1D electrostatic δf particle-in-cell (PIC) formulation in vector-matrix form

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1 1D Vlasov-Poisson equations

$$\begin{aligned}
\frac{\mathrm{d}f_\alpha(x,v,t)}{\mathrm{d}t} &= \partial_t f_\alpha(x,v,t) + v\partial_x f_\alpha(x,v,t) + \frac{Z_\alpha E(x,t)}{m_\alpha}\partial_v f_\alpha(x,v,t) \\
&= 0 \ , \qquad (1) \\
\partial_x E(x,t) &= 4\pi \sum_\alpha Z_\alpha n_\alpha(x,t) \ , \qquad (2) \\
n_\alpha(x,t) &\equiv \int_{-\infty}^{\infty} f_\alpha(x,v,t)\mathrm{d}v \ . \qquad (3)
\end{aligned}$$

α indicates species. f is particle distribution. Z is charge. m is mass. n is density. E is electrostatic field.

2 δf formulation

Decompose quantities into equilibrium part and perturbed part:

$$\begin{aligned}
f_\alpha &= f_{0\alpha} + \delta f_\alpha \ , \qquad (4) \\
n_\alpha &= n_{0\alpha} + \delta n_\alpha \ , \qquad (5) \\
n_{0\alpha} &\equiv \int_{-\infty}^{\infty} f_{0\alpha}\mathrm{d}v \ , \qquad (6) \\
\delta n_\alpha &\equiv \int_{-\infty}^{\infty} \delta f_\alpha \mathrm{d}v \ . \qquad (7)
\end{aligned}$$

Note that equilibrium electrostatic field is zero, E is perturbed field.

Although now multiple options for equilibrium distribution are implemented in `PIC1D-PETSc`, here for simplicity, Maxwellian is taken, which is time-independent and uniform in x:

$$f_{0\alpha} = f_{0\alpha}(v) = \frac{n_{0\alpha}}{\sqrt{2\pi v_{\mathrm{th},\alpha}^2}} \exp\left(\frac{v^2}{2v_{\mathrm{th},\alpha}^2}\right) , \tag{8}$$

$$v_{\mathrm{th},\alpha} \equiv \frac{T_\alpha}{m_\alpha} , \tag{9}$$

$$\partial_t f_{0\alpha} = 0 , \tag{10}$$

$$\partial_x f_{0\alpha} = 0 . \tag{11}$$

δf formulation:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\delta f_\alpha &= -\frac{\mathrm{d}}{\mathrm{d}t} f_{0\alpha} \\ &= -\frac{Z_\alpha}{m_\alpha} E \partial_v f_{0\alpha} , \end{aligned} \tag{12}$$

$$\partial_x E = 4\pi \sum_\alpha Z_\alpha \, \delta n_\alpha . \tag{13}$$

3 δf particle-in-cell (PIC) formulation

Physical particle distribution is carried by marker particles. Each marker particle carries 4 quantities in this case: x, v, p and w. Marker particle equilibrium weight p and perturbed weight w are defined as:

$$p \equiv \frac{f_{0\alpha}}{g_\alpha} , \tag{14}$$

$$w \equiv \frac{\delta f_\alpha}{g_\alpha} , \tag{15}$$

$$\tag{16}$$

where g is marker particle distribution function:

$$g_\alpha(x, v, t) = \sum_{j_\alpha=1}^{N_\alpha} S_x(x - x_{j_\alpha}) S_v(v - v_{j_\alpha}) . \tag{17}$$

N_α is number of marker particles for species α. j_α is marker particle index. x_{j_α} and v_{j_α} are position and velocity of the j_α-th marker particle, respectively. S_x and S_v are shape functions in x and v, respectively. In this PIC formulation, take S_v to be Dirac δ function and S_x to be hat function:

$$S_v(v - v_{j_\alpha}) = \delta(v - v_{j_\alpha}) \ , \tag{18}$$

$$S_x(x - x_{j_\alpha}) = \begin{cases} \frac{h_x - |x - x_{j_\alpha}|}{h_x^2} & |x - x_{j_\alpha}| < h_x \\ 0 & \text{otherwise} \end{cases} \ , \tag{19}$$

where h_x is grid size in x.

Physical particle distribution functions are given by:

$$f_\alpha(x, v, t) = \sum_{j_\alpha=1}^{N_\alpha} p_{j_\alpha} S_x(x - x_{j_\alpha}) S_v(v - v_{j_\alpha}) \ , \tag{20}$$

$$\delta f_\alpha(x, v, t) = \sum_{j_\alpha=1}^{N_\alpha} w_{j_\alpha} S_x(x - x_{j_\alpha}) S_v(v - v_{j_\alpha}) \ . \tag{21}$$

Note that for Maxwellian:

$$\frac{\partial_v f_{0\alpha}}{f_{0\alpha}} = -\frac{v}{v_{\text{th},\alpha}^2} = -\frac{v}{T_\alpha / m_\alpha} \ . \tag{22}$$

δf PIC formulation:

$$\frac{\mathrm{d}x_{j_\alpha}}{\mathrm{d}t} = v_{j_\alpha} \ , \tag{23}$$

$$\frac{\mathrm{d}v_{j_\alpha}}{\mathrm{d}t} = \frac{Z_\alpha}{m_\alpha} E(x_{j_\alpha}) \ , \tag{24}$$

$$\frac{\mathrm{d}p_{j_\alpha}}{\mathrm{d}t} = 0 \ , \tag{25}$$

$$\begin{aligned} \frac{\mathrm{d}w_{j_\alpha}}{\mathrm{d}t} &= -(p_{j_\alpha} - w_{j_\alpha}) \frac{Z_\alpha}{m_\alpha} E(x_{j_\alpha}) \frac{\partial_v f_{0\alpha}}{f_{0\alpha}} \\ &= (p_{j_\alpha} - w_{j_\alpha}) \frac{Z_\alpha}{T_\alpha} E(x_{j_\alpha}) v_{j_\alpha} \ , \end{aligned} \tag{26}$$

$$\partial_x E(x_{j_x}) = 4\pi \sum_\alpha \sum_{j_\alpha} w_{j_\alpha} S_x(x_{j_x} - x_{j_\alpha}) \ , \tag{27}$$

$$E(x_{j_\alpha}) = \sum_{j_x=0}^{N_x - 1} E(x_{j_x}) S_x(x_{j_x} - x_{j_\alpha}) h_x \ . \tag{28}$$

j_x is index for grids in x. Note that j_x starts from 0 for convenience to write the discrete Fourier transform (DFT) equations in the next paragraph.

In this model, x is periodic and the box size is l. Eq. (27) is solved by spectral method. The charge density is given by:

$$\rho(x_{j_x}) = \sum_{\alpha} \sum_{j_\alpha} w_{j_\alpha} S_x(x_{j_x} - x_{j_\alpha}) \ . \tag{29}$$

Fourier expand charge density and electrostatic field:

$$\left\{ \begin{array}{c} \rho(x_{j_x}) \\ E(x_{j_x}) \end{array} \right\} = \sum_{j_k=0}^{N_x-1} \left\{ \begin{array}{c} \rho_{j_k} \\ E_{j_k} \end{array} \right\} \exp\left(i \frac{2\pi}{N_x} j_k j_x \right) \ . \tag{30}$$

The Fourier component coefficients are given by (DFT):

$$\left\{ \begin{array}{c} \rho_{j_k} \\ E_{j_k} \end{array} \right\} = \frac{1}{N_x} \sum_{j_k=0}^{N_x-1} \left\{ \begin{array}{c} \rho(x_{j_x}) \\ E(x_{j_x}) \end{array} \right\} \exp\left(-i \frac{2\pi}{N_x} j_k j_x \right) \ . \tag{31}$$

Plug Eqs. (29) and (30) into Eq. (27) and consider the orthogonality of Fourier harmonics to get:

$$i \frac{2\pi}{l} j_k E_{j_k} = 4\pi \rho_{j_k} \ , \tag{32}$$

$$E_{j_k} = -i \frac{l}{2\pi j_k} 4\pi \rho_{j_k} \ . \tag{33}$$

4 Normalization

In `PIC1D-PETSc`, charge is normalized by proton charge e. Mass is normalized by electron mass m_e. Temperature is normalized by electron temperature T_e. Time is normalized by the reciprocal of electron oscillation frequency $1/\omega_\mathrm{pe}$. Length (l or x) is normalized by electron Debye length λ_De. As a result, velocity is normalized by electron thermal velocity $v_\mathrm{th,e}$. Physical particle distribution function (f or δf) is normalized by electron density over thermal velocity $n_\mathrm{0e}/v_\mathrm{th,e}$. Physical particle density (δn) is normalized by electron density n_0e. Electrostatic field is normalized by $T_\mathrm{e}/(e\lambda_\mathrm{De})$.

The normalized equations have the same form as described in Sec. 3, except that the Poisson equation Eqs. (27), (32) and (33) no longer have the 4π coefficient.

5 Vector-matrix form of δf PIC formulation

As this is a 1D model, all physical quantities are scalars. All vectors mentioned in this section are mathematical vectors. For each species, all particles' x coordinates form a vector of size N_α:

$$\boldsymbol{x}_\alpha \equiv \begin{bmatrix} x_{1,\alpha} \\ x_{2,\alpha} \\ \vdots \\ x_{j_\alpha} \\ \vdots \\ x_{N_\alpha} \end{bmatrix} . \tag{34}$$

Similarly, velocities and weights form vectors of $\boldsymbol{v}_\alpha$, $\boldsymbol{p}_\alpha$ and $\boldsymbol{w}_\alpha$, all of which are of size N_α.

Field quantities E and ρ form vectors $\boldsymbol{E}$ and $\boldsymbol{\rho}$ of size N_x, respectively. For example, $\boldsymbol{E}$ is given by:

$$\boldsymbol{E} \equiv \begin{bmatrix} E(x_1) \\ E(x_2) \\ \vdots \\ E(x_{j_x}) \\ \vdots \\ E(x_{N_x}) \end{bmatrix} . \tag{35}$$

The particle evolution equations, i.e., Eqs. (23)–(26), become:

$$\frac{\mathrm{d}\boldsymbol{x}_\alpha}{\mathrm{d}t} = \boldsymbol{v}_\alpha , \tag{36}$$

$$\frac{\mathrm{d}\boldsymbol{v}_\alpha}{\mathrm{d}t} = \frac{Z_\alpha}{m_\alpha}\boldsymbol{E}_\alpha , \tag{37}$$

$$\frac{\mathrm{d}\boldsymbol{p}_\alpha}{\mathrm{d}t} = 0 , \tag{38}$$

$$\frac{\mathrm{d}\boldsymbol{w}_\alpha}{\mathrm{d}t} = -\frac{Z_\alpha}{T_\alpha}(\boldsymbol{p}_\alpha - \boldsymbol{w}_\alpha) \circ \boldsymbol{E}_\alpha \circ \boldsymbol{v}_\alpha , \tag{39}$$

where $\circ$ is the element-wise multiplication (Hadamard product); $\boldsymbol{E}_\alpha$ is a vector of size N_α, and each element is the electrostatic field at the corresponding

particle's position:

$$\boldsymbol{E}_\alpha = \begin{bmatrix} E(x_{1,\alpha}) \\ E(x_{2,\alpha}) \\ \vdots \\ E(x_{j_\alpha}) \\ \vdots \\ E(x_{N_\alpha}) \end{bmatrix} . \tag{40}$$

The relation between $\boldsymbol{E}_\alpha$ and $\boldsymbol{E}$ can be found from Eq. (28), and is then given by:

$$\boldsymbol{E}_\alpha = \mathbb{S}_\alpha \boldsymbol{E} , \tag{41}$$

where $\mathbb{S}_\alpha$ is the shape matrix of size $N_\alpha \times N_x$ and its elements are given by:

$$(\mathbb{S}_\alpha)_{j_\alpha, j_x} = S_x(x_{j_x} - x_{j_\alpha}) \cdot h_x = \begin{cases} 1 - \frac{|x_{j_x} - x_{j_\alpha}|}{h_x} & |x_{j_x} - x_{j_\alpha}| < h_x \\ 0 & \text{otherwise} \end{cases} . \tag{42}$$

Note that $\mathbb{S}_\alpha$ is a sparse matrix. For the hat shape function, each row of $\mathbb{S}_\alpha$ has two non-zero elements. The charge density vector $\boldsymbol{\rho}$ of size N_x can be found from Eq. (29), and is then given by:

$$\boldsymbol{\rho} = \sum_\alpha Z_\alpha \frac{\mathbb{S}_\alpha^{\mathrm{T}} \boldsymbol{w}_\alpha}{h_x} , \tag{43}$$

where superscript $^{\mathrm{T}}$ indicates matrix transpose.

Because DFT is a linear transform, the DFT of charge density Eq. (31) can be written as:

$$\boldsymbol{\rho}_k = \frac{1}{N_x} \mathbb{F} \boldsymbol{\rho} , \tag{44}$$

where $\mathbb{F}$ is the DFT operator matrix of size $N_x \times N_x$, and its elements are given by:

$$(\mathbb{F})_{j_k, j_x} = \exp\left(-i \frac{2\pi}{N_x} j_k j_x \right) . \tag{45}$$

Note that literally performing the matrix multiplication in Eq. (44) has a complexity $O(N_x^2)$. When the whole spectrum is needed, fast Fourier transform (FFT) should be used instead, which reduces the complexity to $O(N_x \log_2 N_x)$ if N_x is a power of 2. If only a few Fourier components are needed, then only the corresponding rows in $\mathbb{F}$ need to be kept, which is implemented in `PIC1D-PETSc`. Then the electrostatic field in Fourier space

can be found from Eq. (33), and the vector-matrix form is given by (after normalization, the factor 4π does not show up here):

$$\boldsymbol{E}_k = -i \cdot \mathrm{diag}(\boldsymbol{k})^{-1} \boldsymbol{\rho}_k \ , \tag{46}$$

where vector k in full-spectrum case is given by:

$$\boldsymbol{k} = \begin{bmatrix} 0 \\ \frac{2\pi}{l} \\ \frac{2\pi}{l} \cdot 2 \\ \vdots \\ \frac{2\pi}{l} \cdot (N_x - 1) \end{bmatrix} \ ; \tag{47}$$

diag() transforms a vector to a diagonal matrix:

$$\mathrm{diag}(\boldsymbol{y}) = \mathrm{diag}(\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}) \equiv \begin{bmatrix} y_1 & & & \\ & y_2 & & \\ & & \ddots & \\ & & & y_N \end{bmatrix} \ . \tag{48}$$

If only some Fourier components are kept, then the size of $\boldsymbol{k}$ becomes the number of the kept components, and only the corresponding elements show up in $\boldsymbol{k}$. Note that the first element of $\boldsymbol{k}$ is 0, which corresponds to the $k = 0$ zonal component. This would not be a problem when zonal component is excluded from the system. If there is a case when zonal component needs to be kept, it needs special care and cannot be put in $\boldsymbol{E}_k$ and $\boldsymbol{k}$ directly as the matrix inversion $\mathrm{diag}(\boldsymbol{k})^{-1}$ would fail. Finally, the electrostatic field on the real space grid is given by the inverse DFT:

$$\boldsymbol{E} = \mathbb{F}^{\dagger} \boldsymbol{E}_k \ , \tag{49}$$

where † indicates conjugate transpose.