Hyperbolic Quadrature Method of Moments for the one-dimensional kinetic equation

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Considered kinetic model

Kinetic model on $f(t, x, v)$

$$\frac{\partial f}{\partial t} + \nabla \cdot (v f) = S(f)$$

- $\frac{\partial f}{\partial t}$ physical transport
- $S(f)$ Source terms
**Context**

**Considered kinetic model**

**Kinetic model on \( f(t, x, v) \)**

\[
\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} \left( v f \right) = S(f)
\]

- **physical transport**
- **Source terms**

**Gas dynamics**

For example, BGK source term: \( S(f) = -\frac{f - f_{eq}}{Kn} \)

Transition regime: \( 0.01 < Kn < 10 \)

Far from the Maxwellian equilibrium
Considered kinetic model

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\partial_t f + \partial_x \cdot (v f) = S(f)
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**Population of inertial particles in a gas**

for example drag source term: \( S(f) = -\partial_v \cdot \left( \frac{v_g(t, x) - v}{St} f \right) \)

Particle trajectory crossing for large enough particles (and \( St \)): \( f \) is no more a Dirac delta function
Considered kinetic model

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- **Physical transport**
- **Source terms**

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**Population of inertial particles in a gas**

- For example drag source term: \( S(f) = -\partial_v \cdot \left( \frac{v_g(t, x) - v}{St} f \right) \)
- Particle trajectory crossing for large enough particles (and \( St \)): \( f \) is no more a Dirac delta function

- The kinetic model is too costly to solve with direct methods of Monte-Carlo type
- Moments \( \int_{\mathbb{R}} v^k f(t, x, v) dv \) of order \( k \) smaller than 1 or 2 are not enough to represent the distribution.
Moment method

Principle of the method

Write equations on a finite set of moments $\mathbf{m}_N = (m_0, m_1, \ldots, m_N)^t$:

$$\partial_t m_k + \partial_x m_{k+1} = S_k, \quad k = 0, 1, \ldots, N \quad (1)$$

**Closure**: express $m_{N+1}$ (and eventually the source terms $S_k$) as a function of $\mathbf{m}_N$.

**Issues**:
- $(m_0, m_1, \ldots, m_N, m_{N+1})^t$ is realizable
- The system (1) is globally hyperbolic
- Capture equilibrium state

**Strategy**
- Solve the Hamburger truncated moment problem:
  
  find a positive measure $\mu$ such that $\mathbf{m}_N = \int_{\mathbb{R}} (1, \mathbf{v}, \ldots, \mathbf{v}^N)^t d\mu(\mathbf{v})$.

  and set $m_{N+1} = \int_{\mathbb{R}} \mathbf{v}^{N+1} d\mu(\mathbf{v})$
- Give directly $m_{N+1}$
Moment method

**Principle of the method**

Write equations on a finite set of moments $\mathbf{m}_N = (m_0, m_1, \ldots, m_N)^t$:

$$
\partial_t m_k + \partial_x m_{k+1} = S_k, \quad k = 0, 1, \ldots, N
$$

**Closure**: express $m_{N+1}$ (and eventually the source terms $S_k$) as a function of $\mathbf{m}_N$.

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**Examples of closure in the literature**
- Grad closure [Grad, 1949] $\rightarrow$ hyperbolic only around the moments of the maxwellian distribution
- Entropy maximization [Levermore, 1996, Müller and Ruggeri, 1998] $\rightarrow$ high computational cost - not valid on the entire realizability domain
Moment method

Moment space

**Definition**

The \( n^{th} \)-moment space \( \mathcal{M}_n \) is defined by

\[
\mathcal{M}_n = \left\{ \mathbf{m} \in \mathbb{R}^{n+1} \mid \exists \mu \in \mathcal{M}_+(\mathbb{R}), \quad \mathbf{m} = \int_{\mathbb{R}} (1, v, \ldots, v^n)^t d\mu(v) \right\}
\]

If \( \mathbf{m} \) belongs to \( \mathcal{M}_n \), then it is said to be realizable.
If \( \mathbf{m} \) belongs to the interior \( \text{Int} \mathcal{M}_n \) of \( \mathcal{M}_n \), it is said to be strictly realizable.

Characterized by the non-negativity of the **Hankel determinants**: \( n \geq 0 \)

\[
H_{2n} = \begin{vmatrix}
 m_0 & \cdots & m_n \\
 \vdots & \ddots & \vdots \\
 m_n & \cdots & m_{2n}
\end{vmatrix}
\]

**Theorem**

\[
\mathbf{m}_N = (m_0, m_1, \ldots, m_N)^t \text{ strictly realizable } \iff H_{2k} > 0, \quad k \in \{0, 1, \ldots, \left\lfloor \frac{N}{2} \right\rfloor \}
\]

\[
\mathbf{m}_N \in \partial \mathcal{M}_N \cap \mathcal{M}_n \Rightarrow H_0 > 0, \ldots, H_{2k-2} > 0, H_{2k} = 0, \ldots, H_{2\left\lfloor \frac{N}{2} \right\rfloor} = 0, \quad k \leq \left\lfloor \frac{N}{2} \right\rfloor.
\]

In the latter case, the only corresponding measure is a sum of \( k \) weighted Dirac delta functions.

Moment method

Moment space

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If $\mathbf{m}$ belongs to $\mathcal{M}_n$, then it is said to be **realizable**.

If $\mathbf{m}$ belongs to the interior $\text{Int} \, \mathcal{M}_n$ of $\mathcal{M}_n$, it is said to be **strictly realizable**.

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m_0 & \ldots & m_n \\
\vdots & \ddots & \vdots \\
m_n & \ldots & m_{2n}
\end{vmatrix}
$$

First constraints for the strict realizability:

$$
m_0 > 0 \quad m_2 > \frac{m_1^2}{m_0} \quad m_4 > \frac{m_0 m_3^2 - 2m_1 m_2 m_3 + m_3^2}{m_2 m_0 - m_1^2} \quad \ldots
$$
Hyperbolicity

Characteristic polynomial

System on moments

Equations on \( \mathbf{m}_N = (m_0, m_1, \ldots, m_N)^t \):

\[
\partial_t \mathbf{m}_N + \partial_x F(\mathbf{m}_N) = \bar{S}
\]

Characteristic Polynomial

Jacobian matrix

\[
\frac{DF(\mathbf{m}_N)}{D\mathbf{m}_N} =
\begin{pmatrix}
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}
\]

Characteristic polynomial

\[
\bar{P}_{N+1}(X) = X^{N+1} - \sum_{i=0}^{N} \frac{\partial m_{N+1}}{\partial m_i} X^i
\]
Moments - Central moments - Standardized moments

moments:

\[ m_k = \int_{\mathbb{R}} v^k f(v) dv \]

central moments: with \( \rho = m_0, \ u = \frac{m_1}{m_0} \) and \( f^c(c) = \frac{1}{\rho} f(c + u) \)

\[ C_k = \frac{1}{\rho} \int_{\mathbb{R}} (v - u)^k f(v) dv = \int_{\mathbb{R}} c^k f^c(c) dc \]

so that \( C_0 = 1 \) and \( C_1 = 0 \).

standardized moments: with \( \sigma = \sqrt{C_2} \), \( f^s(s) = \frac{\sigma}{\rho} f(u + \sigma s) \)

\[ S_k = \frac{1}{m_0} \int_{\mathbb{R}} \left( \frac{v - u}{\sqrt{C_2}} \right)^k f(v) dv = \int_{\mathbb{R}} s^k f^s(s) ds \]

so that \( S_0 = 1, S_1 = 0 \) and \( S_2 = 1 \).

link:

\[ C_k = \sum_{i=0}^{k} \binom{k}{i} \left( -\frac{m_1}{m_0} \right)^{k-i} m_i, \quad m_k = \rho \left( \sum_{i=2}^{k} \binom{k}{i} u^{k-i} C_i + u^k \right), \quad S_k = \frac{C_k}{(C_2)^{k/2}}. \]
Property of the characteristic polynomial

\[ m_N = (m_0, m_1, \ldots, m_N)^t \] be a realizable moment vector such that \( m_0 > 0 \) and \( C_2 > 0 \).

Linear functional \( \langle \cdot \rangle_{m_N} \) on the space \( \mathbb{R}[X]_N \)

\[ \langle X^k \rangle_{m_N} = m_k, \quad \text{for } k \in \{0, 1, \ldots, N\}. \]

Linear functional \( \langle \cdot \rangle_{S_N} \) associated with the standardized moments \( S_N = (S_0, \ldots, S_N)^t \):

\[ \langle X^k \rangle := \langle X^k \rangle_{S_N} = S_k, \quad \text{for } k \in \{0, 1, \ldots, N\}. \]

Property of the scaled characteristic polynomial

Let us assume that the function \( S_{N+1} \) does not depend on \((m_0, u, C_2)\), i.e., \( S_{N+1}(S_3, \ldots, S_N) \). Then, the following polynomial

\[ P_{N+1}(X) := \overline{P}_{N+1} \left( u + C_2^{1/2} X \right) C_2^{-(N+1)/2} \]

only depends on \((S_3, \ldots, S_N)\), and

\[ \langle P_{N+1} \rangle = 0, \quad \langle P'_{N+1} \rangle = 0, \quad \langle XP'_{N+1} \rangle = 0. \]
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QMOM: Principles of the method

From a strictly realizable moment vector $\mathbf{m}_{2n-1}$

**Reconstruction**

reconstruct the discret measure $\mu = \sum_{i=1}^{n} w_i \delta u_i$
in such a way that

$$\sum_{i=1}^{n} w_i u_i^k = m_k \quad k = 0, 1, \ldots, 2n - 1$$

**Closure**

$$m_{2n} = \int_{\mathbb{R}} v^{2n} d\mu = \sum_{i=1}^{n} w_i u_i^{2n}$$

It is the minimal value for this moment
**QMOM: Principles of the method**

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It is the minimal value for this moment

**Reconstruction**

From the standardized moments $S_{2n-1}$, with $\rho = m_0$, $u = m_1/m_0$, $\sigma = \sqrt{C_2}$

reconstruct the discret measure

$$\mu = \sum_{i=1}^{n} \rho \omega_i \delta u + \sigma c_i$$

in such a way that

$$\sum_{i=1}^{n} \omega_i c_i^k = S_k \quad k = 0, 1, \ldots, 2n - 1$$

**Closure**

$$S_{2n} = \sum_{i=1}^{n} \omega_i c_i^{2n}$$
QMOM: Principles of the method

From a strictly realizable moment vector \( m_{2n-1} \)

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From the standardized moments \( S_{2n-1} \), with \( \rho = m_0, u = m_1/m_0, \sigma = \sqrt{C_2} \)

**Reconstruction**

reconstruct the discret measure

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in such a way that

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\]

**Closure**

\[
S_{2n} = \sum_{i=1}^{n} \omega_i c_i^{2n}
\]

Remarks

- The reconstruction \( \mu \) is the only one possible for the moment vector \( m_{2n} \).
- \( m_{2n} \) is at the boundary of the moment space: \( H_{2n} = 0 \)
**Introduction**

**QMOM**

**HyQMOM**

**Results**

**Conclusion, Perspectives**

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**Principle of the method**

**QMOM: Computation of the weights and abscissas**

\( m_{2n-1} \): strictly realizable moment vector

**Orthogonal polynomials**

Family \((Q_k)_{k=0,...,n}\) of monic orthogonal polynomials for the scalar product \((p, q) \mapsto \langle pq \rangle\) of \(\mathbb{R}_n[X]\).

\[ Q_{k+1}(X) = (X - a_k)Q_k(X) - b_k Q_{k-1}(X) \]

with \(Q_{-1} = 0\) and \(Q_0 = 1\).

The recurrence coefficients \(a_k\) and \(b_k\) can be found from the standardized moments using the Chebyshev algorithm [Chebyshev, 1859, Wheeler, 1974, Gautschi, 2004]

\[
\begin{align*}
    a_k &= \frac{\langle XQ_k^2 \rangle}{\langle Q_k^2 \rangle}, \\
    b_k &= \frac{\langle Q_k^2 \rangle}{\langle Q_{k-1}^2 \rangle} = \frac{H_{2k} H_{2k-4}}{H_{2k-2}^2}.
\end{align*}
\]

example

\[
\begin{align*}
    a_0 &= 0, & a_1 &= S_3, & a_2 &= \frac{S_5 - S_3(2 + S_3^2 + 2H_4)}{H_4} \\
    b_0 &= 1, & b_1 &= 1, & b_2 &= H_4, & b_3 &= H_6 / H_4^2
\end{align*}
\]
QMOM: Computation of the weights and abscissas

\[ m_{2n-1} \]: strictly realizable moment vector

Orthogonal polynomials

Family \((Q_k)_{k=0,\ldots,n}\) of monic orthogonal polynomials for the scalar product \((p, q) \mapsto \langle pq \rangle\) of \(\mathbb{R}_n[X]\).

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The recurrence coefficients \(a_k\) and \(b_k\) can be found from the standardized moments using the Chebyshev algorithm [Chebyshev, 1859, Wheeler, 1974, Gautschi, 2004]

The abscissas \(c_i\) are the zeros of \(Q_n\) and also the eigenvalues of the Jacobi matrix

\[
J_n = \begin{pmatrix}
a_0 & \sqrt{b_1} & \sqrt{b_2} & \cdots & \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-1}} \\
\sqrt{b_1} & a_1 & \sqrt{b_2} & \cdots & \sqrt{b_{n-1}} & a_{n-1} \\
\sqrt{b_2} & \sqrt{b_1} & a_1 & \cdots & \sqrt{b_{n-2}} & a_{n-2} \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
\sqrt{b_{n-2}} & \sqrt{b_{n-1}} & \cdots & \sqrt{b_2} & a_1 & \sqrt{b_1} \\
\sqrt{b_{n-1}} & \sqrt{b_{n-2}} & \cdots & \sqrt{b_1} & a_1 & \sqrt{b_0}
\end{pmatrix}
\]
Hyperbolicity of the QMOM method

Theorem

The QMOM closure $b_n = 0$ induces the following characteristic polynomial $P_{2n} = Q_n^2$ and the system is only weakly hyperbolic.

proof [Chalons et al., 2012, Huang et al., 2020]
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First version of the HyQMOM closure [Fox et al., 2018]

Extension of QMOM, adding one moment and one abscissa for the reconstruction [Fox et al., 2018]

three-node HyQMOM

reconstruction with an additional fixed abscissa \( \mu = w_0 \delta_u + \sum_{i=1}^{2} w_i \delta u_i \) in such a way that

\[
w_0 u^k + \sum_{i=1}^{n} w_i u_i^k = m_k \quad k = 0, 1, \ldots, 4
\]

Closure

in term of the standardized moments: \( S_5 = S_3(2S_4 - S_3^2) \)

Theorem (Hyperbolicity)

Assuming that the vector \( m_4 \) is strictly realizable, then system with the three-node HyQMOM closure is hyperbolic.

Problem

- The generalization to a larger number of moment is not easy
- The eigenvalues of the problem do not tend to the ones of QMOM when \( H_4 \to 0 \)
Idea:
- Instead of looking at a reconstruction or at a closure on $S_{2n+1}$, one looks at $a_n$.
- Have a reduced characteristic polynomial on the form

$$P_{2n+1} = Q_n [(X - \alpha_n)Q_n - \beta_n Q_{n-1}]$$

such that $\beta_n$ tends to zero when $H_{2n} \to 0$.

Theorem:

For all $n = 1, 2, \ldots$; let the monic polynomial $P_{2n+1}$ be given by

$$P_{2n+1} = Q_n [(X - \alpha_n)Q_n - \beta_n Q_{n-1}] \quad \alpha_n, \beta_n \in \mathbb{R}$$

Then, the following statements are equivalent:

(i) $\langle P_{2n+1} \rangle = 0$, $\langle P_{2n+1}' \rangle = 0$ and $\langle XP_{2n+1}' \rangle = 0$.

(ii) $\alpha_n = a_n = \frac{1}{n} \sum_{k=0}^{n-1} a_k$ and $\beta_n = \frac{2n+1}{n} b_n$. 
New HyQMOM closure [Fox and Laurent, 2021]

Theorem

For all \( n = 1, 2, \ldots, 9 \); the scaled characteristic polynomial can be written as

\[
P_{2n+1} = Q_n \left[ (X - \alpha_n)Q_n - \beta_nQ_{n-1} \right]
\]

if and only if the closure on \( S_{2n+1} \), defined through the coefficient \( a_n \), and the coefficients \( \alpha_n \) and \( \beta_n \) are related to the recurrence coefficients \( a_k \) and \( b_k \) by

\[
a_n = \alpha_n = \frac{1}{n} \sum_{k=0}^{n-1} a_k, \quad \beta_n = \frac{2n+1}{n} b_n.
\]

Proof using formal computation with matlab symbolic:
from the \( a_k \) and \( b_k \), \( k = 0, \ldots, n - 1 \) (with \( a_0 = 0, a_1 = 1, b_0 = 1 \))

1. set the closure \( a_n = \frac{1}{n} \sum_{k=0}^{n-1} a_k \)

2. compute the Standardized moments \( S_{2n+1} \) with the reverse Chebyshev algorithm

3. compute the coefficients \( c_k \) of \( P_{2n+1} \)

4. compute the polynomials \( Q_k, k = 0, 1, \ldots, n \)

5. compute \( P_{2n+1} - Q_n \left[ (X - a_n)Q_n - \frac{2n+1}{n} b_nQ_{n-1} \right] \)
New HyQMOM closure

Theorem

For all \( n = 1, 2, \ldots, 9 \); the scaled characteristic polynomial can be written as

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\]

Examples

- \( n = 1 \): \( S_3 = 0 \) (as for the Maxwellian reconstruction)
- \( n = 2 \): \( S_5 = \frac{1}{2} S_3 (5S_4 - 3S_3^2 - 1) \) (different from the previous version: \( S_5 = S_3 (2S_4 - S_3^2) \))
Hyperbolicity - Eigenvalues

**Theorem**

*When $\beta_n > 0$, the $n + 1$ roots of $R_{n+1} = (X - \alpha_n)Q_n - \beta_nQ_{n-1}$ are real-valued and bound and separate the $n$ roots of $Q_n$.*

comes from Christoffel–Darboux formula.

The roots of $P_{2n+1}$ are then the eigenvalues of the two following Jacobi matrices:

$$
\begin{pmatrix}
    a_0 & \sqrt{b_1} & \sqrt{b_2} & \cdots & \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-1}} \\
    \sqrt{b_1} & a_1 & \sqrt{b_2} & \cdots & \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-1}} \\
    \sqrt{b_2} & a_1 & \sqrt{b_2} & \cdots & \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-1}} \\
    \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
    \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-2}} & \cdots & \sqrt{b_{n-1}} & a_{n-2} & \sqrt{b_{n-1}} \\
    \sqrt{b_{n-1}} & a_{n-1} & \sqrt{b_{n-1}} & \cdots & \sqrt{b_{n-1}} & a_{n-1} & \sqrt{b_{n-1}} \\
    a_{n-1} & \sqrt{b_{n-1}} & a_{n-1} & \cdots & \sqrt{b_{n-1}} & a_{n-1} & \sqrt{b_{n-1}} \\
    \sqrt{\beta_n} & a_{n-1} & \sqrt{\beta_n} & \cdots & \sqrt{\beta_n} & a_{n-1} & \sqrt{\beta_n} \\
    \sqrt{\alpha_n} & a_{n-1} & \sqrt{\alpha_n} & \cdots & \sqrt{\alpha_n} & a_{n-1} & \sqrt{\alpha_n}
\end{pmatrix}
$$
Hyperbolicity - Eigenvalues

Theorem

When $\beta_n > 0$, the $n + 1$ roots of $R_{n+1} = (X - \alpha_n)Q_n - \beta_n Q_{n-1}$ are real-valued and bound and separate the $n$ roots of $Q_n$.

comes from Christoffel–Darboux formula.

Example of the evolution of the eigenvalues with $H_{2n}$

$$S_3 = -1$$

$$n = 2$$

$$(S_3, S_4, S_5) = (-1, 5, -8)$$

$$n = 3$$
Theorem

When $\beta_n > 0$, the $n + 1$ roots of $R_{n+1} = (X - \alpha_n)Q_n - \beta_n Q_{n-1}$ are real-valued and bound and separate the $n$ roots of $Q_n$.

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Example of the evolution of the eigenvalues with $H_{2n}$

\[
S_3 = -1
\]

\[
(S_3, S_4, S_5) = (-1, 5, -8)
\]

The moment system with the HyQMOM closure is then hyperbolic, whatever the strictly realizable moment.
Practical Computations

Closure, directly from the moments \( m_{2n} \)

1. Compute the \( (\bar{a}_k)^{n-1}_{k=0} \) and \( (\bar{b}_k)^n_{k=0} \) from \( m_{2n} \) with the Chebyshev algorithm.

2. Set the closure \( \bar{a}_n = \frac{1}{n} \sum_{k=0}^{n-1} \bar{a}_k \).

3. Compute \( m_{2n+1} \) using the reverse Chebyshev algorithm.
Properties - Practical computations

**Practical computations**

**Closure, directly from the moments \( m_{2n} \)**

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**Eigenvalues of the system**

Eigenvalues of the two following Jacobi matrices:

\[
\begin{pmatrix}
\bar{a}_0 & \sqrt{\bar{b}_1} \\
\sqrt{\bar{b}_1} & \bar{a}_1 & \sqrt{\bar{b}_2} \\
& \ddots & \ddots & \ddots \\
& \sqrt{\bar{b}_{n-2}} & \bar{a}_{n-2} & \sqrt{\bar{b}_{n-1}} \\
& & \sqrt{\bar{b}_{n-1}} & \bar{a}_{n-1}
\end{pmatrix},
\begin{pmatrix}
\bar{a}_0 & \sqrt{\bar{b}_1} \\
\sqrt{\bar{b}_1} & \bar{a}_1 & \sqrt{\bar{b}_2} \\
& \ddots & \ddots & \ddots \\
& \sqrt{2n+1} \bar{b}_n & \bar{a}_{n-1} & \sqrt{\frac{2n+1}{n} \bar{b}_n}
\end{pmatrix}
\]
Practical computations

**Closure, directly from the moments \( m_{2n} \)**

1. Compute the \( (\bar{a}_k)_{k=0}^{n-1} \) and \( (\bar{b}_k)_{k=0}^{n} \) from \( m_{2n} \) with the Chebyshev algorithm.

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**Eigenvalues of the system**

Eigenvalues of the two following Jacobi matrices:

\[
\begin{pmatrix}
\bar{a}_0 & \sqrt{\bar{b}_1} & \sqrt{\bar{b}_2} & \cdots & \sqrt{\bar{b}_{n-2}} & \sqrt{\bar{b}_{n-1}} \\
\sqrt{\bar{b}_1} & \bar{a}_1 & \sqrt{\bar{b}_2} & \cdots & \sqrt{\bar{b}_{n-2}} & \sqrt{\bar{b}_{n-1}} \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
\sqrt{\bar{b}_{n-2}} & \sqrt{\bar{b}_{n-2}} & \bar{a}_{n-2} & \sqrt{\bar{b}_{n-1}} & \sqrt{\bar{b}_{n-1}} & \bar{a}_{n-1} \\
\sqrt{\bar{b}_{n-1}} & \sqrt{\bar{b}_{n-1}} & \bar{a}_{n-1} & \sqrt{\bar{b}_{n}} & \sqrt{\bar{b}_{n}} & \bar{a}_{n} \\
\end{pmatrix}
\]

**Reconstruction**

A reconstruction as a sum of weighted Dirac delta function corresponds to the closure. The abscissas and weights can be easily computed from the \( (\bar{a}_k, \bar{b}_k)_{k=0,\ldots,n} \).
Outline

1. Introduction
   - Context
   - Moment method
   - Hyperbolicity

2. QMOM
   - Principle of the method
   - Hyperbolicity

3. HyQMOM
   - First version of HyQMOM
   - New HyQMOM closure
   - Properties - Practical computations

4. Results
   - Configuration
   - Results

5. Conclusion, Perspectives
The 1D Riemann problem

Problem at the kinetic level

\[ \frac{\partial f}{\partial t} + \frac{\partial}{\partial x} (v f) = 0, \]
\[ f(v; 0, x) = M_\sigma(v - \bar{u}(x)) \]

with \( \sigma = 1/3 \)

\[ \bar{u}(x) = \begin{cases} 1 & \text{if } x < 0, \\ -1 & \text{otherwise}. \end{cases} \]

Analytical solution \( f(t, x, v) = M_\sigma(v - \bar{u}(x - vt)) = \begin{cases} M_\sigma(v - 1) & \text{if } v > x/t, \\ M_\sigma(v + 1) & \text{otherwise}. \end{cases} \)

\( t = 0: \)

\[ X=0 \]
The 1D Riemann problem

Problem at the kinetic level

Two homogeneous sprays, with Gaussian distribution and infinite Stokes, crossing.

Problem at the kinetic level

\[ \partial_t f + \partial_x (v f) = 0, \]
\[ f(v; 0, x) = M_\sigma (v - \bar{u}(x)) \]

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Analytical solution

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Moment problem

\[ \partial_t m_k + \partial_x m_{k+1} = 0, \quad k = 0, \ldots, 2n \]

with the initial condition for the standardized moments

\[ \rho(0, x) = 1, \quad u(0, x) = \bar{u}(x), \quad C_2(0, x) = \sigma, \quad \begin{cases} S_{2k-1} = 0, \\ S_{2k} = (2k - 1)S_{2k-2}, \end{cases} \quad k = 2, \ldots, n \]

Numerical scheme: HLL  [Harten et al., 1983]
The 1D Riemann problem - Results

moments - cases n=2,3,4

Good behavior on this hard test case.
The 1D Riemann problem - Results

standardized moments - cases n=2,3,4

Good behavior on this hard test case.
The 1D Riemann problem - Results

first moments - case n=10

Close to the analytical solution.
The 1D Riemann problem - Results

first standardized moments - case n=10

Close to the analytical solution.
The 1D Riemann problem - Convergence

The moment method seems to converge to the solution of the kinetic equation when the number of moments increases.
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Conclusion and Perspectives

Conclusion

- Closure inducing a global hyperbolicity
- Include the Maxwellian distribution
- Good behavior at the boundary of the moment space
- Efficient algorithm to compute the closure and the eigenvalues

THANK YOU FOR YOUR ATTENTION
Conclusion and Perspectives

Conclusion
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Perspectives
- 2D-3D version of the HyQMOM closure
Conclusion and Perspectives

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**Perspectives**
- 2D-3D version of the HyQMOM closure

THANK YOU FOR YOUR ATTENTION
Beyond pressureless gas dynamics: quadrature-based velocity moment models.

Sur l'interpolation par la méthode des moindres carrés.
Also in œuvres I pp. 473–498.


Hyperbolic quadrature method of moments for the one-dimensional kinetic equation.
submitted, https://hal.archives-ouvertes.fr/hal-03171566/.

Conditional hyperbolic quadrature method of moments for kinetic equations.

*Orthogonal Polynomials: Computation and Approximation.*
Oxford University Press, Oxford, UK.
On the kinetic theory of rarefied gases.

On upstream differencing and Godunov-type schemes for hyperbolic conservation laws.

Stability analysis of quadrature-based moment methods for kinetic equations.

Moment closure hierarchies for kinetic theories.

Description of aerosol dynamics by the quadrature method of moments.

Rational Extended Thermodynamics.
Springer-Verlag, New York.

The Moment Problem, volume 277 of Graduate Texts in Mathematics.
Springer, Cham.
References III

Shohat, J. A. and Tamarkin, J. D. (1943). 
*The Problem of Moments.*

Modified moments and Gaussian quadratures.
Chebyshev algorithm

**Three terms recurrence relation** for a sequence \((Q_k)_{k \geq 0}\) of orthogonal polynomials relative to \(\langle ., . \rangle\):

\[
Q_{k+1}(x) = (x - a_k)Q_k(x) - b_k Q_{k-1}(x).
\]


\[
Z_{k,p} = \langle Q_k x^p \rangle
\]

\[
Z_{-1,p} = 0, \quad Z_{0,p} = m_p
\]

\[
Z_{k+1,p} = Z_{k,p+1} - a_k Z_{k,p} - b_k Z_{k-1,p}.
\]

\[
b_0 = m_0, \quad a_0 = \frac{m_1}{m_0}, \quad \forall k > 0 \quad b_k = \frac{Z_{k,k}}{Z_{k-1,k-1}}, \quad a_k = \frac{Z_{k,k+1}}{Z_{k,k}} - \frac{Z_{k-1,k}}{Z_{k-1,k-1}},
\]