Non-Uniform Splines for Semi-Lagrangian Kinetic Simulations of the Plasma Sheath

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Atelier gaine plasma `https://gaine2024.sciencesconf.org`

Joint work with Emily Bourne, Yann Munschy, Virginie Grandgirard, Philippe Ghendrih (CEA Cadarache)
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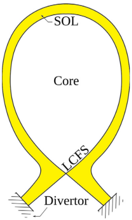
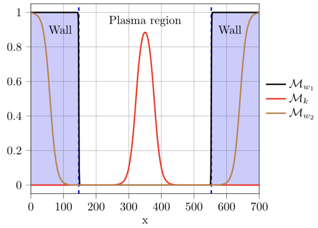
Plasma sheath and interest of non equidistant points

- Plasma sheath: part of hot plasma adjacent to cold wall
- Presence of steep gradient
- Sheath is best described by kinetic: it is far away from Maxwellian distributions
- Main kinetic methods: PIC (Particle in Cell) & eulerian
- Challenges:
  - PIC : low density in the sheath
  - eulerian: Mesh step $<$ Debye length, with domain of one million Debye length

Non-equidistant points in eulerian simulations should help





1D Vlasov-Poisson model

- Two species: $s = e$ (electrons) and $s = i$ (ions)
- **Vlasov** for distribution function $f_s = f_s(t, x, v)$

$$\frac{\partial f_s}{\partial t} + v\frac{\partial f_s}{\partial x} - \frac{q_s}{m_s}\frac{\partial \phi}{\partial x}\frac{\partial f_s}{\partial v} = S_s + C_{ss}$$

- Source term $S_s = S_s(t, x, v)$ for loss of particle in the wall and kinetic source (addition of particles and energy from the body of plasma)
- Collision operator $C_{ss} = C_{ss}(t, x, v)$ (warning with negative values)
- q_s, m_s : charge and mass of species s
- **Poisson** for potential $\phi = \phi(t, x)$

$$-\varepsilon_0\frac{\partial^2 \phi}{\partial x^2} = q_i n_i + q_e n_e,\ n_s = \int f_s dv$$

Simplified model to investigate plasma self-organization in contact with a wall

Conservative laws

- Fluid quantities
  - fluid density $n_s = \int f_s dv$
  - particle flux $\Gamma_s = \int v f_s dv$
  - Reynold's stress $\Pi_s = \int v^2 f_s dv$
  - heat flux $Q_s = \frac{1}{2} \int v^3 f dv$
- Conservation equations (after normalization)
  - particle density

$$\frac{\partial n_s}{\partial t} + \frac{1}{\sqrt{m_s}} \frac{\partial \Gamma_s}{\partial x} = \int S_s + C_{ss} dv$$

  - mean velocity

$$\frac{\partial \Gamma_s}{\partial t} + \frac{1}{\sqrt{m_s}} \left(\frac{\partial \Pi_s}{\partial x} + q_s \frac{\partial \phi}{\partial x} n_s \right) = \int v (S_s + C_{ss}) dv$$

  - kinetic energy

$$\frac{\partial \Pi_s}{\partial t} + \frac{2}{\sqrt{m_s}} \left(\frac{\partial Q_s}{\partial x} + q_s \frac{\partial \phi}{\partial x} \Gamma_s \right) = \int v^2 (S_s + C_{ss}) dv$$

Numerical conservation will be checked comparing left and right hand side

Time discretization with Strang splitting

- X: advection in x
- $V(\phi)$: advection in v
- W: sink 1
- D: sink 2
- K: source
- C: collision
- P: Poisson: $f \to \phi$

We form

$$\mathcal{A}_{\Delta t}(f,\phi) = (W_{\Delta t/2} C_{\Delta t/2} K_{\Delta t/2} D_{\Delta t/2} X_{\Delta t/2} V(\phi)_{\Delta t} X_{\Delta t/2} D_{\Delta t/2} K_{\Delta t/2} C_{\Delta t/2} W_{\Delta t/2}) f$$

and get the second order in time scheme:

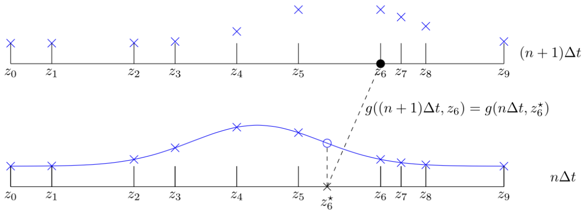
$$\begin{cases} f_{n+1} = \mathcal{A}_{\Delta t}(f_n, P\mathcal{A}_{\Delta t/2}(f_n,\phi_n)) \\ \phi_{n+1} = Pf_{n+1} \end{cases}$$

f_n is an approx of $f_{i/e}$ at time $t_n = n\Delta t$; ϕ_n is the corresp. electric potential

Semi-Lagrangian method

- we are lead to solve 1d advection equation

$$\frac{\partial g}{\partial t} = A\frac{\partial g}{\partial z}$$



- compute foot of characteristic: $z_6^* = z_6 + A\Delta t$
- Interpolate at time $n\Delta t$; here, using splines
- distribution function is assumed to be constant outside of the domain.
  - $\Rightarrow$ if the foot falls outside the domain, boundary value is used
- Indeed, distribution function falls to zero in the wall and tends to zero for $|v|$ large

Splines

- n_c is the number of intervals partitioning domain $[a, b]$
- d is the degree of the splines
- knot vector: $[k_{-d}, \dots, k_{n_c+d}]$, with

$$k_{-d} \leq k_{1-d} \leq \cdots \leq k_0 = a < k_1 \cdots < k_{n_c-1} < k_{n_c} = b \leq \cdots \leq k_{n_c+d-1} \leq k_{n_c+d}$$

- splines are polynomials on each subdomain $[k_i, k_{i+1}]$, for each $i = 0, \dots, n_c - 1$
- basis functions $b_{i,d},\ i = 0, \dots, n_c + d - 1$ defined through
  - $b_{i,0}(x) = \begin{cases} 1, & k_i < x < k_{i+1} \\ 0, & \text{else} \end{cases}$, $i = -d, \dots, n_c + d - 1$
  - for $\ell = 1, \dots, d$ and $i = -d + \ell, \dots, n_c + d - 1$

$$b_{i,\ell}(x) = S(k_{i+\ell} - k_i)(x - k_i)b_{i,\ell-1}(x) + S(k_{i+\ell+1} - k_{i+1})(k_{i+\ell} - x)b_{i+1,\ell-1}(x)$$

    using $S(z) = \begin{cases} 1/z, & z \neq 0 \\ 0, & \text{else} \end{cases}$

- definition ok for x not a knot
- Extension by continuity to knots when possible
- Taking $k_{-d} = \cdots = k_0$ and $k_{n_c} = \cdots = k_{n_c+d}$, $b_{0,d}$ is extended at k_0 to be right continuous and $b_{n_c+d-1,d}$ is extended at k_{n_c} to be left continuous.
- Spline function writes

$$S_d(x) = \sum_{i=0}^{n_c+d-1} c_i b_{i,d}(x)$$

- $c_i,\ i = 0, \dots, n_c + d - 1$ are the coefficients of the splines that are to be determined

Interpolation at Greville points

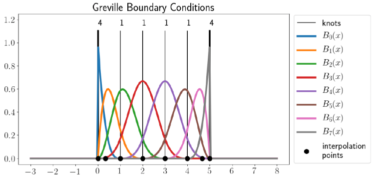
- We define the Greville points

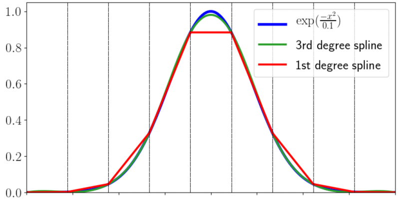
$$x_i = \frac{\sum_{j=1}^{d} k_{i-d+j}}{d}, \ i = 0, \dots, n_c + d - 1$$

- Applying the Schoenberg-Whitney theorem, the interpolation problem

$$S_d(x_i) = y_i, \ i = 0, \dots, n_c + d - 1$$

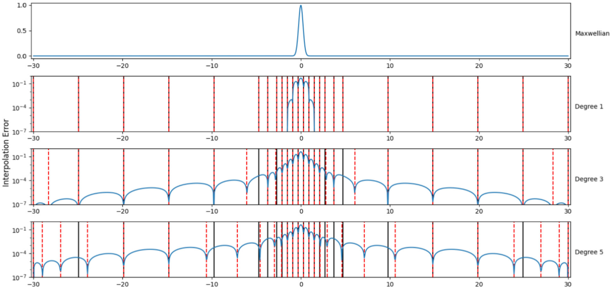
has a unique solution, given values $y_i, \ i = 0, \dots, n_c + d - 1$.





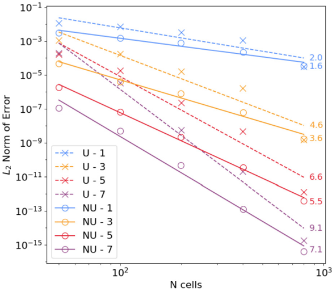
Non uniform grid for the interpolation

- We use a weight function $W(x) = \sqrt{1 + (0.1\frac{\partial u}{\partial x}(x))^2}$ for the interpolation of $u(x)$



Error comparison for interpolation

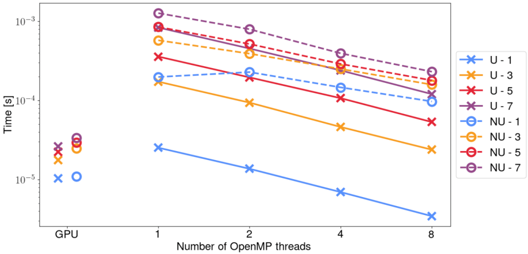
- order increases as degree increases
- order of convergence slightly lower for non uniform grid
- improved choice of points leads to smaller error, except for very large number of points



Efficiency comparison

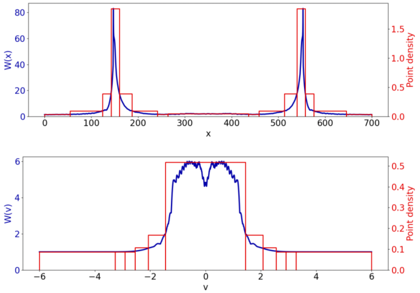
- Backward semi-Lagrangian advection on non-uniform splines is slower than uniform splines
- the cost difference is much smaller on GPU

(U-1 = Uniform splines of degree 1)

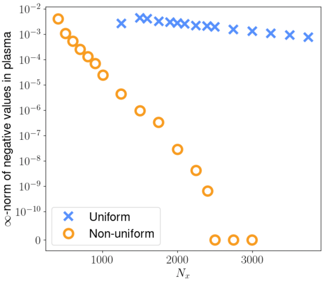


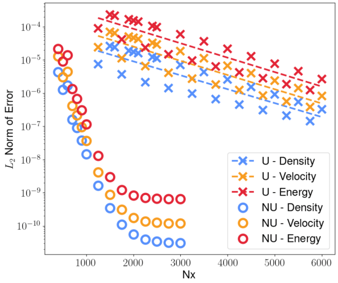
Vlasov-Poisson case

- We replace $\frac{\partial u}{\partial x}(x)$ by an approximation of $L_x \max_{t,v} |\frac{\partial f}{\partial x}(t,x,v)|$
- and similarly for the mesh in v

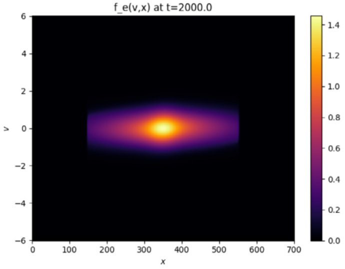


Negative values and conservation errors

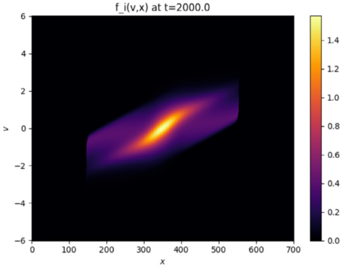




Distribution functions at time $T = 2000$



(a) Electrons



(b) Ions

High order numerical methods for Vlasov-Poisson models of plasma sheaths

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Joint work with Valentin Ayot, Mehdi Badsi, Yann Barsamian, Anaïs Crestetto, Nicolas Crouseilles, Averil Prost and Christian Tayou-Fotso
https://inria.hal.science/hal-03926305

The model

- Vlasov-Poisson model for ions and electrons

$$\begin{cases} \partial_t f_i + v\partial_x f_i - \partial_x \phi \partial_v f_i = \nu f_e \\ \partial_t f_e + v\partial_x f_e + \frac{\partial_x \phi}{\mu} \partial_v f_e = 0 \\ -\lambda^2 \partial_{xx}^2 \phi = \rho = \rho_i - \rho_e = \int f_i - f_e dv \end{cases}$$

- $\nu \geq 0$ is the ionization frequency: rate of creation of ions in presence of electrons
- $\mu = m_e / m_i$ mass ratio between electrons and ions
- $\lambda > 0$ is the Debye length
- $E = -\partial_x \phi$

Numerical method

- splitting scheme

$$\frac{\Delta t}{2}: \quad \begin{cases} \partial_t f_s + v\partial_x f_s = 0 & \text{Linear advection along } x, \\ \lambda^2 \partial_x E = \rho_i - \rho_e & \text{Poisson problem,} \end{cases}$$

$$\frac{\Delta t}{2}: \quad \partial_t f_i = \nu f_e \qquad \text{Ionization,}$$

$$\Delta t: \quad \partial_t f_s + c_s E \partial_v f_s = 0 \quad \text{Linear advection along } v,$$

$$\frac{\Delta t}{2}: \quad \partial_t f_i = \nu f_e \qquad \text{Ionization,}$$

$$\frac{\Delta t}{2}: \quad \begin{cases} \lambda^2 \partial_x E = \rho_i - \rho_e & \text{Poisson problem,} \\ \partial_t f_s + v\partial_x f_s = 0 & \text{Linear advection along } x. \end{cases}$$

- Lagrange interpolation for advection

$$f_j^{n+1} = \sum_{k=-d}^{d+1} f_{j_0+k}^n L_k(\alpha), \; j = 0, \dots, J$$

- $L_k(z) = \prod_{\ell=--d,\ell\neq k}^{d+1} \frac{z-k}{\ell-k}$
- $x_j - a\Delta t = x_{j_0} + \alpha \Delta x$, with $j_0 \in \mathbb{Z}$ and $0 \leq \alpha < 1$
- 0 values for inflow ghost points and outflow ghost points by extrapolation with polynomial fo degree $\leq k_b$, interpolating (x_j, f_j^n) for $j = J - k - b, \dots, J$.

Numerical results

- We take $\lambda = 1/2$, $\mu = 1/100$ and $\nu = 20$.
- Initial conditions:

$$f_i^0(x,v) = mask(x,v)\frac{exp(-v^2/2)}{\sqrt{2\pi}}, \quad f_e^0(x,v) = mask(x,v)\sqrt{\mu}\frac{exp(-\mu v^2/2)}{\sqrt{2\pi}}$$

- $mask(x,v) = \frac{1}{2}\left(tanh(\frac{x-(-0.8)}{0.1}) - tanh(\frac{x-(0.8)}{0.1})\right)$, for satisfying initially the boundary conditions

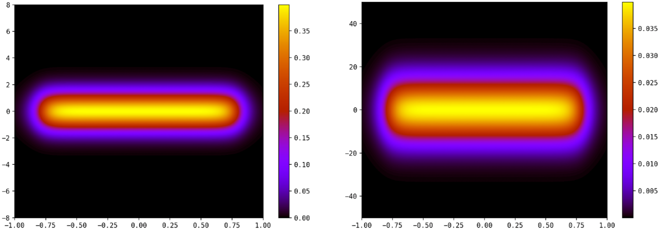


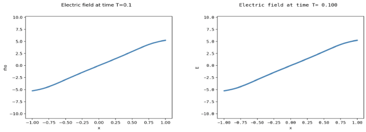
Figure 5: Initial conditions f_i^0 (left) and f_e^0 (right).

Numerical parameters

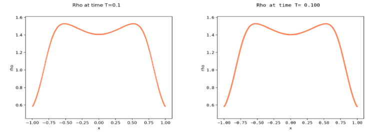
- $d = 8$ and periodic boundary conditions for interpolation in velocity (in v)
- $d = 2$ and $k_b = 1$ for spatial interpolation (in x)
- $v_e \in [-60, 60]$ and $v_i \in [-50, 50]$
- Lagrange interpolation of degree 3 ($d = 1$) for passing from ion velocity mesh to electron velocity mesh (needed for ionization step)

Short time results: $T = 0.1$

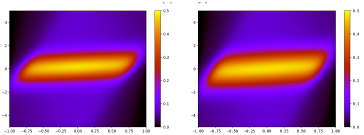
- Comparison with a Finite Difference scheme (left) with $N_x = 512,\ N_{v_i} = N_{v_e} = 513$ and Δt such that CFL condition is satisfied; same grid for v_i and v_e: $[-60, 60]$
- Semi-Lagrangian: $N_x = 1024,\ N_{v_i} = 2049,\ N_{v_e} = 8193,\ \Delta t = 0.00025$



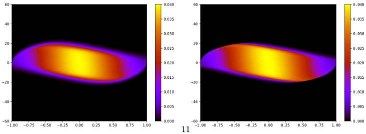
(a) Electric field



(b) Density ρ

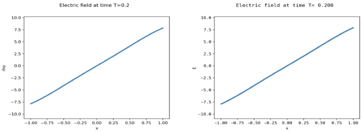


(c) Ion distribution function

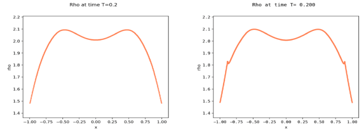


(d) Electron distribution function

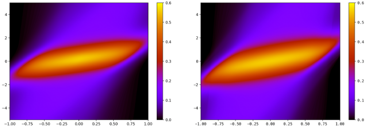
Short time results: $T = 0.2$



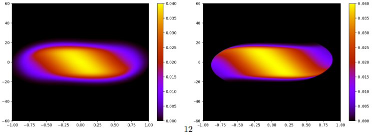
(a) Electric field



(b) Density ρ



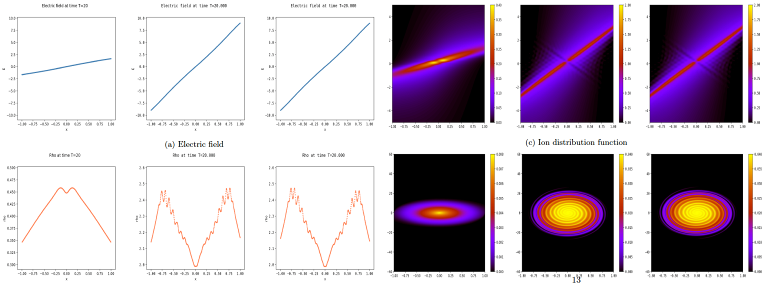
(c) Ion distribution function



(d) Electron distribution function

$T = 20$

- middle: $E(t, 0) = 0$; right: $\int_{-1}^{1} E(t, x)dx = 0$
- Semi-Lagrangian: $N_x = 512,\ N_{v_i} = N_{v_e} = 513,\ \Delta t = 0.00025$



(a) Electric field

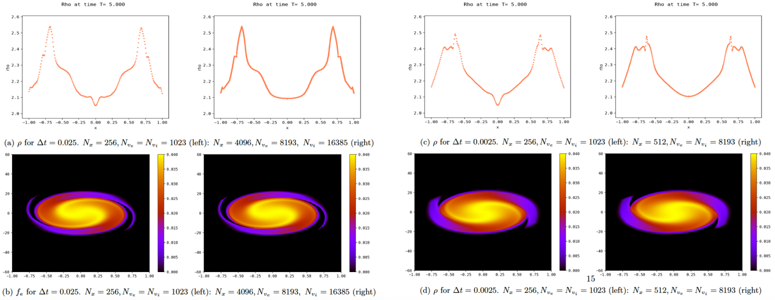
(b) Density ρ

(c) Ion distribution function

(d) Electron distribution function

$T = 5$

- We look for a reference solution
- $\Delta t = 0.025$ (left) $\Delta t = 0.0025$ (right)



(a) ρ for $\Delta t = 0.025$. $N_x = 256, N_{v_e} = N_{v_i} = 1023$ (left): $N_x = 4096, N_{v_e} = 8193$, $N_{v_i} = 16385$ (right)

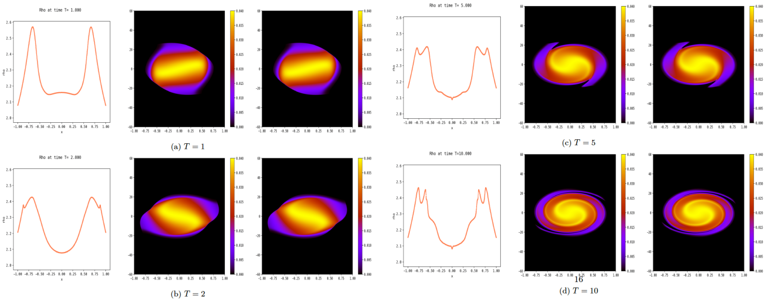
(b) f_e for $\Delta t = 0.025$. $N_x = 256, N_{v_e} = N_{v_i} = 1023$ (left): $N_x = 4096, N_{v_e} = 8193$, $N_{v_i} = 16385$ (right)

(c) ρ for $\Delta t = 0.0025$. $N_x = 256, N_{v_e} = N_{v_i} = 1023$ (left): $N_x = 512, N_{v_e} = N_{v_i} = 8193$ (right)

(d) ρ for $\Delta t = 0.0025$. $N_x = 256, N_{v_e} = N_{v_i} = 1023$ (left): $N_x = 512, N_{v_e} = N_{v_i} = 8193$ (right)

$T = 1, 2, 5$ and 10

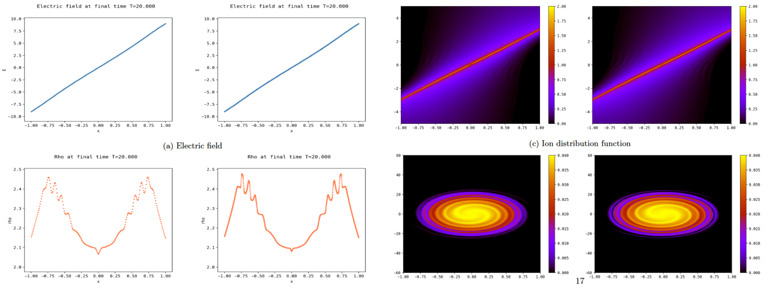
- Density ρ (left); electron distribution function (middle,right)
- $N_x = 1024,\ N_{v_i} = 2049,\ N_{v_e} = 8193$ and $\Delta t = 0.00025$ (left,middle)
- $N_x = 1024,\ N_{v_i} = 2049,\ N_{v_e} = 8193$ and $\Delta t = 0.000025$ (right)



(a) $T = 1$
(b) $T = 2$
(c) $T = 5$
(d) $T = 10$

$T = 20$ again

- left : $N_x = 256,\ N_{v_i} = 2049,\ N_{v_e} = 8193$ and $\Delta t = 0.00025$
- right : $N_x = 1024,\ N_{v_i} = 2049,\ N_{v_e} = 8193$ and $\Delta t = 0.00025$



(a) Electric field

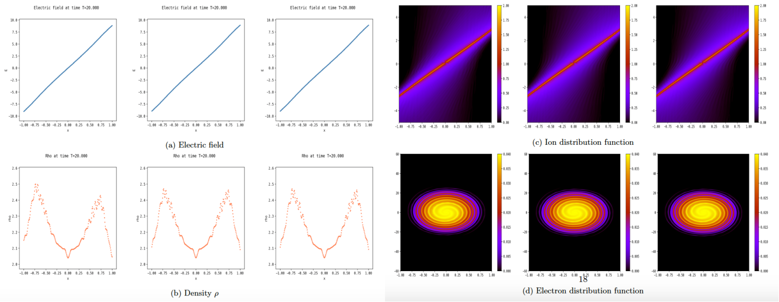
(b) Density ρ

(c) Ion distribution function

(d) Electron distribution function

$T = 20$

- left: $E(t, 0) = 0$
- middle: $E(t, 1) = -E(t, -1)$
- right: $\int_{-1}^{1} E(t, x)dx = 0$



(a) Electric field

(b) Density ρ

(c) Ion distribution function

(d) Electron distribution function

Numerical stability of plasma sheath

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Marseille, november 2024

Joint work with Mehdi Badsi and Laurent Navoret
https://doi.org/10.1051/proc/201864017

Boundary conditions

- Non standard equilibrium `Badsi, Journal of Mathematical analysis and applications , 2017`
- Question:
  - How well is the equilibrium preserved by the numerical scheme?
  - difficulties:
    - two species and realistic mass ratio $\mu = \frac{1}{3672}$
    - treatment of boundary condition with large stencil interpolation

Vlasov-Ampère model

$$\partial_t f_e + v\,\partial_x f_e - \frac{1}{\mu} E\,\partial_v f_e = 0$$

$$\partial_t f_i + v\,\partial_x f_i + \quad E\,\partial_v f_i = 0$$

$$\lambda^2\,\partial_t E = -J$$

current density $J(t,x) = \int_{v\in\mathbb{R}} v\,(f_i(t,x,v) - f_e(t,x,v))\,dv$

Initialization:

- incoming ion distribution:

$$f_{s_i}^{in}(v) = \mathbf{1}_{\{v>0\}}\ \min(1, v^2/\eta)\,\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(v-Z)^2}{2\sigma^2}}$$

  Z : macroscopic ionic velocity

- Initial data: ϕ^{sh}, f_i^{sh}, f_e^{sh}

Difficulties:

- $\omega_p = 1/(\sqrt{\mu}\,\lambda)$ plasma frequencies
- numerical constraint: $\omega_p \Delta t \leqslant 1$

Semi-Lagrangian scheme

- Splitting between advections in space and in velocity

$$(\mathcal{T}) \quad \begin{aligned} &\partial_t f_e + v\,\partial_x f_{s_e} = 0 \\ &\partial_t f_i + v\,\partial_x f_i = 0 \\ &\lambda^2\,\partial_t E = -J, \end{aligned} \qquad (\mathcal{U}) \quad \begin{aligned} &\partial_t f_e - \frac{1}{\mu} E\,\partial_v f_e = 0 \\ &\partial_t f_i + E\,\partial_v f_i = 0 \\ &\lambda^2\,\partial_t E = 0 \end{aligned}$$

- interpolation at the feet of the characteristics

$$f_j^{n+1} = [\Pi f^n]\,(x_j - a\,\Delta t),$$

- local Lagrange interpolation with $(2d+1)$th accuracy

$$[\Pi f]_{|[x_j, x_{j+1}]} = \pi((x_\ell, w_\ell)_{j-d \le \ell \le j+d}).$$

- Second order in time Strang splitting

$$\left\{\left(f^{n+1}_{s,(i,j)}\right)_{i,j}, (E_i^{n+1})_i\right\} = \left[\mathcal{U}_{h,\Delta t/2} \circ \mathcal{T}_{h,\Delta t} \circ \mathcal{U}_{h,\Delta t/2}\right] \{(f^n_{s,(i,j)})_{i,j}, (E_i^n)_i\}$$

- Possible extension to higher order splitting

Difficulties:

- interpolation requires values at **points outside the physical domain**
- Extrapolation of the distribution function
- Entrance: For any $x_i = i\Delta x < 0$

$$f_{(i,j)} = \begin{cases} f(0,0,v_j), & \text{if } v_j \geq 0, \\ 2f_{(0,j)} - f_{(-i,j)}, & \text{if } v_j < 0. \end{cases}$$

- Wall: for any $x_{i+N_x} = (i + N_x)\Delta x > 1$

$$f_{s,(i+N_x,j)} = \begin{cases} 2f_{s,(N_x,j)} - f_{s,(N_x-i,j)} & \text{if } v_j \geq 0, \\ 0 & \text{if } v_j < 0 \end{cases}.$$

→ Dirichlet condition for incoming velocities (with constant values)

→ extension by imparity for leaving velocities (butterfly procedure)

Parameters: $\lambda = 10^{-2}$, $\mu = 1/3672$

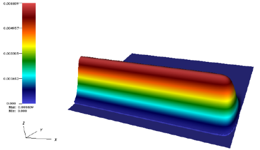
$$d = 8, \quad N_x = 2048, \quad N_v = 4096,$$

velocity domain $[-200, 500]$ for electrons and $[-5, 5]$ for ions

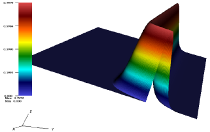
$$\Delta t = 10^{-5}.$$

Numerical simulation: 256 processors, 24 hours, final time $T = 8.03478$

Time $t = 0$



electron distribution



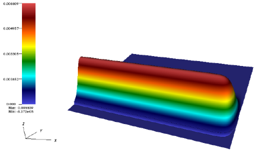
ion distribution

Parameters: $\lambda = 10^{-2}$, $\mu = 1/3672$

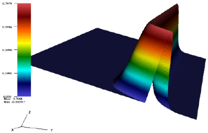
$d = 8, \quad N_x = 2048, \quad N_v = 4096,$
velocity domain $[-200, 500]$ for electrons and $[-5, 5]$ for ions
$\Delta t = 10^{-5}$.

Numerical simulation: 256 processors, 24 hours, final time $T = 8.03478$

Time $t = 4$



electron distribution



ion distribution

Parameters: $\lambda = 10^{-2}$, $\mu = 1/3672$

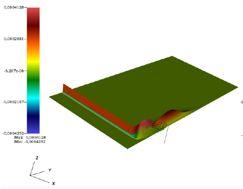
$d = 8, \quad N_x = 2048, \quad N_v = 4096,$

velocity domain $[-200, 500]$ for electrons and $[-5, 5]$ for ions

$\Delta t = 10^{-5}$.

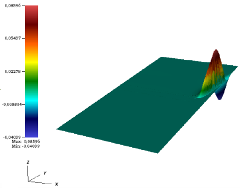
Numerical simulation: 256 processors, 24 hours, final time $T = 8.03478$

Time $t = 4$



error on electron distribution

range: $[-4.252 \times 10^{-4}, 4.128 \times 10^{-4}]$



error on ion distribution

range: $[-4.03 \times 10^{-2}, 8.59 \times 10^{-2}]$

Parameters: $\lambda = 10^{-2}$, $\mu = 1/3672$

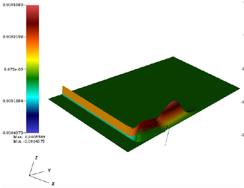
$d = 8, \quad N_x = 2048, \quad N_v = 4096,$

velocity domain $[-200, 500]$ for electrons and $[-5, 5]$ for ions

$\Delta t = 10^{-5}.$

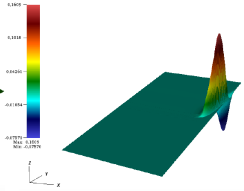
Numerical simulation: 256 processors, 24 hours, final time $T = 8.03478$

Time $t = 8$



error on electron distribution

range: $[-4.375 \times 10^{-4}, 5.589 \times 10^{-4}]$



error on ion distribution

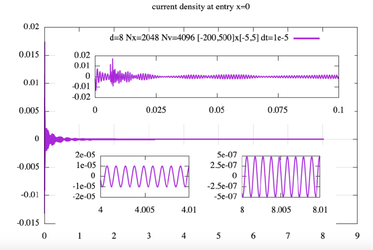
range: $[-7.57 \times 10^{-2}, 1.61 \times 10^{-1}]$

Parameters $\lambda = 10^{-2}$, $\mu = 1/3672$

$d = 8$, $N_x = 2048$, $N_v = 4096$,
velocity domain $[-200, 500]$ for electrons and $[-5, 5]$ for ions
$\Delta t = 10^{-5}$.

Numerical simulation: 256 processors, 24 hours, final time $T = 8.03478$

→ small peak at $t = 0.01$
→ stabilization
→ oscillation plasma $2\pi/\omega_{p,e} = 2\pi(\sqrt{\mu}\,\lambda) = 1 \times 10^{-3}$



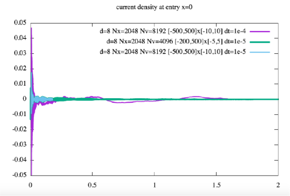
Current density $J(x = 0, t)$

Remarks

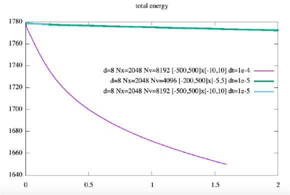
- **Requires small Δt**
  $\to$ $\Delta t = 10^{-4}$ instead of 10^{-5}
  $\to$ longer time simulation
  $\to$ less accurate results

- Requires large N_x and N_v
  $\to$ N_x, N_v divided by 8
  $\to$ instability develops in large time

- Requires high order
  $\to$ $d = 8$ instead of $d = 0$
  $\to$ total energy is dissipated even for large N_v and small Δt



current density $J(t, x = 0)$



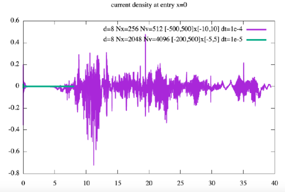
Total energy

Remarks

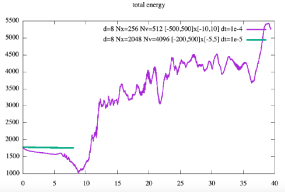
- Requires small Δt
  $\rightarrow$ $\Delta t = 10^{-4}$ instead of 10^{-5}
  $\rightarrow$ longer time simulation
  $\rightarrow$ less accurate results

- **Requires large N_x and N_v**
  $\rightarrow$ N_x, N_v divided by 8
  $\rightarrow$ instability develops in large time

- Requires high order
  $\rightarrow$ $d = 8$ instead of $d = 0$
  $\rightarrow$ total energy is dissipated even for large N_v and small Δt



current density $J(t, x = 0)$



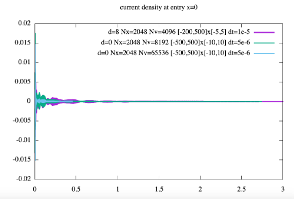
Total energy

Remarks

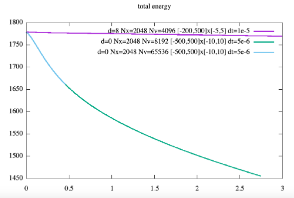
- Requires small Δt
  $\to$ $\Delta t = 10^{-4}$ instead of 10^{-5}
  $\to$ longer time simulation
  $\to$ less accurate results

- Requires large N_x and N_v
  $\to$ N_x, N_v divided by 8
  $\to$ instability develops in large time

- **Requires high order d**
  $\to$ $d = 8$ instead of $d = 0$
  $\to$ total energy is dissipated even for large N_v and small Δt



current density $J(t, x = 0)$



Total energy

Other boundary conditions

- Uncentered interpolation at the boundaries → instabilities (for $d = 4, 5$)
- Butterfly is numerically stable