Poisson Solvers for Self-Consistent Multi-Particle Simulations

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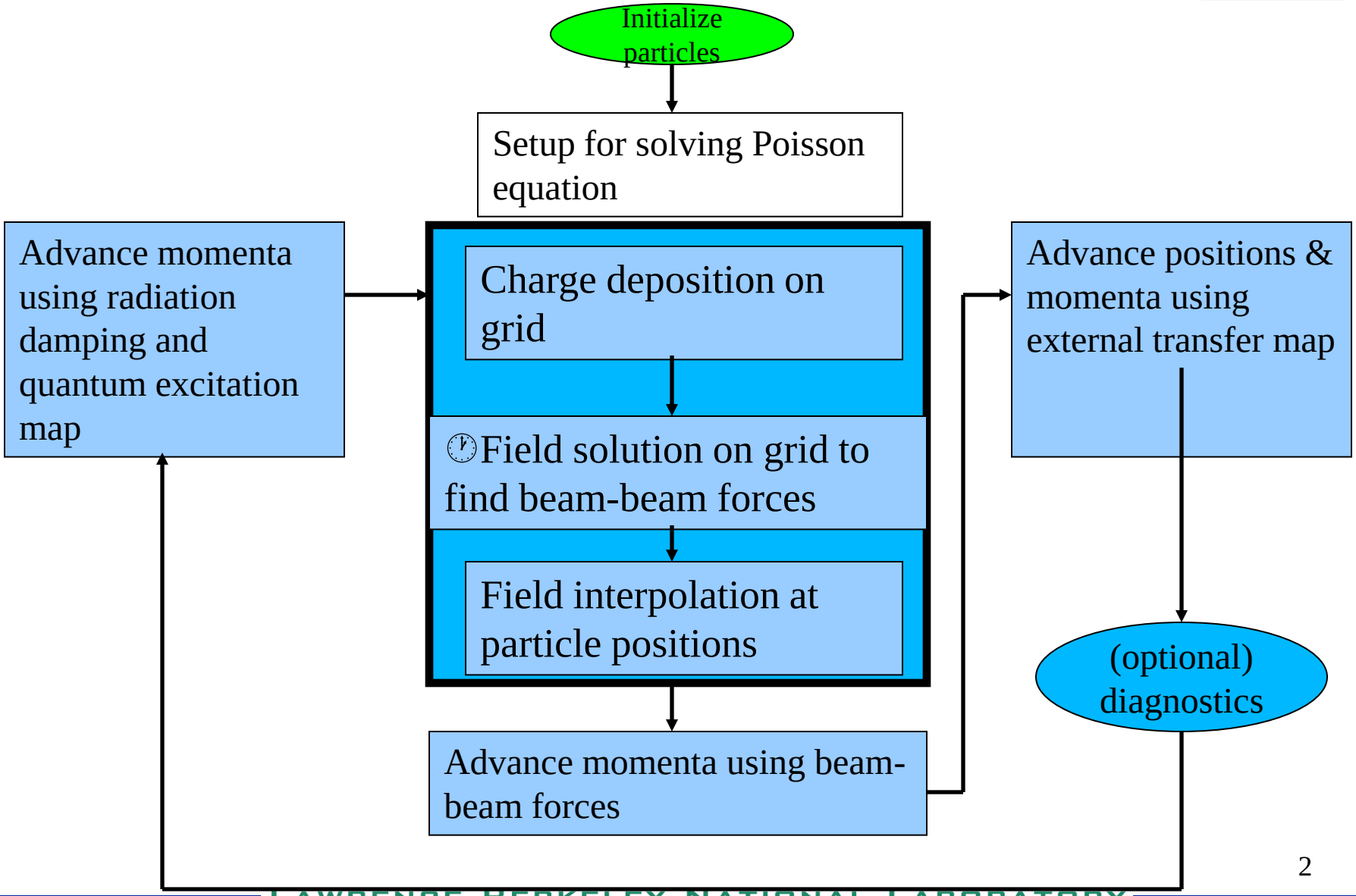
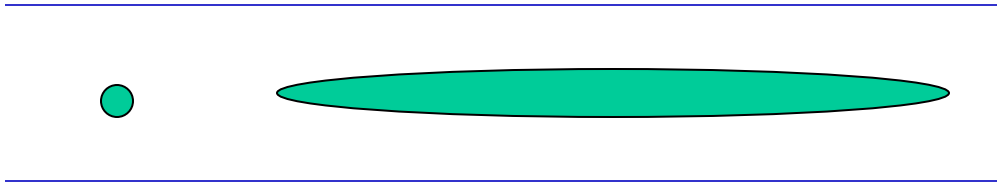
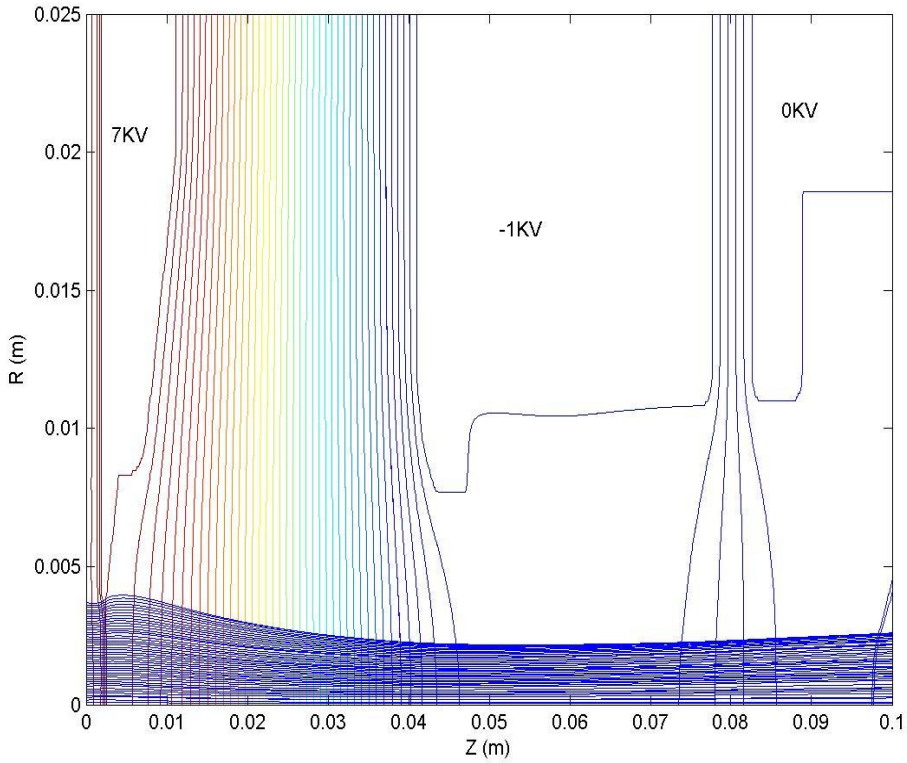
Self-Consistent Multi-Particle Simulations with Particle-In-Cell (PIC) Method



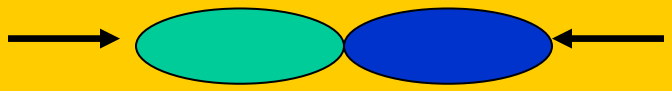
Fast Efficient Poisson Solvers with Different Boundary Conditions Are Needed

geometry in space-charge and beam-beam force calculation

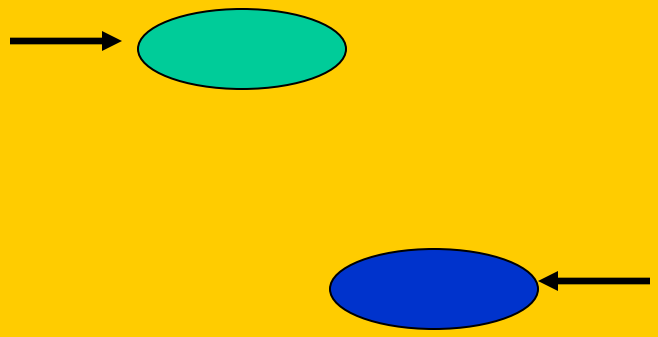




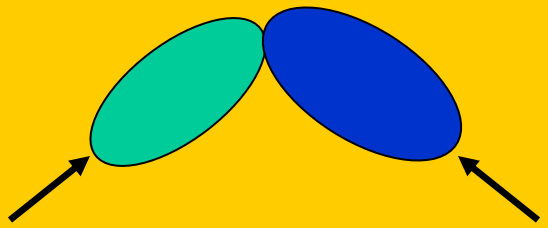
Head-on collision



Long-range collision



Crossing angle collision



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

Fully open boundary conditions

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)

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

$$\mathbf{E} = -\nabla\phi,$$

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

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

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

Direct summation of the convolution scales as N^2 !!
N – number of total grid points ($N_x N_y$)

Green Function Solution of Poisson's Equation (open boundary conditions)

Define a new periodic potential function ϕ_c

$$\phi_c(x_i, y_j) = h_x h_y \sum_{i=1}^{2N_x} \sum_{j=1}^{2N_y} G_c(x_i - x_{i'}, y_i - y_{j'}) \rho_c(x_{i'}, y_{j'}),$$

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

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

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

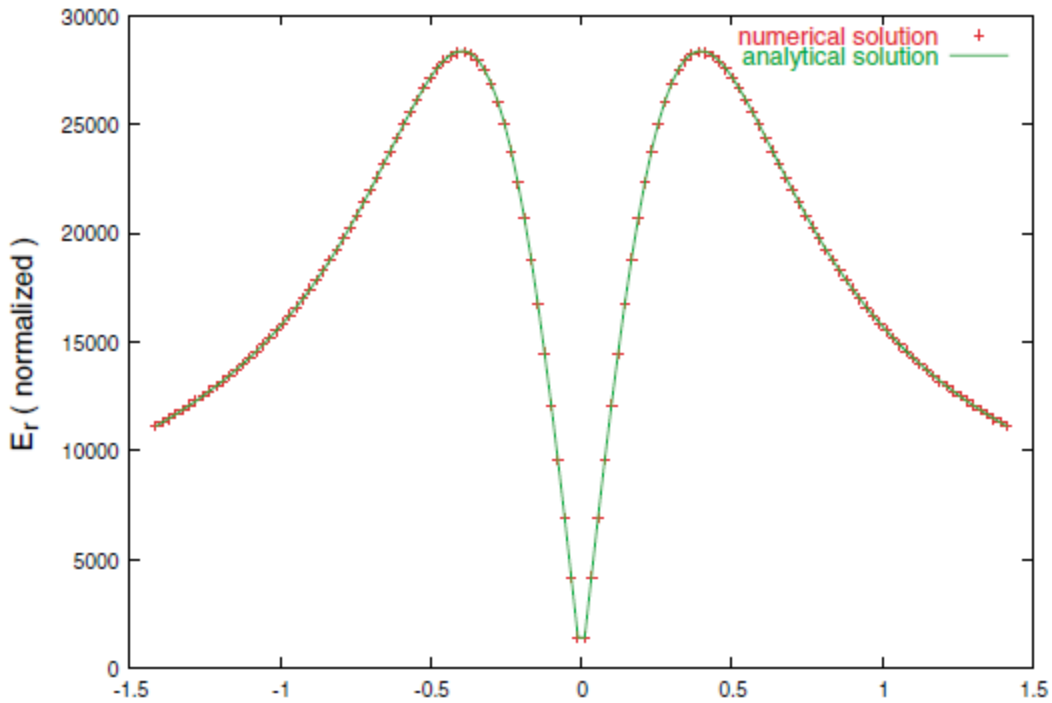
$$G_c(x_i, y_j) = G_c[x_i + 2(L_x + h_x), y_j + 2(L_y + h_y)].$$

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 ϕ_c

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



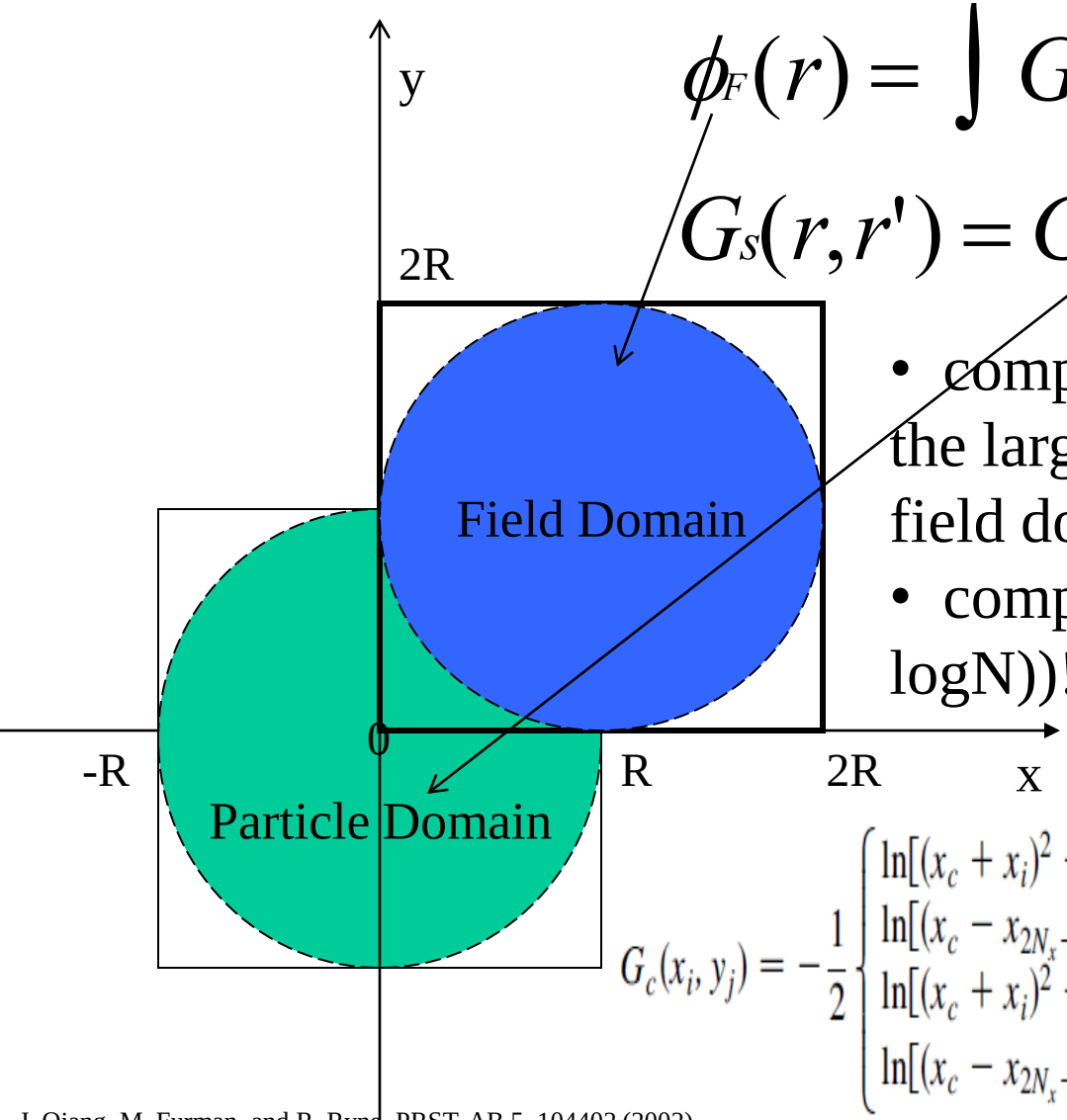
-Ref: Hockney and Easwood, ***Computer Simulation using Particles***, McGraw-Hill Book Company, New York, 1985.

-W. H. Press et al., Numerical Recipes, 1992.

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

$$\phi_F(r) = \int G_s(r,r')\rho(r')dr'$$

$$G_s(r,r') = G(r + r_s, r')$$

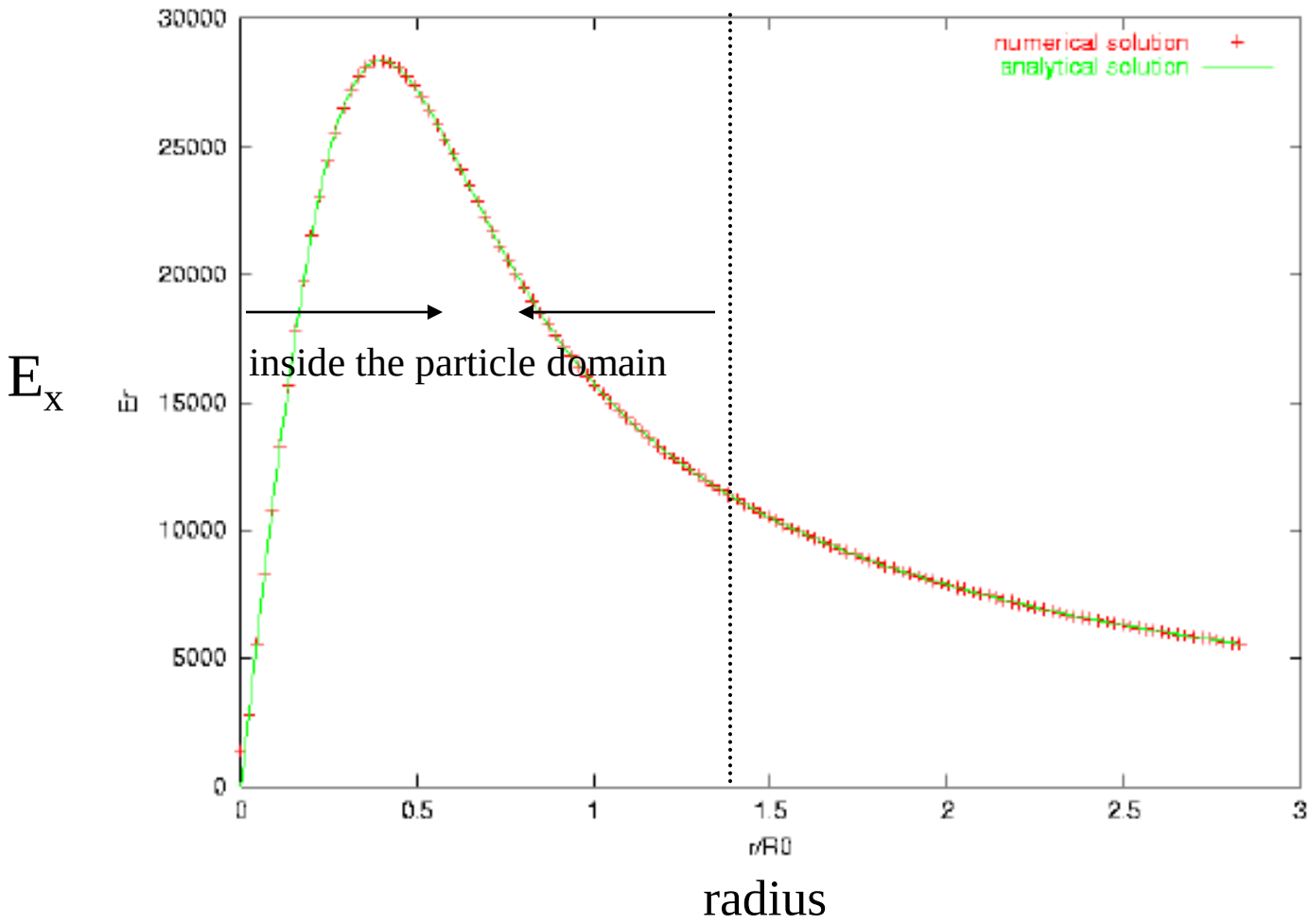


- computational domain covers only the larger one of the particle or the field domain, not both!
- computational cost scales as (O(N logN))!

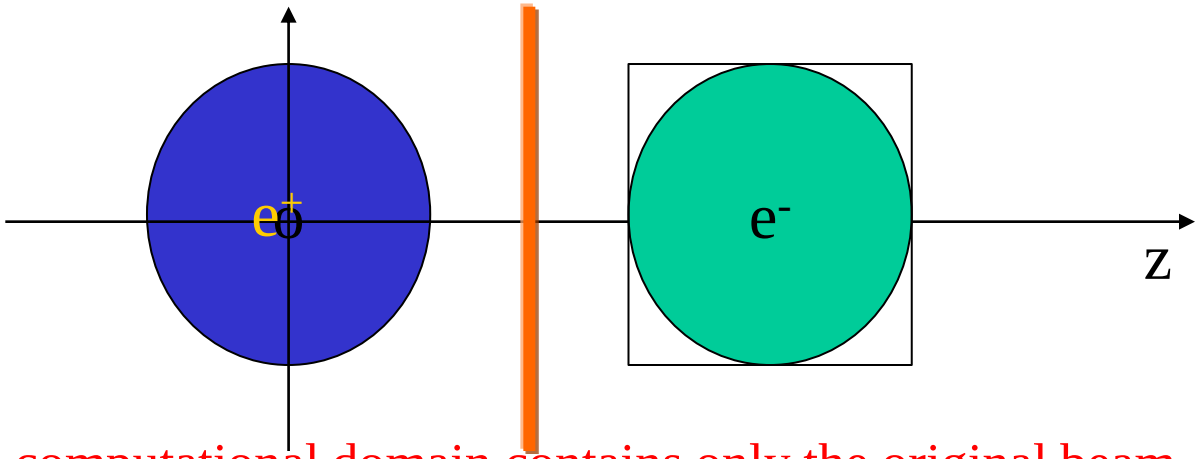
$$G_c(x_i, y_j) = -\frac{1}{2}\begin{cases} \ln[(x_c + x_i)^2 + (y_c + y_j)^2]: & 1 \le i \le N_x, 1 \le j \le N_y, \\ \ln[(x_c - x_{2N_x-i+2})^2 + (y_c + y_j)^2]: & N_x < i \le 2N_x, 1 \le j \le N_y, \\ \ln[(x_c + x_i)^2 + (y_c - y_{2N_y-j+2})^2]: & 1 \le i \le N_x, N_y < i \le 2N_y, \\ \ln[(x_c - x_{2N_x-i+2})^2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

J. Qiang, M. Furman, and R. Ryne, PRST-AB 5, 104402 (2002).

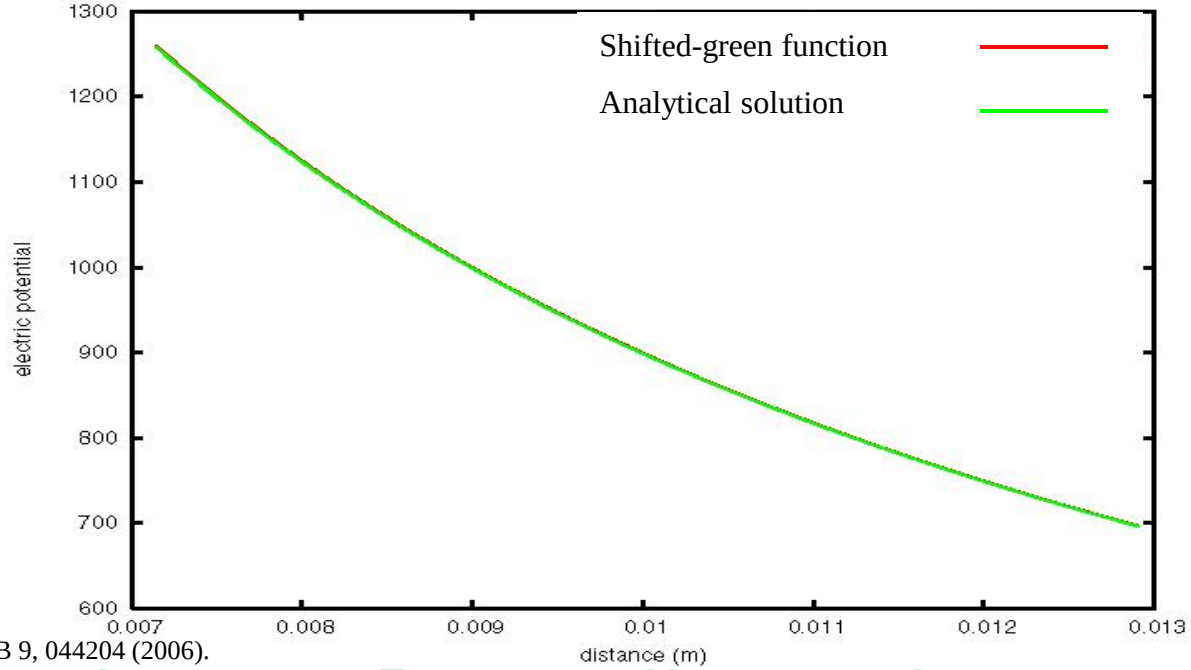
Comparison between Numerical Solution and Analytical Solution (Shifted Green Function)



Efficient Shifted Green Function Method to Calculate Image Space-Charge Effects



computational domain contains only the original beam



J. Qiang, et al., PRST-AB 9, 044204 (2006).

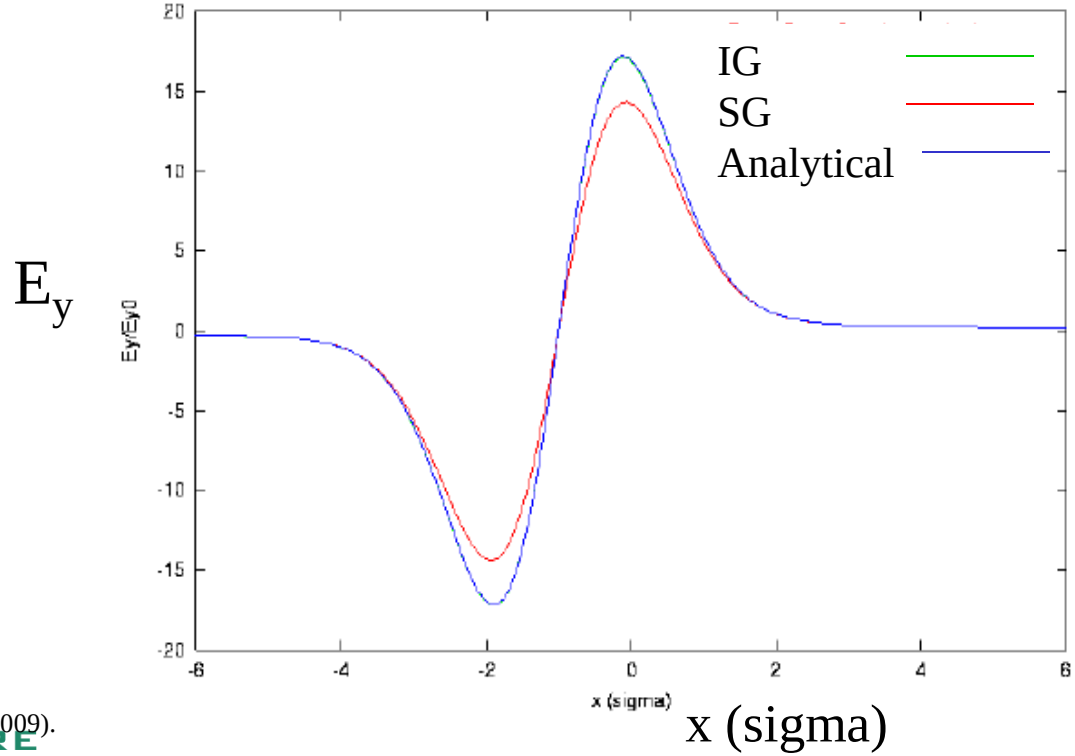
Green Function Solution of Poisson's Equation (Integrated Green Function)

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

no resolution of the Green function is needed

$$\phi_c(r_i) = \sum_{i'=1}^{2N} G_i(r_i - r_{i'})\rho_c(r_{i'}) \qquad G_i(r,r') = \oint G_s(r,r')dr'$$

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



E_y

x (sigma)

K. Ohmi, Phys. Rev. E 62 (2000) 7287.
R. D. Ryne, ICFA Beam DynamicsMini Workshop on Space Charge Simulation, Trinity College, Oxford, 2003
J. Qiang, M. Furman, and R. Ryne, J Comp. Phys. vol. 198, 278 (2004).
V. Ivanov, Int. J. Mod. Phys. A, 24, p. 869 (2009).

FFT based convolution with non-uniform grid

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

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

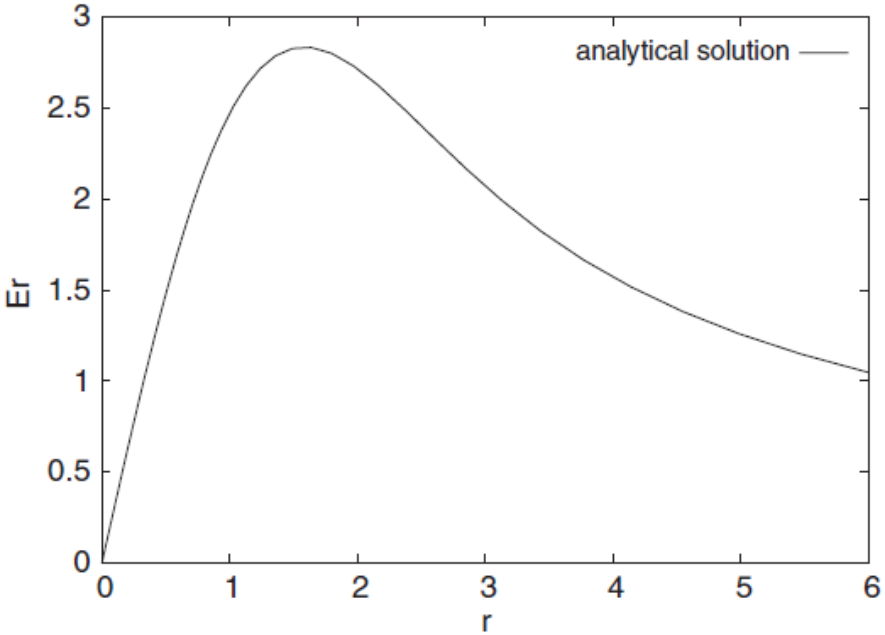
$$s = \frac{1}{k_1}\log\left(\frac{r}{k_2}\right)$$

$$\boxed{G(s,s',\theta,\theta') = -\frac{1}{2}\log(e^{2k_1(s-s')} - 2e^{k_1(s-s')}\cos(\theta-\theta') + 1)}$$

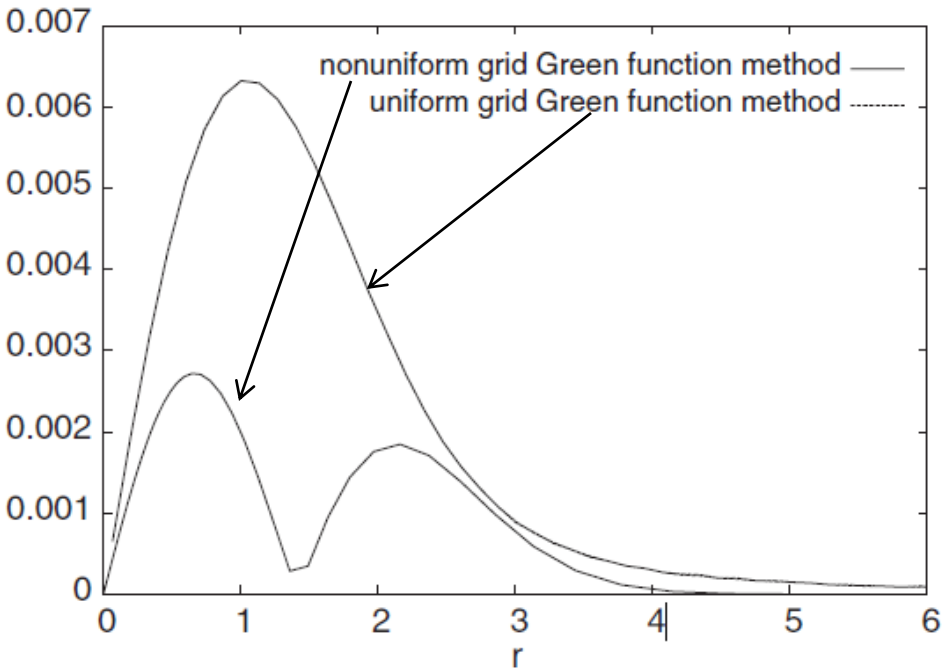
FFT can be used on uniform s-θ grid

J. Qiang et al., NIM-A, 558, p. 351 (2006).

Test of the Non-Uniform Grid FFT Solver



Errors of Er



Spectral-Finite Difference Method (2D open boundary condition)

computational domain covers only the beam by using boundary matching conditions

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

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

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

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\phi_m\right)-\frac{m^2}{r^2}\phi_m=-\frac{\rho_m}{\varepsilon_0}\quad for\quad r\le a$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\phi_m\right)-\frac{m^2}{r^2}\phi_m=0\quad for\quad r>a$$

Solution of Poisson's Equation (Spectral-Finite Difference)

$$For \quad r \le a:$$

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

$$\frac{\partial}{\partial r}\phi_m = 0 \quad for \quad r=0 \quad and \quad m=0$$

$$\phi_m = 0 \quad for \quad r=0 \quad and \quad m>0$$

$$For \quad r \ge a:$$

$$\phi = c\, r^{-m} \qquad m>0$$

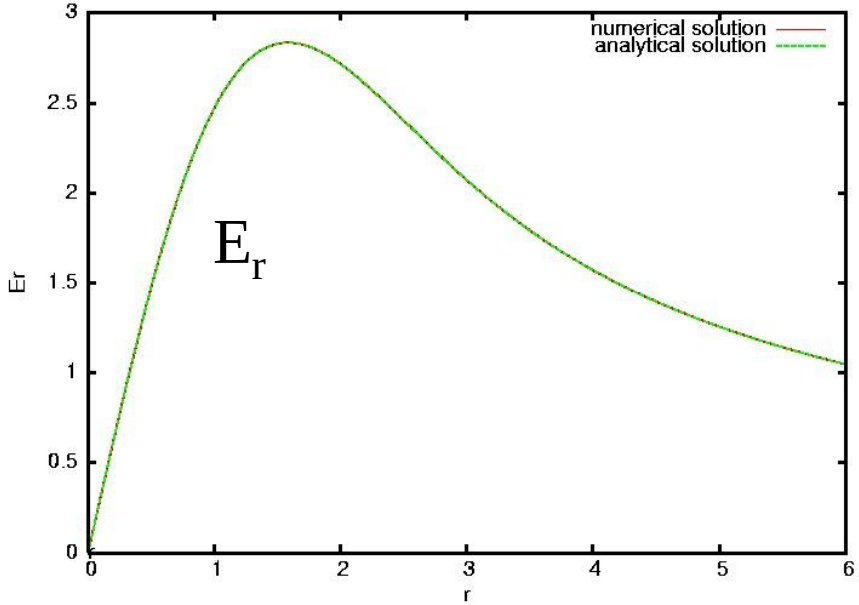
$$\phi = c\ln(r) \qquad m=0$$

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

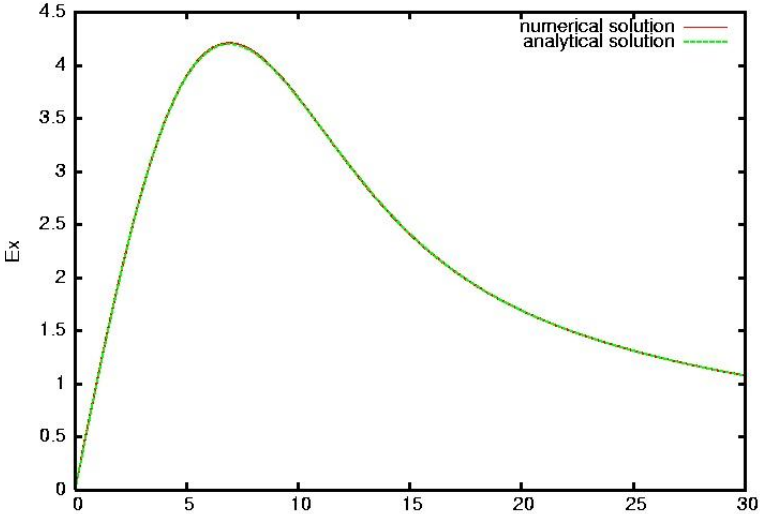
N is the number of radial grid points.

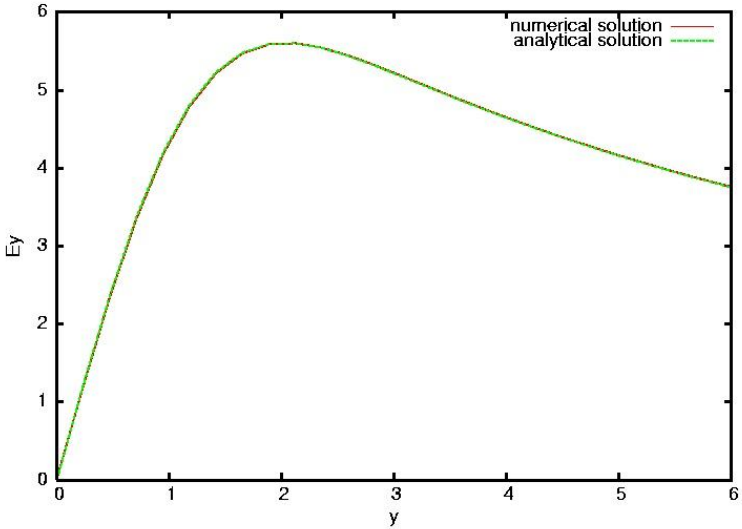
Comparison between Numerical Solution and Analytical Solution

aspect ratio =1



aspect ratio =5





3D Poisson Solver with Transverse Rectangular Pipe

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}=-\frac{\rho}{\epsilon_0}$$

with boundary conditions

$$\begin{aligned}\phi(x=0,y,z) &= 0,\\ \phi(x=a,y,z) &= 0,\\ \phi(x,y=0,z) &= 0,\\ \phi(x,y=b,z) &= 0,\\ \phi(x,y,z=\pm\infty) &= 0,\end{aligned}$$

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

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

where

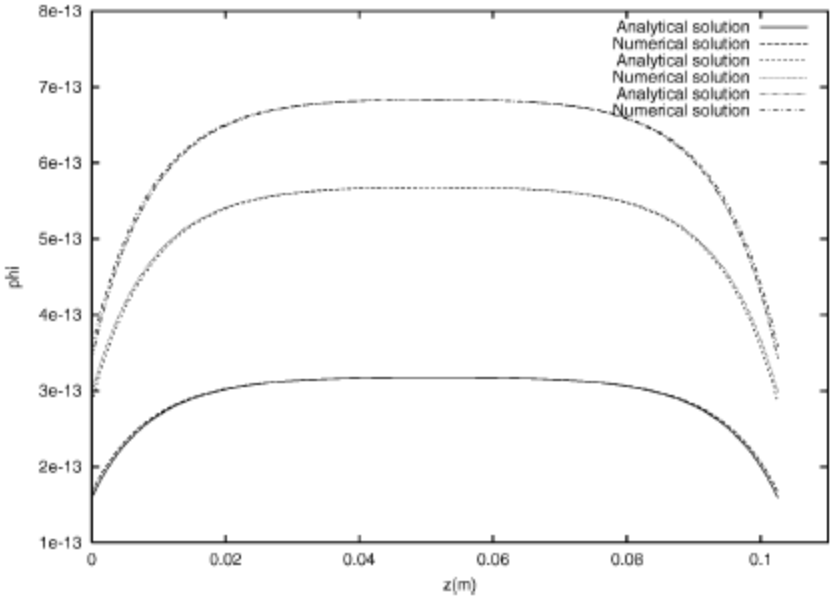
$$\rho^{lm}(z)=\frac{4}{ab}\int_0^a\int_0^b\rho(x,y,z)\sin(\alpha_l x)\sin(\beta_m y),$$

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

$$\frac{\partial^2\phi^{lm}(z)}{\partial z^2}-\gamma_{lm}^2\phi^{lm}(z)=-\frac{\rho^{lm}(z)}{\epsilon_0},$$

$$\frac{\phi_{n+1}^{lm}-2\phi_n^{lm}+\phi_{n-1}^{lm}}{h_z^2}-\gamma_{lm}^2\phi_n^{lm}=-\frac{\rho_n^{lm}}{\epsilon_0},$$

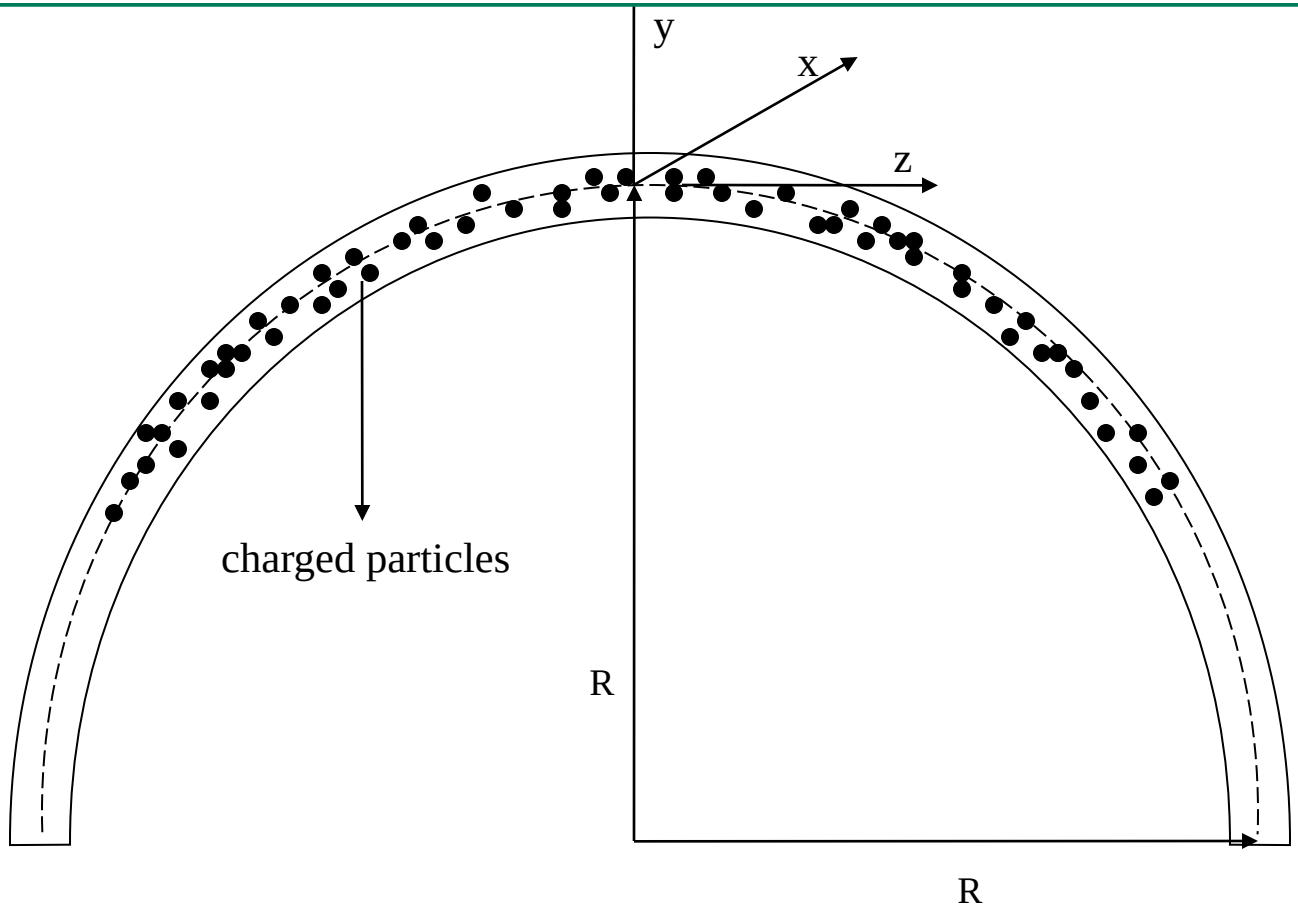
$$\begin{aligned}\phi_{-1}^{lm}&=\exp(-\gamma_{lm}h_z)\phi_0^{lm}, &\quad n=0,\\ \phi_{N+1}^{lm}&=\exp(-\gamma_{lm}h_z)\phi_N^{lm}, &\quad n=N.\end{aligned}$$



J. Qiang, and R. Ryne, Comput. Phys. Comm. 138, p. 18 (2001).

3D Poisson Solver inside a Ring with a Long Bunch

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



J. Qiang, and R. L. Gluckstern, Comput. Phys. Comm. 160, p. 120 (2004).

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

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

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

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

$$\nabla_\perp^2\phi_n + \frac{1}{R}\frac{1}{1+\frac{r\cos(\theta)}{R}}\left(\cos(\theta)\frac{\partial\phi_n}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial\phi_n}{\partial r}\right)$$
$$+ \frac{1}{\left(1+\frac{r\cos(\theta)}{R}\right)^2}\left(\frac{1}{4}\phi_{n-2} - \frac{1}{2}(2n+1)\phi_n + (n+2)(n+1)\phi_{n+2}\right)\frac{1}{A^2} = -\rho_n.$$

$$\nabla_\perp^2\phi_n^1 = -\rho_n,$$

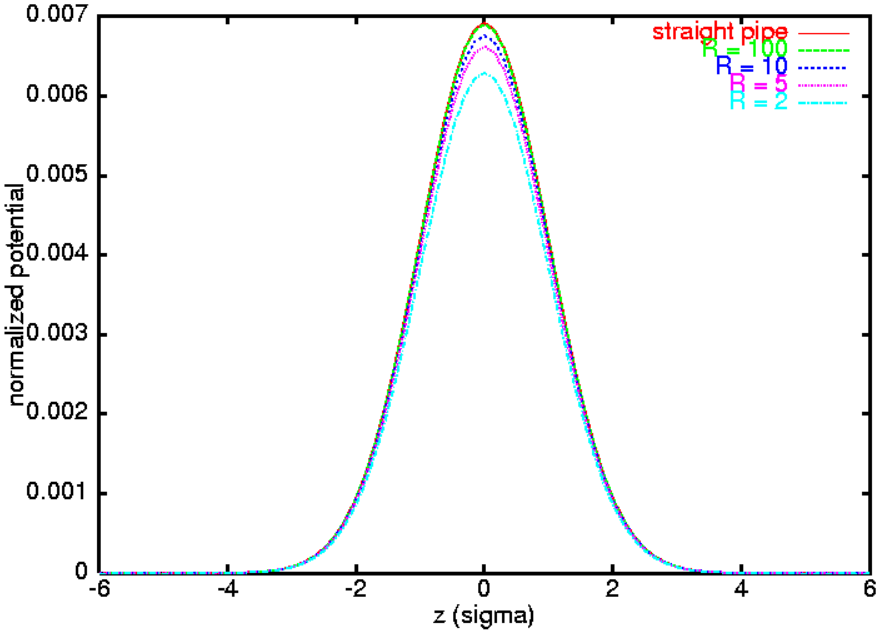
$$\nabla_\perp^2\phi_n^2 = -\rho_n - \frac{1}{R}\frac{1}{1+\frac{r\cos(\theta)}{R}}\left(\cos(\theta)\frac{\partial\phi_n^1}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial\phi_n^1}{\partial r}\right)$$
$$+ \left(\frac{1}{4}\phi_{n-2}^1 - \frac{1}{2}(2n+1)\phi_n^1 + (n+2)(n+1)\phi_{n+2}^1\right)\frac{1}{\left(1+\frac{r\cos(\theta)}{R}\right)^2}\frac{1}{A^2},$$

$$\nabla_\perp^2\phi_n^3 = -\rho_n - \frac{1}{R}\frac{1}{1+\frac{r\cos(\theta)}{R}}\left(\cos(\theta)\frac{\partial\phi_n^2}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial\phi_n^2}{\partial r}\right)$$
$$+ \left(\frac{1}{4}\phi_{n-2}^2 - \frac{1}{2}(2n+1)\phi_n^2 + (n+2)(n+1)\phi_{n+2}^2\right)\frac{1}{\left(1+\frac{r\cos(\theta)}{R}\right)^2}\frac{1}{A^2},$$

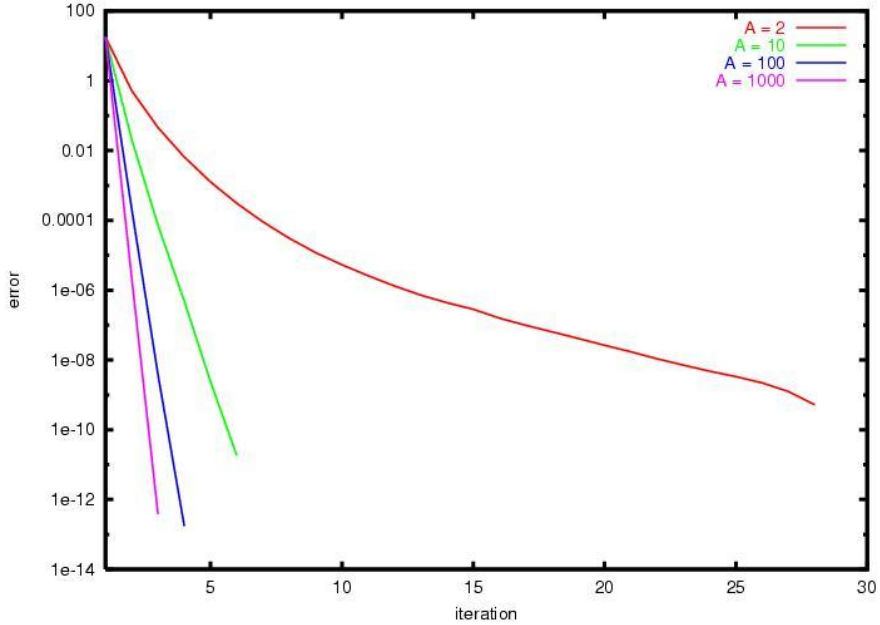
$$\vdots = \vdots.$$

Normalized Electric Potential and Convergence

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

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

$$where:$$

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

$$\varphi(r,\theta,z) = \sum \phi^m(r,z)\exp(-im\theta)$$

$$we\ obtain:$$

$$\frac{\partial^2 \phi^m}{\partial r^2} + \frac{1}{r}\frac{\partial \phi^m}{\partial r} - \frac{m^2}{r^2}\phi^m + \frac{\partial^2 \phi^m}{\partial z^2} = -\frac{\rho^m}{\varepsilon}$$

Multigrid Spectral Finite-Difference Solution of Poisson's Equation in Frenet-Serret Coordinates

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

$where:$

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

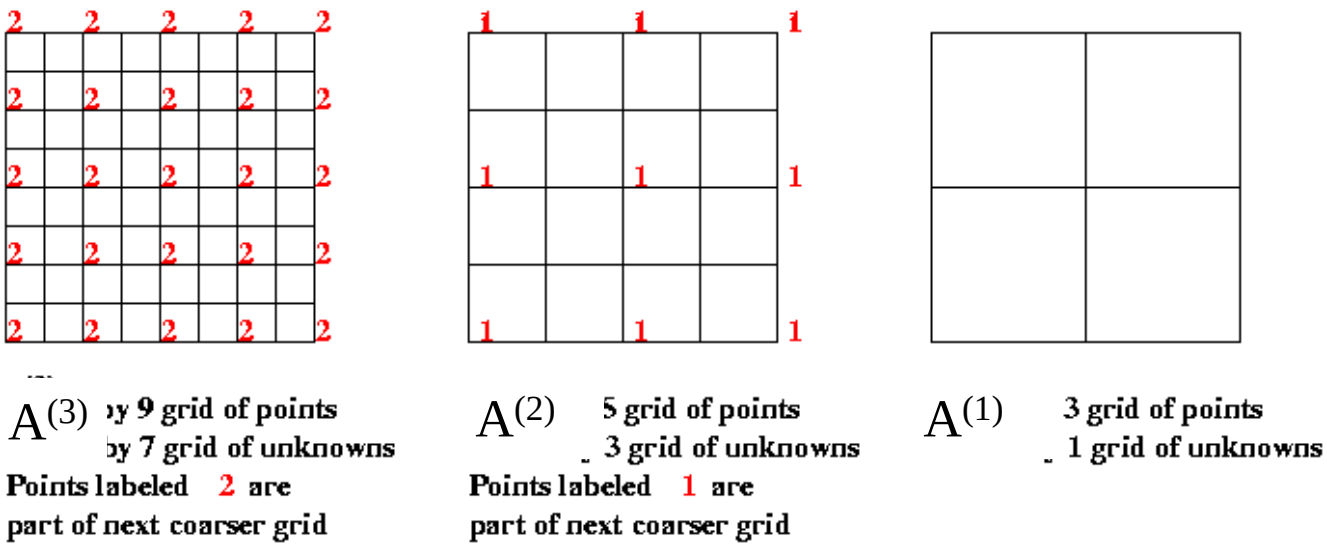
$$\phi(x,y,z)=\sum\phi^m(x,z)\sin(m\pi y/a)$$

$we\ obtain:$

$$\frac{1}{1+hx}\left(\frac{\partial}{\partial x}(1+hx)\frac{\partial\phi^m}{\partial x}+\frac{\partial}{\partial z}\frac{1}{1+hx}\frac{\partial\phi^m}{\partial z}\right)-\frac{m^2\pi^2}{a^2}\phi^m=-\frac{\rho^m}{\varepsilon}$$

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



-W. H. Press et al., Numerical Recipes, 1992.

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

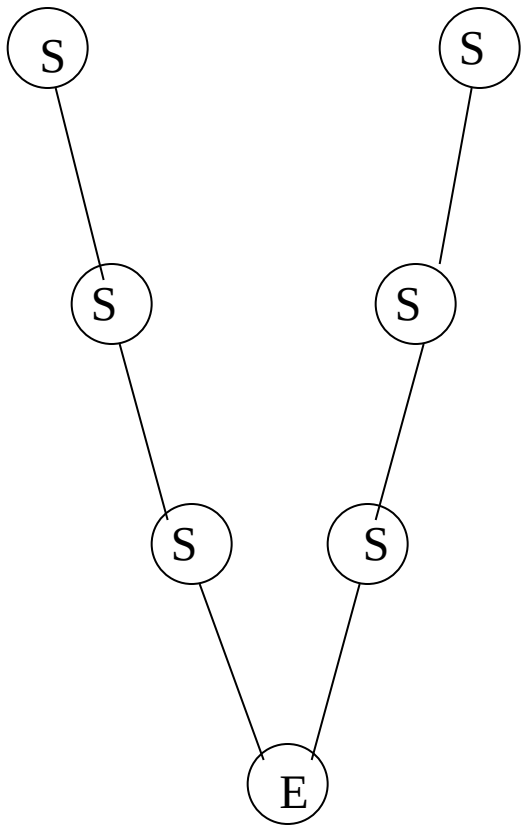
4) Prolongation:

$$\tilde{X}^{(i)} = \tilde{X}^{(i)} + P\,\tilde{X}^{(i+1)}$$

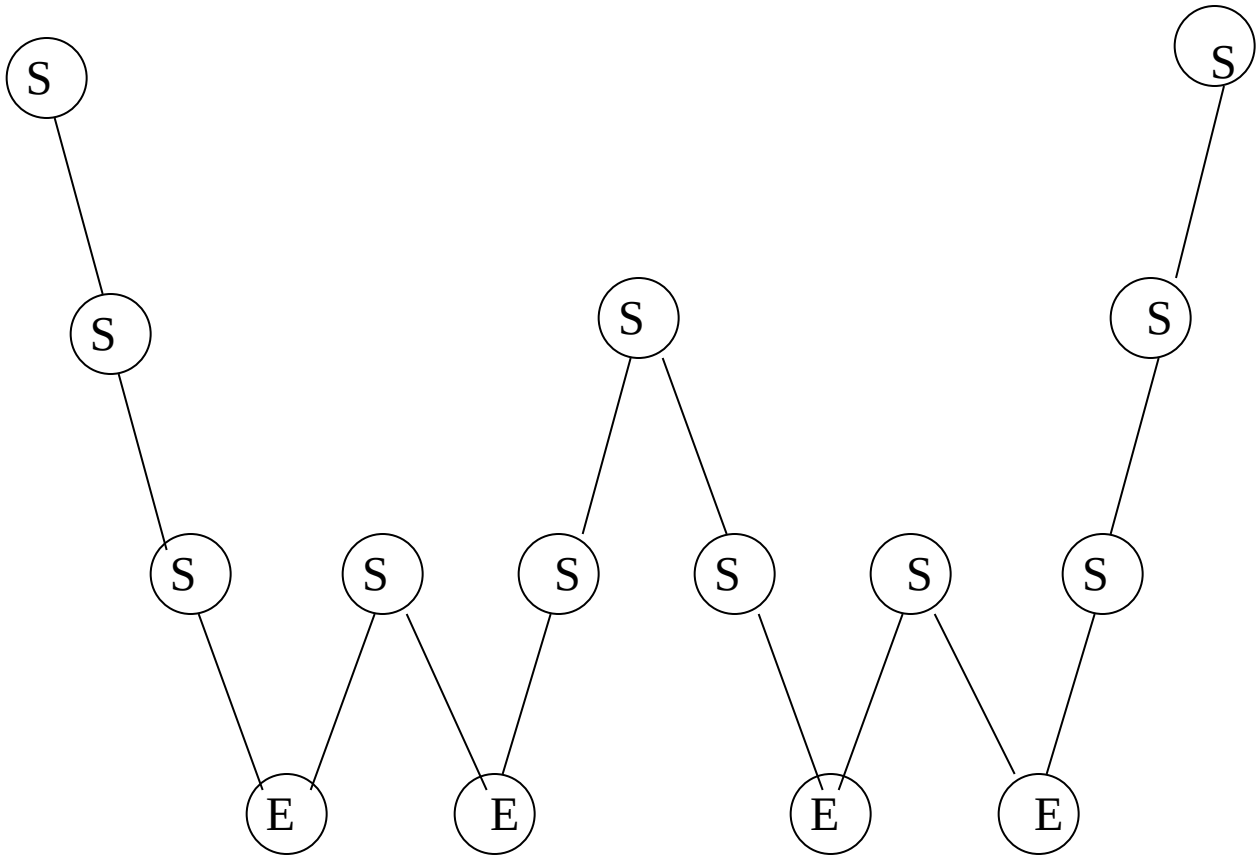
5) Post-smoothing:

$$\tilde{X}^{(i)} = (L^{(i)} + D^{(i)})^{-1} B^{(i)} - (L^{(i)} + D^{(i)})^{-1} U^{(i)} \tilde{X}^{(i)}$$

Multigrid V and W Cycle of Iteration with 4 Grid Levels

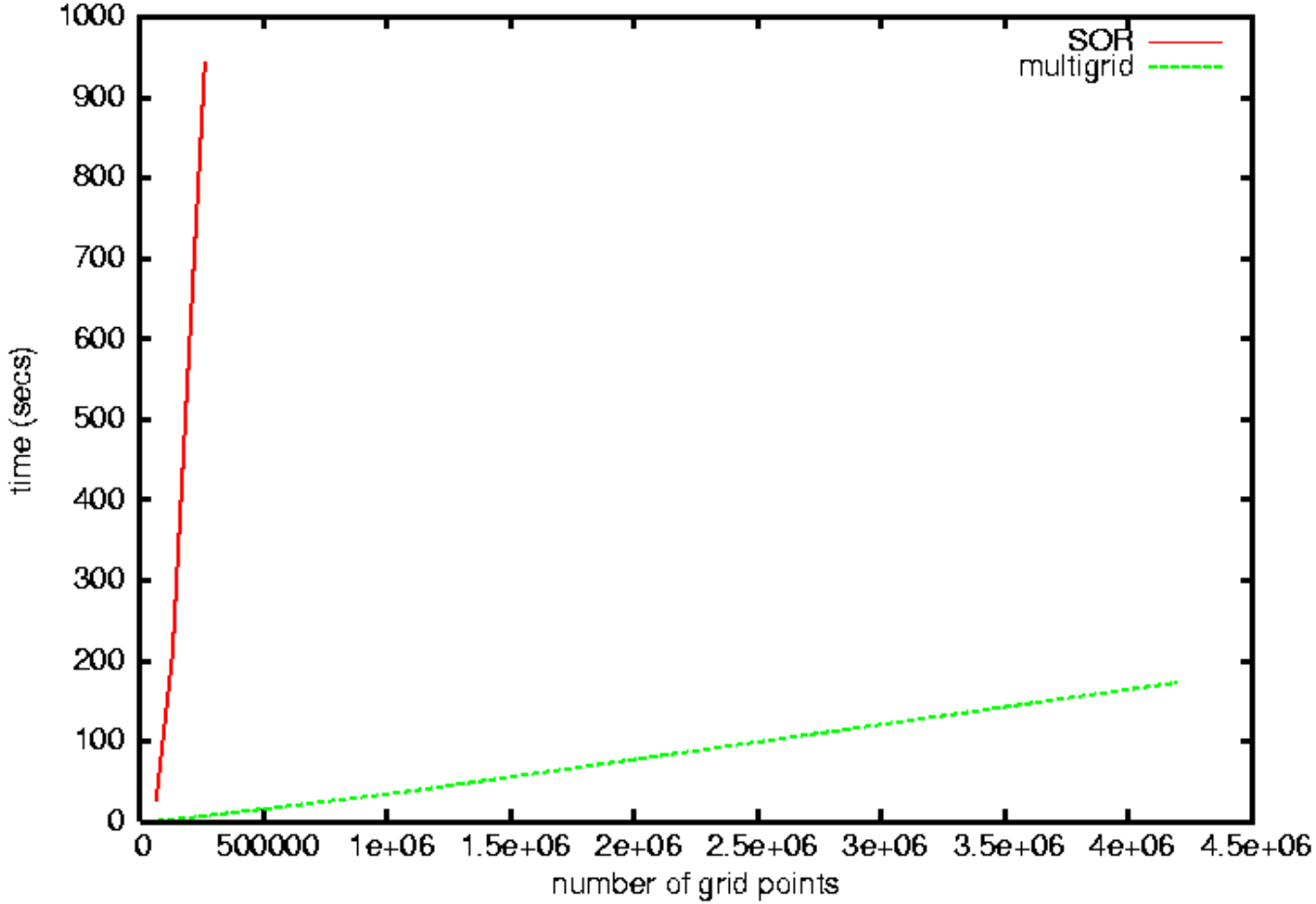


V cycle



W cycle

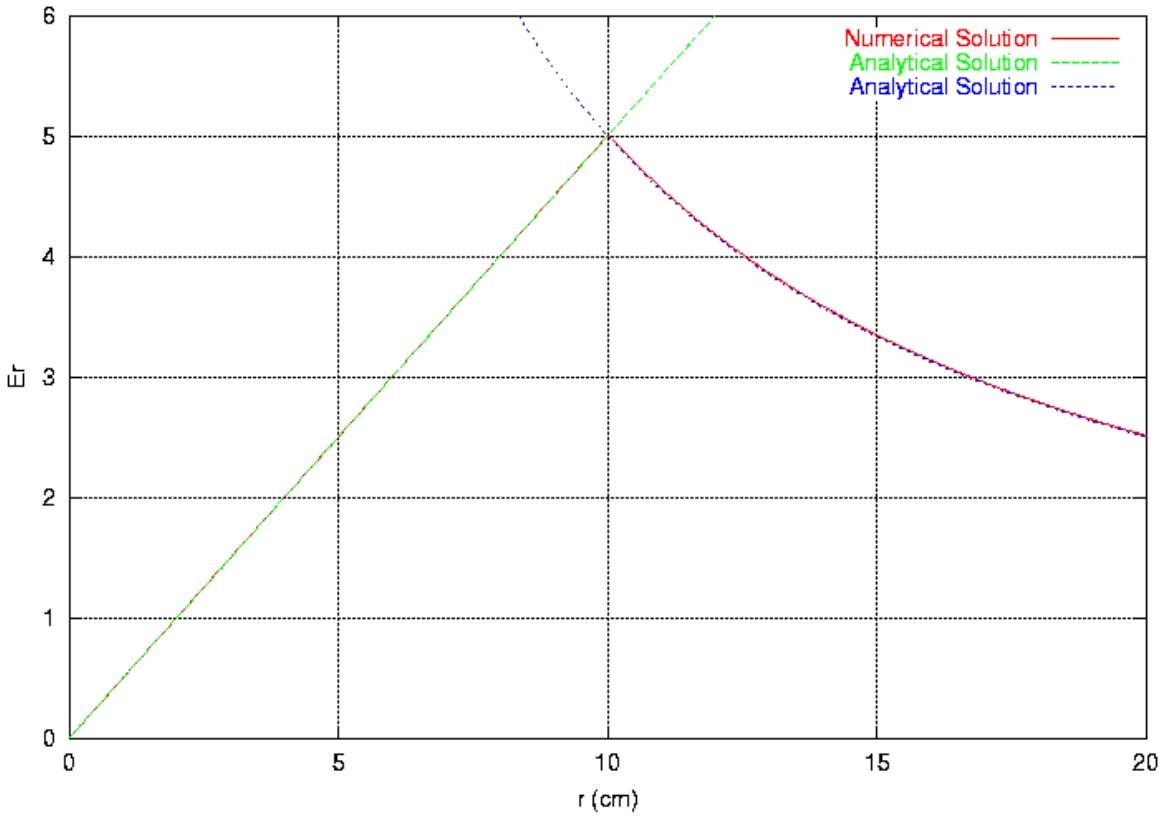
Computing Time vs. Number of Grid Points Using SOR and Multigrid



J. Qiang, D. Todd, D. Leitner, Comput. Phys. Comm. 175. p. 416 (2006).

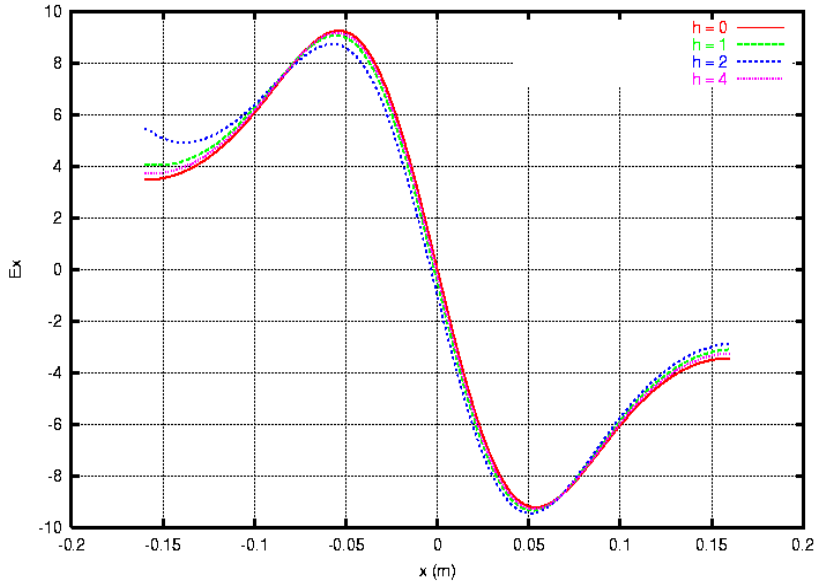
Comparison of the Poisson Solver with Analytical Solution

Radial Electric Field Distribution (uniform cylinder beam)

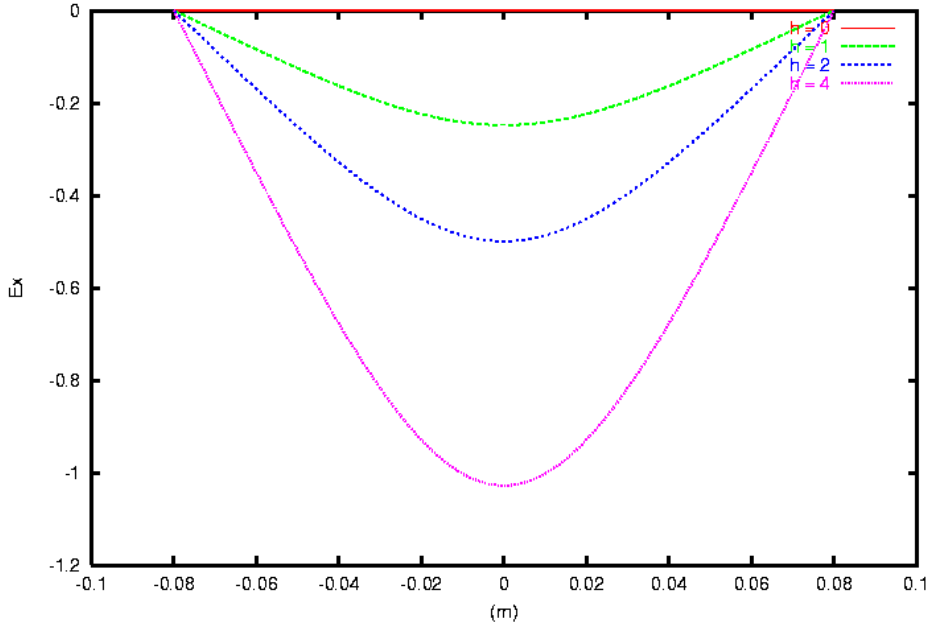


Test of the Poisson Solver with Varying Bending Curvatures

Ex vs. X



Ex vs. Y



Thank you!

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