Numerical Solution of Hyperbolic Moment Equations for the Boltzmann Equation

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Outline

Introduction

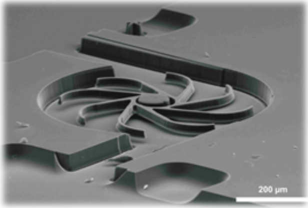
Introduction

Aim

Derive hyperbolic PDE systems for rarefied gas flows

Extension of standard fluid dynamic equations

- Reentry flows
- Micro channel flows



Introduction

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Derive hyperbolic PDE systems for rarefied gas flows

Extension of standard fluid dynamic equations

- Reentry flows
- Micro channel flows

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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Reduction of Complexity

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

Model Order Reduction

Ansatz

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

Reduction of Complexity

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

$$\Downarrow$$

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

Review of Hyperbolic Moment Equations

History of Hyperbolic Moment Equations

Grad's Method [Grad, 1949]

- Galerkin projection with Hermite polynomials, locally hyperbolic

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

- modification of system matrix

Quadrature-Based Moment Equations (QBME) [JK, 2013]

- use of Gaussian quadrature

Operator Projection framework (OP) [Fan, JK et al., 2014]

- application of projections

State of the art

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

$\mathbf{M} := \mathbf{P}\widetilde{\mathbf{M}}\mathbf{P}^T$ projected multiplication matrix

State of the art

Moment equations

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

$\mathbf{P}$ projection matrix

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

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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

$$\partial_t \mathbf{u} + \partial_x \mathbf{F}(\mathbf{u}) = 0$$

Conservative PDE systems

Standard conservative PDE system

$$\partial_t \mathbf{u} + \partial_x \mathbf{F}(\mathbf{u}) = 0$$

Basic Finite Volume scheme

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{F}^*_{\mathbf{i}+\frac{1}{2}} - \mathbf{F}^*_{\mathbf{i}-\frac{1}{2}}\right)$$

- Numerical flux $\mathbf{F}^*_{\mathbf{i}+\frac{1}{2}}$ needed
- Conservation property by design
- Easily extendable to 2D and unstructured grids

Non-conservative PDE systems

Non-conservative PDE system

$$\partial_t \mathbf{u} + \mathbf{A}(\mathbf{u}) \partial_x \mathbf{u} = 0$$

Non-conservative PDE systems

Non-conservative PDE system

$$\partial_t \mathbf{u} + \mathbf{A}(\mathbf{u})\partial_x \mathbf{u} = 0$$

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

$\Rightarrow$ 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 [LeVeque, 1997]

First order scheme

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

- $\mathbf{A} \boldsymbol{\Delta} \mathbf{u}_i$ is called *fluctuation*
- Fluctuations are split $\mathbf{A} \boldsymbol{\Delta} \mathbf{u}_i = \mathbf{A}^- \boldsymbol{\Delta} \mathbf{u}_i + \mathbf{A}^+ \boldsymbol{\Delta} \mathbf{u}_i$
- Similar to flux difference splitting, but without a flux function

Solution of local Riemann problem

$$\mathbf{A}(\mathbf{u}_{i-\frac{1}{2}}) = \mathbf{R} \cdot \mathbf{\Lambda} \cdot \mathbf{R}^{-1}$$

- Wave speeds $\lambda^j = \mathbf{\Lambda}_{jj}$
- Waves $\mathbf{W}^j = \alpha^j \cdot \mathbf{R}^j$
- Wave strengths $\alpha^j = \left(\mathbf{R}^{-1} \mathbf{\Delta u}\right)_j$

Left and right going fluctuations

$$\mathbf{A}^- \mathbf{\Delta u}_i = \sum_p (\lambda^p)^- \mathbf{W}^p$$

$$\mathbf{A}^+ \mathbf{\Delta u}_i = \sum_p (\lambda^p)^+ \mathbf{W}^p$$

Second order extension

Add correction term

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{A}^+ \mathbf{\Delta u}_i + \mathbf{A}^- \mathbf{\Delta u}_{i+1}\right) - \frac{\Delta t}{\Delta x}\left(\widetilde{\mathbf{F}}_{i+1} - \widetilde{\mathbf{F}}_i\right)$$

Second order corrections

$$\widetilde{\mathbf{F}}_i = \frac{1}{2}\sum_p |\lambda_i^p| \left(1 - \frac{\Delta t}{\Delta x}|\lambda_i^p|\right) \widetilde{\mathbf{W}}_i^p$$

Limiter for stability

$$\widetilde{\mathbf{W}}_i^p = \phi\left(\theta_i^p\right) \mathbf{W}_i^p, \quad \theta_i^p = \frac{\mathbf{W}_{i-1}^p \cdot \mathbf{W}_i^p}{\mathbf{W}_i^p \cdot \mathbf{W}_i^p}$$

Summary: Wave propagation scheme

Scheme

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{A}^+\mathbf{\Delta u}_i + \mathbf{A}^-\mathbf{\Delta u}_{i+1}\right) - \frac{\Delta t}{\Delta x}\left(\widetilde{\mathbf{F}}_{i+1} - \widetilde{\mathbf{F}}_i\right)$$

+

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

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- Not exactly second order
- Not extendable to higher order
- Not for unstructured grids

PRICE-C scheme [Canestrelli, 2009]

First order scheme

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

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

FORCE scheme

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{F}^{\mathrm{FORCE}}_{\mathbf{i+\frac{1}{2}}} - \mathbf{F}^{\mathrm{FORCE}}_{\mathbf{i-\frac{1}{2}}}\right)$$

Generalization of Roe matrix

Roe matrix for conservative systems

$$\mathbf{A}_{Roe}\left(\mathbf{u}_L, \mathbf{u}_R\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) = \mathbf{F}\left(\mathbf{u}_R\right) - \mathbf{F}\left(\mathbf{u}_L\right)$$

Non-conservative case

- $\mathbf{A}_{Roe}$ depends on a path ψ between $\mathbf{u}_L$ and $\mathbf{u}_R$
- Example: $\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right) = \mathbf{u}_L + s \cdot \left(\mathbf{u}_R - \mathbf{u}_L\right), s \in [0, 1]$

Extension: Generalized Roe matrix

$$\mathbf{A}_{\psi}\left(\mathbf{u}_L, \mathbf{u}_R\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) = \int_0^1 \mathbf{A}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right) \frac{\partial \psi}{\partial s} ds$$

Generalization of Roe matrix 2

Reduces to standard Roe matrix for conservative case

$$\begin{aligned}
\mathbf{A}_{\psi}\left(\mathbf{u}_L, \mathbf{u}_R\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) &= \int_0^1 \mathbf{A}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right) \frac{\partial \psi}{\partial s} ds \\
&= \int_0^1 \frac{\partial \mathbf{F}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right)}{\partial \psi} \frac{\partial \psi}{\partial s} ds \\
&= \int_0^1 \frac{\partial \mathbf{F}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right)}{\partial s} ds \\
&= \mathbf{F}\left(\psi\left(1, \mathbf{u}_L, \mathbf{u}_R\right)\right) - \mathbf{F}\left(\psi\left(0, \mathbf{u}_L, \mathbf{u}_R\right)\right) ds \\
&= \mathbf{F}\left(\mathbf{u}_R\right) - \mathbf{F}\left(\mathbf{u}_L\right)
\end{aligned}$$

Computation of generalized Roe matrix

$$\mathbf{A}_{\psi}\left(\mathbf{u}_L, \mathbf{u}_R\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) = \int_0^1 \mathbf{A}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right)\frac{\partial \psi}{\partial s} ds$$

- Choose linear path $\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right) = \mathbf{u}_L + s \cdot \left(\mathbf{u}_R - \mathbf{u}_L\right), s \in [0, 1]$
- Use Gaussian quadrature to compute integral

Computation of generalized Roe matrix

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Computation

$$\mathbf{A}_{\psi}\left(\mathbf{u}_L, \mathbf{u}_R\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) = \int_0^1 \mathbf{A}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right)\left(\mathbf{u}_R - \mathbf{u}_L\right) ds$$

$$\implies \mathbf{A}_{\psi}\left(\mathbf{u}_L, \mathbf{u}_R\right) = \int_0^1 \mathbf{A}\left(\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right)\right) ds \approx \sum_{j=1}^{M} \omega_j \mathbf{A}\left(\psi\left(s_j, \mathbf{u}_L, \mathbf{u}_R\right)\right)$$

Complete PRICE-C scheme

First order scheme

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

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

$$\begin{aligned}
\mathbf{A}^-_{i+\frac{1}{2}} &= \frac{1}{4}\left(2\mathbf{A}_\psi\left(\mathbf{u}_i^n, \mathbf{u}_{i+1}^n\right) - \frac{\Delta x}{\Delta t}\mathbf{I} - \frac{\Delta t}{\Delta x}\left(\mathbf{A}_\psi\left(\mathbf{u}_i^n, \mathbf{u}_{i+1}^n\right)\right)^2\right) \\
\mathbf{A}^+_{i-\frac{1}{2}} &= \frac{1}{4}\left(2\mathbf{A}_\psi\left(\mathbf{u}_{i-1}^n, \mathbf{u}_i^n\right) - \frac{\Delta x}{\Delta t}\mathbf{I} - \frac{\Delta t}{\Delta x}\left(\mathbf{A}_\psi\left(\mathbf{u}_{i-1}^n, \mathbf{u}_i^n\right)\right)^2\right)
\end{aligned}$$

Higher order extension

WENO reconstruction in space

$$\mathbf{u}_i \Rightarrow \mathbf{u}_i(x)$$

ADER approach in time

$$\mathbf{u}_i(x,t) = \mathbf{u}(x_i, t^n) + (x - x_i)\frac{\partial \mathbf{u}}{\partial x} + (t - t^n)\frac{\partial \mathbf{u}}{\partial t}$$

$$\frac{\partial \mathbf{u}}{\partial t} = -\mathbf{A}(\mathbf{u})\partial_x \mathbf{u}$$

Integration of PDE over time-space volume and computation of integrals using Gaussian quadrature and reconstruction

Summary: PRICE-C scheme

Scheme

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

+

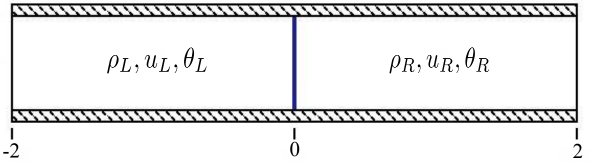
- Extension to arbitrary order
- No eigensystem needed
- For unstructured grids

-

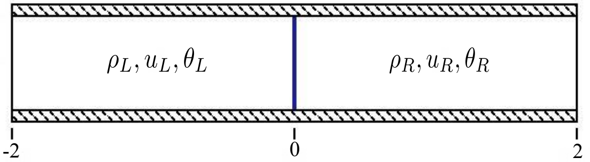
- Higher order difficult to implement
- Added numerical diffusion

Numerical Results

Shock Tube Test Case



Shock Tube Test Case



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

Model Equations

Grad model

$$\mathbf{A}_{\mathrm{Grad}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v \end{pmatrix}$$

HME model

$$\mathbf{A}_{\mathrm{HME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v \end{pmatrix}$$

Model Equations 2

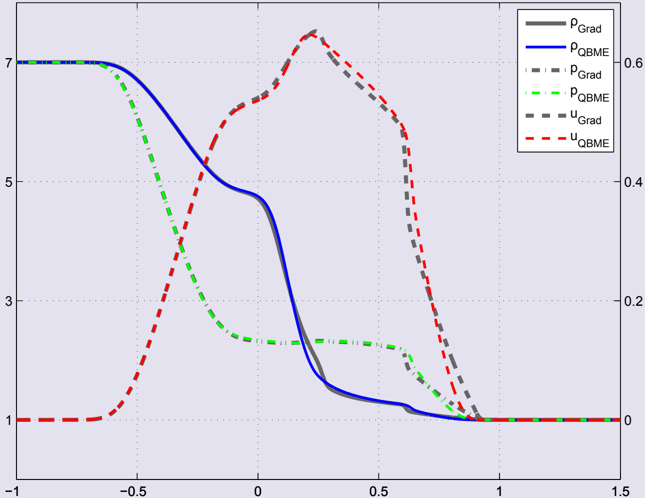
Grad model

$$\mathbf{A}_{\mathrm{Grad}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v \end{pmatrix}$$

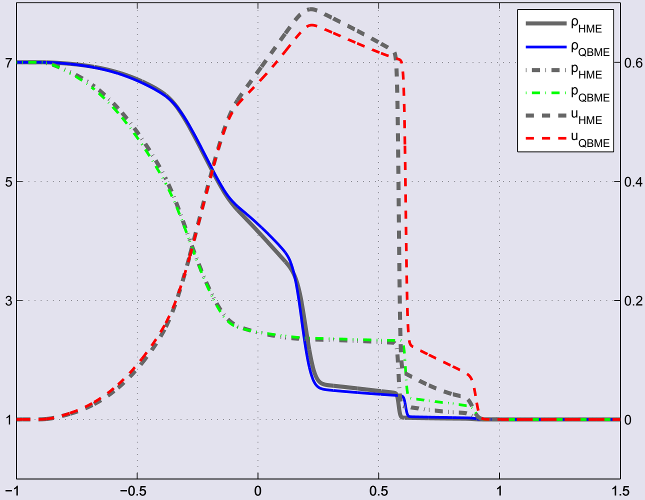
QBME model

$$\mathbf{A}_{\mathrm{QBME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} - \frac{10f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15f_4}{\rho\theta} & v \end{pmatrix}$$

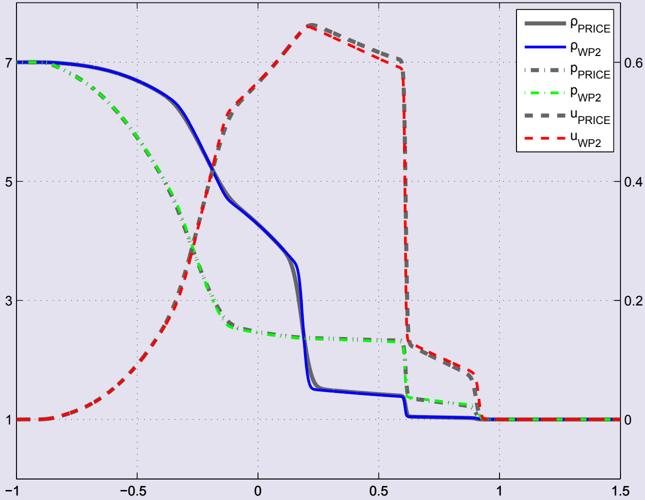
QBME vs Grad, $\mathrm{Kn} = 0.05$



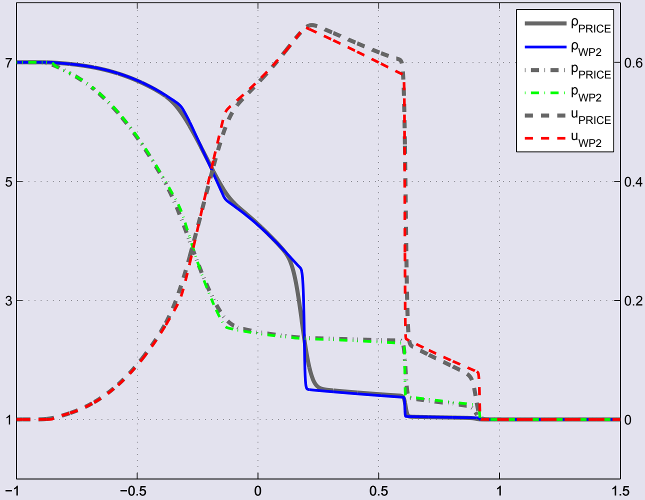
QBME vs HME, $\mathrm{Kn} = 0.5$



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



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



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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Thank you for your attention!

References

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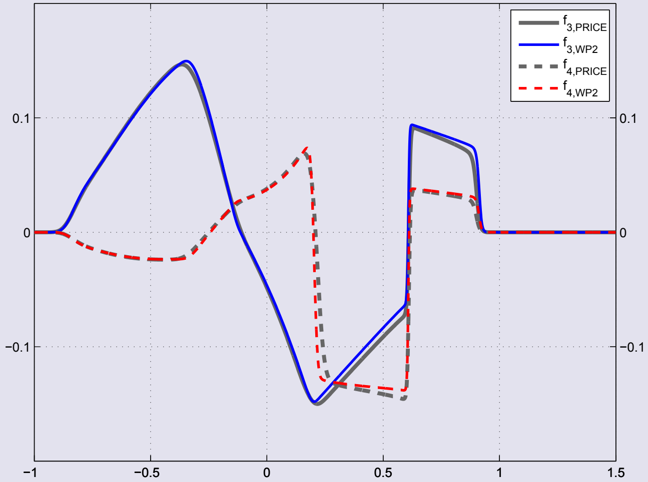
PRICE vs WP f_3, f_4



PRICE vs WP2 f_3, f_4