh-Onsager dissipation function
\vec{S}	-	face vector
S_x, S_y, S_z	-	components of face vector
$\Delta \hat{S}^x, \Delta \hat{S}^y, \Delta \hat{S}^z$	-	Projections of the control volume
U	-	vector of conservative variables
\mathbf{U}_h	-	approximated solution of conservative variables
\mathbf{U}_{BC}	-	boundary state variable
$\mathbf{U}_{h}^{L},\mathbf{U}_{h}^{R}$	-	approximate solution for left and right states
$\mathbf{F}^{\mathrm{inv}}$	-	inviscid flux function
$\mathbf{F}^{\mathrm{vis}}$	-	viscous flux function
N_{E}	-	number of elements
N_F	-	number of faces
N_k	-	number of basis functions
b_k	-	basis function
$\mathbf{H}_{auxiliary}, \mathbf{H}_{auxiliary}^{b}$	-	numerical auxiliary flux, numerical boundary auxiliary flux
$\mathbf{H}_{inviscid}$, $\mathbf{H}^{b}_{inviscid}$	-	numerical inviscid flux, numerical boundary inviscid flux
$\mathbf{H}_{viscous}, \mathbf{H}_{viscous}^{b}$	-	numerical viscous flux, numerical boundary viscous flux
Μ	-	mass matrix
\mathbf{M}^{-1}	-	inverse of mass matrix
R (U)	-	residual vector of U variables
T_e	-	affine sub-parametric transformation

Abbreviation

DG	-	Discontinuous Galerkin
FD	-	Finite difference
FV	-	Finite volume
FE	-	Finite element
SD	-	Spectral difference
SV	-	Spectral volume
CFL	-	Courant–Friedrichs-Lewy number
RK	-	Runge-Kutta
RKDG		Runge-Kutta discontinuous Galerkin
TVB	-	Total variation bounded
TVD	-	Total variation diminishing
BR1	-	First Bassi-Rebay scheme
BR2	-	Second Bassi-Rebay scheme
DOF	-	Degree of freedom
LDG	-	Local discontinuous Galerkin
MPI	-	Message passage interface
SPMD	-	Single program multiple data
NSF	-	Navier-Strokes-Fourier
LTE	-	Local thermal equilibrium
NF	-	Navier-Fourier
NCCR	-	Nonlinear coupled constitutive relations
SVI	-	Shock-vortex interaction
SBI	-	Shock-bubble interaction

Abstract

Development of a 3D discontinuous Galerkin method for the second-order Boltzmann-Curtiss based hydrodynamic models of diatomic and polyatomic gases

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It is well known that in conventional approach, description of diatomic and polyatomic gases is basically the same as the monatomic gas; that is, it is based on the physical laws of conservation (mass, momentum, and energy), with the modified ratio of specific heats, and in conjunction with the first-order constitutive laws, the two-century-old so-called Navier-Stokes-Fourier equation based on a critical assumption made by Stokes in 1845 that the bulk viscosity vanishes. While the Stokes's hypothesis is certainly legitimate in the case of monatomic gases like argon, there is ever increasing evidence that now indicates that this is not the case for non-monatomic gases—like nitrogen (or air) and carbon dioxide—that are far from local thermal equilibrium. Therefore, the study of thermal non-equilibrium effects of diatomic and polyatomic gas flow is extremely important.

The general interest of the present study is to explore the suitable and proper master kinetic equations for describing diatomic and polyatomic gases and to develop computational methods to solve these kinetic equations. First, on the basis of Eu's generalized hydrodynamics and Myong's balanced closure, the second-order constitutive laws are derived from the Boltzmann-Curtiss kinetic equation for diatomic (and linear polyatomic) molecules. Then the topology of

the second-order nonlinear coupled constitutive relations in phase space is investigated for elementary flow situations like compression, expansion, and velocity shear. Lastly, a theoretical and computational attempt is made to highlight the rotational non-equilibrium effects in polyatomic gases by investigating the strong interaction of two important nonequilibrium phenomena in polyatomic gases –compressive shock structure and velocity-shear of the vortex—using the second-order constitutive laws.

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 two-dimensional Riemann problems. The basic structure of this hyperbolic system, such as contact discontinuity, shock wave, and rarefaction wave, were studied numerically. Although modern DG method has been successfully applied for solving the Euler equation, the validity of the Euler equation is restricted to an 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 is developed for solving the first-order Navier-Fourier and second-order Boltzmann-Curtiss based equations. The final judgment on the accuracy of the computational models is obtained through a rigorous study of verification and validation. The first-order and second-order Boltzmann-Curtiss based models are compared with the 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 solutions of first-order and second-order Boltzmann-Curtiss based model in the shock wave structure are considered as a verification study on conservative, primitive and non-conservative variables. A self-contained summary of numerical implementation of various limiters, numerical flux functions, and boundary conditions is provided for the pedagogical purpose.

Also, the three-dimensional Maxwell velocity slip and Smoluchowski temperature jump boundary conditions are provided for arbitrary geometries. Efficient numerical methods for solving non-linear implicit algebraic equations arising from the second-order Boltzmann-Curtiss based constitutive relations are described, and the solutions of the constitutive relations are analyzed in detail.

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

Abstract in Korean

Boltzmann – Curtiss 기반의 이원자·다원자 기체에 관한 2 차 정확도 유체역학 모델을 위한 3D 불연속 Galerkin 기법 개발

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지도교수: 명 노 신

기존의 이원자 및 다원자 기체에 관한 접근 방식은 단일원자 기체와 기본적으로 동일한 것으로 알려져 왔다. 즉, 비열비가 수정된 보존(질량, 운동량, 에너지) 물리 법칙에 기초하고 있으며, 1차 정확도 구성 법칙과 함께 Bulk 점성을 무시하는 Stokes 가정에 근거하여 2 세기 전(1845 년)에 유도된 이른바 Navier-Stokes-Fourier (NSF) 식을 그 근간으로 한다. Stokes 가정은 아르곤과 같은 단일원자 기체의 경우는 확실히 정당화되지만. 국소 열 평형과 거리가 먼 비단일원자 기체 (질소, 또는 공기, 이산화탄소)에는 그렇지 않다. 따라서 이원자와 다원자 기체 흐름의 열 비평형 효과에 대한 연구는 매우 중요하다.

본 연구에서는 이원자와 다원자 기체를 설명하는 적절한 마스터 운동 방정식을 연구하고 이에 기초한 수학적 지배 방정식에 관한 전산기법을 개발하는 것이다. 첫째, Generalized Hydrodynamics 와 Balanced Closure 이론을 기반으로 이원자 및 선형 다 원자 기체에 관한 2 차 정확도 구성 법칙을 Boltzmann-Curtiss 운동 방정식으로부터 유도한다. 위상 공간에서의 비선형 결합 구성 관계식에 관한 Topology 를 압축, 팽창 및 속도 전단류와 같은 기본 흐름의 경우에 대해 분석한다. 다음으로 다원자 기체의 회전 비평 형 효과를 강조하기 위해 다원자 기체의 중요한 두 가지 비평형 현상(충격파 내부 구조와 와류 내부의 속도 전단) 사이의 강한 상호 작용을 이론 및 전산계산을 통해 분석한다.

또한 본 연구에서는 먼저 1 차원과 2 차원의 Riemann 문제 해를 구하기 위해 Euler 시스템에 불연속 Galerkin (DG) 법을 적용하였다. 이 쌍곡선 시스템의 기본 구조 (접촉면, 불연속 충격파, 팽창파)를 수치적으로 연구하였다. 최신 DG 기법은 Euler 방정식을 푸는 데 성공했지만, Euler 방정식의 타당성은 평형 상태에 한정되므로 비평형 유동에는 유효하지 않다.

비평형 기체 유동을 분석하기 위해 1 차 NF와 2 차 Boltzmann-Curtiss 방정식을 풀기 위한 Mixed 기법 기반의 새로운 DG 기법을 개발하였다. 계산 모델의 정확도에 관한 최종 결정은 검증의 엄격한 검토를 통해 얻을 수 있다. 1 차 및 2 차 Boltzmann-Curtiss 모델을 다양한 문제에 적용한 다음 DSMC 의 계산과 실험 결과와 비교하였다. DG 법을 정상 상태 및 비정상 상태의 천이 유동 문제, 보존법칙의 Smooth 및 Stiff 문제를 대해 검증하였다. 보존적, 비보수적인 변수의 검증 연구를 위해 충격파 구조에 대한 1 차 및 2 차 Boltzmann-Curtiss 모델의 해석 해를 고려하였다. 다양한 Limiter, 수치 Flux 함수, 경계 조건의 수치 구현 기법을 요약하였다.

또한 임의의 기하학적 형상에 적용이 가능한 삼차원 Maxwell 미끄럼 및 Smoluchowski 온도 점프 경계 조건을 개발하였다. 2 차 Boltzmann-Curtiss 모델에 기초한 구성 관계식에서 나타나는 비선형 음함수 형태의 대수 방정식을 효율적인 계산하는 방법을 기술하였다.

xxviii

1 차 NF 와 2 차 Boltzmann-Curtiss 기반 Solver 의 계산 비용을 직렬 및 병렬 컴퓨터 시스템에 대해 분석하였다. 2 차 Boltzmann-Curtiss 기반 Solver 는 반복 수치기법에서 나타나는 반복 횟수가 유동 특성과 열적 비평형도에 따라 달라지기 때문에 계산 격자 수에 대해 비선형 거동을 나타내었다. 결론적으로 희박 및 마이크로 스케일 기체에 관한 2 차 정확도 Boltzmann-Curtiss 모델 기반의 비선형 결합 구성 관계식에 대해 불연속 Galerkin 코드는 초 병렬 특성을 보여주었다.

Chapter 1. Introduction

"Thinking should become your capital asset, no matter whatever ups and downs you come across in your life."

- A.P.J Abdul Kalam (1931-2015)

1.1 Objective

When the flow deviates from equilibrium state, the classical continuum description of fluid may not provide accurate information about the flow. Hence, application of kinetic theory, Boltzmann-Curtiss kinetic equation, or methods based on simplified kinetic theory are necessary to describe the flow with an acceptable level of accuracy. This work is motivated to elaborate the diatomic and polyatomic gas flows at equilibrium and far-from-equilibrium states using classical and non-classical constitutive relations derived from the Boltzmann-Curtiss equation kinetic, so-called Boltzmann-Curtiss based models. The Boltzmann-Curtiss based models considered in the present study are derived from Eu's hydrodynamics equations [1-6]. 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-Curtiss based models at a deep level. Accordingly, detailed information on the development of a modal DG method for one-, two-, and three- dimensional systems and application of various 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 a comprehensive explanation on both numerical and mathematical aspects of the DG methods to help researchers in the development of advanced high-order numerical schemes.

1.2 Contents of the thesis

This thesis is organized into following chapters. In Chapter 1, the objective of the present thesis and its contents are presented. Chapter 2 covers the fundamental of the kinetic theory including the classification of flow regimes, bulk viscosity with its applications, definition of microscopic and macroscopic properties based on density distribution, description of Boltzmann kinetic equation as well Boltzmann-Curtiss kinetic equation and Direct Simulation Monte Carlo (DSMC) method. In Chapter 3, derivation of Boltzmann-Curtiss based constitutive models, numerical methods for solving algebraic constitutive relations, and the description of the physical phenomena of the Boltzmann-Curtiss constitutive models are delivered.

In Chapter 4, development of the modal discontinuous Galerkin methods for onedimensional, two-dimensional, and three-dimensional systems is presented. A summary of available high-order CFD methods and categories of spectral methods is reviewed. Later, the efficient discretization of a problem in space and time based on discontinuous Galerkin formulation is discussed in detailed. Also, a detailed explanation of the discretization of inviscid and viscous flux functions, implementation of various boundary conditions as well as positivity preserving and Berth Jespersen limiters are provided.

In Chapter 5, solutions of zero- and first-order Boltzmann-Curtiss based hydrodynamic models for multi-dimensional problems are provided using a modal DG method. Various benchmark problems are solved, and their numerical results are compared with experiment, exact and other numerical solutions. In Chapter 6, the modal DG Solver is employed for solving the second-order Boltzmann-Curtiss based hydrodynamics model for one-dimensional and two-dimensional rarefied and microscale gas flow problems. And, the numerical results are compared with exact, experimental and DSMC method. Chapter 7 deals with the solution of the second-order Boltzmann-Curtiss based hydrodynamic model

for three-dimensional flow problems, and results are compared with experimental data. Chapter 8 provides detailed information on parallelization of DG solvers using single program multi data (SPMD) parallel programming methods. The computational costs of both solvers using serial and parallel solvers based on Boltzmann-Curtiss models are discussed. Finally, Chapter 9 summarizes all the important findings from the present research work and proposes an outlook on further research works. The basics of vector and tensor theory, derivation of conservation laws and constitutive equations, three-dimensional form of second-order Boltzmann-Curtiss based constitutive equations, quadrature rule for numerical integration, a flow chart of developed in-house 3D-DG solver and basics of aerodynamics theory are provided in appendices, followed by a list of references.

Chapter 2. Basics of gas kinetic theory

"Imagination is more important than knowledge."

- Albert Einstein (1879-1955)

In this chapter, we first review the elementary gas kinetic theory of monatomic, diatomic and polyatomic (linear) gases and introduce the nonequilibrium phenomena and bulk viscosity. Then, we shall discuss the classical Boltzmann-Curtiss kinetic equation, which is the fundamental governing equation for processes in dilute gases. We will also discuss one of its direct consequences and standard method — the direct simulation Monte Carlo (DSMC) method. Also, we shall deal with the moments of Boltzmann-Curtiss kinetic equation.

2.1 Gas flow regimes classification

2.1.1 Flow regimes based on Knudsen number

The study of nonequilibrium gases has been treated as a fundamental and challenging research topic in last few decades. The flow of gases at high altitudes, in porous media, in microscale thermo-fluidic devices, in vacuum technology and microelectromechanical systems (MEMS) are of great importance due to their tremendous technological and scientific applications [7, 8], thereby requires a very good understanding of gases in non-equilibrium conditions. The major indicators of nonequilibrium in above cases are high Mach and high Knudsen numbers. Mach number (*M*) can be defined as the ratio of fluid flow speed and sound speed. The deviation of gases from its local equilibrium state can be characterized by Knudsen number (*Kn*) which is usually measured the degree of rarefaction [9, 10]. Typically it is defined as the ratio of the particle molecular mean free path λ_{mean} ,

the average distance that a gas particle travels between successive collision, to the characteristic length scale of flow L,

$$\lambda_{mean} = \frac{\lambda_{mean}}{L}.$$
(2.1)

Generally, the value of Knudsen number is served as the primary parameter to determine the degree of rarefaction and the degree of validity of Boltzmann-based models. Figure 2-1 predicts the classification of gas flow regimes based on the value of the Knudsen number.



Figure 2-1. Flow regime classification based on Knudsen number.

Normally, the gas flow regime is characterized as continuum or hydrodynamics flow regime (for $Kn \le 10^{-3}$), slip flow regime (for $10^{-3} \le Kn \le 10^{-1}$), transition flow regime (for $10^{-1} \le Kn \le 10$), and free molecular regime (for $Kn \ge 10$) [11]. However, this classification has been used widely in gas dynamics community. It may not be suitable for categorizing gas flow regimes in natural form. Also, there is a requirement of at least two parameters for describing a gas flow in continuum fluid dynamics [12]. Therefore, the flow may be classified based on Reynolds number as well the flow velocity. In order to elaborate the gas flows in all flow regimes from equilibrium to highly non-equilibrium states, it may be re-categorized the flow regimes based on the level of deviation from the equilibrium state.

2.1.2 Flow regimes based on Tsien's parameter

In 1946, Tsien [13] suggested a Knudsen number based not on a typical body dimension L but the thickness δ of the boundary layer on the body. Thus

$$Kn_{\delta} = \frac{\lambda}{\delta}.$$
 (2.2)

For a flat plate flow whose length L, the boundary layer thickness is related with Reynolds number Re_L defined as

$$\delta \propto \frac{L}{\sqrt{\text{Re}}}, \text{Re}_L = \frac{\rho \mathbf{u}L}{\mu}, \text{Re}_\delta = \frac{\rho \mathbf{u}\delta}{\mu} \propto \sqrt{\text{Re}}.$$
 (2.3)

Here, ρ is the gas density, **u** is the bulk flow velocity, and μ is the viscosity coefficient. Thus, the Knudsen number Kn_{δ} based on the thickness δ can be represented regarding freestream Mach (*M*) and Reynolds (Re) numbers:



$$Kn_{\delta} = \frac{\lambda}{\delta} = \frac{M}{\operatorname{Re}_{\delta}} = \frac{M}{\sqrt{\operatorname{Re}}}.$$
(2.4)

Figure 2-2. Flow regime classification based on Tsien's parameter.

The non-dimensional parameter $M/\sqrt{\text{Re}}$ may be referred as Tsien's parameter. The flow regime classification based on Tsien's parameter is illustrated in Figure 2-2. The larger value of Tsien's parameter indicates a higher degree of rarefaction and a larger distance from an equilibrium state as shown in Figure 2-2. The flow regime classification based on Tsien's parameter may be characterized as continuum flow regime for $M/\sqrt{\text{Re}} \le 0.01$, slip
flow regime for $0.01 \le M/\sqrt{\text{Re}} \le 1$, rarefied flow regime for $1 \le M/\sqrt{\text{Re}} \le 10$, and freemolecular flow regime for $M/\sqrt{\text{Re}} > 10$. Tsien's parameter reduces to the ordinary Knudsen number defined in Eq. (2.1) for free-molecular flow.

2.1.3 Estimation of mean free path

According to gas kinetic theory, the gas molecules move in a vessel with large velocities even at room temperature. These molecules are considered as particles having finite and small size. As a result, the molecules moving in the space of vessel containing it collide with each other. *The collision between these molecules of a matter is known as a molecular collision*. However, collisions are supposed to be elastic.

The gas molecules are constantly moving in all directions at various speeds. They frequently collide with each other. Therefore, their speeds and directions change. Since these molecules exert no force upon one another except at collision, they move in straight lines with constant speed between two successive collisions. So, the path of a single molecule is a series of short zig-zag paths of different lengths. These are called the free paths of the molecule, and their mean is called mean free path. Hence, the mean free path λ_{mean} is the average distance travelled by a molecule between two successive collisions with other molecules.

For an ideal gas, the mean free path λ_{mean} is a function of number density *n* (molecules per unit volume), and the size of molecules *d* (*d* being the diameter of the molecule):

$$\lambda_{mean} = \frac{1}{\sqrt{2}n\pi d^2}.$$
(2.5)

The relationship between pressure p, temperature T, and the number density n is defined as

$$p = nK_BT, (2.6)$$

where K_B is the Boltzmann constant which is ratio of gas constant R_{gas} and Avogadro number N_A i.e.

$$K_B = \frac{R_{gas}}{N_A}.$$
(2.7)

Using the relations (2.6) and (2.7), the mean free path can be represented as

$$\lambda_{mean} = \frac{K_B T}{\sqrt{2\pi} d^2 p}.$$
(2.8)

2.2 Thermal nonequilibrium phenomena and bulk viscosity

2.2.1 Thermal nonequilibrium phenomena

A gas particle can have various energy modes, including translational, rotational and vibrational modes. A translational mode is described by the random motion of gas particles. In addition to a translational mode, diatomic and polyatomic gas particles can also possess an internal mode, due to the rotation of atoms around an axis, as well as the vibration of atoms along an inter-nuclear axis. The internal modes of diatomic and polyatomic gases—the rotational and vibrational modes—are closely related to thermal non-equilibrium.

The rotational energy is easily excited at room temperature and ubiquitous across whole flow conditions. However, in many gas flow problems, the rotational non-equilibrium effect can be neglected because the relaxation time of rotational energy is extremely short and the equilibrium of rotational mode is usually easy to reach. In the other word, the rotational non-equilibrium effect become important when the flow problem is relevant to small time scale which is comparable to the relaxation time of rotational energy. The effect of vibrational non-equilibrium becomes relevant only in gas flows where the temperature is greater than the vibrational excitation temperature; for example, 1000°K. For this reason, in the study of diatomic and polyatomic gases, the excitation of vibrational degrees of freedom is usually neglected. The rotational non-equilibrium effect can be simply accounted for by introducing the excess normal stress associated with bulk viscosity. The so-called bulk viscosity has a long history, not only in compressible gas dynamics, but also in fluid dynamics in general. For example, the two-century old Navier-Stokes-Fourier equation (called NSF hereafter) is considered to be the *de facto* mathematical equation for every possible flow problem, including compressible gas dynamics. The NSF theory is built upon a critical assumption of the constitutive equations, introduced by Stokes [14] in 1845, that the bulk viscosity vanishes,

$$\mu_{bulk} \equiv \lambda + \frac{2}{3}\mu = 0$$
, equivalently $\lambda = -\frac{2}{3}\mu$. (2.9)

Here μ_{bulk} , λ and μ represent the bulk viscosity, the second coefficient of viscosity and the shear viscosity of the fluid, respectively. The Stokes's hypothesis, mathematically expressed as (2.9), assumes that the dilatational term ($\nabla \cdot \mathbf{u}$) plays no role in the level of the constitutive equation of viscous stress, even though it may play a significant role in the level of conservation laws in general, like compressible gas flows.

Further, the origin of bulk viscosity is often attributed to pure phenomenological observation, such as interpreting it as the dissipation mechanism during a change in volume at a finite rate, rather than resorting to a fundamental microscopic kinetic theory.

While the Stokes's hypothesis is certainly legitimate in the case of monatomic gases like argon, there is ever increasing evidence that now indicates that this is not the case for non-monatomic gases [15-17] —like nitrogen (or air), methane, and carbon dioxide—that are far from local thermal equilibrium. Examples of such cases include the inner structure of strong shock waves, hypersonic entry into the Mars atmosphere, which consists mostly of carbon dioxide, the effects of bulk viscosity on the stability of the early universe, and the bulk viscosity of suspensions [18-20].

It should also be noted that from room temperature acoustic attenuation data, the bulk viscosity for carbon dioxide is known to be three orders of magnitude larger than its shear viscosity, indicating it has a highly dispersive nature which is dependent on frequency. In fact, in a recent experimental study [15] in 2016 on the role of dilatational (longitudinal acoustic) waves in a second-mode instability in the laminar-to-turbulence transition in hypersonic boundary layers, it was observed that, for a real diatomic gas, the growth and decay of the second mode is accompanied by a dilatation process which leads to about a 50% increase in dilatation dissipation, in comparison with the Stokes's hypothesis.

2.2.2 Bulk viscosity derivation from conventional theory

Consider a constant velocity field without the gravity. In this situation, the stress tensor σ is independent from position vector **r**, and the fluid possesses neither the shearing motion nor the shear stresses. Therefore, the stress tensor σ can be written [21, 22] as

$$\boldsymbol{\sigma} = (\text{constant})\mathbf{I}. \tag{2.10}$$

Since the normal stress is independent of an orientation of the surface that is given by normal vector **n**. This is the case for the stress due to the hydrostatic pressure p, which varies with **r** but not with **n**. Then, Eq. (2.10) can be written as

$$\boldsymbol{\sigma} = -p \, \mathbf{I}. \tag{2.11}$$

Here, by convection, compressive stress is negative here producing the minus stress. A fluid motion with a nonzero velocity gradient will possess normal stresses that are not equal to the negative of the hydrostatic pressure. We now subtract the hydrostatic pressure term from σ to obtain the viscous stress tensor τ ,

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - (-p\,\mathbf{I}) = \boldsymbol{\sigma} + p\,\mathbf{I}.\tag{2.12}$$

The viscous stress tensor τ is nonzero only if the fluid possesses a non-zero relative motion. It can be related to the rate-of-strain tensor (rate-of-deformation tensor). Any

second-order tensor can be written as the sum of symmetric and antisymmetric tensors. Then the velocity gradient $\nabla \mathbf{u}$ can be written as

$$\nabla \mathbf{u} = \mathbf{\varepsilon} + \mathbf{\omega}. \tag{2.13}$$

The symmetric tensor ε called the rate-of-strain tensor, is given by

$$\boldsymbol{\varepsilon} = \varepsilon_{ij} = \frac{1}{2} \left[\nabla \mathbf{u} + \left(\nabla \mathbf{u} \right)^T \right] = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \tag{2.14}$$

while, the anti-symmetric part of $\nabla \mathbf{u}$ is the rotation tensor denoted by $\boldsymbol{\omega}$,

$$\boldsymbol{\omega} = \omega_{ij} = \frac{1}{2} \left[\nabla \mathbf{u} - \left(\nabla \mathbf{u} \right)^T \right] = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right).$$
(2.15)

Thus Eq. (2.13) can be written as

$$\nabla \mathbf{u} = \mathbf{d} \mathbf{r} \cdot \boldsymbol{\varepsilon} + \mathbf{d} \mathbf{r} \cdot \boldsymbol{\omega}. \tag{2.16}$$

Eq. (2.16) is associated with a solid body rotation and does not contribute to the viscous stress tensor τ . This means that τ can only depend on the rate-of-strain tensor ε . This tensor, however, is symmetric with six independent components. These components can be further subdivided into those producing a shearing motion and dilatation strain. This later strain is given by the trace of ε i.e.

$$\operatorname{Tr}\left(\boldsymbol{\varepsilon}\right) = \varepsilon_{ii} = \nabla \cdot \mathbf{u}. \tag{2.17}$$

For Newtonian fluids, two assumptions are considered—one is linear relation between τ and ε , and second is isotropic condition (assumptions of linearity and isotropy). Each tensor τ has nine scalar components. The linear assumption means that each τ component is proportional to the nine components of ε . Hence, there are $3^4 = 81$ scalar coefficients that relate two tensors. These coefficients are the components of a fourth order tensor. With a subscript notation, the linear relation is given by

$$\tau_{ii} = C_{ijmn} \varepsilon_{mn}, \qquad (2.18)$$

where C_{ijmn} is called the fourth-order viscosity coefficient tensor. The most general form of an isotropic fourth-order tensor is given by

$$C_{ijmn} = A \,\delta_{ij} \delta_{mn} + B \,\delta_{im} \delta_{jn} + C \,\delta_{in} \delta_{jm}, \qquad (2.19)$$

where, A, B, and C are only coefficients remaining out of the original 81. Then relation (2.18) can be written as

$$\tau_{ij} = \left(\mathbf{A} \,\delta_{ij} \delta_{mn} + \mathbf{B} \,\delta_{im} \delta_{jn} + \mathbf{C} \,\delta_{in} \delta_{jm} \right) \varepsilon_{mn}$$

$$= \mathbf{A} \,\delta_{ij} \delta_{mn} + \mathbf{B} \,\varepsilon_{ij} + \mathbf{C} \,\varepsilon_{ji}.$$
(2.20)

Since $\boldsymbol{\varepsilon}$ is symmetric, this further simplifies to

$$\tau_{ij} = \left(A \,\delta_{ij} \delta_{mn} + B \,\delta_{im} \delta_{jn} + C \,\delta_{in} \delta_{jm} \right) \varepsilon_{mn}$$

$$= A \,\delta_{ij} \delta_{mn} + \left(B + C \right) \varepsilon_{ij}.$$
(2.21)

Now introducing the notation μ and λ for the first (shear) and second viscosity coefficients respectively:

$$\mu = \frac{1}{2} (\mathbf{B} + \mathbf{C}), \quad \lambda = \mathbf{A}.$$

Therefore, the relation (2.21) becomes

$$\tau_{ij} = \lambda \delta_{ij} \varepsilon_{mm} + 2\mu \varepsilon_{ij}, \qquad (2.23)$$

which can be written in tensor form as

$$\boldsymbol{\tau} = 2\boldsymbol{\mu}\boldsymbol{\varepsilon} + \boldsymbol{\lambda} (\nabla \cdot \mathbf{u}) \mathbf{I}. \tag{2.24}$$

From the relations (2.12) and (2.24), we have

$$\boldsymbol{\sigma} = (-p + \lambda \nabla \cdot \mathbf{u})\mathbf{I} + 2\mu\boldsymbol{\varepsilon}. \tag{2.25}$$

This relation can be written in Cartesian form as

$$\sigma_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij}.$$
(2.26)

We emphasize that these equations are restricted to the Newtonian fluid. In case of incompressible flow, $\nabla \cdot \mathbf{u} = 0$ i.e., there is no role of second viscosity coefficient λ in an incompressible flow. For describing the role of λ for a compressible flow, we define the mean pressure \overline{P} as the negative one-third of the sum of the trace of stress tensor $\boldsymbol{\sigma}$ i.e.

$$\overline{P} = -\frac{1}{3} \left(\sigma_{11} + \sigma_{22} + \sigma_{33} \right) = p - \left(\lambda + \frac{2}{3} \mu \right) \nabla \cdot \mathbf{u} = p - \mu_{bulk} \nabla \cdot \mathbf{u},$$
(2.27)

where the bulk viscosity coefficient μ_{bulk} is defined as $\mu_{bulk} \equiv \lambda + \frac{2}{3}\mu$. Replacing the value of λ in term of μ_{bulk} Eq. (2.24) becomes

$$\boldsymbol{\tau} = 2\boldsymbol{\mu} [\nabla \mathbf{u}]^{(2)} + \boldsymbol{\mu}_{bulk} (\nabla \cdot \mathbf{u}) \mathbf{I}, \qquad (2.28)$$

where $[\nabla \mathbf{u}]^{(2)}$ represents the traceless symmetric part of $\nabla \mathbf{u}$ defined by

$$\left[\nabla \mathbf{u}\right]^{(2)} = \frac{1}{2} \left[\nabla \mathbf{u} + \left(\nabla \mathbf{u}\right)^{T}\right] - \frac{1}{3} \left(\nabla \cdot \mathbf{u}\right) \mathbf{I}.$$
(2.29)

The term τ also known as rate-of-shear tensor provides the viscous stresses associated only with a shearing motion. Consequently, the bulk viscosity term provides the viscous stresses due to the dilatational motion. The shear and dilatational stresses are caused by the attractive and repulsive forces between molecules and the collision relaxation of the rotational and vibrational energy modes of polyatomic molecules, respectively. As can be seen from Eq. (2.28), the viscous tensor has an isotropic part and a deviatoric part. By recalling decomposition (2.25), we get the following expression for the complete stress tensor,

$$\boldsymbol{\sigma} = \left(-p + \boldsymbol{\mu}_{bulk} \left(\nabla \cdot \mathbf{u}\right)\right) \mathbf{I} + 2\boldsymbol{\mu} \left[\nabla \mathbf{u}\right]^{(2)}.$$
(2.30)

2.2.3 Physical interpretation of bulk viscosity

The physical interpretation of the bulk viscosity in a gas flow is *associated with the relaxation of internal, rotational and vibrational, modes* of polyatomic molecules. It is well known from kinetic theory and experiments that *bulk viscosity is zero for a monatomic gas* [23]. At room temperature, diatomic gases such as O_2 , N_2 , CO, and NO, are fully excited rotationally but possess negligible vibrational excitation. As a consequence, only rotation contribution to μ_{bulk} , and the bulk viscosity ratio $f_{bulk} \equiv \mu_{bulk}/\mu$ is of unity order i.e. $f_{bulk} \equiv O(\mu)$. The number of collisions required for rotational energy equilibration is about 4 or 5, whereas vibrational energy relaxation typically requires thousands of collisions. Consequently, when the vibration mode(s) is partly or fully excited, f_{bulk} is large compared to unity. For example, at room temperature, CO₂ has a value of about 2000 [24].

The magnitude of this difference between rotational and vibrational relaxation is justified by the kinetic theory [25]. The physical interpretation for the bulk viscosity in dense gas or liquids are different from that of a simple molecular collision relaxation process. For instance, the μ_{bulk} is proportional to the $\sqrt{\rho}$ at relatively large density values [26].

Gas	Argon (Ar)	Nitrogen (N2)	Oxygen (O2)	Hydrogen (H2)	Carbon mono- oxide (CO)	Methane (CH4)	Carbon dioxide (CO2)
Bulk viscosity	0.0	0.8	0.73	35	0.55	1.33	1000
Degree of freedom	3	5	5	5	5	6.4	6.7
Specific heat ratio	1.667	1.4	1.4	1.4	1.4	1.3125	1.2985
Gas constant	208.24	296.913	259.91	4133.668	296.93	518.45	188.87
Viscosity	2.117×10 ⁻⁵	1.656×10 ⁻⁵	1.919×10 ⁻⁵	0.845×10 ⁻⁵	1.635×10^{-5}	1.024×10 ⁻⁵	1.38×10 ⁻⁵
Viscosity index	0.81	0.74	0.77	0.67	0.73	0.84	0.93
Prandtl number	0.667	0.7368	0.7368	0.7368	0.7368	0.7706	0.7767
Molecular diameter (meter)	4.17×10^{-10}	4.17×10^{-10}	4.07×10^{-10}	2.92×10^{-10}	4.19×10^{-10}	4.83×10^{-10}	5.62×10 ⁻¹⁰
Molecular mass (kg)	66.3×10^{-27}	46.5×10 ⁻²⁷	53.12×10^{-27}	3.34×10^{-27}	46.5×10 ⁻²⁷	26.63×10^{-27}	73.1×10 ⁻²⁷

Figure 2-3. Physical paramters of monatomic, diatomic and polyatomic gases.

Physically, the bulk viscosity provides a damping of volumetric vibrations such as might occur during sound absorption. In fluid dynamics, bulk viscosity which plays a central role is related to the number of collisions or time, required for the molecules to achieve internal, vibrational and rotational equilibrium. In present work, we only focus on the rotational contribution to the bulk viscosity. In traditional fluid dynamics theory, the rotational modes of energy are always considered in equilibrium with the translational and completely neglects other internal energy modes. Although there is voluminous literature in gas dynamics and fluid mechanics for the description of transport properties like shear viscosity and specific heat, there is no significant data for the bulk viscosity. A few theoretical and experimental explanation for bulk viscosity has been done [17, 24, 27-32].

These studies are limited to some specific molecules and temperature ranges. The data available in the literature of bulk viscosity of ideal gases tells us that the bulk viscosity ratio f_{bulk} has a variation in temperature and usually has a local maximum. It may be noted that the bulk viscosity treatment has been the subject of controversy for quite some time [16, 32, 33].

2.3 Microscopic properties

2.3.1 Basic molecular properties

A gas molecule can be described based on three molecular parameters—molecular mass *m*, molecular velocity **v**, and effective molecular diameter *d* [1, 34]. The molecular velocity **v** is the sum of bulk velocity **u** and peculiar velocity **C**, i.e., $\mathbf{v} = \mathbf{u} + \mathbf{C}$. There are several quantum energy states ζ^{dof} in a molecule based on the internal degrees of freedoms of the molecule,

$$\zeta^{dof} = 3N - N_m, \tag{2.31}$$

where ζ^{dof} is the degree of freedom, N is the number of gas molecules and N_m is the number of independent relations among molecules. For instance, a monatomic gas molecule has 3 degrees of freedom ($\zeta^{dof} = 3$), since it has only one molecule (N = 1) and there is no independent relation i.e. $N_m = 0$. For a diatomic gas molecule, $\zeta^{dof} = 5$, since the diatomic gas molecule has 3 translational and 2 rotational degrees of freedom. In case of polyatomic gas, $\zeta^{dof} = 7$. The total energy of a system can be written as the sum of kinetic, internal and potential energy,

$$E_{\text{total}} = E_{\text{kinetic}} + E_{\text{internal}} + E_{\text{potential}}, \qquad (2.32)$$

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

$$\mathcal{E}_{\text{total}} = \mathcal{E}_{\text{kinetic}} + \mathcal{E}_{\text{internal}} + \mathcal{E}_{\text{potential}}.$$
(2.33)

The specific energy and total energy are related through the relations

$$E_{\text{total}} = \int_{V} \rho \mathcal{E}_{\text{total}} \, \mathrm{dV}.$$
 (2.34)

The kinetic energy of the molecule moving at velocity **u** is given by:

$$E_{\text{kinetic}} = \frac{1}{2}m\mathbf{u}^2. \tag{2.35}$$

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;

$$\zeta_{\text{internal}}^{dof} = \zeta_{\text{translational}}^{dof} + \zeta_{\text{rotational}}^{dof} + \zeta_{\text{vibrational}}^{dof}.$$
 (2.36)

The translational energy of a gas molecule is defined by

$$E_{\text{translational}} = \frac{1}{2}m\,\mathbf{v}^2.$$
(2.37)

The rotational energy of a gas molecule is defined by

$$E_{\text{rotational}} = \frac{1}{2} I \omega_f^2, \qquad (2.38)$$

where ω_f is the angular frequency of rotation about one of the axes, and *I* is the moment of inertia of the molecule about its center of mass, given by

$$I = \left(\frac{m_1 m_2}{m_1 + m_2}\right) r^2 = \mu_{mass} r^2,$$
(2.39)

where m_1, m_2 are the masses of the atoms that form the molecule, *r* is the atomic separation, and $\mu_{mass} = m_1 m_2 / (m_1 + m_2)$ denotes the reduced mass of the molecule. The magnitude of the molecule's angular momentum about its center of mass is represented by

$$L = I\omega_f, \tag{2.40}$$

which classically can have any value. According to Quantum mechanics, the angular momentum of the molecule has the value

$$L = \sqrt{J(J+1)\hbar}, \quad J = 0, 1, 2, 3.....$$
(2.41)

where *J* is an integer called the rotational quantum number and $\hbar = \frac{h}{2\pi}$, *h* being the Planck constant. Combining the Eqs. (2.38), (2.40), and (2.41) the rotational energy of the molecule is given by

$$E_{\text{rotational}} = \frac{1}{2}I\omega_f^2 = \frac{L^2}{2I} = \frac{\hbar}{2I}J(J+1), \quad J = 0, 1, 2, 3.....$$
(2.42)

The vibrational energy of a gas molecule is given by

$$E_{\text{vibrational}} = \left(\upsilon + \frac{1}{2}\right) h f_{vib}, \quad \upsilon = 0, 1, 2, 3....$$
(2.43)

Here, v is an integer called the vibration quantum number, and f_{vib} the frequency of vibration for the system is defined by

$$f_{vib} = \frac{1}{2\pi} \sqrt{\frac{k_{spring}}{\mu_{mass}}},$$
(2.44)

where k_{spring} is the effective spring constant.

2.3.2 Gas properties

For an ideal gas, the temperature is related to the pressure p and density ρ by the ideal gas law:

$$p = \rho R_{gas} T, \tag{2.45}$$

while, the internal energy of the gas is simply function of temperature only, i.e. $E_{\text{internal}} = E_{\text{internal}}(T)$, which is defined by

$$E_{\text{internal}} = C_v T, \qquad (2.46)$$

where, C_{ν} is the specific heat at constant volume. The gases that obeys Eqs. (2.45) and (2.46) are called calorically or thermally perfect gas. The specific enthalpy of the gas is defined by

$$h = C_p T, \tag{2.47}$$

where C_p is called the specific heat at constant pressure. By the ideal gas law results:

$$C_p - C_v = R_{gas}.$$
 (2.48)

The equation of state of a polytropic gas turns out to depend only on the ratio of the specific heats:

$$\gamma = \frac{C_p}{C_v}.$$
(2.49)

In terms of internal degree of freedom, the specific heat ratio of a gas molecule can be defined as

$$\gamma = \frac{\zeta^{dof} + 5}{\zeta^{dof} + 3} = 1 + \frac{2}{\zeta^{dof} + 3}.$$
(2.50)

The mass of unit molecule and the ordinary gas constant can be defined as

$$m = \frac{W_{gas}}{N_A}, \quad R_{gas} = \frac{K_B}{m}, \tag{2.51}$$

where N_A denotes the Avogadro number and W_{gas} is the molecular weight of the gas. The Prandtl number Pr can be calculated using Eucken's formulation as

$$\Pr = \frac{4\gamma}{9\gamma - 5}.$$
(2.52)

The transport properties of a gas can be defined based on the models which are used for describing the inter-molecular potential forces. In case of power-law model which is a short-range repulsive inter-molecular model, the first coefficient of viscosity μ and the thermal conductivity κ can be defined as

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}}\right)^{s}, \quad \kappa = \kappa_{ref} \left(\frac{T}{T_{ref}}\right)^{s}, \quad (2.53)$$
with
$$\mu_{ref} = \frac{15\sqrt{mK_{B}T_{ref}}}{2d_{ref}^{2}\sqrt{\pi} (5-2s)(7-2s)},$$

$$\kappa_{ref} = \frac{\mu_{ref}C_{p}}{\Pr}, \quad s = \frac{1}{2} + \frac{2}{\nu - 1}.$$

The *s* denotes the viscosity index and ν represents the exponent of the inverse power law for the gas-particle interaction.

2.3.3 Phase density distribution

In kinetic theory, the state of a gas is described by a distribution function $f(\mathbf{v}, \mathbf{r}, t)$ such that the number of particles in a phase space element, $d\mathbf{v}d\mathbf{r}$ at time *t* is given by

$$dN = f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v} d\mathbf{r}, \tag{2.54}$$

where, *N* is the number of molecules. The integration of $f(\mathbf{v}, \mathbf{r}, t)$ in phase space is equal to a number of molecules in the physical space:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\mathbf{v}, \mathbf{r}, t) d\mathbf{v} = N.$$
(2.55)

The phase density distribution function $f(\mathbf{v},\mathbf{r},t)$ is the central quantity in kinetic theory.

2.4 Macroscopic properties

All the macroscopic quantities for diatomic gases can be obtained based on the phase density distribution function $f(\mathbf{v},\mathbf{r},t)$. Therefore, in this section, several important and commonly used definitions in this thesis are defined for simplicity, clarity and helpful to readers.

2.4.1 Density

The density which is the first macroscopic variable is obtained as

$$\rho = \left\langle m f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}, \qquad (2.56)$$

where the symbol $\langle \cdots \rangle$ represents the integration over **v**-space i.e.

$$\langle \cdots \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{v} \cdots$$
 (2.57)

2.4.2 Velocity

Velocity or mass velocity, momentum density, and the mean peculiar velocity are represented as

$$\mathbf{u} = \left\langle \mathbf{v} f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle = \frac{1}{n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{v} f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}, \qquad (2.58)$$

$$\rho \mathbf{u} = \langle m \mathbf{v} f(\mathbf{v}, \mathbf{r}, t) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \mathbf{v} f(\mathbf{v}, \mathbf{r}, t) d\mathbf{v},$$

$$\langle m \mathbf{C} f(\mathbf{v}, \mathbf{r}, t) \rangle = \langle m(\mathbf{v} - \mathbf{u}) f(\mathbf{v}, \mathbf{r}, t) \rangle$$

$$= \langle m \mathbf{v} f(\mathbf{v}, \mathbf{r}, t) \rangle - \langle m \mathbf{u} f(\mathbf{v}, \mathbf{r}, t) \rangle$$

$$= \rho \mathbf{u} - \langle m f(\mathbf{v}, \mathbf{r}, t) \rangle \mathbf{u} = \rho \mathbf{u} - \rho \mathbf{u} = \mathbf{0}.$$
(2.59)

2.4.3 Temperature

Generally, the thermodynamic temperature is known as temperature which can be defined based on the equation of states for an ideal gas (2.45),

$$T = \frac{p}{\rho R_{gas}} = \frac{2}{3} \frac{e_{\text{translational}}}{R_{gas}},$$
(2.61)

(2.60)

where $e_{translational}$ denotes translational energy density. Also, the temperature quantity can be written in terms of probability distribution function as

$$T = \frac{2}{3\rho R_{gas}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2} mC^2 f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}.$$
 (2.62)

In case of diatomic and polyatomic gases, the temperature quantity can be measured for each state of the energy level as

$$T_{\text{translational}} = \frac{2}{3\zeta_{\text{translational}}^{dof}} \frac{m}{K_B} e_{\text{translational}},$$

$$T_{\text{rotational}} = \frac{2}{3\zeta_{\text{rotational}}^{dof}} \frac{m}{K_B} e_{\text{rotational}},$$

$$T_{\text{vibrational}} = \frac{2}{3\zeta_{\text{vibrational}}^{dof}} \frac{m}{K_B} e_{\text{vibrational}}.$$
(2.63)

The overall temperature value in non-equilibrium condition can be calculated on weighted averaging formulation as

$$T_{\text{overall}} = \frac{\zeta_{\text{translational}}^{dof} T_{\text{translational}} + \zeta_{\text{rotational}}^{dof} T_{\text{rotational}} + \zeta_{\text{vibrational}}^{dof} T_{\text{vibrational}}}{\zeta_{\text{translational}}^{dof} + \zeta_{\text{vibrational}}^{dof}} .$$
(2.64)

It may be noted that the temperature specifies the collective thermal state of matter comprising the system and quantifies the physiological perception of coldness and hotness of the body [1]. It is a notion intimately connected with heat and its transfer between bodies in contact. The temperature of a body is quantified if a thermometer is put in thermal equilibrium with the body in question. When the thermometer is standardized to a universal scale, the temperature of the body is given by an absolute temperature.

2.4.4 Energy

The macroscopic internal energy, total energy, and enthalpy for an ideal gas can be defined in thermodynamic equilibrium condition as

$$E_{\text{internal}} = \rho e_{\text{internal}} \approx \rho C_{\nu} T, \qquad (2.65)$$

$$E_{\text{total}} = E_{\text{kinetic}} + E_{\text{internal}} + E_{\text{potential}}$$
$$= \frac{1}{2} \rho \left\| \mathbf{u} \right\|^{2} + \rho C_{\nu} T + \rho g h_{\text{height}} (=0), \qquad (2.66)$$

$$H_{\text{total}} = E_{\text{total}} + \frac{p}{\rho} = \frac{1}{2} \rho \|\mathbf{u}\|^2 + \rho C_v T + \frac{p}{\rho}.$$
 (2.67)

The total energy can be determined through the probability distribution function as

$$E_{\text{total}} = \left\langle \frac{1}{2} m \, \mathbf{v}^2 f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2} m \mathbf{v}^2 f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}.$$
(2.68)

The internal energy state can also be represented based on ensemble averaging and the first moment of single particle probability distribution functions as

$$\rho E_{\text{internal}} = \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f\left(\mathbf{v},\mathbf{r},t\right) \right\rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{1}{2}mC^2 + H_{rot}\right)f\left(\mathbf{v},\mathbf{r},t\right)d\mathbf{v}.$$
(2.69)

2.4.5 Pressure tensor

Pressure tensor, so-called stress 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

$$\mathbf{P} = \left\langle m \operatorname{CC} f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \operatorname{CC} f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}.$$
(2.70)

where C is the peculiar velocity. The pressure tensor P is decomposable into three components: hydrostatic pressure, excess trace part, and traceless part.

$$\mathbf{P} = (p + \Delta)\mathbf{I} + \mathbf{\Pi}. \tag{2.71}$$

Here, **I** is the unit second-rank tensor, p is the hydrostatic pressure, Δ is the excess trace part (excess normal stress), and Π is the traceless part (viscous stress tensor).

2.4.6 Viscous stress tensor

Viscous stress tensor can be defined as the traceless part of the symmetric pressure tensor.

$$\boldsymbol{\Pi} = \boldsymbol{P} - \frac{1}{3} \boldsymbol{I} \operatorname{Tr} \left(\boldsymbol{P} \right) = \left[\boldsymbol{P} \right]^{(2)}.$$
(2.72)

It can be defined based on the moments of distribution function as

$$\mathbf{\Pi} = \left\langle m \left[\mathbf{C} \mathbf{C} \right]^{(2)} f \left(\mathbf{v}, \mathbf{r}, t \right) \right\rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m \left[\mathbf{C} \mathbf{C} \right]^{(2)} f \left(\mathbf{v}, \mathbf{r}, t \right) d\mathbf{v}.$$
(2.73)

Where $[\mathbf{CC}]^{(2)}$ denotes the traceless part of the thermal velocity production tensor \mathbf{CC} defined in Eq. A.32 (Appendix A).

2.4.7 Excess normal stress

Excess normal stress Δ can be defined as the excess trace part of the symmetric pressure tensor **P**,

$$\Delta = \frac{1}{3} \operatorname{Tr}(\mathbf{P}) - p.$$
(2.74)

The statistical mechanical formula for Δ is given as,

$$\Delta = \left\langle \left[\frac{1}{3} m \operatorname{Tr} \left(\mathbf{C} \mathbf{C} \right) - p \right] f \left(\mathbf{v}, \mathbf{r}, t \right) \right\rangle.$$
(2.75)

2.4.8 Hydrostatic pressure

In kinetic theory, the hydrostatic pressure is convecntionally defined [35, 36] as

$$p = \frac{1}{3} \operatorname{Tr}(\mathbf{P}). \tag{2.76}$$

However, this definition of hydrostatic pressure is not valid for all fluids since the stress tensor is a non-equilibrium quantity. Although the definition (2.76) is true in case of dilute gases (i.e., monatomic gas) and it provides zero bulk viscosity i.e. $\mu_{bulk} = 0$ or $\Delta = 0$. But this definition (2.76) is not true for dense fluids (for example, diatomic and polyatomic gases). Therefore, the hydrostatic pressure requires a more careful definition in kinetic theory. According to B.C. Eu [1], "Hydrostatic pressure is an isotropic average of the virial tensor over the local equilibrium distribution which in the case of a dilute monatomic gas is given by the formula

$$p = \left\langle \frac{1}{3} m \operatorname{Tr} (\mathbf{C} \mathbf{C}) f^{0} (\mathbf{v}, \mathbf{r}, t) \right\rangle.$$
(2.77)

where $f^{0}(\mathbf{v},\mathbf{r},t)$ denotes the equilibrium distribution function". In case of dense fluids the virial tensor includes contributions from the intermolecular forces in addition to the kinetic part *m***CC**.

2.4.9 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. The heat flux vector for a diatomic and polyatomic gas reads as,

$$\mathbf{Q} = \left\langle \left[\frac{1}{2} m C^2 + H_{rot} - m \hat{h} \right] \mathbf{C} f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\frac{1}{2} m C^2 + H_{rot} - m \hat{h} \right] \mathbf{C} f\left(\mathbf{v}, \mathbf{r}, t\right) d\mathbf{v}.$$
(2.78)

Here, \hat{h} denotes the enthalpy density defined by

$$\hat{h} = \frac{5}{2m} k_B T + \bar{E}_{rot}, \qquad (2.79)$$

with \overline{E}_{rot} for the average rotational energy density

$$\rho \overline{E}_{rot} = \left\langle H_{rot} f\left(\mathbf{v}, \mathbf{r}, t\right) \right\rangle.$$
(2.80)

2.5 Classical Boltzmann kinetic equation

In kinetic theory, a gas is defined as a collection of many interacting particles. In such a microscopic scale where the collective dynamics of particles describes the macroscopic state of gas, an appropriate kinetic equation is required to precisely describe the underlying micro-dynamics.

The Boltzmann kinetic equation that connects the regime of dynamics with that of thermodynamics has been a milestone in the development of theoretical physics. For describing the kinetics of gas, Boltzmann [37] introduced a probabilistic description for the evolution of a single-particle distribution which anticipated atomistic scattering concepts.

Let $f(\mathbf{v}, \mathbf{r}, t)$ denotes the single particle distribution function where \mathbf{v} , \mathbf{r} , and t represents the particle velocity, position and time, respectively. The distribution function $f(\mathbf{v}, \mathbf{r}, t)$ allows the probability of finding a particle in the range of $\mathbf{v} \sim \mathbf{v} + d\mathbf{v}$ and $\mathbf{r} \sim \mathbf{r} + d\mathbf{r}$ at time t. At infinitesimally small time interval dt, the change in distribution function in small control volume $d\mathbf{v}d\mathbf{r}$ located at phase space (\mathbf{v}, \mathbf{r}) can be written as

$$\left(\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathbf{F}^{\text{external}} \cdot \nabla_{v} f\right) d\mathbf{v} d\mathbf{r} dt, \qquad (2.81)$$

where the higher-order terms of order $O(\Delta t^2)$ are neglected and $\mathbf{F}^{external}$ denotes the vector of external force on unit mass; $\nabla \equiv \frac{\partial}{\partial \mathbf{r}}$, $\nabla_v \equiv \frac{\partial}{\partial \mathbf{v}}$. This expression (2.81) accounts for a change in probability distribution function due to the steaming motion of the particle in the phase space. If there is no collision between molecules, the changes in the single particle distribution $f(\mathbf{v}, \mathbf{r}, t)$ can be interpreted by a single particle Liouville equation which is called the collision-less Boltzmann equation defined by

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{F}^{external} \cdot \nabla_{v}\right) f(\mathbf{v}, \mathbf{r}, t) = 0.$$
(2.82)

Single particle Liouville equation does not contract the information of the system but preserves the information. It describes the evolution of an incompressible probability fluid. However, in reality, the molecules collide each other and probability distribution function change inside the control volume of the phase space due to the inter-molecular collision. Therefore, it is required to find a relationship between the distribution functions $f(\mathbf{v}, \mathbf{r}, t)$ and $f_2(\mathbf{v}_2, \mathbf{r}, t)$ of the colliding molecules.

The collision operator $C(f, f_2)$ is the Boltzmann's lasting contribution to the kinetic theory which is not invariant to the time reversal. It connects the dynamics of the intermolecular 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

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{F}^{external} \cdot \nabla_{v}\right) f(\mathbf{v}, \mathbf{r}, t) = C(f, f_{2}).$$
(2.83)

The collision operator $C(f, f_2)$ 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 collision operator $C(f, f_2)$ using *Stosszahl ansatz* approach, given by

$$C(f,f_2) = \int d\mathbf{v}_2 \int_0^{2\pi} d\varepsilon \int_0^{\infty} db \, b \, \mathbf{v}_r \left(f f_2' - f f_2 \right), \tag{2.84}$$

where f and f_2 are the distribution functions of colliding molecules (and prime denotes the distribution functions after collision); b is the impact parameter of two-body collision between particles; ε denotes the azimuth angle in collision plane which describes the

orientation of the collision plane; and $\mathbf{v}_r = |\mathbf{v} - \mathbf{v}_2|$ represents the relative velocity. Using Eqs. (2.83) and (2.84), the classical Boltzmann kinetic equation is given by

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{F}^{external} \cdot \nabla_{v}\right) f\left(\mathbf{v}, \mathbf{r}, t\right) = \int d\mathbf{v}_{2} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \, b \, \mathbf{v}_{r} \left(ff_{2}^{\prime} - ff_{2}\right).$$
(2.85)

The Boltzmann kinetic equation is well-known in kinetic theory for monatomic gas such as Argon. 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. 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 nonlinearity of the collisional term.

2.6 Classical Boltzmann-Curtiss kinetic equation

In 1981, Curtiss designed a thermodynamically consistent extension of the Boltzmann equation to dilute rigid diatomic gases which is known as namely, the Boltzmann-Curtiss kinetic equation [3, 38, 39]. The mathematical expression of this kinetic equation looks rather similar to the Boltzmann of monatomic gases, contains more terms about the molecular rotation.

Consider the diatomic molecule having a moment of inertia *I* and an angular momentum **j**. The orientation of the angular momentum is specified by the polar angles θ and ϕ and its magnitude is defined by *j*. Since the orientation of the molecules is described by Euler angles α, β and γ . Therefore, polar angles of angular momentum **j** is chosen as $\alpha = \theta, \beta = \phi$. Also, $\psi = \gamma$ is the azimuth specifying the orientation of the molecule in the plane perpendicular to the **j** vector. The unit vector of the body axis is denoted by $\hat{\mathbf{R}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ with polar angles θ and ψ . Then the Boltzmann-

Curtiss kinetic equation for the diatomic molecule can be expressed with the presence of external force [3] as

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{L}_r\right) f\left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t\right) = C(f, f_2).$$
(2.86)

Here, the subscript 2 refers to the second molecule; f represents the distribution function; v is the particle velocity; r is the particle position and \mathbf{L}_r is the internal Liouville operator defined by

$$\mathbf{L}_{r} = \frac{j}{I} \frac{\partial}{\partial \psi} + \left(\boldsymbol{\omega}_{B} \times \mathbf{j}\right) \cdot \frac{\partial}{\partial \mathbf{j}}, \qquad (2.87)$$

Where $\boldsymbol{\omega}_{B}$ is the vector of angular frequency of precession of the angular momentum due to the presence of external force. The $C(f, f_2)$ denotes the collision integral of the binary interaction among the particles and it is given by the expression

$$C(f, f_2) = \iiint d\mathbf{v}_r^* d\mathbf{v}_2 d\Omega_2 d\Omega^* d\Omega_2^* \mathbf{v}_r' \times$$

$$\sigma(\mathbf{v}_r', \mathbf{j}^*, \mathbf{j}_2^* | \mathbf{v}_r, \mathbf{j}, \mathbf{j}_2) (f^* f_2^* - ff_2)$$
(2.88)

where the asterisk denotes the post-collision value; $\mathbf{v}_r = |\mathbf{v} - \mathbf{v}_2|$ denotes the relative velocity, $d\Omega = j \, dj \sin \theta d\theta d\phi d\gamma$ denotes the solid angle of scattering; $\sigma(\mathbf{v}'_r, \mathbf{j}^*, \mathbf{j}^*_2 | \mathbf{v}_r, \mathbf{j}, \mathbf{j}_2)$ represents the collision cross section. In present work, it is assumed that there is no external force which leads $\boldsymbol{\omega}_B = 0$. Then the Boltzmann-Curtiss kinetic equation (2.86) can be expressed as

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) f\left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t\right) = C(f, f_2).$$
(2.89)

According to Curtiss, the distribution function f depends primarily on the free molecular constants of motion and it does not depend on azimuthal angle ψ i.e. on the phase of the rotational motion and depends only weakly on the coordinate **r** so that one may neglect this dependence over distances of the order of molecular dimensions. The conservation laws of

conserved variables, and the evolution equations for non-conserved variables such as the stress vector, excess normal stress, heat flux, can be derived by defining the following velocity moments and then calculating their time derivatives with the help of the Boltzmann-Curtiss kinetic equation.

2.7 Direct Simulation Monte Carlo method

Monte Carlo (MC) method was initially served around sixty years ago 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 [40, 41]. 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 [42]. 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 [43].

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. The capability and the simplicity of the DSMC method persuade many researchers to utilize it as the standard solver for studying non-continuum gas flows. It has been used to study various applications, such as micro gas flows, material processing, acoustics, high-speed gas flows, and gas mixing [44-48].

The conventional DSMC algorithms consider gases as a group of the finite number of particles 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 move based on their own velocities throughout the gas flow without considering the interaction with other particles. Subsequently, if any particle reaches a boundary, the proper action according to the type of boundary condition is 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 *acceptancerejection* method, and finally, the post-collision properties are calculated regarding 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 should be large enough to quantify the number of binary collisions among the 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 [49, 50].

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 [51]. However, Boltzmann kinetic equation cannot elaborate all aspects of DSMC approach [52]. 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 [53] 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 too 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.

2.8 Moments of Boltzmann-Curtiss kinetic equation

2.8.1 Collisional invariants

The Boltzmann-Curtiss collisional integral (2.88) has a special property that it provides to a vanishing integral of a collisional invariant quantity. Consider the integral

$$I[\Psi] = \int d\mathbf{v} \,\Psi C(f, f_2), \qquad (2.90)$$

Substituting of the explicit expression for $C(f, f_2)$ from Eq. (2.88), we get

$$I[\Psi] = \iiint d\mathbf{v} d\mathbf{v}_r^* d\mathbf{v}_2 d\Omega_2 d\Omega^* d\Omega_2^* \mathbf{v}_r' \times$$

$$\sigma (\mathbf{v}_r', \mathbf{j}^*, \mathbf{j}_2^* | \mathbf{v}_r, \mathbf{j}, \mathbf{j}_2) \Psi (f^* f_2^* - f f_2).$$
(2.91)

Since subscripts are dummy indices, they may be interchanged, and the interchange leaves $I[\Psi]$ invariant. Then Eq. (2.91) can be written in the form

$$I[\Psi] = \frac{1}{2} \iiint d\mathbf{v} d\mathbf{v}_r^* d\mathbf{v}_2 d\Omega_2 d\Omega^* d\Omega_2^* \mathbf{v}_r' \times$$

$$\sigma(\mathbf{v}_r', \mathbf{j}^*, \mathbf{j}_2^* | \mathbf{v}_r, \mathbf{j}, \mathbf{j}_2) (\Psi + \Psi_2) (f^* f_2^* - ff_2).$$
(2.92)

The collision process involved in Eq. (2.92) is $(\mathbf{v}, \mathbf{v}_2) \rightarrow (\mathbf{v}^*, \mathbf{v}_2^*)$. On reversal of the collision process, we get

$$I[\Psi] = \frac{1}{2} \iiint d\mathbf{v}^* d\mathbf{v}_r d\mathbf{v}_2^* d\Omega_2^* d\Omega_2 \mathbf{v}_r^{**} \times \sigma(\mathbf{v}_r^{**}, \mathbf{j}, \mathbf{j}_2 | \mathbf{v}_r^{*}, \mathbf{j}^*, \mathbf{j}_2^*) (\Psi^* + \Psi_2^*) (ff_2 - f^* f_2^*).$$

$$(2.93)$$

On adding both Eqs. (2.92) and (2.93) side by side and dividing the result by 2, we obtain

$$I[\Psi] = -\frac{1}{4} \iiint d\mathbf{v}_{r} d\mathbf{v}_{r} d\mathbf{v}_{2} d\Omega_{2} d\Omega^{*} d\Omega_{2}^{*} \mathbf{v}_{r}^{\prime} \times$$

$$\sigma \left(\mathbf{v}_{r}^{\prime}, \mathbf{j}^{*}, \mathbf{j}_{2}^{*} \middle| \mathbf{v}_{r}, \mathbf{j}, \mathbf{j}_{2} \right) \left(\Psi^{*} + \Psi_{2}^{*} - \Psi - \Psi_{2} \right) \left(f^{*} f_{2}^{*} - f f_{2} \right).$$

$$(2.94)$$

If the quantity Ψ is conserved in collision, then

$$\Psi^* + \Psi_2^* - \Psi - \Psi_2 = 0, \qquad (2.95)$$

and the integral $I[\Psi]$ vanishes identically:

$$I[\Psi] = 0. \tag{2.96}$$

Such quantity is called a collision invariant. If the particles are structureless, there are three collisional invariants obeying the relations: mass, momentum, and energy.

2.8.2 Conservation laws

Since the collisional integral vanishes for mass, momentum, and energy of a molecule, it is easy to derive the conservation laws based on Boltzmann-Curtiss kinetic equation (2.89). Defining the macroscopic quantity $\varphi = \left[m, m\mathbf{u}, \frac{1}{2}mC^2 + H_{rot}\right]$ and multiply it into Eq. (2.89) and integrating over velocity space. Then simplifying the equations by considering that φ depends only on the particle position and time, i.e. (\mathbf{r}, t) leads to the differential form of the conservation of mass, momentum, and energy as can be followed by Appendix B,

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E_{total} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ (\rho E_{total} + p) \mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \mathbf{\Pi} + \Delta \mathbf{I} \\ (\mathbf{\Pi} + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$
(2.97)

where E_{total} is the total energy; Π , Δ and \mathbf{Q} are the viscous stress tensor, excess normal stress and heat flux vector which are not defined still now. It must be emphasized that the conservation laws are the exact consequence of Boltzmann-Curtiss kinetic equation, and they are valid for all degree of non-equilibrium. Only after some approximation in the derivation of Π , Δ and \mathbf{Q} , they become approximate. In next chapter, non-conservative variables and the way to obtain an approximate constitutive relation for these variables are discussed in detail.

Chapter 3. Boltzmann-Curtiss based hydrodynamic models

"I believe all complicated phenomena can be explained by simpler scientific principles." - Linus Pauling (1901-1994)

In the previous Chapter, it was shown that the average of an extensive macroscopic quantity $\langle \varphi f \rangle$ could be obtained by taking the first moment of a distribution function times the microscopic quantity $\langle \varphi(\mathbf{v}) \rangle$. It was shown that the conservation laws can be obtained from the moment of Boltzmann-Curtiss 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 the gas consists of non-reacting diatomic molecules. The moment methods are applied to Boltzmann-Curtiss kinetic equation, and the extended hydrodynamic equations for non-conserved variables are derived. Afterwards, these exact but open equations are approximated based on Eu's closure, and Myong's balanced closure and then various Boltzmann-Curtiss based models are obtained.

3.1 The moment method

The general evolution equation for non-conserved variables can be obtained by multiplication of Boltzmann-Curtiss equation (2.89) with $\varphi(\mathbf{v}) = h^{(n)}$ and subsequent integration over velocity space yields

$$\left\langle h^{(n)} \frac{\partial f}{\partial t} \right\rangle + \left\langle h^{(n)} \mathbf{v} \cdot \nabla f \right\rangle + \left\langle h^{(n)} \frac{j}{I} \frac{\partial f}{\partial \psi} \right\rangle = \left\langle h^{(n)} C[f, f_2] \right\rangle.$$
(3.1)

Here the collisional term is not zero, and it is denoted by $\mathbf{\Lambda}^{(n)} = \langle h^{(n)}C[f, f_2] \rangle$. As we need to investigate over velocity, we have to convert the molecular velocity into peculiar velocity and then bring it together with distribution function *f* as

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \left\langle \mathbf{v} \cdot \nabla \left(h^{(n)} f \right) \right\rangle - \left\langle \mathbf{v} f \cdot \nabla h^{(n)} \right\rangle + \left\langle \frac{j}{I} \frac{\partial}{\partial \psi} \left(h^{(n)} f \right) \right\rangle$$

$$- \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(n)} \right\rangle = \mathbf{A}^{(n)}.$$

$$(3.2)$$

The Eq. (3.2) can be simplified as follows,

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \left\langle \left(\mathbf{C} + \mathbf{u} \right) \cdot \nabla \left(h^{(n)} f \right) \right\rangle - \left\langle \left(\mathbf{C} + \mathbf{u} \right) f \cdot \nabla h^{(n)} \right\rangle + \left\langle \frac{j}{I} \frac{\partial}{\partial \psi} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(n)} \right\rangle = \mathbf{\Lambda}^{(n)}.$$
(3.3)

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \mathbf{u} \cdot \nabla \left\langle h^{(n)} f \right\rangle + \left\langle \mathbf{C} \cdot \nabla \left(h^{(n)} f \right) \right\rangle - \left\langle \mathbf{C} f \cdot \nabla h^{(n)} \right\rangle$$

$$- \left\langle \mathbf{u} f \cdot \nabla h^{(n)} \right\rangle + 0 - \left\langle f \frac{j}{\partial t} \frac{\partial}{\partial t} h^{(n)} \right\rangle - \mathbf{A}^{(n)}$$

$$(3.4)$$

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \mathbf{u} \cdot \nabla \left\langle h^{(n)} f \right\rangle + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle - \left\langle h^{(n)} f \left(\nabla \cdot \mathbf{C} \right) \right\rangle$$

$$- \left\langle \mathbf{C} f \cdot \nabla h^{(n)} \right\rangle - \left\langle \mathbf{u} f \cdot \nabla h^{(n)} \right\rangle - \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(n)} \right\rangle = \mathbf{A}^{(n)}.$$

$$(3.5)$$

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \mathbf{u} \cdot \nabla \left\langle h^{(n)} f \right\rangle + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle - \left\langle h^{(n)} f \left(\nabla \cdot \mathbf{C} \right) \right\rangle - \left\langle \mathbf{C} f \cdot \nabla h^{(n)} \right\rangle - \left\langle \mathbf{u} f \cdot \nabla h^{(n)} \right\rangle - \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(n)} \right\rangle = \mathbf{\Lambda}^{(n)}.$$
(3.6)

$$\left\langle \frac{\partial}{\partial t} \left(h^{(n)} f \right) \right\rangle - \left\langle f \frac{\partial}{\partial t} h^{(n)} \right\rangle + \mathbf{u} \cdot \nabla \left\langle h^{(n)} f \right\rangle + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle + \left\langle h^{(n)} f \right\rangle (\nabla \cdot \mathbf{u}) - \left\langle \mathbf{C} f \cdot \nabla h^{(n)} \right\rangle - \left\langle \mathbf{u} f \cdot \nabla h^{(n)} \right\rangle - \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(n)} \right\rangle = \mathbf{\Lambda}^{(n)}.$$
(3.7)

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \left\langle h^{(n)} f \right\rangle + \left\langle h^{(n)} f \right\rangle \cdot \nabla \mathbf{u} + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle$$

$$- \left\langle f \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) h^{(n)} \right\rangle = \mathbf{\Lambda}^{(n)}.$$
(3.8)

Using the definition of substantial time derivative, we have

$$\frac{D}{Dt} \left\langle h^{(n)} f \right\rangle + \left\langle h^{(n)} f \right\rangle \cdot \nabla \mathbf{u} + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle - \left\langle f \left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right) h^{(n)} \right\rangle$$

$$= \mathbf{\Lambda}^{(n)}.$$
(3.9)

Using the mass conservation law, the general evolution equation (3.9) becomes

$$\rho \frac{D}{Dt} \left(\frac{\left\langle h^{(n)} f \right\rangle}{\rho} \right) + \nabla \cdot \left\langle \mathbf{C} h^{(n)} f \right\rangle - \left\langle f \left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right) h^{(n)} \right\rangle = \mathbf{\Lambda}^{(n)}.$$
(3.10)

This general evolution equation can be written [3, 39] as

$$\rho \frac{D}{Dt} \hat{h}^{(n)} + \nabla \cdot \boldsymbol{\Psi}^{(n)} - \boldsymbol{Z}^{(n)} = \boldsymbol{\Lambda}^{(n)}, \qquad (3.11)$$

where $\Psi^{(n)}$, the flux of $\langle h^{(n)}f \rangle$, denotes the high-order moments, $\mathbf{Z}^{(n)}$ represents the kinematic term arising from hydrodynamic streaming effect and $\Lambda^{(n)}$ is the dissipation term which accounts for energy dissipation accompanying the irreversible process. These terms are defined by

$$\hat{h}^{(n)} = \frac{\left\langle h^{(n)} f \right\rangle}{\rho}, \quad \Psi^{(n)} = \left\langle \mathbf{C} h^{(n)} f \right\rangle,$$

$$Z^{(n)} = \left\langle f \left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right) h^{(n)} \right\rangle,$$

$$\mathbf{\Lambda}^{(n)} = \left\langle h^{(n)} C[f, f_2] \right\rangle.$$
(3.12)

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, excess normal stress and heat flux vector, such that

$$h^{(1)} = m [\mathbf{CC}]^{(2)},$$

$$h^{(2)} = \frac{1}{3}mC^{2} - \frac{p}{n},$$

$$h^{(3)} = \left(\frac{1}{2}mC^{2} + H_{rot} - m\hat{h}\right)\mathbf{C}.$$
(3.13)

Using the general evolution equation (3.11), and the respectively molecular expression (3.13), the constitutive relation for shear stress tensor, excess normal stress and heat flux vector can be obtained (see Appendix C) as,

$$\rho \frac{D}{Dt} \left(\frac{\Pi}{\rho} \right) + \nabla \cdot \Psi^{(\Pi)} + 2(p + \Delta) [\nabla \mathbf{u}]^{(2)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} = \Lambda^{(\Pi)},$$
(3.14)

$$\rho \frac{D}{Dt} \left(\frac{\Delta}{\rho} \right) + \nabla \cdot \Psi^{(\Delta)} + 2\gamma' \left(\mathbf{\Pi} + \Delta \mathbf{I} \right) : \nabla \mathbf{u} + \frac{2}{3} \gamma' p \nabla \cdot \mathbf{u} = \Lambda^{(\Delta)},$$
(3.15)

$$\rho \frac{D}{Dt} \left(\frac{\mathbf{Q}}{\rho} \right) + \nabla \cdot \Psi^{(\mathbf{Q})} + \psi^{(P)} : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot (\mathbf{\Pi} + \Delta \mathbf{I}) + (p + \Delta) C_p \nabla T$$

$$+ \mathbf{\Pi} \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} = \Lambda^{(\mathbf{Q})}.$$
(3.16)

The conservation law introduced in Section (2.8.2), together with extended hydrodynamics equations can be written in a complete and compact form,

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho \mathbf{E}_{total} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} + p \mathbf{I} \\ (\rho E_{total} + p) \mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{0} \\ \mathbf{\Pi} + \Delta \mathbf{I} \\ (\Pi + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix},$$

$$\rho \frac{D}{Dt} \begin{bmatrix} \mathbf{\Pi} / \rho \\ \Delta / \rho \\ \mathbf{Q} / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(\Delta)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} + \begin{bmatrix} 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} \\ 2\gamma'(\mathbf{\Pi} + \Delta \mathbf{I}) : \nabla \mathbf{u} \\ \psi^{(P)} : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot (\mathbf{\Pi} + \Delta \mathbf{I}) + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T \end{bmatrix}$$

$$+ \begin{bmatrix} 2(p + \Delta)[\nabla \mathbf{u}]^{(2)} \\ \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u} \\ C_p (p + \Delta) \nabla T \end{bmatrix} = \begin{bmatrix} \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{\Lambda}^{(\Delta)} \\ \mathbf{\Lambda}^{(Q)} \end{bmatrix}.$$
(3.17)

Here $\nabla \cdot \Psi^{(\Pi)}$, $\nabla \cdot \Psi^{(\Delta)}$, and $\nabla \cdot \Psi^{(Q)}$ are the higher-order moment terms with the thermal velocity that can be seen from Eq. (3.12). It is clear that the higher-order moment terms and the intergo-differential collisional terms are not yet defined properly appearing in Eq. (3.17), therefore, these moment equations 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

In Eu's theory [1], the kinetic theory of fluids is intimately 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 this method is the balance equation for the calortropy $\hat{\Psi}$, which is different from the Boltzmann entropy,

$$\rho \hat{\Psi}(\mathbf{r},t) = -k_B \left\langle \left[\ln f^c \left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t \right) - 1 \right] f \left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t \right) \right\rangle.$$
(3.18)

Here the non-equilibrium canonical distribution function f^c represents the thermodynamic branch of the solution of the Boltzmann-Curtiss kinetic equation f. By differentiating the local calortropy density $\hat{\Psi}$ with time and combining it with the Boltzmann-Curtiss equation, the following equation can be obtained:

$$\rho \frac{d\hat{\Psi}}{dt} + \nabla \cdot \left(-k_B \left\langle \mathbf{C} \left(\ln f^c - 1\right) f \right\rangle \right) + k_B \left\langle f \left(\frac{d}{dt} + \mathbf{C} \cdot \nabla \right) \ln f^c \right\rangle = \sigma_c, \qquad (3.19)$$

where $\sigma_c \equiv -k_B \langle \ln f^c C[f, f_2] \rangle$. According to Eu's theory [3], the nonequilibrium canonical distribution function for diatomic gas can be expressed in the exponential form

$$f^{c} = \exp\left[-\frac{1}{K_{B}T}\left(\frac{1}{2}mC^{2} + H_{rot} + \sum_{n=1}^{\infty}X^{(n)}h^{(n)} - \mu_{Normalized}\right)\right],$$
(3.20)

where, $\mu_{Normalized}$ is the normalization factor defined as

$$\exp\left(-\frac{1}{K_{B}T}\mu_{Normalized}\right) = \left\langle \exp\left[-\frac{1}{K_{B}T}\left(\frac{1}{2}mC^{2} + H_{rot} + \sum_{n=1}^{\infty}X^{(n)}h^{(n)}\right)\right] \right\rangle / n,$$
(3.21)

where **C** is the peculiar velocity of the gas particle defined by $\mathbf{C} = \mathbf{v} - \mathbf{u}$, where **v** and **u** being the particle velocity and the average bulk velocity, respectively; *n* is the number density; *T* is the temperature; H_{rot} denotes the rotational Hamiltonian of the molecule; *m* is the molecular mass; K_B is the Boltzmann constant; and $X^{(n)}$, unknown macroscopic quantities, are the conjugate variables to the molecular expressions for moment, $h^{(n)}$. In

physical perspective, 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. On the other hand, in mathematical perspective, it guarantees the non-negativity of the distribution function regardless of the level of approximations. It may be noticed that the number of moments goes to infinity as shown in Eq. (3.20). This is in contrast with common practice in considering only the first 13^{th} moments for monatomic gas and the first 14^{th} moments for diatomic as well as simple polyatomic gases from the outset in the formulation of the theory. For simplicity, after dropping the superscripts *c* in the distribution function, it may be written in short notation for the exponent [54] as

$$f = f^{(0)} \exp(-x), \text{ where } x = \frac{1}{K_B T} \left(\sum_{n=1}^{\infty} X^{(n)} h^{(n)} - \mu_{Normalized} \right).$$
(3.22)

With further introducing of notations and dimensionless variables

$$x_{12} = x_{1} + x_{2}, \ y_{12} = y_{1} + y_{2} = x_{12}^{*}, \ \overline{\sigma}_{c} = \frac{\sigma_{c}}{K_{B}/g}, \ g \equiv \frac{1}{n^{2}d^{2}}\sqrt{\frac{m}{2K_{B}T}},$$
(3.23)
$$\overline{b} = \frac{b}{d}, \ \overline{g}_{12} = g_{12}\sqrt{\frac{m}{2K_{B}T}}, \ w = \mathbb{C}\sqrt{\frac{m}{K_{B}T}}, \ \omega(w) = \frac{1}{(2\pi)^{3/2}}\exp\left(-\frac{1}{2}w^{2}\right),$$
$$\omega_{12}(w, w_{2}) \equiv \frac{1}{(2\pi)^{3}}\exp\left(-\frac{1}{2}w^{2} - \frac{1}{2}w^{2}\right),$$
$$\langle A \rangle_{c} \equiv \int d\hat{\Gamma}_{12}\omega_{12}(w, w_{2})A(w, w_{2}),$$
$$\int d\hat{\Gamma}_{12} \cdots \equiv \int dw \int dw_{2}\int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \ \overline{b} \ \overline{g}_{12} \cdots,$$
$$\int d\Gamma_{12} \cdots \equiv \int dv \int dv_{2}\int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \ b \ g_{12} \cdots.$$

The calortropy production can be expressed as

$$\sigma_{c} \equiv -K_{B} \left\langle \ln f C[f, f_{2}] \right\rangle$$

$$= \frac{1}{T} \left\langle \left(\frac{1}{2} m C^{2} + H_{rot} + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} - \mu_{Normalized} \right) C[f^{(0)} \exp(-x), f_{2}^{(0)} \exp(-x_{2})] \right\rangle$$

$$= \frac{1}{4} K_{B} \int d\mathbf{v} \int d\mathbf{v}_{2} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \, bg_{12} \, f^{(0)} f_{2}^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})]$$

$$= \frac{1}{4T} \int d\Gamma_{12} f^{(0)} f_{2}^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})]$$
(3.25)

or simply

$$\bar{\sigma}_{c} = -\frac{1}{4} \left\langle (x_{12} - y_{12}) \left[\exp(-y_{12}) - \exp(-x_{12}) \right] \right\rangle_{c}.$$
(3.26)

This mathematical expression is suitable for so-called cumulant expansion, and it may be expressed in the form of

$$\overline{\sigma}_{c} = \kappa_{1}^{2} q\left(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots\right), \text{ where } \kappa_{1} = \frac{1}{2} \left\{ \left\langle \left(x_{12} - y_{12}\right)^{2} \right\rangle_{c} \right\}^{1/2},$$

$$q\left(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots\right) \equiv \frac{1}{2\kappa_{1}} \left\{ \exp\left[\sum_{l=1}^{\infty} \frac{\left(-1\right)^{l}}{l!} \kappa_{1}^{(+)}\right] - \exp\left[\sum_{l=1}^{\infty} \frac{\left(-1\right)^{l}}{l!} \kappa_{1}^{(-)}\right] \right\}.$$
(3.27)

This mathematical expression (3.27) guarantees the positivity of the calortropy production regardless of the level of approximations. In addition, when the distribution functions (3.22) is inserted into the definition of calortropy production, the dissipation term is shown to be directly related to the calortropy production σ_c ,

$$\sigma_{c} = -K_{B} \left\langle \ln f C[f, f_{2}] \right\rangle = -K_{B} \left\langle -\frac{1}{k_{B}T} \sum_{n=1}^{\infty} X^{(n)} h^{(n)} C[f, f_{2}] \right\rangle$$

$$= \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \left\langle h^{(n)} C[f, f_{2}] \right\rangle = \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)}$$
(3.28)

Now the explicit form of the dissipation term $\Lambda^{(n)}$ can be derived from Eqs. (3.27) and (3.28) by calculating the first reduced collision integral κ_1 in terms of $X^{(n)}$, as $x = \frac{1}{2} \left(\frac{\infty}{2} + \frac{1}{2}\right)$

performing in
$$\kappa_1$$
 consists of a sum of various moments, $x = \frac{1}{K_B T} \left(\sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right)$, with

the definition $\delta h^{(n)} = h^{(n)} - h^{(n)*}$, etc., κ_1^2 may be expressed as a quadratic form of X and X_2 ,

$$\kappa_{1}^{2} = \frac{1}{4} \sum_{n,l=1}^{\infty} \left\langle \left(X^{(n)} \delta h^{(n)} + X_{2}^{(n)} \delta h_{2}^{(n)} \right) \left(X^{(l)} \delta h^{(l)} + X_{2}^{(l)} \delta h_{2}^{(l)} \right) \right\rangle_{c}.$$
(3.29)

On rearranging of the terms it may become

$$\kappa_1^2 = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)}, \qquad (3.30)$$

where $R_{12}^{(nl)}$ are scalar coefficients made up of collision bracket integrals of $h^{(n)}$ and $h_2^{(l)}$ for an isotropic system of dilute gases. After comparing Eqs. (3.27), (3.28), and (3.30),

$$\overline{\sigma}_{c} = \kappa_{1}^{2} q \Big(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots \Big) = \frac{1}{K_{B}T} g \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)} = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(n)l} X_{2}^{(l)} q \Big(\kappa_{1}^{(\pm)}, \kappa_{2}^{(\pm)}, \cdots \Big),$$
(3.31)

then the dissipation term $\mathbf{\Lambda}^{(n)}$ can be derived as,

$$\boldsymbol{\Lambda}^{(n)} = \frac{K_B T}{g} \sum_{l=1}^{\infty} R_{12}^{(nl)} X_2^{(l)} q\left(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots\right).$$
(3.32)

The unknown conjugate variables $X^{(n)}$ can be achieved by generalizing the equilibrium Gibbs ensemble theory – providing the relationship between thermodynamic variables and the partition functions —to nonequilibrium processes. Such nonequilibrium generalization was developed by Eu [1] and it may be summarized here

$$\frac{\left\langle h^{(n)}f\right\rangle}{\rho} = -K_{B}T\left(\frac{\partial}{\partial X^{(n)}}\ln Z\right),$$
(3.33)
where $Z = \frac{1}{n_{d}}\left\langle \exp\left[-\frac{1}{K_{B}T}\left(\frac{1}{2}mC^{2} + H_{rot} + \sum_{n=1}^{\infty}X^{(n)}h^{(n)}\right)\right]\right\rangle$

After then, $X^{(n)}$ can be calculated in terms of the macroscopic flux $\langle h^{(n)} f \rangle$ by solving the differential equation (3.33). The leading order approximate solutions are known to be

$$X^{(1)} = -\frac{\Pi}{2p}, \ X^{(2)} = -\frac{3}{2}\frac{\Delta}{p}, \ X^{(3)} = -\frac{\mathbf{Q}}{pC_pT}.$$
(3.34)

Finally, the moment equation for the general type of molecules (3.14)-(3.16) can be written by replacing the collisional term with Eq. (3.32) as

$$\rho \frac{D}{Dt} \left(\frac{\Pi}{\rho} \right) + \nabla \cdot \Psi^{(\Pi)} + 2(p + \Delta) [\nabla \mathbf{u}]^{(2)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)}$$
(3.35)

$$= \frac{K_B T}{g} \sum_{l=1}^{\infty} R_{l2}^{(ll)} X_2^{(l)} q\left(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots\right),$$
(3.36)

$$\rho \frac{D}{Dt} \left(\frac{\Delta}{\rho} \right) + \nabla \cdot \Psi^{(\Delta)} + 2\gamma' (\Pi + \Delta \mathbf{I}) : \nabla \mathbf{u} + \frac{2}{3} \gamma' p \nabla \cdot \mathbf{u}$$
(3.36)

$$= \frac{K_B T}{g} \sum_{l=1}^{\infty} R_{l2}^{(2l)} X_2^{(l)} q\left(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots\right),$$
(3.37)

$$\rho \frac{D}{Dt} \left(\frac{\mathbf{Q}}{\rho} \right) + \nabla \cdot \Psi^{(\mathbf{Q})} + (p + \Delta) C_p \nabla T + \Pi \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u}$$
(3.37)

Remarks, the system of Eqs. (3.35)-(3.37) are still exact to the original Boltzmann-Curtiss equation, since the number of terms in dissipation series goes to infinity, and the kinematic high-order term is not yet approximated. Nevertheless, Eqs. (3.35)-(3.37) are in suitable shape for balance treatment in approximating the kinematic high-order term on the left-hand side, and the dissipation term on the right-hand side.

There are some criticisms found in Eu's closures. One of these criticisms is too simplistic treatment of high-order term. In Eu's closure, the high order term $\Psi^{(\Pi)}$ is assumed to be zero i.e. $\Psi^{(\Pi)} = 0$ by setting $\langle mCCCf \rangle = \frac{2}{3}IQ$. This closure suffers a mathematical inconsistency, since $\langle mCCCf \rangle$ is a symmetric tensor, whereas IQ is non-symmetric tensor, leading to a contradiction. This inconsistency in Eu's closure was eventually overcome by a recent balanced closure developed by Myong in 2014 [54].

3.3 Boltzmann-Curtiss based constitutive models via the balance closure

3.3.1 Zero-order Boltzmann-Curtiss based model

The zero-order Boltzmann-Curtiss based model (or Euler constitutive relations) is a direct consequence of assuming flow in an equilibrium state. As a resultant, density distribution function is assumed to be a Maxwellian distribution function. Note that the Maxwellian distribution function is defined [10] as

$$f^{(0)} = n \left(\frac{m}{2\pi K_B T}\right)^{3/2} \exp\left[-\frac{mC^2}{2K_B T}\right].$$
 (3.38)

The statistical formulation of the viscous stress tensor, excess normal stress and the heat flux vector using the Maxwellian distribution has simple and exact solution given as;

$$\Pi = \left\langle h^{(1)} f^{(0)} \right\rangle = 0,$$

$$\Delta = \left\langle h^{(2)} f^{(0)} \right\rangle = 0,$$

$$\mathbf{Q} = \left\langle h^{(3)} f^{(0)} \right\rangle = 0.$$
(3.39)

3.3.2 First-order Boltzmann-Curtiss based model

In the Boltzmann-Curtiss kinetic equation, the left-hand side which demonstrates the change of particles due to the collisionless motion of the particles, changes with a time scale of the order of $nm/2k_BTL$. On the other side, the right-hand side of Boltzmann-Curtiss kinetic equation explains the net change in the number of gas molecules due to intermolecular collisions. Basically, it is described by gain minus loss (exp^(nonequilibrium)-exp^(-nonequilibrium))[55], has the time scale of $n\sigma m/2k_BTL$. According to Eu [1], the time scale of conservative and non-conservative variables are different. The relaxation time of non-conserved variables is much shorter than conserved variables and is found in the order of 10^{-10} seconds. Therefore, the evaluation of non-conserved variables near equilibrium
state becomes linear and cumulant expansion of collisional term recovers the first-order Chapman-Enskog approximation. It is possible to approximate the entropy production and consequently non-conservative evolution equations, such that the viscous stress tensor, the excess normal stress, and the heat flux vector moment equations are linearized by truncating collisional term–considering the first term of cumulant expansion $\frac{K_BT}{g}R_{12}^{(n1)}X_2^{(1)}q(\kappa_1^{(\pm)})$ –and approximating transport process. The approximate dissipation

terms can be written as

$$\boldsymbol{\Lambda}^{(\boldsymbol{\Pi})} = -\frac{p}{\mu} \boldsymbol{\Pi} q_{1st} (k_1),$$

$$\boldsymbol{\Lambda}^{(\Delta)} = -\frac{2}{3} \gamma' \frac{p}{\mu_{bulk}} \Delta q_{1st} (k_1),$$

$$\boldsymbol{\Lambda}^{(\boldsymbol{Q})} = -\frac{pC_p}{k} \boldsymbol{Q} q_{1st} (k_1),$$
(3.40)

where, $q_{1st}(k_1) = 1$, μ , μ_{bulk} and k are the first coefficient of viscosity, the bulk viscosity coefficient and the thermal conductivity derived by Chapman-Enskog transport theory. According to Eu's theory, the non-conserved variables change considerably faster than conserved variables, and they reach to steady state much earlier than the conserved variables. It is valid to simplify the non-conserved equation by omitting the substantial time derivative from the equations as,

$$\nabla \cdot \boldsymbol{\Psi}^{(\boldsymbol{\Pi})} + 2(p + \Delta) [\nabla \mathbf{u}]^{(2)} + 2[\boldsymbol{\Pi} \cdot \nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu} \boldsymbol{\Pi} q_{1st}(k_1), \qquad (3.41)$$

$$\nabla \cdot \boldsymbol{\Psi}^{(\Delta)} + 2\gamma' (\boldsymbol{\Pi} + \Delta \mathbf{I}) : \nabla \mathbf{u} + \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u} = -\frac{2}{3}\gamma' \frac{p}{\mu_{bulk}} \Delta q_{1st}(k_1), \qquad (3.41)$$

$$\nabla \cdot \boldsymbol{\Psi}^{(\mathbf{Q})} + (p + \Delta) C_p \nabla T + \boldsymbol{\Pi} \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} = -\frac{pC_p}{k} \mathbf{Q} q_{1st}(k_1).$$

To close the system of equations (3.41), the high-order moments appearing on the left side of above equations must be known. According to Myong's balanced closure theory [54], and a recent summary of his theory [56], the first-order approximation of collisional terms requires the same order of approximation on the left-hand side of non-conserved moment equations. Therefore, not only $\nabla \cdot \Psi^{(\Pi)}$, $\nabla \cdot \Psi^{(\Delta)}$ and $\nabla \cdot \Psi^{(Q)}$ are required to remove from the first-order constitutive relations, but also $2[\Pi \cdot \nabla \mathbf{u}]^{(2)}$, $2\gamma'(\Pi + \Delta \mathbf{I}): \nabla \mathbf{u}$ and $\Pi \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u}$ are needed to be eliminated for the first-order approximation. Because the thermal velocity appeared in their statistical formulations is the order of two or more which can destroy the balance assumptions on the equations. As a result, the firstorder linear Boltzmann-Curtiss based model (i.e. Navier-Fourier constitutive relation) is given by

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

$$\Delta = -\mu_{bulk} \nabla \cdot \mathbf{u},$$

$$\mathbf{Q} = -k \nabla T.$$
(3.42)

3.3.3 Second-order Boltzmann-Curtiss based model

Previous theoretical and computational studies [57-59] have revealed that the fundamental physics in conditions far from thermal equilibrium is significantly different from the classical physics governed by the first-order Boltzmann-Curtiss based model are valid only in conventional flows near equilibrium. As a consequence, simple modification of first-order Boltzmann-Curtiss based model using transport coefficients, or by introducing velocity-slip and temperature-jump boundary conditions, cannot solve the current bottleneck of problems in the classical first-order (linear uncoupled) laws. Ultimately, the problem demands a completely new development of the non-classical second-order (nonlinear coupled) laws.

Recently, independent of the previous continuum approach, a new development has been reported on the constitutive equations of gases in a thermal nonequilibrium (rarefied and microscale) state from the viewpoint of the moment method applied to the kinetic Boltzmann-Curtiss equation [39] and the so-called balanced closure [54]. An important result obtained from these studies is that the number of places for closing the moment equations is two –kinematic and collision terms—and thus, the order of approximations in handling two terms must be the same, for example, second-order for both kinematic and collision terms. Otherwise, in the case of high Mach number shock structure, the kinematic (stress-strain) coupling term of quadratic nature will grow far faster than the strain rate term due to the destructive interplay, resulting in an imbalance with the first-order dissipation term and eventually a blow-up mathematical singularity. Therefore, to go beyond the first-order accuracy, one must abandon the simple linear relation in the collisional term enjoyed by assuming the simple Maxwellian gas molecule, which was once considered a nice-to-have mathematical coincidence.

As a result of the balanced closure, a second-order nonlinear coupled constitutive relation expressed in a mathematically implicit "sinh" form, which is an exact consequence of the Boltzmann-Curtiss equation of diatomic and polyatomic gases within the second-order accuracy, can be derived [39]as

$$2(p+\Delta)[\nabla \mathbf{u}]^{(2)} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu} \mathbf{\Pi} q_{2nd}(k_1),$$

$$2\gamma'(\mathbf{\Pi} + \Delta \mathbf{I}): \nabla \mathbf{u} + \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u} = -\frac{2}{3}\gamma' \frac{p}{\mu_{bulk}} \Delta q_{2nd}(k_1),$$

$$(p+\Delta)C_p \nabla T + \mathbf{\Pi} \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} = -\frac{pC_p}{k} \mathbf{Q} q_{2nd}(k_1).$$
(3.43)

In this expansion, the second-order dissipation term q_{2nd} , and the first cumulant expansion term k_1 , are given in hyperbolic sine form and a Rayleigh dissipation function, respectively,

$$q_{2nd}(k_{1}) = \frac{\sin k_{1}}{k_{1}},$$

$$k_{1} = \frac{(mK_{B})^{1/4}}{\sqrt{2}d} \frac{T^{1/4}}{p} \left[\frac{\Pi : \Pi}{2\mu} + \gamma' \frac{\Delta^{2}}{\mu_{bulk}} + \frac{\mathbf{Q} \cdot \mathbf{Q} / T}{k} \right]^{1/2}.$$
(3.44)

These algebraic second-order Boltzmann-Curtiss based relations, so-called nonlinear coupled constitutive relations (NCCR), can be solved using an appropriate numerical

method while the conserved variables remain constant during the evaluation process. The remaining task is to solve this algebraic nonlinear system of equations (3.43) beside the conservation of laws using an appropriate numerical method.

3.4 Governing equations for numerical simulation

The conservation laws in three-dimensional form, provide a system of five differential equations including mass, momentum and energy equations. However, the number of unknown field variables is fourteen, namely, ρ , **u**, p, T, E, Π , Δ , and **Q**.

 $\begin{array}{l} \hline \mathbf{Zero-order Boltzmann-Curtiss based model (Euler constitutive relations)} \\ \mu, \mu_{bulk}, k \rightarrow 0, \\ \Pi = 0, \Delta = 0, \mathbf{Q} = 0. \\ \hline \mathbf{First-order Boltzmann-Curtiss based model (Navier-Stokes-Fourier constitutive relations)} \\ \mu, k \rightarrow f(p,T), \mu_{bulk} \rightarrow 0 \\ \Pi = -2\mu [\nabla \mathbf{u}]^{(2)}, \Delta = 0, \mathbf{Q} = -k\nabla T. \\ \hline \mathbf{First-order Boltzmann-Curtiss based model (Navier-Fourier constitutive relations)} \\ \mu, \mu_{bulk}, k \rightarrow f(p,T), \\ \Pi = -2\mu [\nabla \mathbf{u}]^{(2)}, \Delta = -\mu_{bulk} \nabla \cdot \mathbf{u}, \mathbf{Q} = -k\nabla T. \\ \hline \mathbf{Second-order Boltzmann-Curtiss based model (Nonlinear coupled constitutive relations)} \\ \mu, \mu_{bulk}, k \rightarrow f(p,T), \\ 2(p + \Delta) [\nabla \mathbf{u}]^{(2)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu} \prod \frac{\sinh k_1}{k_1} \\ 2\gamma' (\Delta \mathbf{I} + \Pi) : \nabla \mathbf{u} + \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u} = -\frac{2}{3}\gamma' \frac{p}{\mu_{bulk}} \Delta \frac{\sinh k_1}{k_1} \\ (p + \Delta) C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} + C_p \Pi \cdot \nabla T = -\frac{C_p p}{k} \mathbf{Q} \frac{\sinh k_1}{k_1}. \end{array}$

Figure 3-1. A glance of Boltzmann-Curtiss based consitutive models up to second order.

The non-conservative variables $(\Pi, \Delta, \mathbf{Q})$ can be read from the second-order Boltzmann-Curtiss based constitutive relations which is introduced in Figure 3-1. The thermodynamic state variables — density, pressure, and temperature — can be obtained from the equations of states. In dilute gas conditions, mean molecular spacing ($\delta = n^{-1/3}$) is much bigger than molecular diameter *d*. Therefore, the gas is assumed to be calorically perfect that behaves ideally,

$$p = nK_{B}T = (\gamma - 1)\rho\left(E_{total} - \frac{1}{2}\mathbf{u}\mathbf{u}\right).$$
(3.45)

where K_B is the Boltzmann constant, *n* is the number density, and $\gamma = C_p/C_v$ is the specific heat ratio. In addition to 14 field unknown variables, there are few more unknown which are related to the microscopic gas properties, so-called transport coefficients; the first coefficient of viscosity μ , the coefficient of bulk viscosity μ_{bulk} , the coefficient of thermal conductivity κ , and the second coefficient of viscosity λ . They may be calculated from either inter-molecular force relations or Chapman-Enskog relations.

3.4.1 Conservative form of the conservation laws

The D – dimension conservation laws for diatomic and polyatomic gases without source term can be represented in differential form as,

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}}(\mathbf{U}) + \nabla \cdot \mathbf{F}^{\text{vis}}(\mathbf{U}, \nabla \mathbf{U}) = 0 \quad \text{in} [(t, \Omega): t \in (0, \infty), \Omega \in \mathbb{R}], \quad (3.46)$$
$$\mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0(\mathbf{x}) \quad \text{in} \Omega \in \mathbb{R}.$$

Here $\mathbf{U} \in \mathbb{R}^{(\mathcal{D}+2)}$ is a vector of conservative variables – mass per unit volume, momentum vector and energy – which are continuously differentiable in the computational domain Ω . The $\mathbf{F}^{inv} \in \mathbb{R}^{(\mathcal{D}+2)\times\mathcal{D}}$ and $\mathbf{F}^{vis} \in \mathbb{R}^{(\mathcal{D}+2)\times\mathcal{D}}$ are the inviscid and viscous flux functions, respectively. The inviscid flux function which is also known as convective flux is related to convective transport of macroscopic quantities in the fluid. The viscous flux function contains the viscous stresses and heat diffusion terms.

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E_{total} \end{bmatrix}, \quad \mathbf{F}^{inv} = \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + \rho \mathbf{I} \\ (\rho E_{total} + \rho \mathbf{I}) \mathbf{u} \end{bmatrix}, \quad \mathbf{F}^{vis} = \begin{bmatrix} 0 \\ \Pi + \Delta \mathbf{I} \\ (\Pi + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix}$$
(3.47)

3.4.2 Dimensionless form of the governing equations

In order to study under different conditions around the same geometry and moreover, in order to reduce the error due to the finite precision of computers, we have to make sure that all the used flow variables are approximate of the same order of magnitude. This process can be performed by normalizing the governing equations. There are many different non-dimensionalization procedures. In this thesis, we are introducing the following variables and parameters to make the conservation laws (3.47) in dimensionless form,

$$t^{*} = \frac{t}{t_{ref}}, \quad \mathbf{x}^{*} = \frac{\mathbf{x}}{L}, \quad \rho^{*} = \frac{\rho}{\rho_{ref}}, \quad \mathbf{u}^{*} = \frac{\mathbf{u}}{u_{ref}}, \quad p^{*} = \frac{p}{p_{ref}}, \quad T^{*} = \frac{T}{T_{ref}}, \quad (3.48)$$
$$\mu^{*} = \frac{\mu}{\mu_{ref}}, \quad k^{*} = \frac{k}{k_{ref}}, \quad C_{p}^{*} = \frac{C_{p}}{C_{p_{ref}}}, \quad E^{*} = \frac{E}{E_{ref}}, \\ \Pi^{*} = \frac{\Pi}{\Pi_{ref}}, \\ \mathbf{Q}^{*} = \frac{\mathbf{Q}}{\mathbf{Q}_{ref}}, \quad \nabla^{*} = L\nabla.$$

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

$$t_{ref} = \frac{L}{u_{ref}}, \ E_{ref} = u_{ref}^2, \ \Pi_{ref} = \frac{\mu_{ref} u_{ref}}{L}, \ \mathbf{Q}_{ref} = \frac{k_{ref} \Delta T_{ref}}{L}.$$
(3.49)

Here *L* denotes the characteristics length, ΔT_{ref} denotes $T_w - T_{ref}$ or $T_{ref} - T_w$, where T_w is the wall temperature. Putting dimensionless variables from Eqs. (3.38)-(3.39) into Eq. (3.47) and divide it through by the leading dimensional coefficient resulting dimensionless form of the conservation laws for diatomic and polyatomic gas, after dropping the asterisks

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}} \left(\mathbf{U} \right) + \nabla \cdot \mathbf{F}^{\text{vis}} \left(\mathbf{U}, \nabla \mathbf{U} \right) = 0, \qquad (3.50)$$

with the dimensionless form of conservative variables, inviscid, and viscous flux vector defined as,

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E_{total} \end{bmatrix}, \mathbf{F}^{\text{inv}} = \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} + \frac{1}{N_{\delta} \operatorname{Re}} p \mathbf{I} \\ \left(\rho E_{total} + \frac{1}{N_{\delta} \operatorname{Re}} p \mathbf{I} \right) \mathbf{u} \end{bmatrix}, \mathbf{F}^{\text{vis}} = \frac{1}{\operatorname{Re}} \begin{bmatrix} 0 \\ \Pi + \Delta \mathbf{I} \\ (\Pi + \Delta \mathbf{I}) \cdot \mathbf{u} + \frac{1}{Ec \operatorname{Pr}} \mathbf{Q} \end{bmatrix}.$$
(3.51)

Here the fluid dynamic dimensionless parameters – Mach number M, Reynolds number Re, Prandtl number Pr, Knudsen number Kn, composite number N_{δ} , Eckert number Ec – are defined as

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

$$Kn = \frac{\lambda_{ref}}{L}, \quad N_{\delta} = \frac{\mu_{ref} u_{ref}}{p_{ref} L}, \quad \varepsilon = \frac{\Delta T_{ref}}{T_{ref} Ec \operatorname{Pr}}.$$
(3.52)

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

$$\mu = T^{s}, \ \mu_{bulk} = f_{bulk} \mu, \ k = T^{s},$$
(3.53)

where $s = \frac{1}{2} + \frac{2}{\nu - 1}$, ν is the exponent of the inverse power laws.

The second-order Boltzmann-Curtiss based constitutive relations can be reduced in dimensionless form as

$$\hat{\boldsymbol{\Pi}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \left(1 + f_{bulk}\hat{\boldsymbol{\Delta}}\right)\hat{\boldsymbol{\Pi}}_{1st} + [\hat{\boldsymbol{\Pi}}\cdot\nabla\hat{\boldsymbol{u}}]^{(2)},$$

$$\hat{\boldsymbol{\Delta}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \hat{\boldsymbol{\Delta}}_{1st} + \frac{3}{2}f_{bulk}\left(\hat{\boldsymbol{\Pi}} + f_{bulk}\hat{\boldsymbol{\Delta}}\boldsymbol{I}\right):\nabla\hat{\boldsymbol{u}},$$

$$\hat{\boldsymbol{Q}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \left(1 + f_{bulk}\hat{\boldsymbol{\Delta}}\right)\hat{\boldsymbol{Q}}_{1st} + \hat{\boldsymbol{\Pi}}\cdot\hat{\boldsymbol{Q}}_{1st} + \frac{1}{2\Pr}\hat{\boldsymbol{Q}}\cdot\nabla\hat{\boldsymbol{u}}.$$
(3.54)

Here the caret \land over a symbol represents a quantity with the dimension of the ratio of the stress to the pressure, and, f_{bulk} denotes the ratio of the bulk viscosity to the shear viscosity.

$$\hat{\boldsymbol{\Pi}} = \frac{N_{\delta}}{p} \boldsymbol{\Pi}, \quad \hat{\boldsymbol{\Delta}} = \frac{N_{\delta}}{p} \boldsymbol{\Delta}, \quad \hat{\boldsymbol{Q}} = \frac{N_{\delta}}{p} \frac{\boldsymbol{Q}}{\sqrt{T/(2\varepsilon)}}, \quad (3.55)$$

$$\nabla \hat{\boldsymbol{u}} = -2\mu \frac{N_{\delta}}{p} \nabla \boldsymbol{u}, \quad \nabla \hat{T} = -2k \frac{N_{\delta}}{p} \frac{\nabla T}{\sqrt{T/(2\varepsilon)}}, \quad \varepsilon = \frac{1}{Ec \operatorname{Pr}} \frac{1}{T_r/\Delta T}.$$

The values of $\hat{\Pi}_{1st}$, $\hat{\Delta}_{1st}$, and $\hat{\mathbf{Q}}_{1st}$ are the reduced form of the first-order Boltzmann-Curtiss based constitutive relations, defined as

$$\hat{\boldsymbol{\Pi}}_{1\text{st}} = -2\mu \left[\nabla \hat{\boldsymbol{u}} \right]^{(2)},$$

$$\hat{\boldsymbol{\Delta}}_{1\text{st}} = -\mu_{bulk} \nabla \cdot \hat{\boldsymbol{u}},$$

$$\hat{\boldsymbol{Q}}_{1\text{st}} = -\kappa \nabla \hat{T}.$$
(3.56)

The nonlinear coupling factor $q_{2nd}(c\hat{R})$ and dimensionless form of the dissipation function \hat{R} which was derived from the Rayleigh–Onsager dissipation function [1], given as

$$q_{2nd}\left(c\hat{R}\right) \equiv \frac{\sinh\left(c\hat{R}\right)}{c\hat{R}}, \ \hat{R}^{2} \equiv \hat{\Pi} : \hat{\Pi} + \frac{2\gamma'}{f_{bulk}}\hat{\Delta}^{2} + \hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}},$$

$$c^{2} = \frac{2\sqrt{\pi}}{5} \mathbf{A}_{2}\left(\nu\right)\Gamma\left[4 - \frac{2}{\nu - 1}\right].$$
(3.57)

The constant *c* defined in Eq. (3.57) has a value between 1.0138 (Maxwellian) and 1.2232 ($\nu = 3$), where ν is the exponent of the inverse power law for the gas-particle interaction potential and Γ denotes the gamma function.

In the rest part of present work, *non-dimensional equations are utilized, and the asterisk symbol is omitted in order to condense the notations*. To solve equations using advanced numerical methods. A numerical method for solving algebraic constitutive relations is provided in the next subsections of this chapter.



Figure 3-2. Comparison of stress tensor for first-order (top) and second-order (bottom) Boltzmann-Curtiss constitutive models.

3.4.3 Topology of the second-order Boltzmann-Curtiss constitutive model

In order to study the nature of rotational nonequilibrium based on a various range of bulk viscosities, the non-conserved variables obtained by the first-order linear constitutive model and the second-order Boltzmann-Curtiss based constitute model are compared. The f_{bulk} values for argon, nitrogen, and carbon dioxide gases are taken 0.0, 0.8, and 1000, respectively from Figure 2-3.

A significant comparison of the non-conservative stress quantity for first-order and second-order constitutive models has been made based on various bulk viscosity f_{bulk} values as shown in Figure 3-2. It is obvious that the response of the first-order constitutive model to the applied stress and thermal forces are linear whereas the second-order constitutive model behaves nonlinearly. For first-order linear model, the viscous stress

tensor is not a function of thermal force. Therefore, the influence of thermal forces are negligible and the stress values are found to be symmetry with respect to the adiabatic line. However, in the case of second-order constitutive model – due to strong coupling between non-conserved variables through the Rayleigh-Onsager function \hat{R} – the viscous stress tensor is a function of both shear force and thermal force. Thus, stress values are changing nonlinearly with respect to thermal forces, although stress tensor is more influenced by the stress forces in comparison to the thermal forces. Similarly to the first-order model, the monotonicity of the solution is preserved and the solution has symmetrical behavior with respect to the adiabatic line. As the f_{bulk} value increases, the influence of thermal forces reduces and the stress forces play a dominant role due to a significant contribution of $f_{bulk} \nabla \cdot \mathbf{u}$ in the compression and expression term. Therefore, the thermal forces become weaker and shear forces become stronger at a higher f_{bulk} value.

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 3-3. Comparison of excess normal stress for first-order (top) and second-order (bottom) Boltzmann-Curtiss constitutive models.

Figure 3-3 illustrates a comparison between first-order and second-order constitutive models based on excess normal stress for various gases. In the case of monatomic gas, the role of the excess normal stress is negligible i.e. $\Delta = 0$ due to $f_{bulk} = 0$. Therefore, the influence of thermal force and stress force disappear. In the first-order constitutive equation, excess normal stress has a similar pattern like stress tensor but different in magnitudes of thermal forces (Figure 3-2 and Figure 3-3). In the case of diatomic gases, where $f_{bulk} \neq 0$, the effect of rotational nonequilibrium is considerable significant due to bulk viscosity. When $f_{bulk} = 0.8$, the excess normal stress does not preserve the monotonicity behavior but it contains symmetry behavior along with an adiabatic line. When bulk viscosity increases to 1000, the excess normal stress approaches to monotonicity behavior.



Figure 3-4. Comparison of heat flux for first-order (top) and second-order (bottom) Boltzmann-Curtiss constitutive models.

Similar to stress tensor, heat flux plays a vital role in the constitutive model for describing the physics of flow behavior. Figure 3-4 shows a comparison between first order and second order constitutive models based on heat flux quantity for various gases. In the first order constitutive model, the heat flux shows a linear and monotone behavior with respect to thermal force while it does not under influence of stress forces. On the other hand, the second order model demonstrates the nonlinear behavior of heat flux constitutive relations with respect to both forces. It is sensible that at $f_{bulk} = 0$, the heat flux is affected by the thermal force almost twice than the stress forces and a high nonlinearity behavior is found near the origin. As the bulk viscosity increases to $f_{bulk} = 0.8$, the influence of stress forces which are far from the origin, is faded and the heat flux is followed an asymmetry behavior with respect to the stress-free line. The heat flux cover fully asymmetry and take shape like a shark finning at a higher bulk viscosity value, $f_{bulk} = 1000$.



Figure 3-5. Comparison of Rayleigh-Onsager dissipation parameter for first-order (top) and second-order (bottom) Boltzmann-Curtiss constitutive models.

Figure 3-5 illustrates a comparison between computed Rayleigh-Onsager dissipation parameter \hat{R} , using the first-order and second-order constitutive models based on various gases. As it is well known that \hat{R} implicitly represents the degree of thermal nonequilibrium for a process. In the first-order model, at $f_{bulk} = 0.0$ and $f_{bulk} = 0.8$, the dissipation parameter having a circular shape which presents a uniform distribution of thermal nonequilibrium along the thermal stress and stress forces in all directions. At higher bulk viscosity value $f_{bulk} = 1000$, the dissipation parameter shows higher thermal nonequilibrium effects along stress tensor in comparison of thermal forces. On the other hand, in second-order Boltzmann-Curtiss based model, the deviation from equilibrium state due to thermal stress forces is not equally distributed. 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 to influence the flow.

3.5 An analysis on the second-order Boltzmann-Curtiss based constitutive model

3.5.1 One-dimensional compression-expansion constitutive relation

Considering the one-dimensional shock structure problem for diatomic and polyatomic gases in which the flow only evolves in *x*-direction, the second-order Boltzmann-Curtiss based constitutive relations (3.54) can be reduced [39] as,

$$\hat{\Pi}_{xx}q_{2nd}\left(c\hat{R}\right) = \left(\hat{\Pi}_{xx} + f_{bulk}\hat{\Delta} + 1\right)\hat{\Pi}_{xx_{1st}},$$

$$\hat{\Delta}q_{2nd}\left(c\hat{R}\right) = \left[3\left(\hat{\Pi}_{xx} + f_{bulk}\hat{\Delta}\right) + 1\right]\hat{\Delta}_{1st},$$

$$\hat{Q}_{x}q_{2nd}\left(c\hat{R}\right) = \left(\hat{\Pi}_{xx} + f_{bulk}\hat{\Delta} + 1\right)\hat{Q}_{x_{1st}} + \frac{3}{4\Pr}\hat{Q}_{x}\hat{\Pi}_{xx_{1st}},$$
(3.58)

where

$$\hat{R} = \sqrt{\left(\frac{3}{2}\hat{\Pi}_{xx}^{2} + \frac{4}{5}\frac{\hat{\Delta}^{2}}{f_{bulk}} + \hat{Q}_{x}^{2}\right)},$$

$$\hat{\Delta}_{1st} = \frac{3}{4}f_{bulk}\hat{\Pi}_{xx_{1st}}.$$
(3.59)

The normal stress in y- and z- directions are defined as $\hat{\Pi}_{yy} = \hat{\Pi}_{zz} = -\frac{1}{2}\hat{\Pi}_{xx}$ due to the traceless property of viscous stress tensor. The relation between the xx-component of the shear stress and the excess normal stress can be obtained by combining the first two equations of (3.58) as,

$$\hat{\Delta} = \frac{1}{8f_{bulk}} \Big[\Big(9f_{bulk}^2 - 4 \Big) \hat{\Pi}_{xx} - 4 + \sqrt{D} \Big],$$
(3.60)

where

$$D = \left(81f_{bulk}^4 + 72f_{bulk}^2 + 16\right)\hat{\Pi}_{xx}^2 + \left(32 - 24f_{bulk}^2\right)\hat{\Pi}_{xx} + 16.$$
(3.61)



Figure 3-6. Second-order model (diatomic and monatomic) relative to the first-order model in the compression-expansion flow. The horizontal and vertical axes represent the strain (force) term and the normal stress, respectively (Reproduced with permission from Myong [39]).

Figure 3-6 illustrates the general features of the second-order constitutive relations (3.58) for diatomic and polyatomic gases in the one-dimensional compression-expansion. The second-order constitutive model gives the asymmetrical behavior of normal stress for the rapid expansion and compression of a gas, as shown in Figure 3-6. Even though the details of the second-order constitutive models for monatomic and diatomic and polyatomic gases are different, the general patterns remain unchanged. Figure 3-6 shows the free-molecular asymptotic behavior with increasing degree of expansion and velocity-shear, satisfying $\hat{\Pi}_{xx} + \hat{\Delta} \rightarrow -1$ or $\Pi_{xx} + \Delta + p \rightarrow 0$. Previous studies [39, 54, 60] showed that the solutions of the second-order constitutive models were well-posed (existence, uniqueness, and continuous dependence on the data) for all inputs on thermodynamic forces.

3.5.2 One-dimensional shear-velocity constitutive relation

Considering the one-dimensional shear dominant flow problem where the flow only evolves in *x*-direction, and the temperature gradients are negligible, and velocity components are assumed zero in *y*- and *z*- directions. The reduced form of the second-order Boltzmann-Curtiss based constitutive relations (3.54) can be derived as,

$$\hat{\Pi}_{xx}q_{2nd}\left(c\hat{R}\right) = -\frac{2}{3}\hat{\Pi}_{xy}\hat{\Pi}_{xy_{1st}}$$

$$\hat{\Pi}_{xy}q_{2nd}\left(c\hat{R}\right) = \left(\hat{\Pi}_{xx} + f_{bulk}\hat{\Delta} + 1\right)\hat{\Pi}_{xy_{1st}},$$

$$\hat{\Delta}q_{2nd}\left(c\hat{R}\right) = 3f_{bulk}\hat{\Pi}_{xy}\hat{\Pi}_{xy_{1st}},$$
(3.62)

The above mentioned relation (3.62) yields an equation of one variable $\hat{\Pi}_{xx}$ and additional equation for $\hat{\Delta}$ as,

$$\hat{\Pi}_{xx}q_{2nd}^{2}\left(c\hat{R}\right) = -\frac{2}{3} \left[\left(1 - \frac{9}{2}f_{bulk}^{2}\right)\hat{\Pi}_{xx} + 1 \right]\hat{\Pi}_{xy_{1st}}, \qquad (3.63)$$

$$\hat{\Delta} = -\frac{9}{2} f_{bulk} \hat{\Pi}_{xx}, \qquad (3.64)$$

where

$$\hat{R} = \sqrt{\left(3\hat{\Pi}_{xx}\left[\left(1 + \frac{45}{4}f_{bulk}^{2}\right)\hat{\Pi}_{xx} - 1\right]\right)},$$
(3.65)

which follows from the stress constraint

$$\hat{\Pi}_{xy} = sign(\hat{\Pi}_{xy_{1st}}) \left[-\frac{3}{2} \left[\left(1 - \frac{9}{2} f_{bulk}^2 \right) \hat{\Pi}_{xx} + 1 \right] \hat{\Pi}_{xx} \right]^{1/2}.$$
(3.66)

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

The general features of the second-order constitutive relations (3.62) for diatomic and polyatomic gases in the one-dimensional shear flow are illustrated in Figure 3-7. It is obvious that as the shear velocity gradient becomes very large, the shear stresses predicted by the second-order constitutive model become very small, compared to the first-order constitutive model, as shown in Figure 3-7. 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 $(\hat{\Pi}_{yy})$ and shear $(\hat{\Pi}_{yy})$ stress.



Figure 3-7. Second-order model (diatomic and monatomic) relative to the first-order model in the shear flow. The horizontal and vertical axes represent the strain (force) term and the shear and normal stress, respectively (Reproduced with permission from Myong [39]).

3.6 Numerical Solver of the second-order Boltzmann-Curtiss based constitutive relations: iterative method

The second-order Boltzmann-Curtiss based constitutive relations (3.54) consist of 10 nonlinear implicit algebraic equations of the non-conserved variables (Π_{xx} , Π_{xy} , Π_{xz} , Π_{yy} , Π_{yz} , Π_{yz} , Π_{zz} , Δ , Q_x , Q_y , Q_z) for known 14 variables (p, T, ∇u , ∇v , ∇w). Owing to the highly nonlinear terms, it appears to be daunting task to develop a proper numerical method for solving the nonlinear system of equations. In present work, these nonlinear system of equations can be solved by the method of iterations based on previous studies [39, 60].

In the case of the three-dimensional problems, the stress and heat flux components $(\Pi_{xx}, \Pi_{xy}, \Pi_{xz}, \Delta, Q_x)$ on a line in the physical plane induced by thermodynamic forces such as velocity gradients (u_x, v_x, w_x, T_x) and temperature gradient (T_x) can be approximated as the sum of three solvers: first on $(u_x, 0, 0, T_x)$ second on $(0, v_x, 0, 0)$, and third on $(0, 0, w_x, 0)$. Thus the stress and heat flux $(\Pi_{xx}, \Pi_{xy}, \Pi_{xz}, \Delta, Q_x)$ in case of *x*-direction can be decomposed as function of (u_x, v_x, w_x, T_x) as,

$$f(u_x, v_x, w_x, T_x) = f_1(u_x, 0, 0, T_x) + f_2(0, v_x, 0, 0) + f_3(0, 0, w_x, 0).$$
(3.67)

The iteration procedures can be designed individually for these solvers as follows. In the first solver on $(u_x, 0, 0, T_x)$ which represents the compression-expansion of diatomic and polyatomic gases, the stress and heat flux (Π_{xx}, Δ, Q_x) can be determined based on positive $\hat{\Pi}_{xx_{1st}}$ and $\hat{Q}_{x_{1st}}$ as,

$$\hat{R}_{n+1} = \frac{1}{c} \sinh^{-1} \left[c \sqrt{Y_n} \right], \tag{3.68}$$

where

$$Y_{n} = \left(1 + \hat{\Pi}_{xx_{n}} + f_{bulk}\hat{\Delta}_{n}\right)^{2}\hat{R}_{1st}^{2} + 4\left(\hat{\Pi}_{xx_{n}} + f_{bulk}\hat{\Delta}_{n}\right)\left[1 + 2\left(\hat{\Pi}_{xx_{n}} + f_{bulk}\hat{\Delta}_{n}\right)\right]\frac{4}{5f_{bulk}}\hat{\Delta}_{1st}^{2}$$
(3.69)

and

$$\hat{\Pi}_{xx_{n+1}} = \frac{\left(1 + \hat{\Pi}_{xx_n} + f_{bulk} \hat{\Delta}_n\right) \hat{\Pi}_{xx_{1st}}}{\sqrt{Y_n}} \hat{R}_{n+1},$$

$$\hat{Q}_{x_{n+1}} = \frac{\hat{Q}_{x_{1st}}}{\hat{\Pi}_{xx_{1st}}} \hat{\Pi}_{xx_{n+1}}.$$
(3.70)

For the negative $\hat{\Pi}_{_{xx_{1st}}}$ and $\hat{Q}_{_{x_{1st}}}$, the stress and heat flux can be calculated as,

$$\hat{\Pi}_{xx_{n+1}} = \frac{\left(1 + f_{bulk}\hat{\Delta}_{n}\right)\hat{\Pi}_{xx_{1st}}}{q\left(c\hat{R}_{n}\right) - \hat{\Pi}_{xx_{1st}}},$$

$$\hat{Q}_{x_{n+1}} = \frac{\hat{Q}_{x_{1st}}}{\hat{\Pi}_{xx_{1st}}}\hat{\Pi}_{xx_{n+1}}.$$
(3.71)

Since the equations are invariant under a transformation $\hat{Q}_x \leftrightarrow -\hat{Q}_x$, only two cases satisfying $\hat{\Pi}_{xx}\hat{Q}_x > 0$ are considered. In these expressions, $\hat{\Pi}_{xx_1}$, $\hat{\Delta}_1$, \hat{Q}_{x_1} are the initial guess solution given by the equations

$$\hat{\Pi}_{xx_{1}} = \frac{\sinh^{-1}(c\hat{R}_{1st})}{c\hat{R}_{1st}}\hat{\Pi}_{xx_{1st}},$$

$$\hat{\Delta}_{1} = \frac{\sinh^{-1}(c\hat{R}_{1st})}{c\hat{R}_{1st}}\hat{\Delta}_{1st},$$

$$\hat{Q}_{x_{1}} = \frac{\sinh^{-1}(c\hat{R}_{1st})}{c\hat{R}_{1st}}\hat{Q}_{x_{1st}}.$$
(3.72)

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

$$\hat{R}_{n+1} = \frac{1}{c} \sinh^{-1} [cY_n], \qquad (3.73)$$

$$\hat{\Pi}_{xx_{n+1}} = \frac{2(3 - \sqrt{D_{n+1}})}{3(4 + 45f_{bulk}^2)},$$

where

$$Y_{n} = \left[2 \left\{ 1 + \left(1 - \frac{9}{2} f_{bulk}^{2} \right) \hat{\Pi}_{xx_{n}} \right\} \left\{ 1 - \left(1 + \frac{45}{4} f_{bulk}^{2} \right) \hat{\Pi}_{xx_{n}} \right\} \right]^{1/2} \hat{\Pi}_{xy_{0}},$$

$$D_{n+1} = 12 \left(1 + \frac{45}{4} f_{bulk}^{2} \right) \hat{R}_{n+1}^{2} + 9.$$
(3.74)

Noted that, the term Y_n is well defined for any f_{bulk} greater than the critical value $\sqrt{2}/3$. The $\hat{\Delta}$ and $\hat{\Pi}_{xy}$ can be determined by using Eq. (3.64) and the stress constraint (3.66). When $0 \le f_{bulk} < \sqrt{2}/3$, the $\hat{\Pi}_{xx}$ can be calculated by replacing the following algorithm,

$$\hat{\Pi}_{xx_{n+1}} = -\frac{2\hat{\Pi}_{xy_0}^2}{3q^2 \left(c\hat{R}_n\right) + \left(2 - 9f_{bulk}^2\right)\hat{\Pi}_{xy_0}^2},$$
(3.75)

where

$$\hat{R}_{n} = \left[3\hat{\Pi}_{xx_{n}}\left[\left(1 + \frac{45}{4}f_{bulk}^{2}\right)\hat{\Pi}_{xx_{n}} - 1\right]\right]^{1/2}.$$
(3.76)

These solvers and their outcomes can be summarized [61] as following :

$f_1(u_x,0,0,T_x)$	$f_2(0,v_x,0,0)$	$f_3(0,0,w_x,0)$
$\hat{\Pi}_{xx-1x}, \hat{\Pi}_{yy-1x} = -\frac{1}{2}\hat{\Pi}_{xx-1x},$ $\hat{\Pi}_{xy-1x} = \hat{\Pi}_{xz-1x} = 0,$ $\hat{\Pi}_{zy-1x} = 0, \hat{\Pi}_{zz-1x} = -\frac{1}{2}\hat{\Pi}_{xx-1x},$ $\hat{Q}_{x} = \hat{Q}_{x-1x}, \hat{\Delta}_{1-x} = \hat{\Delta},$	$\hat{\Pi}_{xx-2x}, \hat{\Pi}_{xy-2x},$ $\hat{\Pi}_{xz-2x} = \hat{\Pi}_{yz-2x} = 0,$ $\hat{\Pi}_{yy-2x} = -2\hat{\Pi}_{xx-2x},$ $\hat{\Pi}_{zz-2x} = \hat{\Pi}_{xx-2x},$ $\hat{Q}_{x-2x} = 0, \hat{\Delta}_{2-x} = 0,$	$\hat{\Pi}_{xx-3x}, \hat{\Pi}_{xz-3x}, \\\hat{\Pi}_{xy-3x} = \hat{\Pi}_{yz-3x} = 0, \\\hat{\Pi}_{yy-3x} = \hat{\Pi}_{xx-3x}, \\\hat{\Pi}_{zz-3x} = -2\hat{\Pi}_{xx-3x}, \\\hat{Q}_{x-3x} = 0, \hat{\Delta}_{3-x} = 0.$

Similarly, it is possible to evaluate the value of stress and heat flux in other two primary directions. In the case of *y*-direction, the stress and heat flux $(\Pi_{yx}, \Pi_{yy}, \Pi_{yz}, \Delta, Q_y)$ on a line in the physical plane induced by thermodynamic forces (velocity and temperature gradients) can be approximated as the sum of three solvers:

$$f(u_{y}, v_{y}, w_{y}, T_{y}) = f_{1}(0, v_{y}, 0, T_{y}) + f_{2}(u_{y}, 0, 0, 0) + f_{3}(0, 0, w_{y}, 0).$$
(3.77)

Here,

$$\begin{array}{c|c} f_1(0,v_y,0,T_y) & f_2(u_y,0,0,0) & f_3(0,0,w_y,0) \\ \hline \hat{\Pi}_{yy-1y}, \hat{\Pi}_{xx-1y} = -\frac{1}{2}\hat{\Pi}_{yy-1y}, & \hat{\Pi}_{xy-2y}, \hat{\Pi}_{yy-2y}, & \hat{\Pi}_{yy-2y}, \\ \widehat{\Pi}_{xy-1y} = \hat{\Pi}_{xz-1y} = 0, & \hat{\Pi}_{xz-2y} = \hat{\Pi}_{yz-2y} = 0, \\ \hline \hat{\Pi}_{zy-1y} = 0, \hat{\Pi}_{zz-1y} = -\frac{1}{2}\hat{\Pi}_{yy-1y}, & \hat{\Pi}_{zz-2y} = -2\hat{\Pi}_{yy-2y}, & \hat{\Pi}_{xx-3y} = \hat{\Pi}_{yy-3y}, \\ \hline \hat{Q}_y = \hat{Q}_{y-1y}, \hat{\Delta}_{1-y} = 0, & \hat{Q}_{y-2y} = 0, \hat{\Delta}_{2-y} = 0, \\ \hline \end{pmatrix}$$

In case of *z*-direction, the decomposed stress and heat flux $(\Pi_{zx}, \Pi_{zy}, \Pi_{zz}, \Delta, Q_z)$ can be calculated as,

$$f(u_z, v_z, w_z, T_z) = f_1(0, 0, w_z, T_y) + f_2(u_z, 0, 0, 0) + f_3(0, v_z, 0, 0).$$
(3.78)

$f_1(0,w_z,0,T_z)$	$f_2(u_z, 0, 0, 0)$	$f_3(0,v_z,0,0)$
$\hat{\Pi}_{zz-1z}, \hat{\Pi}_{xx-1z} = -\frac{1}{2}\hat{\Pi}_{zz-1z},$ $\hat{\Pi}_{xy-1z} = \hat{\Pi}_{xz-1z} = 0,$ $\hat{\Pi}_{zy-1z} = 0, \hat{\Pi}_{yy-1z} = -\frac{1}{2}\hat{\Pi}_{zz-1z},$ $\hat{Q}_{z-1z} = \hat{Q}_{z}, \hat{\Delta}_{1-z} = 0,$	$\hat{\Pi}_{xz-2z}, \hat{\Pi}_{zz-2z},$ $\hat{\Pi}_{xy-2z} = \hat{\Pi}_{yz-2z} = 0,$ $\hat{\Pi}_{xx-2z} = -2\hat{\Pi}_{zz-2z},$ $\hat{\Pi}_{zz-2z} = \hat{\Pi}_{zz-2z},$ $\hat{Q}_{z-2z} = 0, \hat{\Delta}_{2-z} = 0,$	$\hat{\Pi}_{zz-3z}, \hat{\Pi}_{yz-3z},$ $\hat{\Pi}_{xy-3z} = \hat{\Pi}_{xz-3z} = 0,$ $\hat{\Pi}_{xx-3z} = \hat{\Pi}_{zz-3z},$ $\hat{\Pi}_{yy-3z} = -2\hat{\Pi}_{zz-3z},$ $\hat{Q}_{z-3z} = 0, \hat{\Delta}_{3-z} = 0.$

Finally, we will have

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

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

$$\Pi = \frac{p}{N_{\delta}} \hat{\Pi}, \ \Delta = \frac{p}{N_{\delta}} \hat{\Delta}, \ \mathbf{Q} = \frac{p}{N_{\delta}} \sqrt{T/(2\varepsilon)} \hat{\mathbf{Q}},$$

$$\nabla \mathbf{u} = -\frac{p}{2\mu N_{\delta}} \nabla \hat{\mathbf{u}}, \ \nabla T = \frac{p\sqrt{T/(2\varepsilon)}}{kN_{\delta}} \nabla \hat{T}.$$
(3.79)

3.7 Breakdown parameters

The continuum (or near-equilibrium) breakdown parameter is essential in quantifying the gas flow regions in which the linear Navier-Stokes-Fourier hypothesis is no longer valid. There were several breakdown parameters appearing in the literature.

3.7.1 Bird's breakdown parameter

Bird [62] first proposed a semi-empirical parameter based on the spatial derivative of flow properties such as density, pressure, temperature or velocity magnitude, for steady state expanding flows.

$$B = M \sqrt{\frac{\gamma \pi}{8}} \frac{\lambda_{mean}}{\rho} \left| \frac{d\rho}{ds} \right|$$
(3.80)

where M is the *local* Mach number. The spatial gradient along the streamline, can be calculated in Cartesian coordinates as follows:

$$\frac{d\rho}{ds} = \frac{d\rho}{dx}\frac{u}{\sqrt{u^2 + v^2 + w^2}} + \frac{d\rho}{dy}\frac{v}{\sqrt{u^2 + v^2 + w^2}} + \frac{d\rho}{dz}\frac{w}{\sqrt{u^2 + v^2 + w^2}},$$
(3.81)

where u, v, and w represents the x-, y- and z-directional velocities, respectively. Moreover, if the other flow properties χ like the temperature and the velocity, are introduced in order to take both viscous effect and heat transfer into account, the following breakdown parameters B_{χ} (e.g. B_D , B_V and B_T) can be calculated:

$$B_{\chi} = M \sqrt{\frac{\gamma \pi}{8}} \frac{\lambda_{mean}}{\chi} \left| \frac{d\chi}{ds} \right|.$$
(3.82)

Then, by considering all the parameters, a breakdown parameters B_{max} can be defined by

$$B_{\max} \equiv \max\left(B_D, B_T, B_V\right). \tag{3.83}$$

In case of steady expanding flows, it was known that the value of B of about 0.05 is a good criterion for identifying the near-equilibrium breakdown.

3.7.2 Boyd's breakdown parameter

However, it was soon recognized that there might be a problem when the Mach number approaches to zero at stagnation points. Boyd *et al.* [63] carried out an extensive numerical investigation of one-dimensional normal shock waves and two-dimensional bow shocks using DSMC and CFD results in order to determine an appropriate breakdown parameter. The gradient length local (GLL) Knudsen number,

$$Kn_{GLL} = \frac{\lambda_{mean}}{\chi} \left| \frac{d\chi}{dl} \right|, \tag{3.84}$$

where *l* is some distance between two points in the flow field, was introduced and demonstrated to provide a better indication of continuum breakdown than *B* for compression-dominated hypersonic flows. The distance *l* was taken approximately along the line of the steepest gradients in the flow properties. For simplicity, $d\chi/dl$ was evaluated by $\nabla \chi$. Then, the parameter is reduced to

$$Kn_{\chi} = \frac{\lambda_{mean}}{\chi} |\nabla \chi| = \frac{\lambda_{mean}}{\chi} \sqrt{\left(\frac{d\chi}{dx}\right)^2 + \left(\frac{d\chi}{dy}\right)^2 + \left(\frac{d\chi}{dz}\right)^2}.$$
(3.85)

Also, by considering all the flow properties, the following breakdown parameter Kn_{max} can be derived:

$$Kn_{\max} \equiv \max\left(Kn_D, Kn_T, Kn_V\right). \tag{3.86}$$

It is apparent that there is a direct relationship between Eqs. (3.82) and (3.85);

$$B_{\chi} = M \sqrt{\frac{\gamma \pi}{8}} \cos \theta \, K n_{\chi} \,. \tag{3.87}$$

where θ is the angle between gradient $\nabla \chi$ and the flow direction.

3.7.3 Rayleigh-Onsagar's breakdown parameter

The primary objective of the near-equilibrium breakdown parameter is to quantify the gas flow regions according to the breakdown of the linear hypothesis in the Navier-Stokes-Fourier constitutive relation. Therefore, the problem of finding such a parameter is essentially related to the knowledge of when the (first-order) Newtonian hypothesis breaks down, which in turn demands the derivation of the second-order non-Newtonian constitutive relation.

A systematic method to derive the second-order non-Newtonian constitutive relation from the Boltzmann-Curtiss kinetic equation was recently developed by Myong [39, 64]. According to him, the resulting second-order constitutive relations (3.43) can be summarized in steady-state case as follows,

$$2(p+\Delta)[\nabla \mathbf{u}]^{(2)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu}\Pi q_{2nd}(k_1),$$
(3.88)
where, $q_{2nd}(k_1) = \frac{\sin k_1}{k_1}, k_1 \equiv \frac{(mK_B)^{1/4}}{\sqrt{2}d} \frac{T^{1/4}}{p} \left[\frac{\Pi : \Pi}{2\mu} + \gamma' \frac{\Delta^2}{\mu_{bulk}} + \frac{\mathbf{Q} \cdot \mathbf{Q} / T}{k}\right]^{1/2}.$

Note that, the first-order cumulant expansion takes a form of hyperbolic sine function whose argument is given in terms of a quadratic function. Then the function k_1 can be shown nothing but the Rayleigh-Onsagar dissipation function \hat{R} and is readily used to identify what regions are expected to derive significantly from near-local equilibrium assumption since it measures the level of calortropy production in irreversible process [64, 65];

$$\hat{R} = \frac{N_{\delta}}{p} \left(\boldsymbol{\Pi} : \boldsymbol{\Pi} + \frac{2\gamma'}{\mu_{bulk}} \Delta^2 + \frac{2\varepsilon}{T} \mathbf{Q} \cdot \mathbf{Q} \right)^{1/2}$$
(3.89)
where $N_{\delta} = \sqrt{\frac{2\gamma}{\pi}} Kn \cdot M$, $\varepsilon = \frac{1}{Ec \operatorname{Pr}} \left| \frac{T_w}{T_r} - 1 \right|$, $Ec = \frac{(\gamma - 1)M^2}{|T_w/T_r - 1|}$.

Here, N_{δ} , ε are the reference values, while p, T, Π, \mathbf{Q} are the local values. The new nearequilibrium breakdown parameter (3.89) is shown to avoid the problem in the Bird's parameter that the Mach number approaches to zero at stagnation points. Further, it takes both viscous stress and heat transfer into account within a single framework [64].

The distributions of the near-equilibrium breakdown parameters $B_{\text{max}}, Kn_{\text{max}}, \hat{R}$ based on Bird, Boyd and Rayleigh-Onsagar dissipation function are calculated in multidimensional hypersonic rarefied gas flows around a cylinder. Argon gas is considered as working gas for all cases. Figure 3-8 compares the distributions of three near-equilibrium breakdown parameters for the first-order (NSF) and the second-order (NCCR) Boltzmann-Curtiss based constitutive models. It can be noticed that 1) there exist two distinctive regions of gaseous compression and expansion in the frontal and rear parts of the cylinder, respectively; 2) the level of breakdown parameters is high at the bow shock structure and at the rear part of cylinder; and (3) the first-order model in general predicts high than the second-order model in the level of parameters. In addition, it can be found that all three breakdown parameters produce qualitatively similar results, but new and Bird's parameters predict more similar distributions.



Figure 3-8. Comparison of the breakdown parameters in hypersonic rarefied gas flow with M=5.48, Kn=0.5 [64].

Chapter 4. Discontinuous Galerkin method

"Mathematics is the language with which God wrote the universe."

— Galileo Galilei (1564-1642)

In this chapter, numerical methods for solving the highly nonlinear partial differential equations are discussed in details. We first provide the brief summary of available numerical methods used in modern CFD, then the literature survey of discontinuous Galerkin (DG) method is provided. The space discontinuous Galerkin discretization of the compressible Navier-Stokes equations is discussed along with problem definition in DG framework, elemental transformation to the computational space, the foundation of basis functions, numerical integration, numerical inviscid and viscous fluxes, and numerical boundary conditions. Finally, we discuss the crucial part of DG method—implementation of limiters.

4.1 Numerical methods for modern CFD

4.1.1 Finite difference method

The Finite difference (FD) method is the oldest and the simplest discretization approach for a conservation law based upon the differential form of partial differential equations (PDEs) to be solved. In FD method, a discrete approximation is obtained using Taylor series expansion approach for the occurring derivatives and replacing the analytical derivatives with the discrete ones. It results in a discrete problem that can be solved numerically. In this method, a topologically square network of lines is used to construct the discretization of the PDEs. There are some excellent references for describing these methodologies in [66-69]. The great strengths of the FD method are that, they are easy to program and that they are extremely efficient in terms of computational cost. Due to their well-efficiency and well-analyzed numerical properties, FD method is often used for numerically sensitive and computationally costly problems, such as laminar-turbulent transition [70, 71]. High order versions of the FD method are easy to construct since the accuracy of the method is determined by the accuracy of the estimation of the discrete derivative [72]. There are some major drawbacks of the FD method. For examples, it is mainly applicable for structured grids and it is unable to preserve the conservative nature of the governing equations. However, this method can be implemented on unstructured grids using the reconstruction of a polynomial function [73], but it is a very complex problem for unstructured grids. Moreover, a high-order FD method requires smooth and regular grids for geometrically complex configurations regarding for stability issues [74].

4.1.2 Finite element method

The main idea behind the finite element (FE) method is somewhat different than the finite difference discretization techniques discussed previously. The finite element method takes the differential equations, multiply them by an arbitrary test function, and integrate them by parts. The approximate solution is constructed as a linear combination of the so-called basis (ansatz) functions, which are the piecewise polynomials. The choice of the basis and test function space adjudicates upon which type of FE method is obtained. There are some typical versions of FE methods: the Galerkin, Petrov-Galerkin, and Least-squares [75]. The finite element methods can be classified into two main classes of schemes, continuous and discontinuous methods. In contrast to the continuous finite element method, the discontinuous method needs no global continuity requirement for ansatz and test functions leading to the frequently-used term discontinuous finite element method. The

approximation space is not a subspace of the continuous solution space. In other words, the element is nonconforming.

For the convection-dominated Navier-Stokes equations, the continuous FE method typically produces oscillations which can be handled by adding artificial dissipation terms to the formulation. There are various techniques for selecting the stabilization terms. In the streamline upwind Petrov-Galerkin [76] method, a stabilizing term is added in the weak formulation. As a result, it creates an upwind effect by weighting more heavily the upwind stream nodes within each element. A variety of other methodologies have been proposed to provide additional stability to the convection terms, monotone discrete systems and ease of implementation. A disadvantage of the conforming FE discretization compared to FD and FV is, that if explicit discretization in time is used, a coupled system of equations has to be solved for every time step. This is due to the coupling of the degrees of freedom at cell interfaces, where continuity requirements have to be fulfilled.

4.1.3 Finite volume method

The finite volume (FV) method is very famous numerical scheme in the CFD community. The FV method is based on the integral formulation of the conservation laws. In contrast to FD method, the FV method evaluates the fluxes through the discretization element boundaries. There are various views for selecting numerical fluxes. An upwind method is a very popular approach to convection-dominated problems [77, 78], where the flux choice is based on characteristics of wave propagation.

The higher order versions of the FV method are generally obtained with the help of a so-called reconstruction procedure [79, 80], whereas an intermediate higher-order solution is constructed out of the piecewise constant element data of adjacent cells. The cells, which are included in the reconstruction, are depicted as the reconstruction stencil of the method. The problem with high-order FV methods working on unstructured grids is, that the

reconstruction stencil (especially in 3D) becomes extremely large [81] and the resulting scheme would be extremely complex to program, and more importantly, would be expensive in terms of CPU time. In general, real high-order is only achieved on relatively smooth and regular grids. A further drawback is, that due to the increased stencil, such a scheme is not suited for efficient parallelization because the stencil is quite large for the reconstruction and consequently a lot of information has to be exchanged between the parallel nodes. The same holds for high order FD methods. To conclude, in principle, FV methods are approved schemes for the simulation of flows around complex geometries, but a fundamental problem is to construct a high order scheme working on unstructured grids.

4.1.4 High order spectral method

In recent years, the high order numerical methods in computational fluid dynamics (CFD) have been widely used to effectively resolve complex flows that particularly require highly accurate treatment, such as wave propagation problems, vortex-dominated flows including high-lift configurations and flows over blunt bodies, flows with complex shock interactions, transitional flow over airfoils, as well as large eddy simulate on and direct numerical simulation of turbulence, all of which are difficult to simulate appropriately via classical low-order methods whose use in academia and industry remains widespread up to the present date.

A class of schemes especially efficient for practical CFD applications are the so-called spectral/*hp* methods. Regarding the terminology, in a broad sense, the so-called "spectral" methods are those in which the numerical solution is represented by series of (modal) functions. In general, the solution accuracy enhances when the number of such modal functions is increased. In some approaches, the entire domain is represented by a single mesh element and the solution is represented entirely by one (large) function series. For

general applications, however, the hp methods are preferred, where the domain of interest is divided into a number of elements of typical size h and the solution within each element is represented individually through a local function series, normally consisting of a polynomial of maximum degree p.

The choice of the polynomial space function is the main feature that distinguishes highorder 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 flux reconstruction (FR) approach. An excellent reference for the explanation of spectral methods is [80].

4.2 Discontinuous Galerkin method

The discontinuous Galerkin Method is probably the famous and most developed highorder accurate method for arbitrary type grids. It is now emerging as a new class of methods in the field of the numerical solution of partial differential equations representing conservation laws. It was originally developed by Reed and Hill [82] in 1973 for a steady conservation law, namely the neutron transport problem. In 1978, this method was first time used for unsteady advection laws by Van Leer [83]. Le Saint and Raviart [84] in 1975, first analyzed DG for linear hyperbolic problems, derived a priori error estimates and proved rates of convergence. A major contribution to the development of the Runge-Kutta DG (RKDG) methods for linear and nonlinear hyperbolic conservation laws were made by Cockburn and Shu [85-88]. The RKDG method is an essentially high-order Finite Element method using ideas of the high-order Finite Volume method, such as exact or approximate Riemann solvers to evaluate numerical fluxes, in order to handle discontinuities at the cell interfaces. A more comprehensive historical overview of DG methods can be found in a review article by Cockburn et al.[89].

From the last decades, the development of DG has gradually shifted to convectiondiffusion problems. The RKDG method was recently extended to handle convectiondiffusion systems by Cockburn and Shu [90]. Bassi and Rebay demonstrated the high-order accurate DG discretization for the compressible Euler and Navier-Stokes equations [91, 92]. Motivated by pioneering work of Bassi and Rebay for compressible Navier-Stokes equations, various approaches for the discretization of the diffusion equation were developed. These include the local DG (LDG) approach [93], interior penalty (IP) approach[94], and Baumann and Oden (BO) approach[95]. An interesting overview and study within a unifying framework of all these approaches can be found in Arnold et al.[96], where their consistency, stability, and order of accuracy are discussed. The order of accuracy of all these approaches for the diffusion equation is limited to p + 1, with p the degree of the solution polynomials. The local DG approach developed by Cockburn and Shu provides the stability and convergence with error estimates. The LDG approach may handle higher order (≥ 2) derivatives such as the viscous second order terms in the Navier-Stokes equation. Recently, Dumbser et al. [41] introduced the ADER-DG approach, which couples the ADER [89] with the spatial DG approach. With the aid of ADER, they developed arbitrary high-order schemes for hyperbolic conservation laws not only in space but also in time.

Many other researchers made significant contributions to the various aspect of DG methods. A quadrature-free DG formulation was investigated by Atkins and Shu [97]. An analysis based on the wave propagation properties of the DG method was performed by Hu et al. [98]. A simplified treatment of curved wall boundaries for the Euler equations with the DG method was proposed by Krivodonova and Berger [99]. A significant

contribution in space-time implicit DG methods for hyperbolic conservation laws were done by Lowrie et al. [100], Van der Vegt and its co-authors [101-103]. In the area of DG method based turbulent flow simulations, a very little experience has been gained to till date. Collis performed a numerical study of DG for the simulation of turbulent flows with the aid of direct numerical simulation (DNS) [104]. The application of DG to the Reynolds-Averaged-Navier-Stokes (RANS) equations has only been reported by Bassi and Rebay [105]. For closure of the RANS equations, they use the fully coupled $k - \omega$ turbulence model equations. Later, Bassi and Rebay extended their solution algorithm, where reliability conditions were added to the ω - equation in order to increase the numerical robustness of the method [106].

4.3 Problem definition in DG framework

In order to construct a DG discretization system for \mathcal{D} – dimension conservation laws (3.50), let's consider a bounded domain $\Omega \in \mathbb{R}^{\mathcal{D}}$ with boundary $\partial \Omega$. The boundary is decomposed into a region of Dirichlet boundary $\partial \Omega_D$ and a region of Neumann boundary $\partial \Omega_N$ i.e., $\partial \Omega = \partial \Omega_D \bigcup \partial \Omega_N$,

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}} (\mathbf{U}) + \nabla \cdot \mathbf{F}^{\text{vis}} (\mathbf{U}, \nabla \mathbf{U}) = 0,$$

$$\mathbf{U}(\mathbf{x}) = \mathbf{U}_0 (\mathbf{x}), \quad \text{at } t = t_0,$$

$$\mathbf{U}(\mathbf{x}) = g_D (\mathbf{x}), \quad \text{for all } \mathbf{x} \in \partial \Omega_D,$$

$$\mathbf{U}(\mathbf{x}) = g_N (\mathbf{x}), \quad \text{for all } \mathbf{x} \in \partial \Omega_N,$$
(4.1)

where g_D and g_N are the 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. The $\mathbf{U} \in \mathbb{R}^{D+2}$ is the vector of conservative variables; $\mathbf{F}^{inv} \in \mathbb{R}^{(D+2) \times D}$ is the inviscid flux tensor; and $\mathbf{F}^{vis} \in \mathbb{R}^{(D+2) \times D}$ is the viscous flux tensor. Since the spatial discretization of governing equation (4.1) cannot be accomplished with the standard DG method due to the presence of higher order derivatives in viscous terms. Therefore, a mixed DG formulation developed by Xiao and Myong [58, 107] is employed to discretize the governing equation. In this formulation, an auxiliary variable vector Θ is introduced to handle the second-order derivatives in viscous stress and heat flux. Therefore, the auxiliary variable vector Θ can be defined as the derivative of either primitive or conservative variables **U**. In order to apply the mixed DG formulation, Eq. (4.1) can be rewritten as a coupled system for **U** and Θ as

$$\begin{cases} \Theta - \nabla \mathbf{U} = \mathbf{0}, \\ \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}} (\mathbf{U}) + \nabla \cdot \mathbf{F}^{\text{vis}} (\mathbf{U}, \Theta) = \mathbf{0}. \end{cases}$$
(4.2)

It may be noticed that the introduction of an extra set of equations for the auxiliary variables leads to additional computational cost that is the main drawback of the mixed DG formulations.

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 is utilized and auxiliary equations are solved besides the primary equations.

4.3.1 Discontinuous Galerkin spatial discretization

In order to discretize the coupled system of equations (4.2), the domain Ω can be approximated by Ω_h such that $\Omega_h \to \Omega$ as $h \to 0$. Accordingly, the approximated domain Ω_h is tessellated into a collection of N_E arbitrary non-overlapping elements Ω_e such that $\mathcal{T}_h = \{\Omega_e\}$. In present thesis, the discretization elements Ω_e are lines in one-dimensional, triangles/rectangular in two-dimensional and tetrahedrons in three-dimensional spaces.

The boundaries of every element $\partial \Omega_e$ are divided into two parts: interfaces-oriented boundaries Γ_F^e and element-oriented boundaries Γ_B^e . The collection of the interfaces and boundary faces of the tessellated domain \mathcal{T}_h are denoted by I_h and \mathcal{B}_h , respectively.

$$I_{h} = \bigcup_{\substack{\forall j \in \Omega_{e} \\ \forall e \in \mathcal{T}_{h}}} \Gamma_{F_{j}}^{e}, \quad \mathcal{B}_{h} = \bigcup_{\substack{\forall j \in \Omega_{e} \\ \forall e \in \mathcal{T}_{h}}} \Gamma_{B_{j}}^{e},$$
(4.3)

where $\Gamma_{F_j}^e$ denotes the j^{th} face of the local element Ω_e . Consider the finite element space (broken space) \mathbf{V}_h defined by

$$\mathbf{V}_{h} = \left\{ \boldsymbol{\upsilon}_{h} \in \left[L^{2} \left(\boldsymbol{\Omega}_{h} \right) \right]^{\mathcal{D}+2} : \boldsymbol{\upsilon}_{h} \big|_{\boldsymbol{\Omega}_{e}} \in \left[\mathbb{P}^{k} \left(\boldsymbol{\Omega}_{e} \right) \right]^{\mathcal{D}+2} \quad \forall \boldsymbol{\Omega}_{e} \in \mathcal{T}_{h} \right\},$$
(4.4)

for some polynomial degree $k \ge 0$, being $\mathbb{P}^k(\Omega_e)$ the space of polynomial functions of degree at most k on the element Ω_e and $L^2(\Omega_h)$ represents the space of functions, which are squared Lebesgue integrable over the approximated domain Ω_h .

If the space of the polynomial functions are defined appropriately in a standard 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 with corresponding polynomial functions of degree k as,

$$\mathbf{U}_{h^{e}}\left(\mathbf{x},t\right) = \sum_{k=1}^{N_{k}} U_{h^{e}}^{k}\left(t\right) b_{k}\left(\mathbf{x}\right),$$

$$\mathbf{\Theta}_{h^{e}}\left(\mathbf{x}\right) = \sum_{k=1}^{N_{k}} \Theta_{h^{e}}^{k} b_{k}\left(\mathbf{x}\right).$$
(4.5)

Here the expansion coefficients $U_{h^e}^k(t)$ and $\Theta_{h^e}^k$ denote the degree of freedom of the numerical solution and of the test function in an element Ω_e , respectively, and N_k denotes the number of basis functions required for approximating the smooth and continuous

solution inside the space of the polynomial functions. The N_k +1 basis functions $b_k(\mathbf{x})$ are a base for the polynomial functions \mathbb{P}^k . The exact solution of the conservative variables and their derivatives can be approximated by the numerical solution obtained in every element as follows

$$\mathbf{U}(\mathbf{x},t) \approx \mathbf{U}_{h} = \bigoplus_{e=1}^{N_{E}} U_{h}^{e}(\mathbf{x},t) = \left\{ U_{h}^{1} + U_{h}^{2} + \dots + U_{h}^{N_{E}} \right\},$$

$$\mathbf{\Theta}(\mathbf{x}) \approx \mathbf{\Theta}_{h} = \bigoplus_{e=1}^{N_{E}} \Theta_{h}^{e}(\mathbf{x}) = \left\{ \Theta_{h}^{1} + \Theta_{h}^{2} + \dots + \Theta_{h}^{N_{E}} \right\}.$$
(4.6)

4.3.2 Elemental formulation

Taking the product of the conservation laws with vector υ , and the auxiliary equations with tensor τ and then integrating over the solution domain, we obtain its weighted residual form

$$\begin{cases} \int_{\Omega} \tau(\Theta - \nabla \mathbf{U}) d\Omega = 0, \\ \int_{\Omega} \upsilon \left(\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}} (\mathbf{U}) + \nabla \cdot \mathbf{F}^{\text{vis}} (\mathbf{U}, \Theta) \right) d\Omega = 0. \end{cases}$$
(4.7)

Now we perform integration by parts using Gaussian divergence theorem on the advection and viscous term and we get the basic form of the DG approach for the system of conservation law – the weak formulation of the problem (4.2),

$$\begin{cases} \int_{\Omega} \boldsymbol{\tau} \boldsymbol{\Theta} d\Omega - \oint_{\partial \Omega} \boldsymbol{\tau} \mathbf{U} \cdot \mathbf{n} \, d\sigma + \int_{\Omega} \nabla \boldsymbol{\tau} \cdot \mathbf{U} d\Omega = 0, \\ \int_{\Omega} \left(\upsilon \frac{\partial \mathbf{U}}{\partial t} \right) d\Omega + \oint_{\partial \Omega} \upsilon \mathbf{F}^{\text{inv}} (\mathbf{U}) \cdot \mathbf{n} \, d\Gamma - \int_{\Omega} \nabla \upsilon \cdot \mathbf{F}^{\text{inv}} (\mathbf{U}) \, d\Omega \\ + \oint_{\partial \Omega} \upsilon \mathbf{F}^{\text{vis}} (\mathbf{U}, \boldsymbol{\Theta}) \cdot \mathbf{n} \, d\Gamma - \int_{\Omega} \nabla \upsilon \cdot \mathbf{F}^{\text{vis}} (\mathbf{U}, \boldsymbol{\Theta}) \, d\Omega = 0, \end{cases}$$
(4.8)

where **n** represents the outward normal vector. Splitting the volume integral over Ω_h into sum of the integrals over the local elements Ω_e and using the divergence theorem, Eq. (4.8) leads to the elemental formulation of the governing equations as

$$\begin{cases}
\sum_{\Omega_{e}} \left[\int_{\Omega_{e}} \tau \Theta d\Omega_{e} - \oint_{\partial\Omega_{e}} \tau \mathbf{U} \cdot \mathbf{n} \, d\Gamma_{e} + \int_{\Omega_{e}} \nabla \tau \cdot \mathbf{U} d\Omega_{e} \right] = 0 \\
\sum_{\Omega_{e}} \left[\int_{\Omega_{e}} \left(\upsilon \frac{\partial \mathbf{U}}{\partial t} \right) d\Omega_{e} + \oint_{\partial\Omega_{e}} \upsilon \mathbf{F}^{\text{inv}} (\mathbf{U}) \cdot \mathbf{n} \, d\Gamma_{e} - \int_{\Omega_{e}} \nabla \upsilon \cdot \mathbf{F}^{\text{inv}} (\mathbf{U}) d\Omega_{e} \\
+ \oint_{\partial\Omega_{e}} \upsilon \mathbf{F}^{\text{vis}} (\mathbf{U}) \cdot \mathbf{n} \, d\Gamma_{e} - \int_{\Omega_{e}} \nabla \upsilon \cdot \mathbf{F}^{\text{vis}} (\mathbf{U}) d\Omega_{e} \\
\end{bmatrix} = 0.$$
(4.9)

Here $d\Gamma_e$ denotes the boundaries of the local element.

The solution **U** inside each element is approximated by a linear combination of the test function υ . In addition, if we choose the same discontinuous test functions and ansatz functions for the solution of the auxiliary variable Θ as for the solution **U** itself i.e. $\tau_h = \upsilon_h = b_k(\mathbf{x})$, we obtain the following semi-discrete system of k equations for the generic element Ω_e :

$$\begin{cases} \int_{\Omega_{e}} b_{k} \Theta_{h} d\Omega_{e} - \oint_{\partial\Omega_{e}} b_{k} \mathbf{U}_{h} \cdot \mathbf{n} d\Gamma_{e} + \int_{\Omega_{e}} \nabla b_{k} \cdot \mathbf{U}_{h} d\Omega_{e} = 0, \\ \frac{\partial}{\partial t} \int_{\Omega_{e}} b_{k} \mathbf{U}_{h} d\Omega_{e} + \oint_{\partial\Omega_{e}} b_{k} \left(\mathbf{F}^{\text{inv}} \left(\mathbf{U}_{h} \right) + \mathbf{F}^{\text{vis}} \left(\mathbf{U}_{h}, \Theta_{h} \right) \right) \cdot \mathbf{n} d\Gamma_{e} \\ - \int_{\Omega_{e}} \nabla b_{k} \cdot \left(\mathbf{F}^{\text{inv}} \left(\mathbf{U}_{h} \right) + \mathbf{F}^{\text{vis}} \left(\mathbf{U}_{h}, \Theta_{h} \right) \right) d\Omega_{e} = 0. \end{cases}$$
(4.10)

The system of equations introduced in Eq. (4.10) is not solvable since the degree of freedom related to every element is not linked to the degree of freedoms in another element of Ω_h . Thus, establishing a weak inter-element connection though introducing an appropriate monotone numerical fluxes at interfaces and boundaries of elements Ω_e is essential to obtain an approximate spectral solution.

4.3.3 Weak DG formulation

In order to handle the discontinuities occurring in the boundary integral of Eq. (4.10), we have to approximate the physical fluxes using the following numerical fluxes such as
$$\begin{aligned} & \oint_{\partial \Omega_{e}} b_{k} \mathbf{U}_{h} \cdot \mathbf{n} d\Gamma_{e} &\approx \oint_{\partial \Omega_{e}} b_{k} \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) \cdot \mathbf{n} d\Gamma_{e}, \\ & \oint_{\partial \Omega_{e}} b_{k} \mathbf{F}^{inv} \left(\mathbf{U}_{h} \right) \cdot \mathbf{n} d\Gamma_{e} &\approx \oint_{\partial \Omega_{e}} b_{k} \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) \cdot \mathbf{n} d\Gamma_{e}, \\ & \oint_{\partial \Omega_{e}} b_{k} \mathbf{F}^{vis} \left(\mathbf{U}_{h}, \Theta_{h} \right) \cdot \mathbf{n} d\Gamma_{e} &\approx \oint_{\partial \Omega_{e}} b_{k} \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \Theta_{h}^{L}, \mathbf{U}_{h}^{R}, \Theta_{h}^{R} \right) \cdot \mathbf{n} d\Gamma_{e}. \end{aligned} \tag{4.11}$$

Here the $(\cdot)^{L}$ and $(\cdot)^{R}$ notation is used to indicate the trace value taken from the interior and exterior of the element, respectively. If we split the element boundary integrals into inner face integrals and domain boundary face integrals, we finally arrive at the mixed weak DG formulation of the conservation laws (4.2) on the local element Ω_{e} :

$$\begin{cases} \int_{\Omega_{e}} b_{k} \Theta_{h} d\Omega_{e} \\ -\sum_{e \in \partial \Omega_{e} \setminus \partial \Omega} \oint b_{k} \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) \cdot \mathbf{n} d\Gamma_{e} \\ -\sum_{e \in \partial \Omega_{e} \cap \partial \Omega} \oint b_{k} \mathbf{H}_{auxiliary}^{b} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) \cdot \mathbf{n} d\Gamma_{e} + \int_{\Omega_{e}} \nabla b_{k} \cdot \mathbf{U}_{h} d\Omega_{e} = 0, \\ \frac{\partial}{\partial t} \int_{\Omega_{e}} b_{k} \mathbf{U}_{h} d\Omega_{e} \\ +\sum_{e \in \partial \Omega_{e} \setminus \partial \Omega} \oint b_{k} \left(\mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) + \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \mathbf{O}_{h}^{L}, \mathbf{U}_{h}^{R}, \Theta_{h}^{R} \right) \right) \cdot \mathbf{n} d\Gamma_{e} \\ + \sum_{e \in \partial \Omega_{e} \cap \partial \Omega} \oint b_{k} \left(\mathbf{H}_{inviscid}^{b} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{R} \right) + \mathbf{H}_{viscous}^{b} \left(\mathbf{U}_{h}^{L}, \mathbf{O}_{h}^{L}, \mathbf{U}_{h}^{R}, \Theta_{h}^{R} \right) \right) \cdot \mathbf{n} d\Gamma_{e} \\ - \int_{\Omega_{e}} \nabla b_{k} \cdot \left(\mathbf{F}^{inv} \left(\mathbf{U}_{h} \right) + \mathbf{F}^{vis} \left(\mathbf{U}_{h}, \Theta_{h} \right) \right) d\Omega_{e} = 0. \end{cases}$$

$$(4.12)$$

The resulting formulation is called a two-step mixed-DG method in which the test functions, accordingly to Galerkin method are chosen to equal to the basis (ansatz) functions. In mixed DG method, the auxiliary equations are initially solved at beginning of every step, then the gradients of primary variables Θ_{h^e} are updated based on the global solutions U_{h^e} at current time step. Afterwards, the primary system is solved, using the values of Θ_{h^e} obtained from step one.

All the boundary conditions are be imposed in a weak manner. We construct an exterior boundary state $\mathbf{U}_{h}^{b}(\mathbf{U}_{h}^{L},\mathbf{U}_{BC})$, which is a function of the interior state \mathbf{U}_{h}^{L} and the known

physical boundary data \mathbf{U}_{BC} . Hence the numerical boundary flux is computed as $\mathbf{U}_{h}^{b}(\mathbf{U}_{h}^{L},\mathbf{U}_{BC})$,

$$\mathbf{H}_{auxiliary}^{b} = \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right),
\mathbf{H}_{inviscid}^{b} = \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right),
\mathbf{H}_{viscous}^{b} = \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \Theta_{h}^{L}, \mathbf{U}_{h}^{b}, \Theta_{h}^{b} \right).$$
(4.13)

In this work, we implemented the approximate Riemann solvers of Lax-Friedrich solver for inviscid numerical flux $\mathbf{H}_{inviscid}$. Moreover, the choice of the fluxes $\mathbf{H}_{auxiliary}$ and $\mathbf{H}_{viscous}$ is the crucial part of the weal formulation for DG methods for higher order derivatives, since there is no counterpart or experience from the Finite Volume method. Therefore, the choice of numerical fluxes $\mathbf{H}_{auxiliary}$ and $\mathbf{H}_{viscous}$ for different approaches has been adopted from the theoretical and numerical studies of purely diffusive model problems.

All the integrals appearing in the elemental equations are calculated by means of numerical quadrature rule with a number of integration points consistent with the accuracy required. By assembling all the elemental information in Eq. (4.12), it leads to a system of ordinary differential equations (ODEs) in time which can be written as

$$\mathbf{M}\frac{d\mathbf{U}}{dt} = \mathbf{R}(\mathbf{U}) \tag{4.14}$$

where \mathbf{M} is the mass matrix, \mathbf{U} is the global vector of the degree of freedom, and \mathbf{R} is the residual vector. The elements of mass matrix is defined as

$$\mathbf{M} = \int_{E} b_k b_j d\Omega. \tag{4.15}$$

In case of orthogonal basis functions

$$\mathbf{M} = \int_{E} b_{k} b_{j} d\Omega = 0, \quad k \neq j,$$
(4.16)

Thus the elemental mass matrices possess diagonal form.

4.4 Elemental transformation to computational space

4.4.1 One-dimensional elemental transformation

For one-dimensional problems, the local element Ω_e are equally spaced $\Delta x = x_{i+1} - x_i$ and the space coordinate x in element Ω_e is linked to the local spatial coordinate ξ in a standard element $\Omega_e^{st} \in [-1,1]$, see Figure 4-1, under the affine sub-parametric transformation $T_e: \Omega_e \to \Omega_e^{st}$ defined by

$$\xi = 2 \frac{x - x_i}{x_{i+1} - x_i} - 1, \qquad \forall x \in \Omega_e.$$

$$(4.17)$$

The Jacobian of this transformation is given by

$$\mathbf{J}_{\mathbf{x} \to \mathbf{\xi}} = \frac{\partial x}{\partial \xi} = \frac{\Delta x}{2}.$$
(4.18)

The inverse of the transformation $T_e^{-1}: \Omega_e^{st} \to \Omega_e$ is given by

$$x = \frac{1-\xi}{2}x_i + \frac{1+\xi}{2}x_{i+1}, \qquad \forall \xi \in \Omega_e^{st}.$$
(4.19)

In addition, the space coordinate x in element Ω_e may be transformed to the local spatial coordinate ξ in a standard element $\Omega_e^{st} \in [0,1]$, as defined in Figure 4-2, under the affine sub-parametric transformation $T_e: \Omega_e \to \Omega_e^{st}$,

$$\xi = \frac{x - x_i}{x_{i+1} - x_i}, \qquad \forall x \in \Omega_e.$$
(4.20)

In this case, the Jacobian of this transformation can be evaluated as

$$\mathbf{J}_{\mathbf{x}\to\mathbf{\xi}} = \frac{\partial x}{\partial\xi} = \Delta x. \tag{4.21}$$

While the inverse of the transformation $T_e^{-1}: \Omega_e^{st} \to \Omega_e$ is given by

$$x = (1 - \xi) x_1 + \xi x_2, \qquad \forall \xi \in \Omega_e^{st}.$$
(4.22)



Figure 4-1. Transformation from physical line elment to computational standard element in interval [-1,1].



Figure 4-2. Transformation from physical line elment to computational standard element in interval [0,1].

4.4.2 Two-dimensional elemental transformation

Rectangular element

A reference or standard rectangular element Ω_e^{st} is defined using a local Cartesian coordinate system $(\xi, \eta) \in [-1, 1]$ as defined in Figure 4-3. The reference (standard) rectangular element can be mapped from the computational space (ξ, η) to an arbitrary rectangular element in the physical space (x, y) under the linear transformation $T_e: \Omega_e^{st} \to \Omega_e$ defined by

$$x = \frac{1}{2} [(1 - \xi) x_1 + (1 + \xi) x_2],$$

$$y = \frac{1}{2} [(1 - \eta) y_1 + (1 + \eta) y_2],$$
(4.23)

where $(x_1, y_1), (x_2, y_2), (x_3, y_3)$, and (x_4, y_4) are the physical coordinates of the vortices of Ω_e . The Jacobian of this mapping is given by

$$\mathbf{J}_{\mathbf{x}\to\mathbf{\xi}} = \frac{\partial(x,y)}{\partial(\xi,\eta)} = \frac{1}{4} \begin{bmatrix} x_2 - x_1 & 0\\ 0 & y_2 - y_1 \end{bmatrix} = \frac{1}{4} \mathbf{A}_e^{\text{rectangle}}, \tag{4.24}$$

where $A_e^{\text{rectangle}}$ is the area of the rectangle element Ω_e . The inverse of the transformation $T_e^{-1}: \Omega_e \to \Omega_e^{\text{st}}$ is given by

$$\xi = \frac{1}{\Delta x} (2x - x_1 - x_2)$$

$$\eta = \frac{1}{\Delta y} (2y - y_1 - y_2)$$
(4.25)

where $\Delta x = x_2 - x_1$, and $\Delta y = y_2 - y_1$.

Triangular element

A reference triangle can be mapped from the physical space (x, y) to computational space (ξ, η) with the linear transformation $T_e: \Omega_e^{st} \to \Omega_e$

$$x = (1 - \xi - \eta) x_1 + \xi x_2 + \eta x_3,$$

$$y = (1 - \xi - \eta) y_1 + \xi y_2 + \eta y_3,$$
(4.26)

while the Jacobian of the transformation is given by

$$J = \left| \frac{\partial(x, y)}{\partial(\xi, \eta)} \right| = \left| \frac{\partial x}{\partial \xi} \quad \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} \quad \frac{\partial y}{\partial \eta} \right| = x_1 \left(y_2 - y_3 \right) + x_2 \left(y_3 - y_1 \right) + x_3 \left(y_1 - y_2 \right) = 2\Delta_{tri}.$$

$$(4.27)$$



Figure 4-3. Transformation from physical rectangular elment to computational standard rectangular element in interval [-1,1].



Figure 4-4. Transformation from physical triangular element to computational triangular element in interval [0,1].

Here, Δ_{tri} is the area of physical triangle element which is given by

$$\Delta_{tri} = \frac{1}{2} \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}$$

$$= \frac{1}{2} \Big[x_1 (y_2 - y_3) + x_2 (y_3 - y_1) + x_3 (y_1 - y_2) \Big].$$
(4.28)

The inverse transformation from computational space to physical space $T_e^{-1}: \Omega_e \to \Omega_e^{st}$ is given by



Figure 4-5. Transformation from physical tetraherdral element to computational tetraherdral element in interval [0,1].

4.4.3 Three-dimensional elemental transformation

A tetrahedral element in physical space (x, y, z) can be transformed to a canonical reference tetrahedral in a computational space (ξ, η, ζ) system under the linear mapping $T_e: \Omega_e^{st} \to \Omega_e$ as shown in Figure 4-5. The coordinate transformation $(x, y, z) \to (\xi, \eta, \zeta)$

is given as

$$\Upsilon = \{ (\xi, \eta, \zeta) | 0 \le \xi \le 1; \ 0 \le \eta \le 1 - \xi; \ 0 \le \zeta \le 1 - \xi - \eta \},$$
(4.30)

such that

$$x(\xi,\eta,\zeta) = (1-\xi-\eta-\zeta)x_{1} + \xi x_{2} + \eta x_{3} + \zeta x_{4},$$

$$y(\xi,\eta,\zeta) = (1-\xi-\eta-\zeta)y_{1} + \xi y_{2} + \eta y_{3} + \zeta y_{4},$$

$$z(\xi,\eta,\zeta) = (1-\xi-\eta-\zeta)z_{1} + \xi z_{2} + \eta z_{3} + \zeta z_{4}.$$
(4.31)

The Jacobian of the transformation is given as

$$J_{x \to \xi} = \left| \frac{\partial (x, y, z)}{\partial (\xi, \eta, \zeta)} \right| = \left| \begin{array}{ccc} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{array} \right| = \left| \begin{array}{ccc} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{array} \right| = 6\Omega_{tet}.$$
(4.32)

The inverse transformation $(\xi, \eta, \zeta) \rightarrow (x, y, z)$ is given as

$$\begin{split} \xi &= \frac{1}{J_{x \to \xi}} \begin{vmatrix} x - x_1 & x_3 - x_1 & x_4 - x_1 \\ y - y_1 & y_3 - y_1 & y_4 - y_1 \\ z - z_1 & z_3 - z_1 & z_4 - z_1 \end{vmatrix} \\ &= \frac{1}{6\Omega_{tet}} [x_1 (y_4 z_3 - y_3 z_4) + x_3 (y_1 z_4 - y_4 z_1) + x_4 (y_3 z_1 - y_1 z_3) + x_4 \{y_1 (z_3 - z_4) + y_3 (z_4 - z_1) + y_4 (z_1 - z_3)\} + y_1 \{x_1 (z_4 - z_3) + x_3 (y_4 - y_1) + x_4 (y_1 - y_3)\}], \\ &\qquad x \{y_1 (z_4 - z_3) + x_3 (y_4 - y_1) + x_4 (y_1 - y_3)\}], \\ &\eta = \frac{1}{J_{x \to \xi}} \begin{vmatrix} x_2 - x_1 & x - x_1 & x_4 - x_1 \\ y_2 - y_1 & y - y_1 & y_4 - y_1 \\ z_2 - z_1 & z - z_1 & z_4 - z_1 \end{vmatrix} \\ &= \frac{1}{6\Omega_{tet}} [y_1 (x_4 z_2 - x_2 z_4) + y_3 (x_1 z_4 - x_4 z_1) + y_4 (x_2 z_1 - x_1 z_2) + x_4 \{y_1 (z_2 - z_4) + x_3 (z_4 - z_1) + x_4 (y_2 - y_1)\}], \\ &\zeta &= \frac{1}{J_{x \to \xi}} \begin{vmatrix} x_2 - x_1 & x_3 - x_1 & x - x_1 \\ y_2 - y_1 & y_3 - y_1 & y - y_1 \\ z_2 - z_1 & z_3 - z_1 & z - z_1 \end{vmatrix} \\ &= \frac{1}{6\Omega_{tet}} [z_1 (x_3 y_2 - x_2 y_3) + z_2 (x_1 y_3 - x_3 y_1) + z_3 (x_2 y_1 - x_1 y_2) + x_4 \{y_1 (z_2 - z_3) + y_2 (z_3 - z_1) + y_3 (z_1 - z_2)\} + y_4 \{x_1 (z_3 - z_2) + x_3 (z_1 - z_3) + x_3 (z_2 - z_1)\} + y_4 \{x_1 (z_3 - z_2) + x_3 (z_1 - z_3) + x_3 (z_2 - z_1)\} + y_4 \{x_1 (z_3 - z_2) + x_3 (z_1 - z_3) + x_3 (z_2 - z_1)\} + z_4 \{x_1 (y_2 - y_3) + x_2 (y_3 - y_1) + x_3 (y_1 - y_2)\}]. \end{split}$$

Note that, Ω_{tet} is the volume of real tetrahedral in *xyz*-system

$$\Omega_{tet} = \frac{1}{6} \begin{vmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{vmatrix}.$$
(4.34)

With respect to the coordinate transformation into the computational space (ξ, η, ζ) , we have

$$dxdydz = J_{x \to \xi} d\xi d\eta d\zeta, \qquad (4.35)$$

and the transformation gradients of the form

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} & \frac{\partial \zeta}{\partial x} \\ \frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} & \frac{\partial \zeta}{\partial y} \\ \frac{\partial \xi}{\partial z} & \frac{\partial \eta}{\partial z} & \frac{\partial \zeta}{\partial z} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{pmatrix}.$$
(4.36)

4.5 Foundation of basis functions

The choice of the basis functions is ambiguous and has a little contribution to the accuracy, but no effect on the overall results of the DG method. Both orthogonal and non-orthogonal basis functions have been used. Apart from being orthogonal and non-orthogonal, basis function may be modal and nodal. In this thesis, we employed modal basis function, with increasing order of accuracy, higher order polynomials are included in the approximation which are in hierarchical nature. It means that $b_0, b_1 \cdots b_{N_k-2}$ are included along with the b_{N_k-1} basis functions in $N_k - 1$ order approximation. With the modal expansion, the position of the degree of freedom $U_{h^e}^k$ in the reference domain is not important. The approximation solution can be defined in terms of modal expansion as,

$$\mathbf{U}_{h^{e}}\left(\mathbf{x},t\right) = \sum_{k=1}^{N_{k}} U_{h^{e}}^{k}\left(t\right) b_{k}\left(\mathbf{x}\right),\tag{4.37}$$

where, $b_k(\mathbf{x})$ is the Jacobi polynomials. The alternate of modal basis functions are the *nodal* basis functions, which apart from increasing the mode of polynomial, increase the nodes on which to evaluate the degree of freedom. Nodal basis functions are not hierarchical meaning the basis functions for an N_k –1 accuracy cannot be constructed from the $b_0, b_1 \cdots b_{N_k-2}$ basis functions. Also the reconstruction of the approximate solution is different. In nodal basis function, the position of the degree of freedom $U_{h'}^k$ in the reference domain is important as a particular node corresponds to a particular basis function. Hence information about the position of the degree of freedom is stored in the solution array. In term of nodal expansion, the approximation solution can be defined as,

$$\mathbf{U}_{h^{e}}\left(\mathbf{x},t\right) = \sum_{k=1}^{N_{k}} U_{h^{e}}^{k}\left(t\right) l_{k}\left(\mathbf{x}\right),\tag{4.38}$$

where $l_k(\mathbf{x})$ is the Lagrangian polynomials defined as

$$l_{k}(x) = \sum_{j=0, j \neq k}^{n} \frac{\left(x - x_{j}\right)}{\left(x_{k} - x_{j}\right)}$$

$$= \frac{\left(x - x_{0}\right)\left(x - x_{1}\right)\cdots\left(x - x_{k-1}\right)\left(x - x_{k+1}\right)\cdots\left(x - x_{n}\right)}{\left(x_{k} - x_{0}\right)\left(x_{k} - x_{1}\right)\cdots\left(x_{k} - x_{k-1}\right)\left(x_{k} - x_{k+1}\right)\cdots\left(x_{k} - x_{n}\right)}.$$
(4.39)

In the present thesis, we use orthogonal *Jacobi polynomials* $P_n^{\alpha,\beta}(\xi)$ which is also called hypergeometric polynomials. These are defined as the polynomial solutions of the Strum-Liouville problem which can be given as

$$(1-\xi^2)\frac{d^2y}{d\xi^2} + \left[\beta - \alpha - (\alpha + \beta + 2)\xi\right]\frac{dy}{d\xi} = n(n+\alpha + \beta + 1)\xi.$$

$$(4.40)$$

In the interval [-1, 1], the Jacobi polynomials can be expressed as

$$P_{n}^{\alpha,\beta}\left(\xi\right) = \frac{\left(-1\right)^{n}}{2^{n}n!} \left(1+\xi\right)^{\alpha} \left(1+\xi\right)^{-\beta} \frac{d^{n}}{d\xi^{n}} \left\{ \left(1-\xi\right)^{\alpha+n} \left(1-\xi\right)^{\beta+n} \right\}, \quad \alpha,\beta > -1$$
(4.41)

The Jacobi Polynomials have the orthogonal property

$$\int_{-1}^{1} P_{i}^{\alpha,\beta}\left(\xi\right) P_{j}^{\alpha,\beta}\left(\xi\right) \left(1+\xi\right)^{\alpha} \left(1+\xi\right)^{\beta} d\xi = \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i\neq j. \end{cases}$$
(4.42)

The Legendre polynomials $P_n^{0,0}(\xi)$, which are a generalisation form of the *Jacobi* polynomials (by setting $\alpha = \beta = 0$) can be given by

$$L_{n}(\xi) = P_{n}^{0,0}(\xi) = \frac{(-1)^{n}}{2^{n}n!} \frac{d^{n}}{d\xi^{n}} (1-\xi^{2})^{n}.$$
(4.43)

Polynomial order, <i>p</i>	0	1	2	3	4	5
1-dimensional	1	2	3	4	5	6
2-dimensional	1	3	6	10	15	21
3-dimensional	1	4	10	20	35	56

Figure 4-6. Number of required basis (polynomial) functions up to 5th order.

4.5.1 Number of required basis functions

The total number of required basis function for a reconstruction of a complete set bases of order p is a function of degree p and dimension D:

$$N_{p} = N(p, \mathcal{D}) = \frac{\prod_{k=1}^{\mathcal{D}} (p+k)}{\mathcal{D}!}.$$
(4.44)

For instance, the number of required basis function of order p in arbitrary-dimension is given by

$$N_{p} = \begin{cases} (p+1), & \text{if } \mathcal{D} = 1, \\ \frac{(p+1)(p+2)}{2}, & \text{if } \mathcal{D} = 2, \\ \frac{(p+1)(p+2)(p+3)}{6}, & \text{if } \mathcal{D} = 3. \end{cases}$$
(4.45)

Figure 4-6 provides the required number of basis functions for one-dimensional, twodimensional and three-dimensional discontinuous Galerkin method.



Figure 4-7. Modes of one-dimensional Legendre basis functions up to 5th order.



Figure 4-8. Modes of one-dimensional scaled Legendre basis functions up to 5th order.

4.5.2 Basis functions for one-dimensional problem

Due to different features as orthogonality and recursive formula, Legendre polynomials are mainly used. In one-dimensional DG method, Legendre polynomials are used as the basis functions such as,

$$b_i = P_i^{0,0}(\xi). \tag{4.46}$$

The one-dimensional Legendre basis functions up to 5^{th} order are defined in Eq. (4.47) and their modes are given in Figure 4-7

$$b_{0}(\xi) = 1, \qquad (4.47)$$

$$b_{1}(\xi) = \xi, \qquad (4.47)$$

$$b_{2}(\xi) = \frac{1}{2}(3\xi^{2} - 1), \qquad (4.47)$$

$$b_{3}(\xi) = \frac{1}{2}(5\xi^{3} - 3\xi), \qquad (4.47)$$

$$b_{3}(\xi) = \frac{1}{2}(5\xi^{3} - 3\xi), \qquad (4.47)$$

$$b_{3}(\xi) = \frac{1}{2}(3\xi^{2} - 1), \qquad (4.47)$$

$$b_{5}(\xi) = \frac{1}{2}(3\xi^{2} - 1), \qquad (4.47)$$

$$b_{5}(\xi) = \frac{1}{2}(3\xi^{2} - 1), \qquad (4.47)$$

$$b_{5}(\xi) = \frac{1}{2}(3\xi^{2} - 1), \qquad (4.47)$$

The scaled Legendre polynomials are defined as:

$$\mathcal{L}_{n}(\xi) = \frac{2^{n}(n!)^{2}}{(2n)!} P_{n}^{0,0}(\xi).$$
(4.48)

The one-dimensional scaled Legendre basis functions $b_i(\xi) = \mathcal{L}_n(\xi)$ up to 5th order are given in Eq. (4.49) and their modes are plotted in Figure 4-8.

$$b_{0}(\xi) = 1, \qquad (4.49)$$

$$b_{1}(\xi) = \xi, \qquad (4.49)$$

$$b_{2}(\xi) = \xi^{2} - \frac{1}{3}, \qquad (4.49)$$

$$b_{3}(\xi) = \xi^{3} - \frac{3}{5}\xi, \qquad (4.49)$$

$$b_{3}(\xi) = \xi^{3} - \frac{3}{5}\xi, \qquad (4.49)$$

$$b_{3}(\xi) = \xi^{3} - \frac{3}{5}\xi, \qquad (4.49)$$

$$b_{5}(\xi) = \xi^{5} - \frac{10}{9}\xi^{2} + \frac{3}{35}, \qquad (4.49)$$

4.5.3 Basis functions for two-dimensional problem

4.5.3.1 Basis functions for rectangular elements

An orthogonal basis for the rectangular element can be constructed as a tensor product of the so-called principal function defined as

$$\psi_{i}^{a}(\xi) = \mathcal{L}_{i}(\xi) = \frac{2^{n}(i!)^{2}}{(2i)!} P_{i}^{0,0}(\xi),$$

$$\psi_{j}^{b}(\eta) = \mathcal{L}_{j}(\eta) = \frac{2^{n}(j!)^{2}}{(2j)!} P_{j}^{0,0}(\eta),$$
(4.50)

where $\mathcal{L}_i(\xi)$ and $\mathcal{L}_j(\eta)$ are the scaled Legendre polynomials. With the definitions of the principal functions ψ_i^a and ψ_j^b , the rectangular basis functions are constructed as their tensor product

$$b_k(\xi,\eta) = \psi_i^a(\xi)\psi_j^b(\eta). \tag{4.51}$$

The two-dimensional scaled Legendre basis functions for rectangular element up to 4th order are defined in Eq. (4.52) and their modes are represented in Figure 4-9.

$$b_{0}(\xi,\eta) = 1, \qquad b_{1}(\xi,\eta) = \xi,$$

$$b_{2}(\xi,\eta) = \eta, \qquad b_{3}(\xi,\eta) = \xi^{2} - \frac{1}{3},$$

$$b_{4}(\xi,\eta) = \xi\eta, \qquad b_{5}(\xi,\eta) = \eta^{2} - \frac{1}{3},$$

$$b_{6}(\xi,\eta) = \xi^{3} - \frac{3}{5}\xi, \qquad b_{7}(\xi,\eta) = \left(\xi^{2} - \frac{1}{3}\right)\eta,$$

$$b_{8}(\xi,\eta) = \xi\left(\eta^{2} - \frac{1}{3}\right), \qquad b_{9}(\xi,\eta) = \eta^{3} - \frac{3}{5}\eta,$$

$$b_{10}(\xi,\eta) = \xi^{4} - \frac{6}{7}\xi^{2} + \frac{3}{35}, \qquad b_{11}(\xi,\eta) = \left(\xi^{3} - \frac{3}{5}\xi\right)\eta,$$

$$b_{12}(\xi,\eta) = \left(\xi^{2} - \frac{1}{3}\right)\left(\eta^{2} - \frac{1}{3}\right), \qquad b_{13}(\xi,\eta) = \xi\left(\eta^{3} - \frac{3}{5}\eta\right),$$

$$b_{14}(\xi,\eta) = \eta^{4} - \frac{6}{7}\eta^{2} + \frac{3}{35}.$$

(4.52)



Figure 4-9. Complete scaled Legendre polynomial space, based on Pascal's triangle, for full standard rectangular expansion up to 4th order.



Figure 4-10. Complete scaled Legendre polynomial space, based on Pascal's triangle, for full standard triangular expansion up to 4th order.

4.5.3.2 Basis functions for triangular elements

An orthogonal basis for the triangle can be constructed as a generalized tensor product of the so-called principal functions defined as

$$\psi_{i}^{a}(z) = P_{i}^{0.0}(z), \qquad (4.53)$$
$$\psi_{ij}^{b}(z) = \left(\frac{1-z}{2}\right)^{i} P_{j}^{2i+1,0}(z).$$

The basis functions for the standard triangle element are defined using the principle functions as

$$b_{k}(\xi,\eta) = \psi_{i}^{a} \left(\frac{2\xi}{1-\eta} - 1\right) \psi_{ij}^{b}(-1+2\eta).$$
(4.54)

The two-dimensional hierarchical basis functions for the standard triangle element up to 4^{th} order are defined in Eq. (4.55) and their modes are presented in Figure 4-10.

$$\begin{aligned} b_{1}(\xi,\eta) &= 1, \\ b_{2}(\xi,\eta) &= -1 + 2\xi + \eta, \\ b_{3}(\xi,\eta) &= -1 + 3\eta, \\ b_{4}(\xi,\eta) &= 6\xi^{2} + 6\xi(-1+\eta) + (-1+\eta)^{2}, \\ b_{5}(\xi,\eta) &= (-1+2\xi+\eta)(-1+5\eta), \ b_{6}(\xi,\eta) &= 1 + 2\eta(-4+5\eta), \\ b_{7}(\xi,\eta) &= (10\xi^{2}+10\xi(-1+\eta) + (-1+\eta)^{2})(-1+2\xi+\eta), \\ b_{8}(\xi,\eta) &= (6\xi^{2}+6\xi(-1+\eta) + (-1+\eta)^{2})(-1+7\eta), \\ b_{9}(\xi,\eta) &= (-1+2\xi+\eta)(1+3\eta(-4+7\eta)), \\ b_{10}(\xi,\eta) &= -1+5\eta(3+\eta(-9+7\eta)), \\ b_{11}(\xi,\eta) &= 70\xi^{4}+140\xi^{3}(-1+\eta) + 90\xi^{2}(-1+\eta)^{2}+20\xi(-1+\eta)^{3}+(-1+\eta)^{4}, \\ b_{12}(\xi,\eta) &= (10\xi^{2}+10\xi(-1+\eta) + (-1+\eta)^{2})(-1+2\xi+\eta)(-1+9\eta), \\ b_{13}(\xi,\eta) &= (6\xi^{2}+6\xi(-1+\eta) + (-1+\eta)^{2})(1+4\eta(-4+9\eta)), \\ b_{14}(\xi,\eta) &= (-1+2\xi+\eta)(-1+21(1-2\eta)^{2}\eta), \\ b_{15}(\xi,\eta) &= 1+2\eta(-12+7\eta(9+\eta(-16+9\eta))). \end{aligned}$$

4.5.4 Basis functions for three-dimensional problem

An orthogonal basis for the tetrahedral element can be constructed as a generalized tensor product of the so-called principal functions defined as

$$\begin{split} \psi_{i}^{a}(z) &= P_{i}^{0,0}(z), \\ \psi_{ij}^{b}(z) &= \left(\frac{1-z}{2}\right)^{i} P_{j}^{2i+1,0}(z), \\ \psi_{ijk}^{c}(z) &= \left(\frac{1-z}{2}\right)^{i+j} P_{k}^{2i+2j+2,0}(z). \end{split}$$
(4.56)

The basis functions b_k for the standard tetrahedral element are defined in terms of the principle functions as

$$b_k\left(\xi,\eta,\zeta\right) = \psi_i^a \left(\frac{2\xi}{1-\eta-\zeta} - 1\right) \psi_{ij}^b \left(\frac{2\eta}{1-\zeta} - 1\right) \psi_{ijk}^c \left(-1 + 2\zeta\right).$$

$$(4.57)$$

The three-dimensional hierarchical basis functions for tetrahedral element up to secondorder are given as:

$$b_{1}(\xi,\eta,\zeta) = 1, \qquad (4.58)$$

$$b_{2}(\xi,\eta,\zeta) = -1 + 2\xi + \eta + \zeta, \\b_{3}(\xi,\eta,\zeta) = -1 + 3\eta + \zeta, \\b_{4}(\xi,\eta,\zeta) = -1 + 4\zeta, \\b_{5}(\xi,\eta,\zeta) = (-1 + 2\xi + \eta + \zeta)(-1 + 5\eta + \zeta), \\b_{6}(\xi,\eta,\zeta) = (-1 + 2\xi + \eta + \zeta)(-1 + 6\zeta), \\b_{7}(\xi,\eta,\zeta) = (-1 + 3\eta + \zeta)(-1 + 6\zeta), \\b_{8}(\xi,\eta,\zeta) = 6\xi^{2} + 6\xi(-1 + \eta + \zeta) + (-1 + \eta + \zeta)^{2}, \\b_{9}(\xi,\eta,\zeta) = 10\eta^{2} + 8\eta(-1 + \zeta) + (-1 + \zeta)^{2}, \\b_{10}(\xi,\eta,\zeta) = 1 + 5\zeta(-2 + 3\zeta).$$

4.5.5 Derivatives of basis functions

In case of one-dimensional problems, the basis functions are defined as

$$b_k(x) = b_k(x(\xi)). \tag{4.59}$$

Then the derivatives of the basis function in the computational domain are given by

$$\frac{\partial b_k}{\partial x} = \frac{\partial b_k}{\partial \xi} \frac{\partial \xi}{\partial x}.$$
(4.60)

In case of two-dimensional problems, the basis functions b_k are defined as

$$b_k(x, y) = b_k(x(\xi, \eta), y(\xi, \eta)).$$

$$(4.61)$$

Then the derivatives of the basis function in the computational domain are given as

$$\frac{\partial b_k}{\partial x} = \frac{\partial b_k}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial b_k}{\partial \eta} \frac{\partial \eta}{\partial x},$$

$$\frac{\partial b_k}{\partial y} = \frac{\partial b_k}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial b_k}{\partial \eta} \frac{\partial \eta}{\partial y}.$$
(4.62)

In case of three-dimensional problems, the basis function b_k is defined as

$$b_k(x, y, z) = b_k(x(\xi, \eta, \zeta), y(\xi, \eta, \zeta), z(\xi, \eta, \zeta)).$$

$$(4.63)$$

Then the derivatives of the basis function in the computational domain are given as

$$\frac{\partial b_{k}}{\partial x} = \frac{\partial b_{k}}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial b_{k}}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial b_{k}}{\partial \zeta} \frac{\partial \zeta}{\partial x},$$

$$\frac{\partial b_{k}}{\partial y} = \frac{\partial b_{k}}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial b_{k}}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial b_{k}}{\partial \zeta} \frac{\partial \zeta}{\partial y},$$

$$\frac{\partial b_{k}}{\partial z} = \frac{\partial b_{k}}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial b_{k}}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial b_{k}}{\partial \zeta} \frac{\partial \zeta}{\partial z}.$$
(4.64)

4.5.6 Evaluation of mass Matrix

In section (4.3), the elemental mass matrix M is introduced. The integration required for the elements M is performed in the three-dimensional computational domain

$$M = \int_{\Omega} b_i(x, y, z) b_j(x, y, z) dx dy dz$$

$$= \int_{\xi} \int_{\eta} \int_{\zeta} b_i(\xi, \eta, \zeta) b_j(\xi, \eta, \zeta) |\mathbf{J}_{\mathbf{x} \to \mathbf{\xi}}| d\xi d\eta d\zeta$$

$$= |\mathbf{J}_{\mathbf{x} \to \mathbf{\xi}}| C_{ij}.$$

$$(4.65)$$

Here $|\mathbf{J}_{\mathbf{x}\to\mathbf{\xi}}|$ denotes the transformation Jacobian. Since, the orthogonal basis function are employed in present work, therefore, the constant C_{ij} can be defined as

$$C_{ij} = \begin{cases} \int_{\xi} \int_{\eta} \int_{\zeta} \left(b_i \left(\xi, \eta, \zeta\right) \right)^2 d\xi d\eta d\zeta, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$
(4.66)



Figure 4-11. A plot of the computed mass matrix for complete orthogonal polynomial space up to 4th order for full tetrahedral expansion.

4.6 Numerical integration in computational domain

In many cases, it is not possible to integrate the expression in closed form. Therefore numerical integration must, therefore, be utilized. If one is using sophisticated elements, it is almost always necessary to use numerical integration. Similarly, if the application is complicated, e.g., the solution of a nonlinear ordinary differential equation, then even simple one-dimensional elements can require numerical integration. Many analysts have found that the use of numerical integration simplifies the programming of the element matrices. This results from the fact that lengthy algebraic expressions are avoided and thus the chance of algebraic and/or programming errors is reduced. There are many numerical

integration methods available. Only those methods commonly used in finite element applications will be considered here.

In discontinuous Galerkin weak formulation (4.12), the surface and volume integrals are needed to be a weighted 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.

4.6.1 Numerical integration in one-dimensional space

The Gaussian quadrature of order N_q for the standard interval [-1, 1] is given as follows:

$$\int_{-1}^{1} f\left(\xi\right) d\xi \approx \sum_{i=1}^{N_q} \omega_i f\left(\xi_i\right),\tag{4.67}$$

where ξ_i and ω_i are the Gaussian quadrature points and weights, respectively. Noted that a Gaussian quadrature using N_q points may provide the exact integral if $f(\xi)$ is a polynomial of order $2N_q - 1$ or less. The Gaussian quadrature points and weights of order N_q in interval [-1, 1] are provided in Table E.1 (9.2.4Appendix E). In addition the numerical integration of a polynomial function $f(\xi)$ on a reference line of unit length [0, 1] is approximated as

$$\int_{0}^{1} f\left(\xi\right) d\xi \approx \sum_{i=1}^{N_{q}} \omega_{i} f\left(\xi_{i}\right).$$

$$(4.68)$$

The quadrature points and weights of the unit reference line in interval [0, 1] are provided in Table E.2 (9.2.4Appendix E). Figure 4-12 shows the distribution of the Gauss-Legendre quadrature points inside and over the one-dimensional master element.



Figure 4-12. Number of required quadrature points for integrating inside and over onedimensional master element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials.

4.6.2 Numerical integration in two-dimensional space

Integration on standard quadrilateral (square) element $Q_{st} = \{(\xi, \eta): -1 \le \xi, \eta \le 1\}$ usually relies on tensor product of the one-dimensional Gaussian quadrature formulas defined in Eq. (4.67). Thus, the application of Eq. (4.67) to a two-dimensional integral on a standard quadrilateral element on $[-1,1] \times [-1,1]$ yields the approximation

$$\iint_{\mathcal{Q}_{sr}} f\left(\xi,\eta\right) d\xi d\eta = \int_{-1-1}^{1} f\left(\xi,\eta\right) d\xi d\eta \approx \sum_{i=1}^{N_q} \sum_{j=1}^{N_q} \omega_i \omega_j f\left(\xi_i,\eta_j\right),\tag{4.69}$$

where ξ_i , η_j the quadrature are points and ω_i , ω_j are the weights of the respective quadrature points of order N_q . Figure 4-13 shows the distribution of the Gauss-Legendre quadrature points inside and over the two-dimensional master triangular element.



Figure 4-13. Number of required quadrature points for integrating inside and over the two-dimensional master triangular element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials.

In case of two-dimensional standard triangle (unit triangle) element $T_{st} = \{(\xi, \eta) : 0 \le \xi, \eta, \xi + \eta \le 1\}$ integration may be calculated by using tensor product-type Gaussian quadrature formula, but it may be less efficient [108]. The integration of the standard triangular element on $[0,1] \times [0,1]$ can be evaluated by symmetric quadrature formula defined in [108, 109] as

$$\iint_{T_{st}} f\left(\xi,\eta\right) d\xi d\eta = \int_{0}^{1} \int_{0}^{1-\xi} f\left(\xi,\eta\right) d\xi d\eta \approx \frac{1}{2} \sum_{i=1}^{N_q} \omega_i f\left(\xi_i,\eta_i\right),\tag{4.70}$$

where (ξ_i, η_i) are the quadrature points located inside the standard triangle, ω_i are the normalized weights with respect to the triangle area and N_q is the number of quadrature points. Noted that the resulting quadrature should use as less as a possible number of quadrature points to achieve as high as possible accuracy, we also would like the quadrature points to possess some kind of symmetry. The typical points for symmetric quadrature rules on the unit triangle are provided in Table E.3 (9.2.4Appendix E). Figure 4-14 shows the distribution of the Gauss-Legendre quadrature points inside and over the two-dimensional master rectangular element.



Figure 4-14. Number of required quadrature points for integrating inside and over the two-dimensional master rectangular element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials.

Distribution of all quadrature points



Figure 4-15 Number of required quadrature points for numerical integration in a three-dimensional tetrahedron element for (a) p=0, (b) p=1, and (c) p=2 order of space polynomials.

4.6.3 Numerical integration in three-dimensional space

In present work, we are using the standard tetrahedral (unit tetrahedral) element $Tet_{st} = \{(\xi, \eta, \zeta): 0 \le \xi, \eta, \zeta, \xi + \eta + \zeta \le 1\}$ for three-dimensional simulations. The integration of the standard tetrahedral element may be evaluated by symmetric quadrature formula defined in [108, 110] as

$$\iiint_{Tet_{st}} f\left(\xi,\eta,\zeta\right) d\xi d\eta d\zeta = \int_{0}^{1} \int_{0}^{1-\xi} \int_{0}^{1-\xi-\eta} f\left(\xi,\eta,\zeta\right) d\xi d\eta d\zeta$$

$$= \frac{1}{6} \sum_{i=1}^{N_{q}} \omega_{i} f\left(\xi_{i},\eta_{i},\zeta_{i}\right).$$

$$(4.71)$$

The symmetric quadrature points for a unit tetrahedral element are given in Table E.4 (9.2.4Appendix E). Figure 4-15 shows the distribution of the symmetric quadrature points inside and over the surface in the three-dimensional master tetrahedral element.

4.7 Initialization of DG solver

Let the initial condition be defined in the physical space Ω as

$$\mathbf{U}(\mathbf{x},0) = \mathbf{U}_0(\mathbf{x}) \tag{4.72}$$

Replacing the left-hand side with the approximation solution

$$\mathbf{U}_{h}\left(\mathbf{x},0\right) = \mathbf{U}_{0}\left(\mathbf{x}\right) \tag{4.73}$$

where, as previously defined

$$\mathbf{U}_{h}\left(\mathbf{x},t\right) = \sum_{i=1}^{N_{p}} \mathbf{U}_{i}\left(t\right) b_{i}\left(\mathbf{x}\right)$$
(4.74)

Casting this into the weak form, multiplying Eq. (4.73) by the test function and integrating over the element of the domain

$$\int_{\Omega} \mathbf{U}_{h}(\mathbf{x},0) b_{i}(\mathbf{x}) d\Omega = \int_{\Omega} \mathbf{U}_{0}(\mathbf{x}) b_{i}(\mathbf{x}) d\Omega$$
(4.75)

From the Eqs. (4.74) and (4.75), we get

$$\int_{\Omega} \left(\sum_{i=1}^{N_p} \mathbf{U}_i(0) b_i(\mathbf{x}) \right) b_j(\mathbf{x}) d\Omega = \int_{\Omega} \mathbf{U}_0(\mathbf{x}) b_i(\mathbf{x}) d\Omega, \qquad (4.76)$$

factoring out the degree of freedom,

$$\mathbf{U}_{i}(0) \cdot \int_{\Omega} b_{i}(\mathbf{x}) b_{j}(\mathbf{x}) d\Omega = \int_{\Omega} \mathbf{U}_{0}(\mathbf{x}) b_{i}(\mathbf{x}) d\Omega$$
(4.77)

where the integral on the left-hand side of Eq. (4.77) is the mass matrix

$$\mathbf{M} = \int_{\Omega} b_i(\mathbf{x}) b_j(\mathbf{x}) d\Omega.$$
(4.78)

Thus, finally the initialization becomes

$$\mathbf{U}_{i}(0) = \frac{1}{\mathbf{M}} \int_{\Omega} \mathbf{U}_{0}(\mathbf{x}) b_{i}(\mathbf{x}) d\Omega.$$
(4.79)

4.8 Time discretization of the problem

The spatial discretization of the governing Eq. (4.14) with discontinuous Galerkin method results to a system of semi-discrete ordinary differential equation in time

$$\mathbf{M}\frac{d\mathbf{U}}{dt} = \mathbf{R}(\mathbf{U}),\tag{4.80}$$

where **M** is the mass matrix, **U** is the global vector of the degree of freedom, and **R** is the residual vector. In our present work, explicit time scheme of the solution is performed with high-order strong stability preserving (SSP) Runge-Kutta methods that preserve the monotonicity of the spatial discretization in any norm or semi-norm coupled with first-order forward Euler time stepping. The explicit third-order accurate SSP Runge-Kutta method proposed by Shu and Osher [111] is employed,

$$\mathbf{U}^{(1)} = \mathbf{U}^{n} + \Delta t \, \mathbf{M}^{-1} \mathbf{R} \left(\mathbf{U}^{n} \right), \tag{4.81}$$
$$\mathbf{U}^{(2)} = \frac{3}{4} \mathbf{U}^{n} + \frac{1}{4} \mathbf{U}^{(1)} + \frac{1}{4} \Delta t \, \mathbf{M}^{-1} \mathbf{R} \left(\mathbf{U}^{(1)} \right),$$
$$\mathbf{U}^{n+1} = \frac{1}{3} \mathbf{U}^{n} + \frac{2}{3} \mathbf{U}^{(2)} + \frac{2}{3} \Delta t \, \mathbf{M}^{-1} \mathbf{R} \left(\mathbf{U}^{(2)} \right),$$

where \mathbf{M}^{-1} is the inverse of the mass matrix.

4.8.1 Time step calculation

The time step value Δt for nonlinear system of differential equations can be given by

$$\Delta t_I = CFL \frac{\Omega_I}{\left(\hat{\Lambda}_{inv}^x + \hat{\Lambda}_{inv}^y + \hat{\Lambda}_{inv}^z\right)_I + C\left(\hat{\Lambda}_{vis}^x + \hat{\Lambda}_{vis}^y + \hat{\Lambda}_{vis}^z\right)_I}.$$
(4.82)

Here, *CFL* is the Courant–Friedrichs-Lewy condition (*CFL* \leq 1). The inviscid spectral radii are defined as

$$\hat{\Lambda}_{inv}^{x} = (|u|+c)\Delta \hat{S}^{x}, \qquad (4.83)$$

$$\hat{\Lambda}_{inv}^{y} = (|v|+c)\Delta \hat{S}^{y}, \qquad \hat{\Lambda}_{inv}^{z} = (|w|+c)\Delta \hat{S}^{z},$$

and the viscous spectral radii are given by

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

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

$$\hat{\Lambda}_{vis}^{z} = \max\left(\frac{4}{3\rho}, \frac{\gamma}{\rho}\right) \left(\frac{\mu}{\Pr}\right) \frac{\left(\Delta S^{z}\right)^{2}}{\Omega}.$$
(4.84)

Here, the *C* denotes the constant parameter that is set to be zero for zero-order Boltzmann-Curtiss based model; 2 for first-order Boltzmann-Curtiss based model; and 4 for secondorder Boltzmann-Curtiss based model. The variables $\Delta \hat{S}^x$, $\Delta \hat{S}^y$, and $\Delta \hat{S}^z$, illustrate the projections of the control volume on the y-z, x-z and x-y planes, respectively. These may be defined as

$$\Delta \hat{S}^{x} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{x}|_{J}, \quad \Delta \hat{S}^{y} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{y}|_{J}, \quad \Delta \hat{S}^{z} = \frac{1}{2} \sum_{J=1}^{N_{F}} |S_{z}|_{J}, \tag{4.85}$$

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

4.9 Numerical flux functions

Due to the discontinuous space and individual elements, the numerical flux function provides the necessary communication of flow information between elements on the "left" and "right" sides of a given interface. Traditionally, with the local element Ω_e and

corresponding outward unit normal traditionally designated as the *L*-side and the neighbor element is designated as the *R*-side. At a minimum, the numerical flux function must satisfy the consistency relations

$$\mathbf{H}(\mathbf{U}_{h},\mathbf{U}_{h}) = \mathbf{H}(\mathbf{U}_{h}), \qquad (4.86)$$
$$\mathbf{H}(\mathbf{U}_{h}^{L},\mathbf{U}_{h}^{R}) = -\mathbf{H}(\mathbf{U}_{h}^{R},\mathbf{U}_{h}^{L}).$$

For the viscous flux function treatment, various schemes exist which are provided in depthdiscussion by Arnold [112]. In this thesis, we employed first Bassi-Rebay scheme (BR1) for viscous flux treatment. In this scheme, a central discretization is proposed for the auxiliary as well as the viscous fluxes:

$$\mathbf{H}_{auxiliary}\left(\mathbf{U}_{h}^{L},\mathbf{U}_{h}^{R}\right) = \frac{1}{2}\left(\mathbf{U}_{h}^{L} + \mathbf{U}_{h}^{R}\right),$$

$$\mathbf{H}_{viscous}\left(\mathbf{U}_{h}^{L},\boldsymbol{\Theta}_{h}^{L},\mathbf{U}_{h}^{R},\boldsymbol{\Theta}_{h}^{R}\right) = \frac{1}{2}\left(\mathbf{F}^{vis}\left(\mathbf{U}_{h}^{L},\boldsymbol{\Theta}_{h}^{L}\right) + \mathbf{F}^{vis}\left(\mathbf{U}_{h}^{R},\boldsymbol{\Theta}_{h}^{R}\right)\right).$$
(4.87)

On the other hand, the inviscid flux normal trace is constructed with the theory of the Finite Volume (FV) method—well known Riemann problem. Many choices exist in literature, such as Lax-Friedrichs, Roe, van Leer, Harten-Lax-van Leer, exact Godunov and many others. However, in contrast to FV methods, the particular choice of flux function becomes less important for at least two reasons. First, the interface integral does not carry the entire burden for the element update. Second, the inter-element solution jumps become increasingly small at an exponential rate with increasing order of the DG approximating space. Therefore, due consideration must be given to the sophistication, difficulty of implementation, and cost of computation. It turns out that the Lax-Friedrichs flux performs quite well compared to other traditional and more complex functions. The function is given by

$$\mathbf{H}_{inviscid}\left(\mathbf{U}_{h}^{L},\mathbf{U}_{h}^{R}\right) = \frac{1}{2} \left[\mathbf{F}^{inv}\left(\mathbf{U}_{h}^{L}\right) + \mathbf{F}^{inv}\left(\mathbf{U}_{h}^{R}\right)\right] + \frac{1}{2}\lambda_{max}\left(\mathbf{U}_{h}^{L} - \mathbf{U}_{h}^{R}\right),\tag{4.88}$$

where λ_{max} is the spectral radius (maximum eigenvalue) of the flux Jacobian

$$J = \left| \frac{\partial \mathbf{F}^{\text{inv}}}{\partial \mathbf{U}} \right|,\tag{4.89}$$

along the direction **n** normal to the edge and is equal to:

$$\lambda_{\max} = \mathbf{V} \cdot \mathbf{n} + C_{sound} = |\mathbf{V}| + C_{sound}.$$
(4.90)

Here, C_{sound} is the sound speed.

4.10 Numerical boundary conditions

According to the flow conditions which have to be found at specific regions of the computational domain, the appropriate boundary conditions have to implement to the system of the governing equations. The numerical implementation of the boundary conditions is tricky and it demands special attention. The accuracy of the simulation, the rate of residual convergence, and stability of the numerical solver are strongly dependent on the implementation of the boundary conditions.

All boundary conditions may be imposed weakly. For this purpose, we construct an exterior boundary state variable $\mathbf{U}_{h}^{b}(\mathbf{U}_{h}^{L},\mathbf{U}_{BC})$, which is a function of interior state \mathbf{U}_{h}^{L} and the known physical boundary data \mathbf{U}_{BC} .

4.10.1 Far-field boundary

Two requirements must be satisfied in numerical implementation of the far-field boundary conditions: first, the cutting of the physical domain should not have any considerable effect on the flow solution as compared to the unbounded domain and second, any outgoing noise should have no influence on the flow field. Inadequate truncation of the domain can lead to a severe slowdown of steady-state convergence rate. This issue is more sensible in the simulation of subsonic and transonic flow problems which are naturally elliptic and parabolic.

Based on the concept of characteristics variables, all information are transported into the computational domain along the characteristics waves when the 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

$$\mathbf{U}_{h}^{b} = \begin{pmatrix} \rho_{\infty} \\ (\rho \mathbf{u})_{\infty} \\ (\rho E)_{\infty} \end{pmatrix}$$
(4.91)

where the subscript ∞ denotes the free-stream values. In addition, the numerical flux functions — auxiliary, inviscid, and viscous – can be approximated as

$$\mathbf{H}_{auxiliary}^{b} = \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right),$$

$$\mathbf{H}_{inviscid}^{b} = \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right),$$

$$\mathbf{H}_{viscous}^{b} = \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \Theta_{h}^{L}, \mathbf{U}_{h}^{b}, \Theta_{h}^{b} \right).$$
(4.92)

4.10.2 Inviscid wall boundary

In case of an inviscid flow, the fluid slips over the surface and it does not penetrate into the wall. Since there is no friction force, the velocity vector must be tangent to the surface e.g., there is no flow normal to the surface, i.e.

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0},\tag{4.93}$$

where \mathbf{u} is the velocity of flow on the boundary, and \mathbf{n} is the unit outer normal vector on the boundary. The inviscid flux function is computed by adjusting the wall velocity to have zero normal component. While the viscous and auxiliary flux function are zero by default.

$$\mathbf{U}_{h}^{b} = \begin{pmatrix} \boldsymbol{\rho}^{L} \\ \mathbf{u}^{L} - 2(\mathbf{u}^{L} \cdot \mathbf{n})\mathbf{n} \\ \boldsymbol{\rho}^{L} E^{L} \end{pmatrix}, \qquad (4.94)$$

and

$$\mathbf{H}_{auxiliary}^{b} = \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right) = 0,
\mathbf{H}_{inviscid}^{b} = \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right) = 0,
\mathbf{H}_{viscous}^{b} = \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \mathbf{\Theta}_{h}^{L}, \mathbf{U}_{h}^{b}, \mathbf{\Theta}_{h}^{b} \right) = 0.$$
(4.95)

4.10.3 No-slip viscous wall boundary

In no-slip wall where a viscous fluid passes a solid wall, the relative velocity between a solid wall and fluid attachment to the surface is assumed to be zero. Therefore, the physical velocity on the solid should be defined such that,

$$\mathbf{u}^b - \mathbf{u}^{solid} = 0. \tag{4.96}$$

The solid temperature should be given explicitly if the wall boundary maintains the temperature. However, if heat flux vector is prescribed at wall, the normal heat flux on the wall should be defined as

$$\mathbf{q}^{solid} = \mathbf{n} \cdot \mathbf{q}^b. \tag{4.97}$$

For Navier-Fourier (NF) equations where Fourier law is employed for calculating heat flux vector, the normal gradient of temperature on the surface must set zero for adiabatic wall boundary condition as,

$$\mathbf{n} \cdot \nabla T^{b} = n_{i} \frac{\partial T^{L}}{\partial x_{i}}.$$
(4.98)

The most straight forward method to define no-slip boundary condition is to use following relations for adiabatic wall

$$\mathbf{U}_{h}^{b} = \begin{pmatrix} \rho^{L} \\ 0 \\ \rho^{L} E^{L} \end{pmatrix}, \qquad (4.99)$$
$$\Theta_{h}^{b} = \Theta_{h}^{L} - C_{11} \left(\mathbf{U}_{h}^{L} - \mathbf{U}_{h}^{b} \right) \mathbf{n}^{L}.$$

and

$$\mathbf{H}_{auxiliary}^{b} = \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right), \\
\mathbf{H}_{inviscid}^{b} = \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right), \\
\mathbf{H}_{viscous}^{b} = \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \Theta_{h}^{L}, \mathbf{U}_{h}^{b}, \Theta_{h}^{b} \right).$$
(4.100)

4.10.4 Viscous slip wall boundary

4.10.4.1 Langmuir velocity slip and temperature jump boundary

The velocity slip and temperature jump boundary conditions on the surface are necessary for the studying the rarefied and microscale gas flows. Among the various slip models, the Langmuir slip model based on the physical adsorption isotherm can be employed to model the slip effects[55, 113]. This boundary condition is considered that not only recovers the predictability but also facilitates a hydrodynamic treatment of the entire density regime with a single formalism. This present method takes the interfacial gas—surface molecule interaction into account. A fraction $\alpha (0 \le \alpha \le 1)$ of molecules reaching thermal equilibrium with wall can be expressed in dimensional form, as

$$\alpha = \begin{cases} \frac{\beta_{slip} p}{1 + \beta_{slip} p}, & \text{for monatomic gas,} \\ \frac{\sqrt{\beta_{slip} p}}{1 + \sqrt{\beta_{slip} p}}, & \text{for diatomic gas,} \end{cases}$$
(4.101)

where *p* is the surface pressure and the parameter β_{slip} depends on the wall temperature T_w as well as interfacial interaction parameters. By considering the gas-surface molecular interaction process as a chemical reaction, the parameter β_{slip} can be expressed as,

$$\beta_{slip} = \sqrt{\frac{\pi}{32}} \frac{\pi}{c^2} \frac{T_{ref}}{T_w} \exp\left(\frac{De}{k_B T_w}\right) \frac{1}{p_{ref} K n},$$
(4.102)

where *c* is the gas constant of the exponent of the inverse power law of the particle interaction potential, p_{ref} and T_{ref} are reference pressure and temperature, *Kn* is the global Knudsen number, and *De* is the heat of adsorption, for example, De = 5,255 J/mol for Ar-Al molecular interaction model. The velocity slip and temperature jump boundary conditions in the Langmuir model are determined according to the fraction, α ,

$$\mathbf{u} = \alpha \mathbf{u}_{w} + (1 - \alpha) \mathbf{u}_{g}, \qquad (4.103)$$
$$T = \alpha T_{w} + (1 - \alpha) T_{g}.$$

Here, **u** is velocity vector, \mathbf{u}_w is the wall velocity vector, \mathbf{u}_g and T_g are the gas velocity vector and temperature at the reference location.

4.10.4.2 Maxwell slip wall boundary

In 1879, Maxwell proposed a velocity slip boundary condition known as Maxwell velocity slip boundary condition[114, 115]. In this boundary condition, he related the tangential gas velocity slip \mathbf{u}_{slip} to the tangential shear stress $\Pi_{tangential}$ and the tangential heat flux $\mathbf{Q}_{tangential}$. This slip boundary condition can be expressed in tensor form [115] as,

$$\mathbf{u}_{slip} - \mathbf{u}_{wall} = -\left(\frac{2 - \sigma_{v}}{\sigma_{v}}\right) \frac{\lambda_{mean}}{\mu} \Pi_{tangential} - \frac{3}{4} \frac{\Pr(\gamma - 1)}{\gamma p} \mathbf{Q}_{tangential}$$
(4.104)

where the tangential shear stress $\Pi_{tangential}$ and the tangential heat flux $Q_{tangential}$ are defined at the surface as,

$$\boldsymbol{\Pi}_{\text{tangential}} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S}, \quad \mathbf{Q}_{\text{tangential}} = \mathbf{Q} \cdot \mathbf{S}.$$
(4.105)

Here, Π and \mathbf{Q} is the stress tensor and the heat flux vector along the surface; \mathbf{n} denotes unit outward normal vector; tensor \mathbf{S} which defined as $\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$, removes normal components at any non-scalar field, for example, velocity, so that slip only occurs in the tangential direction to the surface. The symbol \mathbf{I} denotes the identity tensor and \otimes represents the dyadic product between two vectors defined in equation (A.18) of 9.2.4Appendix A; Pr is the Prandtl number; and \mathbf{u}_{wall} is the wall velocity. The tangential momentum accommodation coefficient is denoted by σ_v ($0 \le \sigma_v \le 1$) which determines the proportion of the molecules reflected from the surface purely diffusely or purely specularly according to $\sigma_v = 1$ and $\sigma_v = 0$, respectively. In the notation given in Eq. (4.105), the Maxwell velocity slip boundary condition becomes,

$$\mathbf{u}_{slip} - \mathbf{u}_{wall} = -\left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \frac{\lambda_{mean}}{\mu} (\mathbf{n} \cdot \mathbf{\Pi}) \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) - \frac{3}{4} \frac{\Pr(\gamma - 1)}{\gamma p} \mathbf{Q} \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}).$$
(4.106)

Generally, the stress tensor Π and heat flux Q are defined for Newtonian fluid as

$$\mathbf{\Pi} = \begin{bmatrix} \Pi_{xx} & \Pi_{xy} & \Pi_{xz} \\ \Pi_{yx} & \Pi_{yy} & \Pi_{yz} \\ \Pi_{zx} & \Pi_{zy} & \Pi_{zz} \end{bmatrix},$$
(4.107)
$$\mathbf{Q} = \begin{bmatrix} \mathcal{Q}_x, \mathcal{Q}_y, \mathcal{Q}_z \end{bmatrix}^T.$$

Using Eq. (4.107), the Maxwell slip boundary condition, (4.106) becomes as

$$\mathbf{u}_{s} - \mathbf{u}_{w} = -\left(\frac{2-\sigma_{v}}{\sigma_{v}}\right) \frac{\lambda_{mean}}{\mu} \begin{bmatrix} \left(1-n_{x}^{2}\right)\theta_{1} - n_{x}n_{y}\theta_{2} - n_{x}n_{z}\theta_{3} \\ -n_{y}n_{x}\theta_{1} + \left(1-n_{y}^{2}\right)\theta_{2} - n_{y}n_{z}\theta_{3} \\ -n_{z}n_{x}\theta_{1} - n_{z}n_{y}\theta_{2} + \left(1-n_{z}^{2}\right)\theta_{3} \end{bmatrix}$$

$$-\frac{3}{4} \frac{\Pr(\gamma-1)}{\gamma p} \begin{bmatrix} \left(1-n_{x}^{2}\right)Q_{x} - n_{x}n_{y}Q_{y} - n_{x}n_{z}Q_{z} \\ -n_{y}n_{x}Q_{x} + \left(1-n\right)_{y}^{2}Q_{y} - n_{y}n_{z}Q_{z} \\ -n_{z}n_{x}Q_{x} - n_{z}n_{y}Q_{y} + \left(1-n_{z}^{2}\right)Q_{z} \end{bmatrix},$$

$$(4.108)$$

where

$$\theta_{1} = \Pi_{xx}n_{x} + \Pi_{xy}n_{y} + \Pi_{xz}n_{z}$$

$$\theta_{2} = \Pi_{yx}n_{x} + \Pi_{yy}n_{y} + \Pi_{yz}n_{z}$$

$$\theta_{3} = \Pi_{zx}n_{x} + \Pi_{zy}n_{y} + \Pi_{zz}n_{z}$$
(4.109)

4.10.5 Symmetry boundary

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

$$\mathbf{n} \cdot \nabla \mathbf{U} = 0, \qquad (4.110)$$
$$\mathbf{n} \cdot \nabla (\mathbf{u} \cdot t) = \mathbf{n} \cdot \nabla (\mathbf{u} \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})) = 0, \qquad (4.110)$$
$$t \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla (\mathbf{u} \cdot \mathbf{n}) = 0,$$

where *t* denotes a tangential vector to the symmetry boundary.

4.10.6 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. Considering behavior of the characteristics waves, the boundary operator can be defined as,

$$\mathbf{U}_{h}^{b} = \begin{pmatrix} \rho^{L} \\ \rho^{L} \mathbf{u}^{L} \\ \rho^{L} E^{L} \end{pmatrix}, \qquad (4.111)$$
$$\Theta_{h}^{b} = \Theta_{h}^{L} - C_{11} \left(\mathbf{U}_{h}^{L} - \mathbf{U}_{h}^{b} \right) \mathbf{n}^{L}.$$

The numerical inviscid, viscous and auxiliary flux functions can also be approximated as

$$\mathbf{H}_{auxiliary}^{b} = \mathbf{H}_{auxiliary} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right), \\
\mathbf{H}_{inviscid}^{b} = \mathbf{H}_{inviscid} \left(\mathbf{U}_{h}^{L}, \mathbf{U}_{h}^{b} \right), \\
\mathbf{H}_{viscous}^{b} = \mathbf{H}_{viscous} \left(\mathbf{U}_{h}^{L}, \Theta_{h}^{L}, \mathbf{U}_{h}^{b}, \Theta_{h}^{b} \right).$$
(4.112)

4.11 Implementation of limiters

4.11.1 Positivity preserving limiter

In DG scheme, numerical solutions may lead to negative density and pressure during the time marching. But, physically, the density and the pressure should be positive. Therefore, the positivity preserving limiter is needed to enforce positive pressure and density at every element. Recently, Zhang and Shu proposed [116] positivity preserving limiters for compressible Euler equations on rectangular meshes in DG method and also, extended this method to unstructured triangular meshes [117]. According to Zhang and Shu, the solution coefficients are limited in such a way, so that the accuracy is maintained for smooth solutions while the DG scheme remains conservative and limiting for positivity of density and pressure is performed locally at each element. The first step is to limit the density field at every element. So, start with defining a small value $\omega = \min(10^{-13}, \overline{\rho}, \overline{p})$ based on the mean value of the computed density and pressure in the target cell. Then, the positivity of density checks by computing and finding the minimum value of density, ρ_{\min} looping over the quadrature points in the local elements. The limited coefficient θ_1 is then evaluated as

$$\theta_{1} = \min\left(\frac{\bar{\rho} - \omega}{\bar{\rho} - \rho_{\min}}, 1\right)$$
(4.113)

The high order components of the density variable are then limited by

$$\mathbf{U}_{h}\left(\mathbf{x},t\right) = U_{j}^{0}\left(t\right)\varphi_{0}\left(\mathbf{x}\right) + \theta_{1}\sum_{i=1}^{k}U_{j}^{i}\left(t\right)\varphi_{i}\left(\mathbf{x}\right).$$

$$(4.114)$$

The second step is to preserve the pressure at each local element. This requires the scaling of all high order moments of the solution of all conservative variables with θ_2 . For computing the value of θ_2 , it requires to solve the quadratic equation

$$p\left[\left(1-t\right)\overline{W}+t\,\overline{\mathbf{U}}\right]=\omega,\quad 0\le t\le 1.$$
(4.115)

where \overline{W} is the mean solution and \overline{U} is the conservative variables with limited density solution. Then, pick the minimum value of *t* among all the quadrature points as θ_2 . The limited coefficient $\theta_2 = \min(t_1, t_2)$. The high order components of conservative variables are limited by

$$\mathbf{U}_{h}\left(\mathbf{x},t\right) = U_{j}^{0}\left(t\right)\varphi_{0}\left(\mathbf{x}\right) + \theta_{2}\sum_{i=1}^{k}U_{j}^{i}\left(t\right)\varphi_{i}\left(\mathbf{x}\right)$$

$$(4.116)$$

4.11.2 The Barth Jespersen limiter

In the context of DG methods, a slope limiter is post-processing filter that constraints a polynomial basis function to stay within certain bounds. Barth and Jespersen [118] proposed an algorithm based on the unstructured grid for piecewise-linear data. Given a

cell average $\overline{\mathbf{U}}_h = \mathbf{U}_c$ and the gradient $(\nabla \mathbf{U})_c$, the goal is to determine the maximum admissible slope for a constrained reconstruction of the form,

$$\mathbf{U}_{h}\left(\mathbf{x}\right) = \mathbf{U}_{c} + \alpha_{e}\left(\nabla\mathbf{U}\right)_{c} \cdot \left(\mathbf{x} - \mathbf{x}_{c}\right), \qquad 0 \le \alpha_{e} \le 1, \ \mathbf{x} \in \Omega_{e}.$$
(4.117)

Bath and Jespersen define the correction factor α_e so that the final solution values at a number of control points $\mathbf{x}_i \in \partial \Omega_e$ or in one of its neighbors Ω_a having a common boundary with Ω_e . That is,

$$\mathbf{U}_{e}^{\min} \leq \mathbf{U}(\mathbf{x}_{i}) \leq \mathbf{U}_{e}^{\max}, \quad \forall i.$$
(4.118)

Due to linearity, the solution \mathbf{U}_h attains its extrema at the vertices \mathbf{x}_i of the cell Ω_e . To enforce condition (4.118), the correction factor α_e is defined as

$$\alpha_{e} = \min \begin{cases} \min \left\{ 1, \frac{\mathbf{U}_{e}^{\max} - \mathbf{U}_{c}}{\mathbf{U}_{i} - \mathbf{U}_{c}} \right\}, & \text{if } \mathbf{U}_{i} - \mathbf{U}_{c} > 0, \\ 1, & \text{if } \mathbf{U}_{i} - \mathbf{U}_{c} = 0, \\ \min \left\{ 1, \frac{\mathbf{U}_{e}^{\min} - \mathbf{U}_{c}}{\mathbf{U}_{i} - \mathbf{U}_{c}} \right\}, & \text{if } \mathbf{U}_{i} - \mathbf{U}_{c} < 0, \end{cases}$$
(4.119)

where $\mathbf{U}_{h}(\mathbf{x}) = \mathbf{U}_{c} + (\nabla \mathbf{U})_{c} \cdot (\mathbf{x} - \mathbf{x}_{c})$ is the unconstrained solution value at \mathbf{x}_{i} .
Chapter 5. Solutions of zero and first-order Boltzmann-Curtiss based hydrodynamic models

"All of physics is either impossible or trivial. It is impossible until you understand it, and then it becomes trivial."

— Ernest Rutherford (1871-1937)

This chapter is devoted to a series of applications for laminar flows based on zero-order, and first-order Boltzmann-Curtiss based hydrodynamic models i.e. Euler, and Navier-Fourier are provided. This chapter is divided into three sections based on one-dimensional, two-dimensional and three-dimensional benchmark problems. In case of one-dimensional problems, the different Riemann test cases are assessed within DG framework and compared to the exact solutions. In case of two-dimensional problems, the different inviscid Riemann test cases—double Mach reflection, forward facing step, shock-vortex interaction and bubble-shock interaction, are simulated for checking solver accuracy. Finally, in three-dimensional problems, various Riemann benchmark are simulated. A subsonic flow past a sphere is simulated at $\alpha = 0^{\circ}$ and validated with experimental results. Finally, a transonic flow over a G400 aircraft is simulated with angle of attack, $\alpha = 0^{\circ}$.

5.1 One-dimensional problems

5.1.1 One-dimensional Riemann problem

The test cases introduced by Toro[119] are well suited and often used as first test cases for the validation of inviscid CFD codes because exact solutions can easily be found for the respective problems. These test cases are performed for capturing the wave configurations. The computational domain is $\Omega = [0,1]$ and 200 points are considered for all simulations. All cases are initial value problem (IVP), characterized by discontinuous conditions for flow variables which are prescribed in Figure 5-1.

Problem	Left state			Right State			Final time (sec.)	Discontinuity position
	Density	Pressure	Velocity	Density	Pressure	Velocity		
Sod shock tube problem	1.0	1.0	0.0	0.125	0.1	0.0	0.25	0.5
Lax shock tube problem	0.445	3.528	0.698	0.5	0.571	0.0	0.14	0.5
123 problem	1.0	-2.0	0.4	1.0	2.0	0.4	0.15	0.5
Blast wave problem	1.0	1000.0	0.0	1.0	0.01	0.0	0.012	0.5

Figure 5-1. Initial conditions of various one-dimensional Riemann test cases.

The ratio of specific heats is $\gamma = 1.4$, and the initial discontinuity is located at x = 0.5 for these problems. The Zero Gradient boundary condition is employed. The exact solution of these problems can be found in [119]. The density, pressure, and velocity distributions for the exact solutions and numerical solutions are presented in Figure 5-2 and Figure 5-3. We observed that the numerical solutions of these Riemann problems are in good agreement with the exact solution.



Figure 5-2. One-dimensional Riemann problem: Sod shock tube problem (left): the density, pressure, velocity distribution contours at t=0.25, and Lax shock tube problem (right): the density, pressure, velocity distribution contours at t=0.14.



Figure 5-3. One-dimensional Riemann problem: 123 problem (left): the density, pressure, velocity distribution contours at t=0.15, and blast wave problem (right): the density, pressure, velocity distribution contours at t=0.012.

5.2 Two-dimensional problems

5.2.1 Two-dimensional double Mach reflection problem

The double Mach reflection problem is a standard test problem for shock capturing schemes. It originated by experimental and numerical studies of reflections of planar shock waves from wedges. This problem was extensively studied by Woodward and Colella for the inviscid flow [120]. In this problem, the shock wave has a strength with Mach number of 10, which is initially positioned at x = 0, and hits a 30^o ramp with the x-axis. The initial pre-shock and post-shock conditions is

$$(\rho, u, v, p) = \begin{cases} (8, 8.25, 0, 116.5), & \text{if } -0.25 \le x \le 0 \\ (1.4, 0, 0, 1), & \text{if } 0 \le x \le 3.0. \end{cases}$$
(5.1)

The computational domain is $\Omega = [-0.25,3] \times [0,1]$, and the implemented boundary conditions (inflow, outflow and reflected wall) are shown in Figure 5-4.



Figure 5-4. Two-dimensional double Mach refelction problem: computational domain and intial configuration.

The final simulation time is considered as t = 0.2. The post-shock condition is imposed from x = -0.25 to x = 0 whereas a reflecting boundary condition is enforced from x = 0to x = 3.0 at the bottom. For the top boundary condition, the fluid variables are defined as to exactly follow the evolution of the Mach 10 shock wave. The inflow and outflow conditions are imposed for the left and right side of the computational domain. The density distributions with mesh size h = 1/150 are shown in Figure 5-5. This modal DG scheme resolves the flow structure under the Mach stem clearly.



Figure 5-5. Two-dimensional double Mach reflection problem: density distribution contours at t=0.2.



Figure 5-6. Two-dimensional forward facing step problem: computational domain.



Figure 5-7. Two-dimensional forward facing step problem: density contours at various time step.

5.2.2 Two-dimensional forward facing step problem

The forward facing step problem which is also known as Mach reflection problem was also proposed by Woodward and Colella [120] for the inviscid flow. The computational domain is $\Omega = [0,3] \times [0,1]/[0.6,3] \times [0,0.2]$ as shown in Figure 5-6, which is covered by unstructured triangular mesh. The Mach step is located at x = 0.6 with height 0.2 in the tunnel. Initially, a right-moving flow with Mach 3 is imposed in the whole computational domain. The reflective boundary conditions are applied on the upper and along the walls of the tunnel, and inflow and outflow boundary conditions are imposed at the entrance and the exit. The corner of the step is the center of a rarefaction fan, which is a singularity point. For minimizing this numerical error generated at corner, the meshes near the corner are refined. The density distributions with h = 1/200 at various times are presented in Figure 5-7. It may be noted that the resolution is improved with this mesh refinement, especially for the slip line started from the triple point.

5.2.3 Two-dimensional shock-vortex interaction problem

In this test case, we are considering the interaction of a vortex with a steady shock wave. The shock-vortex interaction (SVI) problem proposed by Rault [121], is a good benchmark problem for a high order numerical scheme. It is usually followed by a complex flow pattern with both smooth features and discontinuous waves. The computational domain is $[0,2]\times[0,1]$, and a normal strong shock wave with Mach M_s is located at x = 0.5, as shown in Figure 5-8.

The flow is from the left to the right direction. The upstream state of the pre-shock region is given by $(\rho, u, v, p) = (1, M_s \sqrt{\gamma}, 0, 1)$ and the downstream value in the post-shock region are computed through the Rankine-Hugoniot condition. A composite vortex,

rotating clockwise direction, is initially located at $(x_c, y_c) = (0.25, 0.5)$ with an angular velocity

$$v_{\theta} = \begin{cases} u_m \frac{r}{a} & \text{if } r \leq a, \\ u_m \frac{a}{a^2 - b^2} \left(r - \frac{b^2}{r} \right) & \text{if } a < r \leq b, \\ 0 & \text{if } r > b. \end{cases}$$
(5.2)

Here, u_m is the maximum tangential velocity, $r = \sqrt{(x - x_c)^2 + (y - y_c)^2}$ is the distance from the vortex core (x_c, y_c) , and the radii of the inner and the outer annular region are given as (a,b) = (0.075, 0.175). The strength of the vortex is measured by M_v , where $M_v = u_m/a$ and *a* is the sound speed calculated from the upstream flow condition. Inside the vortex, the density and pressure are the functions of the temperature (*T*) and the upstream state of the normal shock.

$$\rho = \rho_0 \left(\frac{T}{T_0}\right)^{\frac{1}{\gamma - 1}}, \quad p = p_0 \left(\frac{T}{T_0}\right)^{\frac{\gamma}{\gamma - 1}}, \tag{5.3}$$

where the temperature at the left state of T_0 is calculated by the ideal gas law $p = \rho RT$ with gas constant R = 1. The temperature inside the vortex is obtained after solving the ordinary differential equation

$$\frac{dT}{dr} = \frac{\gamma - 1}{R\gamma} \frac{v_{\theta}^2(r)}{r}.$$
(5.4)

In the present computation, we are considering two different simulation problem: weak SVI with $M_s = 1.2$ and $M_v = 0.5$ and strong SVI with $M_s = 1.5$ and $M_v = 0.7$. The computed solutions of these two test cases are presented in Figure 5-9 and Figure 5-10.



Figure 5-8. Two-dimensional shock-vortex interaction problem: computational domain.



Figure 5-9. Two-dimensional shock-vortex interaction problem: computed (a) vorticity and (b) density distribution contours with shock Mach =1.2, Vortex Mach =0.5 at t=2.5.





(b) Density contours

Figure 5-10. Two-dimensional shock-vortex interaction problem: computed (a) vorticity and (b) density distribution contours with shock Mach =1.5, Vortex Mach =0.7 at t=2.5.

5.2.4 Two-dimensional shock-bubble interaction problem

The developed DG solver is applied to the prediction of shock-bubble interaction (SBI) problem. The schematic diagram of the SBI problem is illustrated in Figure 5-11. The computational domain is $\Omega = [0,3] \times [-0.5, 0.5]$. The diameter of the bubble is D = 0.5 and it is centered at $(x_c, y_c) = (1.75, 0)$. A left running shock wave is initially located at x = 2.5. The initial value of post-shocked region is $(\rho, u, v, p) = (1.38, -0.39, 0, 1.57)$, the initial flow condition of bubble is $(\rho, u, v, p) = (0.138, 0, 0, 1.0)$, and the flow condition of the pre-shocked region is $(\rho, u, v, p) = (1.0, 0, 0, 1.0)$. The right boundary is set to be inflow; and the other boundaries, namely, left, upper and bottom are set to be outflow. For the numerical simulation, we have considered 1000×1000 points over rectangular meshes.



Figure 5-11. Two-dimensional shock-bubble interaction (SBI) problem: schematic diagram of computational domain.

The numerical schlieren images for the flow field evolution at various time steps are reported in Figure 5-12. The density and velocity of the post-shocked region are determined from the Rankine-Hugoniot jump condition.



Figure 5-12. Two-dimensional shock-bubble interaction (SBI) problem: schlieren images for flow field evolution at various times.

5.3 Three-dimensional problems

5.3.1 Three-dimensional Sod shock tube problem

The shock tube problem or Sod problem introduced by Gary A. Sod in 1978 [122] is frequently used to test the accuracy of computational methods. An analytical solution is infact available, therefore, it is possible to compare numerical results with it and understand the strengths and weaknesses of the scheme implemented. A shock tube consists of a pipe with rectangular cross-section filled with a fluid (or a gas) with a diaphragm splitting the tube into two halves as shown in Figure 5-13. The diaphragm is numerically simulated as a discontinuity in different fluid conditions (temperature, pressure, and density) across that specific surface. Generally, the left side of the tube has higher values for the fluid properties. Given such initial conditions, the system is allowed to evolve in time. Two waves are generated and can be seen in all the physical variables. A shock wave will move towards the right (low-pressure region), and a refractive wave will move to the left (highpressure region). A contact discontinuity (moving towards the right side) separates the two regions and is visible in density and temperature (or energy) only as shown in Figure 5-14.



Figure 5-13. Three-dimensional Sod shock tube problem: schematic diagram and initial configuration.



Figure 5-14. Three-dimensional Sod shock tube problem: produced different waves after broken diaphragm.

In present work, the classical Sod shock tube on a one-dimensional unstructured mesh to assess the ability of the numerical methods to capture one-dimensional simple wave is considered as a standard benchmark problem. We select a computational domain, defined by $[0,1] \times [0,0.1] \times [0,0.01]$. The unstructured tetrahedral mesh are used for our computations and contains 98801 tetrahedral elements with mesh size h = 0.01. It provides an equivalent one-dimensional resolution of 100 elements. The Dirichlet boundary conditions are imposed in *x*-direction, whereas the periodic boundary conditions are imposed in *y* and *z* directions. The initial condition is defined as follows:

$$(\rho, u, v, w, p) = \begin{cases} (1, 0, 0, 0, 1), & \text{if } x \le 0.5 \\ (0.125, 0, 0, 0, 0.1), & \text{if } x > 0.5. \end{cases}$$
(5.5)

The ratio of specific heats is $\gamma = 1.4$ and the initial discontinuity is located at x = 0.5. The computed final time is considered at t = 0.2 sec. The computed density and pressure distributions for the Sod shock tube problem in three-dimension, two-dimension and one-dimension representation are shown in Figure 5-15. The x-component of the computed density and pressure distributions are compared with the exact solutions and found in good agreement as shown Figure 5-15 (bottom)







Figure 5-15. Three-dimensional Sod shock tube problem: the computed density (left) and pressure (right) distributions in three-dimensional view (upper); two-dimensional view (middle) and one-dimensional profiles (bottom) at t=0.2.



Figure 5-16. Three-dimensional Riemann 123 problem: the computed density (left) and pressure (right) distributions in three-dimensional view (upper); two-dimensional view (middle) and one-dimensional profiles (bottom) at t=0.15.

5.3.2 Three-dimensional 123 problem

The next validation test case, so-called the *Riemann 123 problem*, has a solution consisting of two strong rarefactions and a trivial stationary contact discontinuity; the pressure is very small (close to vacuum) and this can lead to difficulties in the iteration scheme to find pressure numerically. This benchmark problem is also useful in assessing the performance of numerical methods for low-density flows [123].

For the numerical simulations, we select a computational domain, defined by $[-0.5, 0.5] \times [-0.03, 0.03] \times [0, 0.01]$. The unstructured tetrahedral mesh are used for our computations and contains 22318 tetrahedral elements with mesh size h = 0.01. It provides an equivalent one-dimensional resolution of 100 elements. The Dirichlet boundary conditions are imposed in *x*-direction, whereas the periodic boundary conditions are imposed in *y* and *z* directions. The initial condition is defined as follows:

$$(\rho, u, v, w, p) = \begin{cases} (1, -2.0, 0.0, 0.0, 0.4) & \text{for } x \le 0, \\ (1.0, 2.0, 0.0, 0.0, 0.4) & \text{otherwise } x > 0. \end{cases}$$
(5.6)

The ratio of specific heats is $\gamma = 1.4$ and the initial discontinuity is located at x = 0. The computed final time is considered at t = 0.15 sec. The computed density and pressure distributions for the 123 problem in three-dimension, two-dimension and one-dimension representation are shown in Figure 5-16. The x-component of the computed density and pressure distributions are compared with the exact solutions and found in good agreement as shown in Figure 5-16 (bottom).

5.3.3 Three-dimensional explosion problem

To validate the present numerical scheme in three spatial dimensions, we have considered a spherical explosion problem. This problem is important, as it involves the propagation of the waves which is not aligned with the Cartesian grid.



Figure 5-17. Three-dimensional explosion problem: initial configuration at t = 0 sec.



Figure 5-18. Three-dimensional explosion problem: the computed density contours at t = 0.2 sec.

The computational domain is the one-eighth of a sphere whose radius is one. The problem setup represents a multi-dimensional extension of the classical Sod problem [122], with initial conditions

$$(\rho, u, v, w, p) = \begin{cases} (1, 0, 0, 0, 1), & \text{for } r \le R, \\ (0.125, 0, 0, 0, 0, 1) & \text{for } r > R, \end{cases}$$
(5.7)

where $r = \sqrt{x^2 + y^2 + z^2}$ is the radial coordinate, while R = 0.5 denotes the radius of the initial discontinuity. The computational domain consists of the fine grid with a huge mesh 898,582 unstructured tetrahedral. Figure 5-17 illustrates the initial configuration of the explosion problem, while the computed density contours at t = 0.2 have been reported in Figure 5-18. Since the problem is spherically symmetric, the reference solution can be obtained solving an equivalent one-dimensional PDE in the radial direction with geometric source term [119].

5.3.4 Three-dimensional double Mach reflection problem

The next benchmark problem in the three-dimensional simulation is the double Mach reflection problem which is first extensively studied by Woodward and Colella [120] for the inviscid flow. This is one of the most well-known benchmark problems for high-resolution shock-capturing schemes. For this problem, the computational domain is $\Omega = [-0.3,3] \times [0,2] \times [0,0.05]$, and a solid wall lies at the bottom of the computational domain starting from x = 0. The unstructured tetrahedral mesh are used for our computations and contains 1023663 tetrahedral elements with mesh size h = 0.01. This test problem involves a strong moving shock with Mach 10 in a perfect gas with $\gamma = 1.4$ which hits a ramp at 30 degree with x-axis. The initial and post-shock conditions are

$$(\rho, u, v, w, p) = \begin{cases} (8.0, 8.25, 0.0, 0.0, 116.5) & \text{for } x \le 0.0, \\ (1.0, 0.0, 0.0, 0.0, 1.0) & \text{for } x > 0.0. \end{cases}$$
(5.8)

The final simulation time is considered as t = 0.2. The post-shock condition is imposed from x = -0.25 to x = 0 whereas a reflecting boundary condition is enforced from x = 0to x = 3.0 at the bottom. For the top boundary condition, the fluid variables are defined as to exactly follow the evolution of the Mach 10 shock wave. The inflow and outflow conditions are imposed on the left and right side of the computational domain. The computed density distributions are shown in Figure 5-19.



Figure 5-19. Three-dimensional double Mach reflection problem: computed density contours.

5.3.5 Three-dimensional forward facing step problem

Another classical three-dimensional benchmark problem for high-resolution shockcapturing discontinuous Galerkin scheme consists in the forward facing step problem, also called the Mach 3 wind tunnel test. It has also been proposed originally by Woodward, and Collela [120]. The computational domain is given by $\Omega = [0,3] \times [0,1] \setminus [0.6,3] \times [0,0.2]$ which consists 1251048 unstructured tetrahedral meshes. The initial condition is a uniform flow at Mach number M = 3 moving to the right. In $\rho(x, y, 0) = 1, p(x, y, 0) = 1/\gamma, u(x, y, 0) = 3,$ variables particular, the flow v(x, y, 0) = 0, w(x, y, 0) = 0 are employed at initial conditions. The ratio of specific heats is set to $\gamma = 1.4$. Simulations are carried out until t = 3.0 sec. Reflective boundary conditions are applied on the upper and lower boundary of the domain and inflow/outflow boundary conditions are applied at the entrance/exit. At the corner of the step, there is a singularity, which is properly resolved with the second-order modal DG scheme using grid refinement. The computed density distributions with second order modal threedimensional DG method are depicted in Figure 5-20. One can observe that the secondorder scheme provides a much better resolution of the physical instability and roll up of the contact line compared to the standard second order scheme. This indicates that the use of higher order schemes may be appropriate to enhance resolution and to reduce numerical viscosity for small-scale turbulent structures.



Figure 5-20. Three-dimensional forward facing step problem: computed density contours.

5.3.6 Three-dimensional transonic flow over a G400 aircraft

The test case of a transonic gas flows past a complete G400 aircraft at a free stream Mach number M = 0.84 and an angle of attack of $\alpha = 0^{\circ}$ is chosen in order to assess the performance of the three-dimensional modal DG method in computing complex geometric configurations. In this test case, laminar flow is considered in contrast to turbulent flow, as it is the smooth flow of a fluid over a surface. Moreover, engineers want to design aircraft

with the laminar flow over their wings to make them more aerodynamic and efficient. Here, the G400 configuration includes the fuselage, wings, horizontal and vertical tails and two jet engines. For numerical simulations, the unstructured tetrahedral grids are used, containing 2,010,878 elements and 366,684 grid points. In present test case, the full aircraft is modeled, as shown in Figure 5-21. The computed pressure coefficient value, the pressure contours on the wing and the streamlines over the aircraft are shown in Figure 5-22, Figure 5-23 and Figure 5-24, respectively.



Figure 5-21. Three-dimensional transonic flow over a G400 aircraft: computational domain with tetrahedral unstructured grids.



Figure 5-22. Three-dimensional transonic flow over a G400 aircraft: computed C_p value.



Figure 5-23. Three-dimensional transonic flow over a G400 aircraft: pressure contours on wing.



Figure 5-24. Three-dimensional transonic flow over a G400 aircraft: computed streamlines.

5.3.7 Three-dimensional subsonic viscous flow past a sphere

A viscous flow past a sphere at a freestream Mach number of 0.3, and an angle of attack 0° , and a Reynolds number of 118 is considered in this benchmark problem. This problem has been studied both experimentally [124] and numerically [125]. An adiabatic wall is assumed in this benchmark problem. Figure 5-25 shows the computational grid used in this test case, consisting of 98,000 tetrahedral elements, and 25344 grid points.



Figure 5-25. Three-dimensional subsonic viscous flow past a sphere: computational domain with unstructured tetrahedral mesh with 98,000 elements and 25,344 grid points.



(a) Present computational results

(b) Experimental results

Figure 5-26. Three-dimensional subsonic viscous flow past a sphere: computed streamlines of the flow field (left) and from experiment (right) at Mach =0.3, Re=118 and AoA=0 degree.

The computational streamlines obtained by the modal DG (P=2) method are compared with experimental streamlines in Figure 5-26, where steady separation bubble is readily observed in both plots and the size of the separation region in the computation agrees very well with that of the experiment. The computed Mach contours and streamlines in the flow field at different Reynolds numbers 25.5 and 133 with Mach =0.3 are shown in Figure 5-27. The numerical results show that at low Reynolds number, the viscous effects are important in a large area. A small recirculating zone (or vortex ring) develops close to the rear

stagnation points at about Re=25.5, as shown in Figure 5-27 (a). With further increase in the Reynolds number, this recirculating zone or wake expands, as shown in Figure 5-27 (b).



Figure 5-27. Three-dimensional subsonic viscous flow past a sphere: computed Mach contours and streamlines at Mach =0.3, (a) Re=25.5, and (b) Re=133.

Chapter 6. Solution of second-order Boltzmann-Curtiss based hydrodynamic models: 1D and 2D problems

"Dream is not that which you see while sleeping it is something that does not let you sleep" -A.P.J. Abdul Kalam (1931-2015)

In case that flow deviates from local thermal equilibrium state, application of the moment method into the classical Boltzmann-Curtiss equations leads to Boltzmann-Curtiss 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-Curtiss based models. Therefore, solutions of the Boltzmann-Curtiss based models are compared with each other, the solution of the DSMC method, and experimental data. Firstly, One-dimensional shock structure is simulated using Boltzmann-Curtiss based model and the results are compared with experiments. Then the flow over a cylinder is studied in detail. Then, a comparative analysis of different slip boundary conditions is provided using Navier-Fourier (i.e., first-order Boltzmann-Curtiss-based) equation. Finally, a flow over a sphere is simulated using modal DG method.

6.1 One-diemensional compression dominant problem: shock structure

The shock wave structure is one of the most fundamental problems in kinetic theory of gases and it is considered as a major stumbling block for theoreticians for the last decades [126-132]. For example, it has a big impact on the overall flow patterns around hypersonic

aerospace vehicles at high altitude [133]. The stationary shock wave structure problem is defined as very thin (order of mean free path; in other words, Knudsen number close to 1.0) stationary gas flow region between supersonic and subsonic downstream. The upstream and downstream states, denoted by the subscripts 1 and 2, respectively, are determined by the so-called Rankine-Hugoniot condition:

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} = \frac{(\gamma+1)M_1^2}{(\gamma-1)M_1^2 + 2},$$

$$\frac{p_2}{p_1} = 1 + \frac{2\gamma}{\gamma+1} (M_1^2 - 1),$$

$$\frac{T_2}{T_1} = \frac{\left[2\gamma M_1^2 - (\gamma-1)\right] \left[(\gamma-1)M_1^2 + 2\right]}{(\gamma-1)^2 M_1^2}.$$
(6.1)

For comparison of various results of shock structure, the following parameters are very useful. The inverse of the shock density thickness $(1/\delta)$, and the shock temperaturedensity separation (Δ_s) , which measures the separation between density and temperature profiles are defined as

$$\frac{1}{\delta} = \frac{1}{\left(\bar{\rho}_{2} - \bar{\rho}_{1}\right)} \left| \frac{d\bar{\rho}}{dx} \right|_{\max},$$

$$\Delta_{s} = \left[x \left(\bar{\rho} = 0.5 \right) - x \left(\bar{T} = 0.5 \right) \right],$$
(6.2)

where $\overline{\rho}$ and \overline{T} are the normalized density and temperature profiles defined as

$$\bar{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1}, \ \bar{T} = \frac{T - T_1}{T_2 - T_1}.$$
(6.3)

The central position x = 0 is defined as the location where the local variables (i.e. density, temperature, velocity) becomes equal to the arithmetic average of the upstream and downstream variables.

The density solution of viscous shock structure for argon gas ($f_{bulk} = 0$) and nitrogen gas ($f_{bulk} = 0.8$) with four different Mach stream conditions are shown in Figure 6-1 and Figure 6-2, respectively. The zero-order solutions are way off from the experiment, while the quasi-linear hydrodynamic model, the first-order and the second-order Boltzmann-Curtiss 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- Curtiss based solution is very close to the experiments.



Figure 6-1. One-dimensional shock structure problem: normalized density profile for argon gas at four different flow stem Mach numbers.



Figure 6-2. One-dimensional shock structure problem: normalized density profile for nitrogen gas at four different flow stem Mach numbers.

The shock density thickness is known as one of the important parameters on the accuracy of the models, therefore, the solution of Boltzmann-Curtiss based models for argon gas and nitrogen gas are compared with experimental data [134]. It is obvious from Figure 6-3 that second-order Boltzmann-based method can precisely capture the shock-density thickness for all Mach number regimes.



Figure 6-3. One-dimensional shock structure problem: computed inverse shock density thickness profile for (a) argon, and (b) nitrogen gas.

6.2 Two-dimensional hypersonic flow past a cylinder

To demonstrate the capability of the second-order Boltzmann-Curtiss based constitutive model, a viscous compressible flow past a cylinder is simulated for both hypersonic rarefied [135] and low-speed microscale [136]. The two-dimensional DG code was validated for various benchmark problems of viscous compressible gas flow. A monatomic argon gas with Pr=2/3 and s=0.75 was chosen as the working gas. In our previous studies [58, 137], the numerical results were compared with the DSMC method. Unstructured triangular grid with approximately 90,000 computation cells refined with a ratio of 1.06 near the wall to capture the physics is used for the DG simulations. The farfield boundary condition was imposed on the outer boundary of the computational domain while the Langmuir boundary condition [57,126, 127] was applied to the solid wall. The power law model was used for calculating the transport properties [60]. On the other hand, in the DSMC simulation, the VHS inter-particle collision model and the fully diffusive wall boundary condition were implemented. Approximately 2,000,000 particles were used

with at least 50 particles per each cell. The time step and the cell size were set one-tenth of mean collision time and one-fifth of the free-stream mean free path, respectively[138].



Figure 6-4. Validation of second-order Boltzmann-Curtiss based model (NCCR) with the DSMC in density distribution for (a) M = 5.48, Kn = 0.05, and (b) M = 0.1, Kn = 0.1 [58, 137].

In Figure 6-4, a comparison of the DG code with DSMC solutions for rarefied and microscale gas flow around a circular cylinder is shown for both cases of high-speed rarefied (M=5.48, Kn=0.05) and low-speed microscale (M=0.1, Kn=0.1) problems. The results show that the numerical solutions of the second-order Boltzmann-Curtiss based constitutive model are in close agreement with the simulated solutions of DSMC. In the high-speed case, the flow consists of a compressive bow shock structure, a stagnation region near the frontal part of the cylinder, and a gaseous expansion region near the rear part of the cylinder. The density remains initially constant in the free-stream region and then experiences a rapid change across the bow shock wave, whose value is very close to the theoretical prediction given by the Rankine–Hugoniot relations. Further, the shock thickness and general flow pattern are very similar. In the low-speed case, the flow consists of smooth compression and stagnation regions near the frontal part of the cylinder, and a microstate wave is the cylinder, and a gaseous case, the flow consists of the shock wave, whose value is very close to the theoretical prediction given by the Rankine–Hugoniot relations. Further, the shock thickness and general flow pattern are very similar. In the low-speed case, the flow consists

modest expansion region near the rear part of the cylinder. The solution of second-order Boltzmann-Curtiss based constitutive model is smooth in the low-speed regime, whereas the DSMC solution contains non-negligible statistical fluctuations.



Figure 6-5. Comparison of normalized density contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen numbers.



Figure 6-6. Comparison of Mach contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen numbers.

The two-dimensional DG solver is applied to simulate the hypersonic flow (Mach=5.48) around a circular cylinder from the continuum regime (Kn=0.005) to transition regime (Kn=0.5) at argon gas [137]. The first-order Boltzmann-Curtiss model results are compared with the second-order Boltzmann-Curtiss model results for three different Knudsen numbers (Kn) in Figure 6-5 and Figure 6-6. The contours show that the flow fields vary significantly as the Knudsen number increases from 0.005 to 0.5. At Kn = 0.005, the

discrepancies between the first order and the second-order Boltzmann-Curtiss model results turn out to be negligible, as shown in Figure 6-5(a) and Figure 6-6(a). As the Knudsen number increases to 0.05, however, non-negligible deviations begin to appear, as seen in Figure 6-5(b) and Figure 6-6(b). As the Knudsen number increases further to 0.5, well within the transition regime, significant deviations are present all over the flow field, as shown in Figure 6-5(c) and Figure 6-6(c). There are two distinctive regions of compression and expansion in the frontal and rear parts of the cylinder, respectively. A most notable difference is the structure of the stand-off shock wave in the frontal parts; a thicker and broader shock structure in the second-order Boltzmann-Curtiss model in comparison with the first-order Boltzmann-Curtiss model.



Figure 6-7. Comparison of the degree of non-equilibrium contours for the first-order and the second-order Boltzmann-Curtiss model at Mach=5.48 with various Knudsen numbers.

Further, from the contours of the degree of thermal nonequilibrium measured by the Rayleigh–Onsager dissipation function (3.57) as described in Figure 6-7, significant deviations from the LTE assumption can be observed in the compressive bow shock region and the expansive rear part of the cylinder. Because of this, most of the gaps between the first-order and the second-order Boltzmann-Curtiss models are observed in these regions. It can also be noted that the degree of gaseous expansion near the rear part of the cylinder predicted by the first-order Boltzmann-Curtiss model is considerably higher than that of

the second-order Boltzmann-Curtiss model. This over-estimation of the degree of thermal non-equilibrium in the first-order Boltzmann-Curtiss model may explain the poor performance of the first-order Boltzmann-Curtiss model in high Knudsen and Mach number flows.



Figure 6-8. Pressure coefficient distribution around a cylinder at various Knudsen numbers for (a) the first-order, and (b) the second-order Boltzmann-Curtiss models [137].



Figure 6-9. Normalized wall shear stress distribution around a cylinder at various Knudsen numbers for (a) the first-order, and (b) the second-order Boltzmann-Curtiss models [137].

Figure 6-8 illustrates the pressure coefficient distributions around the cylinder predicted by the first-order Boltzmann-Curtiss model and the second-order Boltzmann-

Curtiss model at three different Knudsen numbers. The pressure coefficient values estimated by the second-order Boltzmann-Curtiss model at Kn = 0.5 is considerably different from that of NSF, since the degree of thermal non-equilibrium is non-negligible in one-eighth of the frontal part of the cylinder. Figure 6-9 shows a comparison of the distribution of the normalized wall shear stress around the cylinder predicted by the first-order Boltzmann-Curtiss model and the second-order Boltzmann-Curtiss model. A significant reduction in viscous shear stress across the surface of the cylinder is observed for the second-order Boltzmann-Curtiss model, in particular, in the case of Kn = 0.5 in the transition regime. This is due to the shear-thinning property of the second-order Boltzmann-Curtiss model as shown in Figure 3-7, that is, smaller effective viscosity at high Knudsen number.

6.3 Two-dimensional hypersonic flow over a rectangular block

The next two-dimensional test case is conducted to investigate the effects of the inflow Knudsen number (Kn) on hypersonic nonequilibrium rarefied flows over a rectangular block. The free stream flow consists of argon gas ($f_{bulk} = 0$) with Mach number of 5.48 (flow speed of 525.59 m/s), an angle of attack $\alpha = 30^{\circ}$, a temperature of 26.6 K and four various free-stream Knudsen numbers 0.0001, 0.01, 0.1, and 1.0 in continuum to transition regimes. The wall temperature of the block is considered as 293.15 K. Figure 6-10 shows contours of Mach number, normalized density, and streamlines for the second-order Boltzmann-Curtiss model at various Knudsen numbers. The contours show that the flow fields vary significantly as the Knudsen number increases from 0.001 to 1.0. It is shown that in the case of Kn=0.0001, which corresponds to the continuum regime, a strong detached bow shock is developed starting from the front of the rectangular block and extending to both



(d) *Kn*=1.0

Figure 6-10. Mach contours (Left), normalized density contours (middle), and streamlines (right) over a rectangular block for the second-order Boltzmann-Curtiss based model at Mach=5.48, AoA=30 degree with various Knudsen numbers.
sides symmetrically. In the shock wave region, the velocity decreases sharply from hypersonic to subsonic.

With the increase of the value of Kn, the flow gets closer to the slip regime. At the same time, the disturbed flow-field gradually expands outward and the shock layer becomes thicker, while the detached distance gets larger and the shock intensity gets weaker. When Kn reaches to transition regime (Kn=0.1), the shock wave almost disappears and the velocity diminishes slowly from the free-stream value to zero on the surface. Meanwhile, the inner flow-field structure shrinks to the front part of the rectangular block, and a large arc-expansion region is formed. When Kn rises continually, it belongs to the transitional flow regime and free-molecular flow regime.

6.4 Shock-vortex interaction problem

The interaction between shock waves and vortical flows has received considerable attention in gas dynamics and aeroacoustics. It includes the fuel-air mixing enhancement in the combustion [139], helicopter blades operating at supercritical speeds [140], the 'shock noise' generation in the design of advanced jet engines [141], combustion instability [142], and so on. In such flows, when a number of shock waves interact with vortices, the coupling between them dominates the flow field and yields a complicated flow pattern. Due to this complexity, the disturbance is generated which propagates along with shock waves and brings out a distortion phenomenon between shock waves and vortices. The interaction alters or destroys the shock waves and the vortical flow structure.

The shock-vortex interaction (called SVI hereafter) has been the subject of extensive study, since it is one of the most simplified models of the interaction between shock waves and vortical flows. Over the last decades, the significant efforts have been devoted to interpret the physical phenomena for SVI through experiment, theoretical analysis, and numerical simulations. Hollingsworth and Richards[143] carried out an early experiment and showed that SVI produces a cylindrical acoustic wave, consisting of alternating compression and rarefaction regions around the circumference. Later, the circumferential pressure distribution of the acoustic wave was measured by Dosanjh and Weeks [144]. A linear theory was proposed by Ribner [145] for describing the sound production mechanism and its quadrupolar nature in SVI. Ellzey *et al.*[146] investigated numerically SVI and found two acoustic waves in a quadrupolar nature. Subsequently, Inoue and Hattori [147] identified a third acoustic wave generated in planar SVI. Grasso and Pirozzoli [148] examined the interaction of a shock wave with a cylindrical vortex and investigated the dependence of shock distortion and vortex compression on the shock and vortex strength. Later, Zhang *et al.*[149] conducted a numerical study on SVI with strong vortex and found the multistage features of acoustic shock waves. Recently, the multiple acoustic waves, quadrupolar in nature and successively out of phase, were captured in the numerical simulation of SVI by Chatterjee and Vijayraj [150].

In this study, encouraged by these developments, we aim to investigate the nonequilibrium effects of diatomic and polyatomic gases on SVI problem based on the secondorder constitutive model of the Boltzmann-Curtiss kinetic equation. *To the best knowledge of authors, no attempt has been made in past to investigate the non-equilibrium effects of the rotational mode in diatomic and polyatomic gases (at micro besides macro levels) on SVI problem.* Further, the present study may be regarded as the first theoretical and computational attempt of investigating the strong interaction of two important nonequilibrium phenomena in diatomic and polyatomic gases—compressive shock structure and velocity-shear of the vortex—on the basis of a fundamental microscopic Boltzmann-Curtiss kinetic theory and subsequent second-order constitutive equations, without resorting to pure phenomenological theory.

6.4.1 Problem definition

A schematic diagram of the flow model for the simulations of a shock wave interacting with a single vortex is depicted in Figure 6-11. The computational domain is prescribed to be rectangular ($x_l \le x \le x_r$, $y_b \le y \le y_u$). Two computational domains with different sizes are used in this work; one is a domain with size of $x_r = -x_l = 0.0008$ m, $y_u = -y_b = 0.0008$ m used for simulation of micro SVI cases; the other one is a domain with size of $x_r = -x_l = 0.1$ m, $y_u = -y_b = 0.1$ m used for simulation of macro SVI cases. Here, a moving shock wave and clockwise-rotating stationary vortices are considered. The shock wave moves from left to right with respect to the initial shock wave in the computational domain. The location of the centre of vortex is prescribed to be (0, 0) in the computational domain.



Figure 6-11. Schematic diagram of the flow model for shock-vortex interaction problem. A vortex is formed by prescribing its initial flow to be that of a composite vortex [121, 151]. The composite vortex model consists of two regions; an inner core region and surrounding region where the velocity gradually approaches to zero. The rotational centre of the vortex is initially stationary and a velocity distribution between a core radius r_1 and an outer radius r_2 is prescribed before starting a simulation. In this flow, the maximum

tangential velocity is found at the core radius while the tangential velocity outside the outer radius $(r > r_1)$ is set to zero. Inside the core $(r \le r_1)$, the velocity goes linearly to zero at r = 0. The size of the core radius r_1 has a significant effect on the flow field. Therefore, we consider the core radius from 8λ to 1000λ with a step of 2λ , where from now on the symbol $\lambda (= 6.26 \times 10^{-6} \text{ m})$ represents a mean free path at initial condition.

The tangential velocity distribution of clockwise-rotating vortex is defined as follows,

$$u_{\theta} = \begin{cases} u_{m} \frac{r}{r_{1}}, & r \leq r_{1} \\ u_{m} \frac{r_{1}}{r_{1}^{2} - r_{2}^{2}} \left(r - \frac{r_{2}^{2}}{r} \right), & r_{1} \leq r \leq r_{2} \\ 0, & r > r_{2} \end{cases}$$
(6.4)

where u_{θ} is the azimuthal component of velocity, and u_m denotes the maximum tangential velocity. The temperature and the pressure in the quiescent field surrounding the vortex are also prescribed. Inside the vortex, the pressure, the density and the energy are determined by balancing the pressure gradients with the centripetal force as defined in equations (5.3)-(5.4).

In general, the flow fields generated by interactions between the shock wave and vortices are largely affected by the three flow parameters; the Mach number of incoming shock wave and rotating vortex, M_s and M_v defined by the maximum tangential velocity of vortex, and the core radius r_1 . These flow parameters are chosen to demonstrate the effects of shock wave, vortex strength and vortex size on the interaction. The Mach number of incoming shock wave M_s is considered from 1.5 to 3.5 with a step of 0.5, while the Mach number of vortex M_v ranges from 0.6 (weak vortex) to 1.0 (strong vortex). The

baseline case for our computation is an incoming shock Mach number of $M_s = 2.5$, a vortex Mach number of $M_v = 1.0$ and vortex core radius $r_1 = 10\lambda$ and $r_2 = 2r_1$.

6.4.2 Important physical quantities in SVI Problem

6.4.2.1 Sound pressure

The sound pressure defined below is used to examine the basic structure of vortex deformation;

$$\Delta p = \frac{p - p_s}{p_s},\tag{6.5}$$

where p is the local pressure and p_s is the pressure after shock wave.

6.4.2.2 Rayleigh-Onsager dissipation function

The Rayleigh-Onsager dissipation function is used to measure the degree of nonequilibrium in flow fields;

$$\hat{R}^2 \equiv \hat{\Pi} : \hat{\Pi} + \frac{2\gamma'}{f_{bulk}} \hat{\Delta}^2 + \hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}}.$$
(6.6)

6.4.2.3 Vorticity

The vorticity plays a vital role in deeper understanding of the interaction of a vortex with the shock wave. It can be defined as

$$\Omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}.$$
(6.7)

6.4.2.4 Enstrophy evolution

The physical phenomena of vorticity generation or attenuation during the interaction can be explained by monitoring the time evolution of the enstrophy. The time evolution of the enstrophy may be defined as the area integral of the square of the vorticity in the flow field [151],

Enstrophy
$$(t) = \int_{\partial A} \Omega_z^2(x, y, t) dx dy,$$
 (6.8)

where ∂A is the area of computational domain.

6.4.2.5 Dissipation rate evolution

The viscous effects of diatomic and polyatomic gases may be investigated by introducing the area-weighted dissipation rate of kinetic energy

Dissipation rate
$$(t) = \int_{\partial A} E(x, y, t) dx dy.$$
 (6.9)

Here E(x, y, t) denotes the dissipation rate per unit volume and is defined as

$$E(x, y, t) = -((\Pi_{xx} + \Delta)S_{xx} + \Pi_{xy}S_{xy} + \Pi_{yx}S_{yx} + (\Pi_{yy} + \Delta)S_{yy}),$$
(6.10)

where Π_{ij} is the viscous shear stress, Δ is the excess normal stress and S_{ij} is the strain rate defined as $S_{ij} = \partial u_i / \partial x_j$.

6.4.2.6 Vorticity transportation

The transport equation of vorticity can describe dominant physics in SVI as it contains several physically distinctive quantities [121, 151]. The transport equation of vorticity can be written as; in two dimensional case,

$$\frac{\partial\Omega_{z}}{\partial t} = -\Omega_{z} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{1}{\rho^{2}} \left(\frac{\partial\rho}{\partial x} \frac{\partial p}{\partial y} - \frac{\partial\rho}{\partial y} \frac{\partial p}{\partial x} \right) + \left[\frac{\partial}{\partial y} \left(\frac{1}{\rho} \frac{\partial}{\partial x} \left(\Pi_{xx} + \Delta \right) + \frac{1}{\rho} \frac{\partial\Pi_{xy}}{\partial y} \right) - \frac{\partial}{\partial x} \left(\frac{1}{\rho} \frac{\partial\Pi_{yx}}{\partial x} + \frac{1}{\rho} \frac{\partial}{\partial y} \left(\Pi_{yy} + \Delta \right) \right) \right].$$
(6.11)

There are three important dynamic processes for the vorticity component, Ω_z ; (i) vorticity generation through the dilatation strain rate, (ii) baroclinic generation through the interaction of pressure and density gradients, and (iii) viscous vorticity generation through the viscous effects. The net area-weighted vorticity generation is defined as

Net vorticity
$$(x, y, t) = \int_{\partial A} \frac{\partial \Omega_z}{\partial t} dx dy.$$
 (6.12)

The net area-weighted dilatational vorticity generation is computed as follows:

Dilatational vorticity
$$(x, y, t) = -\int_{\partial A} \Omega_z \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dx dy.$$
 (6.13)

The net area-weighted baroclinic vorticity generation is given as

Baroclinic vorticity
$$(x, y, t) = \int_{\partial A} \frac{1}{\rho^2} \left(\frac{\partial \rho}{\partial x} \frac{\partial p}{\partial y} - \frac{\partial \rho}{\partial y} \frac{\partial p}{\partial x} \right) dx dy.$$
 (6.14)

The net area-weighted viscous vorticity generation is expressed as

Viscous vorticity
$$(x, y, t) = \int_{\partial A} \frac{\partial}{\partial y} \left(\frac{1}{\rho} \frac{\partial}{\partial x} (\Pi_{xx} + \Delta) + \frac{1}{\rho} \frac{\partial \Pi_{xy}}{\partial y} \right) dx dy$$

$$- \int_{\partial A} \frac{\partial}{\partial x} \left(\frac{1}{\rho} \frac{\partial \Pi_{yx}}{\partial x} + \frac{1}{\rho} \frac{\partial}{\partial y} (\Pi_{yy} + \Delta) \right) dx dy.$$
(6.15)



Figure 6-12. Grid refinement study: density contours in macro SVI.



Figure 6-13. Grid refinement study: density (upper) and pressure (below) profiles at center-line of computational domain in macro SVI.

6.4.3 Grid refinement and validation of numerical solver

To evaluate the quality of the computational results, a grid refinement study is carried out by computing a macro SVI test case with $M_s = 2.0$, $M_v = 0.8$, $r_1 = 1000\lambda$ for argon gas. A sequence of grids is considered: 100×100 , 200×200 , 400×400 and 800×800 . Density contours of macro SVI at 1000 nanosecond are compared in Figure 6-12. In addition, the density and pressure profiles at center-line of computational domain are plotted for various grid points as shown in Figure 6-13. The results show that there is no significant difference between results obtained by 400×400 and 800×800 .grids, implying that 800×800 .grids are very close to asymptotic range. Based on this finding, all the computations are carried out on 800×800 .grids.



Figure 6-14. First-order Botlzmann-Curtiss constitutive model (Navier-Fourier) validation: circumferential distribution of the pressure amplitude in macro SVI (Air gas).

In order to verify the reliability and accuracy of present computational model and numerical DG solver, we compared the computational results with the experimental data of Dosanjh and Weeks [152], the theoretical result of Ribner [145], and the computational results of Ellzey *et al.*[146] and Inoue and Hattori [147]. The conditions for this benchmark case are set based on the experimental study of Dosanjh and Weeks [152]; $M_s = 1.29, M_v = 0.39, \gamma = 1.4$. Figure 6-14 shows the comparison of the circumferential distributions of the pressure amplitude defined as $(p_2 - p_p)/p_s$, where p_p, p_2 , and p_s denote the peak pressure of the precursor, the peak pressure of the second sound, and pressure behind the shock wave, respectively. As seen from Figure 6-14, the present result is very close to both the computational results of Ellzey *et al.*[146] and Inoue and Hattori [147]. This indicates that the present numerical code is able to compute the flow-fields in macro SVI accurately.



Figure 6-15. Second-order Boltzmann-Curtiss based constitutive model validation: time evolution of area-weighted enstrophy in micro SVI (Argon gas).

In order to further check the present the second-order Boltzmann-Curtiss-based constitutive model, three different cases of micro SVI investigated by Koffi *et al.*[151] are considered. Argon gas in its quiescent state surrounding the vortex at an initial temperature of 273 K and an initial pressure of 1013 Pa is considered. The core radius varies from 8λ to 12λ . In Figure 6-15, the time of the enstrophy is compared with the DSMC results. It can be shown that the present results, including the general trend of the enstrophy change with time, were found very close to the DSMC results.

6.4.4 Effects of diatomic and polyatomic gases on SVI

In this section, we investigate physics of macro and micro SVI in diatomic and polyatomic gases, in particular, in relation to the non-equilibrium effects. Emphasis is placed on sound generation mechanism, vorticity transport, enstrophy evolution, and dissipation rate evolution. Three types of vortices are chosen for extensive studies including transonic vortex with $M_v = 1.0$ followed by two types of subsonic vortices with $M_v = 0.6$ and $M_v = 0.8$. For given vortex Mach number, the core radius increases from 8λ to 1000λ with a step of 2λ . The incident shock Mach number M_s increases from 1.5

to 3.5 with a step of 0.5. Three gases are considered to investigate the non-equilibrium effects of diatomic and polyatomic gases; argon $(f_{bulk} = 0.0)$, nitrogen $(f_{bulk} = 0.8)$, and methane $(f_{bulk} = 1.33)$.



Figure 6-16. Time evolution of sound pressure for macro SVI.

6.4.4.1 Sound generation mechanism in SVI for diatomic and polyatomic gases

A. Sound generation mechanism in macro SVI

Figure 6-16 displays the time evolution of sound pressure in the macro SVI with conditions $M_s = 2.0, M_v = 0.8, r_1 = 1000\lambda$, and $f_{bulk} = 1.33$. The symbol \oplus denotes the compression region while \ominus presents the rarefaction region. As the incident shock wave interacts with the outer flow field of the clockwise-rotating composite vortex, the lower and upper portions of the incident shock wave are diffracted around the vortex. Two

diffracted shocks, fast diffracted shock (FD) and slow diffracted shock (SD) are connected by the refracted shock (RF), which passes through the vortex core as shown in Figure 6-16 (a). A rarefaction region appears in the upper portion where the shock propagation is promoted by the vortex velocity, while a compression region appears in the lower portion where the shock propagation is deterred by the vortex velocity. As a result, a precursor is generated first as seen in Figure 6-16(a). With development of interaction, the incident shock wave passes though the vortex core and is distorted into S shape, as shown in Figure 6-16(b). New rarefaction and compression regions appear outside of compression and rarefaction regions, respectively. This process of interaction shows that the precursor changes from the initially dipolar to quadrupolar nature consisting of compressions and rarefactions along the circumferential direction.

Figure 6-16(c) shows that, when the incident shock wave passes through the vortex flow field, a Mach reflection configuration with two reflection shocks MR1 and MR2 which propagate upward and downward, respectively, is generated. Because of the clockwise rotation of the vortex, both the strength and propagating velocity of MR2 is larger than that of MR1. At the same time, a second acoustic wave appears behind the precursor, which also displays a quadrupolar nature. The Mach stem MS accelerates relative to the two incident shocks waves SW1 and SW2, and the shock front again becomes approximately planar as shown in Figure 6-16(d). A shocklet type shock wave C1 is also observed at the opposite side of vortex core which merges with the planar shock front part as seen in Figure 6-16(e) and Figure 6-16(f). Further, another two reflection shocks MR3 and MR4 moving upward and downward, respectively, are formed. Finally, a third sound wave with a quadrupolar nature is generated by the compressed vortex as shown in Figure 6-16(f).



Figure 6-17. Time evolution of sound pressure for micro SVI.

B. Sound generation mechanism in micro SVI

Figure 6-17 displays the time evolution of sound pressure in the micro SVI with conditions $M_s = 2.0$, $M_v = 0.8$, $r_1 = 10\lambda$, and $f_{bulk} = 1.33$. As the incident shock wave interacts with the outer flow field of the micro vortex, the lower and upper portion of the shock wave are diffracted slowly around the vortex as seen in Figure 6-17(a). One rarefaction region is developed in upper and lower portions of the incident shock wave. When the incident shock wave approaches to the vortex core, a compression region is generated between two rarefaction regions. Also, a Mach stem MS and two reflected shock waves MR1 and MR2 are formed as shown in Figure 6-17(b). Later, as the incident shock wave passes through the vortex core, new rarefaction and compression regions appear outside the rarefaction regions in the upper portion of shock wave, as shown in Figure

6-17(c). Because the vortex rotates in clockwise direction, the deformed incident shock wave SW1 moves upward and one compression region is developed near the upper side of vortex core, as shown in Figure 6-17(d). For the same reason, the strength of reflected shock wave MR2 is stronger than that of MR1. Further, two additional shock waves MR3 and MR4 are formed and one rarefaction region comes out near the vortex core, as demonstrated in Figure 6-17(e). This rarefaction region moves upward near the compression region and a second sound wave is generated, as seen in Figure 6-17(f).

Overall, the results show that the micro SVI has similar evolution pattern of sound pressure with the macro SVI. However, due to enhanced viscous dissipations in micro SVI, the pattern is much more smeared including the incident, reflected and newly formed shock waves. For the similar reason, *it was observed that the quadrupolar acoustic wave structures, which are typical in the macro SVI, disappear in the micro SVI.* From the Ribner's linearized theory of SVI [145] which predicts the quadrupolar acoustic wave in macro SVI, the pressure jump varies around the vortex and generates a quadrupole field. The interaction also causes a 1/r potential flow around the vortex core and the pressure of this potential flow field can be expressed as

$$p \sim \frac{u_{\rm m}}{\rm V} \left(\frac{r_{\rm l}}{at}\right)^{1/2}.$$
(6.16)

Here V is the upstream velocity of the shock. The expression (6.16) conforms that, when the radius of the vortex core r_1 is very small, the pressure jump is greatly weakened in the micro SVI. As a result, the quadrupolar acoustic wave disappears in the micro SVI.

6.4.4.2 Effects of diatomic and polyatomic gases on the macro and micro SVI

Here we investigate the effects of diatomic and polyatomic gases on the macro and micro SVI. For this purpose, we select three gases: monatomic argon $(f_{bulk} = 0.0)$,

diatomic nitrogen $(f_{bulk} = 0.8)$, and linear polyatomic methane $(f_{bulk} = 1.33)$. We consider basically two types of the SVI problem: macro SVI with $r_1 = 1000\lambda$, $M_v = 0.8$, and micro SVI with $r_1 = 10\lambda$, $M_v = 0.8$ for $M_s = 1.5$, 2.0, 3.0.



Figure 6-18. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom): sound pressure contours.

A. Sound Pressure

Figure 6-18 displays the effects of diatomic and polyatomic gases on the sound pressure in macro and micro SVI at time t = 1000 ns. Due to the strong shock vortex interaction, a Mach reflection configuration is developed in all cases. It is observed in monatomic case $(f_{bulk} = 0.0)$ that a second sound wave and two reflected shock waves MR1 and MR2 are generated in the macro SVI, as seen in Figure 6-18(a). In addition, a small shocklet type wave C1 appears at the opposite side of the vortex core and near a compression region. When the f_{bulk} value increases to 0.8, two additional reflected shock waves MR3 and MR4 are formed and the shocklet wave C1 becomes larger in comparison with the monatomic case, as shown in Figure 6-18(b). Moreover, the expansion of reflected shock waves is stronger than that of reflected shock waves in monatomic case. This difference is maybe due to the substantial contribution of the dilatational term appearing in constitutive relations for diatomic gases. As the f_{bulk} value increases further to 1.33, an additional (third) sound wave is generated as shown in Figure 6-18(c). The expansion region of the sound waves becomes larger with increasing f_{bulk} . It is also observed that the size of the shocklet wave C1 increases and begins to merge with reflected shock waves of quadrupolar nature. On the other hand, the sound pressure pattern in the micro SVI is notably different from the macro SVI. First, the quadrupolar acoustic wave structure, which is the main feature of the macro SVI. Such the micro SVI. Nevertheless, faster propagation of incident shock wave with increasing f_{bulk} (equivalently, decreasing γ) is observed in both of macro and micro SVI, since the shock propagation speed is affected by the specific heat ratio of gases, regardless of macro or micro condition.

B. Vorticity distribution

Figure 6-19 illustrates the effects of diatomic and polyatomic gases on the vorticity distribution in macro and micro SVI for $M_s = 2.0$ at time t=1000 ns. It can be easily observed that there are significant differences in vorticity distribution for different gases after interaction. For instance, as already explained in the subsection of sound pressure, two additional reflected shock waves MR3 and MR4 are clearly formed in the macro SVI in case of diatomic and polyatomic gases. Furthermore, in the macro SVI, two branches of a vertical wave (SL1 and SL2) emanating from the vortex core are formed and it becomes strong with increasing Mach shock number, but becomes weak with increasing f_{bulk} value.

Note that this (vorticity and density related) wave was completely unseen in any of sound pressure contours.



Figure 6-19. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom): vorticity contours.

In present simulations, a composite vortex has negative vorticity in its core and positivity vorticity in the outside so that the total circulation produced by the regions may be zero. After the interaction, the vortex is deformed in horizontally stretched form in macro SVI, while it remains in circular shape and is squeezed in the longitudinal direction in micro SVI. In macro SVI with small f_{bulk} value, it is observed that the inner core of the vortex with negative vorticity is stretched and the outer annular region with positive vorticity begins to detach from the inner core, as shown in Figure 6-19(a). This stretching is more pronounced for large f_{bulk} values as seen from Figure 6-19(b)(c). It is also found

that, with increasing f_{bulk} value, the domain of negative vorticity increases, owing to an enhanced vorticity generation.



Figure 6-20. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom): degree of thermal non-equilibrium contours.

C. Degree of thermal non-equilibrium

Figure 6-20 shows the effects of diatomic and polyatomic gases on the degree of thermal non-equilibrium in macro and micro SVI at time t=1000 ns. The thermal non-equilibrium parameter R defined in (6.6) is calculated in order to examine what regions are expected to deviate significantly from the local equilibrium state during interaction. As expected, it is observed that the degree of thermal non-equilibrium is very high in micro SVI case compared with macro SVI. The macro SVI shows in general low degree of deviation from thermal equilibrium and the deviation is mostly confined inside the shock and vortex regions. In contrast, the micro SVI is significantly affected by non-equilibrium process in

all type of gases and the deviation occurs inside much more broader domain. It is apparent that non-equilibrium process associated with the micro SVI affects large portion of the flow field. This result confirms the essence of the difference between macro and micro SVI. Moreover, by comparing Figure 6-19 and Figure 6-20, it can easily be noticed that, while both of the vorticity and the non-equilibrium parameter based on the Rayleigh-Onsager dissipation function can describe the essential features in macro SVI quite effectively, the non-equilibrium parameter is much more effective than the vorticity in case of micro SVI.



Figure 6-21. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom): time evolution of enstrophy.

D. Evolution dynamics

Figure 6-21 illustrates the effects of diatomic and polyatomic gases on the time evolution of enstrophy in macro and micro SVI. It can be seen that the enstrophy during interaction is substantially enhanced with increasing f_{bulk} value in both of macro and micro SVI. However, a different pattern of enstrophy evolution is observed in macro and micro SVI. In macro SVI, the enstrophy increases until 400 ns and then remains fairly constant, as shown in Figure 6-21(a). On the other hand, in micro SVI, the enstrophy decreases rapidly until 250 ns and, after that, it increases briefly in 250-350 ns. Then it decreases slowly for

the remainder of interaction, as shown in Figure 6-21(b). The effects of diatomic and polyatomic gases can be further examined through the time evolution of dissipation rate in Figure 6-22. It can be noticed that the effect of rotational mode in gases on the dissipation rate is reversed depending on macro or micro conditions. Figure 6-22(a) indicates an increase in dissipation rate with increasing f_{bulk} value in macro SVI, whereas Figure 6-22(b) shows the opposite trend in case of micro SVI, a decrease in dissipation rate with increasing f_{bulk} value.



Figure 6-22. Diatomic and polyatomic gas effects on macro SVI (top) and micro SVI (bottom): time evolution of dissipation rate.

E. Summary of macro and micro SVI in diatomic and polyatomic gases

Several major effects of diatomic an polyatomic gases on shock-vortex interaction were identified; for example, generation of additional reflected shock waves MR3 and MR4 observed in both macro and micro SVI for non-monatomic gases. A significant increase in enstrophy is also observed with increasing f_{bulk} value in both macro and micro SVI. Furthermore, the macro and micro SVI show distinct flow field features. It is interesting to notice that the quadrupolar acoustic wave structure, which is essential phenomenon in macro SVI, is not observed in any case of micro SVI. Finally, the degree of thermal non-

equilibrium is found very high in micro SVI in comparison with macro SVI and consequently the non-equilibrium parameter is much more effective in describing the essential features in micro SVI.

Cases	Shock Mach	Vortex Mach	Core radius (r_1)
	$(M_{\rm s})$	$(M_{ m v})$	
1	1.5	1.0	8λ
2	1.5	1.0	12λ
3	2.5	1.0	8λ
4	2.5	1.0	12λ

TABLE I. Simulation cases for flow pattern and vortex deformation (nitrogen).

6.4.5 Characteristics of micro SVIs in diatomic and polyatomic gases

6.4.5.1 Vortex deformation through a shock wave

Vortex deformation by incident shock wave is a basic flow feature of the micro SVI. To analyse this physical phenomenon, four cases were selected, as summarized in Table I. These cases were chosen to demonstrate the effects of shock wave strength and vortex size on the interaction, and they may be considered as representative of the micro SVI. The first two cases involve a relatively weak shock wave, a vortex ($M_s = 1.5, M_v = 1.0$), and different vortex sizes $r_1 = 8\lambda$, 12λ . In contrast, the last two cases involve a strong shock wave, a vortex ($M_s = 2.5, M_v = 1.0$), and different vortex sizes $r_1 = 8\lambda$, 12λ . Nitrogen gas, a major component of air, was considered as a representative diatomic gas for the study of the micro SVI.

Figure 6-23 shows four snapshots of the sound pressure contours generated in the micro SVI with different incoming shock Mach numbers and vortex sizes. The positive value of the sound pressure denotes the compression region, whereas the negative value denotes the rarefaction region. The results show that five regions, two rarefication and three compression regions, are generated after the interaction in all cases. These regions are strongly dependent on the strength of the incoming shock wave. For example, the first two cases 1 and 2 produce three weak compression regions, while the last two cases 3 and 4 produce three strong compression regions, which are located between the two rarefaction regions. It can also be observed that stronger compression and rarefaction regions are produced at larger vortex sizes. It is interesting to note that the quadrupolar acoustic wave structure, which is the prime feature in the macro SVIs, is not found in any case of micro SVI.



Figure 6-23. Vortex deformation in micro SVI: sound pressure contours with $M_{y}=1.0$.

The results show that vortex deformation produced by an incident shock wave is strongly dependent on the strength of the interaction. In this context, the information about the vorticity evolution during the interaction may be very helpful. It can be obtained by examining the evolution dynamics of the net production and dissipation of vorticity.



Figure 6-24. Vortex deformation in micro SVI: time evolution of (a) Enstrophy and, (b) dissipation rate with $M_v = 1.0$.

6.4.5.2 Evolution dynamics of micro SVIs

Figure 6-24 displays the time evolution of enstrophy and dissipation rate for all cases 1-4. A substantial attenuation of enstrophy with time is found in all cases, as shown in Figure 6-24(a). The results show that the first two cases 1 and 2 with a weak shock wave produce an enstrophy pattern that is different from the last two cases 3 and 4 which have a strong shock wave. It may be noted that the shock wave in cases 1 and 2 starts to interact actively with the vortex around 200 ns and completes around 600 ns. Moreover, a monotonic decrease in enstrophy is found throughout the interaction process.

On the other hand, in cases 3 and 4, a brief increase in enstrophy is observed during the interaction process (250-400 ns). This difference can also be confirmed in the time evolution of the dissipation rate as shown in Figure 6-24(b). The dissipation rate in cases 1 and 2 remains relatively constant over time during the entire weak interaction process, whereas the dissipation rate in cases 3 and 4 experiences a substantial increase during the strong interaction process.



Figure 6-25. Vortex deformation in micro SVI: time evolution of (a) net vorticity, (b) net dilatational vorticity, (c) net baroclinic vorticity and, (d) net viscous vorticity with $M_v = 1.0$.

The reason behind this gap may be that the viscous stress dominates the flow structure during the interaction [153]. Strong interaction with a high shock Mach number or a large vortex size causes strong viscous effects and a large dissipation rate, whereas weak interaction with a low shock Mach number or small vortex size yields weak viscous effects and a low dissipation rate. This is one of the major features of the micro SVI in diatomic nitrogen gas, and is also in qualitative agreement with the conclusion for a monatomic gas [153].

The results of the enstrophy and the dissipation rate show that their evolution dynamics are strongly dependent on the strength of the interactions. Therefore, in order to obtain a better understanding of the physics of the interaction, we conducted a detailed study of the vorticity transportation during the interaction.

Figure 6-25 illustrates the net vorticity and three components of vorticity transportation for cases 1-4. The results show that the net vorticity and all components reach significant values during the interaction and diminish shortly after passing the vortex. It can be observed that, during the interaction, viscous vorticity generation is the most dominant mechanism, followed by dilatational vorticity and baroclinic vorticity generations. In addition, the viscous effects play a more dominant role in the interaction for strong shock waves (cases 3 and 4), resulting in a significant increase in the dissipation rate, as shown in Figure 6-25(b).

6.4.5.3 Comparison of first- and second-order constitutive models in the SVI problem

Figure 6-26 and Figure 6-27 illustrate a comparison between the first- and second-order constitutive models for a micro SVI. For this purpose, we selected three different incoming shock Mach numbers: $M_x = 1.5$, 2.5, 3.5 with the same vortex Mach number $M_v = 1.0$ and the vortex radius $r_i = 10\lambda$. Figure 6-26 shows that the flow field structures (sound pressure contours) in the first- and second-order constitutive models are non-negligibly different, in particular, for high shock Mach numbers. It may be noted that the second-order constitutive model produces stronger compression and rarefaction regions than the first-order constitutive model. The similar pattern was found in the time evolution of the enstrophy and dissipation rates shown in Figure 6-27. While a notable difference was found in the enstrophy, the difference was much more pronounced in the dissipation rate. At a high shock Mach number $M_x = 3.5$, the increase in the dissipation rate was 2600 Pa m²/s in the

first-order constitutive model, while the increase was drastically reduced to 1200 Pa m²/s in the second-order constitutive model, as shown in Figure 6-27(b). At a low shock Mach number $M_s = 1.5$, the increase was found to be 100 Pa m²/s in the first-order constitutive model, while it became negligible in the second-order constitutive model.



Figure 6-26. Comparison of first-order (upper) and second-order (bottom) constitutive models on micro SVI: sound pressure contours with different incoming shock Mach number and $M_v = 1.0$, $r_1 = 10\lambda$.

Figure 6-28 illustrates a comparison between the first-order constitutive models (standard Navier-Stokes-Fourier and Navier-Fourier without Stokes's hypothesis) and second-order constitutive model for a polyatomic (methane) gas on micro SVI with $M_s = 2.0, M_v = 0.8, r_i = 10\lambda$. It is observed that the standard Navier-Stokes-Fourier model predicts more degree of thermal non-equilibrium in comparison to Navier-Fourier and second-order models. It can be observed that the standard Navier-Stokes-Fourier model predicts higher degree of thermal non-equilibrium in comparison with the Navier-Fourier and second-order models.



Figure 6-27. Comparison of first-order and second-order constitutive models for diatomic (nitrogen) gas on micro SVI: time evolution of (a) enstrophy and, (b) dissipation rate with $M_v = 1.0$, $r_1 = 10\lambda$.



Navier-Stokes-Fourier ($f_b=0$) Navier-Fourier ($f_b=1.33$) Second-order model ($f_b=1.33$) **Figure 6-28.** Comparison of the classical first-order Navier-Stokes-Fourier, first-order Navier-Fourier and second-order models for polyatomic (methane) gas on micro SVI: degree of non-equilibrium contours with $M_s = 2.0$, $M_v = 0.8$, $r_1 = 10\lambda$.

6.4.5.4 Summary of characteristics of the micro SVI

The general flow field in a micro SVI, including vortex deformation and the compression and rarefaction regions, is highly dependent of the strength of the incoming shock wave and vortex, and the size of vortex. During the interaction, the viscous vorticity generation was found to be the most dominant factor in the net vorticity transportation process, followed by the generation of dilatational vorticity and baroclinic vorticity.

Finally, the first- and second-order constitutive models yielded a significant difference in the time evolution of enstrophy and dissipation rate in the micro SVI, especially for high shock Mach numbers.

Chapter 7. Solution of second-order Boltzmann-Curtiss based hydrodynamic models: 3D problems

"Dream is not that which you see while sleeping it is something that does not let you sleep" -A.P.J. Abdul Kalam (1931-2015)

This chapter is devoted to demonstrate the capability of the second-order Boltzmann-Curtiss based constitutive model for three-dimensional real-life aeronautical applications. We first conduct a numerical investigation for analyzing effects of no-slip and slip boundary conditions on the hypersonic flow past a sphere. Then, the solution of the firstorder and second-order constitutive models for hypersonic gas flows over a sphere are provided in transition regime. A laminar supersonic gas flows over a flat plate is simulated for second-order constitutive model. Finally, the three-dimensional hypersonic gas flows around a suborbital re-entry vehicle, IXV is investigated.

7.1 Hypersonic flow over a sphere: effect of slip boundary condition

One of the challenging issues in the simulation of rarefied flows using continuum method is to model slip effect accurately. In order to study slip boundary effects, it is necessary to make sure that the no-slip boundary condition is prescribed accurately. Hypersonic flow over a three-dimensional sphere at Mach 5.48 and Knudsen number 0.0001 is considered as the 3D benchmark problem. The computational domain consists 546,702 unstructured tetrahedral elements. A comparison between no-slip and viscous slip boundary conditions is shown in Figure 7-1. The second-order Maxwell velocity slip boundary condition is performed as a viscous slip boundary condition. The numerical

results indicate that the velocity slip effect is dominant and no wake appears in case of slip boundary condition.



(a) No slip boundary (b) Viscous Slip boundary (Maxwell)

Figure 7-1. Hypersonic flow over sphere: slip boundary effects at M = 5.48, Kn=0.0001.

7.2 Hypersonic flow over a sphere: second-order Boltzmann-Curtiss solutions

The numerical results obtained for second-order Boltzmann-Curtiss model using the 3D DG method are compared with the solution of first-order Boltzmann-Curtiss model at Mach of 5.48 and Knudsen number of 0.1. Argon gas with $f_{bulk} = 0$ is performed for the numerical simulations. The computed Mach contours of hypersonic flow past a sphere are shown in Figure 7-2.



Figure 7-2. Computed Mach contours of hypersonic flow over sphere: a comparison between first-order and second-order Boltzmann-Curtiss based constitutive models at Mach=5.48, Kn = 0.1.

7.3 Three-dimensional supersonic flow over a flat plate

We choose the supersonic flow over a flat plate with zero pressure gradient as a next test case. It is intended to assess the accuracy of the numerical solution obtained by the modal 3D-DG scheme for high Reynolds number flow. The laminar boundary layer over a unit flat plate is considered. In this case, the free-stream Mach number is 4.37, and the Reynolds number is 5.0×10^6 . The unstructured tetrahedral meshes are used to compute the flat plate boundary layer as shown in Figure 7-3. The computational domain contains 428053 number of tetrahedral elements and 80058 grid points. Argon gas is considered as working gas. The computed Mach number contours for the second-order constitutive model in 3D laminar flow over the flat plate are presented in Figure 7-4.



Figure 7-3. Three-dimensional supersonic gas flows over a flat plate problem: computational domain with unstructured tetrahedral elements.



(b) Mach contours in 2-D view

Figure 7-4. Three-dimensional supersonic gas flows over a flat plate problem: Mach contours with M=4.36 and $Re = 5.0 \times 10^6$.



Figure 7-5. Three-dimensional hypersonic flow past a re-entry vehicle: computational domain with unstructured tetrahedral meshes.

7.4 Three-dimensional hypersonic gas flow past a re-entry vehicle

The next benchmark case is considered as three-dimensional hypersonic gas flows past a suborbital re-entry vehicle, Intermediate eXperimental Vehicle (IXV) of the European Space Agency (ESA). The computational domain consists 978,445 number of unstructured tetrahedral elements as shown in Figure 7-5. The flow conditions for the hypersonic case are Mach =5.0, Kn = 0.2 and two different angles of attack (AoA) =15 and 45 degrees. The numerical simulations are performed on argon gas with $f_{bulk} = 0.0$. Comparisons of the computed Mach number contours are presented in Figure 7-6. The numerical result shows that there is no much substantial difference between numerical solutions of the first-order and second-order constitutive models, since the degree of thermal non-equilibrium is not high. However, it can be noticed from the Mach contours that some non-equilibrium effects begin to show up in the bow shock structure and in the rear part of the vehicle where the rapid expansion occurs. Besides these findings, the current results demonstrate that the three-dimensional numerical simulations of the second-order constitutive model are possible for hypersonic rarefied flows like re-entry vehicles with complex geometrical configuration.



(c) First-order model (AoA= 45°)



Figure 7-6. Three-dimensional hypersonic flow past a re-entry vehicle: computed Mach contours for first- and second-order Boltzmann-Curtiss based constitutive models at Mach =5.0 and Kn=0.2 and AoA =15 degree (upper) and AoA =45 degree.

Chapter 8. Parallelization of DG Solver

"Dream is not that which you see while sleeping it is something that does not let you sleep." -A.P.J. Abdul Kalam (1931-2015)

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. As mentioned before, the compact form of DG discretization makes it ideally suited for the implementation on parallel computers due to its local nature. In this chapter, we cover our parallelization strategy into the DG program design process from the beginning on, which enormously reduces the later coding complexity. We use the Message Passing Interface (MPI) library for parallel communication, which guarantees maximal flexibility for parallel programming. In the following the methodology—|domain decomposition, data structures and communication of the parallelization is presented. In the present chapter, the main focus is on the computational cost of the modal DG method for solving the conservation laws in conjunction with the first-order and second-order constitutive laws. The computational cost of the Navier-Stokes-Fourier (NSF) and secondorder Boltzmann-Curtiss based model is investigated in the serial and parallel frameworks [137].

8.1 Background

The DG method is compact and highly parallelizable due to the local nature of the discretization. The solution is approximated independently in each element, where interelement 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 study, a single program multiple data (SPMD) parallel model using a message-passing-interface (MPI) library was employed to parallelize the present mixed modal explicit DG method. The MPI library guarantees the maximal flexibility of the parallel programming, portability and scalability of the distributed memory parallel architectures [154]. 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 sub-sections.

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 [155]. 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 [155]. 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 sphere shown in Figure 8-2.



Figure 8-2 Tetrahedral mesh partition using ParMETIS; different colors represent subdomains owned by different processors.

8.3 Communication process

The current 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. In this study, 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 [156] as summarized in Figure 8-3.



Figure 8-3. Flow chart of DG parallel algorithm.

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 8-4 Data communication through Gaussian quadrature points for (a) DG piecewise constant scheme, and (b) DG higher-order approximation (data package is the solution information).



Figure 8-5 Non-blocking communication pattern (Isend and Irecv block diagram).

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, nonblocking 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.

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. The block diagram of the DG communication algorithm is shown in Figure 8-5. 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 [137]. After the solution converges, each of the processors plots its solution for post-processing purposes. However, it is noticeable in Figure 8-6(a) 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. A merging subroutine was devised for better post-processing of the solutions of parallel computations. In this

subroutine, all subdomain results were exported into a unified single domain for the purpose of better visualization. The DG approximate solutions are sought in the finite element space and thus the 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 its own solution, all the solutions are needed to be interpolated to the node for post processing software like TECPLOT. Otherwise, the biased interpolation that does consider all the neighbors of the node can result in very poor visualization as demonstrated in Figure 8-6(a). In order to avoid such shortcoming, the merging of sub-domains was performed for post processing after terminating parallel processing, as shown in Figure 8-6(b). In this process, as the spatial polynomial function is defined in least square space and the solution in each element is calculated locally, the results are irrespective of the number of processors.



Figure 8-6. Merging of the sub-domains for post-processing of the solutions: pressure contour of unified merged domain.

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 [157]. The definition of speed-up (S_p) was

established by Amdahl's law [158]. 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

$$S_p = \frac{t_s}{t_p},\tag{8.1}$$

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-Curtiss based models

The computational cost of Boltzmann-Curtiss based constitutive models measured empirically using serial modal DG solvers for various cases with different numbers of elements are shown in Figure 8-7. It can be seen that the computational cost of secondorder 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 second-order Boltzmann-Curtiss based model increases exponentially with the increasing number of elements, and it is higher than that of the first-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 the solution at added Gaussian quadrature points on the element interfaces, and inside the volume of the elements.



Figure 8-7 Computational cost of solving (a) the first-order Boltzmann-Curtiss constitutive relations, and (b) the second-order Boltzmann-Curtiss constitutive relations [137].

8.7 Parallel performance of Boltzmann-Curtiss based models

Figure 8-8 illustrates the speed-up of the piecewise constant and piecewise linear 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 piecewise linear approximation. Figure 8-9 shows the relative efficiency of the parallel code for piecewise constant and piecewise linear DG approximations, respectively. The communication

overload increases as the number of processors increases, and, as a result, the required runtime 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 speed-up of the piecewise linear polynomial expansion 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 piecewise linear DG schemes are highly parallelizable and a better choice for parallelization.



Figure 8-8 Parallel speed-up, S_p for the first-order Boltzmann-Curtiss constitutive model with (a) DG piecewise constant, and (b) DG piecewise linear scheme [137].

Figure 8-10 depicts the rate of cost reduction in the parallel second-order and first-order Boltzmann-Curtiss based solvers. In the ideal case, the first-order Boltzmann-Curtiss based solver approaches a linear reduction of computational cost, which is compatible with the Amdahl's law [158]. On the other hand, very surprisingly, the computational cost of the second-order Boltzmann-Curtiss based solver reduces much faster, almost exponentially, as the number of processors increases. This super-parallel performance is due to the nonlinear behavior of the cost of the second-order Boltzmann-Curtiss based solver, which demands less computational effort for *smaller* numbers of elements, as illustrated in Figure 8-9(b). Therefore, decomposing the domain into several sub-domains will boost the convergence rate. Put another way, the extra cost incurred from the iterative solver on implicit algebraic the second-order Boltzmann-Curtiss based constitutive model becomes negligible for the parallel computations with larger processors. Finally, Figure 8-10 shows the normalized computational cost of the parallel second-order and first-order Boltzmann-Curtiss based solvers for different numbers of processors. It is obvious that the cost of the second-order Boltzmann-Curtiss based solver reduces with a much higher rate than that of the first-order Boltzmann-Curtiss based solver, for both the piecewise constant and piecewise linear approximations. It is also shown that the cost rate of the first-order Boltzmann-Curtiss based solver decreases slowly with the increasing number of processors, and may approach to a constant rate earlier than the second-order Boltzmann-Curtiss based solver.



Figure 8-9 Parallel relative efficiency, *E* for the first-order Boltzmann-Curtiss constitutive model with (a) DG piecewise constant, and (b) DG piecewise linear scheme.



Figure 8-10. Comparison of the cost reduction between the first-order and second-order Boltzmann-Curtiss constitutive model parallel solvers with argon gas [137].

Chapter 9. Conclusion and future works

"Two things are infinite: the universe and human stupidity; and I'm not sure about the universe." - Albert Einstein (1879-1955)

9.1 Conclusion of present thesis

The research work reported in this thesis is focused on the computational study of nonequilibrium transport phenomena based on Boltzmann-Curtiss based constitutive models for diatomic and polyatomic gases. Starting from Eu's moment equations for diatomic and polyatomic gases derived in the framework of irreversible thermodynamics, the origin of the Boltzmann-Curtiss 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-dimension, two-dimension, and three-dimension 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-Curtiss based model can be significantly reduced by employing parallel algorithms, owing to a super-parallel performance of the nonlinear coupled constitutive solver of the second-order Boltzmann-Curtiss based model.

Further, the discontinuous Galerkin method has been extensively studied as the basic numerical scheme for solving the Boltzmann-Curtiss based models. It is shown that the DG method is suitable for solving the conservation laws together with the BoltzmannCurtiss based constitutive models. The mixed type DG methods were developed for solving one-dimensional, two-dimensional and three-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.

Several boundary value problems have also been studied using the modal DG method; forward facing step flow, double Mach reflection, shock-vortex interaction, bubble-shock interaction, one-, two- and three-dimensional Riemann problems, and external flow over a cylinder, rectangular box, sphere, IXV vehicle and G400 aircraft. It was found that solutions of the second-order Boltzmann-Curtiss 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.

9.2 Scope of future works

After the development of modal discontinuous Galerkin method for the conservation laws in conjunction with the first-order and second-order Boltzmann-Curtiss based constitutive relations for diatomic and polyatomic gases, the present research work can be extended in the following directions as future works:

9.2.1 Study on various numerical solvers for viscous-dominant problems

For viscous-dominant problems, the stability of numerical solver may be reduced due to the appearance of spurious oscillations near boundaries and discontinuities. Hence, it is necessary to further improve the stability of the DG solver for studying viscous-dominant problems. Our next step is to develop a three-dimensional local discontinuous Galerkin (LDG) and the implemented the second Bassi-Rebay scheme (BR2) scheme in our modal DG solver.

9.2.2 Vibrational nonequilibrium effects on gas flow problems

Due to the high temperatures generated by the compression in the inlet and isolator of a scramjet engine, the thermal energy of the flow will easily reach levels where there would be significant vibrational excitation at equilibrium as shown in Figure 9-1. Shocks and turbulent mixing can induce significant nonequilibrium effects owing to the relatively slow relaxation of vibrational energy. For example, the vibrational relaxation times of N_2 can easily exceed the residence time of the flow within a cruise-missile-scale scramjet engine. It is not known, however, how significant levels of vibrational non-equilibrium will impact turbulent mixing and reaction rates for the case of hydrogen or hydrocarbon combustion. Our next step may be towards to investigate the vibrational nonequilibrium effects on gas flow problems.



Figure 9-1. Contributions of the specific heat capacity to the temperature and degrees of freedom or modes.

9.2.3 Study of rarefied gas flows between rotating concentric cylinders

An isothermal gas flow between two concentric rotating cylinders is a classical fluid dynamics problem that is explained for the no-slip cases in many literatures [159].

However, under certain rarefied conditions the flow between the cylinders can exhibit highly non-intuitive behavior. For example, if the outer cylinder is stationary and the inner cylinder is rotating, it is possible for the velocity profile to become *inverted*, i.e., the velocity will *increase* from the inner to the outer cylinder wall. Therefore, the next step in developing more accurate constitutive model may be studied to investigate non-equilibrium effects associated with the Knudsen layers on the rarefied gas flows between two concentric rotating cylinders.

9.2.4 Unsteady turbulent flow problems

The study of turbulent nature in flowing fluids is one the most important and curious problems in all of classical physics [160, 161]. The most of fluid flows are turbulent, and at the same time fluids occur, and in many cases represent the dominant physics, on all macroscopic scales throughout the known universe-from the interior of biological cells, to circulatory and respiratory systems of living creatures, to countless technological devices and household appliances of modern society, to geophysical and astrophysical phenomena including planetary interiors, oceans and atmospheres and stellar physics, and finally to galactic and even super-galactic scales. And, despite the widespread occurrence of fluid flow, and the ubiquity of turbulence, the problem of turbulence remains to this day the last unsolved problem of the classical mathematical physics. Some of the key elements of turbulence are that it occurs over a large range of length and time scales, at high Reynolds number, and is fully three-dimensional and time-dependent. Turbulent flows are much more irregular and intermittent in contrast with laminar flow, and turbulence typically develops as an instability of laminar flow. For a real (i.e. viscous) fluid, these instabilities result from the interactions of the non-linear inertial terms and the viscous terms contained in the Navier-Stokes equations, which are very complex due to the fact that turbulence is rotational, three-dimensional, and time-dependent. Hence, high-order DG method would be a helpful tool for the investigations on unsteady turbulent flow problems that will be our next future research works.

Appendix A. Basics of vector and tensor theory

In this appendix, a basic theory of vector and tensor calculus is provided with mathematical definitions [162-164].

Scalar and vectors

- Scalar. A scalar refers to a quantity which is characterized by its only magnitude. For example, distance, temperature, density, pressure, etc.
- Vector. A vector represents a physical quantity which is characterized by its direction and its magnitude. The length of the vector represents the magnitude, while its direction is denoted with the unit vector along its axis. For example, force, velocity, momentum, etc.

Unit vector definition

Cartesian coordinate system. Let us consider a Cartesian coordinate system in threedimensional Euclidean space. We will denote the coordinates by

$$x_1 = x, \quad x_2 = y, \quad x_3 = z$$
 (A.1)

and the unit vectors so-called, basis vectors in the positive axes

$$\mathbf{e} = (e_1, e_2, e_3) = (\mathbf{i}, \mathbf{j}, \mathbf{k}) = \begin{cases} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \end{cases}.$$
(A.2)

* Kronecker delta symbol. The scalar product of the basis vectors are

$$e_i \cdot e_j = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$
(A.3)

These basis vectors form an orthonormal system. This can be written in a compact form by defining so called Kronecker delta function δ_{ii} . Hence

$$e_i \cdot e_j = \delta_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
 (A.4)

The cross product of two unit vectors can be performed using a special tensor so called the *permutation* or *Levi-Civita* tensor.

$$e_i \times e_j = \varepsilon_{ijk} e_k = \begin{cases} 1 & \text{for even permuations} \\ -1 & \text{for odd permuations} \\ 0 & \text{for any repeated index} \end{cases}$$
(A.5)

Vector definition and its properties

◆ A vector can be defined in three dimensional array. For example,

$$\mathbf{u} = (u_1, u_2, u_3)^T,$$

$$\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)^T.$$
(A.6)

✤ Any vector can be defined in terms of unit vectors 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.7)

Scalar or inner product of two vectors. The scalar or inner product of two vectors is the product of their lengths and the cosine of the smallest angle between them. If

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos \theta = u \, v \cos \theta,$$

where $u = \|\mathbf{u}\| = \sqrt{u_1^2 + u_2^2 + u_3^2}, \quad v = \|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + v_3^2}.$ (A.8)

Dot product of two vectors. The dot product of two vectors results in a scalar defined as

$$\mathbf{u} \cdot \mathbf{v} = \sum_{i} u_{i} v_{i} = u_{1} v_{1} + u_{2} v_{2} + u_{3} v_{3} \dots$$
(A.9)

Cross product of two vectors. The cross product of two vectors u and v can be defined

as

$$\mathbf{u} \times \mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix}.$$
 (A.10)

The magnitude of cross product $|\mathbf{u} \times \mathbf{v}|$ can be written as

$$|\mathbf{u} \times \mathbf{v}| = \|\mathbf{u}\| \|\mathbf{v}\| \sin \theta \,\mathbf{n},\tag{A.11}$$

where \mathbf{n} is the unit vector normal to \mathbf{u} and \mathbf{v} .

***** Dyadic product of two vectors. If **u** and **v** are vectors such as $\mathbf{u} = (u_1, u_2, u_3)^T$ and

 $\mathbf{v} = (v_1, v_2, v_3)^T$. Then the dyadic product of **u** and **v** is defined by

$$\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}^{T} = \begin{bmatrix} u_{1} \\ u_{2} \\ u_{3} \end{bmatrix} \begin{bmatrix} v_{1} & v_{2} & v_{3} \end{bmatrix} = \begin{bmatrix} u_{1}v_{1} & u_{1}v_{2} & u_{1}v_{3} \\ u_{2}v_{1} & u_{2}v_{2} & u_{2}v_{3} \\ u_{3}v_{1} & u_{3}v_{2} & u_{3}v_{3} \end{bmatrix}.$$
 (A.12)

★ Vector differential operator *del*. The vector differential operator ∇ (read as *del* or *nabla*) is defined as

$$\nabla \equiv \frac{\partial}{\partial x_1} e_1 + \frac{\partial}{\partial x_2} e_2 + \frac{\partial}{\partial x_3} e_3 \equiv \sum_i \frac{\partial}{\partial x_i} e_i.$$
(A.13)

• Gradient of scalar function. If ϕ is a scalar function, the gradient of ϕ , denoted by $\nabla \phi$ is defined as follows

grad
$$\phi = \nabla \phi = \frac{\partial \phi}{\partial x_i} e_i = \frac{\partial \phi}{\partial x_1} e_1 + \frac{\partial \phi}{\partial x_2} e_2 + \frac{\partial \phi}{\partial x_3} e_3.$$
 (A.14)

Gradient of vector field. If u is a vector field, the gradient of u can be defined in index notation as

grad
$$\mathbf{u} = \nabla \otimes \mathbf{u} = \frac{\partial u_i}{\partial x_j} e_i \otimes e_j.$$
 (A.15)

This can be written as

$$\operatorname{grad} \mathbf{u} = \nabla \otimes \mathbf{u} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{bmatrix} \equiv \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}.$$
(A.16)

★ Divergence of vector field. If $\mathbf{u} = (u_1, u_2, u_3)^T$ is the vector field, the divergence of \mathbf{u} (denoted by $\nabla \cdot \mathbf{u}$ or div \mathbf{u}) is defined as

$$\nabla \cdot \mathbf{u} = \operatorname{div} \mathbf{u} = \left(\sum_{i} \frac{\partial}{\partial x_{i}} e_{i}\right) \cdot \mathbf{u} = \frac{\partial u_{1}}{\partial x_{1}} + \frac{\partial u_{2}}{\partial x_{2}} + \frac{\partial u_{3}}{\partial x_{3}}.$$
 (A.17)

• Dyadic product of normal vectors. If $\mathbf{n} = (n_1, n_2, n_3)$ denotes the normal vector on the

surface, the dyadic product $\mathbf{n} \otimes \mathbf{n}$ may be defined as

$$\mathbf{n} \otimes \mathbf{n} = \begin{bmatrix} n_1 n_1 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2 n_2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3 n_3 \end{bmatrix} = \begin{bmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2^2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3^2 \end{bmatrix}.$$
(A.18)

Tensor definition and its properties

✤ 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 A_{ij} has 9 components, a third order tensor A_{ijk} has 27 quantities, and fourth-order tensor 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.19)

 \clubsuit A second order unit tensor ${\bf I}$ can be defined as

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
 (A.20)

\diamond The tensor Π can be defined in terms of unit vectors as

$$\mathbf{\Pi} = \sum_{j=1}^{3} \sum_{i=1}^{3} \mathbf{\Pi}_{ij} e_i \otimes e_j.$$
(A.21)

✤ The addition of two tensors is a tensor of a the same rank

$$\mathbf{\Pi} + p\mathbf{I} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} + \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix}$$

$$= \begin{bmatrix} \Pi_{11} + p & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} + p & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} + p \end{bmatrix} = \Pi_{ij} + p\delta_{ij}.$$
(A.22)

✤ Product of a tensor and a vector. The product of a tensor Π and a vector u is a vector which is defined as

$$\mathbf{v} = \mathbf{\Pi} \cdot \mathbf{u} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} \Pi_{11}u_1 + \Pi_{12}u_2 + \Pi_{13}u_3 \\ \Pi_{21}u_1 + \Pi_{22}u_2 + \Pi_{23}u_3 \\ \Pi_{31}u_1 + \Pi_{32}u_2 + \Pi_{33}u_3 \end{bmatrix},$$
(A.23)

which can be also expressed in index notation as

$$v_i = \prod_{ij} u_j. \tag{A.24}$$

The product of $\Pi.u\neq u.\Pi$, 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.25)

Alternatively, using index notation

$$v_j = u_i \Pi_{ij}. \tag{A.26}$$

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.27)

Product of two tensors. The product of two tensors results a tensor of 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.28)

The index notation of this product is

$$B_{ij} = \prod_{ik} \nabla_k u_j \tag{A.29}$$

Inner product of two tensors. The inner product (contraction) of two tensors of second rank results a scalar quantity as

$$\mathbf{A}:\mathbf{B}=A_{ij}B_{ij} \tag{A.30}$$

The component form of the inner product of two second-order tensor is

$$\mathbf{A} : \mathbf{B} = A_{11}B_{11} + A_{12}B_{12} + A_{13}B_{13} + A_{21}B_{21} + A_{22}B_{22} + A_{23}B_{23} + A_{31}B_{31} + A_{32}B_{32} + A_{33}B_{33}.$$
(A.31)

✤ Trace-free part of a symmetrical tensor. The trace-free part of a symmetrical tensor

A 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.32)

Consequently, the trace-free part of the velocity gradient tensor is defined as

$$\left[\nabla \mathbf{u}\right]^{(2)} = \frac{1}{2} \left[\nabla \mathbf{u} + \nabla \mathbf{u}^{T}\right] - \frac{1}{3} \left(\nabla \cdot \mathbf{u}\right) \mathbf{I}$$
(A.33)

Alternatively, the index notation is given by

$$\left[\nabla \mathbf{u}\right]_{ij}^{(2)} = \frac{1}{2} \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{1}{3} \left(\frac{\partial u_k}{\partial x_k} \right) \delta_{ij}$$
(A.34)

The trace-free part of $\mathbf{\Pi} \cdot \nabla \mathbf{u}$ can also be defined as

$$\left[\boldsymbol{\Pi} \cdot \nabla \mathbf{u}\right]_{ij}^{(2)} = \frac{1}{2} \left[\Pi_{ik} \frac{\partial u_j}{\partial x_k} + \Pi_{jk} \frac{\partial u_i}{\partial x_k} \right] - \frac{1}{3} \delta_{ij} \Pi_{lk} \frac{\partial u_l}{\partial x_k}.$$
(A.35)

Tensor relations on the surface

✤ Tensor relations on the surface. A traction vector on the surface S = (I − n ⊗ n) is a second-order tensor which can be defined as

$$\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2^2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3^2 \end{bmatrix},$$
(A.36)
$$\mathbf{S} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \equiv \begin{bmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_2 n_1 & 1 - n_2^2 & -n_2 n_3 \\ -n_3 n_1 & -n_3 n_2 & 1 - n_3^2 \end{bmatrix}.$$

★ Gradient operator to the surface. 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.37)

after multiplication and simplification, it reads as

$$\nabla_{s}T = (\nabla T) \cdot \mathbf{S} = \begin{bmatrix} \frac{\partial T}{\partial x_{1}} \\ \frac{\partial T}{\partial x_{2}} \\ \frac{\partial T}{\partial x_{3}} \end{bmatrix} \begin{bmatrix} 1 - n_{1}^{2} & -n_{1}n_{2} & -n_{1}n_{3} \\ -n_{2}n_{1} & 1 - n_{2}^{2} & -n_{2}n_{3} \\ -n_{3}n_{1} & -n_{2}n_{3} & 1 - n_{3}^{2} \end{bmatrix}.$$
(A.38)

* Tangential velocity on the surface. 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.39)

★ Tangential stress vector. The tangent stress vector $\vec{\tau} = (\mathbf{n} \cdot \mathbf{\Pi}) \cdot \mathbf{S}$ on the surface can be

defined as

$$\vec{\boldsymbol{\tau}} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S} = \begin{bmatrix} \Pi_{11}n_1 + \Pi_{12}n_2 + \Pi_{13}n_3 \\ \Pi_{21}n_1 + \Pi_{22}n_2 + \Pi_{23}n_3 \\ \Pi_{31}n_1 + \Pi_{32}n_2 + \Pi_{33}n_3 \end{bmatrix} \begin{bmatrix} 1 - n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_2n_1 & 1 - n_2^2 & -n_2n_3 \\ -n_3n_1 & -n_3n_2 & 1 - n_3^2 \end{bmatrix}.$$
(A.40)

Alternatively, it can be written in more specific form as

$$\vec{\boldsymbol{\tau}} = (\mathbf{n} \cdot \boldsymbol{\Pi}) \cdot \mathbf{S} = \begin{bmatrix} \Pi_{11}n_1 + \Pi_{12}n_2 + \Pi_{13}n_3 \\ \Pi_{21}n_1 + \Pi_{22}n_2 + \Pi_{23}n_3 \\ \Pi_{31}n_1 + \Pi_{32}n_2 + \Pi_{33}n_3 \end{bmatrix} \begin{bmatrix} 1 - n_1^2 & -n_1n_2 & -n_1n_3 \\ -n_2n_1 & 1 - n_2^2 & -n_2n_3 \\ -n_3n_1 & -n_3n_2 & 1 - n_3^2 \end{bmatrix}.$$
(A.41)
$$\vec{\boldsymbol{\tau}} = \begin{bmatrix} (1 - n_1^2)\theta_1 - n_1n_2\theta_2 - n_1n_3\theta_3 \\ -n_2n_1\theta_1 + (1 - n_2^2)\theta_2 - n_2n_3\theta_3 \\ -n_3n_1\theta_1 - n_3n_2\theta_2 + (1 - n_3^2)\theta_3 \end{bmatrix},$$
(A.42)

where

$$\begin{aligned}
\theta_1 &= \Pi_{11} n_1 + \Pi_{12} n_2 + \Pi_{13} n_3 \\
\theta_2 &= \Pi_{21} n_1 + \Pi_{22} n_2 + \Pi_{23} n_3 \\
\theta_3 &= \Pi_{31} n_1 + \Pi_{32} n_2 + \Pi_{33} n_3.
\end{aligned}$$
(A.43)

***** The Π : $\mathbf{n} \otimes \mathbf{n}$ can be defined as

$$\mathbf{\Pi} : \mathbf{n} \otimes \mathbf{n} = \begin{bmatrix} \Pi_{11} & \Pi_{11} & \Pi_{11} \\ \Pi_{11} & \Pi_{11} & \Pi_{11} \\ \Pi_{11} & \Pi_{11} & \Pi_{11} \end{bmatrix} : \begin{bmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_2 n_1 & n_2^2 & n_2 n_3 \\ n_3 n_1 & n_3 n_2 & n_3^2 \end{bmatrix}$$
(A.44)

which can be written in more simplified form as

$$\mathbf{\Pi} : \mathbf{n} \otimes \mathbf{n} = \Pi_{11} n_1^2 + \Pi_{12} n_1 n_2 + \Pi_{13} n_1 n_3 + \Pi_{21} n_2 n_1 + \Pi_{22} n_2^2 +$$

$$\Pi_{23} n_2 n_3 + \Pi_{31} n_3 n_1 + \Pi_{32} n_3 n_2 + \Pi_{33} n_3^2.$$
(A.45)

♦ The normal heat flux $q_n = \mathbf{q} \cdot \mathbf{n}$ and tangential heat flux vector $\vec{q}_t = \mathbf{q} \cdot \mathbf{S}$ can be defined

as

$$q_{n} = \mathbf{q} \cdot \mathbf{n} = q_{1}n_{1} + q_{2}n_{2} + q_{3}n_{3}$$
(A.46)
$$\vec{q}_{t} = \mathbf{q} \cdot \mathbf{S} = \begin{bmatrix} q_{1} \\ q_{2} \\ q_{3} \end{bmatrix} \cdot \begin{bmatrix} 1 - n_{1}^{2} & -n_{1}n_{2} & -n_{1}n_{3} \\ -n_{2}n_{1} & 1 - n_{2}^{2} & -n_{2}n_{3} \\ -n_{3}n_{1} & -n_{3}n_{2} & 1 - n_{3}^{2} \end{bmatrix}$$

or simply

$$\vec{\mathbf{q}}_{t} = \left(\left(1 - n_{1}^{2} \right) q_{1} - n_{1} n_{2} q_{2} - n_{1} n_{3} q_{z} \right) \mathbf{e}_{1} + \left(-n_{2} n_{1} q_{1} + \left(1 - n_{2}^{2} \right) q_{2} - n_{2} n_{3} q_{3} \right) \mathbf{e}_{2} + \left(-n_{3} n_{1} q_{1} - n_{3} n_{2} q_{2} + \left(1 - n_{3}^{2} \right) q_{3} \right) \mathbf{e}_{3}.$$
(A.47)

of velocity vector, $\mathbf{n} \cdot (\nabla \mathbf{u})^T$ can be defined as

$$\mathbf{n} \cdot \nabla \mathbf{u} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} n_x + \frac{\partial u_2}{\partial x_1} n_2 + \frac{\partial u_3}{\partial x_1} n_3 \\ \frac{\partial u_1}{\partial x_2} n_x + \frac{\partial u_2}{\partial x_2} n_2 + \frac{\partial u_3}{\partial x_2} n_3 \\ \frac{\partial u_1}{\partial x_3} n_x + \frac{\partial u_2}{\partial x_3} n_2 + \frac{\partial u_3}{\partial x_3} n_3 \end{bmatrix}$$
(A.48)

$$\mathbf{n} \cdot \left(\nabla \mathbf{u}\right)^{T} = \begin{bmatrix} n_{1} \\ n_{2} \\ n_{3} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} & \frac{\partial u_{2}}{\partial x_{1}} & \frac{\partial u_{3}}{\partial x_{1}} \\ \frac{\partial u_{1}}{\partial x_{2}} & \frac{\partial u_{2}}{\partial x_{2}} & \frac{\partial u_{3}}{\partial x_{2}} \\ \frac{\partial u_{1}}{\partial x_{3}} & \frac{\partial u_{2}}{\partial x_{3}} & \frac{\partial u_{3}}{\partial x_{3}} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} n_{1} + \frac{\partial u_{1}}{\partial x_{2}} n_{2} + \frac{\partial u_{1}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{2}}{\partial x_{1}} n_{1} + \frac{\partial u_{2}}{\partial x_{2}} n_{2} + \frac{\partial u_{2}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{3}}{\partial x_{1}} n_{1} + \frac{\partial u_{3}}{\partial x_{2}} n_{2} + \frac{\partial u_{3}}{\partial x_{3}} n_{3} \end{bmatrix}$$
(A.49)

✤ The dilatation of velocity vector $\mathbf{I}(\nabla \cdot \mathbf{u})$ is defined as

$$\mathbf{I}(\nabla \cdot \mathbf{u}) = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} & 0 & 0 \\ 0 & \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} & 0 \\ 0 & 0 & \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \end{bmatrix}.$$
 (A.50)

$$\mathbf{n} \cdot \mathbf{I} \left(\nabla \cdot \mathbf{u} \right) = \begin{bmatrix} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_1 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_2 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_3 \end{bmatrix}.$$
(A.51)

♦ The vector $(\mathbf{n} \cdot \nabla \mathbf{u}) \cdot \mathbf{S}$ can be defined as

$$\left(\mathbf{n} \cdot \nabla \mathbf{u}\right) \cdot \mathbf{S} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} n_1 + \frac{\partial u_2}{\partial x_1} n_2 + \frac{\partial u_3}{\partial x_1} n_3\\ \frac{\partial u_1}{\partial x_2} n_1 + \frac{\partial u_2}{\partial x_2} n_2 + \frac{\partial u_3}{\partial x_2} n_3\\ \frac{\partial u_1}{\partial x_3} n_1 + \frac{\partial u_2}{\partial x_3} n_2 + \frac{\partial u_3}{\partial x_3} n_3 \end{bmatrix} \cdot \begin{bmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3\\ -n_2 n_1 & 1 - n_2^2 & -n_2 n_3\\ -n_3 n_1 & -n_3 n_2 & 1 - n_3^2 \end{bmatrix}$$
(A.52)

This equation is written in shorten hand form as

$$(\mathbf{n} \cdot \nabla \mathbf{u}) \cdot \mathbf{S} = \begin{bmatrix} (1 - n_1^2) \alpha_1 - n_1 n_2 \alpha_2 - n_1 n_3 \alpha_3 \\ -n_1 n_2 \alpha_1 + (1 - n_2^2) \alpha_2 - n_1 n_3 \alpha_3 \\ -n_1 n_3 \alpha_1 - n_2 n_3 \alpha_2 + (1 - n_3^2) \alpha_3 \end{bmatrix}$$
(A.53)

where

$$\alpha_{1} = \frac{\partial u_{1}}{\partial x_{1}} n_{1} + \frac{\partial u_{2}}{\partial x_{1}} n_{2} + \frac{\partial u_{3}}{\partial x_{1}} n_{3}$$

$$\alpha_{2} = \frac{\partial u_{1}}{\partial x_{2}} n_{1} + \frac{\partial u_{2}}{\partial x_{2}} n_{2} + \frac{\partial u_{3}}{\partial x_{2}} n_{3}$$

$$\alpha_{3} = \frac{\partial u_{1}}{\partial x_{3}} n_{1} + \frac{\partial u_{2}}{\partial x_{3}} n_{2} + \frac{\partial u_{3}}{\partial x_{3}} n_{3}.$$
(A.54)

• The vector $(\mathbf{n} \cdot (\nabla \mathbf{u})^T) \cdot \mathbf{S}$ can be defined as

$$\left(\mathbf{n} \cdot \left(\nabla \mathbf{u}\right)^{T}\right) \cdot \mathbf{S} = \begin{bmatrix} \frac{\partial u_{1}}{\partial x_{1}} n_{1} + \frac{\partial u_{1}}{\partial x_{2}} n_{2} + \frac{\partial u_{1}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{2}}{\partial x_{1}} n_{1} + \frac{\partial u_{2}}{\partial x_{2}} n_{2} + \frac{\partial u_{2}}{\partial x_{3}} n_{3} \\ \frac{\partial u_{3}}{\partial x_{1}} n_{1} + \frac{\partial u_{3}}{\partial x_{2}} n_{2} + \frac{\partial u_{3}}{\partial x_{3}} n_{3} \end{bmatrix} \cdot \begin{bmatrix} 1 - n_{1}^{2} & -n_{1}n_{2} & -n_{1}n_{3} \\ -n_{2}n_{1} & 1 - n_{2}^{2} & -n_{2}n_{3} \\ -n_{3}n_{1} & -n_{3}n_{2} & 1 - n_{3}^{2} \end{bmatrix},$$
(A.55)

This above equation can be written in shorten form as

$$\left(\mathbf{n} \cdot (\nabla \mathbf{u})^{T}\right) \cdot \mathbf{S} = \begin{bmatrix} (1 - n_{1}^{2})\beta_{1} - n_{1}n_{2}\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{2}\beta_{1} + (1 - n_{2}^{2})\beta_{2} - n_{1}n_{3}\beta_{3} \\ -n_{1}n_{3}\beta_{1} - n_{2}n_{3}\beta_{2} + (1 - n_{3}^{2})\beta_{3} \end{bmatrix},$$
(A.56)

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.57)

♦ The vector $(\mathbf{n} \cdot \mathbf{I}(\nabla \cdot \mathbf{u})) \cdot \mathbf{S}$ can be calculated as follows

$$\left(\mathbf{n} \cdot \mathbf{I} \cdot (\nabla \cdot \mathbf{u}) \right) \cdot \mathbf{S} = \begin{bmatrix} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_1 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_2 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_2 \\ \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) n_3 \end{bmatrix} \cdot \begin{bmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_2 n_1 & 1 - n_2^2 & -n_2 n_3 \\ -n_3 n_1 & -n_3 n_2 & 1 - n_3^2 \end{bmatrix},$$
(A.58)

which can be written in shorten hand form as

$$\left(\mathbf{n}\cdot\mathbf{I}\cdot\left(\nabla\cdot\mathbf{u}\right)\right)\cdot\mathbf{S} = \begin{bmatrix} n_{1}\left(1-n_{1}^{2}\right)\omega-n_{1}n_{2}^{2}\omega-n_{1}n_{3}^{2}\omega\\ -n_{2}n_{1}^{2}\omega+n_{2}\left(1-n_{2}^{2}\right)\omega-n_{2}n_{3}^{2}\omega\\ -n_{3}n_{1}^{2}\omega-n_{3}n_{2}^{2}\omega+n_{3}\left(1-n_{3}^{2}\right)\omega \end{bmatrix},$$
(A.59)

where

$$\omega = \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right). \tag{A.60}$$

Appendix B. Derivation of conservation laws from Boltzmann-Curtiss kinetic equation

In this appendix, conservation laws for diatomic and polyatomic gases are derived from the Boltzmann-Curtiss kinetic equation based on Eu's work [1, 3]. The Boltzmann-Curtiss kinetic equation for the diatomic and polyatomic gas particles without external body force can be read from (2.89) as,

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) f\left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t\right) = C[f, f_1].$$
(B.1)

Let's define the few of the macroscopic quantities appearing in the balance closure based on the statistical mechanical formula as follows:

number density	: $n = \left\langle f\left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t\right) \right\rangle$	(B.2)
density	: $\rho = \langle m f(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t) \rangle$	
momentum	: $\rho \mathbf{u} = \langle m \mathbf{v} f(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t) \rangle$	
energy	: $\rho E_{total} = \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f(\mathbf{v},\mathbf{r},\mathbf{j},\psi,t)\right\rangle$	
stress tesnor	: $\mathbf{P} = \langle m \mathbf{C} \mathbf{C} f(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t) \rangle$	
shear stress tensor	: $\mathbf{\Pi} = \left\langle m [\mathbf{CC}]^{(2)} f(\mathbf{v},\mathbf{r},\mathbf{j},\psi,t) \right\rangle$	
excess normal stress	: $\Delta = \left\langle \left(\frac{1}{3} \operatorname{Tr}(m \mathbf{C} \mathbf{C}) - \frac{p}{n}\right) f(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t) \right\rangle$	
heat flux vector	$: \mathbf{Q} = \left\langle \left(\frac{1}{2}mC^2 + H_{rot} - m\hat{h}\right) \mathbf{C} f\left(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t\right) \right\rangle.$	

Here the peculiar velocity is defined by $\mathbf{C} = \mathbf{v} - \mathbf{u}$. It is imported to note that $(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t)$ are the independent variables, and whereas the peculiar velocity is not independent from space and time. The Boltzmann-Curtiss equation (B.1) can be rewritten in the form of peculiar velocity as,

$$\frac{Df}{Dt} + \mathbf{C}\frac{\partial f}{\partial \mathbf{x}} + \frac{j}{I}\frac{\partial f}{\partial \psi} = C[f, f_1], \tag{B.3}$$

where the substantial time derivative is defined by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \tag{B.4}$$

According to Curtiss [38], the distribution function f does not depend on the azimuthal angle ψ i.e. on the phase of rotational motion, and it depends only weakly on the gas molecule position **r** so that one may neglect this dependence over distance of the order of molecular dimensions.

Mass conservation

Multiplication of Boltzmann-Curtiss equation with $\varphi = m$ and then subsequent integration over velocity space yields

$$\left\langle m\frac{\partial f}{\partial t}\right\rangle + \left\langle m\mathbf{v}\cdot\nabla f\right\rangle + \left\langle m\frac{j}{I}\frac{\partial f}{\partial\psi}\right\rangle = \left\langle mC[f,f_1]\right\rangle$$
(B.5)

Due to conservation of mass collisional integral vanishes, then

$$\left\langle m\frac{\partial f}{\partial t}\right\rangle + \left\langle m\mathbf{v}\cdot\nabla f\right\rangle + \left\langle m\frac{j}{I}\frac{\partial f}{\partial\psi}\right\rangle = 0.$$
 (B.6)

The expression (B.6) can be written as

$$\frac{\partial}{\partial t} \langle mf \rangle + \nabla \cdot \langle m\mathbf{v}f \rangle + \left\langle m\frac{j}{I}\frac{\partial f}{\partial \psi} \right\rangle = 0, \tag{B.7}$$

Using Curtiss's assumption and statistical definition of density and momentum (B.2), the expression (B.7) becomes

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \right) = 0. \tag{B.8}$$

Momentum conservation

Multiplication of Boltzmann-Curtiss equation with $\varphi = m\mathbf{u}$ and subsequent integration over velocity space yields

$$\left\langle m\mathbf{v}\frac{\partial f}{\partial t}\right\rangle + \left\langle m\mathbf{v}\mathbf{v}\cdot\nabla f\right\rangle + \left\langle m\mathbf{v}\frac{j}{I}\frac{\partial f}{\partial\psi}\right\rangle = \left\langle m\mathbf{v}C[f,f_1]\right\rangle.$$
(B.9)

where $\langle m\mathbf{v}C[f, f_1] \rangle = 0$ due to collision invariant property. Since we need to integrate over velocity, therefore we have to convert molecular velocity into peculiar velocity and then bring it with *f* as

$$\frac{\partial}{\partial t} \langle m\mathbf{v}f \rangle + \nabla \cdot \langle m\mathbf{v}\mathbf{v}f \rangle + \left\langle m\mathbf{v}\frac{j}{I}\frac{\partial f}{\partial \psi} \right\rangle = 0$$
(B.10)

Using Curtiss's assumption and $\mathbf{C} = \mathbf{v} - \mathbf{u}$, the above expression (B.10) can be written as

$$\frac{\partial}{\partial t} \langle m \mathbf{v} f \rangle + \nabla \cdot \langle m \mathbf{v} \mathbf{v} f \rangle + 0 = 0$$
(B.11)

where the term $\nabla \cdot \langle m \mathbf{v} \mathbf{v} f \rangle$ can be simplified as

$$\nabla \cdot \langle m\mathbf{v}\mathbf{v}f \rangle = \nabla \cdot \langle m(\mathbf{C} + \mathbf{u})(\mathbf{C} + \mathbf{u})f \rangle$$

$$= \nabla \cdot \langle m\mathbf{C}Cf \rangle + \nabla \cdot \langle m\mathbf{C}\mathbf{u}f \rangle + \nabla \cdot \langle m\mathbf{u}Cf \rangle + \nabla \cdot \langle m\mathbf{u}\mathbf{u}f \rangle$$

$$= \nabla \cdot \langle m\Big[[\mathbf{C}C]^{(2)} - \frac{1}{3} \operatorname{Tr}(\mathbf{C}C)\mathbf{I} \Big]f \rangle + 0 + 0 + \nabla \cdot \langle mf \rangle \mathbf{u}\mathbf{u}$$

$$= \nabla \cdot \langle m[\mathbf{C}C]^{(2)}f \rangle - \nabla \cdot \langle \frac{1}{3} \operatorname{Tr}(m\mathbf{C}C)f \rangle \mathbf{I} + \nabla \cdot (\rho\mathbf{u}\mathbf{u})$$

$$= \nabla \cdot \mathbf{\Pi} - \nabla \cdot \langle \frac{1}{3} \operatorname{Tr}(m\mathbf{C}C)f \rangle \mathbf{I} + \nabla \cdot (\rho\mathbf{u}\mathbf{u})$$

From the statistical definition of excess normal stress (B.2), we have

$$\Delta = \left\langle \left(\frac{1}{3} \operatorname{Tr}(m \operatorname{CC}) - \frac{p}{n}\right) f \right\rangle = \left\langle \frac{1}{3} \operatorname{Tr}(m \operatorname{CC}) f \right\rangle - \frac{p}{n} \left\langle f \right\rangle$$
or
$$\left\langle \frac{1}{3} \operatorname{Tr}(m \operatorname{CC}) f \right\rangle = \Delta + p$$
(B.13)

With help of (B.13), the expression (B.12) can be re-written as

$$\nabla \cdot \langle m\mathbf{v}\mathbf{v}f \rangle = \nabla \cdot \mathbf{\Pi} - \nabla \cdot (\Delta + p)\mathbf{I} + \nabla \cdot (\rho \mathbf{u}\mathbf{u})$$

$$= \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla \cdot ((\Delta + p)\mathbf{I} + \mathbf{\Pi})$$

$$= \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla \cdot \mathbf{P}$$
(B.14)

where the stress tensor **P** is defined by $\mathbf{P} = (\Delta + p)\mathbf{I} + \mathbf{\Pi}$. Using the statistical definition of

momentum and (B.14) in (B.11), finally, we have

$$\frac{\partial}{\partial t}\rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I}) + \nabla \cdot (\mathbf{\Pi} + \Delta \mathbf{I}) = 0.$$
(B.15)

Energy conservation

Multiplication of Boltzmann-Curtiss equation with $\varphi = \left(\frac{1}{2}mC^2 + H_{rot}\right)$ and subsequent

integration over velocity space yields

$$\left\langle \left(\frac{1}{2}mC^{2} + H_{rot}\right)\frac{\partial f}{\partial t} \right\rangle + \left\langle \left(\frac{1}{2}mC^{2} + H_{rot}\right)\mathbf{v}\cdot\nabla f \right\rangle$$

$$+ \left\langle \left(\frac{1}{2}mC^{2} + H_{rot}\right)\frac{j}{I}\frac{\partial f}{\partial\psi} \right\rangle = \left\langle \left(\frac{1}{2}mC^{2} + H_{rot}\right)C[f, f_{1}] \right\rangle.$$

$$(B.16)$$

Using collisional invariant property for conservation of total energy zero i.e. $\left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)C[f, f_1] \right\rangle = 0$ and Curtiss assumption, Eq. (B.16) becomes

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)\mathbf{v} \cdot \nabla f \right\rangle = 0.$$
(B.17)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \left\langle \frac{1}{2}mC^2 \mathbf{v} \cdot \nabla f \right\rangle + \left\langle H_{rot} \mathbf{v} \cdot \nabla f \right\rangle = 0.$$
(B.18)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \left\langle \frac{1}{2}m\mathbf{v}\left(C^2 \cdot \nabla f\right) \right\rangle + \left\langle \mathbf{v}\left(H_{rot} \cdot \nabla f\right) \right\rangle = 0.$$
(B.19)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^{2} + H_{rot}\right)f \right\rangle + \left\langle \frac{1}{2}m\mathbf{v}\nabla\cdot\left(C^{2}f\right) \right\rangle - \left\langle \frac{1}{2}m\mathbf{v}\left(f\cdot\nabla C^{2}\right) \right\rangle + \nabla\cdot\left\langle\mathbf{v}H_{rot}f\right\rangle - \left\langle\mathbf{v}f\left(\nabla\cdot H_{rot}\right)\right\rangle = 0.$$
(B.20)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \nabla \cdot \left\langle \frac{1}{2}m\mathbf{v}C^2f \right\rangle - \left\langle m\mathbf{v}\mathbf{C}f \cdot (\nabla \cdot \mathbf{C}) \right\rangle$$

$$+ \nabla \cdot \left\langle \mathbf{v}H_{rot}f \right\rangle + 0 = 0.$$
(B.21)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \nabla \cdot \left\langle \frac{1}{2}m(\mathbf{C} + \mathbf{u})C^2f \right\rangle$$

$$+ \left\langle m(\mathbf{C} + \mathbf{u})\mathbf{C}f \right\rangle \cdot (\nabla \cdot \mathbf{u}) + \nabla \cdot \left\langle (\mathbf{C} + \mathbf{u})H_{rot}f \right\rangle = 0.$$
(B.22)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}m\mathbf{C}^{2} + H_{rot}\right)f \right\rangle + \nabla \cdot \left\langle \frac{1}{2}m\mathbf{C}\mathbf{C}^{2}f \right\rangle + \nabla \cdot \mathbf{u} \left\langle \frac{1}{2}m\mathbf{C}^{2}f \right\rangle$$

$$+ \left\langle m\mathbf{C}\mathbf{C}f \right\rangle \cdot \left(\nabla \cdot \mathbf{u}\right) + \mathbf{u} \left\langle m\mathbf{C}f \right\rangle \cdot \nabla \mathbf{u} + \nabla \cdot \left\langle \mathbf{C}H_{rot}f \right\rangle + \nabla \cdot \left\langle \mathbf{u}H_{rot}f \right\rangle = 0.$$
(B.23)

$$\frac{\partial}{\partial t} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \nabla \cdot \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)Cf \right\rangle$$

$$+ \nabla \cdot \mathbf{u} \left\langle \left(\frac{1}{2}mC^2 + H_{rot}\right)f \right\rangle + \left\langle m\mathbf{C}\mathbf{C}f \right\rangle \cdot (\nabla \cdot \mathbf{u}) = 0.$$
(B.24)

Since $\langle m\mathbf{C}f \rangle = 0$. Using statistical definition from (B.2), the above equation becomes

$$\frac{\partial}{\partial t} \rho E_{total} + \nabla \cdot \left[\left(\rho E \right) \mathbf{u} + \mathbf{Q} \right] + \mathbf{P} : \nabla \mathbf{u} = 0.$$
(B.25)
or,
$$\frac{\partial}{\partial t} \rho E_{total} + \nabla \cdot \left[\left(\rho E_{total} + p \right) \mathbf{u} \right] + \nabla \cdot \left[\left(\Pi + \Delta \mathbf{I} \right) \cdot \mathbf{u} + \mathbf{Q} \right] = 0.$$

Thus all the conservation law (B.8), (B.15) and (B.25) can be written in compact form as

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E_{total} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} + p \mathbf{I} \\ (\rho E_{total} + p) \mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \mathbf{\Pi} + \Delta \mathbf{I} \\ (\mathbf{\Pi} + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$
(B.26)

Finally, the compact form of all conservation laws (B.26) can be written in terms of substantial time derivative, which are an exact consequence of the Boltzmann-Curtiss equation for diatomic and polyatomic gases, as

$$\rho \frac{D}{Dt} \begin{bmatrix} 1/\rho \\ \mathbf{u} \\ E_{total} \end{bmatrix} + \nabla \cdot \begin{bmatrix} -\mathbf{u} \\ p\mathbf{I} \\ p\mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \mathbf{\Pi} + \Delta \mathbf{I} \\ (\mathbf{\Pi} + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$
(B.26)

Appendix C. Derivation of constitutive equations from Boltzmann-Curtiss kinetic equation

In this appendix, the constitutive equations for diatomic and polyatomic gases are derived from the Botlzmann-Cutiss kinetic equations. In the case of the original Boltzmann-Curtiss kinetic equation of a monatomic gas, the derivation of constitutive equations can be found in orgional Eu's work [1] and in Myong's work [54, 60]. The general evolution equation for diatomic and polyatomic gases can be deduced from Boltzmann-Curtiss kinetic equation (3.11) as found in [3, 5, 39] written as

$$\rho \frac{D}{Dt} \hat{\psi}^{(n)} + \nabla \cdot \Psi^{(n)} - Z^{(n)} = \Lambda^{(n)}, \qquad (C.1)$$

where $\Psi^{(n)}$, the flux of $\langle \psi^{(n)} f \rangle$, denotes the high-order moments, $Z^{(n)}$ represents the kinematic term arising from hydrodynamic streaming effect and $\Lambda^{(n)}$ is the dissipation term which accounts for energy dissipation accompanying the irreversible process. These terms are defined by

$$\hat{\psi}^{(n)} = \frac{\left\langle \psi^{(n)} f \right\rangle}{\rho}, \quad \Psi^{(n)} = \left\langle \mathbf{C} \psi^{(n)} f \right\rangle,$$

$$Z^{(n)} = \left\langle f \left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right) \psi^{(n)} \right\rangle,$$

$$\Lambda^{(n)} = \left\langle \psi^{(n)} C[f, f_1] \right\rangle.$$
(C.2)

Shear stress balance equation

For $\psi^{(1)} = m [\mathbf{CC}]^{(2)}$, where *m* is the mass of gas molecule and $[]^{(2)}$ denotes the traceless symmetric part, the constitutive equation for shear stress tensor $\mathbf{\Pi} = \langle m [\mathbf{CC}]^{(2)} f \rangle$ can be derived from the general evolution equation (C.1):

$$\rho \frac{D}{Dt} \hat{\psi}^{(1)} + \nabla \cdot \Psi^{(1)} - Z^{(1)} = \Lambda^{(1)}, \qquad (C.3)$$

which can be written as

$$\rho \frac{D}{Dt} \left(\frac{\Pi}{\rho} \right) + \nabla \cdot \Psi^{(\Pi)} - Z^{(\Pi)} = \Lambda^{(\Pi)}.$$
(C.4)

The kinematic term $Z^{(\Pi)}$ can be simplified as

$$Z^{(\mathbf{II})} = \left\langle f\left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) \psi^{(1)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} \psi^{(1)} \right\rangle + \left\langle f \mathbf{C} \cdot \nabla \psi^{(1)} \right\rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} \psi^{(1)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} m[\mathbf{CC}] \right\rangle + \left\langle f \mathbf{C} \cdot \nabla m[\mathbf{CC}] \right\rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} m[\mathbf{CC}] \right\rangle$$

$$= -2 \left[\mathbf{J} \frac{D\mathbf{u}}{Dt} \right] - 2(p + \Delta) [\nabla \mathbf{u}]^{(2)} - 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 0.$$
(C.5)
(C.5)

where $\mathbf{J} = \langle m\mathbf{C}f \rangle$ denotes the diffusion flux which can be neglected for single species relation [1] i.e. $\mathbf{J} = \langle m\mathbf{C}f \rangle = 0$. Then the constitutive relation for shear stress tensor can be written as

$$\rho \frac{D}{Dt} \left(\frac{\Pi}{\rho} \right) + \nabla \cdot \Psi^{(\Pi)} + 2(\rho + \Delta) [\nabla \mathbf{u}]^{(2)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} = \Lambda^{(\Pi)}.$$
(C.6)

Excess normal stress balance equation

For $\psi^{(2)} = mC^2/3 - p/n$, where *n* is the number density, the constitutive equation for excess normal stress $\Delta = \langle (mC^2/3 - p/n)f \rangle$ can be derived from the general evolution equation (C.1):

$$\rho \frac{D}{Dt} \hat{\psi}^{(2)} + \nabla \cdot \Psi^{(2)} - Z^{(2)} = \Lambda^{(2)}, \qquad (C.7)$$

which can be written as

$$\rho \frac{D}{Dt} \left(\frac{\Delta}{\rho} \right) + \nabla \cdot \Psi^{(\Delta)} - Z^{(\Delta)} = \Lambda^{(\Delta)}.$$
(C.8)

Here the kinematic term for excess normal stress, $Z^{(\Delta)}$ can be simplified as

$$Z^{(\Delta)} = \left\langle f\left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) \psi^{(2)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} \psi^{(2)} \right\rangle + \left\langle f \mathbf{C} \cdot \nabla \psi^{(2)} \right\rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} \psi^{(2)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} \left(\frac{1}{3}mC^{2} - \frac{p}{n}\right) \right\rangle + \left\langle f \mathbf{C} \cdot \nabla \left(\frac{1}{3}mC^{2} - \frac{p}{n}\right) \right\rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} \left(\frac{1}{3}mC^{2} - \frac{p}{n}\right) \right\rangle$$
(C.9)
(C.9)

which can be simplified based on Eu [1, 6]

$$Z^{(\Delta)} = -2\gamma' \left(\mathbf{\Pi} + \Delta \mathbf{I} \right) : \nabla \mathbf{u} - \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u}$$
(C.10)

Thus the constitutive relation for excess normal stress may be written as

$$\rho \frac{D}{Dt} \left(\frac{\Delta}{\rho} \right) + \nabla \cdot \Psi^{(\Delta)} + 2\gamma' \left(\mathbf{\Pi} + \Delta \mathbf{I} \right) : \nabla \mathbf{u} + \frac{2}{3} \gamma' p \nabla \cdot \mathbf{u} = \Lambda^{(\Delta)}.$$
(C.11)

Heat balance equation

For $\psi^{(3)} = \left(mC^2/2 + H_{rot} - m\hat{h} \right) \mathbf{C}$, where H_{rot} , \hat{h} denote the rotational Hamiltonian of the molecule and the enthalpy density per unit mass, respectively, the constitutive equation for heat flux vector $\mathbf{Q} = \left\langle \left(mC^2/2 + H_{rot} - m\hat{h} \right) \mathbf{C}f \right\rangle$ can be derived from the general evolution equation (C.1):

$$\rho \frac{D}{Dt} \hat{\psi}^{(3)} + \nabla \cdot \Psi^{(3)} - Z^{(3)} = \Lambda^{(3)}, \qquad (C.12)$$

which can be written as

$$\rho \frac{D}{Dt} \left(\frac{\mathbf{Q}}{\rho} \right) + \nabla \cdot \boldsymbol{\Psi}^{(\mathbf{Q})} - \boldsymbol{Z}^{(\mathbf{Q})} = \boldsymbol{\Lambda}^{(\mathbf{Q})}.$$
(C.13)

Here the kinematic term for heat flux vector $Z^{(Q)}$ can be simplified (for this purpose, reader may be referred reference [3]) as,

$$Z^{(\mathbf{Q})} = \left\langle f\left(\frac{D}{Dt} + \mathbf{C} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi}\right) \psi^{(3)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} \psi^{(3)} \right\rangle + \left\langle f \mathbf{C} \cdot \nabla \psi^{(3)} \right\rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} \psi^{(3)} \right\rangle$$

$$= \left\langle f \frac{D}{Dt} \left(\frac{1}{2}mC^{2} + H_{rot} - m\hat{h}\right) \mathbf{C} \right\rangle + \left\langle f \mathbf{C} \cdot \nabla \left(\frac{1}{2}mC^{2} + H_{rot} - m\hat{h}\right) \mathbf{C} \right\rangle$$

$$+ \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} \left(\frac{1}{2}mC^{2} + H_{rot} - m\hat{h}\right) \mathbf{C} \right\rangle$$

$$= -\psi^{(P)} : \nabla \mathbf{u} - \frac{d\mathbf{u}}{dt} \cdot (\mathbf{\Pi} + \Delta \mathbf{I}) - (p + \Delta)C_{p}\nabla T - \mathbf{\Pi} \cdot C_{p}\nabla T - \mathbf{Q} \cdot \nabla \mathbf{u}.$$

$$(C.14)$$

Thus the constitutive relation for heat flux vector may be written as

$$\rho \frac{D}{Dt} \left(\frac{\mathbf{Q}}{\rho} \right) + \nabla \cdot \Psi^{(\mathbf{Q})} + \psi^{(p)} : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot \left(\mathbf{\Pi} + \Delta \mathbf{I} \right)$$

$$+ \left(p + \Delta \right) C_p \nabla T + \mathbf{\Pi} \cdot C_p \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} = \Lambda^{(\mathbf{Q})}.$$
(C.15)

Finally, the constitutive equations, all of which are an exact consequence of the Boltzmann-Curtiss equation, can be expressed in compact form:

$$\rho \frac{D}{Dt} \begin{bmatrix} \mathbf{\Pi} / \rho \\ \Delta / \rho \\ \mathbf{Q} / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(\Delta)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} + \begin{bmatrix} 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} \\ 2\gamma'(\mathbf{\Pi} + \Delta \mathbf{I}) : \nabla \mathbf{u} \\ \psi^{(P)} : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot (\mathbf{\Pi} + \Delta \mathbf{I}) + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T \end{bmatrix} + \begin{bmatrix} 2(p + \Delta)[\nabla \mathbf{u}]^{(2)} \\ \frac{2}{3}\gamma' p \nabla \cdot \mathbf{u} \\ C_p (p + \Delta) \nabla T \end{bmatrix} = \begin{bmatrix} \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{\Lambda}^{(\Delta)} \\ \mathbf{\Lambda}^{(Q)} \end{bmatrix}.$$
(C.16)

Appendix D. Three-dimensional form of secondorder Boltzmann-Curtiss based constitutive equations

In this appendix, the second-order Botlzmann-Curtiss based consituitve equations for diatomic and polyatomic gases which are developed by Myong [39, 54, 60, 65] based on original Eu's work [1, 3] and Myong's balance closure [54] are expanded into fully three-dimensional form. The second order Boltzmann-Curtiss based constitutive equations (3.54) are given by

$$\hat{\boldsymbol{\Pi}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \left(1 + f_{bulk}\hat{\boldsymbol{\Delta}}\right)\hat{\boldsymbol{\Pi}}_{1st} + [\hat{\boldsymbol{\Pi}}\cdot\nabla\hat{\boldsymbol{u}}]^{(2)}, \qquad (D.1)$$

$$\hat{\boldsymbol{\Delta}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \hat{\boldsymbol{\Delta}}_{1st} + \frac{3}{2}f_{bulk}\left(\hat{\boldsymbol{\Pi}} + f_{bulk}\hat{\boldsymbol{\Delta}}\boldsymbol{I}\right):\nabla\hat{\boldsymbol{u}},$$

$$\hat{\boldsymbol{Q}}q_{2nd}\left(c\hat{\boldsymbol{R}}\right) = \left(1 + f_{bulk}\hat{\boldsymbol{\Delta}}\right)\hat{\boldsymbol{Q}}_{1st} + \hat{\boldsymbol{\Pi}}\cdot\hat{\boldsymbol{Q}}_{1st} + \frac{1}{2\Pr}\hat{\boldsymbol{Q}}\cdot\nabla\hat{\boldsymbol{u}}.$$

where $\hat{\Pi}_{lst}$, $\hat{\Delta}_{lst}$, and $\hat{\mathbf{Q}}_{lst}$ are calculated by the Newtonian law of shear and bulk viscosity and the Fourier of heat conduction, respectively,

$$\begin{aligned} \mathbf{\Pi}_{\text{ist}} &= -2\mu \left[\nabla \mathbf{u} \right]^{(2)}, \\ \Delta_{\text{ist}} &= -\mu_{\text{bulk}} \nabla \cdot \mathbf{u} = -f_{\text{bulk}} \mu \nabla \cdot \mathbf{u}, \\ \mathbf{Q}_{\text{ist}} &= -\kappa \nabla T. \end{aligned}$$
(D.2)

Defining the proper parameters such as

$$\hat{\boldsymbol{\Pi}} = \frac{N_{\delta}}{p} \boldsymbol{\Pi}, \ \hat{\boldsymbol{\Delta}} = \frac{N_{\delta}}{p} \boldsymbol{\Delta}, \ \hat{\boldsymbol{Q}} = \frac{N_{\delta}}{p} \frac{\boldsymbol{Q}}{\sqrt{(T/2\varepsilon)}}, \nabla \hat{\boldsymbol{u}} = -2\mu \frac{N_{\delta}}{p} \nabla \boldsymbol{u},$$

$$\varepsilon = \frac{1}{\Pr Ec} \frac{\Delta T_{ref}}{T_{ref}}, \ q(cR) = \frac{\sinh(c\hat{R})}{c\hat{R}}, \ \hat{R}^{2} = \hat{\boldsymbol{\Pi}} : \hat{\boldsymbol{\Pi}} + \frac{2\gamma'}{f_{bulk}} \hat{\boldsymbol{\Delta}}^{2} + \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{Q}}$$
(D.3)

Since, $\nabla \hat{\mathbf{u}} = -2\mu \frac{N_{\delta}}{p} \nabla \mathbf{u}$ leads to $\nabla \mathbf{u} = \left(-\frac{1}{2\mu}\right) \frac{p}{N_{\delta}} \nabla \hat{\mathbf{u}}$. Thus we get the stress tensor in

the following form
$$\hat{\boldsymbol{\Pi}}_{lst} = \left[\nabla \hat{\boldsymbol{u}}\right]^{(2)}.\tag{D.4}$$

Therefore, the constitute relation (D.1) becomes

$$\hat{\boldsymbol{\Pi}}_{\text{2nd}} q\left(c\hat{R}\right) = \left(1 + f_{bulk} \,\hat{\Delta}\right) \left[\nabla \hat{\boldsymbol{u}}\right]^{(2)} + \left[\hat{\boldsymbol{\Pi}} \cdot \nabla \hat{\boldsymbol{u}}\right]^{(2)}, \qquad (D.5)$$

$$\hat{\Delta}_{\text{2nd}} q\left(c\hat{R}\right) = \hat{\Delta}_{1\text{st}} + \frac{3}{2} f_{bulk} \left(\hat{\boldsymbol{\Pi}} + f_{bulk} \,\hat{\Delta}I\right) : \nabla \hat{\boldsymbol{u}},$$

$$\hat{\boldsymbol{Q}}_{\text{2nd}} q\left(c\hat{R}\right) = \left(1 + f_{bulk} \,\hat{\Delta}\right) \hat{\boldsymbol{Q}}_{1\text{st}} + \hat{\boldsymbol{\Pi}} \cdot \hat{\boldsymbol{Q}}_{1\text{st}} + \frac{1}{2 \operatorname{Pr}} \hat{\boldsymbol{Q}} \cdot \nabla \hat{\boldsymbol{u}}.$$

Since,

$$\Delta_{1st} = -f_{bulk} \ \mu \nabla \cdot \mathbf{u} = -f_{bulk} \ \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \tag{D.6}$$
or
$$\Delta_{1st} = -f_{bulk} \ \mu \left(-\frac{1}{2\mu} \right) \frac{p}{N_{\delta}} \left(\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} \right),$$
or
$$\frac{p}{N_{\delta}} \Delta_{1st} = \frac{f_{bulk}}{2} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right),$$

Thus, the excess normal can be represented as

$$\hat{\Delta}_{1st} = \frac{f_{bulk}}{2} \left(\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} \right), \tag{D.7}$$

The traceless symmetric part of $\nabla \mathbf{u}$ i.e. $[\nabla \mathbf{u}]^{(2)}$ can be expressed in tensor form as

$$\left[\nabla \mathbf{u}\right]^{(2)} = \frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = \frac{1}{2} \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}.$$
 (D.8)

Then its components are defined, after simplification as

$$\begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{xx}^{(2)} = \frac{2}{3} \frac{\partial u}{\partial x} - \frac{1}{3} \left(\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \quad \begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{yy}^{(2)} = \frac{2}{3} \frac{\partial v}{\partial y} - \frac{1}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right),$$
(D.9)
$$\begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{zz}^{(2)} = \frac{2}{3} \frac{\partial w}{\partial z} - \frac{1}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right), \quad \begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{xy}^{(2)} = \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right),$$
$$\begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{xz}^{(2)} = \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right), \quad \begin{bmatrix} \nabla \mathbf{u} \end{bmatrix}_{yz}^{(2)} = \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right),$$

The traceless symmetric part of coupling between shear stress and velocity gradient

 $\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)}$ can be expressed as,

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{xx}^{(2)} = \left(\Pi_{xx} \frac{\partial u}{\partial x} + \Pi_{xy} \frac{\partial u}{\partial y} + \Pi_{xz} \frac{\partial u}{\partial z} \right) - \alpha,$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{yy}^{(2)} = \left(\Pi_{yx} \frac{\partial v}{\partial x} + \Pi_{yy} \frac{\partial v}{\partial y} + \Pi_{yz} \frac{\partial v}{\partial z} \right) - \alpha,$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{zz}^{(2)} = \left(\Pi_{zx} \frac{\partial w}{\partial x} + \Pi_{zy} \frac{\partial u}{\partial y} + \Pi_{zz} \frac{\partial w}{\partial z} \right) - \alpha,$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{xy}^{(2)} = \frac{1}{2} \left(\Pi_{xx} \frac{\partial v}{\partial x} + \Pi_{xy} \frac{\partial u}{\partial x} + \Pi_{yx} \frac{\partial v}{\partial y} + \Pi_{yy} \frac{\partial u}{\partial y} + \Pi_{zx} \frac{\partial v}{\partial z} + \Pi_{zy} \frac{\partial u}{\partial z} \right),$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{xz}^{(2)} = \frac{1}{2} \left(\Pi_{xx} \frac{\partial w}{\partial x} + \Pi_{xz} \frac{\partial u}{\partial x} + \Pi_{xy} \frac{\partial w}{\partial y} + \Pi_{yz} \frac{\partial u}{\partial y} + \Pi_{xz} \frac{\partial w}{\partial z} + \Pi_{zz} \frac{\partial u}{\partial z} \right),$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{xz}^{(2)} = \frac{1}{2} \left(\Pi_{xx} \frac{\partial w}{\partial x} + \Pi_{xz} \frac{\partial v}{\partial x} + \Pi_{yy} \frac{\partial w}{\partial y} + \Pi_{yz} \frac{\partial v}{\partial y} + \Pi_{zz} \frac{\partial w}{\partial z} + \Pi_{zz} \frac{\partial u}{\partial z} \right),$$

$$\left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]_{yz}^{(2)} = \frac{1}{2} \left(\Pi_{xy} \frac{\partial w}{\partial x} + \Pi_{xz} \frac{\partial v}{\partial x} + \Pi_{yy} \frac{\partial w}{\partial y} + \Pi_{yz} \frac{\partial v}{\partial y} + \Pi_{yz} \frac{\partial w}{\partial z} + \Pi_{zz} \frac{\partial v}{\partial z} \right),$$

where

$$\alpha = \frac{1}{3} \left[\Pi_{xx} \frac{\partial u}{\partial x} + \Pi_{xy} \frac{\partial v}{\partial x} + \Pi_{xz} \frac{\partial w}{\partial x} + \Pi_{yx} \frac{\partial u}{\partial y} + \Pi_{yy} \frac{\partial v}{\partial y} + \Pi_{yz} \frac{\partial w}{\partial y} + \Pi_{zz} \frac{\partial w}{\partial z} + \Pi_{zz} \frac{\partial w}{\partial z} \right].$$
(D.11)

Therefore, the full expended component-wise form of second order Boltzmann-Curtiss based constitutive relations for diatomic gas is given by

$$\hat{\Pi}_{xx} q_{2nd} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \left[\frac{2}{3} \frac{\partial \hat{u}}{\partial x} - \frac{1}{3} \left(\frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} \right) \right] +$$

$$\left(\hat{\Pi}_{xx} \frac{\partial \hat{u}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial \hat{u}}{\partial y} + \hat{\Pi}_{xz} \frac{\partial \hat{u}}{\partial z} \right) - \hat{\alpha},$$

$$\hat{\Pi}_{xx} q_{2nd} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \left[\frac{2}{3} \frac{\partial \hat{u}}{\partial x} - \frac{1}{3} \left(\frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} \right) \right] +$$

$$\left(\hat{\Pi}_{xx} \frac{\partial \hat{u}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial \hat{u}}{\partial y} + \hat{\Pi}_{xz} \frac{\partial \hat{u}}{\partial z} \right) - \hat{\alpha},$$

$$(D.12b)$$

$$\hat{\Pi}_{zz} q_{2nd} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \left[\frac{2}{3} \frac{\partial \hat{w}}{\partial z} - \frac{1}{3} \left(\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} \right) \right] + \left(\hat{\Pi}_{zx} \frac{\partial w}{\partial x} + \hat{\Pi}_{zy} \frac{\partial w}{\partial y} + \hat{\Pi}_{zz} \frac{\partial w}{\partial z} \right) - \hat{\alpha},$$
(D.12c)

$$\hat{\Pi}_{xy} q_{2nd} \left(c\hat{R} \right) = \frac{1}{2} \left(1 + f_{bulk} \hat{\Delta} \right) \left(\frac{\partial \hat{u}}{\partial y} + \frac{\partial \hat{v}}{\partial x} \right) +$$

$$\frac{1}{2} \left(\hat{\Pi}_{xx} \frac{\partial \hat{v}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial \hat{u}}{\partial x} + \hat{\Pi}_{yx} \frac{\partial \hat{v}}{\partial y} + \hat{\Pi}_{yy} \frac{\partial \hat{u}}{\partial y} + \hat{\Pi}_{zx} \frac{\partial \hat{v}}{\partial z} + \hat{\Pi}_{zy} \frac{\partial \hat{u}}{\partial z} \right),$$

$$\hat{\Pi}_{xz} q_{2nd} \left(c\hat{R} \right) = \frac{1}{2} \left(1 + f_{bulk} \hat{\Delta} \right) \left(\frac{\partial \hat{u}}{\partial z} + \frac{\partial \hat{w}}{\partial x} \right) +$$

$$\frac{1}{2} \left(\hat{\Pi}_{xx} \frac{\partial \hat{w}}{\partial x} + \hat{\Pi}_{xz} \frac{\partial \hat{u}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial \hat{w}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial \hat{u}}{\partial y} + \hat{\Pi}_{xz} \frac{\partial \hat{w}}{\partial z} + \hat{\Pi}_{zz} \frac{\partial \hat{u}}{\partial z} \right),$$
(D.12e)
$$(D.12e)$$

$$\hat{\Pi}_{yz} q_{2nd} \left(c\hat{R} \right) = \frac{1}{2} \left(1 + f_{bulk} \hat{\Delta} \right) \left(\frac{\partial \hat{v}}{\partial z} + \frac{\partial \hat{w}}{\partial y} \right) +$$

$$\frac{1}{2} \left(\hat{\Pi}_{xy} \frac{\partial \hat{w}}{\partial x} + \hat{\Pi}_{xz} \frac{\partial \hat{v}}{\partial x} + \hat{\Pi}_{yy} \frac{\partial \hat{w}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial \hat{v}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial \hat{w}}{\partial z} + \hat{\Pi}_{zz} \frac{\partial \hat{v}}{\partial z} \right),$$
(D.12f)

$$\hat{\Delta}q_{2nd}\left(c\hat{R}\right) = \frac{f_{bulk}}{2} \left(\frac{\partial\hat{u}}{\partial x} + \frac{\partial\hat{v}}{\partial y} + \frac{\partial\hat{w}}{\partial z}\right) +$$

$$\frac{3}{2} f_{bulk} \left[\left(\hat{\Pi}_{xx} + f_{bulk} \hat{\Delta}\right) \frac{\partial\hat{u}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial\hat{u}}{\partial y} + \hat{\Pi}_{xz} \frac{\partial\hat{u}}{\partial z} \right] +$$

$$\frac{3}{2} f_{bulk} \left[\hat{\Pi}_{xy} \frac{\partial\hat{v}}{\partial x} + \left(\hat{\Pi}_{yy} + f_{bulk} \hat{\Delta}\right) \frac{\partial\hat{v}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial\hat{v}}{\partial z} \right] +$$

$$\frac{3}{2} f_{bulk} \left[\hat{\Pi}_{xz} \frac{\partial\hat{w}}{\partial x} + \hat{\Pi}_{yz} \frac{\partial\hat{w}}{\partial y} + \left(\hat{\Pi}_{zz} + f_{bulk} \hat{\Delta}\right) \frac{\partial\hat{w}}{\partial z} \right] +$$

$$\hat{Q}_{x} q_{2\mathrm{nd}} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \hat{Q}_{x_{\mathrm{ist}}} + \left(\hat{\Pi}_{xx} \hat{Q}_{x_{\mathrm{ist}}} + \hat{\Pi}_{xy} \hat{Q}_{y_{\mathrm{ist}}} + \hat{\Pi}_{xz} \hat{Q}_{z_{\mathrm{lst}}} \right) + \qquad (\mathrm{D.12h})$$

$$\frac{1}{2 \mathrm{Pr}} \left(\hat{Q}_{x} \frac{\partial \hat{u}}{\partial x} + \hat{Q}_{y} \frac{\partial \hat{u}}{\partial y} + \hat{Q}_{z} \frac{\partial \hat{u}}{\partial z} \right),$$

$$\hat{Q}_{y} q_{2\mathrm{nd}} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \hat{Q}_{y_{\mathrm{ist}}} + \left(\hat{\Pi}_{xy} \hat{Q}_{x_{\mathrm{ist}}} + \hat{\Pi}_{yy} \hat{Q}_{y_{\mathrm{lst}}} + \hat{\Pi}_{yz} \hat{Q}_{z_{\mathrm{lst}}} \right) + \qquad (\mathrm{D.12h})$$

$$\frac{1}{2\Pr}\left(\hat{Q}_x\frac{\partial\hat{v}}{\partial x}+\hat{Q}_y\frac{\partial\hat{v}}{\partial y}+\hat{Q}_z\frac{\partial\hat{v}}{\partial z}\right),$$

$$\hat{Q}_{z} q_{2nd} \left(c\hat{R} \right) = \left(1 + f_{bulk} \hat{\Delta} \right) \hat{Q}_{z_{1st}} + \left(\hat{\Pi}_{xz} \hat{Q}_{x_{1st}} + \hat{\Pi}_{yz} \hat{Q}_{y_{1st}} + \hat{\Pi}_{zz} \hat{Q}_{z_{1st}} \right) +$$

$$\frac{1}{2 \operatorname{Pr}} \left(\hat{Q}_{x} \frac{\partial \hat{w}}{\partial x} + \hat{Q}_{y} \frac{\partial \hat{w}}{\partial y} + \hat{Q}_{z} \frac{\partial \hat{w}}{\partial z} \right).$$
(D.12j)

Here,

$$\hat{Q}_{x_{\text{lst}}} = -\kappa \frac{\partial \hat{T}}{\partial x}, \quad \hat{Q}_{y_{\text{lst}}} = -\kappa \frac{\partial \hat{T}}{\partial y}, \quad \hat{Q}_{z_{\text{lst}}} = -\kappa \frac{\partial \hat{T}}{\partial z}, \quad (D.13)$$

$$\begin{split} \hat{R}^{2} &= \hat{\Pi} : \hat{\Pi} + \frac{2\gamma'}{f_{bulk}} \hat{\Delta}^{2} + \hat{Q} \cdot \hat{Q} \\ &= \hat{\Pi}_{xx}^{2} + \hat{\Pi}_{yy}^{2} + \hat{\Pi}_{zz}^{2} + 2\left(\hat{\Pi}_{xy}^{2} + \hat{\Pi}_{xz}^{2} + \hat{\Pi}_{yz}^{2}\right) + \frac{2\gamma'}{f_{bulk}} \hat{\Delta}^{2} + \left(Q_{x}^{2} + Q_{y}^{2} + Q_{z}^{2}\right) \\ &= 2\left(\hat{\Pi}_{xx}^{2} + \hat{\Pi}_{yy}^{2} + \hat{\Pi}_{xx} \hat{\Pi}_{yy} + \hat{\Pi}_{xy}^{2} + \hat{\Pi}_{xz}^{2} + \hat{\Pi}_{yz}^{2}\right) + \frac{2\gamma'}{f_{bulk}} \hat{\Delta}^{2} + \left(Q_{x}^{2} + Q_{y}^{2} + Q_{z}^{2}\right), \\ &\text{since } \hat{\Pi}_{zz} = -\left(\hat{\Pi}_{xx} + \hat{\Pi}_{yy}\right), \end{split}$$
(D.14)

$$\hat{\alpha} = \frac{1}{3} [\hat{\Pi}_{xx} \frac{\partial \hat{u}}{\partial x} + \hat{\Pi}_{xy} \frac{\partial \hat{v}}{\partial x} + \hat{\Pi}_{xz} \frac{\partial \hat{w}}{\partial x} + \hat{\Pi}_{yx} \frac{\partial \hat{u}}{\partial y} + \hat{\Pi}_{yy} \frac{\partial \hat{v}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial \hat{w}}{\partial y} + \hat{\Pi}_{yz} \frac{\partial \hat{w}}{\partial y} + \hat{\Pi}_{zz} \frac{\partial \hat{w}}{\partial z} + \hat{\Pi}_{zz} \frac{\partial \hat{w}}{\partial z}].$$
(D.15)

Appendix E. Quadrature points for numerical integration

In this appendix, the quadrature points for numberical integration are provided in one-, two- and three-dimensional spaces [109, 110, 165].

Order (p)	Points (N_q)	ξ	\mathcal{O}
1	1	0.00000000000000000	2.00000000000000000
2	2	-0.5773502691896257	1.0000000000000000
		0.5773502691896257	1.0000000000000000
3	3	-0.7745966692414834	0.555555555555555556
		0.00000000000000000	0.8888888888888888888888888888888888888
		0.7745966692414834	0.55555555555555556
4	4	-0.8611363115940526	0.3478548451374538
		-0.3399810435848563	0.6521451548625461
		0.3399810435848563	0.6521451548625461
		0.8611363115940526	0.3478548451374538
5	5	-0.9061798459386640	0.2369268850561891
		-0.5384693101056831	0.4786286704993665
		0.00000000000000000	0.5688888888888888889
		0.5384693101056831	0.4786286704993665
		0.9061798459386640	0.2369268850561891
6	6	-0.9324695142031521	0.1713244923791704
		-0.6612093864662645	0.3607615730481386
		-0.2386191860831969	0.4679139345726910
		0.2386191860831969	0.4679139345726910
		0.6612093864662645	0.3607615730481386
		0.9324695142031521	0.1713244923791704

Table E.1: Gaussian quadrature points and weights for line in [-1, 1] space

Table E.2: Gaussian quadrature points and weights for line in [0, 1] space

Order (p)	Points (N_q)	ξ	ω
1	1	0.50000000000000000	1.00000000000000000
2	2	0.2113248654051871	0.50000000000000000
		0.7886751345948129	0.50000000000000000
3	3	0.1127016653792583	0.27777777777777778
		0.50000000000000000	0.4444444444444444
		0.8872983346207417	0.27777777777777778
4	4	0.0694318442029737	0.1739274225687269
		0.3300094782075719	0.3260725774312731
		0.6699905217924281	0.3260725774312731
		0.9305681557970263	0.1739274225687269
5	5	0.0469100770306680	0.1184634425280945
		0.0230765344947158	0.2393143352496832
		0.50000000000000000	0.2844444444444444
		0.7692346550528415	0.2393143352496832
		0.9530899229693319	0.1184634425280945

Order (p)	Points (N_q)	ξ	η	ω
1	1	0.33333333333333333	0.33333333333333333	1.00000000000000
2	3	0.166666666666667	0.166666666666667	0.3333333333333333
		0.66666666666666	0.16666666666667	0.33333333333333333
		0.16666666666666	0.666666666666667	0.3333333333333333
3	4	0.200000000000000	0.20000000000000	0.520833333333333
		0.600000000000000	0.20000000000000	0.520833333333333
		0.200000000000000	0.600000000000000	0.520833333333333
		0.33333333333333333	0.33333333333333333	-0.562500000000
4	6	0.09157621350977	0.09157621350977	0.10995174365532
		0.44594849091597	0.10810301816807	0.22338158967801
		0.81684757298046	0.09157621350977	0.10995174365532
		0.44594849091597	0.44594849091597	0.22338158967801
		0.09157621350977	0.81684757298046	0.10995174365532
		0.10810301816807	0.44594849091597	0.22338158967801
5	7	0.10128650732346	0.10128650732346	0.12593918054483
		0.47014206410511	0.05971587178977	0.13239415278851
		0.79742698535309	0.10128650732346	0.12593918054483
		0.47014206410511	0.47014206410511	0.13239415278851
		0.10128650732346	0.79742698535309	0.12593918054483
		0.05971587178977	0.47014206410511	0.13239415278851
		0.33333333333333333	0.33333333333333333	0.2250000000000
6	12	0.06308901449150	0.06308901449150	0.05084490637021
		0.31035245103378	0.05314504984482	0.08285107561837
		0.63650249912140	0.05314504984482	0.08285107561837
		0.87382197101700	0.06308901449150	0.05084490637021
		0.63650249912140	0.31035245103378	0.08285107561837
		0.31035245103378	0.63650249912140	0.08285107561837
		0.06308901449150	0.87382197101700	0.05084490637021
		0.05314504984482	0.63650249912140	0.08285107561837
		0.05314504984482	0.31035245103378	0.08285107561837
		0.24928674517091	0.24928674517091	0.11678627572638
		0.50142650965818	0.24928674517091	0.11678627572638
		0.24928674517091	0.50142650965818	0.11678627572638
7	13	0.06513010290222	0.06513010290222	0.05334723560884
		0.31286549600487	0.04869031542532	0.07711376089026
		0.63844418856981	0.04869031542532	0.07711376089026
		0.86973979419557	0.06513010290222	0.05334723560884
		0.63844418856981	0.31286549600487	0.07711376089026
		0.31286549600487	0.63844418856981	0.07711376089026
		0.06513010290222	0.86973979419557	0.07711376089026
		0.04869031542532	0.63844418856981	0.07711376089026
		0.04869031542532	0.31286549600487	0.05334723560884
		0.26034596607904	0.26034596607904	0.17561525743321
		0.47930806784192	0.26034596607904	0.17561525743321
		0.26034596607904	0.47930806784192	0.17561525743321
		0.3333333333333333333	0.333333333333333333	-0.1495700444677

Table E.3: Symmetric quadrature points and weights for triangle in [0, 1]² space

p	N_q	ξ	η	ζ	ω
1	1	0.25000000000	0.2500000000000	0.250000000000	1.000000000000000
2	4	0.585410196624	0.1381966011250	0.1381966011250	0.25000000000000
		0.138196601125	0.5854101966249	0.1381966011250	0.25000000000000
		0.138196601125	0.1381966011250	0.5854101966249	0.25000000000000
		0.138196601125	0.1381966011250	0.1381966011250	0.25000000000000
3	5	0.25000000000	0.250000000000	0.250000000000	-0.8000000000000
		0.50000000000	0.1666666666666	0.1666666666666	0.45000000000000
		0.166666666666	0.1666666666666	0.1666666666666	0.45000000000000
		0.166666666666	0.1666666666666	0.5000000000000	0.45000000000000
		0.166666666666	0.5000000000000	0.1666666666666	0.45000000000000
4	10	0.568430584196	0.1438564719343	0.1438564719343	0.21776506988041
		0.143856471934	0.1438564719343	0.1438564719343	0.21776506988041
		0.143856471934	0.1438564719343	0.5684305841968	0.21776506988041
		0.143856471934	0.5684305841968	0.1438564719343	0.21776506988041
		0.000000000000	0.50000000000000	0.5000000000000	0.02148995341306
		0.500000000000	0.00000000000000	0.5000000000000	0.02148995341306
		0.500000000000	0.5000000000000	0.00000000000000	0.02148995341306
		0.500000000000	0.00000000000000	0.00000000000000	0.02148995341306
		0.000000000000	0.50000000000000	0.00000000000000	0.02148995341306
		0.000000000000	0.0000000000000	0.5000000000000	0.02148995341306
5	11	0.25000000000	0.2500000000000	0.2500000000000	-0.0789333333333
		0.785714285714	0.0714285714285	0.0714285714285	0.045733333333333
		0.071428571428	0.0714285714285	0.0714285714285	0.045733333333333
		0.071428571428	0.0714285714285	0.7857142857142	0.045733333333333
		0.071428571428	0.7857142857142	0.0714285714285	0.045733333333333
		0.100596423833	0.3994035761668	0.3994035761668	0.149333333333333
		0.399403576166	0.1005964238332	0.3994035761668	0.149333333333333
		0.399403576166	0.3994035761668	0.1005964238332	0.149333333333333
		0.399403576166	0.1005964238332	0.1005964238332	0.149333333333333
		0.100596423833	0.3994035761668	0.1005964238332	0.149333333333333
		0.100596423833	0.1005964238330	0.3994035761668	0.14933333333333
6	15	0.250000000000	0.2500000000000	0.250000000000	0.18170206858254
		0.0000000000000	0.3333333333333333	0.3333333333333333	0.03616071428571
		0.3333333333333333	0.3333333333333333	0.3333333333333333	0.036160/1428571
		0.3333333333333333	0.3333333333333333	0.0000000000000	0.036160/1428571
		0.33333333333333	0.00000000000000	0.3333333333333333	0.036160/14285/1
		0.7272727272727	0.090909090909090	0.090909090909090	0.0698/14945161/
		0.090909090909090	0.090909090909090	0.090909090909090	0.0698/14945161/
		0.090909090909090	0.090909090909090	0.7272727272727	0.0098/14945161/
		0.090909090909090	0.7272727272727	0.090909090909090	0.0698/149451617
		0.4554498464263	0.0000001030/30	0.0000001030/30	0.00509484936832
		0.0000001000/30	0.4334498404203	0.0000001030/30	0.00009484936832
		0.0003301333/30	0.0003301333/30	0.4334498404203	0.00309484936832
		0.0000001000/30	0.4334498404203	0.4334498404203	0.00309484930832
		0.4334498464263	0.0000001030/30	0.4334498464263	0.00509484936832
		0.4334498464263	0.43344984642634	0.0000001030/366	0.00009484936832

 Table E.4: Symmetric quadrature points and weights for tetrahedron in [0, 1]³ space

Appendix F. Flow chart of development of 3D DG solver

In this appendix, the flow chart and detail code structure for the development of in-house 3-D discontinuous Galerkin solver are presented.

1. Flow chart of 3-dimensional discontinuous Galerkin code



Figure F-1. Flow chart of 3D discontinuous Galerkin solver development.



Figure F-2. Global structure of in-house developed 3D discontinuous Galerkin solver.

2. Strucutre details of in-house 3D discontinuous Galerkin solver

2.1. Global structure of in-house 3D discontinuous Galerkin solver

- **4 3D_DG_SOLVER:** This is the main program of ACML-3D-DG solver.
- **DG_RUN:** This is the main subroutine of main program. It contains the following subroutines:

✤ GLOBAL_INPUT

Read the Global input file "Solver_input.txt".

READ_GRID

Read the grid information using "GRID_FILE.NEU"

✤ ALLOCATED_INPUT_DATA

Allocate all the input data using in ACML-3D-DG code.

✤ READ_INFORMATION_INPUT

Read the initial input values and gas information.

✤ READ_BOUNDARY_INPUT

Read the boundary input information for various boundaries likes, Farfield, Solid, Side jet etc.

* MESH_INFORMATION

Making the grid in non-dimensional form, calculating the element volume, surface area, normal & tangential vectors etc.

✤ DG_METHOD

This subroutine is related to DG Solver which contains the following subroutines as shown in Figure F-3.



Figure F-3. Subroutine structure of developed in-house 3D discontinuous Galerkin solver.

2.2. Explanation of subroutine structure of in-house 3D DG Solver

4 MESH_INFORMATION

- **GRID_NON_DIMENSION:** Make grid in non-dimensional form.
- MESH_GLOBAL_VOLUME: Calculate cell volume, cell center, surface normal vectors, tangential vectors etc.
- **ELEMENT_VICINITY:** Find the element connectivity.
- **NODE_VICINITY:** Find the node connectivity.

JG_METHOD

- ALLOCATED_DG_SETUP: Allocate the memory for quadrature points, Basis functions, DG variables and limiters.
- ✤ DG_SETUP_ESSENTAILS
- LOCAL_VPOINTS_INSIDE: Define the quadrature points inside the element.
- **LOCAL_VPOINTS_FACE:** Define the quadrature points over the surface.
- LOCAL_VPOINTS_CENTER: Define the quadrature points in center of the element.
- LOCAL_VPOINTS_CORNER: Define the quadrature points on corner of the element.
- LOCAL_VP_FACE_NEIGHBOR: Define the true quadrature points and position for surface neighbors.
- GLOBAL_VPOINTS_INSIDE: Define the global quadrature points inside the element.
- **GLOBAL_VPOINTS_FACE:** Define the global quadrature points over the surface.
- GLOBAL_VPOINTS_CENTER: Define the global quadrature points in the center of element.
- GLOBAL_VPOINTS_CORNER: Define the global quadrature points on the corner of element.
- BASIS_VPOINTS_INSIDE: Define basis function inside the element at the quadrature points.
- BASIS_VPOINTS_FACE: Define basis function over the face at the quadrature points.
- BASIS_VPOINTS_CORNER: Define basis function over corner of element at quadrature points.

- BASIS_VPOINTS_CORNER: Define basis function over the corner of element at quadrature points
- BASIS_1st_DER_VPOINTS: Define the basis derivative inside the element at quadrature points.
- **DG_INVERSE_BiBj_INTEGRATION:** Define the RHS mass matrix.
- ◆ **DG_REFERENCES:** Define the reference parameters and variables for DG solver.
- DG_INITIALIZATION: Making the equation and variables in nondimensional form and initialize the DG program.
- HIGH_ORDER_LIMITER: Implementation of Positivity preserving limiter, indicator and Berth Jespersen limiter.
- **• DG_TIMESTEP:** Calculating the time step for time marching.





2.3. Explanation of time dependent and time independent solver

4 AUXILARY_TIME_INDEPENDENT_EQUATIONS

- AUXILIARY_SURFACE_INTEGRATION: Calculate the surface integration for auxiliary variables.
- AUXILIARY_BOUNDARY_INTEGRATION: Calculate the boundary integration for auxiliary variables.
- AUXILIARY_VOLUME_INTEGRATION: Calculate the volume integration for auxiliary variables.
- **AUXILIARY_UPDATING:** Update the auxiliary variables.
- **↓ PRIMARY_TIME_DEPENDENT_EQUATIONS**
- **DG_SAVE_OldSTEP_Uh:** Save the old primary variables for further calculation.
- DG_Lu_OPERATOR
- **PRIMARY_SURFACE_INTEGRATION:** Calculate the surface integration for primary variables.
- **PRIMARY_BOUNDARY_INTEGRATION:** Calculate the boundary integration for primary variables.
- **PRIMARY_VOLUME_INTEGRATION:** Calculate the volume integration for primary variables
- **PRIMARY_UPDATING_EQUATIONS:** Update the primary variables.
- **EULER_FORWARD_STPPING:** Implementation for time marching scheme.
- **4 DG_RESIDUAL_CALCULATION:** Calculate the residual for DG solver.
- **4 DG_WRITE_RESTART_FILE:** Write the restart file.
- **4 DG_POST_PROCESS:** Post processing part of DG program.

Appendix G. Computationalcostcomparisonbetween DG and FV methods

In this appendix, we are going to compare the computational cost of each part of discontinuous Galerkin method with Finite volume method in the same number of computational cells in the domain.

Finite volume solution in the cell versus DG solution

In contrast to finite volume, DG expands the solution in the local cells using a series of polynomials. Defining a general framework allows piecewise polynomials of degree approximate the solution of degree $K \in N$ in each element. However, the solution in finite volume is constant at order of accuracy of one and piecewise linear at the order of accuracy of two which do not generated using polynomial series expansion, instead they are using Taylor series to obtain higher order of accuracy.



Figure G-1. General solution of DG method at each local element for different order of accuracy.

In discontinuous Galerkin method the solution is approximated by

$$\mathbf{U}_{h^{e}}\left(\mathbf{x},t\right) = \sum_{k=1}^{N_{k}} U_{h^{e}}^{k}\left(t\right) b_{k}\left(\mathbf{x}\right),\tag{G.1}$$

where, $b_k(\mathbf{x})$ is the relevant values of basis function, N_k denotes the number of basis functions required for approximating the smooth and continuous solution inside the space of the polynomial functions, and $U_{h^e}^k(t)$ denotes the degree of freedom of the numerical solution in an element Ω_e . Therefore, the number of unknown variables for DG method is N_k times bigger than finite volume. It means that the number of equations is going to solve as system of equations increases N_k times. Therefore, the extra computational cost for obtaining the $(2N_k + 1)$ order of accuracy is

$$\operatorname{Cost}_{\operatorname{variables}} = \frac{\prod_{k=1}^{\operatorname{Dimension}} (N_k + k)}{\operatorname{Dimension}!},$$

$$\operatorname{Cost}_{\operatorname{summations}} = \left[\frac{\prod_{k=1}^{\operatorname{Dimension}} (N_k + k)}{\operatorname{Dimension}!} \Theta_{\operatorname{data}} \right] \left(N_{cell} \left(N_{Face} \cdot N_{GP}^{\operatorname{Dimension}-1} + N_{GP}^{\operatorname{Dimension}} \right) \right)$$
(G.2)

If the data structure of computational program is defined properly, this calculation is required to be considered at the beginning of each iteration i.e. $\Theta_{data} \approx 1$. If the computational program is not optimized, then the coefficient value is approximately 4 times, i.e. $\Theta_{data} \approx 4$.

Derivatives calculation

In the case of adventive-convective system of equations we have to calculate the conservative variables derivatives. In contrast to finite volume, DG method does not use least square method or first order gauss method for derivative calculation. In order to have correct and accurate approximation of derivatives we have to use Local DG methods. One of the simplest and straight forward methods we can use is mixed DG formulation which

is introduced by Bassi and Rebay in 1997. However, it demands more computational efforts to solve the extra system of equations beside the original system of equations.

$$\boldsymbol{\Theta}_{h^{e}}\left(\mathbf{x}\right) = \nabla \mathbf{U}_{h^{e}}\left(\mathbf{x},t\right) = \sum_{k=1}^{N_{k}} \boldsymbol{\Theta}_{h^{e}}^{k} b_{k}\left(\mathbf{x}\right)$$
(G.3)

Therefore, the computational cost of these extra calculations can be measured by

Additional Equations = Dimension
$$\cdot N_{Equation} \cdot N_{Basis}$$
 (G.4)
= Dimension $\cdot (Dimension + 2) \cdot N_{Basis}$

$$Cost_{Derivatives} = \frac{\prod_{k=1}^{Dimension} (N_k + k)}{Dimension!},$$

$$Cost_{Auxiliary-Summation} = \begin{bmatrix} \prod_{k=1}^{Dimension} (N_k + k) \\ \frac{k}{Dimension!} \Theta_{data} \end{bmatrix} \left(N_{cell} \left(N_{Face} \cdot N_{GP}^{Dimension-1} + N_{GP}^{Dimension} \right) \right)$$
(G.5)

Numerical Integration Cost

In contrast to finite volume method, DG method uses more degree of freedoms and needs more points to calculate fluxes at the faces. Moreover, there are extra costs in the calculation of each step of DG method because of existence of extra integrals in the weak form of the equations. We have to use quadratic numerical integrations to solve volume and surface integrals. Therefore, it is necessary to define some gauss points on the faces and inside the local elements for solving integrals. This is one of the considerable time consuming part of DG method. The difference between the finite volume and DG methods in the calculation of flux integrals is illustrated in below table:

Finite volume approach	Finite element approach
$Integration_{Surface} = \oint_{\partial\Omega} Flux.ndS$ $Integration_{Volume} = \int_{\Omega} u(x,t)dV = \overline{U}$ $Integration_{Volume} = \int_{\Omega} FluxdV = 0$	$Integration_{Surface} = \oint_{\partial\Omega} Flux.ndS = \sum_{i}^{N_{Gp}} \omega_{i}^{Dimension-1} Flux_{i}$ $Integration_{Volume} = \int_{\Omega} u(x,t)dV = \sum_{i}^{N_{Gp}} \omega_{i}^{Dimension} u_{i} \approx u_{i}^{(0)}$ $Integration_{Volume} = \int_{\Omega} Flux(x,t)dV = \sum_{i}^{N_{Gp}} \omega_{i}^{Dimension} Flux_{i}$
52	52

Therefore the extra cost of DG approach is

$$Cost_{Integration} = N_{GP}^{Dimension-1} + N_{GP}^{Dimension}$$

$$= (4N_k + 2)^{Dimension-1} + (2N_k + 1).$$
(G.6)

Time marching computational cost

To date, most of the DG codes are explicit and their convergence speed is restricted to the value of CFL number. In order to have stable DG solution, it is necessary to reduce CFL number with the weight of $1/(2N_k + 1)$. Therefore the computational cost of each iteration (time step) of DG method is $(2N_k + 1)$ times bigger than first order finite volume scheme, in the case of using forward Euler time step

$$\Delta t = \frac{1}{\left(2N_{k}+1\right)} \cdot \frac{CFL \cdot \Delta x^{cell}}{\left|\lambda_{i}\right|_{conv} + C\left|\lambda_{j}\right|_{Adv}}.$$
(G.7)

Therefore the cost of DG at each time step using Rung-Kutta is

$$Cost_{CFL} = 2N_k + 1,$$

$$Cost_{Temporal} = (Number of RK Steps) \times Cost_{CFL}$$
(G.8)

Simulation two-dimensional problem using DG method with first-order of accuracy

For the first-order of accuracy solution polynomial should be order of zero ($N_k = 0$) and the cost of DG in comparison with FVM is

$Cost_{CFL} = 1,$	$Cost_{Derivatives} = 1,$	$Cost_{DG} = 1$
$Cost_{Variables} = 1,$	$Cost_{Limiter} = 1,$	$\frac{1}{\text{Cost}_{\text{FVM}}}$
$\text{Cost}_{\text{Integration}} = 2$,	$Cost_{Positivity} = 1,$	

However, one can write the computational code wisely in order to avoid non-necessary calculation of volume integration since they are zero. If this issue be considered the cost of DG in comparison with finite volume is 1 which means that both methods have same computational cost.

Simulation two-dimensional problem using DG method with secondorder of accuracy

In order to have a solution with second-order of accuracy we have to use a piecewise linear solution in each cell means that order of polynomial is one ($N_k = 1$). As a result the computational cost of DG in comparison to finite volume is

$Cost_{CFL} = 3,$	$Cost_{Derivatives} = 3,$	$Cost_{DG} = \lceil (3+3) \times 9 \times (1\times 1) \rceil Cost$
$Cost_{Variables} = 3,$	$Cost_{Limiter} = 1,$	$\operatorname{Cost}_{\mathrm{FVM}}$
$\text{Cost}_{\text{Integration}} = 9$,	$Cost_{Positivity} = 1,$	$= 54 Cost_{temporal}$

It means that the computational cost of DG method for obtaining second-order of accuracy is at least 54 times bigger than finite volume simulation with the same order of accuracy. But it may be noticed that this theortical computed DG cost may only 20~25 times in contrast to FVM, as auxiliary variables in DG method is simpler to conservative variables and its computational cost is only 5~10 % of total conservative variables cost.

Appendix H. Basics of aerodynamics theory

In this appendix, the basics concepts of aerodynamic theory such as velocity components of a three dimensional body, total forces, aerodynamic forces, moment forces etc. are presented.

1. Velocity components along the body axes

The orientation of the velocity vector with respect to the body-axes coordinate system establishes two angles of significance in the production of aerodynamic forces and moments, namely, angle of attack, α and sideslip angle, β [166].



Figure H-1. Airframe velocity components.

Consider the velocity vector of the airframe given by V as defined as

$$\mathbf{V} = u\hat{e}_1 + v\hat{e}_2 + w\hat{e}_3 \tag{H.1}$$

where $\hat{e}_1, \hat{e}_2, \hat{e}_3$ are the unit vectors and u, v, w are the velocity components along the x, y, and z axes, respectively, defined as

$$u = V \cos \alpha \cos \beta$$
(H.2)

$$v = V \sin \beta$$

$$w = V \sin \alpha \cos \beta$$

Here $V = |\mathbf{V}| = \sqrt{u^2 + v^2 + w^2}$ is the magnitude of velocity vector **V**. The angle of attack α and angle of sideslip β can be expressed in terms of these body axes velocities

$$\alpha = \tan^{-1} \left(\frac{w}{u} \right)$$
(H.3)
$$\beta = \sin^{-1} \left(\frac{v}{V} \right).$$

2. Total forces on an aerodynamic body

Consider the position of a body particle is given by $\mathbf{r} = \mathbf{r}(x, y, z)$ and acting force on this particle is given by $\mathbf{F} = \mathbf{F}(F_x, F_y, F_z)$. The total forces in each direction due to stress are given as follows [167],

$$dF_{x} = \tau_{xx}n_{x}dydz + \tau_{yx}n_{y}dxdz + \tau_{zx}n_{z}dxdy$$
(H.4)

$$dF_{y} = \tau_{xy}n_{x}dydz + \tau_{yy}n_{y}dxdz + \tau_{zy}n_{z}dxdy$$
dF_z = $\tau_{xz}n_{x}dydz + \tau_{yz}n_{y}dxdz + \tau_{zz}n_{z}dxdy.$

Here τ_{ij} is the stress tensor, and n_x, n_y, n_z are the normal vectors in x, y, z direction, respectively. Thus the stress tensor τ_{ij} for diatomic gas which can be can be calculated using the deformation law for a Newtonian (linear) viscous fluid can be rewritten in terms of bulk viscosity as,

$$\tau_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \delta_{ij} \left(\mu_{bulk} - \frac{2}{3}\mu\right) \mathrm{div}\mathbf{V}.$$
(H.5)

Since $\mu_{bulk} = f_{bulk}\mu$, where f_{bulk} being the ratio of the bulk viscosity to the shear viscosity. Note that the value f_{bulk} for monatomic gas can be assumed zero i.e. $f_{bulk} = 0$. Therefore,

$$\tau_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \delta_{ij} \left(f_{bulk} - \frac{2}{3}\right) \mu \operatorname{div} \mathbf{V}.$$
(H.6)

The components of stress tensor for diatomic gas can be calculated as

$$\begin{aligned} \tau_{xx} &= -p + \mu \left[2 \frac{\partial u}{\partial x} + \left(f_{bulk} - \frac{2}{3} \right) \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] = -p - \left(\Pi_{xx} + \Delta \right), \end{aligned} \tag{H.7a} \\ \tau_{yy} &= -p + \mu \left[2 \frac{\partial v}{\partial y} + \left(f_{bulk} - \frac{2}{3} \right) \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] = -p - \left(\Pi_{yy} + \Delta \right), \end{aligned} \\ \tau_{zz} &= -p + \mu \left[2 \frac{\partial w}{\partial z} + \left(f_{bulk} - \frac{2}{3} \right) \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] = -p - \left(\Pi_{zz} + \Delta \right), \end{aligned} \\ \tau_{xy} &= \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) = -\Pi_{xy}, \end{aligned} \tag{H.7b} \\ \tau_{xz} &= \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) = -\Pi_{xz}, \end{aligned}$$

where Π_{ii} is the normal stress, Π_{ij} is the shear stress and Δ is the excess normal stress. Thus from the relations (H.4) and (H.7a) and (H.7b), the total forces in each direction can be calculated as

$$dF_{x} = \left(-p - \left(\Pi_{xx} + \Delta\right)\right) n_{x} dy dz + \left(-\Pi_{xy}\right) n_{y} dx dz + \left(-\Pi_{xz}\right) n_{z} dx dy$$

$$dF_{y} = \left(-\Pi_{xy}\right) n_{x} dy dz + \left(-p - \left(\Pi_{yy} + \Delta\right)\right) n_{y} dx dz + \left(-\Pi_{yz}\right) n_{z} dx dy$$

$$dF_{z} = \left(-\Pi_{xz}\right) n_{x} dy dz + \left(-\Pi_{yz}\right) n_{y} dx dz + \left(-p - \left(\Pi_{zz} + \Delta\right)\right) n_{z} dx dy.$$
(H.8)

3. Aerodynamic forces in the body axes

Often aerodynamic forces are specified in terms of three mutually perpendicular forces[168]: lift force L (aero-force perpendicular to V), drag force D(aeroforce opposite to V), and side force S. These forces, L, D, and S define an axes system so called flight path axes. These forces can be calculated in terms of total forces as

$$\begin{bmatrix} D\\S\\L \end{bmatrix} = \begin{bmatrix} \cos\beta & -\sin\beta & 0\\ \sin\beta & \cos\beta & 0\\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\alpha & 0 & \sin\alpha\\ 0 & 1 & 0\\ -\sin\alpha & 0 & \cos\alpha \end{bmatrix} \begin{bmatrix} F_x\\F_y\\F_z \end{bmatrix}$$

$$= \begin{bmatrix} \cos\alpha\cos\beta & -\sin\beta & \sin\alpha\cos\beta\\ \cos\alpha\sin\beta & \cos\beta & \sin\alpha\sin\beta\\ -\sin\alpha & 0 & \cos\alpha \end{bmatrix} \begin{bmatrix} F_x\\F_y\\F_z \end{bmatrix}$$

$$= \begin{bmatrix} (\cos\alpha\cos\beta)F_x - (\sin\beta)F_y + (\sin\alpha\cos\beta)F_z\\ (\cos\alpha\sin\beta)F_x + (\cos\beta)F_y + (\sin\alpha\sin\beta)F_z\\ -(\sin\alpha)F_x + (\cos\alpha)F_z \end{bmatrix}$$
(H.9)

Then, we get the drag force D, lateral force S, and lift force L, given below:

$$D = (F_x \cos \alpha + F_z \sin \alpha) \cos \beta - F_y \sin \beta$$
(H.10)

$$S = (F_x \cos \alpha + F_z \sin \alpha) \sin \beta + F_y \cos \beta$$

$$L = -F_x \sin \alpha + F_z \cos \alpha.$$

From the relation (H.10), we can deduce the aerodynamic forces for two dimensional body by using the following assumptions,

$$\beta$$
 = sideslip angle = 0, (H.11)
 S = side force=0,
 F_y = force in y-direction =0,
 A = axial force = F_x ,
 N = normal force = F_z .

Thus, we can have the two dimensional aerodynamic forces defined by

$$D = A\cos\alpha + N\sin\alpha$$
(H.12)
$$L = N\cos\alpha - A\sin\alpha.$$

4. Moment vector on the body

The moment produced by force on the body is given by

$$\mathbf{m} = \mathbf{r} \times \mathbf{F} = \begin{vmatrix} i & j & k \\ x & y & z \\ F_x & F_y & F_z \end{vmatrix}$$
(H.13)
$$= \left(yF_z - zF_y \right) i + \left(zF_x - xF_z \right) j + \left(xF_y - yF_x \right) k.$$



Figure H-2. Moment produced by force on a particle.



Figure H-3. Forces and moments acting on the entire airplane¹

.

Thus,

$$\mathbf{m} = \begin{bmatrix} m_x \\ m_y \\ m_z \end{bmatrix} = \begin{bmatrix} yF_z - zF_y \\ zF_x - xF_z \\ xF_y - yF \end{bmatrix}$$
(H.14)

The force vector is given by

$$\mathbf{F} = \int_{surface} \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} dx dy dz$$
(H.15)

The moment vector is given by

¹ Robert F. Stengel, Aircraft Flight Dynamics, http://www.princeton.edu/~stengel/MAE331Lecture5.pdf

$$\mathbf{m}_{B} = \begin{bmatrix} L_{B} \\ M_{B} \\ N_{B} \end{bmatrix} = \int_{surface} \begin{bmatrix} m_{x} \\ m_{y} \\ m_{z} \end{bmatrix} dx dy dz = \int_{surface} \begin{bmatrix} yF_{z} - zF_{y} \\ zF_{x} - xF_{z} \\ xF_{y} - yF_{x} \end{bmatrix} dx dy dz.$$
(H.16)

5. Center of pressure

Aerodynamic force acts through the center of pressure. The pressure varies around the surface of an object. The center of pressure moves with angle of attack. The center of Pressure, \mathbf{x}_{cp} is the average location of the pressure²

$$\mathbf{x}_{cp} = \frac{\int Surface}{\int Surface} \mathbf{x} \, p(\mathbf{x}) \, dS \tag{H.17}$$

where, $\mathbf{x} = (x, y, z)$ is the position vector of fluid particle on wall and $p(\mathbf{x})$ is the pressure on wall. The coordinate of the "**Center of Pressure**" can be defined as:

$$x_{\rm cp} = \frac{\int\limits_{Surface} x \, p(\mathbf{x}) \, dS}{\int\limits_{Surface} p(\mathbf{x}) \, dS}, \quad y_{\rm cp} = \frac{\int\limits_{Surface} y \, p(\mathbf{x}) \, dS}{\int\limits_{Surface} p(\mathbf{x}) \, dS}, \quad z_{\rm cp} = \frac{\int\limits_{Surface} z \, p(\mathbf{x}) \, dS}{\int\limits_{Surface} p(\mathbf{x}) \, dS}, \quad (H.18)$$

² NASA, https://www.grc.nasa.gov/www/k-12/airplane/cp.html

6. Aerodynamic coefficients

Aerodynamic coefficient	Mathematical expression
Dynamic pressure	$q_{\infty} = \frac{1}{2} \rho_{\infty} V_{\infty}^2$
Pressure coefficient	$C_p = \frac{p - p_{\infty}}{q_{\infty}}$
Drag coefficient	$C_D = \frac{D}{q_{\infty} A_{ref}}$
Lift coefficient	$C_L = \frac{L}{q_{\infty} A_{ref}}$
Lateral force coefficient	$C_{S} = \frac{S}{q_{\infty} A_{ref}}$
Friction coefficient	$C_f = \frac{\tau}{q_{\infty}}, \qquad \tau = \text{tangential stress force}$
Roll moment coefficient	$C_l = \frac{L}{q_{\infty} A_{ref} l_{ref}}$
Pitch moment coefficient	$C_m = \frac{M}{q_{\infty} A_{ref} l_{ref}}$
Yaw moment coefficient	$C_n = \frac{N}{q_{\infty} A_{ref} l_{ref}}$
Heat flux coefficient	$C_h = \frac{Q_{wall}}{q_{\infty}}$

Here, A_{ref} , l_{ref} are the reference surface area and reference length of the body.

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