Moment Methods and Adaptive Spectral Methods in the Gas Kinetic Theory

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Boltzmann equation

- **Boltzmann equation:**

$$\frac{\partial f}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{c} f) = Q(f,f), \qquad t \in \mathbb{R}^+, \quad \boldsymbol{x} \in \mathbb{R}^3, \quad \boldsymbol{c} \in \mathbb{R}^3$$

- **Macroscopic quantities:**
  - Density: $\rho(t,\boldsymbol{x}) = m \int_{\mathbb{R}^3} f(t,\boldsymbol{x},\boldsymbol{c})\,\mathrm{d}\boldsymbol{c}$
  - Velocity: $\boldsymbol{u}(t,\boldsymbol{x}) = \dfrac{m}{\rho(t,\boldsymbol{x})} \int_{\mathbb{R}^3} \boldsymbol{c} f(t,\boldsymbol{x},\boldsymbol{c})\,\mathrm{d}\boldsymbol{c}$
  - Temperature: $T(t,\boldsymbol{x}) = \dfrac{m}{3\rho(t,\boldsymbol{x})R} \int_{\mathbb{R}^3} |\boldsymbol{c} - \boldsymbol{u}(t,\boldsymbol{x})|^2 f(t,\boldsymbol{x},\boldsymbol{c})\,\mathrm{d}\boldsymbol{c}$

- **Equilibrium (Maxwellian):**

$$\mathcal{M}(\boldsymbol{c}) = \frac{\rho}{m(2\pi RT)^{3/2}} \exp\left(-\frac{|\boldsymbol{c}-\boldsymbol{u}|^2}{2RT}\right)$$

Grad's moment method

- **Ansatz:**

$$f(t,\boldsymbol{x},\boldsymbol{c}) = \sum_{n=0}^{N} a_{i_1\cdots i_n}(t,\boldsymbol{x}) c_{i_1}\cdots c_{i_n} \exp\left(-\frac{|\boldsymbol{c}-\boldsymbol{u}(t,\boldsymbol{x})|^2}{2RT(t,\boldsymbol{x})}\right)$$

$$= \sum_{n=0}^{N} a_{i_1\cdots i_n}(t,\boldsymbol{x}) \phi_{i_1\cdots i_n}^{[\boldsymbol{u}(t,\boldsymbol{x}),T(t,\boldsymbol{x})]}(\boldsymbol{c})$$

- **Grad's moment equations:**

$$\int_{\mathbb{R}^3} c_{i_1}\cdots c_{i_n}\left[\partial_t f + \nabla_{\boldsymbol{x}}\cdot(\boldsymbol{c}f)\right]\,\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} c_{i_1}\cdots c_{i_n} Q(f,f)\,\mathrm{d}\boldsymbol{c}$$

$$n = 0,\cdots,N \qquad i_1,\cdots,i_n = 1,2,3$$

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$$n = 0,\cdots,N \qquad i_1,\cdots,i_n = 1,2,3$$

- **Taking moments $\Leftrightarrow$ Taking the inner product:**

$$\int_{\mathbb{R}^3} c_{i_1}\cdots c_{i_n} g(\boldsymbol{c})\,\mathrm{d}\boldsymbol{c} = \left\langle g, \phi_{i_1\cdots i_n}^{[\boldsymbol{u},T]} \right\rangle$$
$$\langle f_1, f_2\rangle = \int_{\mathbb{R}^3} f_1(\boldsymbol{c}) f_2(\boldsymbol{c}) [\phi^{[\boldsymbol{u},T]}(\boldsymbol{c})]^{-1}\,\mathrm{d}\boldsymbol{c}$$

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- **Grad's moment equations:**

$$\mathcal{P}_N^{[\boldsymbol{u},T]}[\partial_t f + \nabla_{\boldsymbol{x}}\cdot(\boldsymbol{c}f)] = \mathcal{P}_N^{[\boldsymbol{u},T]} Q(f,f)$$

where $\mathcal{P}_N^{[\boldsymbol{u},T]}$ is the projection operator onto the space

$$\operatorname{span}\left\{\phi_{i_1\cdots i_n}^{[\boldsymbol{u},T]} \,\middle|\, n=0,\cdots,N\right\} \subset L^2\left(\mathbb{R}^3; [\phi^{[\boldsymbol{u},T]}(\boldsymbol{c})]^{-1}\,\mathrm{d}\boldsymbol{c}\right)$$

- **Taking moments ⇔ Taking the inner product:**

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Hyperbolic moment method

- **Grad's moment equations are not globally hyperbolic!**
- **Grad's moment equations:**

$$\mathcal{P}_N^{[\boldsymbol{u},T]}\partial_t f + \mathcal{P}_N^{[\boldsymbol{u},T]}(c_i\partial_{x_i} f) = \mathcal{P}_N^{[\boldsymbol{u},T]}Q(f,f)$$

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⊕ The system is globally hyperbolic
⊖ The balance law form is lost

Balance law:

$$\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{w})}{\partial x} = \mathbf{P}(\boldsymbol{w})\boldsymbol{w}$$

Weak form:

$$\int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{\varphi}^T \frac{\partial \boldsymbol{w}}{\partial t}\,\mathrm{d}x\,\mathrm{d}t + \int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{\varphi}^T \frac{\partial \boldsymbol{F}(\boldsymbol{w})}{\partial x}\,\mathrm{d}x\,\mathrm{d}t = \int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{\varphi}^T \mathbf{P}(\boldsymbol{w})\boldsymbol{w}\,\mathrm{d}x\,\mathrm{d}t$$

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General first-order quasi-linear system:

$$\frac{\partial \boldsymbol{w}}{\partial t} + \mathbf{A}(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial x} = \mathbf{P}(\boldsymbol{w}) \boldsymbol{w}$$

Weak form:

$$\int_{\mathbb{R}+} \int_{\mathbb{R}} \boldsymbol{\varphi}^T \frac{\partial \boldsymbol{w}}{\partial t} \,\mathrm{d}x \,\mathrm{d}t + \int_{\mathbb{R}+} \int_{\mathbb{R}} \boldsymbol{\varphi}^T \mathbf{A}(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial x} \,\mathrm{d}x \,\mathrm{d}t = \int_{\mathbb{R}+} \int_{\mathbb{R}} \boldsymbol{\varphi}^T \mathbf{P}(\boldsymbol{w}) \boldsymbol{w} \,\mathrm{d}x \,\mathrm{d}t$$

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$$\int_{\mathbb{R}} \boldsymbol{w}^T\boldsymbol{\varphi}\big|_{t=0}\,\mathrm{d}x + \int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{w}^T\frac{\partial\boldsymbol{\varphi}}{\partial t}\,\mathrm{d}x\,\mathrm{d}t - \int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{\varphi}^T\mathbf{A}(\boldsymbol{w})\frac{\partial \boldsymbol{w}}{\partial x}\,\mathrm{d}x\,\mathrm{d}t = -\int_{\mathbb{R}+}\int_{\mathbb{R}} \boldsymbol{\varphi}^T\mathbf{P}(\boldsymbol{w})\boldsymbol{w}\,\mathrm{d}x\,\mathrm{d}t$$

Moment methods and adaptive basis functions

- Ansatz in the moment methods:

$$f(t, \boldsymbol{x}, \boldsymbol{c}) = \sum_{n=0}^{N} a_{i_1 \cdots i_n}(t, \boldsymbol{x}) c_{i_1} \cdots c_{i_n} \exp\left(-\frac{|\boldsymbol{c} - \boldsymbol{u}(t, \boldsymbol{x})|^2}{\sqrt{RT(t, \boldsymbol{x})}} \right)$$

- $\boldsymbol{u}$ and T add adaptivity to the basis functions!

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- $\boldsymbol{u}$ and T add adaptivity to the basis functions!
- General route chart for adaptive methods:

SOLVE (EVOLVE) → ADAPT MESH → UPDATE SOLUTION

- Application in the kinetic theory:
  - SOLVE:

$$\bar{f}^{n+1} = f^n - \Delta t \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{c} f^n) + \Delta t Q(f^n, f^n)$$

  - ADAPT MESH:

$$\boldsymbol{u}^{n+1} = \frac{\langle \boldsymbol{c} \bar{f}^{n+1} \rangle}{\langle \bar{f}^{n+1} \rangle} \qquad T^{n+1} = \frac{\langle |\boldsymbol{c}-\boldsymbol{u}^{n+1}|^2 \bar{f}^{n+1} \rangle}{3R \langle \bar{f}^{n+1} \rangle}$$

  - UPDATE SOLUTION:

$$f^{n+1} = \mathcal{P}_N^{[\boldsymbol{u}^{n+1}, T^{n+1}]} \bar{f}^{n+1}$$

- $\mathcal{P}_N^{[\boldsymbol{u},T]}$ keeps moments up to Nth order $\Rightarrow \mathcal{P}_N^{[\boldsymbol{u}_1,T_1]} \mathcal{P}_N^{[\boldsymbol{u}_2,T_2]} g = \mathcal{P}_N^{[\boldsymbol{u}_1,T_1]} g$

Numerical scheme based on adaptive basis functions

- Discretization of spatial derivative (Lax-Friedrichs):

$$\bar{f}_j^{n+1} = f_j^n - \frac{\Delta t}{\Delta x}(F_{j+1/2}^n - F_{j-1/2}^n) + \Delta t Q(f^n, f^n)$$

$$F_{j+1/2}^n = \frac{1}{2}\left[c_1 f_{j+1}^n + c_1 f_j^n - \frac{\Delta x}{\Delta t}(f_{j+1}^n - f_j^n)\right]$$

- Final scheme:

$$f_j^{n+1} = \mathcal{P}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^{n+1} Q(f^n, f^n)$$

where

$$\mathcal{P}_j^{n+1} = \mathcal{P}_N^{[\boldsymbol{u}_j^{n+1}, T_j^{n+1}]}$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j+1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_{j+1}^n - \mathcal{P}_j^{n+1} f_j^n)\right]$$

$$\tilde{F}_{j,\mathrm{l}}^n = \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j-1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_j^n - \mathcal{P}_j^{n+1} f_{j-1}^n)\right]$$

Relation to the moment methods

$$
\begin{aligned}
f_j^{n+1} &= \mathcal{P}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^{n+1} Q(f^n, f^n) \\
\tilde{F}_{j,\mathrm{r}}^n &= \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j+1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_{j+1}^n - \mathcal{P}_j^{n+1} f_j^n)\right] \\
\tilde{F}_{j,\mathrm{l}}^n &= \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j-1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_j^n - \mathcal{P}_j^{n+1} f_{j-1}^n)\right]
\end{aligned}
$$

What are we really solving?

Relation to the moment methods

$$f_j^{n+1} = \mathcal{P}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^{n+1} Q(f^n, f^n)$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j+1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_{j+1}^n - \mathcal{P}_j^{n+1} f_j^n)\right]$$

$$\tilde{F}_{j,\mathrm{l}}^n = \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 f_{j-1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_j^n - \mathcal{P}_j^{n+1} f_{j-1}^n)\right]$$

What are we really solving?

- Apply $\mathcal{P}_j^n$ to the scheme

Relation to the moment methods

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\begin{aligned}
\mathcal{P}_j^n f_j^{n+1} &= \mathcal{P}_j^n f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^n Q(f^n, f^n) \\
\tilde{F}_{j,\mathrm{r}}^n &= \frac{1}{2}\left[\mathcal{P}_j^n(c_1 f_{j+1}^n) + \mathcal{P}_j^n(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^n f_{j+1}^n - \mathcal{P}_j^n f_j^n)\right] \\
\tilde{F}_{j,\mathrm{l}}^n &= \frac{1}{2}\left[\mathcal{P}_j^n(c_1 f_{j-1}^n) + \mathcal{P}_j^n(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^n f_j^n - \mathcal{P}_j^n f_{j-1}^n)\right]
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\end{aligned}$$

What are we really solving?

- Apply $\mathcal{P}_j^n$ to the scheme
- Rearrange the terms:

$$\mathcal{P}_j^n \left(\frac{f_j^{n+1} - \frac{1}{2}(f_{j-1}^n + f_{j+1}^n)}{\Delta t} + \frac{c_1 f_{j+1}^n - c_1 f_{j-1}^n}{2\Delta x} \right) = \mathcal{P}_j^n Q(f^n, f^n)$$

Relation to the moment methods

$$\mathcal{P}_j^n f_j^{n+1} = \mathcal{P}_j^n f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^n Q(f^n, f^n)$$
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- Grad's moment equations:

$$\mathcal{P}_N^{[\boldsymbol{u},T]}\left[\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{c} f)\right] = \mathcal{P}_N^{[\boldsymbol{u},T]} Q(f,f)$$

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$$\mathcal{P}_j^n f_j^{n+1} = \mathcal{P}_j^n f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^n Q(f^n, f^n)$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2}\left[\mathcal{P}_j^n(c_1 f_{j+1}^n) + \mathcal{P}_j^n(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^n f_{j+1}^n - \mathcal{P}_j^n f_j^n)\right]$$

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We are solving Grad's moment equations!

- Apply $\mathcal{P}_j^n$ to the scheme
- Rearrange the terms:

$$\mathcal{P}_j^n \left(\frac{f_j^{n+1} - \frac{1}{2}(f_{j-1}^n + f_{j+1}^n)}{\Delta t} + \frac{c_1 f_{j+1}^n - c_1 f_{j-1}^n}{2\Delta x} \right) = \mathcal{P}_j^n Q(f^n, f^n)$$

- Grad's moment equations:

$$\mathcal{P}_N^{[\boldsymbol{u},T]}\left[\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{c} f)\right] = \mathcal{P}_N^{[\boldsymbol{u},T]} Q(f,f)$$

Another idea of using adaptive basis functions

$$f_{j-1}^n \qquad f_j^n \qquad f_{j+1}^n$$

$$\mathcal{P}_j^n f_{j-1}^n \qquad \mathcal{P}_j^n f_{j+1}^n$$

$$F_{j,\mathrm{l}}^n = \frac{1}{2}\left[c_1(\mathcal{P}_j^n f_{j-1}^n + f_j^n) - \frac{\Delta x}{\Delta t}(f_j^n - \mathcal{P}_j^n f_{j-1}^n)\right] \qquad F_{j,\mathrm{r}}^n = \frac{1}{2}\left[c_1(\mathcal{P}_j^n f_{j+1}^n + f_j^n) - \frac{\Delta x}{\Delta t}(f_{j+1}^n - \mathcal{P}_j^n f_j^n)\right]$$

$$\bar{f}_j^{\,n+1} = f_j^n - \frac{\Delta t}{\Delta x}(F_{j,\mathrm{r}}^n - F_{j,\mathrm{l}}^n) + \Delta t \mathcal{P}_j^n Q(f_j^n, f_j^n)$$

$$\boldsymbol{u}_j^{n+1} = \frac{\langle \boldsymbol{c} \bar{f}_j^{\,n+1} \rangle}{\langle \bar{f}_j^{\,n+1} \rangle}, \quad T_j^{n+1} = \frac{\left\langle \left|\boldsymbol{c} - \boldsymbol{u}_j^{n+1}\right|^2 \bar{f}_j^{\,n+1} \right\rangle}{3R\langle \bar{f}_j^{\,n+1} \rangle}$$

$$f_j^{n+1} = \mathcal{P}_j^{n+1} \bar{f}_j^{\,n+1}$$

Relation to the moment methods

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\tilde{F}_{j,\mathrm{r}}^n &= \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 \mathcal{P}_j^n f_{j+1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_{j+1}^n - \mathcal{P}_j^{n+1} f_j^n)\right] \\
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f_j^{n+1} &= \mathcal{P}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^{n+1} Q(f^n, f^n) \\
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\tilde{F}_{j,\mathrm{l}}^n &= \frac{1}{2}\left[\mathcal{P}_j^{n+1}(c_1 \mathcal{P}_j^n f_{j-1}^n) + \mathcal{P}_j^{n+1}(c_1 f_j^n) - \frac{\Delta x}{\Delta t}(\mathcal{P}_j^{n+1} f_j^n - \mathcal{P}_j^{n+1} f_{j-1}^n)\right]
\end{aligned}
$$

What are we really solving?

By applying $\mathcal{P}_j^n$ and rearrangement, we get

$$
\mathcal{P}_j^n \left(\frac{f_j^{n+1} - \frac{1}{2}(f_{j-1}^n + f_{j+1}^n)}{\Delta t} + \frac{c_1 \mathcal{P}_j^n f_{j+1}^n - c_1 \mathcal{P}_j^n f_{j-1}^n}{2\Delta x} \right) = \mathcal{P}_j^n Q(f^n, f^n)
$$

Relation to the moment methods

$$
\begin{aligned}
f_j^{n+1} &= \mathcal{P}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t\, \mathcal{P}_j^{n+1} Q(f^n, f^n) \\
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Hyperbolic moment equations:

$$
\mathcal{P}_N^{[\boldsymbol{u},T]} \left(\partial_t f + c_i \mathcal{P}_N^{[\boldsymbol{u},T]} \partial_{x_i} f \right) = \mathcal{P}_N^{[\boldsymbol{u},T]} Q(f, f)
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\end{aligned}
$$

We are solving hyperbolic moment equations!

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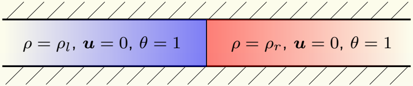
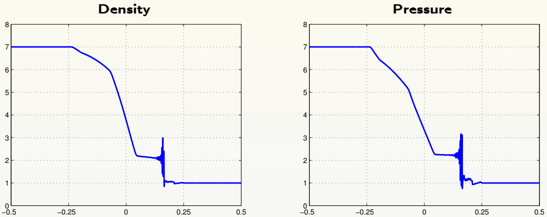
$$
\mathcal{P}_N^{[\boldsymbol{u},T]} \left(\partial_t f + c_i \mathcal{P}_N^{[\boldsymbol{u},T]} \partial_{x_i} f \right) = \mathcal{P}_N^{[\boldsymbol{u},T]} Q(f, f)
$$

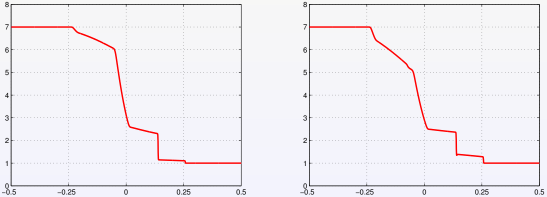
Shock tube problem



Grad:



Hyperbolic:



Collision operator

- **Linearized collision term:**

$$\mathcal{L}(f) = \int_{\mathbb{R}^3} \int_{\boldsymbol{n} \perp \boldsymbol{g}} \int_0^{\pi} K[f/\mathcal{M}]\mathcal{M}(\boldsymbol{c})\mathcal{M}(\boldsymbol{c}_1) g B(g,\chi) \sin\chi \,\mathrm{d}\chi \,\mathrm{d}\boldsymbol{n} \,\mathrm{d}\boldsymbol{c}_1$$

$$K[\psi](\boldsymbol{c},\boldsymbol{c}_1,\boldsymbol{n},\chi) = \psi(\boldsymbol{c}_1') + \psi(\boldsymbol{c}_1') - \psi(\boldsymbol{c}_1) - \psi(\boldsymbol{c})$$

- Ansatz for the distribution function:

$$f(t,\boldsymbol{x},\boldsymbol{c}) = \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{n=0}^{N_l} f_{lmn}(t,\boldsymbol{x}) [RT(t,\boldsymbol{x})]^{-\frac{2n+l+3}{2}} \Phi_{lmn}\left(\frac{\boldsymbol{c} - \boldsymbol{u}(t,\boldsymbol{x})}{\sqrt{RT(t,\boldsymbol{x})}} \right)$$

- Basis functions:

$$\Phi_{lmn}(\boldsymbol{\xi}) = \frac{2^{-l/2}\pi^{-3/4}}{2m} \bar{L}_n^{(l+1/2)}\left(\frac{|\boldsymbol{\xi}|^2}{2}\right) |\boldsymbol{\xi}|^l Y_l^m\left(\frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|}\right) \exp\left(-\frac{|\boldsymbol{\xi}|^2}{2}\right)$$

- Linearized collision operator applied to the ansatz:

$$\mathcal{P}^{[\boldsymbol{u},T]}\mathcal{L}(f) = \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{n=0}^{N} \sum_{n'=0}^{N} a_{lnn'} f_{lmn'} (RT)^{-\frac{2n'+l'+3}{2}} \Phi_{lmn}\left(\frac{\boldsymbol{c}-\boldsymbol{u}}{\sqrt{RT}}\right)$$

The coefficients $a_{lnn'}$

$$\mathcal{P}^{[\boldsymbol{u},T]}\mathcal{L}(f) = \sum_{l=0}^{L}\sum_{m=-l}^{l}\sum_{n=0}^{N}\sum_{n'=0}^{N} a_{lnn'} f_{lmn'} (RT)^{-\frac{2n'+l'+3}{2}} \Phi_{lmn}\left(\frac{\boldsymbol{c}-\boldsymbol{u}}{\sqrt{RT}}\right)$$

- The values of $\tilde{a}_{lnn'} = a_{lnn'}/|a_{200}|$ for Maxwell molecules:

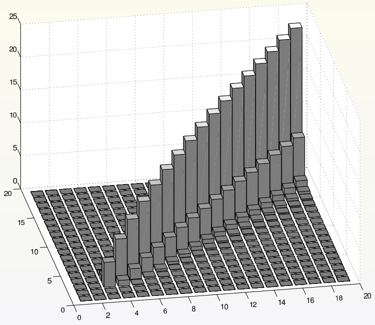
$$\tilde{a}_{0nn'} = \operatorname{diag}\{0, 0, -0.666667, -1, -1.22814, -1.40369, -1.54745, -1.66980, -1.77672, \cdots\}$$
$$\tilde{a}_{1nn'} = \operatorname{diag}\{0, -0.66667, -1, -1.22814, -1.40369, -1.54745, -1.66980, -1.77672, \cdots\}$$
$$\tilde{a}_{2nn'} = \operatorname{diag}\{-1, -1.16667, -1.34222, -1.49147, -1.61932, -1.73098, -1.83018, \cdots\}$$
$$\tilde{a}_{3nn'} = \operatorname{diag}\{-3.08328, -3.22791, -3.42659, -3.62404, -3.80956, -3.98174, -4.14143, \cdots\}$$

- The values of $a_{lnn'}/|a_{200}|$ for hard-sphere molecules:

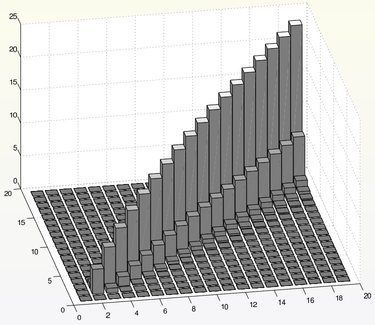
$$a_{0nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -0.666667 & 0.154303 & 0.0181848 & \cdots \\ 0 & 0 & 0.154303 & -1.10714 & 0.282001 & \cdots \\ 0 & 0 & 0.0181848 & 0.282001 & -1.45288 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{1nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -0.666667 & 0.125988 & 0.0128586 & 0.00274147 & \cdots \\ 0 & 0.125988 & -1.07143 & 0.250295 & 0.0305672 & \cdots \\ 0 & 0.0128586 & 0.250295 & -1.40303 & 0.358666 & \cdots \\ 0 & 0.00274147 & 0.0305672 & 0.358666 & -1.68819 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a_{2nn'} = \begin{pmatrix} -1 & 0.133631 & 0.0111359 & 0.0020561 & \cdots \\ 0.133631 & -1.22024 & 0.24256 & 0.0262852 & \cdots \\ 0.0111359 & 0.24256 & -1.47433 & 0.344432 & \cdots \\ 0.0020561 & 0.0262852 & 0.344432 & -1.71982 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{3nn'} = \begin{pmatrix} -1.5 & 0.227284 & 0.0209394 & 0.00420299 & \cdots \\ 0.227284 & -1.64187 & 0.332994 & 0.0373019 & \cdots \\ 0.0209394 & 0.332994 & -1.82502 & 0.42449 & \cdots \\ 0.00420299 & 0.0373019 & 0.42449 & -2.01665 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Coefficients $a_{lnn'}$ for hard-sphere molecules

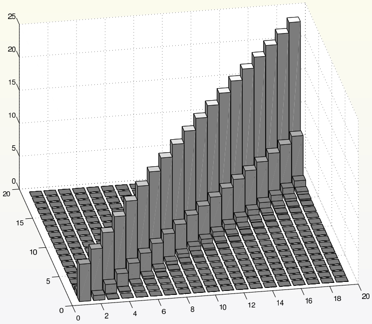


(a) $l = 0$

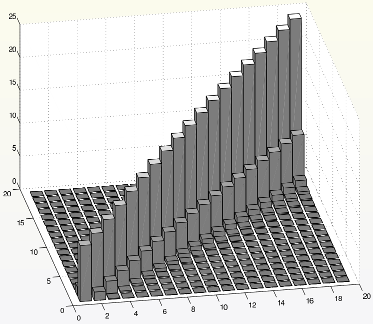


(b) $l = 1$

Coefficients $a_{lnn'}$ for hard-sphere molecules



(c) $l = 2$



(d) $l = 3$

The coefficients $a_{lnn'}$ for inverse-power potentials

- Inverse-power potential with viscosity index 0.72:

$$a_{0nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -0.666667 & 0.0857241 & 0.0145928 & \cdots \\ 0 & 0 & 0.0857241 & -1.05071 & 0.152972 & \cdots \\ 0 & 0 & 0.0145928 & 0.152972 & -1.33463 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{1nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -0.666667 & 0.0699934 & 0.0103186 & 0.00252586 & \cdots \\ 0 & 0.0699934 & -1.0338 & 0.136919 & 0.0243102 & \cdots \\ 0 & 0.0103186 & 0.136919 & -1.31159 & 0.193332 & \cdots \\ 0 & 0.00252586 & 0.0243102 & 0.193332 & -1.53972 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a_{2nn'} = \begin{pmatrix} -1 & 0.0742392 & 0.0089362 & 0.00189439 & \cdots \\ 0.0742392 & -1.19202 & 0.133449 & 0.0209769 & \cdots \\ 0.0089362 & 0.133449 & -1.40633 & 0.187704 & \cdots \\ 0.00189439 & 0.0209769 & 0.187704 & -1.60277 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{3nn'} = \begin{pmatrix} -1.5 & 0.126269 & 0.0168032 & 0.00387244 & \cdots \\ 0.126269 & -1.60731 & 0.183875 & 0.0298685 & \cdots \\ 0.0168032 & 0.183875 & -1.74768 & 0.232508 & \cdots \\ 0.00387244 & 0.0298685 & 0.232508 & -1.89131 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

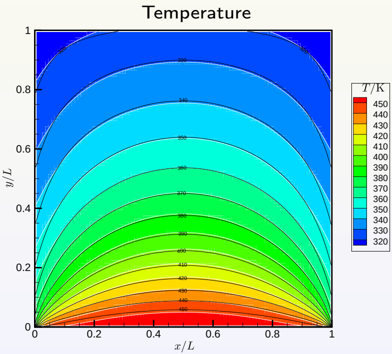
- Inverse-power potential with viscosity index 0.81:

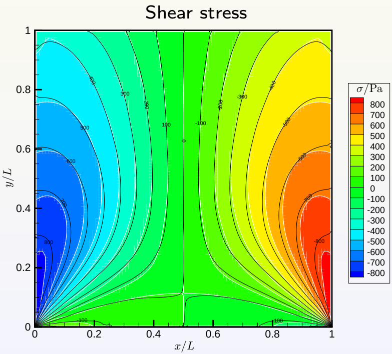
$$a_{0nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -0.666667 & 0.0586353 & 0.0111946 & \cdots \\ 0 & 0 & 0.0586353 & -1.03230 & 0.103809 & \cdots \\ 0 & 0 & 0.0111946 & 0.103809 & -1.29590 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{1nn'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -0.666667 & 0.047875 & 0.00791576 & 0.00203643 & \cdots \\ 0 & 0.047875 & -1.02153 & 0.0931770 & 0.00791576 & \cdots \\ 0 & 0.00791576 & 0.0931770 & -1.28134 & 0.130867 & \cdots \\ 0 & 0.00203643 & 0.0185944 & 0.130867 & -1.49034 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a_{2nn'} = \begin{pmatrix} -1 & 0.0507796 & 0.00685525 & 0.00152732 & \cdots \\ 0.0507796 & -1.18282 & 0.090988 & 0.0160630 & \cdots \\ 0.00685525 & 0.090988 & -1.38322 & 0.127505 & \cdots \\ 0.00152732 & 0.0160630 & 0.127505 & -1.56266 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad a_{3nn'} = \begin{pmatrix} -1.5 & 0.0863680 & 0.0128903 & 0.00312208 & \cdots \\ 0.0863680 & -1.59427 & 0.0128903 & 0.0228829 & \cdots \\ 0.0128903 & 0.125419 & -1.71907 & 0.158046 & \cdots \\ 0.00312208 & 0.0228829 & 0.158046 & -1.84562 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Heated cavity

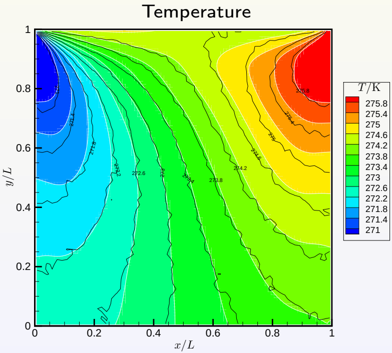
Type of the gas: Maxwell molecules
Temperature of the bottom wall: 600K
Temperature of other walls: 300K
Knudsen number: 0.3
Number of moments: 816 ($\approx 9.34^3$)

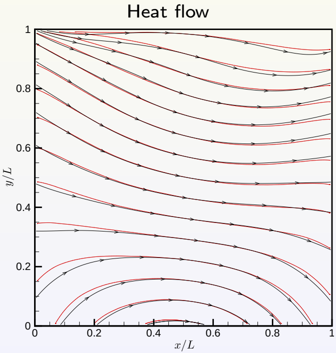




Lid-driven cavity

Type of the gas: Inverse-power-law gas with viscosity index 0.81
Mach number of the top lid: 0.16
Temperature of the walls: 273K
Knudsen number: 1.0
Number of moments: 8436 ($\approx 20.36^3$)





Convergence of the two methods

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↑

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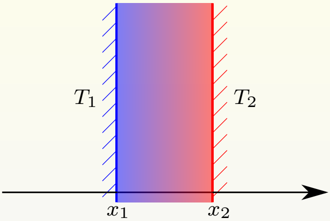
This assumption is too strong...

Heat transfer between plates



Diffuse reflection:

$$f(t,\boldsymbol{x},\boldsymbol{c}) = \frac{\rho^W}{m(2\pi R T^W)^{3/2}} \exp\left(-\frac{|\boldsymbol{c}|^2}{2RT^W}\right), \quad \text{if} \quad \boldsymbol{c}\cdot\boldsymbol{n} < 0$$

where

$$\rho^W = m\sqrt{\frac{2\pi}{RT^W}} \int_{\boldsymbol{c}\cdot\boldsymbol{n}>0} (\boldsymbol{c}\cdot\boldsymbol{n}) f(t,\boldsymbol{x},\boldsymbol{c})\,\mathrm{d}\boldsymbol{c}$$

Heat transfer between plates

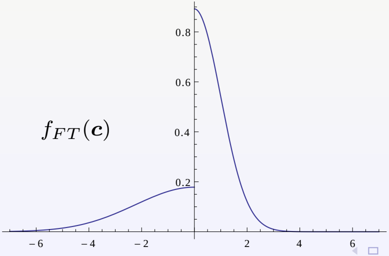
Steady state solution:

- Collisionless case: $(\partial_x f = 0)$

$$f_{FT}(x,\boldsymbol{c}) = \begin{cases} \dfrac{\rho_1}{m(2\pi R T_1)^{3/2}} \exp\left(-\dfrac{|\boldsymbol{c}|^2}{2RT_1}\right) & \text{if } c_1 > 0 \\ \dfrac{\rho_2}{m(2\pi R T_2)^{3/2}} \exp\left(-\dfrac{|\boldsymbol{c}|^2}{2RT_2}\right) & \text{if } c_1 < 0 \end{cases}$$

$$\rho_1\sqrt{T_1} = \rho_2\sqrt{T_2}, \qquad T = \sqrt{T_1 T_2}$$

If $T_1 = 1$ and $T_2 = 5$, then $T = \sqrt{5}$.



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$$\int_{\mathbb{R}^3} [f_{FT}(\boldsymbol{c})]^2 \left(\phi^{[0,T]}(\boldsymbol{c})\right)^{-1} \mathrm{d}\boldsymbol{c}$$
$$\geqslant \frac{\rho_2^2}{m^2(2\pi R T_2)^3} \int_{c_1<0} \exp\left[\left(\frac{1}{2RT} - \frac{1}{RT_2}\right)|\boldsymbol{c}|^2\right] \mathrm{d}\boldsymbol{c} = +\infty$$

$$\boxed{f_{FT}(\boldsymbol{c}) \notin L^2\left(\mathbb{R}^3; \left[\phi^{[\boldsymbol{u},T]}(\boldsymbol{c})\right]^{-1} \mathrm{d}\boldsymbol{c}\right)}$$

From weighted L^2 to normal L^2

- $\mathcal{P}_N^{[\boldsymbol{u},T]} f_{FT}$ is NOT a good approximation of f_{FT}

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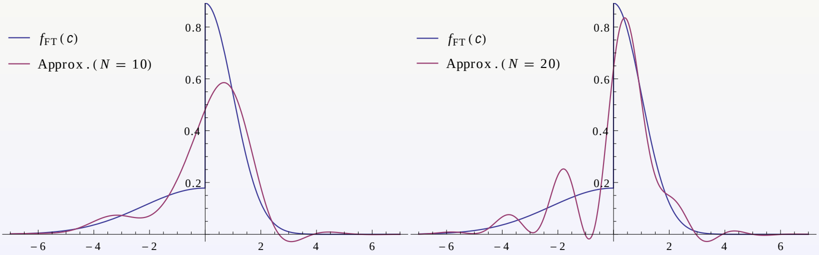

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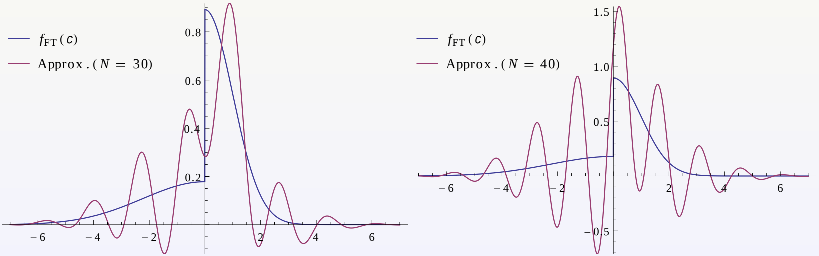
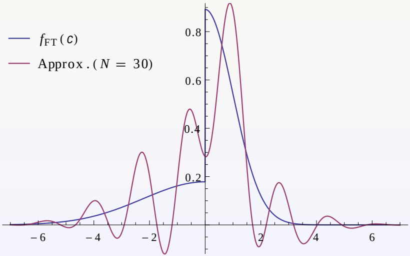
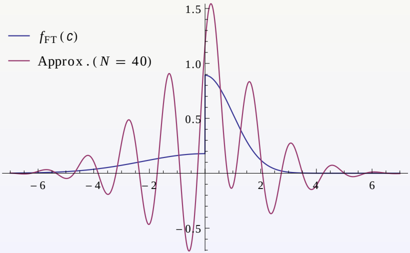


From weighted L^2 to normal L^2

- $\mathcal{P}_N^{[\boldsymbol{u},T]} f_{FT}$ is NOT a good approximation of f_{FT}
- Is there better approximation to f_{FT} in

$$H_N^{[\boldsymbol{u},T]} = \operatorname{span}\left\{ c_{i_1} \cdots c_{i_n} \exp\left(-\frac{|\boldsymbol{c}-\boldsymbol{u}|^2}{2RT}\right) \,\middle|\, n \leqslant N,\ i_1, \cdots, i_n = 1,2,3 \right\} ?$$





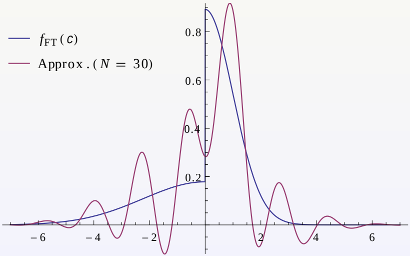
From weighted L^2 to normal L^2

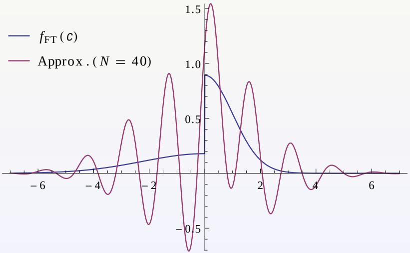
- $\mathcal{P}_N^{[\boldsymbol{u},T]} f_{FT}$ is NOT a good approximation of f_{FT}
- Is there better approximation to f_{FT} in

$$H_N^{[\boldsymbol{u},T]} = \text{span}\left\{ c_{i_1} \cdots c_{i_n} \exp\left(-\frac{|\boldsymbol{c}-\boldsymbol{u}|^2}{2RT} \right) \,\middle|\, n \leqslant N,\ i_1, \cdots, i_n = 1,2,3 \right\}?$$

Yes!

$$\widetilde{\mathcal{P}}_N^{[\boldsymbol{u},T]} f = \mathop{\arg\min}_{g \in H_N^{[\boldsymbol{u},T]}} \|f-g\|_{L^2(\mathbb{R}^3)}$$





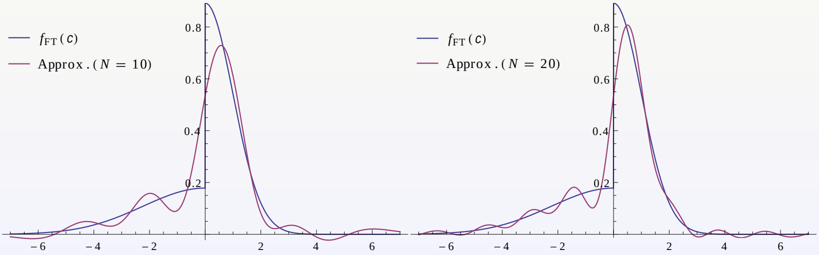
From weighted L^2 to normal L^2

- $\mathcal{P}_N^{[\boldsymbol{u},T]} f_{FT}$ is NOT a good approximation of f_{FT}
- Is there better approximation to f_{FT} in

$$H_N^{[\boldsymbol{u},T]} = \operatorname{span}\left\{ c_{i_1} \cdots c_{i_n} \exp\left(-\frac{|\boldsymbol{c}-\boldsymbol{u}|^2}{2RT} \right) \,\middle|\, n \leqslant N,\ i_1, \cdots, i_n = 1,2,3 \right\} ?$$

Yes!

$$\widetilde{\mathcal{P}}_N^{[\boldsymbol{u},T]} f = \underset{g \in H_N^{[\boldsymbol{u},T]}}{\arg\min} \|f-g\|_{L^2(\mathbb{R}^3)}$$



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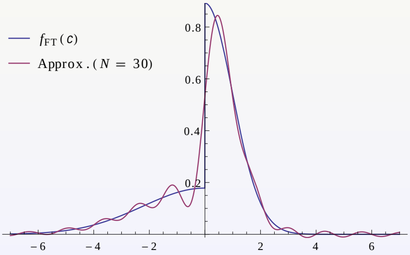

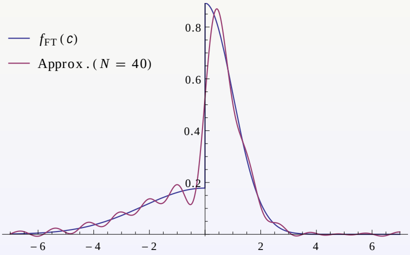

Conservation fix

- The new projection operator $\widetilde{\mathcal{P}}_N^{[\boldsymbol{u},T]}$ does **NOT** preserve moments!
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Fix the conservation:

$$\widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]} f = \underset{g \in H_N^{[\boldsymbol{u},T]}}{\arg\min} \|g - f\|_{L^2(\mathbb{R}^3)}$$

$$\text{subject to } \int_{\mathbb{R}^3} g(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} f(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c}$$

$$\int_{\mathbb{R}^3} c_i g(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} c_i f(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c}$$

$$\int_{\mathbb{R}^3} c_i c_j g(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} c_i c_j f(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c}$$

$$\int_{\mathbb{R}^3} |\boldsymbol{c}|^2 c_i g(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} |\boldsymbol{c}|^2 c_i f(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c}$$

$\widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]}$ does not change density, velocity, pressure tensor and heat flux!

New moment method

$$\widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]}\partial_t f + \widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]}\left(c_i \widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]}\partial_{x_i} f\right) = \widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]} Q(f,f)$$

- If $f(\boldsymbol{c}) \in L^2(\mathbb{R}^3)$ and $f(\boldsymbol{c}) \geqslant 0$ satisfies

$$\int_{\mathbb{R}^3} |\boldsymbol{c}|^3 f(\boldsymbol{c}) \,\mathrm{d}\boldsymbol{c} < +\infty,$$

  then $\widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]} f$ converges to f as $N \to \infty$
- Numerical scheme:

$$f_j^{n+1} = \widehat{\mathcal{P}}_j^{n+1} f_j^n - \frac{\Delta t}{\Delta x}(\tilde{F}_{j,\mathrm{r}}^n - \tilde{F}_{j,\mathrm{l}}^n) + \Delta t \widehat{\mathcal{P}}_j^{n+1} Q(f^n, f^n)$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2}\widehat{\mathcal{P}}_j^{n+1}\left[c_1 \widehat{\mathcal{P}}_j^n f_{j+1}^n + c_1 f_j^n - \frac{\Delta x}{\Delta t}(\widehat{\mathcal{P}}_j^n f_{j+1}^n - f_j^n)\right]$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2}\widehat{\mathcal{P}}_j^{n+1}\left[c_1 \widehat{\mathcal{P}}_j^n f_{j-1}^n + c_1 f_j^n - \frac{\Delta x}{\Delta t}(f_j^n - \widehat{\mathcal{P}}_j^n f_{j-1}^n)\right]$$

Another conservative version

$$\widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]} \partial_t f + \overline{\mathcal{P}}_N^{[\boldsymbol{u},T]} \left(c_i \widehat{\mathcal{P}}_N^{[\boldsymbol{u},T]} \partial_{x_i} f \right) = \overline{\mathcal{P}}_N^{[\boldsymbol{u},T]} Q(f,f)$$

- Definition of $\overline{\mathcal{P}}_N^{[\boldsymbol{u},T]}$:

$$\overline{\mathcal{P}}_N^{[\boldsymbol{u},T]} f = \underset{g \in H_N^{[\boldsymbol{u},T]}}{\arg\min} \|g - f\|_{L^2(\mathbb{R}^3)}$$

$$\text{subject to } \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \boldsymbol{c} \\ |\boldsymbol{c}|^2 \end{pmatrix} g(\boldsymbol{c}) \, \mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \boldsymbol{c} \\ |\boldsymbol{c}|^2 \end{pmatrix} f(\boldsymbol{c}) \, \mathrm{d}\boldsymbol{c}$$

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$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2} \overline{\mathcal{P}}_j^{n+1} \left[c_1 \widehat{\mathcal{P}}_j^n f_{j+1}^n + c_1 f_j^n - \frac{\Delta x}{\Delta t} (\widehat{\mathcal{P}}_j^n f_{j+1}^n - f_j^n) \right]$$

$$\tilde{F}_{j,\mathrm{r}}^n = \frac{1}{2} \overline{\mathcal{P}}_j^{n+1} \left[c_1 \widehat{\mathcal{P}}_j^n f_{j-1}^n + c_1 f_j^n - \frac{\Delta x}{\Delta t} (f_j^n - \widehat{\mathcal{P}}_j^n f_{j-1}^n) \right]$$

Shock structure problem

Initial condition:

$$f_0(x, \boldsymbol{c}) = \begin{cases} \mathcal{M}_{\rho_l, \boldsymbol{u}_l, \theta_l}(\boldsymbol{c}) & \text{if } x < 0 \\ \mathcal{M}_{\rho_r, \boldsymbol{u}_r, \theta_r}(\boldsymbol{c}) & \text{if } x > 0 \end{cases}$$

The initial condition is given by the Rankine-Hugoniot condition:

$$\rho_l = 1 \qquad \boldsymbol{u}_l = \left(\sqrt{\frac{5}{3}} Ma, 0, 0\right)^T \qquad \theta_l = 1$$

$$\rho_r = \frac{4Ma^2}{Ma^2 + 3} \qquad \boldsymbol{u}_r = \frac{\rho_l}{\rho_r} \boldsymbol{u}_l \qquad \theta_r = \frac{(5Ma^2 - 1)(Ma^2 + 3)}{16Ma^2}$$

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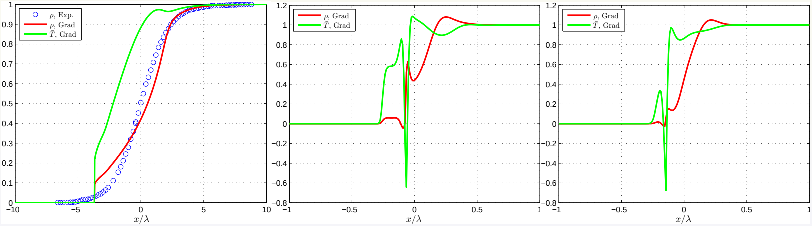
Results of Grad's moment equations for $Ma = 2.31$:



$N = 3$ $N = 6$ $N = 9$

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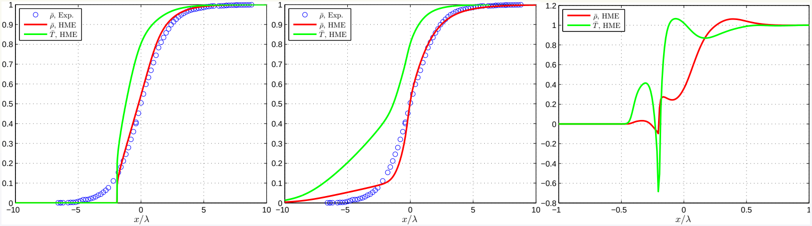
Results of hyperbolic moment equations for $Ma = 2.31$:



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Shock structure problem

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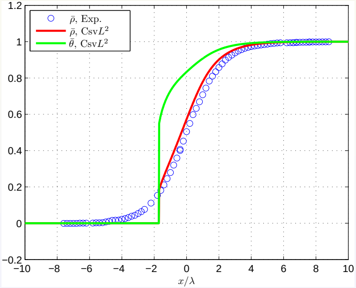
Results of the new moment method for $Ma = 2.31$:



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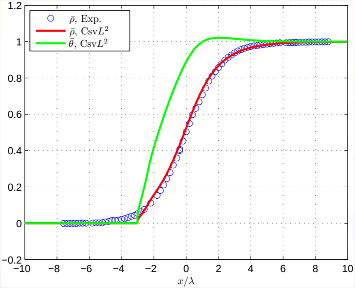

$N = 6$

Shock structure problem

Initial condition:

$$f_0(x, \boldsymbol{c}) = \begin{cases} \mathcal{M}_{\rho_l, \boldsymbol{u}_l, \theta_l}(\boldsymbol{c}) & \text{if } x < 0 \\ \mathcal{M}_{\rho_r, \boldsymbol{u}_r, \theta_r}(\boldsymbol{c}) & \text{if } x > 0 \end{cases}$$

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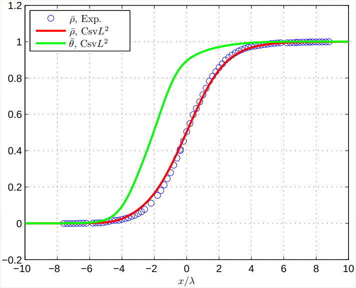

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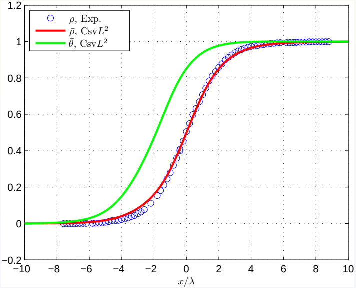

$N = 12$

Conclusion and future work

Conclusion:

- The moment methods can be interpreted as spectral methods with adaptive basis functions
- A reasonable numerical method is developed for the hyperbolic moment equations which do not have a balance-law form
- A new and more robust moment theory is developed with projection operators based on the L^2-norm

Future work:

- Exploration of better adaptive methods
- Use the techniques in the moment method to improve the adaptive spectral method
- More applications

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Thank you!

Email: cai@mathcces.rwth-aachen.de