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

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Outline

Considered kinetic model

Kinetic model on $f(t, \boldsymbol{x}, \boldsymbol{v})$

$$\underbrace{\partial_t f + \partial_{\boldsymbol{x}} \cdot (\boldsymbol{v} f)}_{\text{physical transport}} = \underbrace{\mathcal{S}(f)}_{\text{Source terms}}$$

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Gas dynamics

for example BGK source term: $\mathcal{S}(f) = -\dfrac{f - f_{eq}}{Kn}$

Transition regime : $0.01 < Kn < 10$

Far from the Maxwellian equilibrium

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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 $\int_{\mathbb{R}} \boldsymbol{v}^k f(t, \boldsymbol{x}, \boldsymbol{v}) \mathrm{d}\boldsymbol{v}$ 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 $\mathbf{m}_N = (m_0, m_1, \dots, m_N)^t$:

$$\partial_t m_k + \partial_x m_{k+1} = \mathcal{S}_k, \qquad k = 0, 1, \dots, N \tag{1}$$

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

Issues:

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

Strategy

- Solve the Hamburger truncated moment problem:

  find a positive measure μ such that $\mathbf{m}_N = \int_{\mathbb{R}} (1, v, \dots, v^N)^t \mathrm{d}\mu(v)$.

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

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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
- Quadrature method of moment [McGraw, 1997, Fox, 2008]
  $\rightarrow$ weakly hyperbolic

Moment space

Definition

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

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

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

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

$$\underline{H}_{2n} = \begin{vmatrix} m_0 & \dots & m_n \\ \vdots & & \vdots \\ m_n & \dots & m_{2n} \end{vmatrix},$$

Theorem

$\mathbf{m}_N = (m_0, m_1, \dots, m_N)^t$ *strictly realizable* $\Leftrightarrow \underline{H}_{2k} > 0, \quad k \in \{0, 1, \dots, \left\lfloor \frac{N}{2} \right\rfloor\}$

$\mathbf{m}_N \in \partial\mathcal{M}_N \cap \mathcal{M}_n \Rightarrow \underline{H}_0 > 0, \dots, \underline{H}_{2k-2} > 0, \underline{H}_{2k} = 0, \dots, \underline{H}_{2\left\lfloor \frac{N}{2} \right\rfloor} = 0, k \leq \left\lfloor \frac{N}{2} \right\rfloor.$

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

[Shohat and Tamarkin, 1943, Gautschi, 2004, Schmüdgen, 2017]

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First constraints for the strict realizability:

$$m_0 > 0 \qquad m_2 > \frac{m_1^2}{m_0}$$

$$m_4 > \frac{m_0 m_3^2 - 2 m_1 m_2 m_3 + m_2^3}{m_2 m_0 - m_1^2}$$

$$\ldots$$

Characteristic polynomial

System on moments

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

$$\partial_t \mathbf{m}_N + \partial_x F(\mathbf{m}_N) = \overline{S}$$

Characteristic Polynomial

Jacobian matrix

$$\frac{D\mathbf{F}(\mathbf{m}_N)}{D\mathbf{m}_N} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 \\ \frac{\partial m_{N+1}}{\partial m_0} & \frac{\partial m_{N+1}}{\partial m_1} & \frac{\partial m_{N+1}}{\partial m_2} & \dots & \frac{\partial m_{N+1}}{\partial m_N} \end{pmatrix}.$$

Characteristic polynomial

$$\overline{P}_{N+1}(X) = X^{N+1} - \sum_{i=0}^{N} \frac{\partial m_{N+1}}{\partial m_i} X^i$$

Moments - Central moments - Standardized moments

moments:

$$m_k = \int_{\mathbb{R}} v^k f(v) \mathrm{d}v$$

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

$$C_k = \frac{1}{\rho} \int_{\mathbb{R}} (v-u)^k f(v) \mathrm{d}v = \int_{\mathbb{R}} c^k f^c(c) \mathrm{d}c$$

so that $C_0 = 1$ and $C_1 = 0$.

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

$$S_k = \frac{1}{m_0} \int_{\mathbb{R}} \left(\frac{v-u}{\sqrt{C_2}} \right)^k f(v) \mathrm{d}v = \int_{\mathbb{R}} s^k f^s(s) \mathrm{d}s$$

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

$\mathbf{m}_N = (m_0, m_1, \dots, m_N)^t$ be a realizable moment vector such that $m_0 > 0$ and $C_2 > 0$.

linear functional $\langle . \rangle_{\mathbf{m}_N}$ on the space $\mathbb{R}[X]_N$

$$\langle X^k \rangle_{\mathbf{m}_N} = m_k, \quad \text{for } k \in \{0, 1, \dots, N\}.$$

linear functional $\langle . \rangle_{\mathbf{S}_N}$ associated with the standardized moments $\mathbf{S}_N = (S_0, \dots, S_N)^t$:

$$\langle X^k \rangle := \langle X^k \rangle_{\mathbf{S}_N} = S_k, \quad \text{for } k \in \{0, 1, \dots, N\}.$$

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., $S_{N+1}(S_3, \dots, S_N)$. 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 $(S_3, \dots, S_N)$, and

$$\langle P_{N+1} \rangle = 0, \quad \langle P'_{N+1} \rangle = 0, \quad \langle X P'_{N+1} \rangle = 0.$$

Outline

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

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

It is the minimal value for this moment

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

Reconstruction

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

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

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

Remarks

- The reconstruction μ is the only one possible for the moment vector $\mathbf{m}_{2n}$.
- $\mathbf{m}_{2n}$ is at the boundary of the moment space: $\underline{H}_{2n} = 0$

QMOM: Computation of the weights and abscissas

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

Orthogonal polynomials

Family $(Q_k)_{k=0,\dots,n}$ 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]

$$a_k = \frac{\langle XQ_k^2 \rangle}{\langle Q_k^2 \rangle}, \qquad b_k = \frac{\langle Q_k^2 \rangle}{\langle Q_{k-1}^2 \rangle} = \frac{H_{2k}H_{2k-4}}{H_{2k-2}^2}.$$

example

$$a_0 = 0, \qquad a_1 = S_3, \qquad a_2 = \frac{S_5 - S_3(2 + S_3^2 + 2H_4)}{H_4}$$
$$b_0 = 1, \qquad b_1 = 1, \qquad b_2 = H_4, \qquad b_3 = H_6/H_4^2$$

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

$$\mathbf{J}_n = \begin{pmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{b_{n-2}} & a_{n-2} & \sqrt{b_{n-1}} \\ & & & \sqrt{b_{n-1}} & a_{n-1} \end{pmatrix}$$

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]

Outline

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 $\mathbf{m}_4$ *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 $\underline{H}_4 \to 0$

New HyQMOM closure [Fox and Laurent, 2021]

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

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

such that β_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

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

Then, the following statements are equivalent:

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

(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

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

if and only if the closure on S_{2n+1}, defined through the coefficient a_n, and the coefficients α_n and β_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 $a_n = \dfrac{1}{n}\sum_{k=0}^{n-1} a_k$
2. compute the Standardized moments $\mathbf{S}_{2n+1}$ 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 $P_{2n+1} - Q_n\left[(X - a_n)Q_n - \dfrac{2n+1}{n} b_n Q_{n-1}\right]$

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

Examples

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

Hyperbolicity - Eigenvalues

Theorem

When $\beta_n > 0$, the $n+1$ roots of $R_{n+1} = (X - \alpha_n)Q_n - \beta_n Q_{n-1}$ 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:

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

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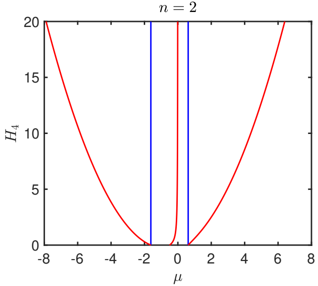
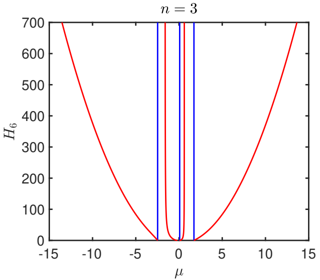
Example of the evolution of the eigenvalues with H_{2n}

$S_3 = -1$



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



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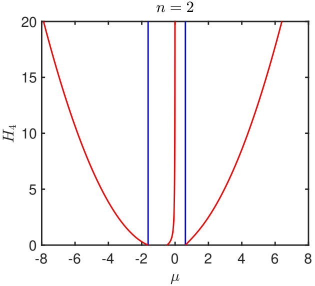

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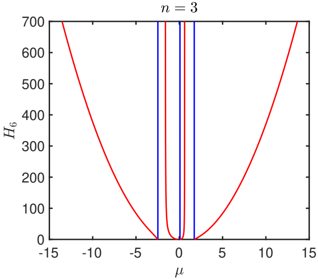

The moment system with the HyQMOM closure is then hyperbolic, whatever the strictly realizable moment.

Practical computations

Closure, directly from the moments $\mathbf{m}_{2n}$

1. compute the $(\bar{a}_k)_{k=0}^{n-1}$ and $(\bar{b}_k)_{k=0}^{n}$ from $\mathbf{m}_{2n}$ with the Chebyshev algorithm
2. set the closure $\bar{a}_n = \dfrac{1}{n}\displaystyle\sum_{k=0}^{n-1} \bar{a}_k$
3. compute m_{2n+1} using the reverse Chebyshev algorithm

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Eigenvalues of the system

eigenvalues of the two following Jacobi matrices:

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

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Eigenvalues of the system

eigenvalues of the two following Jacobi matrices:

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

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 $(\bar{a}_k, \bar{b}_k)_{k=0,\dots,n}$.

Outline

The 1D Riemann problem

problem at the kinetic level

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

Problem at the kinetic level

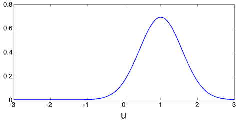
$$\partial_t f + \partial_x (v\, f) = 0,$$
$$f(v; 0, x) = \mathcal{M}_\sigma(v - \bar{u}(x))$$

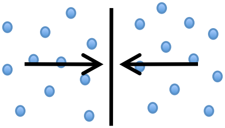
with $\sigma = 1/3$

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

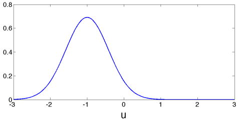
Analytical solution $f(t,x,v) = \mathcal{M}_\sigma(v - \bar{u}(x - vt)) = \begin{cases} \mathcal{M}_\sigma(v-1) & \text{if } v > x/t, \\ \mathcal{M}_\sigma(v+1) & \text{otherwise.} \end{cases}$

$t = 0$:





X=0



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moment problem

$$\partial_t m_k + \partial_x m_{k+1} = 0, \quad k = 0, \dots, 2n$$

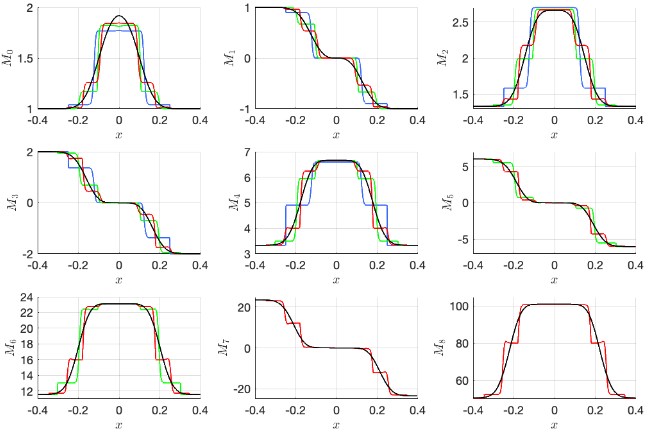
with the initial condition for the standardized moments

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

numerical scheme: HLL [Harten et al., 1983]

The 1D Riemann problem - Results

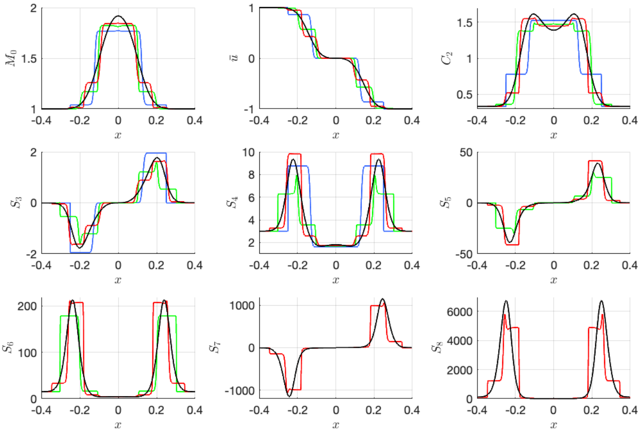
moments - cases n=2,3,4



Good behavior on this hard test case.

The 1D Riemann problem - Results

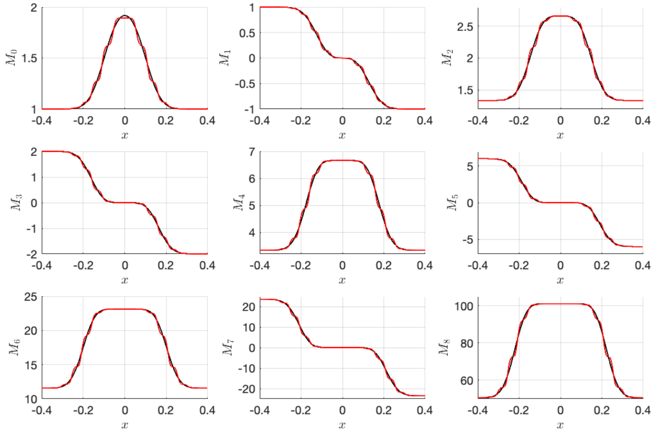
standardized moments - cases n=2,3,4



Good behavior on this hard test case.

The 1D Riemann problem - Results

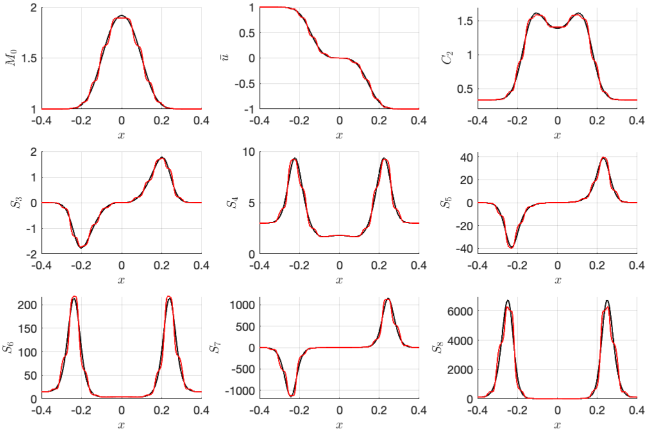
first moments - case n=10



Close to the analytical solution.

The 1D Riemann problem - Results

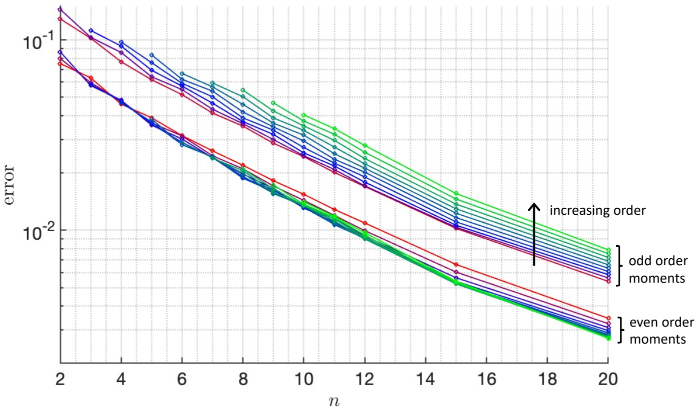
first standardized moments - case n=10



Close to the analytical solution.

The 1D Riemann problem - Convergence

error on the moments



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

Outline

Conclusion and Perspectives

Conclusion

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- Include the Maxwellian distribution
- Good behavior at the boundary of the moment space
- Efficient algorithm to compute the closure and the eigenvalues

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THANK YOU FOR YOUR ATTENTION

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Chebyshev algorithm

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

$$Q_{k+1}(x) = (x - a_k)Q_k(x) - b_k Q_{k-1}(x).$$

Chebyshev algorithm [Chebyshev, 1859, Wheeler, 1974, Gautschi, 2004]

$Z_{k,p} = \langle Q_k X^p \rangle$

$$Z_{-1,p} = 0, \qquad Z_{0,p} = m_p$$

$$Z_{k+1,p} = Z_{k,p+1} - a_k Z_{k,p} - b_k Z_{k-1,p}.$$

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