From Discrete Velocity Method to Moment Method

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Outline

1. Introduction
2. Discrete Velocity Model
3. Moment Method
4. Numerical Example
5. Conclusion Remarks
Kinetic theory: Boltzmann equation

In kinetic theory, the Boltzmann equation reads:

\[
\frac{\partial f}{\partial t} + \sum_{d=1}^{D} \xi_d \frac{\partial f}{\partial x_d} = Q(f, f),
\]

(1)

where \( f(t, x, \xi) \) is the distribution function, \((t, x, \xi) \in \mathbb{R}^+ \times \mathbb{R}^D \times \mathbb{R}^D\), and \( Q(f, f) \) is the collision term with a quadratic expression typically given by

\[
Q(f, f) = \int_{\mathbb{R}^D} \int_{S^{D-1}} (f' f'_* - f f_*) |(\xi - \xi_*) \cdot n| \, d\xi_* \, dn,
\]

where \( f_* = f(\xi_*), \quad f' = f(\xi'), \quad f'_* = f(\xi'_*). \)
Maxwellian and Macroscopic Variables

Maxwellian:

\[
f_M(\xi) = \frac{1}{(2\pi\theta)^{D/2}} \exp \left( -\frac{|\xi - \mathbf{u}|^2}{2\theta} \right).
\]  

The macroscopic variables:

\[
\rho = \int_{\mathbb{R}^D} f \, d\xi,
\]

\[
\rho \mathbf{u} = \int_{\mathbb{R}^D} \xi f \, d\xi,
\]

\[
\rho |\mathbf{u}|^2 + D\rho \theta = \int_{\mathbb{R}^D} |\xi|^2 f \, d\xi.
\]  

For BGK model, the collision term \( Q(f, f) \) reads:

\[
Q(f, f) = \frac{1}{\tau} (f_M - f),
\]

where \( \tau \) is relaxation time.
Hierarchy of solution techniques for the Boltzmann equation

- Solution of the Boltzmann Equation
  - Analytic: Simpliest Flow Problems
    - Direct Simulation Monte Carlo Method
  - Approximate: General Flow Problems
    - Direct or particulate -flow Approches
      - Discrete Velocity Method
    - Extented Hydrodynamics Approches
      - Chapman-Enskog Expansion Technique
      - Grad-type Method of Moments
Discrete Velocity Model

Using the value on finite velocity points

\[ \hat{f}_\alpha(x, t) = f(x, \xi_\alpha; t) \]

to approximate distribution function, where \( \alpha \) is a multi-dimensional index.

Examples for 1D case:
Choose the velocity points as

\[ \xi_k = k \Delta \xi, \quad k = 0, \pm 1, \pm 2, \cdots, \pm (N - 1), \]

or

\[ \xi_k = c_k, \quad k = 1, \cdots, N, \quad \text{satisfying} \ Hc_N(c_k) = 0, \]

etc.
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Discrete Velocity Model: Basic Framework

Let us consider 1D case: give a group of discrete velocity points

\[ \xi_0 < \xi_1 < \cdots < \xi_{N-1} < \xi_N, \quad \xi_k \in \mathbb{R} \]

We get the system as:

\[ \frac{\partial \hat{f}_k}{\partial t} + \xi_k \frac{\partial \hat{f}_k}{\partial x} = Q_k^{BGK}(f), \quad k = 0, \cdots, N, \]

where \( \hat{f}_k \) is a function of \( x \) and \( t \):

\[ \hat{f}_k(x, t) \longrightarrow f(x, \xi_k; t), \]

\[ Q_k^{BGK}(f) \longrightarrow Q^{BGK}(f)(\xi_k). \]
Discrete Velocity Model: Basic Framework

Discrete velocity model (DVM):

\[
\frac{\partial \hat{f}_k}{\partial t} + \xi_k \frac{\partial \hat{f}_k}{\partial x} = Q^{BGK}_k(f), \quad k = 0, \ldots, N.
\]

- Hyperbolic system: locally well-posedness;
- Wave speeds: \( \xi_k \);
- H-theorem for BGK;
- Implementation: convenient (LBM);

- Computational cost?
**Discrete Velocity Model: Basic Framework**

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Computational cost?
Discrete Velocity Model: Basic Framework

Computational cost: equidistant velocity points

Number of points \( \geq \frac{\sup_{x,t} |u(x, t)|}{\sqrt{\inf_{x,t} \theta(x, t)}} \)
Discrete Velocity Model: Basic Framework

Computational cost: equidistant velocity points

Number of points > $\frac{\sup_{x,t} |u(x,t)|}{\sqrt{\inf_{x,t} \theta(x,t)}}$
How to improve the efficiency of DVM?

- Best discrete velocity point?

Gauss-Hermite interpolating point: zeros of Hermite polynomials.

$$\xi_k = c_k, \text{ satisfying } He_N(c_k) = 0.$$
Discrete Velocity Model: Efficiency?

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  \[ \xi_k = c_k, \quad \text{satisfying } He_N(c_k) = 0. \]
Discrete Velocity Model: Efficiency?

How to improve the efficiency of DVM?

- Best discrete velocity point?
- Adaptive configuration of the velocity points?
  - Choose the mean velocity as the center.
    \[ \xi_k = c_k + u. \]
  - The higher the temperature, the greater the distance.
    Take the temperature as normalization factor.
    \[ \xi_k = \sqrt{\theta} c_k + u. \]

- How many points is enough?
  Computational capacity vs Requirement.
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\[ \theta = \frac{1}{2} \]

\[ \theta = 2 \]
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- The higher the temperature, the greater the distance.
  Since the Maxwellian reads
  \[ f_M = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{|\xi - u|^2}{2\theta}\right), \]
  Take the temperature as normalization factor.
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Smart Discrete Velocity Method

Let $c_k$, $k = 0, \ldots, M$ be the $k$-th zeros of $H_{e_{M+1}}$. Then we choose the interpolating points:

$$
    \xi_k = \sqrt{\theta} c_k + u,
$$

$$
    \hat{f}_k(t, x) = f(t, x, \xi_k),
$$

which satisfy the Boltzmann equation

$$
    \frac{\partial \hat{f}_k}{\partial t} + \frac{\partial \xi_k \hat{f}_k}{\partial x} = Q_k^{BGK}(f), \quad k = 0, \ldots, M.
$$

(4)

Attention: $\xi_k$ is dependent on $t$ and $x$.

Number of Degrees of Freedom?

$u, \theta, \hat{f}_k, \quad k = 0, \ldots, M.$

M+3?

Restricted condition:

$$
    \sum_{k=0}^{M} w_k \xi_k \hat{f}_k = \rho u, \quad \sum_{k=0}^{M} w_k \xi_k^2 \hat{f}_k = \rho u^2 + \rho \theta.
$$

(5)

where $w_k$ is integral weight.
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where \( w_k \) is integral weight.
From function values to moments

Define the moments as

$$F_k = \frac{1}{k!} \int_{\mathbb{R}} f \xi^k \, d\xi, \quad k \in \mathbb{N}. \quad (6)$$

Discrete form of the first $M + 1$ moments:

$$F_k = \frac{1}{k!} \sum_{i=0}^{M} w_i \hat{f}_i \xi_i^k, \quad k = 0, \ldots, M. \quad (7)$$

**Remind:** The algebraic accuracy of $n$-point Gauss-Hermite integral formula is $2n - 1$.

Let $\hat{f} = (\hat{f}_0, \ldots, \hat{f}_M)^T$, and $F = (F_0, \ldots, F_M)^T$, then

$$F = A \hat{f},$$

where $A = (\xi_i^k w_j / j!)$. Particularly, $F_1 = \rho u$, $F_2 = (\rho u^2 + \rho \theta) / 2$. 
From function values to moments

Define the moments as

\[ F_k = \frac{1}{k!} \int_{\mathbb{R}} f(x) x^k \, dx, \quad k \in \mathbb{N}. \]  

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From function values to moments

The following two sets of variables are equivalent:

\[ V_M = \{ u, \theta, \hat{f}_0, \ldots, \hat{f}_M \} \iff F_M = \{ u, \theta, F_0, \ldots, F_M \} \]

Let study the set \( F_M \).

Using \( F_M \) to approximate \( f \) is equivalent to

\[ \sum_{k=0}^{M} g_k \xi^k \exp\left(-\frac{|\xi - u|^2}{2\theta}\right) \to f, \]

where \( g_k, k = 0, \ldots, M \) satisfy
From function values to moments

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where \( g_k, k = 0, \ldots, M \) satisfy

\[
F = \left( \int_{\mathbb{R}} \xi^i \exp\left(-\frac{|\xi - u|^2}{2\theta}\right) d\xi \right)_{(M+1) \times (M+1)} \begin{pmatrix} g_0 \\ g_1 \\ \vdots \\ g_M \end{pmatrix}
\]
From function values to moments

The following two sets of variables are equivalent:

\[ \mathcal{V}_M = \{u, \theta, \hat{f}_0, \ldots, \hat{f}_M\} \leftrightarrow \mathcal{F}_M = \{u, \theta, F_0, \ldots, F_M\} \]

Let study the set \( \mathcal{F}_M \).

Using \( \mathcal{F}_M \) to approximate \( f \) is equivalent to

\[
\sum_{k=0}^{M} g_k \xi^k \exp\left(-\left(\frac{\xi - u}{2\theta}\right)^2\right) \to f,
\]

where \( g_k \), \( k = 0, \ldots, M \) satisfy

\[
F = \left(\int_\mathbb{R} \xi^{i+j} \exp\left(-\left(\frac{\xi - u}{2\theta}\right)^2\right) d\xi\right)_{(M+1) \times (M+1)}
\]
Orthogonal polynomials

The orthogonal polynomials for the weight \( w^{[\theta]}(v) = \frac{1}{\sqrt{2\pi\theta}} \exp(-\frac{v^2}{2\theta}) \) and integration interval \( \mathbb{R} \) are **Generalized Hermite polynomials**, defined as

\[
He_k^{[\theta]}(v) = \frac{(\theta v)^k}{w^{[\theta]}(v)} \frac{d^k}{dv^k} w^{[\theta]}(v). \tag{8}
\]

- **Recurrence relations:**
  \( He_0^{[\theta]}(v) = 1, \quad He_1^{[\theta]}(v) = v/\theta, \quad \theta He_n^{[\theta]+1}(v) = vHe_n^{[\theta]}(v) - nHe_n^{[\theta]}(v); \)

- **First few terms:**
  \[
  He_0^{[\theta]}(v) = 1, \quad He_1^{[\theta]}(v) = v/\theta, \\
  He_2^{[\theta]}(v) = (v^2 - \theta)/\theta^2, \quad He_3^{[\theta]}(v) = (v^3 - 3\theta v)/\theta^3, \\
  He_4^{[\theta]}(v) = (v^4 - 6\theta v^2 + 3\theta^2)/\theta^4, \quad He_5^{[\theta]}(v) = (v^5 - 15\theta v^3 + 10\theta^2 v)/\theta^5.
  \]

- **Orthogonality:**
  \[
  \int_{\mathbb{R}} He_m^{[\theta]}(v) He_n^{[\theta]}(v) w^{[\theta]}(v) \, dv = m!\theta^m \delta_{mn}.
  \]
Orthogonal polynomials

Consider the weighted generalized Hermite polynomials

$$\mathcal{H}_{k,\theta}(v) = (-1)^k \frac{d^k}{dx^k} w^{[\theta]} = w^{[\theta]} H_k^{[\theta]}(v). \quad (9)$$

- Recursive relations: \( \theta \mathcal{H}_{n+1}^{[\theta]}(v) = v \mathcal{H}_n^{[\theta]}(v) - n \mathcal{H}_{n-1}^{[\theta]}(v) \);
- Orthogonality: \( \int_{\mathbb{R}} H_m^{[\theta]}(v) H_n^{[\theta]}(v) 1/w^{[\theta]}(v) \, dv = m!\theta^m \delta_{mn} \).
- Differential relations:

$$\frac{d \mathcal{H}_{k}^{[\theta(\tau)]}(v(\tau))}{d\tau} = -\mathcal{H}_{k+1}^{[\theta(\tau)]} \frac{dv(\tau)}{d\tau} + \frac{1}{2} \mathcal{H}_{k+1}^{[\theta(\tau)]} \frac{d\theta(\tau)}{d\tau}. $$
Moments

Consider

\[ f_{h,M} = \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \rightarrow f, \]

where

\[ f_k = \frac{\theta^k}{k!} \int_{\mathbb{R}} f \mathcal{H}_k^{[\theta]}(\xi - u) \frac{1}{w^{[\theta]}(\xi - u)} \, d\xi. \]

\( \hat{f}_k \) and \( f_k \) are related with the Hermite transformation.

Restricted condition:

\[ f_1 = 0, \quad f_2 = 0. \]
Moments

Consider

\[ f_{h,M} = \sum_{k=0}^{M} f_k H_k^\theta(\xi - u) \rightarrow f, \]

where

\[ f_k = \frac{\theta^k}{k!} \int_{\mathbb{R}} f H_k^\theta(\xi - u) \frac{1}{w[\theta](\xi - u)} \, d\xi. \]

The relation of \( \hat{f}_k \) and \( f_k \)?

\[ \hat{f}_k = f_{h,M}(\xi_k) = \sum_{k=0}^{M} f_k H_k^\theta(\xi_k - u). \]

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\( \hat{f}_k \) and \( f_k \) are related with the Hermite transformation.

Restricted condition:

\[ f_1 = f_3 = \ldots = f_{2n-1} = 0. \]
Moments
Consider
\[ f_{h,M} = \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \rightarrow f, \]
where
\[ f_k = \frac{\theta^k}{k!} \int_{\mathbb{R}} f \mathcal{H}_k^{[\theta]}(\xi - u) \frac{1}{w^{[\theta]}(\xi - u)} \, d\xi. \]
\( \hat{f}_k \) and \( f_k \) are related with the Hermite transformation.

Hermitian transformation between \( \hat{f}_k(x, t) \) and \( f_k(x, t) \):
\[
\begin{bmatrix}
\hat{f}_0 \\
\hat{f}_1 \\
\vdots \\
\hat{f}_M
\end{bmatrix} =
\begin{bmatrix}
\mathcal{H}_0^{[\theta]}(\sqrt{\theta}c_0) & \mathcal{H}_1^{[\theta]}(\sqrt{\theta}c_0) & \cdots & \mathcal{H}_M^{[\theta]}(\sqrt{\theta}c_0) \\
\mathcal{H}_0^{[\theta]}(\sqrt{\theta}c_1) & \mathcal{H}_1^{[\theta]}(\sqrt{\theta}c_1) & \cdots & \mathcal{H}_M^{[\theta]}(\sqrt{\theta}c_1) \\
\vdots & \vdots & \ddots & \vdots \\
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f_0 \\
f_1 \\
\vdots \\
f_M
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\[ f_{h,M} = \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \rightarrow f, \]

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\( \hat{f}_k \) and \( f_k \) are related with the Hermite transformation.

Restricted condition:

\[ f_1 = 0, \quad f_2 = 0. \]
Revelation from DVM

- Hyperbolic system: ??
- Wave speeds: $\xi_k = u + \sqrt{\theta} c_k$ ??
- H-theorem for BGK ??
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- H-theorem for BGK ??
Evolution Equation

Let us go back to the Hermite expansion:

\[
f_{h,M}(t, x, \xi) = \sum_{k=0}^{M} f_k(x, t) \mathcal{H}_k^{[\theta]}(\xi - u). \tag{10}
\]

The 1D Boltzmann equation reads:

\[
\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \frac{1}{\tau}(f_M - f). \tag{11}
\]

Particularly,

\[f_M = f_0 \mathcal{H}_0^{[\theta]}(\xi - u), \quad f_0 = \rho, \quad f_1 = f_2 = 0, \quad f_3 = q/3 \text{ heat flux.}\]

Substitute (10) into (11)?
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\[ \frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \frac{1}{\tau} (f_M - f). \] (11)

Particularly,

\[ f_M = f_0 \mathcal{H}_0^{[\theta]}(\xi - u), \quad f_0 = \rho, \quad f_1 = f_2 = 0, \quad f_3 = q/3 \text{ heat flux.} \]

Substitute (10) into (11)?
Evolution Equation

Let us go back to the Hermite expansion:

$$f_{h,M}(t, x, \xi) = \sum_{k=0}^{M} f_k(x, t) \mathcal{H}_k^{[\theta]} (\xi - u).$$  \hspace{1cm} (10)

The 1D Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \frac{1}{\tau} (f_M - f).$$  \hspace{1cm} (11)

Particularly,

$$f_M = f_0 \mathcal{H}_0^{[\theta]} (\xi - u), \quad f_0 = \rho, \quad f_1 = f_2 = 0, \quad f_3 = q/3 \text{ heat flux.}$$

Substitute (10) into (11)?
Grad’s Moment System

Substitute (10) into (11),

\[
\frac{\partial}{\partial t} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) + \xi \frac{\partial}{\partial x} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) = -\frac{1}{\tau} \sum_{k=3}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi-u).
\]

and make a directly expansion to have

\[
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, \tag{12a}
\]

\[
\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} + \rho u \frac{\partial u}{\partial x} = 0, \tag{12b}
\]

\[
\frac{1}{2} \rho \frac{\partial \theta}{\partial t} + \frac{1}{2} \rho u \frac{\partial \theta}{\partial x} + \frac{\partial q}{\partial x} + p \frac{\partial u}{\partial x} = 0, \tag{12c}
\]

\[
\frac{\partial f_k}{\partial t} - f_{k-1} \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + (k+1) f_k \frac{\partial u}{\partial x} + \left( \frac{1}{2} \theta f_{k-3} + \frac{k-1}{2} f_{k-1} \right) \frac{\partial \theta}{\partial x} - \frac{3}{\rho} \frac{\partial f_{k-2}}{\partial x} + \theta \frac{\partial f_{k-1}}{\partial x} + u \frac{\partial f_k}{\partial x} + (k+1) \frac{\partial f_{k+1}}{\partial x} = -\frac{1}{\tau} f_k, \quad \text{for } k \geq 3,
\]

where \( p = \rho \theta, q = 3 f_3 \).
Grad’s Moment System

Substitute (10) into (11),

\[
\frac{\partial}{\partial t} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) + \xi \frac{\partial}{\partial x} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) = -\frac{1}{\tau} \sum_{k=3}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u). 
\]

Recursive relation:
\[ \theta \mathcal{H}_{n+1}^{[\theta]}(v) = v \mathcal{H}_n^{[\theta]}(v) - n \mathcal{H}_{n-1}^{[\theta]}(v); \]

Differential relation:
\[ \frac{d \mathcal{H}_k^{[\theta(\tau)]}(v(\tau))}{d\tau} = -\mathcal{H}_k^{[\theta(\tau)]} \frac{dv(\tau)}{d\tau} + \frac{1}{2} \mathcal{H}_k^{[\theta(\tau)]} \frac{d\theta(\tau)}{d\tau}. \]

and make a directly expansion to have

\[
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, 
\]
\[ (12a) \]
\[
\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} + \rho u \frac{\partial u}{\partial x} = 0, 
\]
\[ (12b) \]
\[
\frac{1}{2} \rho \frac{\partial \theta}{\partial t} + \frac{1}{2} \rho u \frac{\partial \theta}{\partial x} + \frac{\partial q}{\partial x} + p \frac{\partial u}{\partial x} = 0, 
\]
\[ (12c) \]
Grad’s Moment System

Substitute (10) into (11),

$$\frac{\partial}{\partial t} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) + \xi \frac{\partial}{\partial x} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) = -\frac{1}{\tau} \sum_{k=3}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u).$$

and make a directly expansion to have

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0,$$

(12a)

$$\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} + \rho u \frac{\partial u}{\partial x} = 0,$$

(12b)

$$\frac{1}{2} \frac{\partial \theta}{\partial t} + \frac{1}{2} \frac{\partial \theta}{\partial x} + \frac{\partial q}{\partial x} + p \frac{\partial u}{\partial x} = 0,$$

(12c)

$$\frac{\partial f_k}{\partial t} - f_{k-1} \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + (k+1)f_k \frac{\partial u}{\partial x} + \left( \frac{1}{2} \theta f_{k-3} + \frac{k-1}{2} f_{k-1} \right) \frac{\partial \theta}{\partial x},$$

$$- \frac{3}{\rho} f_{k-2} \frac{\partial f_3}{\partial x} + \theta \frac{\partial f_{k-1}}{\partial x} + u \frac{\partial f_k}{\partial x} + (k+1) \frac{\partial f_{k+1}}{\partial x} = -\frac{1}{\tau} f_k,$$

for $k \geq 3$,

where $p = \rho \theta$, $q = 3f_3$. 
Grad’s Moment System

Substitute (10) into (11),

\[
\frac{\partial}{\partial t} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) + \xi \frac{\partial}{\partial x} \left( \sum_{k=0}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u) \right) = - \frac{1}{\tau} \sum_{k=3}^{M} f_k \mathcal{H}_k^{[\theta]}(\xi - u).
\]

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\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, \tag{12a}
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\[
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\]

\[
\frac{1}{2} \rho \frac{\partial \theta}{\partial t} + \frac{1}{2} \rho \theta \frac{\partial \theta}{\partial x} + \frac{\partial q}{\partial x} + p \frac{\partial u}{\partial x} = 0, \tag{12c}
\]

\[
\frac{\partial f_k}{\partial t} - f_{k-1} \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + (k + 1) f_k \frac{\partial u}{\partial x} + \left( \frac{1}{2} \theta f_{k-3} + \frac{k - 1}{2} f_{k-1} \right) \frac{\partial \theta}{\partial x} - \frac{3}{\rho} f_{k-2} \frac{\partial f_3}{\partial x} + \theta \frac{\partial f_{k-1}}{\partial x} + u \frac{\partial f_k}{\partial x} + (k + 1) \frac{\partial f_{k+1}}{\partial x} = - \frac{1}{\tau} f_k, \quad \text{for } k \geq 3,
\]

where \( p = \rho \theta, q = 3 f_3 \).
The Moment System

In quasi-linear formation: let \( w_M = (\rho, u, \theta, f_3, \cdots, f_M)^T \in \mathbb{R}^{M+1} \), \( M \in \mathbb{N} \) and \( M \geq 2 \), \( f_{M+1} = 0 \)

\[
\frac{\partial w_M}{\partial t} + A_M \frac{\partial w_M}{\partial x} = Qw, \tag{13}
\]

where \( A_M \) is a lower Hessenberg matrix as

\[
\begin{pmatrix}
 u & 0 & 0 & \cdots & 0 \\
 \theta/\rho & u & 0 & \cdots & 0 \\
 0 & 2\theta & u & \cdots & 0 \\
 0 & 4f_3 & \rho\theta/2 & \cdots & 0 \\
 -\theta f_3/\rho & 5f_4 & 3f_3/2 & \cdots & 0 \\
 \cdots & \cdots & \cdots & \cdots & \cdots \\
 -\theta f_M-2/\rho & Mf_M-1 & \frac{1}{2}[ (M-2)f_{M-2} + \theta f_{M-4} ] & \cdots & 0 \\
 -\theta f_M-1/\rho & (M+1)f_M & \frac{1}{2}[ (M-1)f_{M-1} + \theta f_{M-3} ] & \cdots & 0 \\
 \end{pmatrix}
\]

Question:

- Is the system (13) hyperbolic? \( \iff A_M \) is diagonalizable with real eigenvalues?
- Are \( u + c_k\sqrt{\theta} \), \( k = 0, \cdots, M \), the eigenvalues of \( A_M \)? \( \iff \) The eigenvalues of \( A_M \) are zeros of \( He_M^{[\theta]}(u - u) \)?
The Moment System

In quasi-linear formation: let \( \mathbf{w}_M = (\rho, u, \theta, f_3, \cdots, f_M)^T \in \mathbb{R}^{M+1}, \) \( M \in \mathbb{N} \) and \( M \geq 2, \) \( f_{M+1} = 0 \)

\[
\frac{\partial \mathbf{w}_M}{\partial t} + \mathbf{A}_M \frac{\partial \mathbf{w}_M}{\partial x} = \mathbf{Qw},
\]

(13)

where \( \mathbf{A}_M \) is a lower Hessenberg matrix as

\[
\begin{pmatrix}
    u & \rho & 0 & \cdots & 0 \\
    \theta / \rho & u & 2\theta & \cdots & 0 \\
    0 & 4f_3 & u & \cdots & 0 \\
    0 & 5f_4 & \rho \theta / 2 & \cdots & 0 \\
    -\theta f_3 / \rho & \cdots & \cdots & \cdots & \cdots \\
    -\theta f_{M-2} / \rho & \cdots & \cdots & \cdots & \cdots \\
    -\theta f_{M-1} / \rho & \cdots & \cdots & \cdots & \cdots \\
    \cdots & \cdots & \! (M+1)f_M & \cdots & \cdots \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix}
\]

Question:

- Is the system (13) hyperbolic? \( \iff \mathbf{A}_M \) is diagonalizable with real eigenvalues?
- Are \( u + c_k \sqrt{\theta}, \) \( k = 0, \cdots, M, \) the eigenvalues of \( \mathbf{A}_M? \) \( \iff \) The eigenvalues of \( \mathbf{A}_M \) are zeros of \( \mathcal{H}_{M+1}^{[\theta]}(u - u) \)?
The Moment System

In quasi-linear formation: let \( \mathbf{w}_M = (\rho, u, \theta, f_3, \cdots, f_M)^T \in \mathbb{R}^{M+1} \), \( M \in \mathbb{N} \) and \( M \geq 2 \), \( f_{M+1} = 0 \)

\[
\frac{\partial \mathbf{w}_M}{\partial t} + \mathbf{A}_M \frac{\partial \mathbf{w}_M}{\partial x} = \mathbf{Qw}, \tag{13}
\]

where \( \mathbf{A}_M \) is a lower Hessenberg matrix as

\[
\begin{pmatrix}
  u & \rho & 0 & \cdots & 0 \\
  \theta / \rho & u & \rho \theta / 2 & \cdots & 0 \\
  0 & 2\theta & u & \cdots & 0 \\
  0 & 4f_3 & 3f_3/2 & \cdots & 0 \\
  -\theta f_3 / \rho & 5f_4 & \cdots & \cdots & 0 \\
  -\theta f_{M-2} / \rho & Mf_{M-1} & \frac{1}{2}[(M-2)f_{M-2} + \theta f_{M-4}] & \cdots & 0 \\
  -\theta f_{M-1} / \rho & (M+1)f_M & \frac{1}{2}[(M-1)f_{M-1} + \theta f_{M-3}] & \cdots & 0 \\
  \end{pmatrix}
\]

Question:

- Is the system (13) hyperbolic? \( \iff \mathbf{A}_M \) is diagonalizable with real eigenvalues?
- Are \( u + c_k\sqrt{\theta} \), \( k = 0, \cdots, M \), the eigenvalues of \( \mathbf{A}_M \)? \( \iff \) The eigenvalues of \( \mathbf{A}_M \) are zeros of \( H_{\theta}^{[\theta]}(\rho - u) \)?
The Moment System

Theorem 1

*The characteristic polynomial of $A_M$ is*

$$He_M^{[\theta]} (\lambda - u)$$

$$- \frac{(M + 1)!}{2 \rho} \left[ \left( (\lambda - u)^2 - \theta \right) f_{M-1} + 2(\lambda - u) f_M \right].$$
The Moment System

Theorem 1
The characteristic polynomial of $A_M$ is

$$He_{M+1}^{[\theta]} (\lambda - u)$$

$$-\frac{(M + 1)!}{2\rho} \left[ ((\lambda - u)^2 - \theta) f_{M-1} + 2(\lambda - u)f_M \right].$$
Regularization of Moment System

We raised the following problem:

Find \( M + 1 \) functions \( a_j = a_j(w_M), j = 0, \cdots, M, \) such that

\[
\begin{align*}
\lambda I - A_M - \sum_{j=0}^{M} a_j E_{M+1,j} &= H e^{[\theta]}_{M+1} (\lambda - w) \\

\end{align*}
\]

where \( E_{ij} \) is a \((M + 1) \times (M + 1)\) matrix, with only the \((i, j)\)-th entry nonzero, and equals to 1.

The answer of this problem is unique as:

\[
\begin{align*}
a_1 &= 0, \\
a_2 &= -(M + 1) f_M, \\
a_3 &= -\frac{M + 1}{2} f_{M-1}. \quad (14) \\

a_j &\equiv 0, \quad j = 4, \cdots, M + 1, \quad (15)
\end{align*}
\]
Regularization of Moment System

We raised the following problem:

Find $M + 1$ functions $a_j = a_j(w_M)$, $j = 0, \cdots, M$, such that

$$\lambda I - A_M - \sum_{j=0}^{M} a_j E_{M+1,j} = He_{M+1}^{(0)} (\lambda - w)$$

where $E_{ij}$ is a $(M+1) \times (M+1)$ matrix, with only the $(i, j)$-th entry nonzero, and equals to 1.

The answer of this problem is unique as:

$$a_1 = 0, \quad a_2 = -(M + 1)f_M, \quad a_3 = -\frac{M + 1}{2}f_{M-1}. \quad (14)$$

$$a_j \equiv 0, \quad j = 4, \cdots, M + 1, \quad (15)$$
Regularization of Moment System

**Definition 2**
The regularization term based on the characteristic speed correction is denoted as
\[
R_M \triangleq \frac{M + 1}{2} \left( 2 f_M \frac{\partial u}{\partial x} + f_{M-1} \frac{\partial \theta}{\partial x} \right).
\] (16)

**Theorem 3**
The moment system
\[
\frac{\partial w_M}{\partial t} + \hat{A}_M \frac{\partial w_M}{\partial x} = 0, \quad \hat{A}_M \frac{\partial w_M}{\partial x} = A_M \frac{\partial w_M}{\partial x} - R_M e_{M+1}
\] (17)

is strictly hyperbolic if \( \theta > 0 \), and its characteristic speeds are
\[
\xi_j = u + c_j \sqrt{\theta}, \quad j = 1, \ldots, M + 1.
\] (18)
Regularization of Moment System

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(18)
Regularization of Moment System

\[
\frac{\partial f_M}{\partial t} - f_{M-1} \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + (M + 1) f_M \frac{\partial u}{\partial x} + \left( \frac{1}{2} \theta f_{M-3} + \frac{M - 1}{2} f_{M-1} \right) \frac{\partial \theta}{\partial x} - \frac{3}{\rho} f_{M-2} \frac{\partial f_3}{\partial x} + \theta \frac{\partial f_{M-1}}{\partial x} + u \frac{\partial f_M}{\partial x} + (M + 1) \frac{\partial f_{M+1}}{\partial x} = 0
\]

The regularization makes

\[
\frac{\partial f_{M+1}}{\partial x} = -f_M \frac{\partial u}{\partial x} - \frac{1}{2} f_{M-1} \frac{\partial \theta}{\partial x}.
\]

A nonlocal state equation!

Let us recall the Euler equations for ideal gas (Gamma law)

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0, \\
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0,
\end{align*}
\]
Regularization of Moment System

\[
\frac{\partial f_M}{\partial t} - f_{M-1} \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + (M + 1) f_M \frac{\partial u}{\partial x} + \left( \frac{1}{2} \theta f_M - 3 + \frac{M - 1}{2} f_{M-1} \right) \frac{\partial \theta}{\partial x} \\
- \frac{3}{\rho} f_{M-2} \frac{\partial f_3}{\partial x} + \theta \frac{\partial f_{M-1}}{\partial x} + u \frac{\partial f_M}{\partial x} + (M + 1) \frac{\partial f_{M+1}}{\partial x} = 0
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\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} &= 0.
\end{align*}
\]
Regularization of Moment System

The regularization makes

\[
\frac{\partial f_{M+1}}{\partial x} = -f_M \frac{\partial u}{\partial x} - \frac{1}{2} f_{M-1} \frac{\partial \theta}{\partial x}. \tag{19}
\]

The distribution function

\[
f_h(x, \xi; t) = \sum_{k=0}^{M} f_k(x, t) \mathcal{H}_{\theta, k}(v)
\]

should be revised to

\[
\sum_{k=0}^{M} f_k(x, t) \mathcal{H}_{\theta, k}(v) - f_{M+1}(x, t) \mathcal{H}_{\theta, M+1}(v)
\]

where \(f_{M+1}(x, t)\) satisfied (19).

A nonlocal state equation!

Let us recall the Euler equations for ideal gas (Gamma law)

\[
\begin{align*}
\partial_t u + u \partial_x u + \frac{1}{\gamma} \partial_x p &= 0, \\
\partial_t \rho + \partial_x (\rho u) &= 0, \\
\partial_t s + \partial_x (\rho u s) &= 0,
\end{align*}
\]
Regularization of Moment System

The regularization makes

\[
\frac{\partial f_{M+1}}{\partial x} = -f_M \frac{\partial u}{\partial x} - \frac{1}{2} f_{M-1} \frac{\partial \theta}{\partial x}.
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Let us recall the Euler equations for ideal gas (Gamma law)

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\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} &= 0,
\end{align*}
\]

with the state equation giving the pressure as

\[ p = \rho^\gamma \exp(s), \quad s \text{ is the entropy.} \]
Regularization of Moment System

The regularization makes

$$\frac{\partial f_{M+1}}{\partial x} = -f_M \frac{\partial u}{\partial x} - \frac{1}{2} f_{M-1} \frac{\partial \theta}{\partial x}. \tag{19}$$

A nonlocal state equation!

Let us recall the Euler equations for ideal gas (Gamma law)

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0, \\
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0, \\
\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} &= 0,
\end{aligned}$$

with the state equation giving the pressure as

$$p = \rho^\gamma \exp(s), \quad s \text{ is the entropy.}$$
Characteristic wave

Theorem 4

The right eigenvector of $A_M$ with eigenvalue $u + c_j \sqrt{\theta}$ is

$$r_j = (r_{j,1}, \cdots, r_{j,M+1})^T, \quad j = 1, \cdots, M + 1,$$

(20)

where $r_{j,k}$ is defined as

$$r_{j,1} = \rho, \quad r_{j,2} = c_j \sqrt{\theta}, \quad r_{j,3} = (c_j^2 - 1)\theta,$$

$$r_{j,k} = \frac{He_{k-1}(c_j)}{(k - 1)!} \rho \theta^{\frac{k-1}{2}} - \frac{c_j^2 - 1}{2} \theta f_{k-3} - c_j \sqrt{\theta} f_{k-2}, \quad k = 4, \cdots, M + 1.$$

Corollary 5

Each characteristic field of the hyperbolic system (17) is either genuinely nonlinear or linearly degenerate.
Characteristic wave

Theorem 4
The right eigenvector of $A_M$ with eigenvalue $u + c_j \sqrt{\theta}$ is

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$$r_{j,k} = \frac{He_{k-1}(c_j)}{(k-1)!} \frac{c_j^2 - 1}{2} \theta f_{k-3} - c_j \sqrt{\theta} f_{k-2}, \quad k = 4, \cdots, M + 1.$$

Corollary 5
Each characteristic field of the hyperbolic system (17) is either genuinely nonlinear or linearly degenerate.
Characteristic wave

**Theorem 6**

*The Riemann invariants for the \( j \)-family for system (17) are*

\[
R_1 = \rho \theta^{-1/(c_j^2-1)}, \quad R_2 = u - \frac{2c_j}{c_j^2 - 1} \sqrt{\theta},
\]

\[
R_k = C_{k,0} \rho \theta^{k/2} + \sum_{i=3}^{k} C_{k,i} f_i \theta^{(k-i)/2}, \quad k = 3, \ldots, M. \tag{21}
\]

\[
C_{k,k} = 1, \quad C_{k,k-1} = \frac{2c_j}{c_j^2 - 1}, \quad C_{k,0} = \frac{2}{(1-c_j^2)k-2} \sum_{i=3}^{k} \frac{He_i(c_j)}{i!} C_{k,i},
\]

\[
C_{k,i} = \frac{1}{k-i} \left( C_{k,i+2} + C_{k,i+1} \frac{2c_j}{c_j^2 - 1} \right), \quad i = 3, \ldots, k-2.
\]
Characteristic wave

Theorem 7

For hyperbolic moment system (17), the type of wave of the $j$-th family can be determined by the value of $c_j$ and the macroscopic velocities or pressures on both sides of the wave:

<table>
<thead>
<tr>
<th>Type of Wave</th>
<th>Velocity Condition</th>
<th>Pressure Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact discontinuity</td>
<td>$c_j = 0, u^L = u^R$</td>
<td>$c_j = 0, p^L = p^R$</td>
</tr>
<tr>
<td>Rarefaction wave</td>
<td>$c_j \neq 0, u^L &lt; u^R$</td>
<td>$c_j &gt; 0, p^L &lt; p^R$; $c_j &lt; 0, p^L &gt; p^R$</td>
</tr>
<tr>
<td>Shock wave</td>
<td>$c_j \neq 0, u^L &gt; u^R$</td>
<td>$c_j &gt; 0, p^L &gt; p^R$; $c_j &lt; 0, p^L &lt; p^R$</td>
</tr>
</tbody>
</table>
Classical DVM in the Moment Method point of view

We define generalized “moment”s as

\[ f_k(x, t) \triangleq \int_{\mathbb{R}} f(x, \xi; t) \psi_k^k(\xi) \, d\xi \]

where \( \xi_{k+1/2} = (\xi_k + \xi_{k+1})/2 \) and

\[ \psi_k^k(\xi) = \begin{cases} 
1, & \xi \in [\xi_{k-1/2}, \xi_{k+1/2}], \\
0, & \text{otherwise}.
\end{cases} \]

Then

\[ f_h(x, \xi; t) = \sum_{k=0}^{N} f_k(x, t) \psi_k^k(\xi), \]

and the discrete velocity model is recovered as the system of the “moment”s \( f_k \)

\[ \frac{\partial f_k}{\partial t} + \xi_k \frac{\partial f_k}{\partial x} = Q_k(f_h, f_h). \]
Classical DVM in the Moment Method point of view

We define generalized “moment”s as

$$f_k(x, t) \triangleq \int_{\mathbb{R}} f(x, \xi; t) \psi^k(\xi) \, d\xi$$

where $$\xi_{k+1/2} = (\xi_k + \xi_{k+1})/2$$ and

$$\psi^k(\xi) = \begin{cases} 1, & \xi \in [\xi_{k-1/2}, \xi_{k+1/2}], \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$f_h(x, \xi; t) = \sum_{k=0}^{N} f_k(x, t) \psi^k(\xi),$$

and the discrete velocity model is recovered as the system of the “moment”s $$f_k$$

$$\frac{\partial f_k}{\partial t} + \xi_k \frac{\partial f_k}{\partial x} = Q_k(f_h, f_h).$$
Cavity Flow

- Monatomic gas: argon (with mass $m = 6.63 \times 10^{-26}$ kg).
- $U_w = 50 \text{m/s}$, and $T_{wall} = T_0 = 273K$.
- Shakhov collision model is used, and relaxation time:
  \[ \tau = \sqrt{\frac{2}{\pi}} \frac{Kn}{\theta \omega}, \quad w = 0.81. \]
- 200 $\times$ 200 grid points for spatial discretization.
- Different Knudsen number $Kn$ is studied.
Cavity Flow with $Kn = 0.1$

Figure 1: Cavity at $Kn = 0.1$. (a) Temperature $T = \theta T_0$ contours with $M = 20$, black lines: DSMC, white lines and background: MM. (b) Heat flux with $M = 20$, red dash-dot line: DSMC, blue line: MM.
Cavity Flow with $Kn = 0.5$

Figure 2: Cavity at $Kn = 0.5$. (a) Temperature $T = \theta T_0$ contours with $M = 25$, black lines: DSMC, white lines and background: MM. (b) Heat flux with $M = 25$, red dash-dot line: DSMC, blue line: MM.
Cavity Flow with $Kn = 1$

Figure 3: Cavity at $Kn = 1$. (a) Temperature $T = \theta T_0$ contours with $M = 25$, black lines: DSMC, white lines and background: MM. (b) Heat flux with $M = 25$, red dash-dot line: DSMC, blue line: MM.
Cavity Flow with $Kn = 8$

Figure 4: Cavity at $Kn = 8$. (a) Temperature $T = \theta T_0$ contours with $M = 35$, black lines: DSMC, white lines and background: MM. (b) Heat flux with $M = 35$, red dash-dot line: DSMC, blue line: MM.
Conclusion Remarks

- The moment method is actually a discrete velocity model with adaptive velocity points;

- Appropriate closure has to be made to achieve the globally hyperbolicity, thus local well-posedness;

- The moment method may have an improved efficiency in the approximation since it is a spectral expansion.
Conclusion Remarks

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Conclusion Remarks

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Thank You

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Reference:

1 1D result: Z.-N. Cai, Y.-W. Fan and R. Li, Globally Hyperbolic Regularization of Grad’s Moment System in One Dimensional Space, Communications in Math Sciences, 11(2), 2012, pp. 547-571.

2 nD result: Z.-N. Cai, Y.-W. Fan and R. Li, Globally Hyperbolic Regularization of Grad’s Moment System, Accepted by Communications on Pure and Applied Mathematics.