A discontinuous-Galerkin implementation of the entropy-based moment closure

Experiments with linear transport in slab geometry

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A linear kinetic equation in slab geometry

$$\partial_t \psi + \mu \partial_x \psi + \sigma_{\mathrm{a}} \psi = \sigma_{\mathrm{s}} \mathcal{C}(\psi) \qquad \begin{matrix} x \in (x_{\mathrm{L}}, x_{\mathrm{R}}) \\ \mu \in [-1, 1] \end{matrix}$$

where $\psi = \psi(t, x, \mu) \geq 0$ is a *kinetic density* and the collision operator $\mathcal{C}$ is linear, for example isotropic scattering:

$$\mathcal{C}(\psi)(t, x, \mu) = \frac{1}{2} \langle \psi(t, x, \cdot) \rangle - \psi(t, x, \mu) \quad \text{where} \quad \langle \phi \rangle = \int_{-1}^{1} \phi(\mu) d\mu.$$

H-Theorem: The entropy

$$H(t) = \int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}} \int_{-1}^{1} \eta(\psi(t, x, \mu)) d\mu dx$$

satisfies $\frac{d}{dt} H(t) \leq 0$.

Moments

- One challenge of numerically simulating (general) kinetic equations is the large state space: typically space is three-dimensional and the velocity variable is two- or three-dimensional.
- In particular, the only velocity information an application usually requires are the *moments*: angular averages against basis functions $m_0(\mu), m_1(\mu), \ldots, m_N(\mu)$:

$$u_i(t,x) := \langle m_i \psi(t,x,\cdot) \rangle \,, \quad \text{or altogether} \quad \mathbf{u}(t,x) = \langle \mathbf{m} \psi(t,x,\cdot) \rangle \,.$$

- The basis functions are typically polynomials, so the zero-th order moment gives a local mass density, the first-order moment gives a bulk velocity, and the second-order moment gives energy or temperature.

The “naïve” spectral method for angular discretization

The typical spectral ansatz is

$$\psi(t, x, \mu) \simeq \sum_{i=0}^{N} \alpha_i(t, x) m_i(\mu) = \mathbf{m}(\mu)^T \boldsymbol{\alpha}(t, x).$$

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One "justification" for the form of this ansatz is that

$$\mathbf{m}^T \boldsymbol{\alpha} = \operatorname{argmin}\{\langle \phi^2 \rangle : \langle \mathbf{m}\phi \rangle = \mathbf{u}\};$$

and it's also nice that the map from the coefficients $\boldsymbol{\alpha}$ to the moments $\mathbf{u}$ is simply linear:

$$\boldsymbol{\alpha} \mapsto \langle \mathbf{m}\mathbf{m}^T \boldsymbol{\alpha} \rangle = \langle \mathbf{m}\mathbf{m}^T \rangle \boldsymbol{\alpha} = \mathbf{u}$$

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Problems (in the context of kinetic equations):

- Not necessarily positive.
- This discretization may not satisfy the H-Theorem

Instead, let's choose an ansatz of the form

$$\psi(t,x,\mu) \simeq \operatorname{argmin}\{\langle \eta(\phi)\rangle : \langle \mathbf{m}\phi\rangle = \mathbf{u}(t,x)\},$$

The solution to this problem is $\hat{\psi}_{\mathbf{u}} = \eta'_*(\mathbf{m}^T\hat{\boldsymbol{\alpha}}(\mathbf{u}))$, where the coefficients $\hat{\boldsymbol{\alpha}}(\mathbf{u})$ are the Legendre multipliers which solve the dual problem

$$\hat{\boldsymbol{\alpha}}(\mathbf{u}) := \operatorname{argmin}\{\big\langle \eta_*(\mathbf{m}^T\boldsymbol{\alpha})\big\rangle - \mathbf{u}^T\boldsymbol{\alpha}\}.$$

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This defines a (now nonlinear) diffeomorphism

$$\boldsymbol{\alpha} \mapsto \big\langle \mathbf{m}\eta_*'(\mathbf{m}^T \boldsymbol{\alpha}) \big\rangle \equiv \mathbf{u}$$

between the expansion coefficients (in $\mathbb{R}^{N+1}$) and the moments (in the map's range (more later)).

Now perform the Galerkin projection step, requiring that the PDE holds on the subspace spanned by $\{m_0(\mu), m_1(\mu), \ldots, m_N(\mu)\}$:

$$\partial_t \psi + \mu \partial_x \psi + \sigma_{\mathrm{a}} \psi = \sigma_{\mathrm{s}} \mathcal{C}(\psi)$$

$$\downarrow \psi \simeq \eta_*'(\mathbf{m}^T \boldsymbol{\alpha}) \downarrow$$

$$\partial_t \left\langle \mathbf{m} \eta_*'(\mathbf{m}^T \boldsymbol{\alpha}) \right\rangle + \partial_x \left\langle \mu \mathbf{m} \eta_*'(\mathbf{m}^T \boldsymbol{\alpha}) \right\rangle + \sigma_{\mathrm{a}} \left\langle \mathbf{m} \eta_*'(\mathbf{m}^T \boldsymbol{\alpha}) \right\rangle$$
$$= \sigma_{\mathrm{s}} \left\langle \mathbf{m} \mathcal{C}(\eta_*'(\mathbf{m}^T \boldsymbol{\alpha})) \right\rangle$$

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or equivalently in moment variables

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) + \sigma_\mathrm{a} \mathbf{u} = \sigma_\mathrm{s} \mathbf{r}(\mathbf{u}) \tag{1}$$

where $\mathbf{f}(\mathbf{u}) := \left\langle \mu \mathbf{m} \eta_*'(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u})) \right\rangle$ and

$$\mathbf{r}(\mathbf{u}) := \left\langle \mathbf{m} \mathcal{C}(\eta_*'(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u}))) \right\rangle .$$

This is a hyperbolic PDE in conservative form!

Back to those two problems with the spectral method

- Using the Maxwell-Boltzmann entropy

$$\eta(z) = z \log z - z,$$

whose Legendre transform is $\eta_*(y) = \exp(y)$, gives the ansatz

$$\hat{\psi}_{\mathbf{u}} = \eta'_*(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u})) = \exp(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u})).$$

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Positive!

- The relevant local entropy for this discretization is $h(\mathbf{u}(t,x)) := \left\langle \eta \left(\hat{\psi}_{\mathbf{u}(t,x)} \right) \right\rangle$. For $\mathbf{u}$ satisfying the moment PDE (1), one can show that

$$\frac{d}{dt} \int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}} h(\mathbf{u}(t,x)) dx \leq 0.$$

Starting to think about numerics

- To simulate this system numerically, we need to choose the moment equations (1) because they are in conservative form.
- However, since the flux $\mathbf{f}(\mathbf{u})$ and collision term $\mathbf{r}(\mathbf{u})$ are written in terms of the multipliers

  $$\mathbf{f}(\mathbf{u}) := \left\langle \mu \mathbf{m} \eta'_*(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u})) \right\rangle \text{ and } \mathbf{r}(\mathbf{u}) := \left\langle \mathbf{m} \mathcal{C}(\eta'_*(\mathbf{m}^T \hat{\boldsymbol{\alpha}}(\mathbf{u}))) \right\rangle$$

  so whenever we need to evaluate $\mathbf{f}$ or $\mathbf{r}$, we need to compute $\hat{\boldsymbol{\alpha}}(\mathbf{u})$. This is typically done by numerically solving the dual problem.
- But before we try to solve the dual problem we better make sure a solution exists . . .

Since our ansatz has the form $\exp(\mathbf{m}^T\boldsymbol{\alpha})$, the map $\mathbf{u} \mapsto \hat{\boldsymbol{\alpha}}(\mathbf{u})$ can only be defined for

$$\mathbf{u} \in \left\{ \left\langle \mathbf{m} \exp(\mathbf{m}^T\boldsymbol{\alpha}) \right\rangle : \boldsymbol{\alpha} \in \mathbb{R}^{N+1} \right\} \subsetneq \mathbb{R}^{N+1}$$

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In our case, this is equal to the *realizable set*

$$\mathcal{R} := \left\{ \mathbf{u} \in \mathbb{R}^{N+1} : \exists \phi > 0 \text{ such that } \mathbf{u} = \langle \mathbf{m}\phi \rangle \right\}.$$

Example: let $\mathbf{m}(\mu) = (1, \mu)^T$, then since $|\mu| \leq 1$,

$$|\langle \mu\phi \rangle| \leq \langle |\mu|\phi \rangle \leq \langle \phi \rangle \quad \iff \quad |u_1| \leq u_0.$$

Problem: errors from the space-time discretization may produce nonrealizable numerical solution!

A high-order spatial method: RKDG

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = \mathbf{s}(\mathbf{u})$$

In cell I_j, project a numerical solution $\mathbf{u}_h(t,x)$ onto the test space span$\{\varphi_k\}$:

$$\begin{aligned}\partial_t \int_{I_j} \mathbf{u}_h(t,x)\varphi_k(x)\,dx &+ \mathbf{f}(\mathbf{u}_h(t,x^-_{j+1/2}))\varphi_k(x^-_{j+1/2}) \\ &- \mathbf{f}(\mathbf{u}_h(t,x^+_{j-1/2}))\varphi_k(x^+_{j-1/2}) \\ &- \int_{I_j} \mathbf{f}(\mathbf{u}_h(t,x))\partial_x\varphi_k(x)\,dx \\ &= \int_{I_j} \mathbf{s}(\mathbf{u}_h(t,x))\varphi_k(x)\,dx\end{aligned}$$

DG Ansatz

The DG ansatz in spatial cell $I_j = (x_{j-1/2}, x_{j+1/2})$ is

$$\begin{aligned}\mathbf{u}(t,x) \simeq \mathbf{u}_h(t,x) &:= \sum_{k=0}^{n} \hat{\mathbf{u}}_j^{(k)}(t)\varphi_k(x) \text{ for } x \in I_j,\\ &= \bar{\mathbf{u}}_j(t) + \sum_{k=1}^{n} \hat{\mathbf{u}}_j^{(k)}(t)\varphi_k(x)\end{aligned}$$

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You need a numerical flux,

$$\mathbf{f}\left(\mathbf{u}_h\left((x_{j+1/2}^{\pm}\right)\right) \simeq \hat{\mathbf{f}}\left(\mathbf{u}_h\left(t, x_{j+1/2}^{-}\right), \mathbf{u}_h\left(t, x_{j+1/2}^{+}\right)\right),$$

and we use Lax-Friedrich:

$$\hat{\mathbf{f}}(\mathbf{v}, \mathbf{w}) = \frac{1}{2}\left(\mathbf{f}(\mathbf{v}) + \mathbf{f}(\mathbf{w}) - (\mathbf{w} - \mathbf{v})\right).$$

Realizability of the cell-means

- Assuming
  - the moments at each spatial quadrature point are realizable and that
  - we use an SSP-RK time integrator

  one can show that the cell means $\bar{\mathbf{u}}_j(t)$ remain realizable under the CFL condition

$$\frac{\Delta t}{\Delta x} < w_Q(1 - (\sigma_\mathrm{a} + \sigma_\mathrm{s})\Delta t).$$

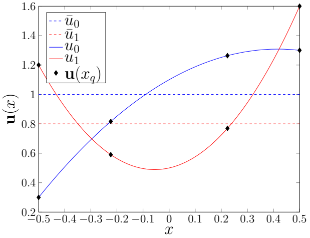
- But previous work (e.g. with Euler equations) has shown that we should expect the moments at the spatial quadrature points of high-order solutions to leave the realizable set.

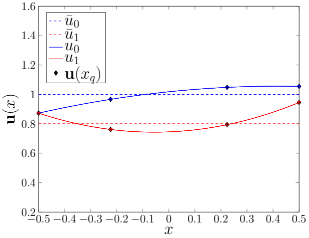
Linear scaling limiter

- Previous work with Euler equations has used a linear scaling limiter to ensure positivity: Here one replaces the moments at the quadrature points $\mathbf{u}_q = \mathbf{u}(t, x_q)$ with

$$\mathbf{u}_q^{\theta} = (1-\theta)\mathbf{u}_q + \theta\bar{\mathbf{u}} = \bar{\mathbf{u}} + (1-\theta)\sum_{k=1}^{n} \hat{\mathbf{u}}^{(k)}\varphi_k(x_q)$$

where θ is the smallest number in $[0, 1]$ such that $\mathbf{u}_q \in \mathcal{R}$.





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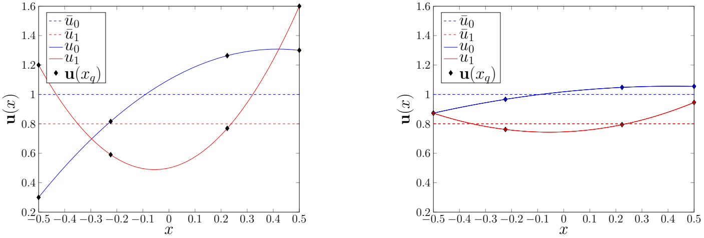
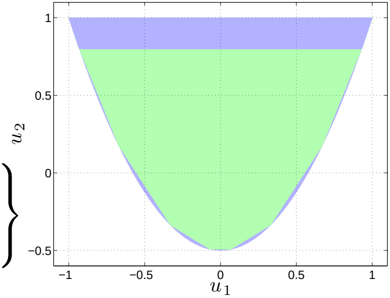


- But how to find θ? The boundary of $\mathcal{R}$ is in general complicated enough in 1D and not even well understood in higher dimensions . . .

Quadrature realizability

Realizability with respect to a quadrature $\mathcal{Q}$ introduces a smaller set:

$$\mathcal{R}_{\mathcal{Q}} := \left\{ \mathbf{u} : \mathbf{u} = \sum_{\mu_i \in \mathcal{Q}} w_i \mathbf{m}(\mu_i) f_i,\ f_i > 0 \right\}$$



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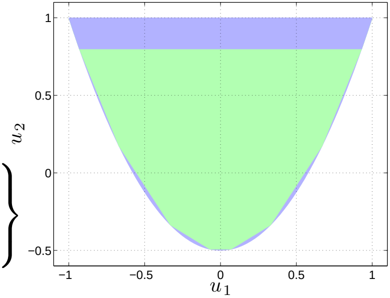


This set is characterized by

$$\begin{aligned} \mathcal{R}_{\mathcal{Q}}\big|_{u_0<1} &= \mathrm{int}\ \mathrm{co}\left\{ \{\mathbf{m}(\mu_\mathrm{i})\}_{\mu_\mathrm{i} \in \mathcal{Q}}, \mathbf{0} \right\} \\ &= \left\{ \mathbf{u} \in \mathbb{R}^{N+1} : \; \mathbf{a}_i^T \mathbf{u} < b_i, i \in \{1, \ldots, d\} \right\}, \end{aligned}$$

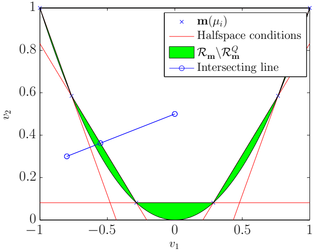
Linear scaling limiter

Thus we can compute θ for each facet

$$\mathbf{a}_i^T(\theta_{qi}\bar{\mathbf{u}} + (1-\theta_{qi})\mathbf{u}_q) = b_i \quad \iff \quad \theta_{qi} = \frac{b_i - \mathbf{a}_i^T\mathbf{u}_q}{\mathbf{a}_i^T(\bar{\mathbf{u}} - \mathbf{u}_q)}.$$

For the q-th quadrature point take

$$\theta_q := \begin{cases} 0 & \nexists \theta_{qi} \in [0,1], \\ \max\{\theta_{qi} : \theta_{qi} \in [0,1]\} & \text{else;} \end{cases}$$



then for the j-th cell take

$$\theta := \max\{\theta_q : x_q \in I_j\}.$$

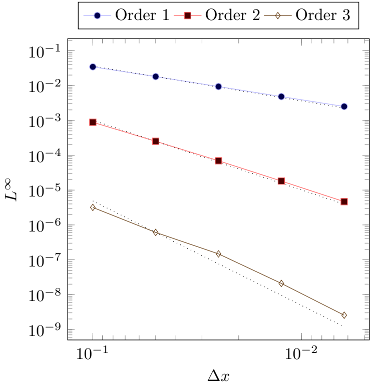
Thus $\mathbf{u}_q \in \mathcal{R}_\mathcal{Q}$ at *each* quadrature point without changing the cell mean.

The rest of the scheme

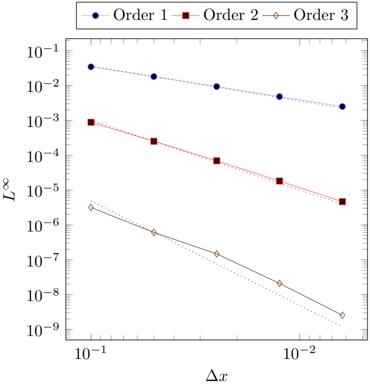
Off-the-shelf stuff:

- Gauss-Lobatto spatial quadrature
- Standard TVBM slope limiter applied to the characteristic fields
- SSP$(3,3)$ RK time integration: a convex combination of Euler steps

Convergence tests



(a) L^1



(b) L^∞

Numerical Results: Plane Source

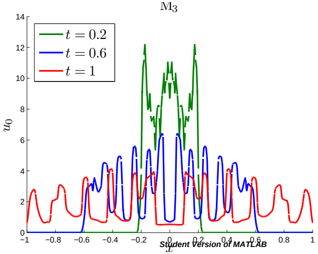
Infinite domain: $x \in (-\infty, \infty)$

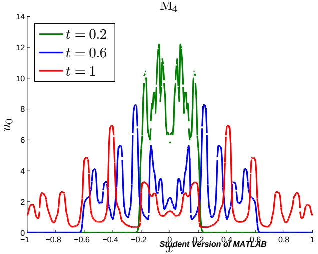
Initial condition: $\psi(t = 0, x, \mu) = 0.5\delta(x)$

Purely scattering medium: $\sigma_{\mathrm{a}} = 0$, $\sigma_{\mathrm{s}} = 1$

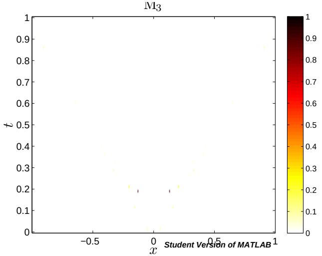
Realizability limiter action in the plane source problem

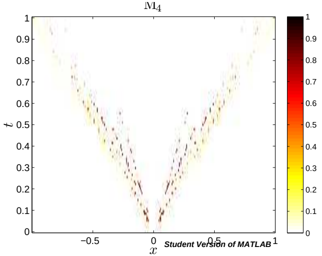
Time slices of the solution





Value of θ from the limiter





Numerical Results: Two-Beam Instability

Bounded domain: $x \in (x_{\mathrm{L}}, x_{\mathrm{R}}) = (-0.5, 0.5)$

Boundary conditions:

$$\psi(t, x_{\mathrm{L}}, \mu) = \exp(-10(\mu - 1)^2)$$
$$\psi(t, x_{\mathrm{R}}, \mu) = \exp(-10(\mu + 1)^2)$$

Initially empty:

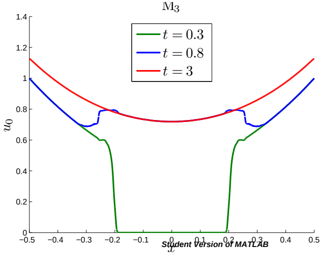
$$\psi(t = 0, x, \mu) = 0$$

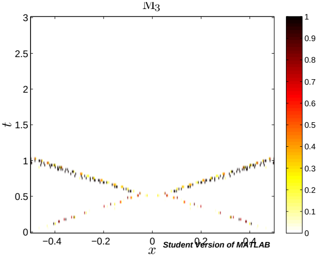
Purely absorbing medium:

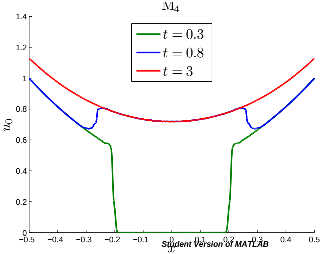
$$\sigma_{\mathrm{a}} = 2 \ , \ \sigma_{\mathrm{s}} = 0$$

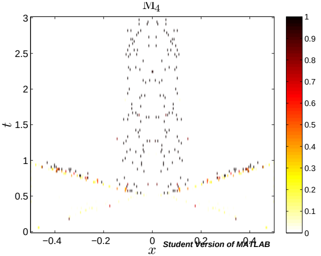
Realizability limiter action in the two-beam instability

Time slices of the solution | Value of θ from the limiter









Parting thoughts

- Entropy-based moment models are an interesting twist on spectral methods which take advantage of structure in kinetic equations at the cost of introducing nonlinearity into the numerical scheme.
- To use a high-order DG method in space, we introduce a linear scaling limiter for the realizable set which is simple to implement and extends to arbitrary dimensions.
- We confirmed expected results on benchmark problems.
- Future work: implementation for 2D and 3D problems (in space). The main challenge here is that the number of facets of $\mathcal{R}_{\mathcal{Q}}$ grows exponentially with the number of moments and the number of quadrature points.