Fast Boundary Element Methods for plasma simulation

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Vlasov–Poisson system

The Vlasov-Poisson system for the distribution function

$$f : (0, \infty) \times \mathbb{R}^3_x \times \mathbb{R}^3_v \to (0, \infty)$$

of electrons in a plasma with positive background charge reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f - E \cdot \nabla_v f = 0,$$
$$E = -\nabla_x \phi,$$
$$-\Delta_x \phi = \frac{1}{\beta} \left[1 - \int_{\mathbb{R}^3} f \, \mathrm{d}v \right],$$

where

$$\beta = \left(\frac{\lambda_D}{L_0} \right)^2, \quad \lambda_D = \sqrt{\frac{\varepsilon_0 k_B T_0}{n_0 e^2}}.$$

Direct Simulation Monte Carlo

We discretise f with N_p *macroparticles*,

$$f(t,x,v) \approx \sum_{i=1}^{N_p} w_i \, \delta_{x_i(t)}(x) \, \delta_{v_i(t)}(v).$$

The Vlasov equation now is a system of ODEs,

$$\begin{aligned} \dot{x}_i &= v_i, \\ \dot{v}_i &= -E(x_i), \end{aligned}$$

$i = 1, \ldots, N_p$.

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grid-free!

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$i = 1, \ldots, N_p$.

$$-\Delta\phi = \frac{1}{\beta}\left[1 - \sum_{j=1}^{N_p} w_j \delta_{x_j}\right]$$

$\rightarrow$ Use Boundary Element Methods for the Poisson equation

Representation formula

Let $\Omega \subset \mathbb{R}^3_x$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$. The solution u of

$$\begin{aligned} -\Delta u &= g_V \quad \text{in } \Omega, \\ \gamma_0 u &= g_D \quad \text{on } \Gamma, \end{aligned}$$

admits the *representation formula*

$$\begin{aligned} u(x) =& \int_\Gamma \gamma_{0,y} U(x,y) \gamma_1 u(y) \, \mathrm{d}S_y - \int_\Gamma \gamma_{1,y} U(x,y) g_D(y) \, \mathrm{d}S_y \\ &+ \int_\Omega U(x,y) g_V(y) \, \mathrm{d}y, \\ =& (\tilde{V}\gamma_1 u)(x) - (W g_D)(x) + (\tilde{N} g_V)(x), \quad x \in \Omega, \end{aligned}$$

where

$$U(x,y) = \frac{1}{4\pi} \frac{1}{|x-y|}, \quad x \neq y \in \mathbb{R}^3.$$

Boundary Integral Equations

Taking the Dirichlet trace γ_0 of the representation formula, we get an *integral equation on* Γ for $t = \gamma_1 u$,

$$Vt = \left(\frac{1}{2} + K\right) g_D - N_0 g_V,$$

where

$$Vt(x) = \int_\Gamma \gamma_{0,y} U(x,y) t(y) \, \mathrm{d}S_y, \quad x \in \Gamma,$$

is symmetric and *positive definite*,

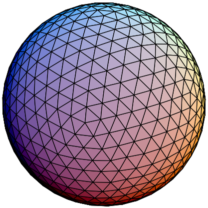
$$Kg_D(x) = \text{p.v.} \int_\Gamma \gamma_{1,y} U(x,y) g_D(y) \, \mathrm{d}S_y, \quad x \in \Gamma,$$

and

$$N_0 g_V(x) = \int_\Omega U(x,y) g_V(y) \, \mathrm{d}y, \quad x \in \Gamma.$$

Boundary Element Methods

We discretise the surface Γ with N_Γ elements, M_Γ nodes, and mesh size h.



Employing a *Galerkin Method* with discontinuous ansatz functions for the Neumann trace t and continuous functions for g_D,

$$t \approx \sum_{k=1}^{N_\Gamma} (t_h)_k \, \varphi_k^0, \quad g_D \approx \sum_{i=1}^{M_\Gamma} (g_h)_i \, \varphi_i^1,$$

leads to the discrete system

$$V_h t_h = \left(\frac{1}{2} M_h + K_h \right) g_h - \underline{N}_0.$$

Approximation error

For sufficiently regular data (g_V, g_D) we have

$$\|\gamma_1 u - t_h\|_{L^2(\Gamma)} \leq C_1 h,$$

where h is the mesh size of the boundary discretisation. This implies the pointwise estimates

$$|u(x) - u_h(x)| \leq C_2(x) h^3,$$
$$|\nabla u(x) - \nabla u_h(x)| \leq C_3(x) h^3$$

for $x \in \Omega$.

- No loss of convergence rate for the gradient!
- Very well suited for the computation of the electric field.

Application to the particle system

The crucial part is the evaluation of the Newton potential $\tilde{N}$,

$$\tilde{N}g_V(x) = \int_\Omega U(x,y)g_V(y)\,\mathrm{d}y,$$

but for our plasma

$$g_V = \frac{1}{\beta}\left[1 - \sum_{j=1}^{N_p} w_j \delta_{x_j}\right]$$

and therefore

$$\tilde{N}g_V(x) = \frac{1}{\beta}\int_\Omega U(x,y)\,\mathrm{d}y - \frac{1}{\beta}\sum_{j=1}^{N_p} w_j U(x,x_j).$$

The remaining volume integral is avoided by the use of a special solution for the background charge.

Application to the particle system

For the particle system, we solve

$$\begin{aligned} -\Delta\phi &= -\frac{1}{\beta}\sum_{j=1}^{N_p} w_j \delta_{x_j} && \text{in } \Omega, \\ \gamma_0 \phi &= g_D - \phi_b && \text{on } \Gamma, \end{aligned}$$

where $\phi_b(x) = -1/(6\beta)|x|^2$, $x \in \Omega$. We have

$$E(x_i) = \sum_{\substack{j=1 \\ j\neq i}}^{N_p} \frac{w_j}{4\pi\beta}\frac{x_i - x_j}{|x_i - x_j|^3} \qquad \text{grid-free}$$

$i = 1, \ldots, N_p$.

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$$- \nabla\phi_b(x_i) \qquad \text{grid-free}$$

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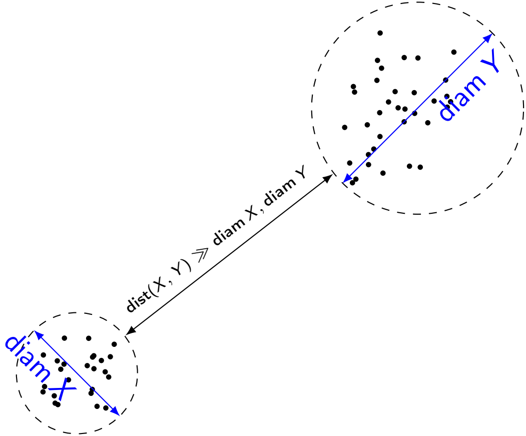
$i = 1, \ldots, N_p$.

- No volume mesh is needed for the evaluation of E.
- Computational complexity for E is in $\mathcal{O}(N_p^2 + N_\Gamma N_p)$.

Hierarchical approximation

The direct summation is

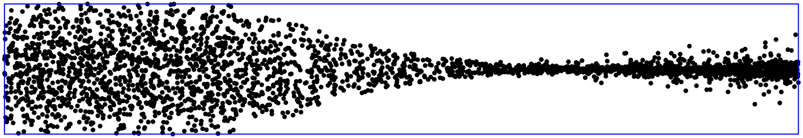
- very expensive, $\mathcal{O}(N_p^2)$ complexity,
- not needed for particles which are "far apart" (in the far field)



Goal: Reduction of complexity from $\mathcal{O}(N_p^2)$ to $\mathcal{O}(rN_p)$, $r \ll N_p$.

Hierarchical approximation

We subdivide the particles by a nested cluster tree



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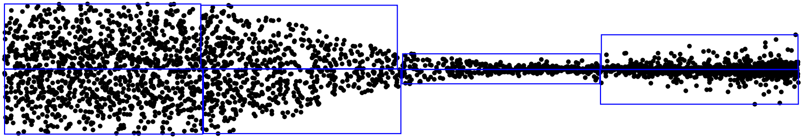

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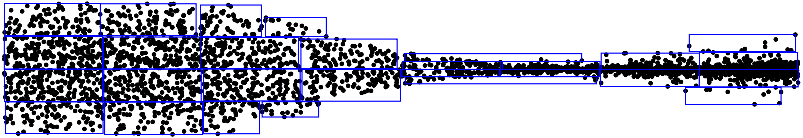

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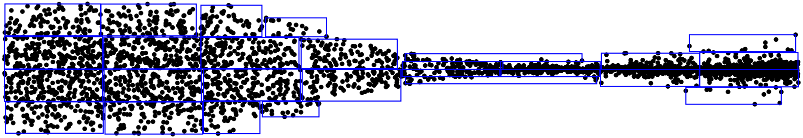


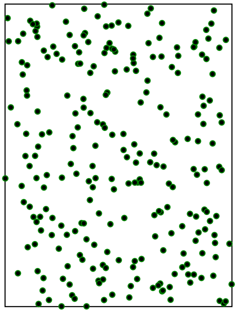
The far field is characterised by the admissibility condition

$$\max\{\operatorname{diam} X, \operatorname{diam} Y\} \leq \eta \operatorname{dist}(X, Y)$$

for clusters X and Y with a constant $\eta > 0$.

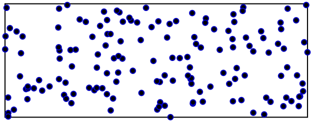
Hierarchical approximation

For admissible clusters (X, Y) the evaluation of U is replaced by interpolation



X

$$\begin{pmatrix} U(x_1, y_1) & U(x_1, y_2) & \dots & U(x_1, y_q) \\ U(x_2, y_1) & U(x_2, y_2) & \dots & U(x_2, y_q) \\ \vdots & \vdots & & \vdots \\ U(x_{p-1}, y_1) & U(x_{p-1}, y_2) & \dots & U(x_{p-1}, y_q) \\ U(x_p, y_1) & U(x_p, y_2) & \dots & U(x_p, y_q) \end{pmatrix}$$



Y

Hierarchical approximation

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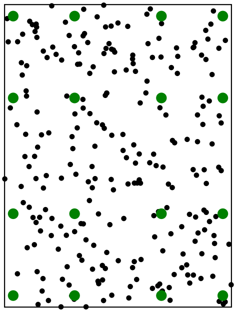
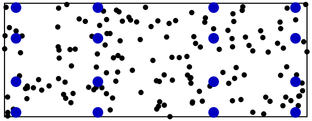


X

$$V_X \begin{pmatrix} U(\xi_1, \zeta_1) & \dots & U(\xi_1, \zeta_r) \\ \vdots & & \vdots \\ U(\xi_r, \zeta_1) & \dots & U(\xi_r, \zeta_r) \end{pmatrix} W_Y^\top$$



Y

V_X and W_Y are interpolation matrices at the positions of the particles.

Hierarchical approximation

- The matrices V_X, W_Y are independent of the interpolated function.
  $\rightarrow$ simultaneous evaluation of vector-valued functions.
- Only small leaf matrices are needed.
  $\rightarrow$ Computation on the fly while iterating through the cluster tree.
  $\rightarrow$ Reduction of complexity from $\mathcal{O}(N_p^2)$ to $\mathcal{O}(rN_p)$, $r \ll N_p$.
- The same techniques apply for the approximation of BEM matrices.

Numerical examples

- The system of ODEs

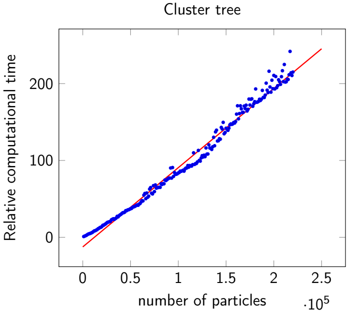
$$\dot{x}_i = v_i,$$
$$\dot{v}_i = -E(x_i), \quad i = 1, \dots, n,$$

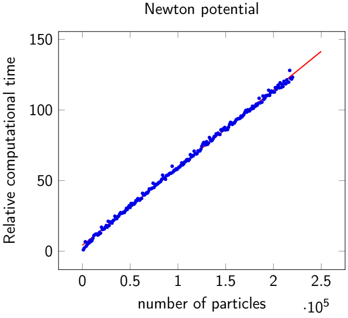
is integrated by the Leapfrog scheme

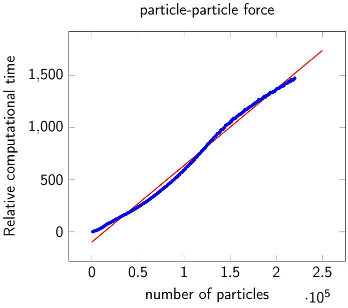
$$\begin{aligned} \mathbf{V}_{t+1/2} &= \mathbf{V}_t - \frac{\Delta t}{2}\mathbf{E}_t, \\ \mathbf{X}_{t+1} &= \mathbf{X}_t + \Delta t \mathbf{V}_{t+1/2}, \\ \mathbf{V}_{t+1} &= \mathbf{V}_{t+1/2} - \frac{\Delta t}{2}\mathbf{E}_{t+1}, \end{aligned}$$

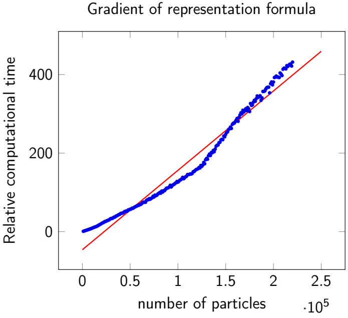
which is second order and time-reversible.

Computational timing for E

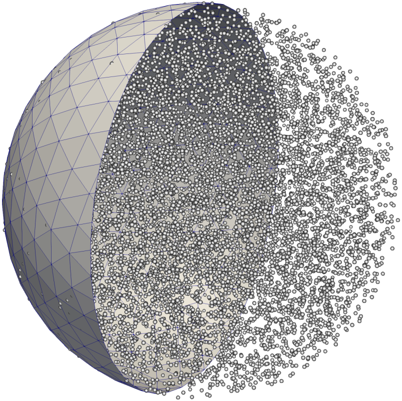






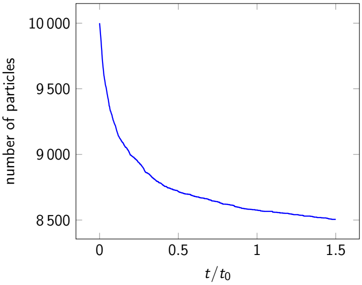


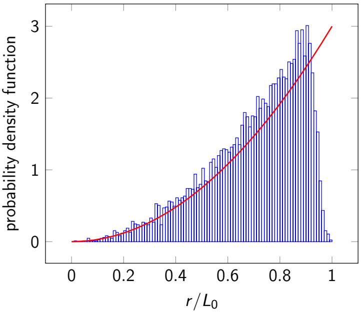
Plasma sheath



- Initially, 10 000 particles are distributed uniformly inside the unit sphere.
- The particles are absorbed at the boundary.
- Homogeneous Dirichlet boundary conditions for ϕ.
- The surface is triangulated with 1280 triangles.

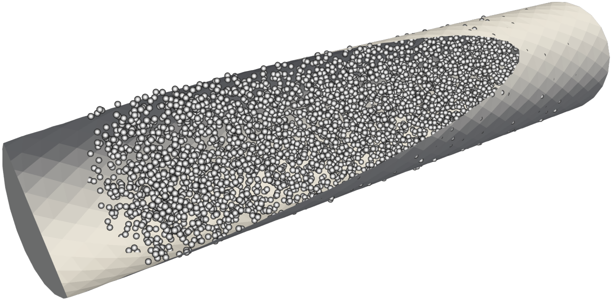
Plasma sheath





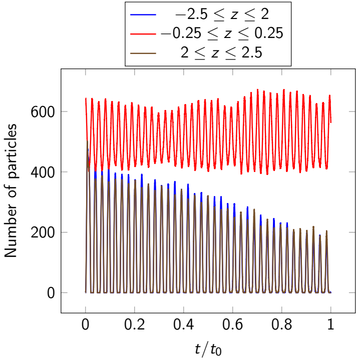
Absorbed particles leave a positive net charge near the boundary.
$\rightarrow$ Potential barrier for slow particles.
$\rightarrow$ Particles are confined to the interior.
$\rightarrow$ Number of particles is (nearly) stationary.

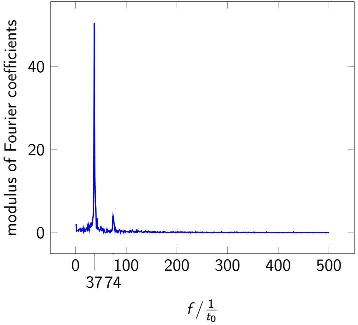
Plasma oscillation



- Initially, 5 000 particles are distributed uniformly in the middle of the cylinder, leaving positive net charge at its ends.
- The particles are absorbed at the boundary.
- Homogeneous Dirichlet boundary conditions on the bases, homogeneous Neumann boundary conditions on the rest.
- The surface is triangulated with 2 110 triangles.

Plasma oscillation





The plasma oscillates with a frequency of $3.0 \cdot 10^8\,\frac{1}{\mathrm{s}}$, which is in the order of the plasma frequency

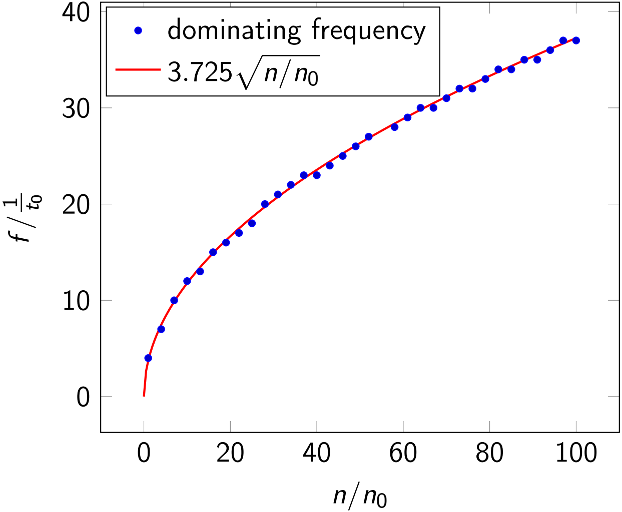
$$\omega_p = \sqrt{\frac{ne^2}{\varepsilon_0 m_e}} \approx 1.8 \cdot 10^8\,\frac{1}{\mathrm{s}}.$$

Plasma oscillation

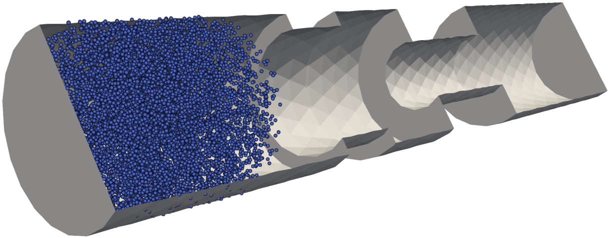
For the plasma frequency, we have

$$\omega_p = C_e \sqrt{n},$$

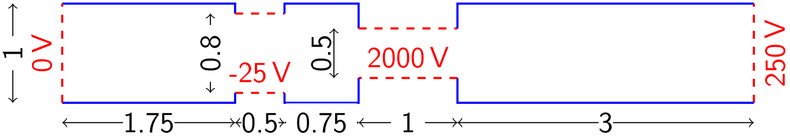
which is observed numerically:



Accelerator



- Initially, 10 000 particles are distributed uniformly in the left cylinder.
- The particles are absorbed at the boundary.
- The surface is triangulated with 2078 triangles.



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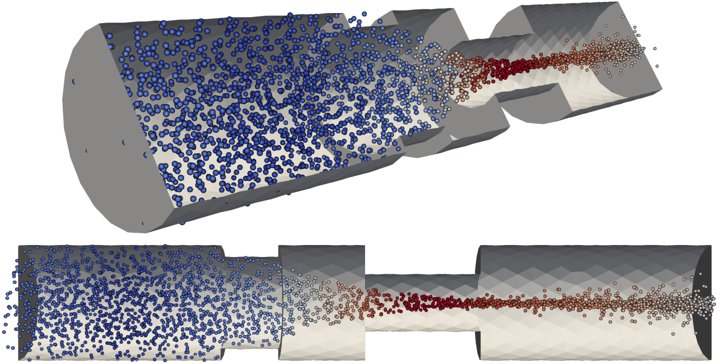

The particle distribution is rotationally symmetric around the symmetry axis of the geometry.

Conclusion

- With BEM,
  - no volume mesh is needed for solving the Vlasov-Poisson system.
  - we can handle complex geometries and mixed boundary value problems.
  - we have the same order of convergence for $E = -\nabla_x \phi$ as for ϕ.
- Combined with hierarchical approximation we obtain an $\mathcal{O}(N_p)$ algorithm.
- The Coulombic interaction is fully resolved by our scheme, especially in the near field.