On the Stability and Numerical Solution of Partially Conservative Hyperbolic Moment Equations

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Introduction

A Short 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]

- use of projections

State of the art

Boltzmann equation

$$\frac{\partial}{\partial t} f + c \frac{\partial}{\partial x} f = 0$$

$$\Downarrow$$

Hyperbolic Moment equations

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

State of the art

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$$\frac{\partial}{\partial t} f + c \frac{\partial}{\partial x} f = 0$$

$$\Downarrow$$

Hyperbolic Moment equations

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

HME Summary

Achievements

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

Problems

- analysis including collision operator
- numerical simulations

Outline

1. Introduction
2. Stability of Hyperbolic Moment Equations
3. Numerical Methods
4. Simulation Results

Stability of Hyperbolic Moment Equations

Stability of Hyperbolic Relaxation System

$$\partial_t \mathbf{u} + \mathbf{A}\partial_x \mathbf{u} = \varepsilon \mathbf{B}\mathbf{u}$$

Stability of Hyperbolic Relaxation System

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Wave ansatz

$$\mathbf{u} = \mathbf{u}_0 \cdot e^{i(kx - \omega t)}, k \in \mathbb{R}, \omega \in \mathbb{C}, \quad Im(\omega) \leq 0 \text{ for stability}$$

Stability of Hyperbolic Relaxation System

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Stability analysis

$$\begin{aligned} -i\omega \mathbf{u} + ik\mathbf{A}\mathbf{u} &= \varepsilon \mathbf{B}\mathbf{u} \\ \left(k\mathbf{A} + i\varepsilon\mathbf{B} - \omega\mathbf{I}\right)\mathbf{u} &= \mathbf{0} \end{aligned}$$

Stability of Hyperbolic Relaxation System

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Stability analysis

$$\begin{aligned} -i\omega\mathbf{u} + ik\mathbf{A}\mathbf{u} &= \varepsilon\mathbf{B}\mathbf{u} \\ (k\mathbf{A} + i\varepsilon\mathbf{B} - \omega\mathbf{I})\,\mathbf{u} &= \mathbf{0} \end{aligned}$$

$$\omega = EV(k\mathbf{A} + i\varepsilon\mathbf{B})$$

$\Rightarrow k\mathbf{A} + i\varepsilon\mathbf{B}$ needs to have only eigenvalues with negative imaginary part

Instability of HME, [Zhao, Yong et al., 2015]

"Stability Analysis of a Globally Hyperbolic Moment System in One Dimension"

HME with BGK

$$\partial_t \mathbf{w} + \mathbf{D}^{-1}\mathbf{M}\mathbf{D}\partial_x \mathbf{w} \;=\; \varepsilon \mathbf{B}\mathbf{w}$$

Example: $n = 4$

Existence of eigenvalue with positive imaginary part and breakdown of numerical simulation.

Towards Stable Hyperbolic Moment Equations

HME with BGK

$$\partial_t \mathbf{w} + \mathbf{D}^{-1}\mathbf{M}\mathbf{D}\partial_x \mathbf{w} = \varepsilon \mathbf{B}\mathbf{w}$$

Linear stability analysis

$$\begin{aligned}\omega &= EV(k\mathbf{D}^{-1}\mathbf{M}\mathbf{D} + i\varepsilon\mathbf{B}) \\ &= EV(k\mathbf{M} + i\varepsilon\mathbf{D}\mathbf{B}\mathbf{D}^{-1}) \\ &= EV(k\mathbf{M} + i\varepsilon\mathbf{B}\mathbf{D}^{-1})\end{aligned}$$

Towards Stable Hyperbolic Moment Equations

HME with BGK

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Stable for $\mathbf{D} = diag(d_{ii})$!

Grad's Equations

$$\partial_t \mathbf{w} + \mathbf{A}_{\mathrm{Grad}} \partial_x \mathbf{w} = \frac{1}{\tau} \mathbf{B} \mathbf{w}$$

Grad model

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

Hyperbolic Moment Equations

$$\partial_t \mathbf{w} + \mathbf{A}_{\mathrm{HME}} \partial_x \mathbf{w} = \frac{1}{\tau} \mathbf{B} \mathbf{w}$$

HME model

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

Stable Hyperbolic Moment Equations

$$\partial_t \mathbf{w} + \mathbf{A}_{\mathrm{SHME}} \partial_x \mathbf{w} = \frac{1}{\tau} \mathbf{B} \mathbf{w}$$

SHME model

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

Numerical Methods

Conservative PDE systems

Standard conservative PDE system

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

Conservative PDE systems

Standard conservative PDE system

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

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

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

Non-conservative PDE systems

Non-conservative PDE system

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

- 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
- What about partially conservative systems?

$\Rightarrow$ Special numerical methods are needed

Numerical Methods

Wave Propagation scheme [LeVeque, 1997]

- 2^{nd} order upwind type scheme
- Implemented on 2D uniform cartesian grids

Castro scheme [Castro, Pares, 2004]

- Arbitrary order upwind type scheme
- Implemented on 2D unstructured grids

PRICE-C scheme [Canestrelli, 2009]

- Arbitrary order centered scheme
- Implemented on 2D unstructured grids

Non-conservative Numerics

How do we evaluate **A** at a cell boundary?

Non-conservative Numerics

How do we evaluate $\mathbf{A}$ at a cell boundary?

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 Numerics

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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

Reduces to standard Roe matrix for conservative case

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

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

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

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Computation

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

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

Different paths

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

linear path

$$\psi\left(s, \mathbf{u}_L, \mathbf{u}_R\right) = \mathbf{u}_L + s \cdot \left(\mathbf{u}_R - \mathbf{u}_L\right)$$

polynomial path

$$\psi_{-}^{N}\left(s, \mathbf{u}_L, \mathbf{u}_R\right) = \mathbf{u}_L + s^N \cdot \left(\mathbf{u}_R - \mathbf{u}_L\right)$$

$$\psi_{+}^{N}\left(s, \mathbf{u}_L, \mathbf{u}_R\right) = \mathbf{u}_R + (s-1)^N \cdot \left(\mathbf{u}_L - \mathbf{u}_R\right)$$

Castro scheme [Castro, Pares, 2004]

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
- Upwind type scheme, uses eigenvalue information

$$\mathbf{A}^{\pm}_{i+\frac{1}{2}} = \mathbf{A}_\psi\left(\mathbf{u}_i, \mathbf{u}_{i+1}\right)^{\pm} = \mathbf{R}_\psi \cdot \mathbf{\Lambda}^{\pm}_\psi \cdot \mathbf{R}_\psi^{-1}$$

Summary: Castro 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
- For 2D unstructured grids

-

- Eigensystem needed

PRICE-C scheme [Canestrelli, 2009]

First order scheme

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

- Same notation as Castro scheme
- PRImitive CEntered scheme, uses no eigenvalue information
- Reduces to FORCE scheme in the conservative case

FORCE scheme

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

Complete PRICE-C scheme

First order scheme

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

Complete PRICE-C scheme

First order scheme

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

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

Summary: PRICE-C scheme

Scheme

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

+

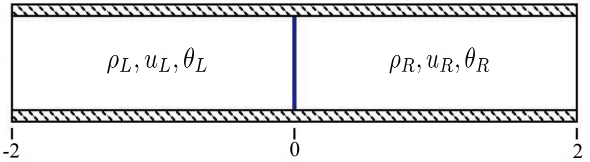
- Extension to arbitrary order
- For 2D unstructured grids
- No eigensystem needed

-

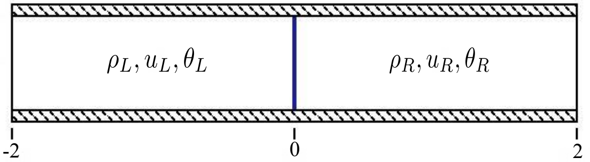
- Added numerical diffusion

Simulation Results

Shock Tube Test Case



Shock Tube Test Case



Riemann problem with BGK collision operator

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

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

- Variable vector $\mathbf{w} = (\rho, u, \theta, f_3, f_4)$
- 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

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

Model Equations 3

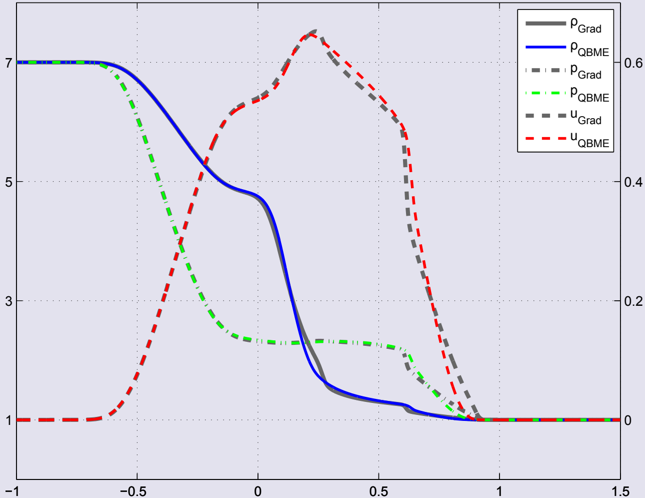
Grad model

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

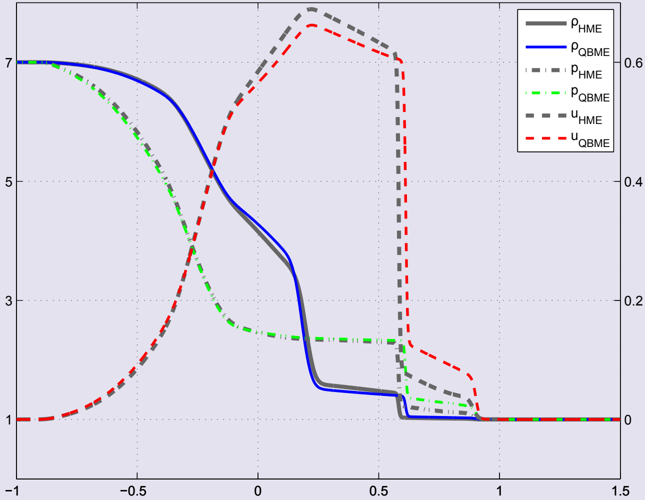
SHME model

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

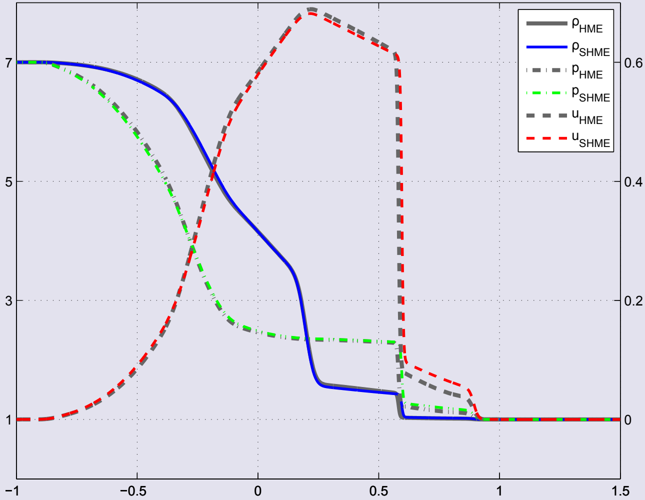
Grad vs QBME, $\mathrm{Kn} = 0.05$



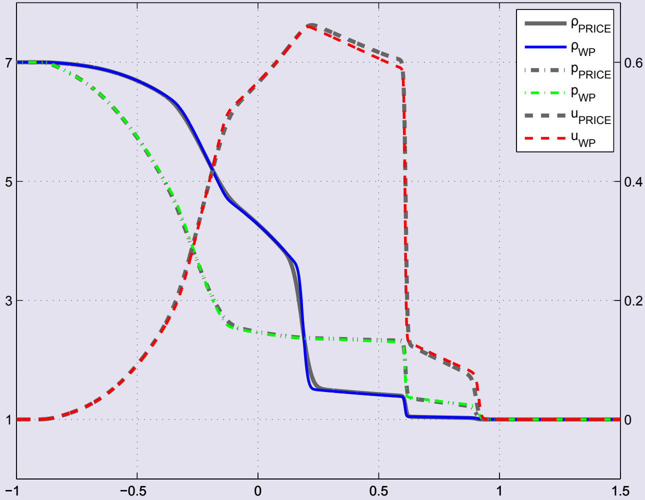
HME vs QBME, $\mathrm{Kn} = 0.5$



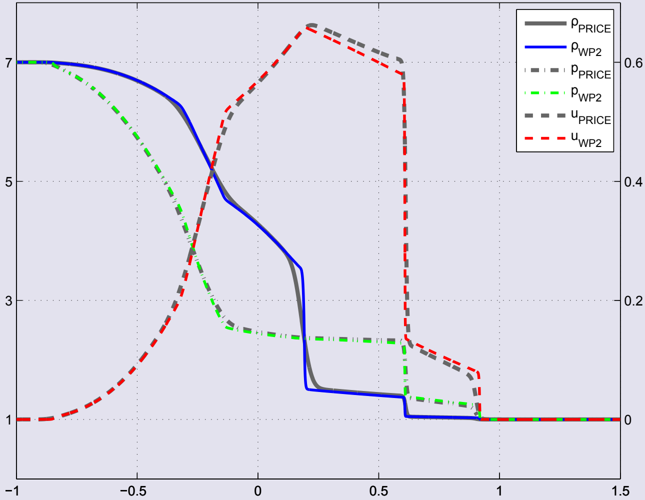
HME vs SHME, $\mathrm{Kn} = 0.5$



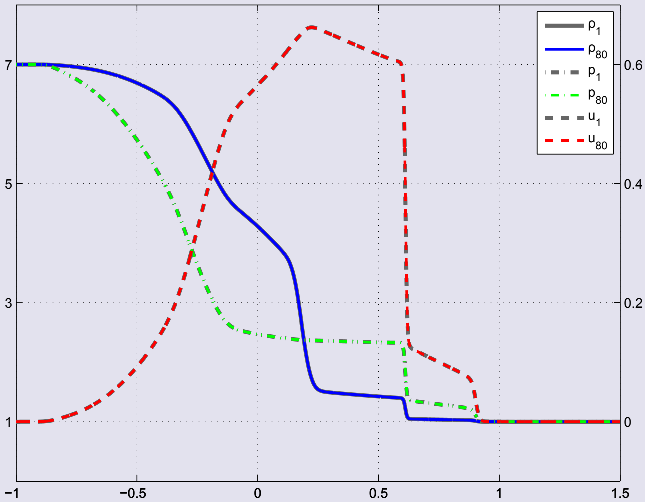
PRICE vs WP/Castro, $\mathrm{Kn} = 0.5$



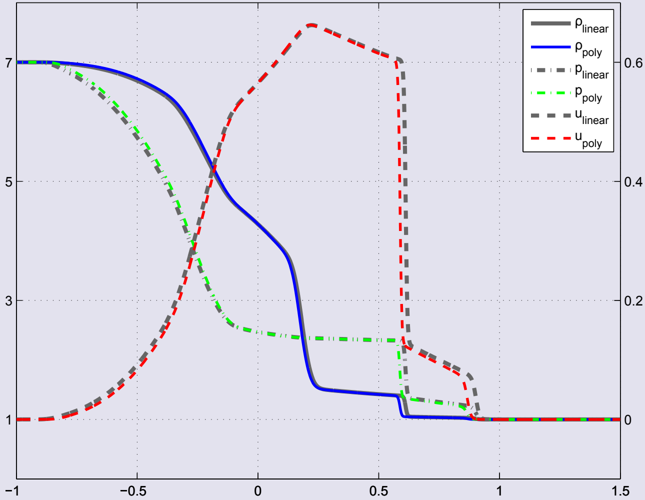
PRICE vs WP2, $\mathrm{Kn} = 0.5$



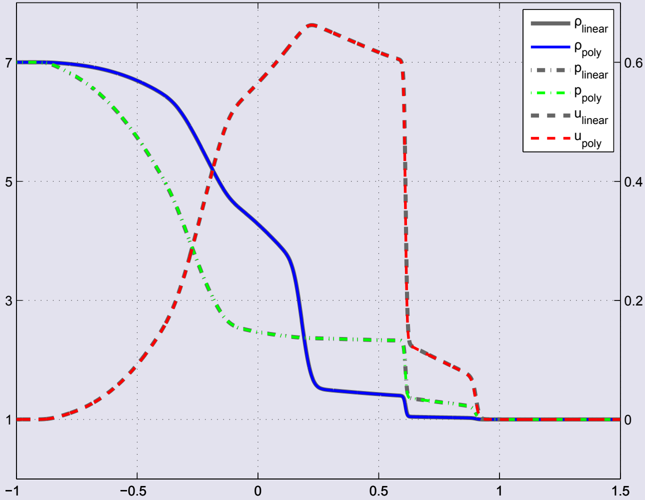
Linear Path, integration 1 vs 80 points



Linear vs Polynomial Path 20 Points



Linear vs Polynomial Path 80 Points



Summary and Further Work

(1) Stability of HME
(2) Non-conservative numerics for HME
(3) Simulation Results of HME

Further Work

- Linear Stability Analysis
- Higher order schemes
- More simulations and test cases

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Thank you for your attention!

References

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