A Thesis for the Degree of Doctor of Philosophy

Computational simulation of Boltzmann-based hydrodynamic models for rarefied and microscale gases and viscoelastic fluids in highly non-equilibrium state

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To begin with, I will lend the words of Sir Isaac Newton's letter to the Hooke in 1675, "*If I have seen further, it is by standing on the shoulders of giants.*" In this sense, I would like to extend my sincere thanks to many giants.

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"The greatest glory in living lies not in falling, but in rising every time we fall."

- Nelson Mandela.

Dedication

To my beloved daughter, wife, and parents

(Thanks for the care and support)

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Nomenclatures

Greek

α	-	angle of attack/viscoelastic model parameter
β	-	side-slip angle/retardation ratio
μ	-	first coefficient of dynamic (shear) viscosity
μ_b	-	coefficient of bulk viscosity
μ_E	-	extensional viscosity
$\mu_{\mathrm{s}}, \mu_{\mathrm{p}}$	-	solvent viscosity, polymeric viscosity
$\mu_{Normalized}$	-	normalized factor
λ	-	second coefficient of viscosity/relaxation time
γ	-	specific heat ratio
κ	-	heat conduction coefficient
$\boldsymbol{\Theta}$	-	vector of auxiliary variable
$\boldsymbol{\Theta}_h$	-	approximated auxiliary variable solution
$\boldsymbol{\Theta}_h^L, \boldsymbol{\Theta}_h^R$		approximated auxiliary solution for left and right state
ξ, η, ζ	-	reference coordinates
ρ	-	density
Γ	-	diffusion coefficient
λ_{mean}	-	mean free path
δ	-	boundary thickness layer of the body
$\boldsymbol{\sigma}, \sigma_{ij}$	-	stress tensor
$\boldsymbol{\tau}, \tau_{ij}, \boldsymbol{\Pi}$	-	viscous stress tensor
$\Pi_{xx}, \Pi_{yy}, \Pi_{zz}, \tau_{xx}, \tau_{yy}, \tau_{zz}$	-	normal stress components
$\Pi_{xy}, \Pi_{xz}, \Pi_{yz}, \tau_{xy}, \tau_{xz}, \tau_{yz}$	-	viscous stress components
Δ	-	excess normal stress
$\boldsymbol{\varepsilon}, \varepsilon_{ij}, \dot{\boldsymbol{\varepsilon}}$	-	symmetric or rate-of-strain tensor
$\dot{\gamma}$	-	shear-rate
$\boldsymbol{\omega}, \omega_{ij}$	-	anti-symmetric tensor
$\nabla \cdot \mathbf{u}$	-	dilatational term
ζ	-	friction coefficient
ζ^{dof}	-	molecular internal degree of freedoms
$\zeta^{dof}_{\mathrm{internal}}$	-	internal energy modes
$\varepsilon_{\mathrm{kinetic}}$	-	specific kinetic energy per unit mass
$\varepsilon_{\mathrm{internal}}$	-	specific internal energy per unit mass
$\varepsilon_{\mathrm{potential}}$	-	specific potential energy per unit mass

$\in$	-	Hencky strain
ω	-	angular frequency
$\boldsymbol{\omega}_B$	-	vector of angular frequency
μ_{mass}	-	reduced mass of molecule
ν	-	exponent of the inverse power law
ψ	-	azimuth angle/distribution function
$\Lambda^{(n)}$	-	dissipation term
$\Psi^{(n)}$	-	high-order moments
$\hat{\Psi}$	-	local calortropy density
σ_c	-	calortropy production
σ_u, σ_T	-	momentum, thermal accommodation coefficients
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 of 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
$\mathbf{J}_{\mathbf{x}\to\boldsymbol{\xi}}$	-	jacobian of transformation
$P_n^{\alpha,\beta}$	-	orthogonal *Jacobi polynomials*
$\boldsymbol{\chi}$	-	flow properties
$\hat{\Lambda}^x_{inv}, \hat{\Lambda}^y_{inv}, \hat{\Lambda}^z_{inv}$	-	inviscid spectral radii
$\hat{\Lambda}^x_{vis}, \hat{\Lambda}^y_{vis}, \hat{\Lambda}^z_{vis}$	-	viscous spectral radii

Latin

L	-	characteristics length scale
T	-	time
Kn	-	Knudsen number based on the characteristic length scale
Kn_δ	-	Knudsen number based on boundary thickness layer
Kn_{GLL}	-	gradient length local-based Knudsen number
N_δ	-	composite number
$B_{\max}$	-	Bird's breakdown parameter

$\mathrm{Kn}_{\max}$	-	Boyd's breakdown parameter
M	-	Mach number
Re	-	Reynolds number
Pr	-	Prandtl number
Ec	-	Eckert number
St	-	Stanton number
We	-	Weissenberg number
$\mathbf{n}$	-	normal vector
$\mathbf{r}$, $\mathbf{x}$	-	position vector
$\mathbf{v}$	-	particle velocity
$\mathbf{u}$	-	bulk velocity vector
u, v, w	-	cartesian components of the velocity vector
$\underset{\sim}{\mathbf{u}}, \underset{\sim}{\mathbf{v}}$	-	microscopic solvent and bead velocities
$\underset{\sim}{R}$	-	end-to-end vector after deformation
$\mathbf{J}$	-	Jacobian matrix
n	-	number density (molecule per unit volume)
d	-	molecular diameter
T	-	overall temperature
T_w	-	wall temperature
p	-	pressure
$\bar{P}$	-	mean pressure
K_B	-	Boltzmann constant
N_A	-	Avogadro number
R_{gas}	-	gas constant
$\mathbf{R}$	-	orthogonal tensor
C_{ijmn}	-	fourth-order viscosity coefficient tensor
f_b	-	ratio of bulk viscosity to shear viscosity
m	-	molecular mass
E_{total}	-	total energy
E_{kineic}	-	kinetic energy
E_{internal}	-	internal energy
$E_{\text{potential}}$	-	potential energy
$E_{\text{viberational}}$	-	vibrational energy
I	-	moment of inertia
$\mathbf{j}$, j	-	angular momentum, magnitude of angular momentum
C_p	-	specific heat at constant pressure
C_v	-	specific heat at constant volume
C_D	-	drag coefficient
C_τ	-	torque coefficient

s	-	viscosity index number
$\mathbf{C}$	-	peculiar velocity/conformation tensor
$H_{total}, h, \hat{h}$	-	total enthalpy, specific enthalpy, enthalpy density
$\mathbf{P}$	-	pressure tensor
$\mathbf{Q}$	-	heat flux vector
Q_x, Q_y, Q_z	-	heat flux components
T_x, T_y, T_z	-	temperature components
$\mathbf{I}$	-	unit tensor
H_{rot}	-	rotational Hamiltonian of the molecule
$\bar{E}_{rot}$	-	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 the hydrodynamic streaming effect
q_{1st}	-	first-order dissipation term
q_{2nd}	-	second-order dissipation term
k_1	-	first cumulant expansion
$\hat{R}$	-	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
$\mathbf{U}$	-	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
$\mathbf{F}^{\text{inv}}$	-	inviscid flux function
$\mathbf{F}^{\text{vis}}$	-	viscous flux function
N_δ	-	non-equilibrium parameter
N_E	-	number of elements
N_F	-	number of faces
N_k	-	number of basis functions

N_1, N_2	-	first and second normal stress difference
b_k	-	basis function
$\mathbf{H}_{auxiliary}, \mathbf{H}^b_{auxiliary}$	-	numerical auxiliary flux, numerical boundary auxiliary flux
$\mathbf{H}_{inviscid}, \mathbf{H}^b_{inviscid}$	-	numerical inviscid flux, numerical boundary inviscid flux
$\mathbf{H}_{viscous}, \mathbf{H}^b_{viscous}$	-	numerical viscous flux, numerical boundary viscous flux
$\mathbf{M}$	-	mass matrix
$\mathbf{M}^{-1}$	-	inverse of the mass matrix
$\mathbf{R}(\mathbf{U})$	-	residual vector of **U** variables
T_e	-	affine sub-parametric transformation
Tr	-	Trouton ratio

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
NVD	-	Normalized variable diagram
CBC	-	Convection boundedness criterion
BAIR	-	Boundedness, accuracy, and interpolative reasonableness
BR1	-	First Bassi-Rebay scheme
BR2	-	Second Bassi-Rebay scheme
DOF	-	Degree of freedom
LDG	-	Local discontinuous Galerkin
NSF	-	Navier-Strokes-Fourier
LTE	-	Local thermal equilibrium
NF	-	Navier-Fourier
NCCR	-	Nonlinear coupled constitutive relations
MD	-	Molecular dynamics
DSMC	-	Direct simulation of Monte Carlo
CCF	-	Cylindrical Couette flow
OREX	-	Orbital Re-entry experiment
HWNP	-	High Weissenberg number problem
BSD	-	Both-side-diffusion
PDPS	-	Positive definiteness preserving scheme
LCR	-	Log conformation tensor representation
SRCR	-	Square root conformation representation

UCM	-	Upper convected derivative
PTT	-	Phan-Thien-Tanner
PS	-	Polystyrene
PAM	-	Polyacrylamides
VOF	-	Volume-of-fluid
CSF	-	Continuum surface force
MULES	-	Multidimensional universal limiter with explicit solution
PISO	-	Pressure-implicit with the splitting of operators
UDS	-	Upwind difference scheme
HRS	-	High-Resolution schemes
HREG	-	High-Resolution equi-gradient scheme
PSD	-	Principal stress difference

Abstract

Computational simulation of Boltzmann-based hydrodynamic models for rarefied and microscale gases and viscoelastic fluids in highly non-equilibrium state

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Fluid flows are governed by a complicated nonlinear system of partial differential equations. In many situations, the mean free path of gas-particle becomes comparable to the characteristic physical length scale or the relaxation time scale for liquid becomes similar to the characteristic time scale, of the flow process. At this stage, the flow processes exhibit non-equilibrium as it significantly deviates from the local state of equilibrium. It is well known that the two-century-old so-called Navier-Stokes-Fourier equations are based on the vital assumptions of local-thermal-equilibrium (made by Stokes in 1845 that the bulk viscosity vanishes), and as a result, their validity may be seriously questioned in states away from the equilibrium. Therefore, it becomes essential to understand the nonlinear flow phenomena associated with these fluids, to design the fluid flow system efficiently and accurately.

The thesis explores the Boltzmann-based hydrodynamic models for describing the rarefied and microscale gas flows, and viscoelastic fluid systems using the higher-order computational methodology. In the first half of the thesis, the second-order constitutive laws based on Eu's generalized hydrodynamics and Myong's balanced closure, for diatomic (and linear polyatomic) gas molecules are presented. A computational attempt is made to investigate the

thermal nonequilibrium associated with different gas types under nonequilibrium conditions. In the next half, the “sinh” second-order nonlinear coupled constitutive relations (NCCR) based on the Rayleigh-Onsager quadratic dissipation for viscoelastic fluid are detailed. Next, a plausible way to overcome the stumbling block of numerical simulations, the so-called High Weissenberg Number Problem (HWNP) is explored.

In this study, the higher-order, *h*-adaptivity scheme, the so-called discontinuous Galerkin (DG) methods were employed for solving the compressible rarefied gas flows to obtain the solution of the two- and three-dimensional flow problems. A summary of numerical implementation of various limiters, numerical flux functions, and boundary conditions is provided for the pedagogical purpose. In the other part of the thesis, the incompressible viscoelastic fluids were solved using the higher-order finite volume schemes in the framework of OpenFOAM. Further briefing on discretization techniques for constitutive equations, high-resolution schemes, the volume-of-fluid method is presented.

The presented methodologies are verified and validated using the analytics, the available experiments, and the existing results. In the case of rarefied gas flows, various benchmark tests using the first- and second-order Boltzmann-Curtiss-based models along with the slip and jump conditions are investigated. The results obtained using the second-order constitutive model with the slip and jump conditions showed better agreement with the existing studies, under the nonequilibrium conditions. Correspondingly, various benchmark tests of viscoelastic fluid using different constitutive models are studied. The results obtained using the viscoelastic “sinh” second-order NCCR model suggested that the HWNP are effectively overcome in comparison with the existing viscoelastic models.