Semi-Lagrangian Formulations for Linear Advection Equations and Applications to Kinetic Equations

Jingmei Qiu

Department of Mathematical and Computer Science
Colorado School of Mines
joint work w/ Chi-Wang Shu
Supported by NSF and AFOSR.

CSCAMM, University of Maryland College Park
Outline

• Background: numerical methods for kinetic equations
• Semi-Lagrangian finite difference methods for linear advection equations
• Simulation results
• Ongoing and future work
The Vlasov-Poisson (VP) system,

\[
\frac{\partial f}{\partial t} + \mathbf{p} \cdot \nabla_x f + \mathbf{E}(t, \mathbf{x}) \cdot \nabla_p f = 0, \quad (1)
\]

\[
\mathbf{E}(t, \mathbf{x}) = -\nabla_x \phi(t, \mathbf{x}), \quad -\Delta_x \phi(t, \mathbf{x}) = \rho(t, \mathbf{x}). \quad (2)
\]

\(f(t, \mathbf{x}, \mathbf{p})\): the probability of finding a particle with velocity \(\mathbf{p}\) at position \(\mathbf{x}\) at time \(t\).

\(\rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \mathbf{p}) d\mathbf{p} - 1\): charge density
Numerical approach: Lagrangian vs. Eulerian vs. semi-Lagrangian

- **Lagrangian**: tracking a finite number of macro-particles. 
  - e.g., PIC (Particle In Cell)

\[
\frac{dx}{dt} = v, \quad \frac{dv}{dt} = E
\]  

- **Eulerian**: fixed numerical mesh 
  - e.g., finite difference WENO, finite volume, finite element, spectral method.

- **Semi-Lagrangian**: 
  - e.g., finite difference, finite volume, finite element, spectral method.
Strang splitting for solving the Vlasov equation

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \mathbf{E}(t, x) \cdot \nabla_v f = 0,
\]

Nonlinear Vlasov equation \(\implies\) a sequence of linear equations.

- 1-D in \(x\) and 1-D in \(v\):

\[
\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial x} = 0, \quad (4)
\]

\[
\frac{\partial f}{\partial t} + \mathbf{E}(t, x) \frac{\partial f}{\partial v} = 0. \quad (5)
\]
SL schemes

1. Solution space: point values, or cell averages, or piecewise polynomials living on fixed Eulerian grid.
2. Evolution: tracking characteristics backward in time.
3. Project the evolved solution back onto the solution space.

Remark: The only error in time comes from tracking characteristics backward in time. The scheme is not subject to CFL time step restriction.
Various formulations of SL finite difference schemes

SL finite difference (point values)

- Scheme I: advective scheme
  the solution is evolved along characteristics (in Lagrangian spirit) approximating advective form of equation
  \[ f_t + af_x = 0. \]

- Scheme II: convective scheme
  the solution is evolved over fixed point (in Eulerian spirit) approximating conservative form of equation
  \[ f_t + (af)_x = 0. \]

* \( a \) being a constant, with possible extension to \( a = a(x, t) \) (relativistic Vlasov equation).
Scheme I: advective scheme

\[ f_{i}^{n+1} = f(x_i, t^{n+1}) = f(x_i^{*}, t^n) = f(x_i - \xi_0 \Delta x, t^n), \quad \xi_0 = \frac{a \Delta t}{\Delta x} \]

When \( \xi_0 \in [0, \frac{1}{2}] \)
Third order example

\[ f_{i}^{n+1} = f_{i}^{n} + ( - \frac{1}{6} f_{i-2}^{n} + f_{i-1}^{n} \cdots + \frac{1}{3} f_{i+1}^{n}) \xi_{0} \]
\[ + \left( \frac{1}{2} f_{i-1}^{n} - f_{i}^{n} + \frac{1}{2} f_{i+1}^{n} \right) \xi_{2}^{2} \]
\[ + \left( \frac{1}{6} f_{i-2}^{n} - \frac{1}{2} f_{i-1}^{n} + \frac{1}{2} f_{i}^{n} - \frac{1}{6} f_{i+1}^{n} \right) \xi_{3}^{3} \]

\( (6) \)

\( \star \) Method 1: apply WENO interpolation on (6).
\( \star \) No mass conservation.
Matrix vector form

\[ f_i^{n+1} = f_i^n + \xi_0 (f_{i-2}^n, f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot A^L_3 \cdot (1, \xi_0, \xi_0^2)', \quad (7) \]

with matrix

\[
A^L_3 = \begin{pmatrix}
-1/6 & 0 & 1/6 \\
1 & 1/2 & -1/2 \\
-1/2 & -1 & 1/2 \\
-1/3 & 1/2 & -1/6
\end{pmatrix}
\]

\[
= \begin{pmatrix}
-1/6 & 0 & 1/6 \\
5/6 & 1/2 & -1/3 \\
1/3 & -1/2 & 1/6 \\
0 & 0 & 0
\end{pmatrix} - \begin{pmatrix}
0 & 0 & 0 \\
-1/6 & 0 & 1/6 \\
5/6 & 1/2 & -1/3 \\
1/3 & -1/2 & 1/6
\end{pmatrix}
\]
Rewrite the advective scheme into a conservative form

\[ f_{i+1}^n = f_i^n - \xi_0 \left( (f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot C_3^L \cdot (1, \xi_0, \xi_0^2)' - (f_{i-2}^n, f_{i-1}^n, f_i^n) \cdot C_3^L \cdot (1, \xi_0, \xi_0^2)' \right) = f_i^n - \xi_0 (\hat{f}_{i+1/2}^n - \hat{f}_{i-1/2}^n) \]

with

\[ C_3^L = \begin{pmatrix} -\frac{1}{6} & 0 & \frac{1}{6} \\ \frac{5}{6} & \frac{1}{2} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{2} & \frac{1}{6} \end{pmatrix} \].

**Method 2:** apply WENO reconstructions on flux functions

\( \hat{f}_{i+1/2}^n \)

**The scheme is locally conservative. However, such splitting can NOT be generalized to equations with variable coefficients.**
Scheme II: conservative scheme

Integrating the conservative form of PDE

\[ f_t + (af)_x = 0, \]

over \([t^n, t^{n+1}]\) at \(x_i\) gives

\[ f_i^{n+1} = f_i^n - \left( \int_{t^n}^{t^{n+1}} af(x, \tau) d\tau \right)_x \bigg|_{x=x_i} \]

\[ = f_i^n - \mathcal{F}_x \bigg|_{x=x_i} \]

\[ = f_i^n - \frac{1}{\Delta x} \left( \hat{\mathcal{F}}_{i+\frac{1}{2}} - \hat{\mathcal{F}}_{i-\frac{1}{2}} \right) + \mathcal{O}(\Delta x^k) \]

where \(\mathcal{F}(x) = \int_{t^n}^{t^{n+1}} af(x, \tau) d\tau\), and \(\hat{\mathcal{F}}_{i \pm \frac{1}{2}}\) are numerical fluxes.
\[ \mathcal{F}(x_i) = \int_{t^n}^{t^{n+1}} af(x_i, \tau) d\tau = \int_{x_i^*}^{x_i} f(\xi, t^n) d\xi, \]

by applying the Divergence Theorem on \( \int_{\Omega} (f_t + (af)_x) dx = 0. \)
\[ \mathcal{F}(x_i) = \int_{t^n}^{t^{n+1}} af(x_i, \tau) d\tau = \int_{x_i^*}^{x_i} f(\xi, t^n) d\xi, \]

by applying the Divergence Theorem on \( \int_{\Omega} (f_t + (af)_x) dx = 0 \).
Let $\mathcal{H}(x)$ to be a function s.t.

$$\mathcal{F}(x) = \frac{1}{\Delta x} \int_{x - \frac{\Delta x}{2}}^{x + \frac{\Delta x}{2}} \mathcal{H}(\xi) d\xi$$

then

$$\mathcal{F}_x \big|_{x=x_i} = \frac{1}{\Delta x} \left( \mathcal{H}(x_{i+\frac{1}{2}}) - \mathcal{H}(x_{i-\frac{1}{2}}) \right).$$

Let numerical fluxes $\hat{\mathcal{F}}_{i\pm\frac{1}{2}} = \mathcal{H}(x_{i\pm\frac{1}{2}})$. 
A first order scheme

\[ f_i^{n+1} = f_i^n - \left( \int_{t^n}^{t^{n+1}} a f(x, \tau) d\tau \right)_x \]

\[ = f_i^n - F_x \]

\[ = f_i^n - \frac{1}{\Delta x} (F(x_i) - F(x_{i-1})), \quad \text{if } a > 0 \]

\[ = f_i^n - \frac{1}{\Delta x} \left( \int_{x_i}^{x_i^*} f(\xi, t^n) d\xi - \int_{x_i^*}^{x_{i-1}^*} f(\xi, t^n) d\xi \right) \]

**Remark.** When \( a \) is a constant and \( cfl < 1 \), the scheme reduces to

\[ f_i^{n+1} = f_i^n - \frac{a \Delta t}{\Delta x} (f_i^n - f_{i-1}^n) \]

which is the first order upwind scheme.
High order WENO reconstructions are applied in the following reconstructions

\[
\left\{ f(x_i, t^n) \right\}_{i=1}^{N} \xrightarrow{\text{WENO}} \left\{ \int_{x_i^*}^{x_i} f(\xi, t^n) d\xi \right\}_{i=1}^{N} \xrightarrow{\text{WENO}} \left\{ \hat{F}_{i+\frac{1}{2}} \right\}_{i=1}^{N}
\]

- Computational expensive: two weno reconstruction procedures
- The reconstruction stencil is widely spread (not compact), leading to instability of algorithm.
\[
\left\{ f(x_i, t^n) \right\}_{i=1}^N \xrightarrow{\text{WENO}} \left\{ \int_{x_i^*}^{x_i} f(\xi, t^n) d\xi \right\}_{i=1}^N \xrightarrow{\text{WENO}} \left\{ \hat{F}_{i+\frac{1}{2}} \right\}_{i=1}^N
\]

\[
\left\{ f(x_i, t^n) \right\}_{i=1}^N \xrightarrow{\text{WENO/ENO}} \left\{ \hat{F}_{i+\frac{1}{2}} \right\}_{i=1}^N
\]
Third order WENO reconstruction when $a = 1$, $dt < dx$.

Consider two substencils

$$S_1 = \{x_{i-1}, x_i\}, \quad S_2 = \{x_i, x_{i+1}\}.$$

Let $\xi = \frac{dt}{dx}$, the third order reconstruction from the three point stencil $\{x_{i-1}, x_i, x_{i+1}\}$

$$\hat{F}_{i+\frac{1}{2}} = \gamma_1 \hat{F}^{(1)}_{i+\frac{1}{2}} + \gamma_2 \hat{F}^{(2)}_{i+\frac{1}{2}}$$

where the linear weights

$$\gamma_1 = \frac{1 - \xi}{3}, \quad \gamma_2 = \frac{2 + \xi}{3},$$
and

\[ \hat{\mathbf{F}}^{(1)}_{i+\frac{1}{2}} = \left(-\left(\frac{3}{2}\xi + \frac{1}{2}\xi^2\right)f^n_i + \left(\frac{1}{2}\xi + \frac{1}{2}\xi^2\right)f^n_{i-1}\right)dx \]

\[ \hat{\mathbf{F}}^{(2)}_{i+\frac{1}{2}} = \left(\left(-\frac{1}{2}\xi + \frac{1}{2}\xi^2\right)f^n_i - \left(\frac{1}{2}\xi + \frac{1}{2}\xi^2\right)f^n_{i+1}\right)dx \]

_Idea of WENO:_ adjust the linear weighting \( \gamma_i \) to a nonlinear weighting \( w_i \), such that

- \( w_i \) is very close to \( \gamma_i \), in the region of smooth structures,
- \( w_i \) weights little on a non-smooth sub-stencil.
• Smoothness indicator:

\[ \beta_1 = (f^n_{i-1} - f^n_i)^2, \quad \beta_2 = (f^n_i - f^n_{i+1})^2 \]

• Nonlinear weights

\[ \tilde{w}_1 = \gamma_1 / (\epsilon + \beta_1)^2, \quad \tilde{w}_2 = \gamma_2 / (\epsilon + \beta_2)^2 \]

• Normalized nonlinear weights \( w_i \):

\[ w_1 = \tilde{w}_1 / (\tilde{w}_1 + \tilde{w}_2), \quad w_2 = \tilde{w}_2 / (\tilde{w}_1 + \tilde{w}_2) \]
Summary of scheme II

Method 3

1. Reconstruction numerical fluxes $\hat{F}_{i\pm1/2}$ from WENO/ENO reconstruction of $\{f_i^n\}_{i=1}^N$.

2. $f_i^{n+1} = f_i^n - \frac{1}{\Delta x} (\hat{F}_{i+1/2} - \hat{F}_{i-1/2}),$

* Compare with the method of line approach (Runge Kutta time discretization), the time integration of the PDE here is exact.
* The scheme can be extended to accommodate extra large time step evolution and to the case of variable coefficient $a(x, t)$. 
• **Method 1 & 2:**
  • Approximates the advective form of PDE
  • Frame of reference: Lagrangian
  • Method 2 is the conservative formulation of Method 1 for equations with constant coefficients
  • Method 1 can be generalized to equations with variable coefficients

• **Method 3:**
  • Approximates the conservative form of PDE
  • Frame of reference: Eulerian
  • conservative scheme
  • extends to equations with variable coefficients
Numerical Simulations

Method 1, 2, 3 with fifth order WENO reconstruction

- Linear advection equation
- Rigid body rotation
- Vlasov Poisson system
Linear transport: $u_t + u_x + u_y = 0$

Table: Order of accuracy with $u(x, y, t = 0) = \sin(x + y)$ at $T = 20$. $dt = 1.1dx = 1.1dy$.

<table>
<thead>
<tr>
<th>mesh</th>
<th>method 1 error</th>
<th>order</th>
<th>method 2 error</th>
<th>order</th>
<th>method 3 error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>20×20</td>
<td>6.03E-4</td>
<td>–</td>
<td>8.28E-4</td>
<td>–</td>
<td>7.94E-4</td>
<td>–</td>
</tr>
<tr>
<td>40×40</td>
<td>2.24E-5</td>
<td>4.75</td>
<td>2.62E-5</td>
<td>4.97</td>
<td>2.51E-5</td>
<td>4.98</td>
</tr>
<tr>
<td>60×60</td>
<td>3.10E-6</td>
<td>4.88</td>
<td>3.44E-6</td>
<td>5.00</td>
<td>3.29E-6</td>
<td>5.01</td>
</tr>
<tr>
<td>80×80</td>
<td>7.50E-7</td>
<td>4.93</td>
<td>8.16E-7</td>
<td>5.00</td>
<td>7.80E-7</td>
<td>5.00</td>
</tr>
</tbody>
</table>
Rigid body rotation:

\[ u_t - yu_x + xu_y = 0 \]

**Figure:** Initial profile and numerical solution of method 1 from the numerical mesh 100 × 100, \( dt = 1.1dx = 1.1dy \) at \( T = 12\pi \)
Rigid body rotation:
\[ u_t - y u_x + x u_y = 0 \]

Figure: Method 2 and 3 with the numerical mesh 100 × 100, \( dt = 1.1 dx = 1.1 dy \) at \( T = 12\pi \).
Rigid body rotation:

\[ u_t - yu_x + xu_y = 0 \]

Figure: Method 1 (left) and 3 (right).
Rigid body rotation:

\[ u_t - y u_x + x u_y = 0 \]

**Figure:** Method 1 (left) and 3 (right).
Consider the VP system with initial condition,

$$f(x, v, t = 0) = \frac{1}{\sqrt{2\pi}} (1 + \alpha \cos(kx)) \exp(-\frac{v^2}{2})$$, \hspace{1cm} (8)
Weak Landau damping:

\[ \alpha = 0.01, \ k = 2 \]

Figure: Time evolution of \( L^2 \) norm of electric field.
Weak Landau damping (cont.)

Figure: Time evolution of $L^1$ (upper left) and $L^2$ (upper right) norm, discrete kinetic energy (lower left), entropy (lower right).
Strong Landau damping: $\alpha = 0.5, \, k = 2$

**Figure:** Time evolution of the $L^2$ norm of the electric field.
Strong Landau damping (cont.)

Figure: Time evolution of $L^1$ (upper left) and $L^2$ (upper right) norm, discrete kinetic energy (lower left), entropy (lower right).
Two-stream instability

Consider the symmetric two stream instability, the VP system with initial condition

\[ f(x, \nu, t = 0) = \frac{2}{7\sqrt{2\pi}}(1 + 5\nu^2)(1 + \alpha((\cos(2kx) + \cos(3kx))/1.2 + \cos(kx))\exp(-\frac{\nu^2}{2}) , \]

with \( \alpha = 0.01, \ k = 0.5 \) and the length of domain in \( x \)-direction \( L = \frac{2\pi}{k} \).
Figure: Two stream instability $T = 53$. The numerical solution of method 1 (left) and Method 3 (right) with the numerical mesh $64 \times 128$. 
Figure: Third order semi-Lagrangian WENO method. Two stream instability $T = 53$. The numerical mesh is $64 \times 128$ (left) and $256 \times 512$ (right).
Figure: Time development of $L^1$ (upper left) and $L^2$ (upper right) norm, discrete kinetic energy (lower left), entropy (lower right).
Ongoing and future work

- **Algorithm:**
  - Equations of variable coefficients
  - Truly multi-dimensional formulation of semi-Lagrangian scheme evolving point values.

- **Application**
  - advection in incompressible flow
  - relativistic Vlasov equations
SL for linear advection with applications to kinetic Equations

Jingmei Qiu

Introduction

Proposed method

SL finite difference I
SL finite difference II
Comparison

Simulation results

Summary

THANK YOU!