Comparison of Numerical Solutions for the Boltzmann Equation and Different Moment Models

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Outline

Introduction

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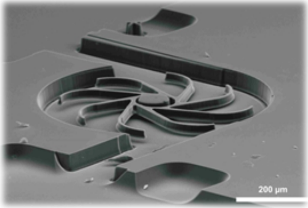
Aim

Derive hyperbolic PDE systems for rarefied gas flows

Extension of standard fluid dynamic equations

- Reentry flows
- Micro channel flows



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Importance of Hyperbolicity

- Well-posedness and stability of the solution

Rarefied Gas Dynamics I

Goal

solve and simulate flow problems involving rarefied gases

Knudsen number

distinguish flow regimes by orders of the *Knudsen* number $Kn = \frac{\lambda}{L}$

- λ is the mean free path length
- L is a reference length

Flow regimes

- $Kn \leq 0.1$: continuum model; Navier-Stokes Equation and extensions
- $Kn \geq 0.1$: rarefied gas; Boltzmann Equation or Monte-Carlo simulations

Rarefied Gas Dynamics II

Applications for large $Kn = \frac{\lambda}{L}$

- large λ: rarefied gases, atmospheric reentry flights
- small L: micro-scale applications, Knudsen pump, MEMS

Tasks

- computation of mass flow rates
- calculation of shock layer thickness
- accurate prediction of heat flux

Boltzmann Transport Equation

$$\frac{\partial}{\partial t} f(t, \mathbf{x}, \mathbf{c}) + c_i \frac{\partial}{\partial x_i} f(t, \mathbf{x}, \mathbf{c}) = S(f)$$

PDE for particles' *probability density function* $f(t, \mathbf{x}, \mathbf{c})$

- Describes change of f due to transport and collisions
- Collision operator S
- Usually a 7-dimensional phase space

Model Order Reduction

Ansatz

$$f(t, \mathbf{x}, \mathbf{c}) = \sum_{i=0}^{M} f_i(t, \mathbf{x}) \mathcal{H}_i^{\rho, \mathbf{v}, \theta}(\mathbf{c})$$

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One PDE for $f(t, \mathbf{x}, \mathbf{c})$ that is 7-dimensional

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Reduction of Complexity

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$$\Downarrow$$

System of PDEs for $\rho(t, \mathbf{x}), \mathbf{v}(t, \mathbf{x}), \theta(t, \mathbf{x}), f_i(t, \mathbf{x})$ that is 4-dimensional

Hyperbolic Moment Equations

Grad's Method [Grad, 1949]

Galerkin Approach

- Standard method
- Multiplication with test function and integration

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$$\partial_t \mathbf{u}_M + \mathbf{A}_{\mathrm{Grad}} \partial_x \mathbf{u}_M = 0,$$

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$\Rightarrow$ Loss of hyperbolicity

Hyperbolic Moment Equations (HME) [Cai et al., 2012]

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$\Rightarrow$ Globally hyperbolic for every state vector $\mathbf{u}_M$

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Operator Projection Framework

Moment equations

$$\mathbf{D}\frac{\partial}{\partial t}\mathbf{w} + \mathbf{M}\mathbf{D}\frac{\partial}{\partial x}\mathbf{w} = 0$$

$\mathbf{P}$ projection matrix

$\mathbf{w} := \mathbf{P}\widetilde{\mathbf{w}}$ projected flow variables

$\mathbf{D} := \mathbf{P}\widetilde{\mathbf{D}}\mathbf{P}^T$ projected derivative matrix

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Model Summary

Properties

- globally hyperbolic system
- multiple spatial dimensions
- rotational invariance
- single framework includes all theories

Problems

- analysis of system including collision operator
- numerical simulations

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Numerical Methods

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- HME and QBME are partially-conservative systems

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$\Rightarrow$ Special numerical methods are needed

Non-Conservative Numerical Methods

Wave Propagation scheme [LeVeque, 1997]

- Upwind type scheme
- First order and almost second order
- Implemented on 2D uniform cartesian grids

PRICE-C scheme [Canestrelli, 2009]

- Centered scheme
- First order and arbitrary order
- Implemented on 2D unstructured grids

Non-Conservative Variables

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$$\mathbf{w} = \mathbf{B}^{-1}(\mathbf{u}) \Leftrightarrow \mathbf{u} = \mathbf{B}(\mathbf{w})$$

Transformed non-conservative PDE system

$$\partial_t \mathbf{w} + \frac{\partial \mathbf{B}(\mathbf{w})}{\partial \mathbf{w}}^{-1} \mathbf{A}(\mathbf{B}(\mathbf{w})) \frac{\partial \mathbf{B}(\mathbf{w})}{\partial \mathbf{w}} \partial_x \mathbf{w} = 0$$

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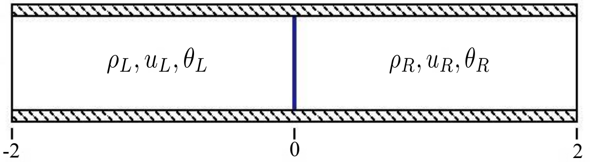
Primitive vs partially conserved variables

- Primitive variables: $\mathbf{u} = (\rho, v, \theta, f_3, f_4)$
- Partially conserved variables: $\mathbf{w} = \left(\rho, \rho v, \rho\left(v^2 + \theta\right), f_3, f_4\right)$

Numerical Results

Shock Tube Test Case



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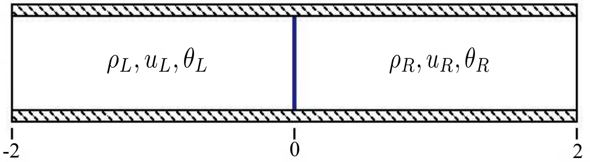


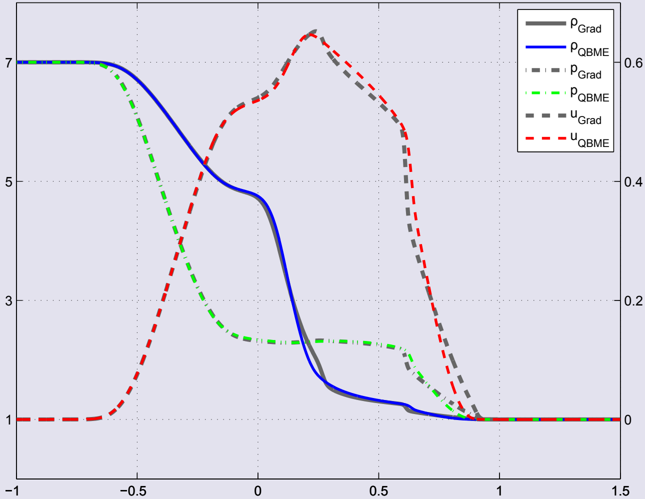
Riemann problem with BGK collision operator

$$\partial_t \mathbf{u} + \mathbf{A}\partial_x \mathbf{u} = -\frac{1}{\tau}\mathbf{P}\mathbf{u}, \quad x \in [-2, 2]$$

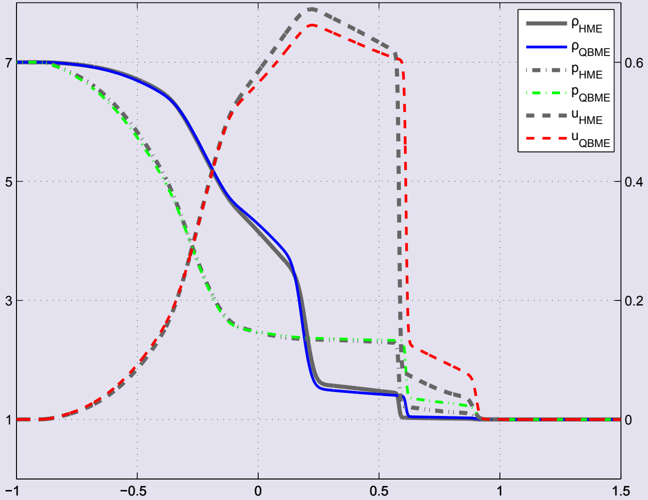
$$\rho_L = 7, \rho_R = 1$$

- Variable vector $\mathbf{u} = (\rho, v, \theta, f_3, f_4)$
- Relaxation time $\tau = \frac{\mathrm{Kn}}{\rho} \Rightarrow$ non-linear

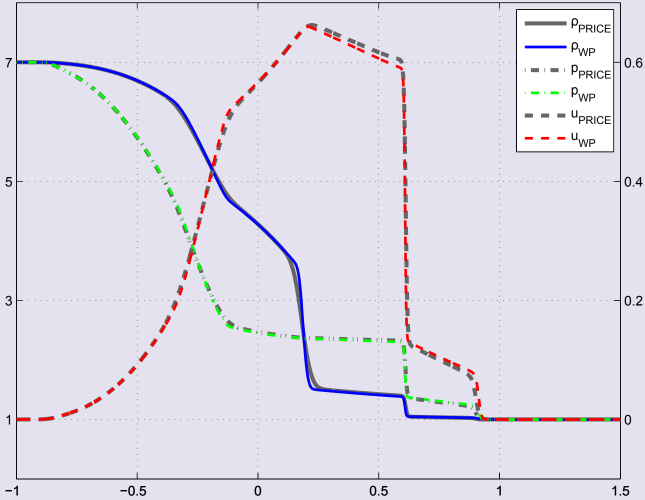
QBME vs Grad, $\mathrm{Kn} = 0.05$



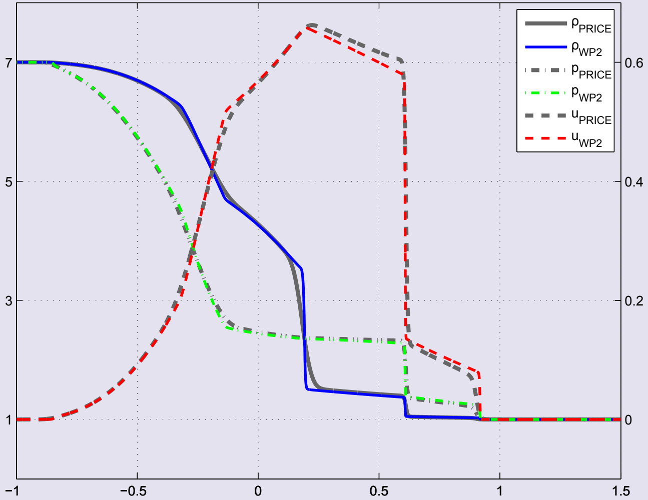
QBME vs HME, $\mathrm{Kn} = 0.5$



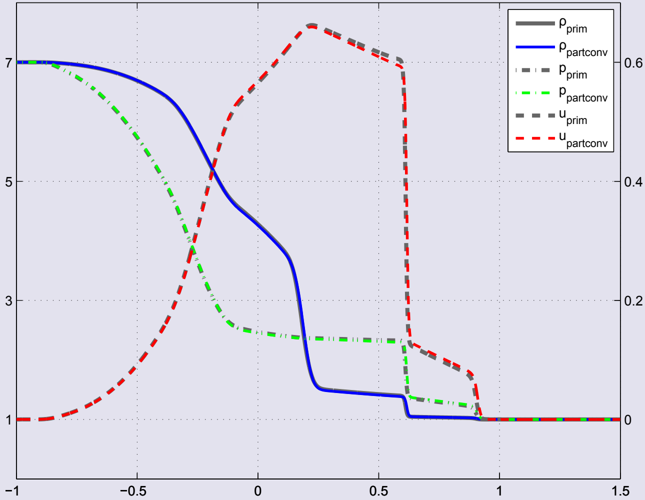
PRICE vs WP, $\mathrm{Kn} = 0.5$



PRICE vs WP2, $\mathrm{Kn} = 0.5$



Primitive vs Partially Conserved, $\mathrm{Kn} = 0.5$



Summary and Further Work

Summary

- Equations: QBME, HME
- Numerics: Wave Propagation, PRICE
- Results: Comparison of models, numerical schemes, variable sets

Differences between models are larger than between numerical schemes

Further Work

- More simulations and test cases
- Higher order PRICE scheme

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Thank you for your attention!

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