Positivity-Preserving Discontinuous Galerkin Schemes for Linear Vlasov-Boltzmann Transport Equations

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Outline

1. Introduction
2. RKDG Methods for Linear BTE
3. The Positivity-Preserving DG Methods for Linear BTE
4. Numerical Results
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1. Introduction

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The Linear Vlasov-Boltzmann Transport Equations (BTE)

\[
\frac{\partial f}{\partial t} + v f_x - \frac{e}{m} E(t, x) f_v = Q\sigma(f), \quad \text{in } \mathbb{R}^d_x \times \mathbb{R}^d_v
\]

with the collision kernel

\[
Q\sigma(f) = \int_{v' \in \mathbb{R}^d} (\sigma(x, v, v') f' - \sigma(x, v', v) f) dv',
\]

The scattering function satisfies

- \(\sigma(x, v, v') \geq 0\)
- \(\sigma(x, v, v') = k(x, v, v') M(v)\)
- \(k(x, v, v') = k(x, v', v)\) and \(M(v)\) is the stationary pdf.
- \(\nu(x, v) = \int_{\mathbb{R}^d_{v'}} \sigma(x, v', v) dv' < K\), the collision frequency.
Properties

Theorem

(Herau, 2006) For relaxation model, we have

\[ \| f(t, x, v) - \mathcal{M}(x, v) \|_{B^2(\mathbb{R}^{2d})} \leq 3 \exp(-\lambda t) \| f_0 - \mathcal{M} \|_{B^2(\mathbb{R}^{2d})}, \]

where \( \| f \|_{B^2}^2 = \int |f|^2 \mathcal{M}^{-1} dx dv. \)

Theorem

\[ \int Q_\sigma(f) \mathcal{G}(\frac{f}{M}) dv \leq 0, \quad \text{for all } \mathcal{G}(\cdot) \uparrow. \]
Properties

Corollary

(1) (Mass conservation)

\[ \int Q_\sigma(f) \, dv = 0. \]

(take \( G = 1 \))

(2) (\( L^1 \) contraction)

\[ \frac{d}{dt} \| f \|_{L^1(D_u^d \times D_x^d)} \leq 0. \]

(take \( G = \text{sgn}(\frac{f}{M}) \))

(3) (Positivity) The solution to the initial value problem is positive for all times if the initial probability \( f_0 = f(0, x, v) \) is positive.

(take \( G = \frac{1}{2} (\text{sgn}(\frac{f}{M}) - 1) \))
A Very Short History of DG

- Invented by Reed and Hill (73) for neutron transport. Lesaint and Raviart (74).
- RKDG method by Cockburn and Shu (89, 90,...) for conservation laws.
- Elliptic and Parabolic problems, (IP methods), Babuška et al. (73), Wheeler (78), Arnold (79), Bassi and Rebay (97), Cockburn and Shu (98), Arnold et al. (02)...
The Main Advantages of DG

- Use of FVM framework, convection-dominated problems.
- Flexibility with the mesh. (hanging nodes, nonconforming mesh)
- Highly parallelizable.
- Polynomials of different degrees in different elements, even non-polynomial basis.
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The Scheme

- Selection of the computational domain
- Define the inflow face as $\Gamma^- = \bigcup_i \{ F_0^+ \cup F_{L_i}^- \}$, and suppose $f_h = f^{in}$ on $\Gamma^-$. Define $\Gamma^0 = \bigcup_i \{ F_{V_i}^- \cup F_{V_i}^- \}$.
- The finite element space is defined as

\[ V_h^k = \{ \phi_h \in L^2(\Omega_D) : \forall K \in T_h(\Omega_D), \phi_h|_K \in P^k(K) \} \]
The Scheme

The semi-discrete DG methods seek \( f_h \in V_h^k \) such that for all test function \( w_h \in V_h^k \),

\[
(\partial_t f_h, w_h)_{T_h} + A(f_h, w_h) = L(w_h),
\]

where

\[
A(f_h, w_h) \equiv -(f_h, \alpha \cdot \nabla w_h)_{T_h} + \langle \hat{f}_h, w_h \alpha \cdot n \rangle_{\partial T_h \setminus \Gamma - \Gamma^0} - \langle Q_\sigma(f_h), w_h \rangle_{T_h}
\]

and

\[
L(w_h) \equiv -\langle f^{in}, w_h \alpha \cdot n \rangle_{\Gamma^-}
\]

\( \hat{f}_h \) is the upwind numerical flux, \( \hat{f}_h = f_h^- \), where

\[
f_h^-(z) = \lim_{\delta \downarrow 0} f_h(z - \delta \alpha(z)).
\]

We use total variation diminishing (TVD) high-order Runge-Kutta methods to solve the method of lines ODE resulting from the semi-discrete scheme.
Properties

Assuming periodic bc, we have the following properties for the semi-discrete DG scheme.

- **Mass conservation.**
  \[
  \frac{d}{dt} \int_{\Omega_D} f_h dv dx = 0.
  \]
  (Take \( w_h = 1 \).)

- **\( L^2 \) stability.**
  \[
  \| f_h(t) \|_{L^2(\Omega_D)} \leq \exp(C t) \| f_h(0) \|_{L^2(\Omega_D)},
  \]
  where \( C = C(\text{diam}(\Omega_D)) \).
  (Take \( w_h = f_h \).)
Properties

- $L^2$ error estimate for general unstructured meshes.

$$\|f_h(t, \cdot, \cdot) - f(t, \cdot, \cdot)\|_{L^2(\Omega_D)} \leq C \sqrt{t} h^{k+\frac{1}{2}} |f|_{H^{k+1}(\Omega_D)},$$

where $C = C(\text{diam}(\Omega_D), ||\alpha||_{W^{1,\infty}(\Omega_D)})$ and $C$ does not depend on $h$ or $t$. (C. Mouhot and L. Neumann, 2006)

- $L^2$ decay of numerical solution towards equilibrium.

$$\|f_h(t, \cdot, \cdot) - \mathcal{M}\|_{L^2(\Omega_D)} \leq C \sqrt{t} h^{k+\frac{1}{2}} |f|_{H^{k+1}(\Omega_D)} + 3e^{-\lambda t} ||f_0 - \mathcal{M}||_{B^2(\mathbb{R}^d)},$$

where $C = C(\text{diam}(\Omega_D), ||\alpha||_{W^{1,\infty}(\Omega_D)}).$
Properties for $V^0_h$

The scheme with piecewise constant approximation is monotone.

- $L^1$ Stability.
  \[ \| f_h(t) \|_{L^1(\Omega_D)} \leq \| f_h(0) \|_{L^1(\Omega_D)} \]  \hspace{1cm} (1)

- Positivity-preserving.
  If $f_h(t = 0) \geq 0$, the solution remains positive:
  \[ f_h(t, x, v) \geq 0, \quad \text{for } t \in [0, T] \text{ for } x, v \in \Omega_D. \]

Not true for high order schemes.
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Motivation

We want a scheme that
- conserves mass
- preserves positivity
- is high order
- simple to implement
The Limiter (Zhang & Shu, 2009)

- on each cell $K_{ij}$, evaluate $T_{ij} = \min_{(x,v) \in S_{i,j}} f_h(x, v)$.
- Compute $\tilde{f}_h(x, v) = \theta(f_h(x, v) - \bar{f}_{ij}) + \bar{f}_{ij}$, where
  \[ \theta = \min\{1, |\bar{f}_{ij}| / |T_{ij} - \bar{f}_{ij}|\} \]

It is shown that this is a $(k + 1)$-th order limiter for $P^k$ approximations.
Algorithm Flowchart

With forward Euler time stepping, $t^n$ to $t^{n+1}$

1. $f^n(x)$ with $f^n \geq 0$

2. Limiter

3. $\tilde{f}(x)$ with $\tilde{f}(x) \geq 0$ at some particular points

4. One DG Step

5. $f^{n+1}(x)$ with $\tilde{f}^{n+1} \geq 0$
The Simplified Proof in 1D

The evolution for cell averages for high order scheme is convex combination of low order schemes.
The Simplified Proof in 1D

The evolution for cell averages for high order scheme is convex combination of low order schemes. For $u_t + f(u)_x = 0$, a first order monotone scheme will be

$$u_{j}^{n+1} = u_{j}^{n} - \frac{\Delta t}{\Delta x} \hat{f}(u_{j}^{n}, u_{j+1}^{n}) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1}^{n}, u_{j}^{n}) = G^{\Delta t}(u_{j-1}^{n}, u_{j}^{n}, u_{j+1}^{n})$$
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Consider DG with $V_h^1$, apply test functions as 1, we have the relation for the evolution of cell averages

$$\bar{u}_j^{n+1} = \bar{u}_j^n - \frac{\Delta t}{\Delta x} \hat{f}(u_{j+1/2}^-, u_{j+1/2}^+) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1/2}^-, u_{j-1/2}^+)$$
The Simplified Proof in 1D

The evolution for cell averages for high order scheme is convex combination of low order schemes.

For \( u_t + f(u)_x = 0 \), a first order monotone scheme will be

\[
\begin{aligned}
  u_j^{n+1} &= u_j^n - \frac{\Delta t}{\Delta x} \hat{f}(u_j^n, u_{j+1}^n) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1}^n, u_j^n) = G^\Delta t(u_{j-1}^n, u_j^n, u_{j+1}^n)
\end{aligned}
\]

Consider DG with \( V_h^1 \), apply test functions as 1, we have the relation for the evolution of cell averages

\[
\begin{aligned}
  \bar{u}_j^{n+1} &= \bar{u}_j^n - \frac{\Delta t}{\Delta x} \hat{f}(u_{j+1/2}^-, u_{j+1/2}^+) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1/2}^-, u_{j-1/2}^+)
  \\
  &= \frac{1}{2} (u_{j-1/2}^+ + u_{j+1/2}^-) - \frac{\Delta t}{\Delta x} \hat{f}(u_{j+1/2}^-, u_{j+1/2}^+) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1/2}^+, u_{j-1/2}^-)
  \\
  &\quad - \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1/2}^+, u_{j+1/2}^-) + \frac{\Delta t}{\Delta x} \hat{f}(u_{j-1/2}^-, u_{j-1/2}^+)
  \\
  &= \frac{1}{2} G^2 \Delta t(u_{j-1/2}^-, u_{j-1/2}^+, u_{j+1/2}^-) + \frac{1}{2} G^2 \Delta t(u_{j-1/2}^+, u_{j-1/2}^-, u_{j+1/2}^+)
\end{aligned}
\]
The Proof

\[ Q_\sigma(f) = \int_{v' \in \mathbb{R}^d} (\sigma(x, v, v') f' - \sigma(x, v', v) f) dv', \]

Let

\[ f_h(x_i^\beta, v) = \sum_{\alpha=1}^{k+1} f_h(x_i^\beta, \hat{v}_j^\alpha) L_\alpha \left( \frac{v - v_j}{\Delta v_j} \right), \]

where \( L_\alpha(\cdot) \) are basis functions for Gauss-Lobatto points. Then

\[ \int_{v_j-\frac{1}{2}}^{v_j+\frac{1}{2}} Q_\sigma(f_h)(x_i^\beta, v) dv = \sum_{\alpha=1}^{k+1} \sum_{m=1}^{N_v} f_h(x_i^\beta, \hat{v}_m^\alpha) A_{j,m}^{\alpha,\beta} - f_h(x_i^\beta, \hat{v}_j^\alpha) A_{m,j}^{\alpha,\beta}. \]

and

\[ A_{j,m}^{\alpha,\beta} = \int_{v_j-\frac{1}{2}}^{v_j+\frac{1}{2}} \int_{v_m-\frac{1}{2}}^{v_m+\frac{1}{2}} \sigma(x_i^\beta, v, v') L_\alpha \left( \frac{v' - v_m}{\Delta v_m} \right) dv' dv. \]
The Proof

Fact

(1)

\[\sum_{m=1}^{N_v} A_{j,m}^{\alpha,\beta} \leq C_k K \Delta v_j,\]

(2)

\[A_{j,m}^{\alpha,\beta} \geq 0.\]

for \(P^1\) and true for \(P^k\) when quadratures are used. (not necessary for relaxation)
The Main Result

Theorem

Consider the semi-discrete DG scheme of piecewise $P^k$ polynomials with forward Euler time stepping on a rectangular mesh that is small enough, (i.e. $\max_j \Delta v_j \leq \frac{a_2}{C_k K}$) if at time $t^n$, we have $f_h(x, v) \geq 0$ on the set $S_{i,j} = (S^x_i \otimes \hat{S}^v_j) \cup (\hat{S}^x_i \otimes S^v_j)$ for all $i, j$, where $S$ and $\hat{S}$ denote Gauss and Gauss-Lobatto quadrature points with $L \geq k + 1$ and $N = k + 1$ points respectively. Moreover, if the CFL condition $a_1 \lambda_1 + a_2 \lambda_2 \leq \min_\alpha \hat{w}_\alpha/2$ is satisfied, then we have the cell average at the next time step $t^{n+1}$ will be positive, i.e.

$$\bar{f}_{ij}^{n+1} \geq 0 \quad \text{for all } i, j.$$

If $k > 1$, then we require that $N$ point Gauss-Lobatto quadrature rules when evaluating the collision term. This restriction can be removed for the relaxation model. Without losing of accuracy for $P^1$ solutions and at most half order loss for general $P^k$ solutions, the algorithm guarantees the positivity of $\bar{f}$ and $\tilde{f}(x)$. 
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The Relaxation Model

\[ \frac{\partial f}{\partial t} + \alpha \cdot \nabla f = \frac{1}{\tau} (M_\theta(v) \rho(t, x) - f), \quad (x, v) \in \Omega_D, t \in \mathbb{R}_+ \]

\[ f(t, -L, v) = 0, \quad \text{for } x = -L, \ 0 < v \leq V, \]

\[ f(t, L, v) = 0, \quad \text{for } x = L, \ -V \leq v < 0, \]

\[ f(t, x, v) = 0, \quad \text{for } v = +V, -V, x \in D_x^1 \]

\[ f(0, x, v) = f_0(x, v), \]

with constant collision frequency \( \tau^{-1} = 1 \) and \( \theta = 1 \). We take a cut off domain \( D_v^1 = [-V, V] = [-5, 5], \ D_x^1 = [-L, L] = [-5, 5] \).
Comparison

- Accurary.

Table: The difference of DG schemes with and without the positivity-preserving limiter when using $P^2$ polynomials and third order RK time discretization until $T = 0.1$. $CFL = 0.2$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$L^1$ difference</th>
<th>$L^1$ order</th>
<th>$L^\infty$ difference</th>
<th>$L^\infty$ order</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 X 25</td>
<td>1.98E-5</td>
<td>-</td>
<td>1.04E-3</td>
<td>-</td>
</tr>
<tr>
<td>50 X 50</td>
<td>1.14E-6</td>
<td>4.11</td>
<td>1.46E-4</td>
<td>2.82</td>
</tr>
<tr>
<td>100 X 100</td>
<td>8.95E-8</td>
<td>3.67</td>
<td>2.00E-5</td>
<td>2.87</td>
</tr>
<tr>
<td>200 X 200</td>
<td>3.40E-9</td>
<td>4.72</td>
<td>6.63E-7</td>
<td>4.91</td>
</tr>
</tbody>
</table>
Comparison

Figure: The number of cells (out of 2500 cells) with negative cell averages as a function of time for the traditional RKDG scheme. $50 \times 50$ mesh with $V_h^2$ and third order Runge-Kutta time stepping.
Consider

\[ \mathcal{H}_{\log}(t) = \int_{\Omega_D} H \log H \mathcal{M}(x, v) dxdv , \]

that measures (what we refer to as) \( f \log f \)-decay in time and the quadratic \( H \) functional

\[ \mathcal{H}_2(t) = \int_{\Omega_D} H^2 \mathcal{M} dxdv . \]

Here \( H(t, x, v) = f_h(t, x, v)/\mathcal{M}(x, v) \) is the global relative entropy function.
Decay to Equilibrium

Figure: Decay rate. Left: $\mathcal{H}_{\text{log}}$, right: $\mathcal{H}_2$. Positivity-preserving DG scheme computed on a $50 \times 50$ mesh with piecewise quadratic polynomials and third order Runge-Kutta time stepping.
Solution
Conclusion & Future Work

Related future work includes

- Boltzmann-Poisson systems in semiconductor-device simulations
- Vlasov equations
- implementation in higher dimension, unstructured meshes
- nonlinear equations
The END
Thank you