Poisson Solvers for Self-Consistent Multi-Particle Simulations

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Self-Consistent Multi-Particle Simulations with Particle-In-Cell (PIC) Method

1. Initialize particles

2. Setup for solving Poisson equation

3. Advance momenta using radiation damping and quantum excitation map

4. Advance momenta using beam-beam forces

5. Charge deposition on grid

6. Field solution on grid to find beam-beam forces

7. Field interpolation at particle positions

8. Advance positions & momenta using external transfer map

9. (optional) diagnostics
Fast Efficient Poisson Solvers with Different Boundary Conditions Are Needed

geometry in space-charge and beam-beam force calculation
Different Boundary/Beam Conditions Need Different Efficient Numerical Algorithms

FFT based Green function method:
- Standard Green function: low aspect ratio beam
- Shifted Green function: separated particle and field domain
- Integrated Green function: large aspect ratio beam
- Non-uniform grid Green function: 2D radial non-uniform beam

Spectral-finite difference method:
- 2D open boundary
  - Transverse regular pipe with longitudinal open

Multigrid spectral-finite difference method:
- Transverse irregular pipe
Green Function Solution of Poisson’s Equation (open boundary conditions)

\[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -2\pi \rho(x, y), \]

\[ E = -\nabla \phi, \]

\[ \phi(x, y) = \int G(x, \bar{x}, y, \bar{y}) \rho(\bar{x}, \bar{y}) d\bar{x} d\bar{y}, \]

\[ \phi(x_i, y_j) = h_x h_y \sum_{i'=1}^{N_x} \sum_{j'=1}^{N_y} G(x_i - x_{i'}, y_i - y_{j'}) \rho(x_{i'}, y_{j'}), \]

\[ G(x, y) = -\frac{1}{2} \log(x^2 + y^2) \]

Direct summation of the convolution scales as \( N^2 \)!!

\( N \) – number of total grid points \((N_xN_y)\)
Define a new periodic potential function \( \phi_c \)

\[
\phi_c(x_i, y_j) = h_x h_y \sum_{i=1}^{2N_x} \sum_{j=1}^{2N_y} G_c(x_i - x'_i, y_i - y'_j) \rho_c(x'_i, y'_j),
\]

\[
\rho_c(x_i, y_j) = \begin{cases} 
\rho(x_i, y_j): & 1 \leq i \leq N_x, 1 \leq j \leq N_y, \\
0: & N_x < i \leq 2N_x \text{ or } N_y < j \leq 2N_y,
\end{cases}
\]

\[
G_c(x_i, y_j) = \begin{cases} 
G(x_i, y_j): & 1 \leq i \leq N_x + 1, 1 \leq j \leq N_y + 1, \\
G(x_{2N_x-i+2}, y_j): & N_x + 1 < i \leq 2N_x, 1 \leq j \leq N_y + 1, \\
G(x_i, y_{2N_y-j+2}): & 1 \leq i \leq N_x + 1, N_y + 1 < j \leq 2N_y, \\
G(x_{2N_x-i+2}, y_{2N_y-j+2}): & N_x + 1 < i \leq 2N_x, N_y + 1 < j \leq 2N_y,
\end{cases}
\]

\[
\rho_c(x_i, y_j) = \rho_c[x_i + 2(L_x + h_x), y_j + 2(L_y + h_y)],
\]

\[
G_c(x_i, y_j) = G_c[x_i + 2(L_x + h_x), y_j + 2(L_y + h_y)].
\]
Green Function Solution of Poisson’s Equation (open boundary conditions)

\[ \phi(x_i, y_j) = \phi_c(x_i, y_j), \quad \text{for } i = 1, N_x; j = 1, N_y. \]

Fast Fourier Transform (FFT) can be used to calculate \( \phi_c \)

FFT based summation of the convolution scales as \( N \log(N) \),


Shifted Green Function to Compute Long-Range Beam-Beam or Image Space-Charge Forces

\[
\phi_F(r) = \int G_s(r,r')\rho(r')dr'
\]
\[
G_s(r,r') = G(r + r_s, r')
\]

- Computational domain covers only the larger one of the particle or the field domain, not both!
- Computational cost scales as \((O(N \log N))\)!

\[
G_c(x_i, y_j) = -\frac{1}{2} \begin{cases} 
\ln[(x_c + x_i)^2 + (y_c + y_j)^2]; & 1 \leq i \leq N_x, 1 \leq j \leq N_y, \\
\ln[(x_c - x_{2N_x - i + 2})^2 + (y_c + y_j)^2]; & N_x < i \leq 2N_x, 1 \leq j \leq N_y, \\
\ln[(x_c + x_i)^2 + (y_c - y_{2N_y - j + 2})^2]; & 1 \leq i \leq N_y, N_y < i \leq 2N_y, \\
\ln[(x_c - x_{2N_x - i + 2})^2 + (y_c - y_{2N_y - j + 2})^2]; & N_x < i \leq 2N_x, N_y < i \leq 2N_y.
\end{cases}
\]

Comparison between Numerical Solution and Analytical Solution (Shifted Green Function)

\[ E_x \quad \text{inside the particle domain} \]
Efficient Shifted Green Function Method to Calculate Image Space-Charge Effects

computational domain contains only the original beam

Green Function Solution of Poisson’s Equation
(Integrated Green Function)

Integrated Green (IG) function algorithm for large aspect ratio:

\[ \phi_c(r_i) = \sum_{i'=1}^{2N} G_i(r_i - r_{i'}) \rho_c(r_{i'}) \]

\[ G_i(r, r') = \int G_s(r, r') dr' \]

Comparison between the IG and SG for a beam with aspect ratio of 30

FFT based convolution with non-uniform grid

\[ \phi(r, \theta) = \int G(r, r', \theta, \theta') \rho(r', \theta') r' dr' d\theta' \]

\[ G(r, r', \theta, \theta') = -\frac{1}{2} \log (r^2 - 2rr' \cos(\theta - \theta') + r'^2) \]

\[ s = \frac{1}{k_1} \log \left( \frac{r}{k_2} \right) \]

\[ G(s, s', \theta, \theta') = -\frac{1}{2} \log \left( e^{2k_1(s-s')} - 2e^{k_1(s-s')} \cos(\theta - \theta') + 1 \right) \]

FFT can be used on uniform s-\theta grid

Test of the Non-Uniform Grid FFT Solver

Errors of Er

analytical solution

nonuniform grid Green function method
uniform grid Green function method
Spectral-Finite Difference Method
(2D open boundary condition)

computational domain covers only the beam
by using boundary matching conditions

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \phi \right) + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} \phi \right) = -\frac{\rho}{\varepsilon_0}
\]

\[
\phi(r, \theta) = \sum \phi_m(r)e^{-im\theta}
\]

\[
\rho(r, \theta) = \sum \rho_m(r)e^{-im\theta}
\]

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \phi_m \right) - \frac{m^2}{r^2} \phi_m = -\frac{\rho_m}{\varepsilon_0} \quad \text{for} \quad r \leq a
\]

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \phi_m \right) - \frac{m^2}{r^2} \phi_m = 0 \quad \text{for} \quad r > a
\]
Solution of Poisson’s Equation (Spectral-Finite Difference)

For \( r \leq a \) :

\[
\left(\frac{1}{h^2} + \frac{1}{hr}\right)\phi_m^{n+1} - \left(\frac{2}{h^2} + \frac{m^2}{r^2}\right)\phi_m^n + \left(\frac{1}{h^2} - \frac{1}{hr}\right)\phi_m^{n-1} = -\frac{\rho_m}{\varepsilon_0};
\]

\[
\frac{\partial}{\partial r} \phi_m = 0 \quad \text{for} \quad r = 0 \quad \text{and} \quad m = 0
\]

\[
\phi_m = 0 \quad \text{for} \quad r = 0 \quad \text{and} \quad m > 0
\]

For \( r \geq a \) :

\[
\phi = c \, r^{-m} \quad m > 0
\]

\[
\phi = c \, \ln(r) \quad m = 0
\]

Above Tri-Diagonal Matrix Can be Solved in \( O(N) \)!

\( N \) is the number of radial grid points.
Comparison between Numerical Solution and Analytical Solution

aspect ratio = 1

aspect ratio = 5
3D Poisson Solver with Transverse Rectangular Pipe

\[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = -\frac{\rho}{\varepsilon_0} \]

with boundary conditions
\[ \phi(x = 0, y, z) = 0, \]
\[ \phi(x = a, y, z) = 0, \]
\[ \phi(x, y = 0, z) = 0, \]
\[ \phi(x, y = b, z) = 0, \]
\[ \phi(x, y, z = \pm\infty) = 0, \]

\[ \rho(x, y, z) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \rho^{lm}(z) \sin(\alpha_l x) \sin(\beta_m y), \]
\[ \phi(x, y, z) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \phi^{lm}(z) \sin(\alpha_l x) \sin(\beta_m y), \]

where
\[ \rho^{lm}(z) = \frac{4}{ab} \int_0^a \int_0^b \rho(x, y, z) \sin(\alpha_l x) \sin(\beta_m y), \]
\[ \phi^{lm}(z) = \frac{4}{ab} \int_0^a \int_0^b \phi(x, y, z) \sin(\alpha_l x) \sin(\beta_m y), \]

\[ \frac{\partial^2 \phi^{lm}(z)}{\partial z^2} - \gamma_l^2 \phi^{lm}(z) = -\frac{\rho^{lm}(z)}{\varepsilon_0}, \]
\[ \frac{\phi^{lm}_{n+1} - 2\phi^{lm}_n + \phi^{lm}_{n-1}}{h_z^2} - \gamma_l^2 \phi^{lm}_n = -\frac{\rho^{lm}_n}{\varepsilon_0}, \]
\[ \phi^{lm}_{-1} = \exp(-\gamma_l h_z) \phi^{lm}_0, \quad n = 0, \]
\[ \phi^{lm}_{N+1} = \exp(-\gamma_l h_z) \phi^{lm}_N, \quad n = N. \]

3D Poisson Solver inside a Ring with a Long Bunch

$$\nabla^2 \phi + \frac{1}{R} \left( \frac{1}{1 + \frac{r \cos(\theta)}{R}} \left( \cos(\theta) \frac{\partial \phi}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial \phi}{\partial r} \right) + \frac{1}{(1 + \frac{r \cos(\theta)}{R})^2} \frac{\partial^2 \phi}{\partial z^2} \right) = -\rho.$$


charged particles
Iterative Solution of the Poisson Equation with the Hermite-Gaussian Approximation

\[ \rho(r, \theta, z) = \sum_{n=0}^{N} \rho_n(r, \theta) \mathcal{H}_n(z), \]

\[ \phi(r, \theta, z) = \sum_{n=0}^{N} \phi_n(r, \theta) \mathcal{H}_n(z). \]

\[ \mathcal{H}_n(z) = H_n \left( \frac{z}{A} \right) \exp \left( -\frac{1}{2} \frac{z^2}{A^2} \right) \]

\[ \nabla_\perp^2 \phi_n + \frac{1}{R} \frac{1}{1 + \frac{r \cos(\theta)}{R}} \left( \cos(\theta) \frac{\partial \phi_n}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial \phi_n}{\partial r} \right) \]

\[ + \frac{1}{(1 + \frac{r \cos(\theta)}{R})^2} \left( \frac{1}{4} \phi_{n-2} - \frac{1}{2} (2n + 1) \phi_n + (n + 2)(n + 1) \phi_{n+2} \right) \frac{1}{A^2} = -\rho_n. \]

\[ \nabla_\perp^2 \phi_n^1 = -\rho_n, \]

\[ \nabla_\perp^2 \phi_n^2 = -\rho_n - \frac{1}{R} \frac{1}{1 + \frac{r \cos(\theta)}{R}} \left( \cos(\theta) \frac{\partial \phi_n^1}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial \phi_n^1}{\partial r} \right) \]

\[ + \left( \frac{1}{4} \phi_{n-2}^1 - \frac{1}{2} (2n + 1) \phi_n^1 + (n + 2)(n + 1) \phi_{n+2}^1 \right) \frac{1}{(1 + \frac{r \cos(\theta)}{R})^2} \frac{1}{A^2}, \]

\[ \nabla_\perp^2 \phi_n^3 = -\rho_n - \frac{1}{R} \frac{1}{1 + \frac{r \cos(\theta)}{R}} \left( \cos(\theta) \frac{\partial \phi_n^2}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial \phi_n^2}{\partial r} \right) \]

\[ + \left( \frac{1}{4} \phi_{n-2}^2 - \frac{1}{2} (2n + 1) \phi_n^2 + (n + 2)(n + 1) \phi_{n+2}^2 \right) \frac{1}{(1 + \frac{r \cos(\theta)}{R})^2} \frac{1}{A^2}, \]

\[ \vdots = \vdots. \]
Potential of a beam in a toroidal conducting pipe (aspect ratio = 100)

Norm 1 Errors vs. Number of Iterations
Multigrid Spectral-Finite Difference Solution of the Poisson’s Equation in Cylindrical Coordinates

\[ \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = - \frac{\rho}{\varepsilon} \]

where:

\[ \rho(r, \theta, z) = \sum \rho^m(r, z) \exp(-im\theta) \]

\[ \phi(r, \theta, z) = \sum \phi^m(r, z) \exp(-im\theta) \]

we obtain:

\[ \frac{\partial^2 \phi^m}{\partial r^2} + \frac{1}{r} \frac{\partial \phi^m}{\partial r} - \frac{m^2}{r^2} \phi^m + \frac{\partial^2 \phi^m}{\partial z^2} = - \frac{\rho^m}{\varepsilon} \]
Multigrid Spectral Finite-Difference Solution of Poisson’s Equation in Frenet-Serret Coordinates

\[
\frac{1}{1 + hx} \left( \frac{\partial}{\partial x} (1 + hx) \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial z} \frac{1}{1 + hx} \frac{\partial \phi}{\partial z} \right) + \frac{\partial^2 \phi}{\partial y^2} = -\frac{\rho}{\varepsilon}
\]

where:

\[
\rho(x, y, z) = \sum \rho^m(x, z) \sin(m\pi y / a)
\]

\[
\phi(x, y, z) = \sum \phi^m(x, z) \sin(m\pi y / a)
\]

we obtain:

\[
\frac{1}{1 + hx} \left( \frac{\partial}{\partial x} (1 + hx) \frac{\partial \phi^m}{\partial x} + \frac{\partial}{\partial z} \frac{1}{1 + hx} \frac{\partial \phi^m}{\partial z} \right) - \frac{m^2 \pi^2}{a^2} \phi^m = -\frac{\rho^m}{\varepsilon}
\]
**Multigrid Method to Solve the Poisson Equation**

**Computational Cost ~ O(N)**

- **Concept:**
  - Smooth out the numerical errors on multiple scales

- **How:**
  - Use restriction and prolongation to connect the solutions between level $i$ and $i + 1$
  - Solve the linear system $A^{(i)} X^{(i)} = B^{(i)}$ approximately on each level

Five Basic Operations of a Two-Grid Algorithm

1) Pre-smoothing:
\[ \tilde{X}^{(i)} = (L^{(i)} + D^{(i)})^{-1} B^{(i)} - (L^{(i)} + D^{(i)})^{-1} U^{(i)} \tilde{X}^{(i)} \]

2) Restriction:
\[ B^{(i+1)} = R (B^{(i)} - A^{(i)} \tilde{X}^{(i)}) \]

3) Evaluation: solving the Poisson equation directly

4) Prolongation:
\[ \tilde{X}^{(i)} = \tilde{X}^{(i)} + P \tilde{X}^{(i+1)} \]

5) Post-smoothing:
\[ \tilde{X}^{(i)} = (L^{(i)} + D^{(i)})^{-1} B^{(i)} - (L^{(i)} + D^{(i)})^{-1} U^{(i)} \tilde{X}^{(i)} \]
Multigrid V and W Cycle of Iteration with 4 Grid Levels

V cycle

W cycle
Computing Time vs. Number of Grid Points Using SOR and Multigrid

Comparison of the Poisson Solver with Analytical Solution

Radial Electric Field Distribution (uniform cylinder beam)
Test of the Poisson Solver with Varying Bending Curvatures

Ex vs. X

Ex vs. Y
Thank you!