# High order conservative Semi-Lagrangian schemes for kinetic equations

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# Motivation

Semi-Lagrangian schemes are very effective for the treatment of convection (and drift) terms in kinetic equations.

- They are obtained by integrating the equations along characteristics.
- Large time steps are possible, therefore improving efficiency
- SL scheme may not be not conservatives.

Conservation is very relevant for

- long time behaviour of Vlasov-like equations
- AP property for BGK-type equation (essential for example for capturing shocks)

Purpose of the talk:
Analyze loss of conservation for SL scheme, and propose some techniques that are able to restore conservation.

# BGK model

BGK is a simple model of the Boltzmann transport equation.
$f(x, v, t)$ satisfies

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\kappa}(M(f) - f) \tag{1.1}$$

with local Maxwellian

$$M(f)(x, v, t) = \frac{\rho(x, t)}{\sqrt{(2\pi RT(x, t))^d}} e^{-\frac{|v-U(x,t)|^2}{2RT(x,t)}}$$

$d$: the dimension in velocity, $\kappa$: Knudsen number,
$\rho = \int_{\mathbb{R}^d} f(x, v, t)\, dv$: space density,
$\rho U = \int_{\mathbb{R}^d} v f(x, v, t)\, dv$: momentum density,
$R$: the gas constant, $T$: temperature,
$d\rho RT(x, t) = \int_{\mathbb{R}^d} (v - U(x, t))^2 f(x, v, t)\, dv$.

In spite of its simple structure, it is very relevant:

- as $\kappa \to 0$ its moments satisfy compressible Euler equations $\Rightarrow$ same fluid dynamic limit of the BTE
- with suitable correction (e.g. ES-BGK), it can be constructed to capture the Navier-Stokes behavior for small, non zero, Knudsen number
- it satisfies an H-theorem
- it is much much easier to solve than the full BTE
- it can be adopted as a tool of the construction of very effective schemes for the numerical solution of the BTE when close (but not too much!) to the fluid dynamic limit (Jin-Filbet)
- can be uses to improve Monte Carlo simulation of BTE (Pareschi-Di Marco)
- . . .

# Outline

# SL scheme

Semi-Lagrangian schemes (SL) for the convection part + implicit discretization for the collision part seem natural because:

- no CFL restriction on $\Delta t$ due to convection
- no restriction due to small collision time

We start from the characterstic formulation of the problem

$$\frac{df}{dt} = \frac{1}{\kappa}(M(f) - f), \quad \frac{dx}{dt} = v,$$

subject to the initial condition: $f(x, v, 0) = f_0(x, v)$.

# Simple Semi-Lagrangian scheme

Suppose that the computational domain is
$[x_{\min}, x_{\max}] \times [v_{\min}, v_{\max}] \times [0, t^f] \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+$.

Grid points are denoted by:

- $t^n = n\Delta t$;
- $x_i = x_{\min} + i\Delta x, \ i = 0, ..., N_x$;
- $v_j = v_{\min} + j\Delta v, \ j = 0, ..., N_v$,

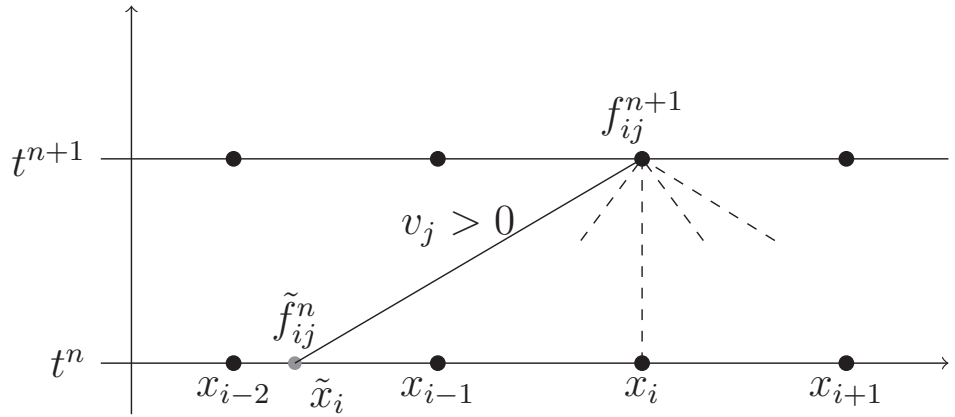
We consider 1D in space and velocity. Let us denote
$f_{ij}^n \approx f(x_i, v_j, t^n)$.

First order semi-Lagrangian implicit Euler scheme:

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}^n + \frac{\Delta t}{\kappa}(M_{i,j}^{n+1} - f_{i,j}^{n+1})$$

where $\tilde{f}_{i,j}^n$ is obtained by linear interpolation from $f_{ij}^n$.

# Simple SL scheme




$M_{i,j}^{n+1}$ is computed imposing it has the same moments of $f^{n+1}$: multiply by $(1, v_j, v_j^2)$ and use the property that
the moments of $M_{ij}^{n+1} - f_{ij}^{n+1}$ vanish:

$$(\rho_i^{n+1}, \rho_i^{n+1} U_i^{n+1}, \rho_i^{n+1} E_i^{n+1}) \approx \sum_j (1, v_j, v_j^2) \tilde{f}_{ij}^{n+1} \Delta v,$$

where $\tilde{f}_{i,j}^{n} \approx f(x_i - v_j \Delta t, v_j, t^n)$.

# Higher order: Runge-Kutta schemes

Runge-Kutta schemes can be adopted for high order in time.
L-stable schemes provide correct fluid dynamic limit.
Example of RK schemes adopted here:

$$RK2 = \begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1\text{-}\alpha & \alpha \\ \hline & 1\text{-}\alpha & \alpha \end{array}, \qquad RK3 = \begin{array}{c|ccc} \gamma & \gamma & 0 & 0 \\ (1+\gamma)/2 & (1-\gamma)/2 & \gamma & 0 \\ 1 & 1-\delta-\gamma & \delta & \gamma \\ \hline & 1-\delta-\gamma & \delta & \gamma \end{array}$$

where

$$\alpha = 1 - \frac{\sqrt{2}}{2}, \quad \gamma = 0.4358665215, \quad \delta = -0.644373171.$$

RK may be expensive due to the high number of interpolations.

# High order: BDF schemes

The BDF (Backward Difference Formula) methods allow same order of accuracy at lower cost.

We use BDF2 and BDF3.
Applying these methods to the Lagrangian formulation of the BGK model we obtain the following schemes:

$$f_{ij}^{n+1} = \frac{4}{3} \overset{(1)}{f}{}_{ij}^{n} - \frac{1}{3} \overset{(2)}{f}{}_{ij}^{n-1} + \frac{\Delta t}{\epsilon}(M_{ij}^{n+1} - f_{ij}^{n+1}) \qquad \text{BDF2}$$

$$f_{ij}^{n+1} = \frac{11}{18} \overset{(1)}{f}{}_{ij}^{n} - \frac{9}{11} \overset{(2)}{f}{}_{ij}^{n-1} + \frac{2}{11} \overset{(3)}{f}{}_{ij}^{n-2} + \frac{\Delta t}{\epsilon}(M_{ij}^{n+1} - f_{ij}^{n+1}) \qquad \text{BDF3}$$

where $\overset{(s)}{f}{}^{n}{}_{ij} = f^n(x_i - s v_j \Delta t, v_j)$, $s = 1, 2, 3$, obtained by interpolation.

# RK2 and BDF2

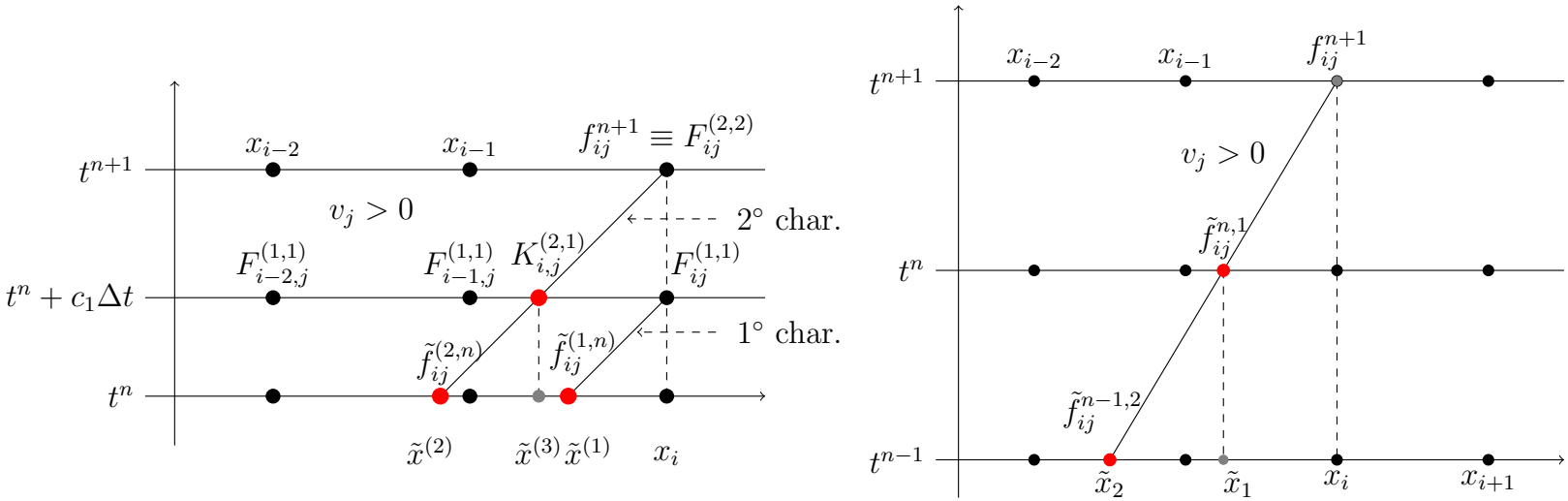



Figure: Left RK2, right BDF2. One has to interpolate in the red circle.

High order in space is obtained by CWENO or by generalized WENO reconstruction (Carlini, Ferretti, R. 2005).

# Conservation of first order scheme - single shock

| $L_1$ relative error | RK1+Linear+CM | | |
|---|---|---|---|
| $(N_x, N_v), CFL = 4$ | Mass | Momentum | Energy |
| $(100, 30)$ | 3.63e-04 | 0.0012 | 0.0021 |
| $(100, 40)$ | 5.54e-08 | 3.26e-07 | 6.03e-07 |
| $(100, 50)$ | 8.55e-13 | 7.81e-12 | 1.43e-11 |
| $(100, 60)$ | 3.55e-14 | 4.96e-14 | 3.89e-14 |
| $(100, 90)$ | 3.24e-14 | 4.82e-14 | 3.77e-14 |
| $(200, 30)$ | 9.10e-04 | 0.0030 | 0.0051 |
| $(200, 40)$ | 1.15e-07 | 6.43e-07 | 1.25e-06 |
| $(200, 50)$ | 1.78e-12 | 1.54e-11 | 2.97e-11 |
| $(200, 60)$ | 7.45e-14 | 8.24e-14 | 7.23e-14 |
| $(200, 90)$ | 7.16e-14 | 7.32e-14 | 7.45e-14 |

Table: $Kn = 10^{-6}$, Conservation error of discrete moments for single shock with velocity domain $[-20, 20]$.

## Remark 2.1

- *The error is small, but prevents construction of AP schemes for Euler equations, since it does not satisfy conservation.*
- *What is the source of error in the first order scheme and how can we fix it?*

**Effect of continuous Maxwellian**

Strong dependence on $N_v$: the use of continuous Maxwellian.
In the classical Maxwellian the parameters $\rho$, $U$, and $T$ are related to $M$ by integration, while numerically they are obtained by discrete summation.
The quadrature formulas are *spectrally accurate*, therefore when the Maxwellian is fully resolved one obtains high accuracy.
Possible solution: use discrete Maxwellian (DM) [Mieussens, 2000]

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# Conservation of high order schemes: RK3

| $L_1$ relative error | Classical RK3+W35+CM | | |
|---|---|---|---|
| $(N_x, N_v)$, $CFL = 2$ | Mass | Momentum | Energy |
| $(100, 42)$ | 1.28e-03 | 1.25e-02 | 1.41e-02 |
| $(100, 50)$ | 1.06e-03 | 1.31e-02 | 1.47e-02 |
| $(100, 60)$ | 1.43e-03 | 1.26e-02 | 1.49e-02 |
| $(100, 90)$ | 1.35e-03 | 1.28e-02 | 1.48e-02 |
| $(200, 42)$ | 1.54e-03 | 1.30e-02 | 1.45e-02 |
| $(200, 50)$ | 1.30e-03 | 1.35e-02 | 1.51e-02 |
| $(200, 60)$ | 1.68e-03 | 1.30e-02 | 1.53e-02 |
| $(200, 90)$ | 1.60e-03 | 1.32e-02 | 1.53e-02 |
| $(400, 42)$ | 1.68e-03 | 1.32e-02 | 1.47e-02 |
| $(400, 50)$ | 1.42e-03 | 1.36e-02 | 1.53e-02 |
| $(400, 60)$ | 1.80e-03 | 1.32e-02 | 1.55e-02 |
| $(400, 90)$ | 1.73e-03 | 1.34e-02 | 1.54e-02 |
| $(800, 60)$ | 1.86e-03 | 1.33e-02 | 1.55e-02 |
| $(800, 90)$ | 1.80e-03 | 1.34e-02 | 1.55e-02 |

Table: $\kappa = 10^{-6}$, Conservation error of discrete moments for single shock problem with velocity domain $[-20, 20]$.

# Conservation of high order schemes: BDF3

| $L_1$ relative error | Classical BDF3+W35+CM | | |
|---|---|---|---|
| $(N_x, N_v)$, $CFL = 2$ | Mass | Momentum | Energy |
| $(100, 42)$ | 1.73e-03 | 1.03e-02 | 1.39e-02 |
| $(100, 50)$ | 1.58e-03 | 1.04e-02 | 1.38e-02 |
| $(100, 60)$ | 1.73e-03 | 1.00e-02 | 1.38e-02 |
| $(100, 90)$ | 1.75e-03 | 1.03e-02 | 1.40e-02 |
| $(200, 42)$ | 2.02e-03 | 1.10e-02 | 1.46e-02 |
| $(200, 50)$ | 1.88e-03 | 1.11e-02 | 1.45e-02 |
| $(200, 60)$ | 2.01e-03 | 1.07e-02 | 1.44e-02 |
| $(200, 90)$ | 2.03e-03 | 1.10e-02 | 1.46e-02 |
| $(400, 42)$ | 2.18e-03 | 1.14e-02 | 1.49e-02 |
| $(400, 50)$ | 2.05e-03 | 1.15e-02 | 1.48e-02 |
| $(400, 60)$ | 2.16e-03 | 1.11e-02 | 1.47e-02 |
| $(400, 90)$ | 2.19e-03 | 1.14e-02 | 1.49e-02 |
| $(800, 60)$ | 2.24e-03 | 1.13e-02 | 1.49e-02 |
| $(800, 90)$ | 2.27e-03 | 1.16e-02 | 1.51e-02 |

Table: $\kappa = 10^{-6}$, Conservation error of discrete moments for single shock problem with velocity domain $[-20, 20]$.

- Why do high order schemes have much larger conservation errors than first order ones?

  Main qualitative difference: in the first order scheme the interpolation weights are the same for all intervals.

  In high order non-oscillatory reconstruction, the interpolation weights depend on the local regularity!

Accuracy in space is obtained by high order reconstruction. Several techniques can be adopted to obtain high order, still avoiding spurious oscillations. They all destroy translation invariance.

- Why do high order schemes have much larger conservation errors than first order ones?
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Accuracy in space is obtained by high order reconstruction. Several techniques can be adopted to obtain high order, still avoiding spurious oscillations. They all destroy translation invariance.

# Lack of conservation of higher order schemes

In the various reconstructions:

- schemes with linear weights are high order, conservative, but do not prevent oscillations
- schemes with non-linear weights (limiters switched on): non-oscillatory but conservation is lost.

Two strategies to restore conservation in SL schemes:

- Conservative correction (S.B. et all, Commun. Comput. Phys. Vol 29. No 1, pp 1-56, 2021)
- Conservative SL reconstruction

First approach has been used to construct conservative schemes. However it presents stability problems, severe CFL restriction.

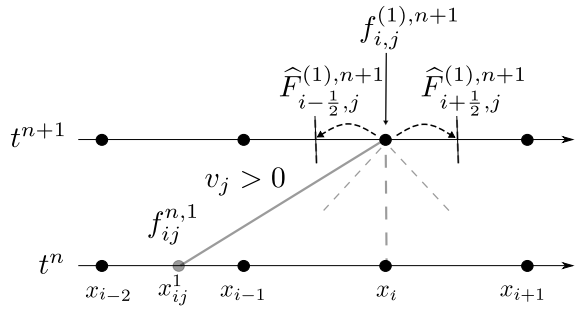
# Conservative correction (first order)

Strategy:

1) We use the discrete Maxwellian, introduced by Mieussens (2000).

2) Conservative correction procedure.

Based on writing $v\partial_x f\big|_{x=x_i} = \left(\widehat{F}_{i+1/2} - \widehat{F}_{i-1/2}\right)/\Delta x$




Representation of the first order scheme.
Black circles: grid nodes, grey circles: interpolation is needed.
Flux values at cell edges are reconstructed from the values at the center

# Conservation error in Sod problem

| $L_1$ relative error | BDF3 | | |
|---|---|---|---|
| $(N_x = 1000, N_v = 30, CFL = 2)$ | Mass | Momentum | Energy |
| Conservative BDF3+W35+DM | 1.57e-13 | 1.06e-13 | 3.68e-12 |
| BDF3+W35+DM | 3.44e-04 | 0.0020 | 0.0010 |

Table: $Kn = 10^{-6}$, Conservation error of discrete moments for Sod test.

Remark Compared to the non-conservative SL schemes, scheme based on conservative correction has severe *CFL* restriction.
In some cases BDF2 and BDF3 require CFL less than 0.45 and 0.35.

# Conservative reconstruction

New *conserv. recon.*, $\Rightarrow$ conservative SL scheme *with no CFL restrictions*.

Example Assume we know cell averages $\bar{u}_i$ of a piecewise smooth function $u(x)$.
Let $u_i(x)$ be its conservative polynomial reconstruction in interval $I_i$ (e.g.CWENO). For a parabola we have:

$$u_i(x) = u_i + u_i'(x - x_i) + \frac{1}{2}u_i''(x - x_i)^2$$

with $u_i, u_i', u_i''$ suitable approximation of the pointwise value of $u$ and its derivatives at cell center.
We want to compute a conservative cell average centered at $x_{i+\theta} := x_i + \theta\Delta x$, $\theta \in [0, 1)$.

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Cho, S. Y., Boscarino, S., Russo, G., Yun, S. B. (2021). Conservative semi-Lagrangian schemes for kinetic equations Part I: Reconstruction. Journal of Computational

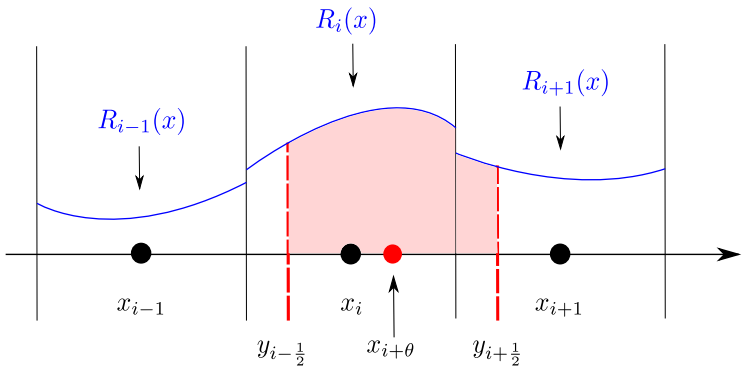
- Generalizing. Given point-wise values $u_i$ on grid points $x_i$, compute a conservative polynomial reconstruction for each cell $I_i = [x_i - \Delta x/2, x_i + \Delta x/2]$:

$$R_i(x) = \sum_{\ell=0}^{k} \frac{R^{(\ell)}}{\ell!}(x - x_i)^\ell$$

  where $R_i^\ell$ is the approximation of the $\ell$-th derivative of $u$, $u^{(\ell)}(x_i)$

- This yields a conservative reconstruction on the spatial domain $R(x) = \sum_i R_i(x)\chi_i(x)$.
- For any $\theta \in [0, 1)$ approximate $\bar{u}(x_i + \theta\Delta x) \approx Q(x_i + \theta\Delta x) := 0$

We integrate in the interval $[y_{i-\frac{1}{2}}, y_{i+\frac{1}{2}}] = [x_{i+(\theta-1/2)\Delta x}, x_{i+(\theta+1/2)\Delta x}]$ whose center is $x_{i+\theta\Delta x}$.




$$\bar{u}(x_{j+\theta}) \approx Q(x_{j+\theta})$$

$$Q(x_{j+\theta}) = \frac{1}{\Delta x} \int_{x_{i+\theta-1/2}}^{x_{i+\theta+1/2}} R_i(x)dx$$

$$Q(x_{j+\theta}) = \frac{1}{\Delta x} \int_{x_{i+\theta-1/2}}^{x_{i+1/2}} R_i(x)dx + \frac{1}{\Delta x} \int_{x_{i+1/2}}^{x_{i+1/2+\theta}} R_i(x)dx$$

# Representation

Integrating from $y_{i-1/2}$ to $y_{i+1/2}$ one obtains

$$Q_{j+\theta} = \frac{1}{\Delta x}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} u_j(x)dx = (1-\theta)u_j + \theta u_{j+1} + \frac{\theta(1-\theta)}{2}(u_j' - u_{j+1}')\Delta x$$
$$+ \frac{1}{24}\Big((1-q(\theta))u_j'' + q(\theta)u_{j+1}''\Big)(\Delta x)^2$$

where $q(\theta) := 3\theta - 6\theta^2 + 4\theta^3$.
Such formulas can be generalized to arbitrary order:

$$Q_{i+\theta} := \sum_{\ell=0}^{k}(\Delta x)^\ell \left(\alpha_\ell(\theta)R_i^{(\ell)} + \beta_\ell(\theta)R_{i+1}^{(\ell)}\right),$$

where $R_i^{(\ell)}$ is the non oscillatory reconstruction of $d^\ell u(x_i)/dx^\ell$, and

$$\alpha_\ell(\theta) = \frac{1-(2\theta-1)^{\ell+1}}{2^{\ell+1}(\ell+1)!}, \quad \beta_\ell(\theta) = \frac{(2\theta-1)^{\ell+1} - (-1)^{\ell+1}}{2^{\ell+1}(\ell+1)!}.$$

Then $Q_{i+\theta}$ denotes the approximation of $\bar{u}(x)$ on $x = x_j + \theta\Delta x$.

- The approximation is non-oscillatory by construction.
- For periodic BC one has
  $\sum_i Q_{i+\theta}$ is independent of $\theta$, $\Rightarrow$ All (global) moments are conserved.
- The same reconstruction from cell averages to cell averages can be used in the framework of finite difference to go from point-wise values to point-wise values (C.W. Shu).

# Conservation error of discrete moments

| $L_1$ relative error | RK3+W35+DM | | |
|---|---|---|---|
| $(N_x, N_v)$ | Mass | Momentum | Energy |
| (160,24) | 2.09e-07 | 7.77e-05 | 9.00e-07 |
| (640,24) | 2.04e-12 | 1.03e-09 | 9.43e-12 |
| (640,60) | 2.19e-12 | 9.90e-10 | 8.96e-12 |

Table: $Kn = 10^{-0}$, Conservation error of discrete moments for Test 1

| $L_1$ relative error | RK3+ Cons.Recon.+DM | | |
|---|---|---|---|
| $(N_x, N_v)$ | Mass | Momentum | Energy |
| (160,24) | 8.88e-15 | 5.54e-13 | 8.85e-15 |
| (640,24) | 4.29e-14 | 4.54e-12 | 3.81e-14 |
| (640,60) | 3.50e-14 | 4.92e-12 | 4.43e-14 |

Table: $Kn = 10^{-0}$, Conservation error of discrete moments for Test 1

| $L_1$ relative error | BDF3 | | |
|---|---|---|---|
| $(N_x = 1000, N_v = 30, CFL = 2)$ | Mass | Momentum | Energy |
| Conservative BDF3+W35+DM | 1.57e-13 | 1.06e-13 | 3.68e-12 |
| BDF3+New+DM | 8.51e-13 | 5.14e-13 | 2.97e-12 |
| BDF3+W35+DM | 3.44e-04 | 0.0020 | 0.0010 |

Table: $Kn = 10^{-6}$, Conservation error of discrete moments for Test 3.

## Remark 4.1

1. *This scheme is conservative even with small number of spatial grids*
2. *The conservative reconstruction can be extended to more dimensions*
3. *Applications to the Vlasov-Poisson system and the BGK model of rarefied gas dynamics:*
   *Cho, S. Y., Boscarino, S., Russo, G., Yun, S. B. (2021). Conservative semi-Lagrangian schemes for kinetic equations Part II: Applications. Journal of Computational Physics.*
4. *As in the case of the non-conservative Semi-Lagrangian schemes, we can use CFL $>$ 4 for various Knudsen numbers.*

# Vlasov-Poisson equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{E}(\mathbf{x}, t) \cdot \nabla_{\mathbf{v}} f = 0, \tag{5.1}$$

and

$$\mathbf{E}(\mathbf{x}, t) = -\nabla_{\mathbf{x}} \phi(\mathbf{x}, t), \quad -\Delta_{\mathbf{x}} \phi(\mathbf{x}, t) = \rho(\mathbf{x}, t) - m, \tag{5.2}$$

$f(\mathbf{x}, \mathbf{v}, t)$: the electron number density in phase space, $\mathbf{E}$: electric field, $\phi$: self-consistent electrostatic potential.
Charge density, $\rho(t, \mathbf{x}) = \int_{\mathbb{R}^{d_v}} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$, $d_v$: dimension in $\mathbf{v}$.
$m$ the ion charge density assumed to be uniformly distributed on the background. 1-D in $\mathbf{x}$ and 1-D in $\mathbf{v}$. Periodic BC in $x$, zero BC at $v$-boundary.

# Conserved quantities

1. Maximum principle:
   $0 \leq f(x, v, t) \leq M, \quad \forall t > 0, \quad \text{provided} \quad 0 \leq f_0(x, v) \leq M.$
2. Conservation of total mass:
   $$\frac{d}{dt} \int_{\mathbb{R}^{d_v}} \int_{\mathbb{R}^{d_x}} f(x, v, t) dx dv = 0.$$
3. Conservation $L^p$ norm $1 \leq p < \infty$:
   $$\|f\|_p = \left( \int_{\mathbb{R}}^{d_v} \int \mathbb{R}^{d_x} |f(x, v, t)|^p dx dv \right)^{\frac{1}{p}}.$$
4. Conservation of energy:
   $$\text{Energy} = \int_{\mathbb{R}^{d_v}} \int_{\mathbb{R}^{d_x}} f(x, v, t) \frac{|v|^2}{2} dx dv + \int_{\mathbb{R}^{d_x}} \frac{E^2(x, t)}{2} dx, \qquad (5.3)$$
5. Conservation entropy:
   $$\text{Entropy} = \int_{\mathbb{R}^{d_v}} \int_{\mathbb{R}^{d_x}} f \log(f) \, dx dv. \qquad (5.4)$$

# Characteristic formulation

Semi Lagrangian methods for VP system

$$\begin{cases} \dfrac{dX}{dt}(t; x, v, t^{n+1}) = V(t; x, v, t^{n+1}), \\ \dfrac{dV}{dt}(t; x, v, t^{n+1}) = E(t, X(t; x, v, t^{n+1})) \end{cases} \tag{5.5}$$

with $(X(t; x, v, t^{n+1}), V(t; x, v, t^{n+1}))$ a characteristic curve which takes the value $(x, v)$ at time $t^{n+1}$. Since the distribution function of the VP system is constant along the particle trajectories, we have

$$f(x, v, t^{n+1}) = f(X(t; x, v, t^{n+1}), V(t; x, v, t^{n+1})). \tag{5.6}$$

To update the solution in this way one has to perform a *shift* in both space and velocity. By adopting a splitting approach, a combination of separate *shifts* in the $x$ and $v$ direction is performed.

Operator splitting is adopted to obtain high order accuracy in time, and the conservative reconstruction that preserves the maximum and minimum of the function is used.
Splitting methods are besed solving separately:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = 0 \quad \text{trasport in space}$$

$$\frac{\partial f}{\partial t} + \mathbf{E}(\mathbf{x}, t) \cdot \nabla_{\mathbf{v}} f = 0, \text{drift in velocity}$$

each equation can be solved along the characteristics.

1. transport step over a time step $\tau > 0$:
   $f(x, v, t + \tau) = e^{t\mathcal{T}} f(x, v, t) = f(x - v\tau, v, t)$
2. Drift step over a time step $\tau > 0$:
   $f(x, v, t + \tau) = e^{t\mathcal{U}} f(x, v, t) = f(x - vE(x, t)\tau, v, t)$

where we denoted by $e^{t\mathcal{T}}$ and $e^{t\mathcal{U}}$ respectively the operators representing a shift along the $x$-axis, and a shift along then $v$-axis.

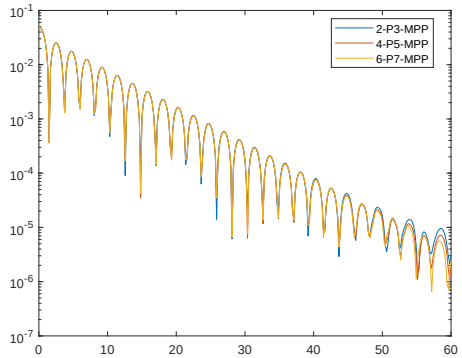
# 1D Long time simulation

Time invariants: $L^p$-norms of the solution total energy and entropy, that should remain constant in time.
We consider two benchmark problems with the following initial data:

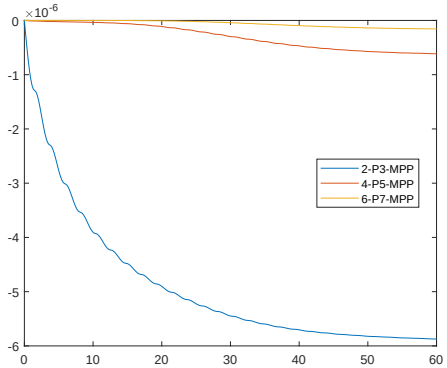
$$f(x, v, 0) = \frac{1}{\sqrt{2\pi}} \left(1 + \alpha \cos(kx)\right) \exp\left(-\frac{v^2}{2}\right),$$

where we use $(\alpha, k) = (0.01, 0.5)$ for *weak Landau damping*, and $(\alpha, k) = (0.5, 0.5)$ for *strong Landau damping*.
For both problems, we impose periodic boundary condition on the physical domain $[-2\pi, 2\pi]$ and zero-boundary condition on velocity domain $[-2\pi, 2\pi]$. Numerical solutions are computed up to final time $t_f = 60$ with a time step determined by CFL$= 6$. The grid size is $N_x = 64$ and $N_v = 128$.

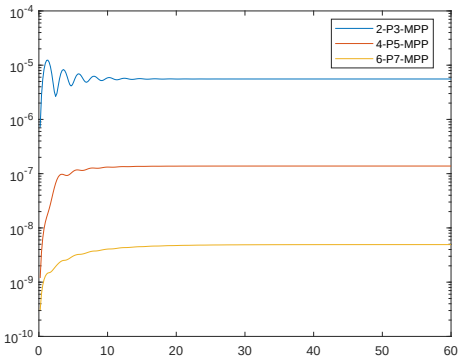
## Weak Landau damping in the 1D Vlasov Poisson. $N_x = 64$, $N_v = 128$



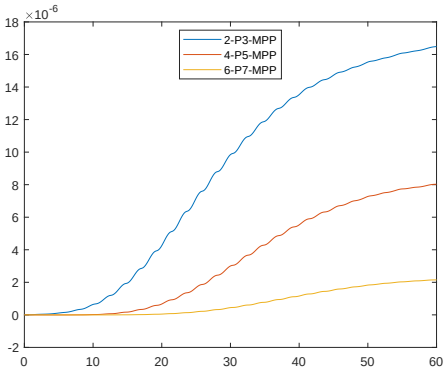

(a) $L^2$-norm of $E$




(b) $\|f^n\|_2 - \|f^0\|_2$

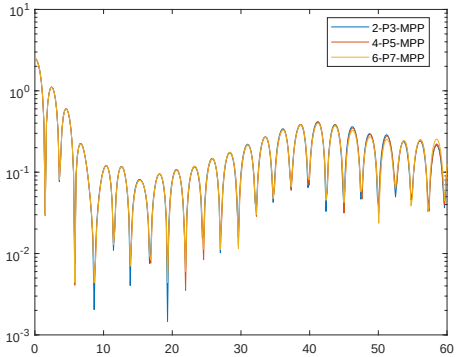



(c) $\left|\text{Energy}(t) - \text{Energy}(0)\right|$

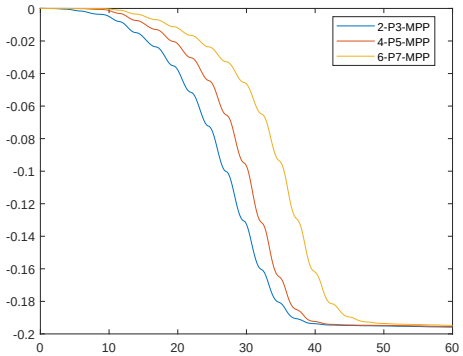



(d) $\text{Entropy}(t) - \text{Entropy}(0)$

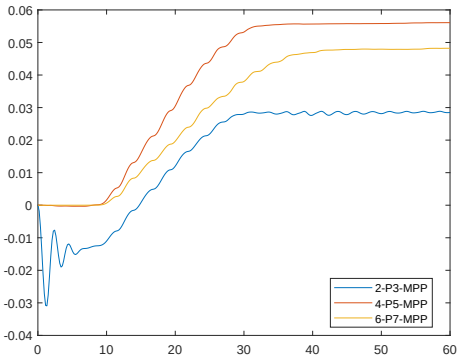
Strong Landau damping in the 1D Vlasov Poisson. $N_x = 64$, $N_v = 128$.



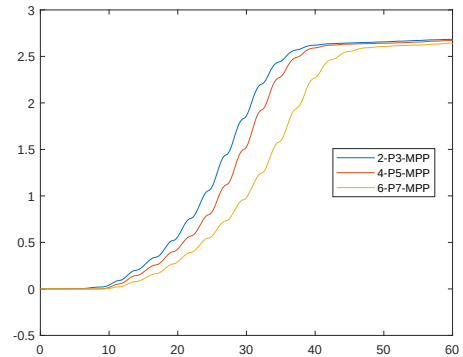

(a) $L^2$-norm of $E$




(b) $\|f^n\|_2 - \|f^0\|_2$




(c) Energy$(t)$−Energy$(0)$




(d) Entropy$(t)$−Entropy$(0)$

# Outline

# Boltzman equation for inert gas mixtures

- The distribution functions of $L$-species inert gases:

$$\{f_s(x, \mathrm{v}, t),\ s = 1, \cdots, L\}$$

defined on $(x, v) \in \mathbb{R}^3 \times \mathbb{R}^3$ at time $t > 0$.

- Boltzmann-type equations for inert gas mixtures:

$$\frac{\partial f_s}{\partial t} + \mathrm{v} \cdot \nabla_x f_s = Q_s, \quad s = 1, \cdots, L,$$

where the collision operator $Q_s$ for $s$-species gas is

$$Q_s = \sum_{k=1}^{L} Q_{sk}(f_s, f_k).$$

The binary collision operator $Q_{sk}$ is defined by

$$Q_{sk}(f_s, f_k) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} d\mathrm{w}\, d\omega\, g_{sk}(|y|, \hat{y} \cdot \omega) \Big[ f_s(\mathrm{v}') f_k(\mathrm{w}') - f_s(\mathrm{v}) f_k(\mathrm{w}) \Big],$$

where $g_{sk}$ is a collision kernel.

In S.B. S-Y- Cho, M. Groppi, G. Russo *BGK Models for inert mixtures: comparison and applications*, Kinetic and Related Models, 2021
The authors briefly recall the three different BGK models for Boltzman equation for inert gas mixtures which have been compared in their kinetic behaviour and then versus the hydrodynamic limits.

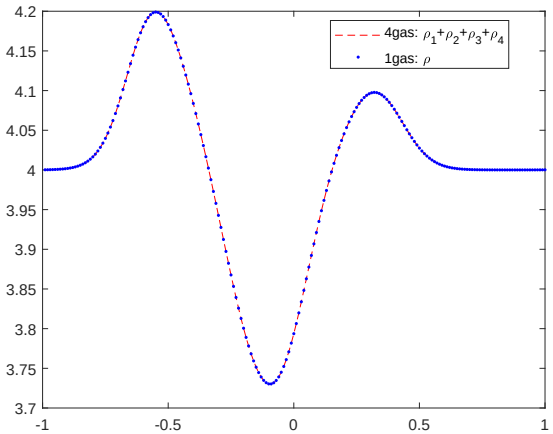
- The BGK model of Andries, Aoki and Perthame (AAP model);
- The BGK model preserving global conservations (GS model) by M. Bisi, M. Groppi and G. Spiga;
- A general consistent BGK model for inert gas mixtures (BBGSP model) by A. V. Bobylev, M. Bisi, M. Groppi, G. Spiga and I. F. Potapenko)

Here we used a conservative semi-Lagrangian method. For the time discretization, we consider an implicit Runge-Kutta method (DIRK) and a backward difference formula (BDF).

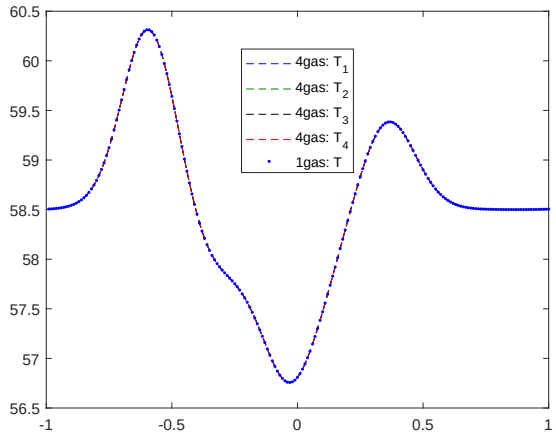
In S.B. S-Y- Cho, M. Groppi, G. Russo *Conservative Semi-Lagrangian Schemes for a general consistent BGK model for inert gas mixtures*, Commun. Math. Sci. 2022
High order conservative semi-Lagrangian scheme fulfills indifferentiability principle and Asymptotic Preserving (AP) property which allows to capture the behavior of hydrodynamic limit models.
**Indifferentiability Principle**: The sum of distribution function $f = \sum_{s=1}^{L} f_s$ obeys the single gas Boltzmann equation if all $m_s$ and collision kernel $g_{sk}$ are identical.

# Indifferentiability principle

BDF3-QCWENO35 for $\varepsilon = 10^{-2}$




(a) Density



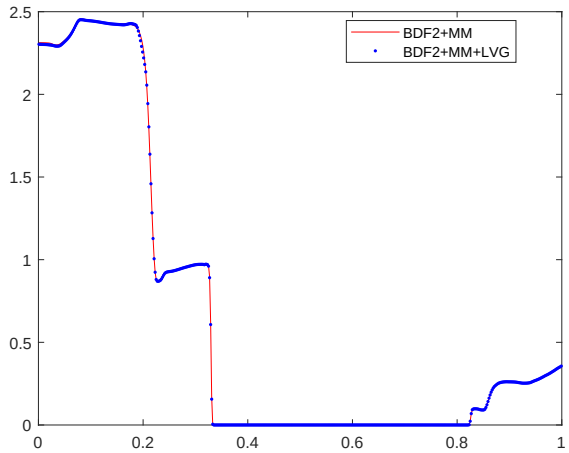

(b) Temperature

# Local Velocity

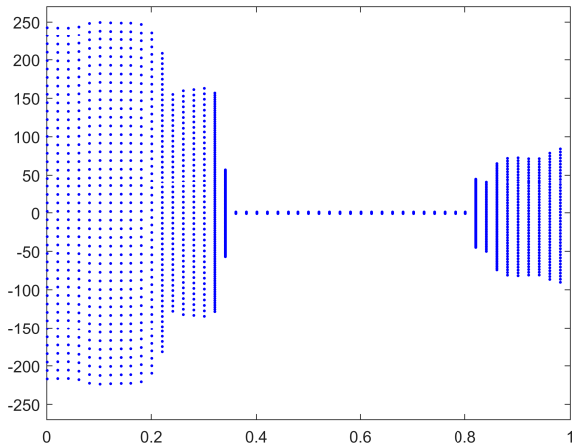
S.B. S.-Y- Cho, G. Russo *A local velocity grid conservative semi-Lagrangian schemes for BGK model*, J. Comput. Phys. 2022
In this paper, we propose a velocity adaptation technique in the semi-Lagrangian framework for BGK model. The velocity grid will be set locally in time and space, according to mean velocity and temperature.
**Motivation:**

- When dealing with high Mach number problems, where large variation of mean velocity and temperature are present in the domain under consideration, the computational cost and memory allocation requirements become prohibitively large.
- Simply applying a local velocity grid approach to the SL schemes may not be conservative.

# Two interacting blast waves




(a) Temperature




(b) Grid points at final time

Figure: Two interacting blast waves. For BDF2+MM scheme we use $N_v = 3800$ for each spatial node, while for a local velocity grid approaches we take an average of $N_v = 45$. We take $\varepsilon = \tau := CT^{\omega}/\rho$ with $C = 1.08 \times 10^{-9}$ as used in [Brull, 2014][1].

[1] Brull, S., Mieussens, L. (2014). Local discrete velocity grids for deterministic rarefied flow simulations. Journal of Computational Physics, 266, 22-46.

# Conclusions

- SL schemes with implicit treatment of collision seem suitable to solve BGK.
- Large time steps can be used, independently on the Knudsen number.
- Conservation is important if we want to have AP schemes for the fluid dynamic limit.
- Two strategies are proposed: conservative correction and conservative SL reconstruction
- Fluid dynamic limit is captured with relatively small number of points in velocity.
- The technique can be adopted to construct conservative SL schemes for the BGK equation, Vlasov-Poisson and other transport equations with similar structure, obtaining better conservation properties.

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Acknowledgments to the PRIN 2017 project

1. Cho, S. Y., B. S., Russo, G., Yun, S. B. *Conservative semi-Lagrangian schemes for kinetic equations Part I: Reconstruction*. J. of Comp. Phys. 2021
2. Cho, S. Y., B. S., Russo, G., Yun, S. B. *Conservative semi-Lagrangian schemes for kinetic equations Part II: Applications*. J. Comput. Phys. 2021
3. S.B. S-Y- Cho, M. Groppi, G. Russo *BGK Models for inert mixtures: comparison and applications*, Kinetic and Related Models, 2021
4. In S.B. S-Y- Cho, M. Groppi, G. Russo *Conservative Semi-Lagrangian Schemes for a general consistent BGK model for inert gas mixtures*, Commun. Math. Sci. 2022
5. S.B. S.-Y- Cho, G. Russo *A local velocity grid conservative semi-Lagrangian schemes for BGK model*, J. Comput. Phys. 2022