Moment Models for Kinetic Equations

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joint work with
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NUMA seminar, KU Leuven

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Content of this talk

1. Moment Equations for Rarefied Gases
2. Moment Equations for Shallow Water Flows
3. Projective Integration for Moment Models

Moment Equations for Rarefied Gases

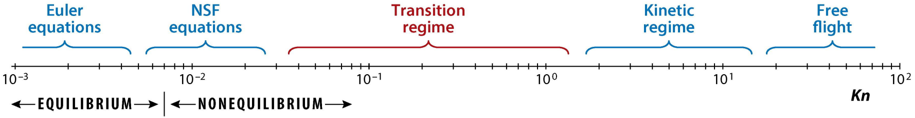
Motivation: Rarefied gases

Task

Simulation of flow problems involving rarefied gases

Characterize a rarefied gas by a large *Knudsen number*

$$\mathrm{Kn} = \frac{\text{mean free path length}}{\text{reference length}} = \frac{\lambda}{L}$$



From Micro and Macro to Meso

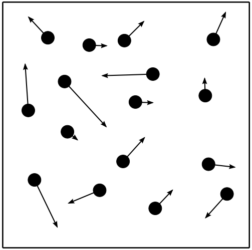
Macroscopic

$$\rho(t,x)$$
$$v(t,x)$$
$$\theta(t,x)$$

Mesoscopic

$$f(t,x,c)$$

Microscopic



Macroscopic

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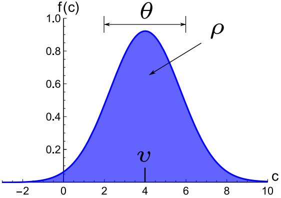
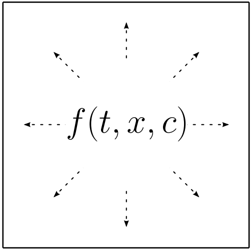
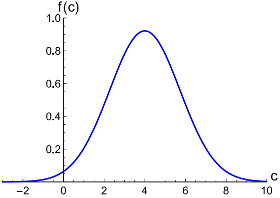
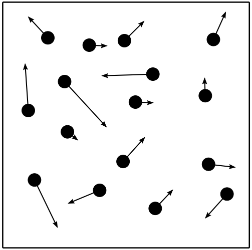


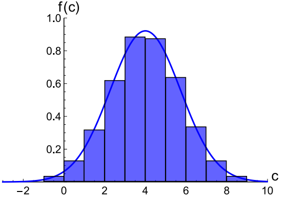
Mesoscopic





Microscopic



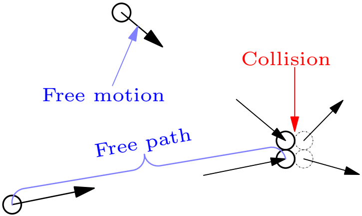


Model: Boltzmann Transport Equation

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

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

- describes change of f due to transport and collisions
- 7-dimensional phase space $(t, x, y, z, c_x, c_y, c_z)$



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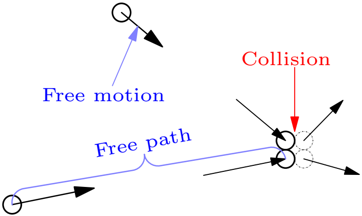
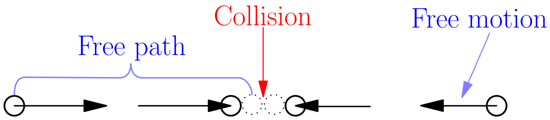


Model: Boltzmann Transport Equation 1D

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

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

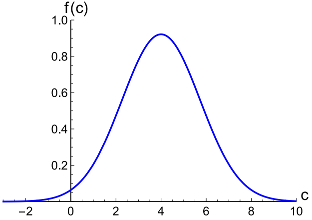
- describes change of f due to transport and collisions
- 3-dimensional phase space (t,x,c)



From $f(t, x, c)$ to moments

Macroscopic quantities

- density $\rho(t, x)$
- velocity $v(t, x)$
- temperature $\theta(t, x)$



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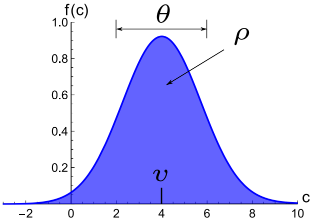
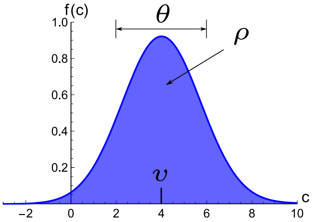


$$
\begin{aligned}
\rho(t,x) &= \int_{\mathbb{R}} f(t,x,c)\,dc \\
\rho(t,x)v(t,x) &= \int_{\mathbb{R}} c\,f(t,x,c)\,dc \\
\frac{1}{2}\rho(t,x)\theta(t,x) + \frac{1}{2}\rho(t,x)v(t,x)^2 &= \int_{\mathbb{R}} \frac{1}{2}c^2\,f(t,x,c)\,dc
\end{aligned}
$$

From $f(t,x,c)$ to moments

Macroscopic quantities

- density $\rho(t,x)$
- velocity $v(t,x)$
- temperature $\theta(t,x)$
- ...



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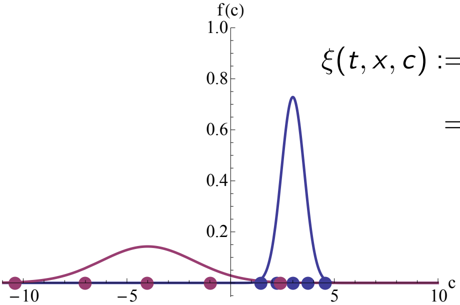
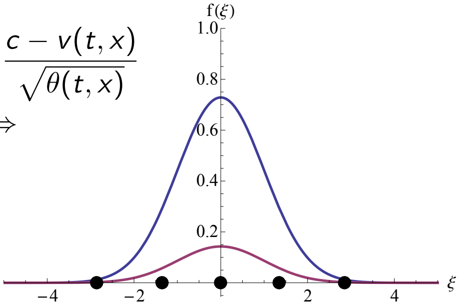
&\vdots
\end{aligned}$$



$$\xi(t,x,c) := \frac{c - v(t,x)}{\sqrt{\theta(t,x)}}$$

$$\Longrightarrow$$



$$f(c) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{(c-v)^2}{2\theta}\right)$$

$$f(\xi) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{\xi^2}{2}\right)$$

Moment method: Grad's method [Grad, 1949]

Grad ansatz: expansion in transformed velocity space

$$f(t,x,c) = \sum_{\alpha=0}^{M} f_\alpha(t,x)\,\phi_\alpha\!\left(\frac{c-v}{\sqrt{\theta}}\right)$$

Galerkin method

Multiplication with test function and integration over c: $\int_{\mathbb{R}} \cdot\, \psi_\alpha(c)\, dc$

Moment method: Grad's method [Grad, 1949]

Grad ansatz: expansion in transformed velocity space

$$f(t,x,c) = \sum_{\alpha=0}^{M} f_\alpha(t,x)\,\phi_\alpha\left(\frac{c-v}{\sqrt{\theta}}\right)$$

Galerkin method

Multiplication with test function and integration over c: $\int_{\mathbb{R}} \cdot\, \psi_\alpha(c)\, dc$

Model reduction

One PDE for $f(t,x,c)$ that is high-dimensional

$$\Downarrow$$

System of PDEs for $\rho(t,x), v(t,x), \theta(t,x), f_\alpha(t,x)$ that is low-dimensional

Grad's moment model

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}(\boldsymbol{u}_M)\,\partial_x \boldsymbol{u}_M = \boldsymbol{S}, \quad \boldsymbol{u}_M = (\rho, v, \theta, f_3, f_4, \ldots, f_M)^T$$

1. **Grad**'s equations [Grad, 1949]

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

Grad's moment model

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}(\boldsymbol{u}_M)\,\partial_x \boldsymbol{u}_M = \boldsymbol{S}, \quad \boldsymbol{u}_M = (\rho, v, \theta, f_3, f_4, \ldots, f_M)^T$$

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Imaginary eigenvalues $\Rightarrow$ Loss of hyperbolicity $\lightning$

Hyperbolic moment models

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}\partial_x \boldsymbol{u}_M = \boldsymbol{S}, \quad \boldsymbol{u}_M = (\rho, v, \theta, f_3, f_4, \dots, f_M)^T$$

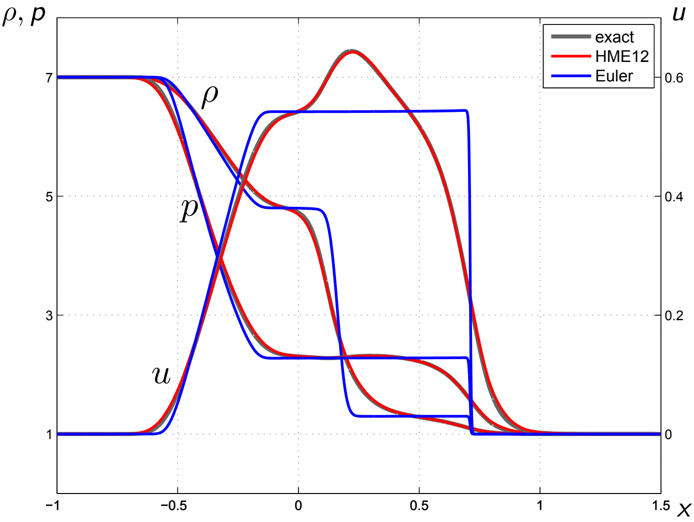
1. Hyperbolic Moment Equations (**HME**) [Cai et al., 2013]
2. Quadrature-Based Moment Equations (**QBME**) [JK, 2013]

$$\boldsymbol{A}_{\mathrm{HME}} \qquad\qquad \boldsymbol{A}_{\mathrm{QBME}}$$

$$\begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v \end{pmatrix}, \quad \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} - \frac{10f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15f_4}{\rho\theta} & v \end{pmatrix}$$

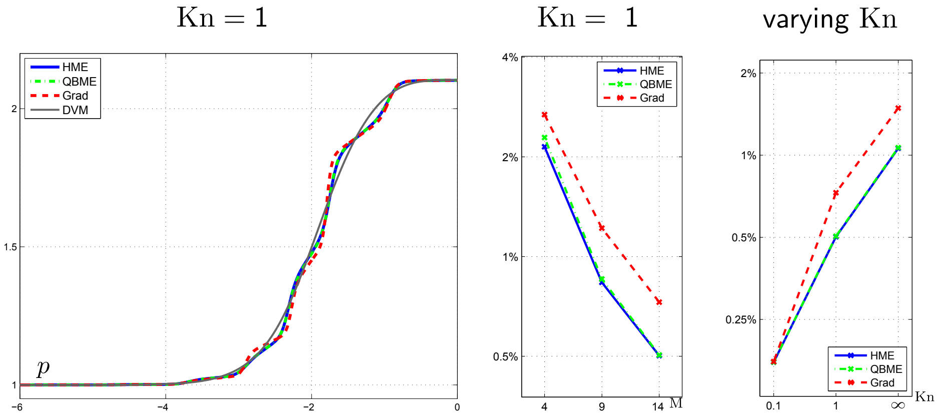
Real eigenvalues $\Rightarrow$ Hyperbolicity for all states $\boldsymbol{u}_M$

Euler vs Moment Equations, $\mathrm{Kn} = 0.05$



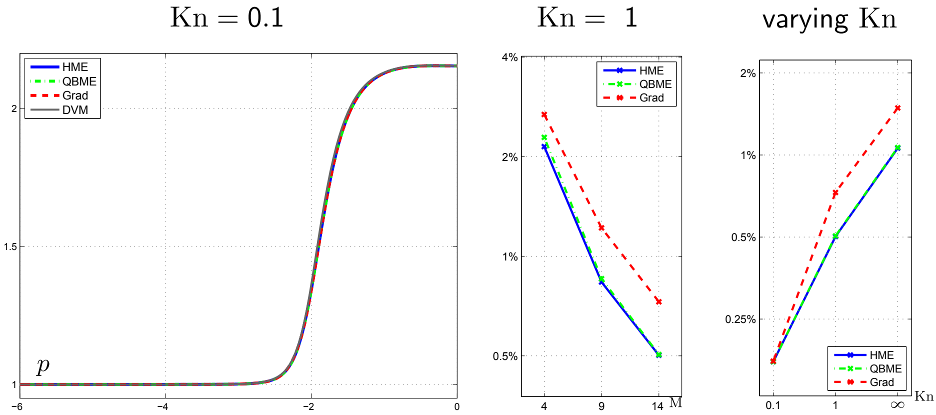
$\Rightarrow$ Moment model yields efficient, yet accurate solution

1D two beam problem



- increased accuracy of hyperbolic models
- convergence with increasing M and decreasing Kn

1D two beam problem



- increased accuracy of hyperbolic models
- convergence with increasing M and decreasing Kn

1. Euler ($\mathrm{Kn} = 0$)

2. QBME $\mathrm{Kn} = 0.001$

3. QBME $\mathrm{Kn} = 0.01$

4. QBME $\mathrm{Kn} = 0.1$

Moment models for the Boltzmann Equation

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}(\boldsymbol{u}_M)\,\partial_x \boldsymbol{u}_M = \boldsymbol{S}, \quad \boldsymbol{u}_M = (\rho, v, \theta, f_3, f_4, \ldots, f_M)^T$$

Extensions

- *nD* case [Cai et al., 2014], [JK, Torrilhon, 2014]

Theoretical background

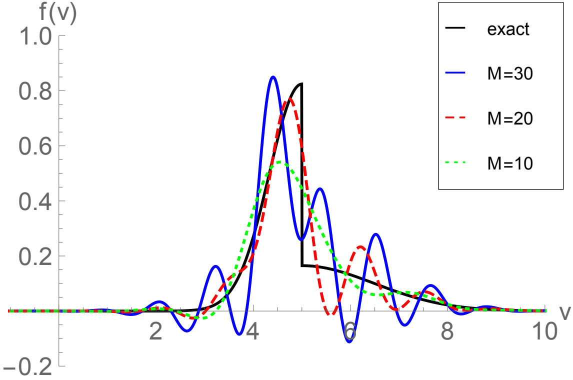
- framework of hyperbolicity [Fan et al., 2016]
- non-conservative Numerics [JK, Torrilhon, 2017]

Applications

- Vlasov-Maxwell [Cai et al., 2015]
- relativistic Boltzmann equation [Kuang, Tang, 2017], ...

Problem: Oscillations for discontinuous f

Polynomial expansion can lead to problems at discontinuities



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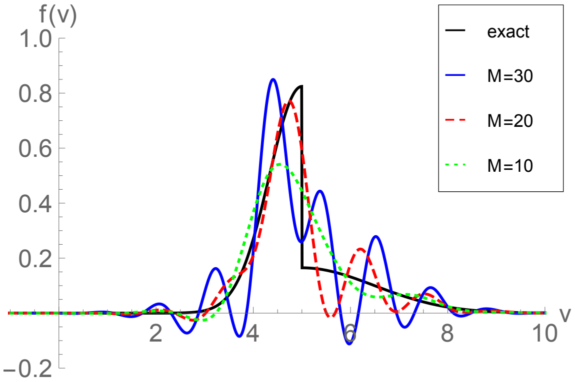
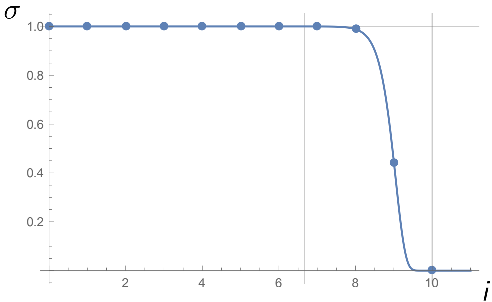


$\Rightarrow$ Filter higher modes of expansion

Filtered moment models [Di et al., 2018]

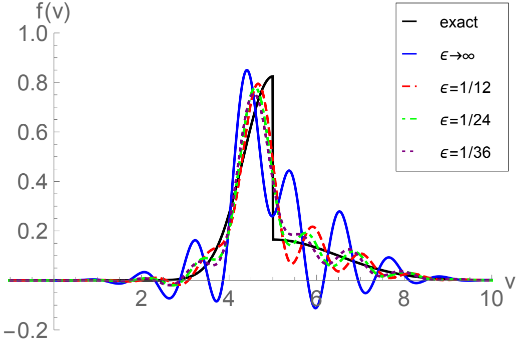
Apply filter function to basis coefficients

$$\widetilde{f_i^n} = \sigma\left(\epsilon, i, \Delta t\right) \cdot f_i^n$$



- keep low-order moments unchanged
- filter high-order moments

Filtered Hermite expansion, $M = 30$

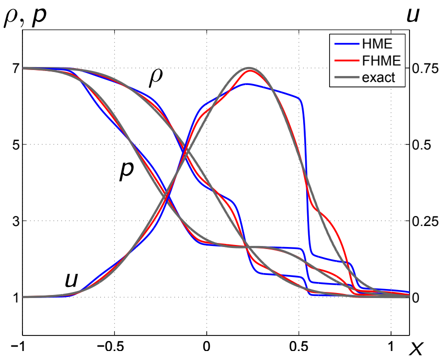


Filtered Hermite expansion minimizes

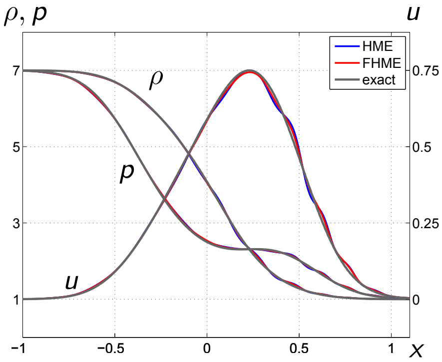
$$J_\sigma(f_M) = \int_{\mathbb{R}} \left((f(c) - f_M(c))^2 + \sigma \cdot (\partial_{cc} f_M(c))^2 \right) \omega(c)^{-1}\, dc$$

$\Rightarrow$ Filter removes oscillations and negativity of f

FHME, $\mathrm{Kn} = 1$, [Fan, JK, submitted]



(a) $M = 6$



(b) $M = 21$

$\Rightarrow$ FHME yields better solution

Summary

$$\widetilde{f_i^n} = \sigma\left(\epsilon, i, \Delta t\right) \cdot f_i^n$$

Filtered HME

- increased accuracy for shock tube, two beam
- almost no computational overhead

Further work

- apply filter to Uncertainty Quantification
- apply filter to other moment models

Moment Equations for Shallow Water Flows

joint work with
Marvin Rominger, Freie Universität Berlin

Meso model: Incompressible Navier-Stokes

Full three-dimensional model

$$\text{Mass:} \qquad \nabla \cdot \boldsymbol{u} = 0$$

$$\text{Momentum:} \qquad \partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma} + g$$

with velocity vector $\boldsymbol{u} = (u, v, w)^T$

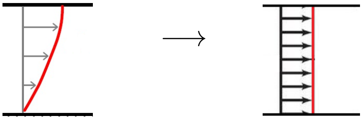
Goal

reduce dimension for shallow flows

Macro model: Shallow Water

Assumption

Velocity profile is constant over height



Velocity components are averaged over height:

$$u_m(t,x) = \frac{1}{h_s - h_b} \int_{h_b}^{h_s} u(z)\ dz$$

$$\partial_t h + \partial_x (h u_m) = 0$$

$$\partial_t (h u_m) + \partial_x \left(h u_m^2 + \frac{1}{2} g h^2 \right) = -hg\partial_x h_b$$

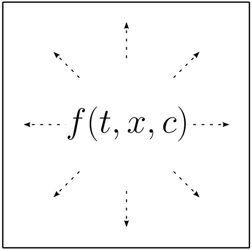
Macroscopic

$\rho(t,x)$

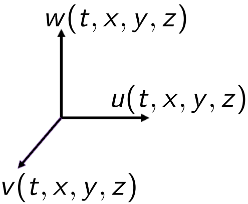
$v(t,x)$

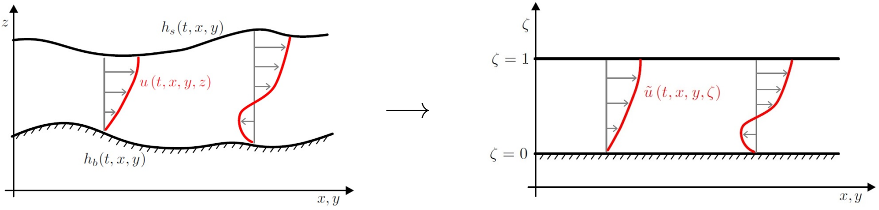
$\theta(t,x)$

Mesoscopic



$u(t,x)$





$$z \mapsto \zeta = \frac{z - h_b}{h_s - h_b} = \frac{z - h_b}{h}$$

Moment model [Torrilhon, Kowalski, 2018]

Moment ansatz: expansion in transformed velocity space

$$u(t,x,\zeta) = \underbrace{u_m(t,x)}_{\text{Mean of } u} + \underbrace{\sum_{j=1}^{N} \alpha_j(t,x)\phi_j(\zeta)}_{\text{Deviation of } u}$$

Galerkin method

Multiplication with test function and integration over ζ: $\int_0^1 \cdot\, \psi_\alpha(\zeta)\, d\zeta$

Model reduction

One PDE for $u(t,x,\zeta)$ that is high-dimensional

$\Downarrow$

System of PDEs for $h(t,x), u_m(t,x), \alpha_j(t,x)$ that is low-dimensional

Shallow Water Moment Equations (SWME) (1)

$N = 0$: Zeroth order system (Shallow water equations):

$$\partial_t \begin{pmatrix} h \\ hu_m \end{pmatrix} + \partial_x \begin{pmatrix} hu_m \\ hu_m^2 + \frac{gh^2}{2} \end{pmatrix} = -\frac{\nu}{\lambda} \begin{pmatrix} 0 \\ u_m \end{pmatrix}$$

$N = 1$: First order system:

$$\partial_t \begin{pmatrix} h \\ hu_m \\ hs \end{pmatrix} + \partial_x \begin{pmatrix} hu_m \\ hu_m^2 + \frac{gh^2}{2} + \frac{1}{3} hs^2 \\ 2hu_m s \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ u_m \partial_x (hs) \end{pmatrix} - \frac{\nu}{\lambda} \begin{pmatrix} 0 \\ u_m + s \\ 3(u_m + s + 4\frac{\lambda}{h} s) \end{pmatrix}$$

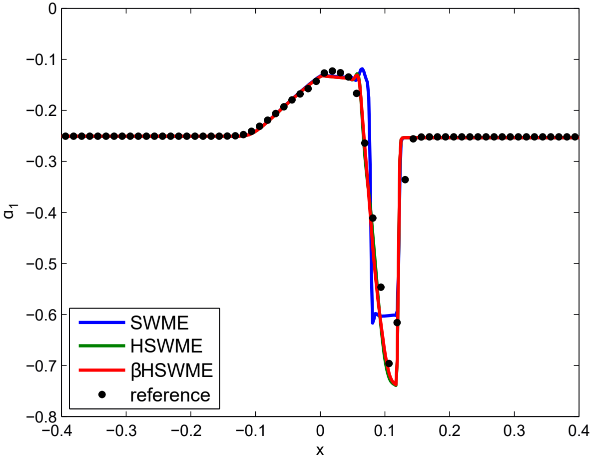
$N = 2$: Second order system:

$$\partial_t \begin{pmatrix} h \\ hu_m \\ hs \\ h\kappa \end{pmatrix} + \partial_x \begin{pmatrix} hu_m \\ hu_m^2 + \frac{gh^2}{2} + \frac{1}{3}hs^2 + \frac{1}{5}h\kappa^2 \\ 2hu_m s + \frac{4}{5}hs\kappa \\ 2hu_m\kappa + \frac{2}{3}hs^2 + \frac{2}{7}h\kappa^2 \end{pmatrix} = \mathbf{Q}\partial_x \begin{pmatrix} h \\ hu_m \\ hs \\ h\kappa \end{pmatrix} - \frac{\nu}{\lambda}\mathbf{P}$$

$$\mathbf{Q} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & u_m - \frac{\kappa}{5} & \frac{s}{5} \\ 0 & 0 & s & u_m + \frac{\kappa}{7} \end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix} 0 \\ u_m + s + \kappa \\ 3(u_m + s + \kappa + 4\frac{\lambda}{h}s) \\ 5(u_m + s + \kappa + 12\frac{\lambda}{h}\kappa) \end{pmatrix}$$

Imaginary eigenvalues $\Rightarrow$ Loss of hyperbolicity $\lightning$

Dam break test instability, $N = 3$



Unstable for SWME, stable for HSWME, β-HSWME

$\Rightarrow$ New hyperbolic models remove instabilities

Dam break test case, convergence

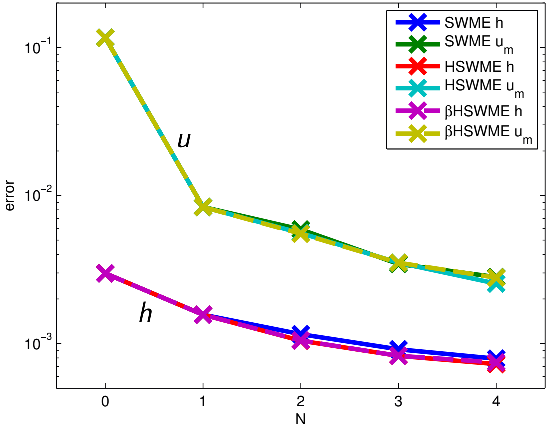


Figure: Error convergence of dam break test case.

$\Rightarrow$ New hyperbolic models show similar convergence

Summary of Shallow Water Moment Equations

$$u(t,x,\zeta) = \underbrace{u_m(t,x)}_{\text{Mean of } u} + \underbrace{\sum_{j=1}^{N} \alpha_j(t,x)\phi_j(\zeta)}_{\text{Deviation of } u}$$

Hyperbolic SWME

- guarantee hyperbolicity
- remove instability
- similar convergence

Further work

- apply filter
- investigate numerics

Projective Integration for Moment Models

joint work with
Giovanni Samaey, KU Leuven

Asymptotic preserving for stiff right-hand side

$$\partial_t \boldsymbol{u} + \boldsymbol{A}(\boldsymbol{u})\partial_x \boldsymbol{u} = \boldsymbol{S}(\boldsymbol{u}), \quad \boldsymbol{u} = (\rho, v, \theta, f_3, f_4, \ldots, f_M)^T$$

$$\boldsymbol{S}(\boldsymbol{u}) = -\frac{1}{\tau}\mathrm{diag}(0,0,0,1,\ldots,1)\,\boldsymbol{u}$$

Asymptotic behavior

- $\tau \to \infty$ collisionless case, free flow
- $\tau \to 0$ continuum case, macroscopic equations sufficient

Asymptotic preserving for stiff right-hand side

$$\partial_t \boldsymbol{u} + \boldsymbol{A}(\boldsymbol{u})\partial_x \boldsymbol{u} = \boldsymbol{S}(\boldsymbol{u}), \quad \boldsymbol{u} = (\rho, v, \theta, f_3, f_4, \dots, f_M)^T$$

$$\boldsymbol{S}(\boldsymbol{u}) = -\frac{1}{\tau}\mathrm{diag}(0,0,0,1,\dots,1)\,\boldsymbol{u}$$

Asymptotic behavior

- $\tau \to \infty$ collisionless case, free flow
- $\tau \to 0$ continuum case, macroscopic equations sufficient

Problem: stiff problem for $\tau \to 0$

Time splitting only second order and not for arbitrary collision terms

$$\partial_t \boldsymbol{u} + \boldsymbol{A}(\boldsymbol{u})\partial_x \boldsymbol{u} = \boldsymbol{S}(\boldsymbol{u})$$

After discretization in space

$$\partial_t \boldsymbol{u} = -D_x(\boldsymbol{u}) + S(\boldsymbol{u})$$

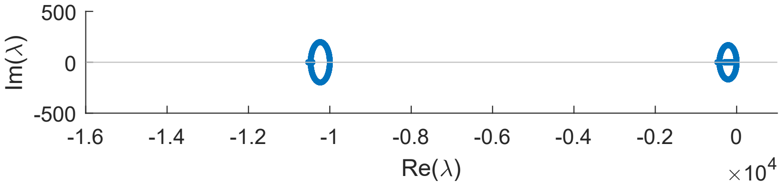
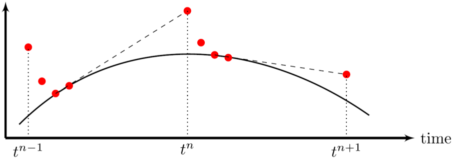


Figure: Spectral gap for $\tau = 10^{-3}$.

Idea: Use Projective Integration for stiff right-hand side

Projective Integration (PI)



1. $K+1$ inner steps:

$$\boldsymbol{u}_M^{n,k+1} = \boldsymbol{u}_M^{n,k} + \delta t D_t \left(\boldsymbol{u}_M^{n,k} \right), \quad k = 0, 1, \ldots, K.$$

2. Extrapolation step:

$$\boldsymbol{u}_M^{n+1} = \boldsymbol{u}_M^{n,K+1} + (\Delta t - (K+1)\delta t) \frac{\boldsymbol{u}_M^{n,K+1} - \boldsymbol{u}_M^{n,K}}{\delta t}.$$

Projective Integration (PI)

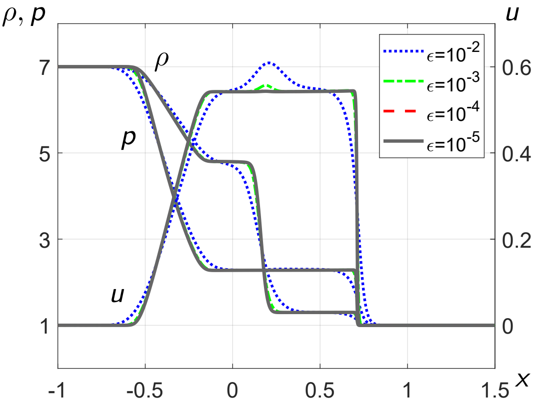
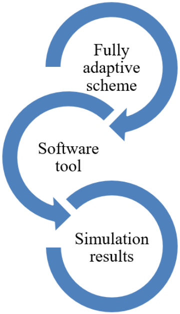


Figure: Shock tube solution using PI

Further work

- higher order numerics and non-linear collision operators
- adaptive PI

Marie Curie project FASTKiT



FASTKiT: Fully Adaptive Simulation Tool for Kinetic Theory

- projective integration for continuum limit
- use adaptive moment model
- extend to adaptivity in space and time

Summary

Moment equations for rarefied gases

- hyperbolic moment equations
- filtered moment equations

Moment Equations for Shallow Water Flows

- hyperbolic shallow water moment equations

Projective Integration for Moment models

- asymptotic preserving method
- Marie Curie FASTKiT

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Thank you for your attention!

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