High Order Semi-Lagrangian Schemes And Operator Splitting For The Boltzmann Equation

Yaman Güçlü ¹  Andrew J. Christlieb ¹  William N.G. Hitchon ²

¹Department of Mathematics, Michigan State University, East Lansing (MI)
²Department of Electrical and Computer Engineering, University of Wisconsin, Madison (WI)

7 June 2013

Issues in Solving the Boltzmann Equation for Aerospace Applications
ICERM topical workshop, Providence (RI), 3-7 June 2013
Contents

1. Model Equations
2. Numerical Challenges
3. Convected Scheme
4. Numerical Results
5. Conclusions
Maxwell-Boltzmann system

Maxwell’s equations:

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \]

\[ \nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \quad \nabla \cdot \mathbf{B} = 0 \]

Sources: charge and current density:

\[
\rho (r, t) = \sum_\alpha q_\alpha n_\alpha (r, t), \quad \mathbf{J} (r, t) = \sum_\alpha q_\alpha n_\alpha (r, t) \mathbf{u}_\alpha (r, t).
\]

Number density and mean velocity of each species:

\[
n_\alpha (r, t) = \int_{\mathbb{R}^3} f_\alpha (r, \mathbf{v}, t) \, d\mathbf{v}, \quad \mathbf{u}_\alpha (r, t) = \frac{1}{n_\alpha (r, t)} \int_{\mathbb{R}^3} \mathbf{v} f_\alpha (r, \mathbf{v}, t) \, d\mathbf{v}.
\]

Boltzmann’s equation for each species:

\[
\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \nabla f_\alpha + \frac{q_\alpha}{m_\alpha} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla \mathbf{v} f_\alpha = \sum_\beta Q_\alpha (f_\alpha, f_\beta) (r, \mathbf{v}, t)
\]
Boltzmann’s equation

Eulerian formulation: \((t, x, v)\) independent variables

\[
\frac{\partial f_\alpha}{\partial t} + v \cdot \nabla f_\alpha + \frac{F_\alpha}{m_\alpha} \cdot \nabla v f_\alpha = \left. \frac{\partial f_\alpha}{\partial t} \right|_{\text{coll}}
\]

Lagrangian formulation: follow trajectory \((x(t), v(t))\) in phase space

\[
\frac{dx}{dt} = v(t), \quad \frac{dv}{dt} = \frac{1}{m_\alpha} F_\alpha (t, x(t), v(t))
\]

• Substituting into Boltzmann’s equation: \(\frac{Df_\alpha}{Dt} = \left. \frac{\partial f_\alpha}{\partial t} \right|_{\text{coll}}\)

• Time rate of change of \(f_\alpha (t, x(t), v(t))\) along phase-space trajectory only determined by collision operator

• Without collisions, \(f_\alpha\) constant along phase-space trajectory: fluid motion in phase-space is incompressible

Semi-Lagrangian method:

• \(f_\alpha (t, x, v)\) lies on Eulerian mesh

• Evolution within time step uses Lagrangian formulation (\textit{method of characteristics})
Modeling challenges

**Weakly Collisional Plasma:**

- Electrons can be far from equilibrium and involved in strongly non-linear processes (e.g. ionization near threshold)
- Multiple species: electrons, multiple ions, neutrals;
- Multiple time and spatial scales;
- Complex geometries, different boundary conditions (perfect/real conductors, dielectrics, absorbing), often time varying and coupled to domain (plasma feedbacks into circuit);
- Complex collisional processes: elastic, inelastic (excitation, ionization, recombination, attachment, dissociation etc.);
- External magnetic fields: electrons may be strongly magnetized, possibly ions too;
- Other important processes: radiation transport, gas-phase chemical reactions, plasma-surface interaction, aggregates (dusty plasmas).

**Challenges for Low-Order Eulerian Codes:**

- For electrons, need high resolution over large velocity mesh
- Impressive memory requirement in multiple dimensions
- Explicit time-stepping imposes non-physical time-step restriction (CFL limit)
- Method of lines (MOL): multistep and multi-stage methods require additional storage
Convected Scheme

The Convected Scheme \(^a\) is a **forward semi-Lagrangian** method for Boltzmann’s equation. Employs operator splitting:

1. **Collision operator** is local in configuration space, solves
   \[
   \frac{\partial f_\alpha}{\partial t} = \frac{\partial f_\alpha}{\partial t} \bigg|_{\text{coll}}
   \]

2. **Ballistic operator** advects \(f_\alpha(t, x, v)\) along characteristic trajectories in phase space according to
   \[
   \frac{Df_\alpha}{Dt} = 0,
   \]
   integrated over a *moving cell* (MC).

\[
\begin{align*}
  f_\alpha(t, x, v) \text{ assumed uniform over MC, allowing for 'area remapping rule'}
\end{align*}
\]

---


Convected Scheme

**PROs:**
- Preserves positivity (good as $f_\alpha > 0$)
- No CFL restriction on $\Delta t$
- Very simple implementation
- Can enforce total energy conservation for stationary electric field

**CONs:**
- Difficult to handle boundary conditions
- **Numerical diffusion**: local remapping error $O(\Delta x^2)$

Reduced Numerical Diffusion

Numerical diffusion mitigated by reducing remapping frequency $\Rightarrow$ “long-lived moving cells” \(^a\). Recently \(^b\), we devised a high-order version of the Convected Scheme, for **neutral gas** kinetics:

**Model equation:** uniform velocity advection: $n_t + u_0 n_x = 0$

**Basic idea:** compensating remapping error by applying small corrections to final position of moving cells prior to remapping $\Rightarrow$ **antidiffusive velocity field**

**Tool:** modified equation analysis, perturbation analysis

---


High-order semi-Lagrangian solution of the Vlasov-Poisson system

**Problem:**
Difficult to construct high-order semi-Lagrangian ballistic operator when mean force is present (no straight trajectories)

**Solution:**
- Further split ballistic operator into separate constant advection operators along $x$ and $v$ \[a\]
- Apply favorite high-order semi-Lagrangian solver to each operator
- Combine operators to high-order in time using Runge-Kutta-Nyström methods \[b, c\]
  (symplectic $\Rightarrow$ energy stable)

---

**References:**


Arbitrarily High-Order Convected Scheme (1)

1D CONSTANT ADVECTION EQUATION

\[
\left( \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right) n(x, t) = 0
\]

- Exact solution (method of characteristics): \( n(x, t + \Delta t) \equiv n(x - u\Delta t, t) \)
- Courant parameter: \( \alpha := u \Delta t / \Delta x \)

**CONVECTED SCHEME UPDATE**

- Discretize time (arbitrary \( \Delta t \)) and space (uniform \( \Delta x \)): \( n_i^k \approx n(x_i, t_k) \)
- Because of uniform \( \Delta x \), solution can be shifted exactly by integer number of cells
- Without loss of generality, assume \( 0 \leq \alpha \leq 1 \)(this is not a CFL limit)
- Under these assumptions, CS update is

\[
n_i^{k+1} = U_{i-1}^k n_{i-1}^k + \left( 1 - U_i^k \right) n_i^k
\]

- As long as \( 0 \leq U_i^k \leq 1 \), CS is **mass** and **positivity preserving**
- With no high-order corrections, \( U(x, t) \equiv \alpha \Rightarrow 1\text{st-order Upwind scheme} \)
- With high-order corrections, \( U(x, t) = [u + \tilde{u}(x, t)] \Delta t / \Delta x = \alpha + \tilde{\alpha}(x, t) \)
- \( \tilde{\alpha}(x, t) \) is **anti-diffusive Courant parameter**
Arbitrarily High-Order Convected Scheme (2)

**LOCAL TRUNCATION ERROR (LTE)**

- **Exact solution**, Taylor expand in space (smooth initial conditions):

  \[
  n(x, t + \Delta t) = n(x, t) + \left( \sum_{p=1}^{N-1} (-\alpha)^p \frac{(\Delta x)^p}{p!} \frac{\partial^p n}{\partial x^p} \right) n(x, t) + O\left(\Delta x^N\right),
  \]

- **CS solution**, Taylor expand in space about \((x, t) = (x_i, t^k)\):

  \[
  n_{CS}(x, t + \Delta t) = n(x, t) + \left( \sum_{p=1}^{N-1} (-1)^p \frac{(\Delta x)^p}{p!} \frac{\partial^p U n}{\partial x^p} \right) U(x, t) n(x, t) + O\left(\Delta x^N\right)
  \]

- We want the local truncation error \(\mathcal{E}(x, t, \Delta t) := n(x, t + \Delta t) - n_{CS}(x, t + \Delta t) = O(\Delta x^N)\), hence we find \(\tilde{\alpha}(x, t)\) by imposing the **order condition**

  \[
  \sum_{p=1}^{N-1} (-\alpha)^p \frac{(\Delta x)^p}{p!} \frac{\partial^p n}{\partial x^p} - \sum_{p=1}^{N-1} (-1)^p \frac{(\Delta x)^p}{p!} \frac{\partial^p (Un)}{\partial x^p} = O(\Delta x^N)
  \]
Arbitrarily High-Order Convected Scheme (3)

HIGH-ORDER CORRECTIONS \(^{\text{a}}\)

- Make the polynomial ansatz

\[
U_n(x, t) = \sum_{q=0}^{N-2} (-1)^q \beta_q(\alpha) (\Delta x)^q \frac{\partial^q n(x, t)}{\partial x^q},
\]

and solve for the unknown polynomials \(\beta_q(\alpha)\);

- Substitute in order condition to find (after algebraic manipulations)

\[
[\tilde{\alpha} n]^k_i = \sum_{q=1}^{N-2} (-1)^q \frac{B_{q+1}(\alpha) - B_{q+1}(0)}{(q + 1)!} (\Delta x)^q \frac{\partial^q n(x, t)}{\partial x^q} \bigg|_i^k,
\]

where \(B_q(\cdot)\) are Bernoulli polynomials;

- Approximate products \((\Delta x)^q \frac{\partial^q n(x, t)}{\partial x^q} \bigg|_i^k\) with error no larger than \(O(\Delta x^{N-1})\), e.g.:

  1. linear polynomial interpolation,
  2. weighted essentially non-oscillatory (WENO) interpolation,
  3. fast Fourier transform (FFT).

Arbitrarily High-Order Convected Scheme (4)

Numerical Implementation \[^3\]

- 6th-order finite difference scheme

\[
\Delta x \frac{\partial n}{\partial x}^k_i \approx \frac{n^k_{i-2} - 8 n^k_{i-1} + 8 n^k_{i+1} - n^k_{i+2}}{12} + O(\Delta x^5),
\]

\[
(\Delta x)^2 \frac{\partial^2 n}{\partial x^2}^k_i \approx \frac{-n^k_{i-2} + 16 n^k_{i-1} - 30 n^k_i + 16 n^k_{i+1} - n^k_{i+2}}{12} + O(\Delta x^6),
\]

\[
(\Delta x)^3 \frac{\partial^3 n}{\partial x^3}^k_i \approx \frac{-n^k_{i-2} + 2 n^k_{i-1} - 2 n^k_{i+1} - n^k_{i+2}}{2} + O(\Delta x^5),
\]

\[
(\Delta x)^4 \frac{\partial^4 n}{\partial x^4}^k_i \approx n^k_{i-2} - 4 n^k_{i-1} + 6 n^k_i - 4 n^k_{i+1} + n^k_{i+2} + O(\Delta x^6),
\]

- 22nd-order pseudo-spectral scheme

\[
U n(x) = \mathcal{F}^{-1} \left[ \sum_{q=0}^{N-2} (-j)^q \beta_q(\alpha) (\xi \Delta x)^q \cdot \mathcal{F}[n](\xi) \right] (x),
\]

\[^{a}\text{Y. G"uc"l"u, A.J. Christlieb and W.N.G. Hitchon. Arbitrarily high order Convected Scheme solution of the Vlasov-Poisson system. Under preparation.}\]
Vlasov in Stationary Field: phase-space vorticity

- Prescribed stationary potential:
  \[ \phi(x) = \frac{1 + \cos(\pi x^2)}{4} + \frac{\sin(\pi x)}{20} \]

- 2D flow field:
  \[ u(x) = \begin{bmatrix} u_1(x_1, x_2) \\ u_2(x_1, x_2) \end{bmatrix} \]

- 2D vorticity:
  \[ \nabla \times u = \left[ \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2} \right] \hat{n}_3 = \Omega(x_1, x_2) \hat{n}_3 \]

For 1D-1V Vlasov, \((x_1, x_2) = (x, v)\) and \((u_1, u_2) = (v, -E(x))\).
Hence the **phase-space vorticity** depends on \(x\) only:

\[ \Omega(x, v) = -\frac{\partial E}{\partial x} - \frac{\partial v}{\partial v} = \frac{\partial^2 \phi}{\partial x^2} - 1 = \Omega(x) \]
Vlasov in Stationary Field: Hamiltonian

- One-particle Hamiltonian:
  \[ H(x, v) = \frac{v^2}{2} - \phi(x) \]
- Hamiltonian is constant of motion: \( H(x(t), v(t)) \equiv c \)
- \( H(x, v) > 0 \) (solid lines): open trajectories
- \( H(x, v) \leq 0 \) (dashed lines): closed trajectories (electrostatic confinement)

If Vlasov solver is energy-stable, confined particles will remain confined.
Vlasov in Stationary Field: steady-state preservation

**INITIAL CONDITIONS**

\[ f(0, x, v) = g(H(x, v) - \min(H)) \]

\[ g(h) = \begin{cases} 
\cos(\pi h)^6 & \text{if } h < 0.5 \\
0.0 & \text{otherwise}
\end{cases} \]
Vlasov in Stationary Field: steady-state preservation

Relative errors in conserved quantities

GRID
\[ N_x = 128 \]
\[ N_v = 128 \]

TIME STEPPING
\[ \Delta t = 0.25 \]
4000 steps

COURANT NO.
\[ C_x \approx 16 \]
\[ C_v \approx 20 \]
GRID
\( N_x = 512 \)
\( N_v = 512 \)

TIME STEPPING
\( \Delta t = 0.5 \)
100+100 steps

COURANT NUMBER
\( C_x \approx 130 \)
\( C_v \approx 160 \)
Vlasov in Stationary Field: filamentation (2)

Relative errors in conserved quantities

- **L1-norm**
- **L2-norm**
- **Total energy**
- **Entropy**

**GRID**
- \( N_x = 512 \)
- \( N_v = 512 \)

**TIME STEPPING**
- \( \Delta t = 0.5 \)
- 100+100 steps

**COURANT NO.**
- \( C_x \approx 130 \)
- \( C_v \approx 160 \)

**Solid blue line:** forward evolution
**Dashed red line:** backward evolution

Y. Güçlü & A.J. Christlieb (MSU), W.N.G. Hitchon (UW)
High Order Semi-Lagrangian For Boltzmann's eq.
Providence, 7 Jun 2013
Vlasov in Stationary Field: filamentation (3)

Relative errors in conserved quantities

- **L1-norm**
  - Grid: $N_x = 1024$
  - $N_v = 1024$

- **L2-norm**

- **Total energy**

- **Entropy**

  - Courant NO.
    - $C_x \approx 130$
    - $C_v \approx 160$

Solid blue line: **forward** evolution

Dashed red line: **backward** evolution

Vlasov-Poisson: linear Landau damping (1)

\[ \text{GRID} \]
\[ N_x = 16 \]
\[ N_v = 256 \]

\[ \text{TIME STEPPING} \]
\[ \Delta t = 0.5 \]
120 steps

\[ \text{COURANT NUMBER} \]
\[ C_x \approx 4.0 \]
\[ C_v \approx 0.2 \]
Vlasov-Poisson: linear Landau damping (2)

\[ f(t,x,v) \text{ at } t = 0, 2, 6, 15, 30, 60 \]

\[ N_x = 16 \quad N_v = 256 \quad \Delta t = 0.5 \quad 120 \text{ steps} \quad [C_x \approx 4.0 \quad C_v \approx 0.2] \]

Vlasov-Poisson: linear Landau damping (3)

Electrostatic energy in domain

GRID
$N_x = 16$
$N_v = 256$

TIME STEPPING
$\Delta t = 0.5$
120 steps

COURANT NUMBER
$C_x \approx 4.0$
$C_v \approx 0.2$
Vlasov-Poisson: linear Landau damping (4)

Relative errors in conserved quantities

- **L1-norm**
- **L2-norm**
- **Total energy**
- **Entropy**

**GRID**
- \(N_x = 16\)
- \(N_v = 256\)

**TIME STEPPING**
- \(\Delta t = 0.5\)
- 120 steps

**COURANT NO.**
- \(C_x \approx 4.0\)
- \(C_v \approx 0.2\)
Vlasov-Poisson: non-linear Landau damping (1)

**GRID**

\[ N_x = 256 \]
\[ N_v = 512 \]

**TIME STEPPING**

\[ \Delta t = 0.5 \]
120 steps

**COURANT NUMBER**

\[ C_x \approx 64 \]
\[ C_v \approx 20 \]
Vlasov-Poisson: non-linear Landau damping (2)

\( N_x = 256 \quad N_v = 512 \quad \Delta t = 0.5 \quad 120 \text{ steps} \quad [C_x \approx 64 \quad C_v \approx 20] 

Y. Güçlü & A.J. Christlieb (MSU), W.N.G. Hitchon (UW) 
High Order Semi-Lagrangian For Boltzmann's eq. 
Providence, 7 Jun 2013
Vlasov-Poisson: non-linear Landau damping (3)

\[ \frac{|E(t)|}{|E(t=0)|} \]

Electrostatic energy in domain

**GRID**

- \( N_x = 256 \)
- \( N_v = 512 \)

**TIME STEPPING**

- \( \Delta t = 0.5 \)
- 120 steps

**COURANT NUMBER**

- \( C_x \approx 64 \)
- \( C_v \approx 20 \)
Relative errors in conserved quantities

- **L1-norm**
  - Time: 0 to 60
  - Y-axis: $10^{-16}$ to $10^{-13}$

- **L2-norm**
  - Time: 0 to 60
  - Y-axis: $10^{-16}$ to $10^{-12}$

- **Total energy**
  - Time: 0 to 60
  - Y-axis: $10^{-8}$ to $10^{3}$

- **Entropy**
  - Time: 0 to 60
  - Y-axis: $10^{-12}$ to $10^{-1}$

---

**GRID**
- $N_x = 256$
- $N_v = 512$

**TIME STEPPING**
- $\Delta t = 0.5$
- 120 steps

**COURANT NO.**
- $C_x \approx 64$
- $C_v \approx 20$
Vlasov-Poisson: two-stream instability (1)

**GRID**

\[ N_x = 256 \]
\[ N_v = 512 \]

**TIME STEPPING**

\[ \Delta t = 0.5 \]

90 steps

**COURANT NUMBER**

\[ C_x \approx 64 \]
\[ C_v \approx 20 \]
Vlasov-Poisson: two-stream instability (2)

\[N_x = 256 \quad N_v = 512 \quad \Delta t = 0.5 \quad 90 \text{ steps} \quad [C_x \approx 64 \quad C_v \approx 20]\]
Vlasov-Poisson: two-stream instability (3)

Relative errors in conserved quantities

![Graph showing L1-norm vs time](image1)

![Graph showing L2-norm vs time](image2)

![Graph showing Total energy vs time](image3)

![Graph showing Entropy vs time](image4)

**GRID**

- $N_x = 256$
- $N_v = 512$

**TIME STEPPING**

- $\Delta t = 0.5$
- 90 steps

**Courant No.**

- $C_x \approx 64$
- $C_v \approx 20$
Vlasov-Poisson: bump-on-tail instability (1)

**GRID**
\[ N_x = 256 \]
\[ N_v = 512 \]

**TIME STEPPING**
\[ \Delta t = 0.5 \]
44 steps

**COURANT NUMBER**
\[ C_x \approx 49 \]
\[ C_v \approx 9.4 \]
Vlasov-Poisson: bump-on-tail instability (2)

\[ N_x = 256 \quad N_v = 512 \quad \Delta t = 0.5 \quad 44 \text{ steps} \quad [C_x \approx 49 \quad C_v \approx 9.4] \]
Vlasov-Poisson: bump-on-tail instability (3)

Relative errors in conserved quantities

GRID
$N_x = 256$
$N_v = 512$

TIME STEPPING
$\Delta t = 0.5$
44 steps

COURANT NO.
$C_x \approx 49$
$C_v \approx 9.4$
Conclusions and Outlook

RECALL:

- Multi-dimensional mesh-based solution of Boltzmann’s eq. for weakly collisional plasmas;
- In standard Eulerian codes, memory requirement is too large (large mesh + RK storage) and time steps are too small (CFL restriction);
- Splitting ballistic and collision operators allows semi-Lagrangian algorithms (no CFL limit);
- Splitting configuration-advection and velocity-advection permits one to use very accurate constant advection solvers (coarser mesh, no more RK storage).

SUMMARY:

- Convected Scheme (CS) is semi-Lagrangian algorithm, mass and positivity preserving;
- Constant advection CS extended to arbitrarily high order (22nd-order version with FFTs);
- 4th-order Runge-Kutta-Nyström operator splitting guarantees energy stability;
- Tested with standard benchmarks for 1D-1V Vlasov-Poisson system;
- Error in total energy conservation bounded until solution is spatially resolved.

FUTURE WORK:

- Implement absorbing boundary conditions (wall recombination);
- Couple to simple collision operator (electron scattering on neutrals);
- Extend to higher dimensions (1D-2V, 2D-3V).
Acknowledgments

This work was partially supported by the following agencies:

- **MICHIGAN STATE UNIVERSITY FOUNDATION**
  SPG-RG100059

- **AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFOSR)**
  FA9550-11-1-0281, FA9550-12-1-0343, FA9550-12-1-0455

- **NATIONAL SCIENCE FOUNDATION (NSF)**
  DMS-1115709