Pseudospectral Finite Difference methods for the Vlasov-Dougherty-Fokker-Planck Equation

Jack Coughlin

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Here we're interested in numerical methods for the equation

$$\partial_t f_\alpha + v \cdot \nabla_x f_\alpha + (E + v \times B) \cdot \nabla_v f_\alpha = \nu_{\alpha\beta} \nabla_v \cdot \left(\frac{T_{\alpha\beta}}{m_\alpha} \nabla_v f + (v - u_{\alpha\beta}) f \right). \tag{1}$$

1 Two-D Two-V

1.1 Fourier discretization in y

We consider periodic domains in y, so that $f(x, y, v_x, v_y) = f(x, y + L, v_x, v_y)$ where L is the domain length. For the periodic direction we propose a pseudospectral Fourier discretization. That is, we look for solutions of the form

$$\begin{aligned} f(x, y, v_x, v_y, t) &= \hat{f}_{k_y}(x, v_x, v_y, t) \sum_{k_y=0}^{N_y-1} e^{2\pi i k_y y / L_y} = \hat{\boldsymbol{f}}(x, v_x, v_y, t)^T \boldsymbol{\phi}(y) \\ E(x, y, t) &= \hat{E}_{k_y}(x, t) \sum_{k_y=0}^{N_y-1} e^{2\pi i k_y y / L_y} = \hat{\boldsymbol{E}}(x, t)^T \boldsymbol{\phi}(y) \end{aligned}$$

so that the wavenumber k_y ranges from 0 to $N_y - 1$.

We ask that (1) is satisfied at a uniform grid of collocation points y_i. The y derivative is to be evaluated pseudospectrally by a Fourier transform to $\hat{f}_{k_y}$, followed by multiplication by $\frac{2\pi i k_y}{L_y}$, followed by an inverse Fourier transform. The nonlinear terms are to be evaluated as follows:

- For a quadratic nonlinearity, first perform the Fourier transform of both factors, then pad the matrix of coefficients with zeros up to $2N_y$. Then transform back to physical space and perform the multiplication pointwise. Then perform another Fourier transform and truncate the result down to N_y modes. Finally, transform back to physical space.
- For a cubic nonlinearity, do the same but with padding up to $3N_y$.

This amount of padding is potentially wasteful, likely you only need 2/3rds this amount (Orszag).

1.2 Finite difference discretization in x, v_x, v_y

We now describe the finite difference discretization of the other dimensions. Each dimension x, v_x, v_y is discretized on a uniform Cartesian grid, with collocation points at cell centers.

$$x \in [a, b], \quad \Delta x = \frac{b - a}{N_x}, \quad x_i = a + i\frac{\Delta x}{2} - \frac{\Delta x}{2}$$

The cell faces are at $x_{i+1/2}$.

1.2.1 Velocity-space Laplacian

The operator ∇_v^2 is discretized using a sixth-order centered finite difference stencil:

$$(\partial_{v_x}^2 f)_i = \frac{f_{i-3}/90 - 3f_{i-2}/20 + 3f_{i-1}/2 - 49f_i/18 + 3f_{i+1}/2 - 3f_{i+2}/20 + f_{i+3}/90}{\Delta v_x^2}.$$

All ghost cells in velocity space are set to zero.

1.2.2 WENO discretization of hyperbolic terms

We discretize a flux term in conservation form,

$$\partial_x F(u)_i = \frac{1}{\Delta x}(\hat{F}_{i+1/2} - \hat{F}_{i-1/2}).$$

The flux is first split into positive (right-going) and negative (left-going) parts, according to the sign of the flux coefficient.

Left-biased stencil: To estimate $u_{i+1/2}$ from $u_{i-2}, u_{i-1}, u_i, u_{i+1}, u_{i+2}$, which are each cell averages over the respective cells, we follow the procedure described in [**?**]. First, form the polynomials

$$\begin{aligned}
P_1(x) &= \mathcal{I}[(x_{i-5/2}, 0), (x_{i-3/2}, u_{i-2}), (x_{i-1/2}, u_{i-2} + u_{i-1}), (x_{i+1/2}, u_{i-2} + u_{i-1} + u_i)] \\
P_2(x) &= \mathcal{I}[(x_{i-3/2}, 0), (x_{i-1/2}, u_{i-1}), (x_{i+1/2}, u_{i-1} + u_i), (x_{i+3/2}, u_{i-1} + u_i + u_{i+1})] \\
P_3(x) &= \mathcal{I}[(x_{i-1/2}, 0), (x_{i+1/2}, u_i), (x_{i+3/2}, u_i + u_{i+1}), (x_{i+5/2}, u_i + u_{i+1} + u_{i+2})].
\end{aligned}$$

Then the 3-wide stencil approximations are

$$u_{i+1/2}^{(1)} = P_1'(x_{i+1/2}) = \frac{u_{i-2}}{3} - \frac{7u_{i-1}}{6} + \frac{11u_i}{6}, \quad u_{i+1/2}^{(2)} = P_2'(x_{i+1/2}) = \frac{-u_{i-1}}{6} + \frac{5u_i}{6} + \frac{u_{i+1}}{3},$$

$$u_{i+1/2}^{(3)} = P_3'(x_{i+1/2}) = \frac{u_i}{3} + \frac{5u_{i+1}}{6} - \frac{u_{i+2}}{6}.$$

The 5-wide reconstruction polynomial is given by the first-derivative of

$$\begin{aligned}
P(x) = \mathcal{I}[&(x_{i-5/2}, 0), (x_{i-3/2}, u_{i-2}), (x_{i-1/2}, u_{i-2} + u_{i-1}), (x_{i+1/2}, u_{i-2} + u_{i-1} + u_i), \\
&(x_{i+3/2}, u_{i-2} + u_{i-1} + u_i + u_{i+1}), (x_{i+5/2}, u_{i-2} + u_{i-1} + u_i + u_{i+1} + u_{i+2})]
\end{aligned}$$

and is

$$\begin{aligned}
u_{i+1/2} = P'(x_{i+1/2}) &= \frac{u_{i-2}}{30} - \frac{13u_{i-1}}{60} + \frac{47u_i}{60} + \frac{9u_{i+1}}{20} - \frac{u_{i+2}}{20} \\
&= \gamma_1 u_{i+1/2}^{(1)} + \gamma_2 u_{i+1/2}^{(2)} + \gamma_3 u_{i+1/2}^{(3)},
\end{aligned}$$

where the linear weights are

$$\gamma_1 = \frac{1}{10}, \quad \gamma_2 = \frac{3}{5}, \quad \gamma_3 = \frac{3}{10}.$$

The smoothness indicators are given by

$$\beta_j = \sum_{l=1}^{k} \Delta x^{2l-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\frac{d^l}{dx^l} p_j(x) \right)^2 \mathrm{d}x,$$

and are

$$\begin{aligned}
\beta_1 &= \frac{13}{12}(u_{i-2} - 2u_{i-1} + u_i)^2 + \frac{1}{4}(u_{i-2} - 4u_{i-1} + 3u_i)^2, \\
\beta_2 &= \frac{13}{12}(u_{i-1} - 2u_i + u_{i+1})^2 + \frac{1}{4}(u_{i-1} - u_{i+1})^2, \\
\beta_3 &= \frac{13}{12}(u_i - 2u_{i+1} + u_{i+2})^2 + \frac{1}{4}(3u_i - 4u_{i+1} + u_{i+2})^2.
\end{aligned}$$

Right-biased stencil Here we use the stencil $[x_{i-1}, x_i, x_{i+1}, x_{i+2}, x_{i+3}]$ to estimate $u_{i+1/2}$. The 3-wide approximations are

$$u^{(1)}_{i+1/2} = P'_1(x_{i+1/2}) = \frac{-u_{i-1}}{6} + \frac{5u_i}{6} + \frac{u_{i+1}}{3}, \quad u^{(2)}_{i+1/2} = P'_2(x_{i+1/2}) = \frac{u_i}{3} + \frac{5u_{i+1}}{6} - \frac{u_{i+2}}{6},$$

$$u^{(3)}_{i+1/2} = P'_3(x_{i+1/2}) = \frac{11u_{i+1}}{6} - \frac{7u_{i+2}}{6} + \frac{u_{i+3}}{6}.$$

The 5-wide reconstruction estimate is

$$\begin{aligned} u_{i+1/2} &= P'(x_{i+1/2}) = -\frac{u_{i-1}}{20} + \frac{9u_i}{20} + \frac{47u_{i+1}}{60} - \frac{13u_{i+2}}{60} + \frac{u_{i+3}}{30} \\ &= \gamma_1 u^{(1)}_{i+1/2} + \gamma_2 u^{(2)}_{i+1/2} + \gamma_3 u^{(3)}_{i+1/2}, \end{aligned}$$

where the linear weights are

$$\gamma_1 = \frac{3}{10}, \quad \gamma_2 = \frac{3}{5}, \quad \gamma_3 = \frac{1}{10}.$$

The smoothness indicators, which this time are computed by integration over the interval $x_{i+1/2}, x_{i+3/2}$, are

$$\beta_j = \sum_{l=1}^{k} \Delta x^{2l-1} \int_{x_{i+1/2}}^{x_{i+3/2}} \left(\frac{d^l}{dx^l} p_j(x) \right)^2 \mathrm{d}x,$$

$$\begin{aligned} \beta_1 &= \frac{13}{12}(u_{i-1} - 2u_i + u_{i+1})^2 + \frac{1}{4}(u_{i-1} - 4u_i + 3u_{i+1})^2 \\ \beta_2 &= \frac{13}{12}(u_i - 2u_{i+1} + u_{i+2})^2 + \frac{1}{4}(u_i - u_{i+2})^2, \\ \beta_3 &= \frac{13}{12}(u_{i+1} - 2u_{i+2} + u_{i+3})^2 + \frac{1}{4}(3u_{i+1} - 4u_{i+2} + u_{i+3})^2. \end{aligned}$$

1.3 Lorentz force flux

For each point (x, y, z), we can compute the velocity-dependent force $E + v \times B$. For the electrostatic approximation, there is then a specific range of coordinates where the acceleration force is positive, depending only on velocity:

$$v_y : v_y B_z > -E_x, \quad v_x : v_x B_z > E_y.$$

In the electrostatic case, this will form a rectangular region of velocity space which may be iterated over efficiently.

Flux in v_x The flux is

$$df_{v_x} = -\frac{1}{\Delta v_x} \left(\hat{F}^+_{i+1/2} - \hat{F}^+_{i-1/2} \right),$$

where $\hat{F}^+_{i+1/2}$ is determined from the left-biased WENO reconstruction procedure.

We will use the linear WENO reconstruction procedure with the linear weights, since we don't expect much "action" in velocity space so to speak. Thus,

$$F^+_{i+1/2} = \frac{F^+_{i-2}}{30} - \frac{13F^+_{i-1}}{60} + \frac{47F^+_i}{60} + \frac{9F^+_{i+1}}{20} - \frac{F^+_{i+2}}{20},$$

and

$$
\begin{aligned}
df_{v_x} &= -\frac{1}{\Delta v_x}\left(\frac{F^+_{i-2}}{30} - \frac{13F^+_{i-1}}{60} + \frac{47F^+_i}{60} + \frac{9F^+_{i+1}}{20} - \frac{F^+_{i+2}}{20}\right.\\
&\qquad \left. -\frac{F^+_{i-3}}{30} + \frac{13F^+_{i-2}}{60} - \frac{47F^+_{i-1}}{60} - \frac{9F^+_i}{20} + \frac{F^+_{i+1}}{20}\right)\\
&= -\frac{1}{\Delta v_x}\left(-\frac{F^+_{i-3}}{30} + \frac{F^+_{i-2}}{4} - F^+_{i-1} + \frac{F^+_i}{3} + \frac{F^+_{i+1}}{2} - \frac{F^+_{i+2}}{20}\right)\\
&= -\frac{1}{\Delta v_x}\left(-\frac{f_{i-3}}{30} + \frac{f_{i-2}}{4} - f_{i-1} + \frac{f_i}{3} + \frac{f_{i+1}}{2} - \frac{f_{i+2}}{20}\right)\max(E_x + v_y B_z, 0)
\end{aligned}
$$

Here, $F_i^+ = (E_x + v_y B_z) f_i$. So the positivity or negativity of the acceleration force is determined for any given set of (x, y, v_y), and we can iterate over the whole range in v_x.

Similarly, for the negative part of the acceleration flux, we have

$$
\begin{aligned}
df_{v_x} &= -\frac{1}{\Delta v_x}\left(-\frac{F^-_{i-1}}{20} + \frac{9F^-_i}{20} + \frac{47F^-_{i+1}}{60} - \frac{13F^-_{i+2}}{60} + \frac{F^-_{i+3}}{30}\right.\\
&\qquad \left. +\frac{F^-_{i-2}}{20} - \frac{9F^-_{i-1}}{20} - \frac{47F^-_i}{60} + \frac{13F^-_{i+1}}{60} - \frac{F^-_{i+2}}{30}\right)\\
&= -\frac{1}{\Delta v_x}\left(\frac{F^-_{i-2}}{20} - \frac{F^-_{i-1}}{2} - \frac{F^-_i}{3} + F^-_{i+1} - \frac{F^-_{i+2}}{4} + \frac{F^-_{i+3}}{30}\right)\\
&= -\frac{1}{\Delta v_x}\left(\frac{f_{i-2}}{20} - \frac{f_{i-1}}{2} - \frac{f_i}{3} + f_{i+1} - \frac{f_{i+2}}{4} + \frac{f_{i+3}}{30}\right)\min(E_x + v_y B_z, 0)
\end{aligned}
$$

At the boundary, we will assume $f_{-2} = f_{-1} = f_0 = 0$.

1.4 Free-streaming flux in x

For $v_x > 0$,

$$
df_x = -\frac{v_x}{\Delta x}\left(-\frac{f_{i-3}}{30} + \frac{f_{i-2}}{4} - f_{i-1} + \frac{f_i}{3} + \frac{f_{i+1}}{2} - \frac{f_{i+2}}{20}\right).
$$

When $v_x \le 0$,

$$
df_x = -\frac{v_x}{\Delta x}\left(\frac{f_{i-2}}{20} - \frac{f_{i-1}}{2} - \frac{f_i}{3} + f_{i+1} - \frac{f_{i+2}}{4} + \frac{f_{i+3}}{30}\right).
$$

1.5 Fokker-Planck collisions

The collision operator is

$$
\begin{aligned}
C(f_\alpha, f_\beta) &= \nu_{\alpha\beta} \nabla \cdot \left(v^2_{t\alpha\beta} \nabla v f_\alpha + (v - u_{\alpha\beta}) f_\alpha\right)\\
&= \frac{\nu_{\alpha\beta} T_{\alpha\beta}}{m_\alpha} \nabla \cdot \left(M_{\alpha\beta} \nabla (M^{-1}_{\alpha\beta} f_\alpha)\right).
\end{aligned}
$$

Here,

$$
v^2_{t\alpha\beta} = \frac{T_{\alpha\beta}}{m_\alpha}, \quad M_{\alpha\beta} = \left(\frac{m_\alpha}{2\pi T_{\alpha\beta}}\right)^{d/2} e^{-\frac{m_\alpha |v - u_{\alpha\beta}|^2}{2T_{\alpha\beta}}}.
$$

If we discretize both derivatives using a centered finite difference scheme of order 2, then we'll have

$$
\begin{aligned}
\partial_{v_x}(M^{-1}f)_i &= \frac{1}{\Delta v_x/2}\left(-\frac{f_{i-1/2}}{2M_{i-1/2}} + \frac{f_{i+1/2}}{2M_{i+1/2}}\right) \\
(M\partial_{v_x}M^{-1}f)_i &= \frac{1}{\Delta v_x/2}\left(-\frac{f_{i-1/2}M_i}{2M_{i-1/2}} + \frac{f_{i+1/2}M_i}{2M_{i+1/2}}\right)
\end{aligned}
$$

$$
\begin{aligned}
\partial_{v_x}(M\partial_{v_x}(M^{-1}f)) &= \frac{1}{\Delta v_x/2}\left(-\frac{(M\partial_{v_x}(M^{-1}f))_{i-1/2}}{2} + \frac{(M\partial_{v_x}(M^{-1}f))_{i+1/2}}{2}\right) \\
&= \frac{1}{\Delta v_x^2/4}\left(\frac{f_{i-1}M_{i-1/2}}{4M_{i-1}} - \frac{f_iM_{i-1/2}}{4M_i} - \frac{f_iM_{i+1/2}}{4M_i} + \frac{f_{i+1}M_{i+1/2}}{4M_{i+1}}\right) \\
&= \frac{1}{\Delta v_x^2}\left(f_{i-1}\frac{M_{i-1/2}}{M_{i-1}} - f_i\left(\frac{M_{i-1/2}+M_{i+1/2}}{M_i}\right) + f_{i+1}\frac{M_{i+1/2}}{M_{i+1}}\right)
\end{aligned}
$$

If we discretize both derivatives using a centered finite difference scheme of order 4, then we do not get any cancellation of the fractional point values such as $f_{i-3/2}$, so we have to compose a stencil from i_{i-2} with itself, and thus end up with a stencil of width 9, which seems excessive.

$$
\begin{aligned}
\partial_{v_x}(M^{-1}f)_i &= \frac{1}{\Delta v_x/2}\left(\frac{f_{i-1}}{12M_{i-1}} - \frac{2f_{i-1/2}}{3M_{i-1/2}} + \frac{2f_{i+1/2}}{3M_{i+1/2}} - \frac{f_{i+1}}{12M_{i+1}}\right), \\
(M\partial_{v_x}(M^{-1}f))_i &= \frac{1}{\Delta v_x/2}\left(\frac{f_{i-1}M_i}{12M_{i-1}} - \frac{2f_{i-1/2}M_i}{3M_{i-1/2}} + \frac{2f_{i+1/2}M_i}{3M_{i+1/2}} - \frac{f_{i+1}M_i}{12M_{i+1}}\right).
\end{aligned}
$$

$$
\begin{aligned}
\partial_{v_x}(M\partial_{v_x}(M^{-1}f)) &= \frac{1}{\Delta v_x/2}\left[\frac{1}{12}(M\partial_{v_x}(M^{-1}f))_{i-1} - \frac{2}{3}(M\partial_{v_x}(M^{-1}f))_{i-1/2}\right. \\
&\qquad \left. + \frac{2}{3}(M\partial_{v_x}(M^{-1}f))_{i+1/2} - \frac{1}{12}(M\partial_{v_x}(M^{-1}f))_{i+1}\right] \\
&= \frac{1}{\Delta v_x^2/4}\left[\left(\frac{f_{i-2}M_{i-1}}{144M_{i-2}} - \frac{1f_{i-3/2}M_{i-1}}{18M_{i-3/2}}\right)\right]
\end{aligned}
$$

Observe that M_i/M_{i+k} is independent of v_y:

$$
\begin{aligned}
\frac{M_i}{M_{i+k}} &= \exp\left(-\frac{((v_x)_i - u)^2}{2T} + \frac{(v_x)_{i+k} - u)^2}{2T}\right) \\
&= \exp\left(\frac{1}{2T}\left[v_{i+k}^2 - v_i^2 + 2u(v_i - v_{i+k}\right]\right) \\
&= \exp\left(\frac{1}{2T}(v_{i+k} - v_i)(v_{i+k} + v_i - 2u)\right)
\end{aligned}
$$