Numerical Solution of Hyperbolic Moment Equations for the Boltzmann Equation

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Introduction
Introduction

Aim

Derive hyperbolic PDE systems for rarefied gas flows

Extension of standard fluid dynamic equations

- Reentry flows
- Micro channel flows
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Derive hyperbolic PDE systems for rarefied gas flows

Extension of standard fluid dynamic equations

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- Micro channel flows

Importance of Hyperbolicity

- Well-posedness and stability of the solution
Goal
solve and simulate flow problems involving rarefied gases

Knudsen number
distinguish flow regimes by orders of the Knudsen number $Kn = \frac{\lambda}{L}$
- $\lambda$ 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
Applications for large $Kn = \frac{\lambda}{L}$

- large $\lambda$: 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

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

PDE for particles’ probability density function \( f(t, x, c) \)

- Describes change of \( f \) due to transport and collisions
- Collision operator \( S \)
- Usually a 7-dimensional phase space
Model Order Reduction

Ansatz

\[ f(t, x, c) = \sum_{i=0}^{M} f_i(t, x) \mathcal{H}^{\rho, v, \theta}_i (c) \]
Model Order Reduction

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\[ f(t, x, c) = \sum_{i=0}^{M} f_i(t, x) \mathcal{H}_{i}^{\rho, v, \theta} (c) \]

Reduction of Complexity

One PDE for \( f(t, x, c) \) that is 7-dimensional
Model Order Reduction

Ansatz

\[ f(t, x, c) = \sum_{i=0}^{M} f_i(t, x) \mathcal{H}_{i}^{\rho, v, \theta}(c) \]

Reduction of Complexity

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

\[ \Downarrow \]

System of PDEs for \( \rho(t, x), v(t, x), \theta(t, x), f_i(t, x) \) that is 4-dimensional
Review of Hyperbolic Moment Equations
History of Hyperbolic Moment Equations

Grad’s Method \([\textit{Grad}, 1949]\)  
- Galerkin projection with Hermite polynomials, locally hyperbolic

Hyperbolic Moment Equations (HME) \([\textit{Cai} \text{ et al.}, 2012]\)  
- modification of system matrix

Quadrature-Based Moment Equations (QBME) \([\textit{JK}, 2013]\)  
- use of Gaussian quadrature

Operator Projection framework (OP) \([\textit{Fan}, \text{JK et al.}, 2014]\)  
- application of projections
State of the art

Moment equations

\[ D \frac{\partial}{\partial t} w + MD \frac{\partial}{\partial x} w = 0 \]

- \( P \) projection matrix
- \( w := P\tilde{w} \) projected flow variables
- \( D := P\tilde{D}P^T \) projected derivative matrix
- \( M := P\tilde{M}P^T \) projected multiplication matrix
State of the art

Moment equations

\[
\frac{\partial}{\partial t} w + D^{-1} M \frac{\partial}{\partial x} w = 0
\]

\(P\) projection matrix

\(w := P\tilde{w}\) projected flow variables

\(D := P\tilde{D}P^T\) projected derivative matrix

\(M := P\tilde{M}P^T\) projected multiplication matrix
Achievements and Problems

Achievements

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

Problems

- analysis of system including collision operator
- numerical simulations
Numerical Methods
Conservative PDE systems

Standard conservative PDE system

\[ \partial_t u + \partial_x F(u) = 0 \]
Conservative PDE systems

Standard conservative PDE system

$$\partial_t u + \partial_x F(u) = 0$$

Basic Finite Volume scheme

$$u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{\Delta x} \left( F_{i+\frac{1}{2}}^{n} - F_{i-\frac{1}{2}}^{n} \right)$$

- Numerical flux $F_{i+\frac{1}{2}}^{n}$ needed
- Conservation property by design
- Easily extendable to 2D and unstructured grids
Non-conservative PDE systems

\[ \partial_t u + A(u) \partial_x u = 0 \]
Non-conservative PDE systems

\[ \partial_t u + A(u) \partial_x u = 0 \]

- Can be written in conservative form iff \( A(u) = \frac{\partial F(u)}{\partial u} \)
- In general no flux function available
- Direct discretization violates conservation property

⇒ Special numerical methods are needed
Numerical Methods

Wave Propagation scheme [LeVeque, 1997]
- Second order
- Upwind type scheme
- Implemented on 2D uniform cartesian grids

PRICE-C scheme [Canestrelli, 2009]
- Arbitrary order
- Centered scheme
- Implemented on 2D unstructured grids
Wave Propagation scheme \cite{LeVeque1997} 

First order scheme 

\[ u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{\Delta x} \left( A^{+}\Delta u_{i} + A^{-}\Delta u_{i+1} \right) \]

- \( A\Delta u_{i} \) is called fluctuation
- Fluctuations are split \( A\Delta u_{i} = A^{-}\Delta u_{i} + A^{+}\Delta u_{i} \)
- Similar to flux difference splitting, but without a flux function
Solution of local Riemann problem

\[ A\left(u_{i-\frac{1}{2}}\right) = R \cdot \Lambda \cdot R^{-1} \]

- Wave speeds \( \lambda^j = \Lambda_{jj} \)
- Waves \( W^j = \alpha^j \cdot R^j \)
- Wave strengths \( \alpha^j = (R^{-1} \Delta u)_j \)

Left and right going fluctuations

\[
\begin{align*}
A^- \Delta u_i &= \sum_p (\lambda^p)^- W^p \\
A^+ \Delta u_i &= \sum_p (\lambda^p)^+ W^p
\end{align*}
\]
Second order extension

Add correction term

\[ u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} (A^+ \Delta u_i + A^- \Delta u_{i+1}) - \frac{\Delta t}{\Delta x} (\tilde{F}_{i+1} - \tilde{F}_i) \]

Second order corrections

\[ \tilde{F}_i = \frac{1}{2} \sum_p |\lambda_i^p| \left( 1 - \frac{\Delta t}{\Delta x} |\lambda_i^p| \right) \tilde{W}_i^p \]

Limiter for stability

\[ \tilde{W}_i^p = \phi (\theta_i^p) W_i^p, \quad \theta_i^p = \frac{W_{i-1}^p \cdot W_i^p}{W_i^p \cdot W_i^p} \]
Summary: Wave propagation scheme

Scheme

\[ u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} \left( A^+ \Delta u_i + A^- \Delta u_{i+1} \right) - \frac{\Delta t}{\Delta x} \left( \bar{F}_{i+1} - \bar{F}_i \right) \]

+ 
  - Almost second order
  - Upwind type scheme
  - Implemented on 2D uniform cartesian grids

- 
  - Not exactly second order
  - Not extendable to higher order
  - Not for unstructured grids
PRICE-C scheme [Canestrelli, 2009]

First order scheme

\[
\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x} \left( A^-_{i+\frac{1}{2}} (\mathbf{u}_{i+1}^n - \mathbf{u}_i^n) + A^+_{i-\frac{1}{2}} (\mathbf{u}_i^n - \mathbf{u}_i^{n-1}) \right)
\]

- Similar notation as wave propagation scheme
- PRImitive CEntered scheme, uses no eigenvalue information
- Reduces to FORCE scheme in the conservative case

FORCE scheme

\[
\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x} \left( \mathbf{F}^{\text{FORCE}}_{i+\frac{1}{2}} - \mathbf{F}^{\text{FORCE}}_{i-\frac{1}{2}} \right)
\]
Generalization of Roe matrix

Roe matrix for conservative systems

\[ A_{Roe}(u_L, u_R)(u_R - u_L) = F(u_R) - F(u_L) \]

Non-conservative case

- \( A_{Roe} \) depends on a path \( \psi \) between \( u_L \) and \( u_R \)
- Example: \( \psi(s, u_L, u_R) = u_L + s \cdot (u_R - u_L), s \in [0, 1] \)

Extension: Generalized Roe matrix

\[ A_{\psi}(u_L, u_R)(u_R - u_L) = \int_0^1 A(\psi(s, u_L, u_R)) \frac{\partial \psi}{\partial s} \, ds \]
Generalization of Roe matrix 2

Reduces to standard Roe matrix for conservative case

\[
A_{\psi} (u_L, u_R) (u_R - u_L) = \int_{0}^{1} A (\psi (s, u_L, u_R)) \frac{\partial \psi}{\partial s} ds
\]

\[
= \int_{0}^{1} \frac{\partial F (\psi (s, u_L, u_R))}{\partial \psi} \frac{\partial \psi}{\partial s} ds
\]

\[
= \int_{0}^{1} \frac{\partial F (\psi (s, u_L, u_R))}{\partial s} ds
\]

\[
= F (\psi (1, u_L, u_R)) - F (\psi (0, u_L, u_R)) ds
\]

\[
= F (u_R) - F (u_L)
\]
Computation of generalized Roe matrix

\[ A_\psi (u_L, u_R) (u_R - u_L) = \int_0^1 A (\psi (s, u_L, u_R)) \frac{\partial \psi}{\partial s} ds \]

- Choose linear path \( \psi (s, u_L, u_R) = u_L + s \cdot (u_R - u_L), s \in [0, 1] \)
- Use Gaussian quadrature to compute integral
Computation of generalized Roe matrix

\[
A_\psi (u_L, u_R) (u_R - u_L) = \int_0^1 A (\psi (s, u_L, u_R)) \frac{\partial \psi}{\partial s} ds
\]

- Choose linear path \( \psi (s, u_L, u_R) = u_L + s \cdot (u_R - u_L), s \in [0, 1] \)
- Use Gaussian quadrature to compute integral

Computation

\[
A_\psi (u_L, u_R) (u_R - u_L) = \int_0^1 A (\psi (s, u_L, u_R)) (u_R - u_L) ds
\]

\[
\implies A_\psi (u_L, u_R) = \int_0^1 A (\psi (s, u_L, u_R)) ds \approx \sum_{j=1}^{M} \omega_j A (\psi (s_j, u_L, u_R))
\]
Complete PRICE-C scheme

First order scheme

\[ u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} \left( A_{i+\frac{1}{2}}^- (u_{i+1}^n - u_i^n) + A_{i-\frac{1}{2}}^+ (u_i^n - u_{i-1}^n) \right) \]
Complete PRICE-C scheme

First order scheme

\[ u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{\Delta x} \left( A_{i+\frac{1}{2}}^{-} (u_{i+1}^{n} - u_{i}^{n}) + A_{i-\frac{1}{2}}^{+} (u_{i}^{n} - u_{i-1}^{n}) \right) \]

\[ A_{i+\frac{1}{2}}^{-} = \frac{1}{4} \left( 2A_{\psi} (u_{i}^{n}, u_{i+1}^{n}) - \frac{\Delta x}{\Delta t} I - \frac{\Delta t}{\Delta x} (A_{\psi} (u_{i}^{n}, u_{i+1}^{n}))^2 \right) \]

\[ A_{i-\frac{1}{2}}^{+} = \frac{1}{4} \left( 2A_{\psi} (u_{i-1}^{n}, u_{i}^{n}) - \frac{\Delta x}{\Delta t} I - \frac{\Delta t}{\Delta x} (A_{\psi} (u_{i-1}^{n}, u_{i}^{n}))^2 \right) \]
Higher order extension

WENO reconstruction in space

\[ u_i \Rightarrow u_i(x) \]

ADER approach in time

\[ u_i(x, t) = u(x_i, t^n) + (x - x_i) \frac{\partial u}{\partial x} + (t - t^n) \frac{\partial u}{\partial t} \]

\[ \frac{\partial u}{\partial t} = -A(u)\partial_x u \]

Integration of PDE over time-space volume and computation of integrals using Gaussian quadrature and reconstruction
Summary: PRICE-C scheme

\[ u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{\Delta x} \left( A_{i+\frac{1}{2}}^{-} (u_{i+1}^{n} - u_{i}^{n}) + A_{i-\frac{1}{2}}^{+} (u_{i}^{n} - u_{i-1}^{n}) \right) \]

+ -

- Extension to arbitrary order
- No eigensystem needed
- For unstructured grids

- Higher order difficult to implement
- Added numerical diffusion
Numerical Results
Shock Tube Test Case

\[ \rho_L, u_L, \theta_L \quad \rho_R, u_R, \theta_R \]
Riemann problem with BGK collision operator

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

\[ \rho_L = 7, \rho_R = 1 \]

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

Grad model

\[
A_{\text{Grad}} =
\begin{pmatrix}
v & \rho & 0 & 0 & 0 \\
\frac{\theta}{\rho} & v & 1 & 0 & 0 \\
0 & 2\theta & v & \frac{6}{\rho} & 0 \\
0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\
-\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v
\end{pmatrix}
\]

HME model

\[
A_{\text{HME}} =
\begin{pmatrix}
v & \rho & 0 & 0 & 0 \\
\frac{\theta}{\rho} & v & 1 & 0 & 0 \\
0 & 2\theta & v & \frac{6}{\rho} & 0 \\
0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\
-\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v
\end{pmatrix}
\]
Model Equations 2

Grad model

\[
A_{\text{Grad}} = \begin{pmatrix}
\nu & \rho & 0 & 0 & 0 \\
\theta & \rho & 1 & 0 & 0 \\
0 & 2\theta & \nu & \frac{\rho}{\theta} & 0 \\
0 & 4f_3 & \rho\theta & \nu & 4 \\
-\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & \nu
\end{pmatrix}
\]

QBME model

\[
A_{\text{QBME}} = \begin{pmatrix}
\nu & \rho & 0 & 0 & 0 \\
\theta & \rho & 1 & 0 & 0 \\
0 & 2\theta & \nu & \frac{\rho}{\theta} & 0 \\
0 & 4f_3 & \rho\theta & -\frac{10f_4}{\theta} & \nu \\
-\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15f_4}{\rho\theta} & \nu
\end{pmatrix}
\]
QBME vs Grad, $Kn = 0.05$
QBME vs HME, $Kn = 0.5$
PRICE vs WP, $Kn = 0.5$
PRICE vs WP2, Kn = 0.5

The graph compares the pressure, density, and velocity profiles for the PRICE and WP2 models at a Knudsen number of 0.5. The results show a close agreement between the two models, with slight variations in the profiles.
### Summary and Further Work

#### Hyperbolic Moment Equations
- QBME, HME
- PDE system in non-conservative form

#### Non-conservative numerics
- Wave propagation scheme
- PRICE-C scheme

#### Further Work
- More simulations and test cases
- Higher order PRICE-C scheme
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- PDE system in non-conservative form

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### Further Work
- More simulations and test cases
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Thank you for your attention!
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