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FAKULTÄT FÜR INFORMATIK UND ELEKTROTECHNIK
UNIVERSITÄT ROSTOCK

FFT-based Algorithms for 3-D Space Charge Calculation

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Outline

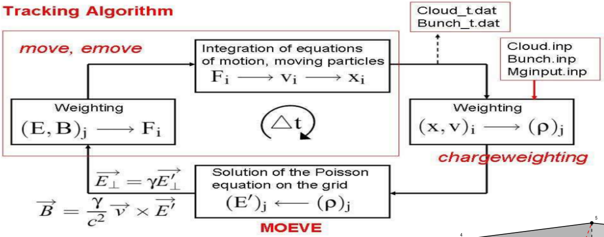
- MOEVE PIC Tracking package
- Space charge effect calculation
- FFT-based algorithms for 3-D space charge calculation
- Advantages and disadvantages
- Space charge including image charge
- Tracking comparison with ASTRA

MOEVE PIC Tracking package

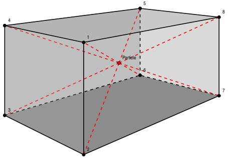
Gains: [Enhanced by A. Markoviḱ, G. Pöplau]

- Simulate the interaction between a positron beam and electron clouds
- Simulate the interaction between an electron bunch and ion clouds
- 3D particle tracking including space charge effect with rectangular (elliptical transverse) cross-section

Tracking algorithm of MOEVE PIC



- cubic computational domain
- Particle-mesh method
- (Non)Eqidistant grid in each axis



[0] PhD.Thesis of A. Markovik

Poisson Equation

The potential φ of the bunch (distribution of macro particles) is calculated from Poisson equation:

$$-\Delta\varphi = \frac{\varrho}{\varepsilon_0} \quad \text{in } \Omega \subset \mathbb{R}^3$$

φ	potential
ϱ	space charge density
Ω	computational domain

$$E = -grad\varphi$$

Boundary conditions:

Dirichlet:

$$\varphi = 0 \text{ on } \partial\Omega$$

Neumann:

$$\frac{\partial\varphi}{\partial n} = \varphi_{\partial\Omega}$$

periodic:

$$\varphi_{-\partial\Omega} = \varphi_{\partial\Omega}$$

open:

$$\frac{\partial\varphi}{\partial n} + \frac{1}{r}\varphi = 0$$

free and mixed boundary conditions.

Numerical methodologies sketch

- Multigrid method:

  MG (multigrid), CG(conjugate gradient), MGCG , SOR (successive over-relaxation), BiCG, BiCGSTAB, PCBiCG

- FFT-based method:

  Spectral method

  GF (Green's function), IGF (Integrated Green's function)

FFT-based method: Spectral Method

Discretization by finite difference provides the following system of linear equations:

$$Lu = f$$

$$L = \begin{pmatrix} -2 & \boxed{N} & 0 & \dots & \boxed{P} \\ 1 & -2 & 1 & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & & 1 & -2 & 1 \\ \boxed{P} & 0 & \dots & \boxed{N} & -2 \end{pmatrix}$$

Dirichlet:	P =0,	N =1
Neumann:	P =0,	N =2
Periodic:	P =1,	N =1

Theorem (Spectral Decomposition, Charles Van Loan, 1992)

If we define the discrete Laplace matrices for the above five boundary conditions as L, there is an invertible matrix V for each boundary condition, such that

$$V^{-1}LV = \Lambda,$$

here Λ is the spectral matrix, which is diagonal.

Dirichlet-Dirichlet: *V=DST,* $\Lambda_{jj} = 4\sin^2(\frac{j\pi}{2n}),\quad j = 1:n-1.$

Dirichlet-Neumann: *V=DST-II,* $\Lambda_{jj} = 4\sin^2(\frac{2j-1}{4n}\pi),\quad j = 1:n.$

Neumann-Dirichlet: *V=DCT-II,* $\Lambda_{jj} = 4\sin^2(\frac{2j-1}{4n}\pi),\quad j = 1:n.$

and

Neumann-Neumann: *V=DCT,* $\Lambda_{jj} = 4\sin^2(\frac{j\pi}{2n}),\quad j = 0:n.$

Periodic: *V=IDFT,* $\Lambda_{jj} = 4\sin^2(\frac{j\pi}{2n}),\quad j = 0:n-1.$

with this factorization of L, we solve the linear system $Lu = f$ as:

$$\begin{aligned}
Lu &= f \\
V\underline{V^{-1}LV}V^{-1}u &= f \\
\Lambda V^{-1}u &= V^{-1}f \\
V^{-1}u &= \Lambda^{-1}V^{-1}f \\
\hat{u} &= \Lambda^{-1}\hat{f} \\
u &= V\Lambda^{-1}V^{-1}f
\end{aligned}$$

3D Situation

The resulting system of linear equations:

$$\left(\frac{1}{h_x^2}(I_{N_z} \otimes I_{N_y} \otimes L_{N_x}) + \frac{1}{h_y^2}(I_{N_z} \otimes L_{N_y} \otimes I_{N_x}) + \frac{1}{h_z^2}(L_{N_z} \otimes I_{N_y} \otimes I_{N_x})\right)u = f$$

Eigenvalues: $\Lambda_{x,y,z} = [\lambda_{i,j,k}]$. $\Rightarrow$ the linear system of equations can be written as:

$$\left(I \otimes I \otimes \frac{1}{h_x^2}\Lambda + I \otimes \frac{1}{h_y^2}\Lambda \otimes I + \frac{1}{h_z^2}\Lambda \otimes I \otimes I\right)(V^{-1} \otimes V^{-1} \otimes V^{-1})u = (V^{-1} \otimes V^{-1} \otimes V^{-1})f$$

$(V^{-1} \otimes V^{-1} \otimes V^{-1})$: three dimensional Fourier-class transform. In the "frequency domain" we have:

$$\hat{u}_{i,j,k} = \frac{1}{\frac{\lambda_i}{h_x^2} + \frac{\lambda_j}{h_y^2} + \frac{\lambda_k}{h_z^2}}\hat{f}_{i,j,k}$$

Standard Green´s function(GF) method

Standard Green's function method:

$$\underbrace{\varphi(x,y,z)}_{\varphi(x_i,y_j,z_k)} = \frac{1}{4\pi\varepsilon_0} \underbrace{\int\int\int}_{\sum\sum\sum} \underbrace{G(x,x',y,y',z,z')}_{G(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'})} \underbrace{\rho(x',y',z')}_{\rho(x_{i'},y_{j'},z_{k'})} \underbrace{dx'dy'dz'}_{h_x h_y h_z}$$

With Green's function:

$$G(x,x',y,y',z,z') = \frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}.$$

Discrete form:

$$\varphi(x_i,y_j,z_k)_{GF} \approx \frac{h_x h_y h_z}{4\pi\varepsilon_0} \sum_{i'=1}^{N_x}\sum_{j'=1}^{N_y}\sum_{k'=1}^{N_z} G(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'})\rho(x_{i'},y_{j'},z_{k'})$$

Integrated Green´s function (IGF) method

Integrated Green's function method [Ji Qiang, 2006]:

$$\underbrace{\varphi(x,y,z)}_{\varphi(x_i,y_j,z_k)} = \underbrace{\frac{1}{4\pi\varepsilon_0}\int\int\int G(x,x',y,y',z,z')\overbrace{\rho(x',y',z')}^{\rho(x_{i'},y_{j'},z_{k'})}dx'dy'dz'}_{\sum\sum\sum \tilde{G}(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'})}$$

With integrated Green's function:

$$\tilde{G}(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'}) = \int_{x_{i'}-h_x/2}^{x_{i'}+h_x/2}\int_{y_{j'}-h_y/2}^{y_{j'}+h_y/2}\int_{z_{k'}-h_z/2}^{z_{k'}+h_z/2} G(x_i,x',y_j,y',z_k,z')dx'dy'dz'$$

Discrte form:

$$\varphi(x_i,y_j,z_k)_{IGF} \approx \frac{1}{4\pi\varepsilon_0}\sum_{i'=1}^{N_x}\sum_{j'=1}^{N_y}\sum_{k'=1}^{N_z}\rho(x_{i'},y_{j'},z_{k'})\tilde{G}(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'})$$

Extensions:

[R. W. Hockney and J. W. Eastwood, 1994]

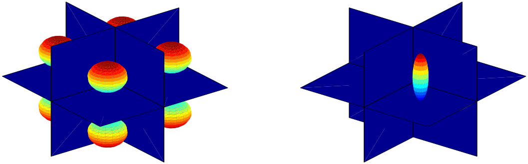


Figure: The expansion of Green's function (Left side) and the expansion of charge density (Right side).

The expansion of Green's function is called **real even** symmetry expansion.
Example: $[x_0, x_1, x_2, x_3] \rightarrow [x_0, x_1, x_2, x_3, x_2, x_1]$.

The expansion of charge density, **zeros** expansion:
$[\rho_0, \rho_1, \ldots, \rho_{N-1}, \rho_N] \rightarrow [\rho_0, \rho_1, \ldots, \rho_N, 0, \ldots, 0]$.

$$\varphi(x_i, y_j, z_k) \approx \frac{h_x h_y h_z}{4\pi\varepsilon_0} \sum_{i'=1}^{N_x} \sum_{j'=1}^{N_y} \sum_{k'=1}^{N_z} G(x_i - x_{i'}, y_j - y_{j'}, z_k - z_{k'}) \rho(x_{i'}, y_{j'}, z_{k'}) \Longrightarrow$$

$$\varphi(x_i, y_j, z_k) \approx \frac{h_x h_y h_z}{4\pi\varepsilon_0} \sum_{i'=1}^{2N_x-2} \sum_{j'=1}^{2N_y-2} \sum_{k'=1}^{2N_z-2} G_{ex}(x_i - x_{i'}, y_j - y_{j'}, z_k - z_{k'}) \rho_{ex}(x_{i'}, y_{j'}, z_{k'})$$

The **convolution theorem**, which is:

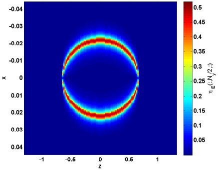
$$\mathfrak{F}\{G * \rho\} = \mathfrak{F}G \bullet \mathfrak{F}\rho$$

reveals that

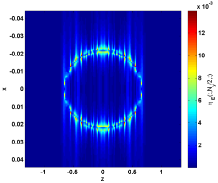
$$\varphi_{i,j,k} = \frac{h_x h_y h_z}{4\pi\varepsilon_0} \mathfrak{F}^{-1}\{[\mathfrak{F}G_{ex}]_{i,j,k} \bullet^* [\mathfrak{F}\rho_{ex}]_{i,j,k}\}$$

or

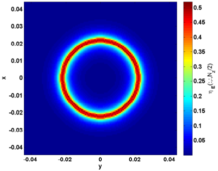
$$\varphi_{i,j,k} = \frac{1}{4\pi\varepsilon_0} \mathfrak{F}^{-1}\{[\mathfrak{F}\tilde{G}_{ex}]_{i,j,k} \bullet^* [\mathfrak{F}\rho_{ex}]_{i,j,k}\}$$



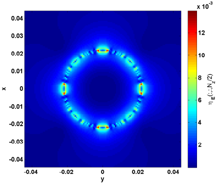
(a) GF at $(:, \frac{N_y}{2}, :)$



(b) IGF at $(:, \frac{N_y}{2}, :)$



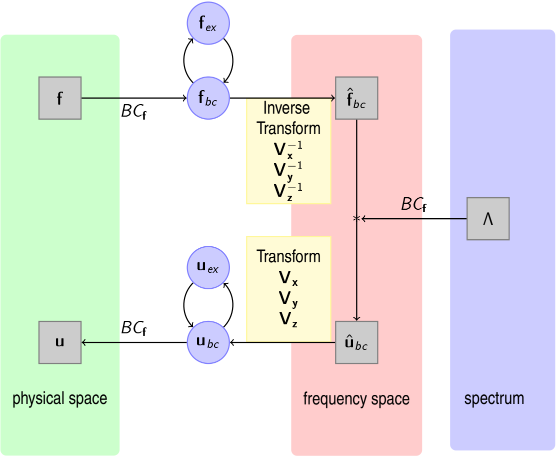
(c) GF at $(:, :, \frac{N_z}{2})$



(d) IGF at $(:, :, \frac{N_z}{2})$

Figure : Comparison of $\eta_E(i, j, k)$ for the two Green's function methods in Example 1. GF (a) (c), IGF (b) (d) .

FFT-based algorithms for 3-D space charge calculation



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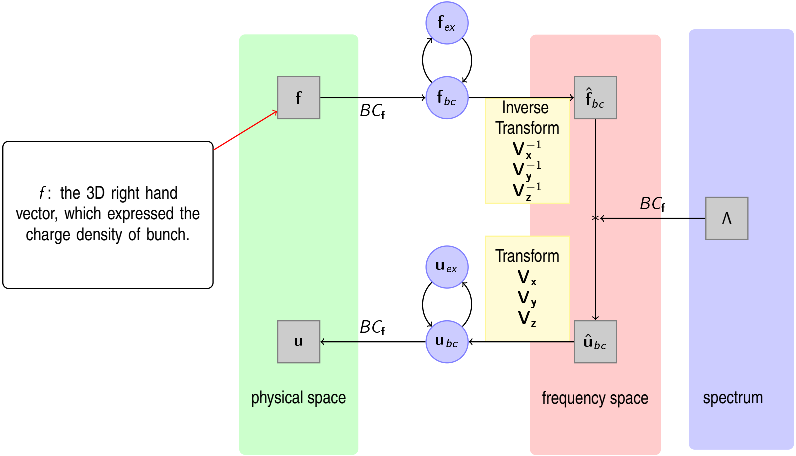

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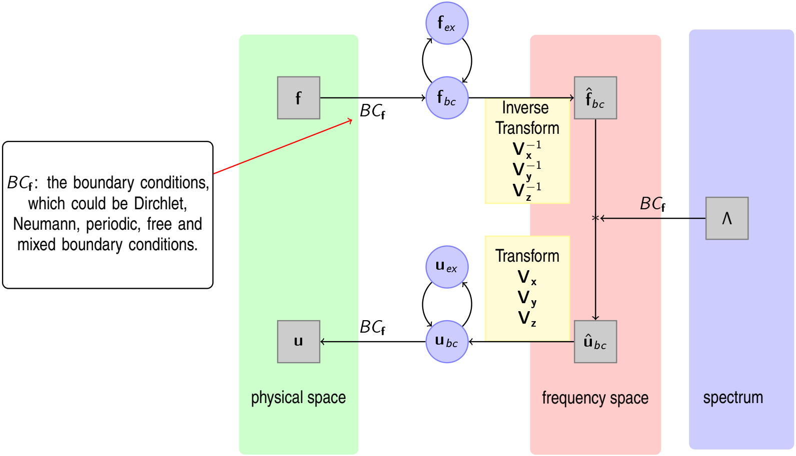

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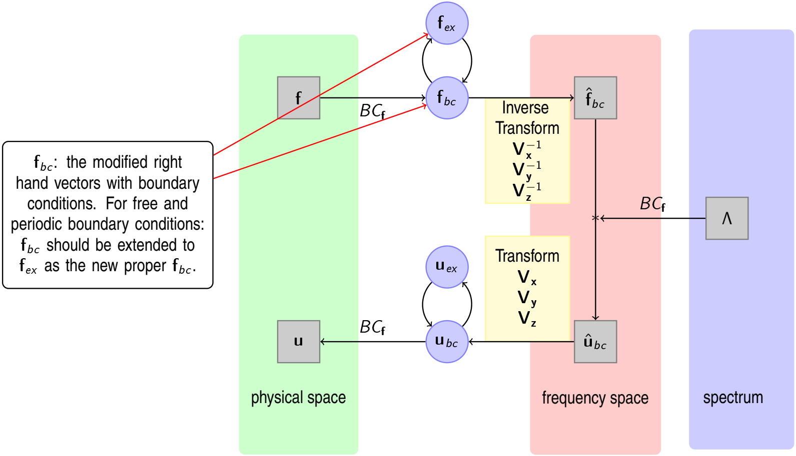

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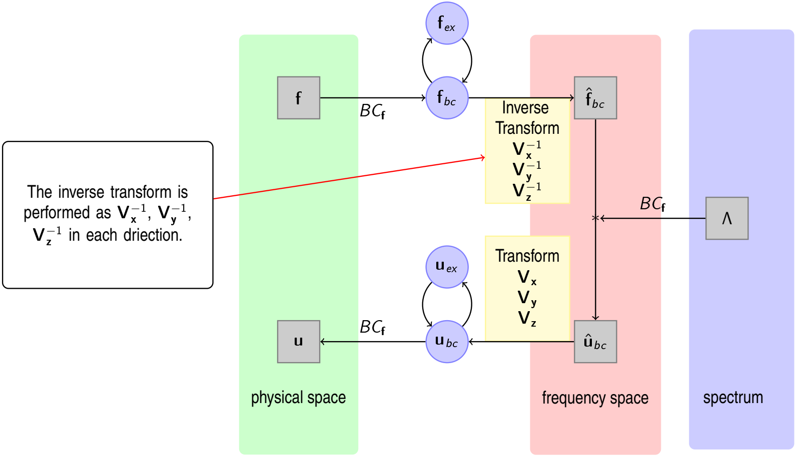

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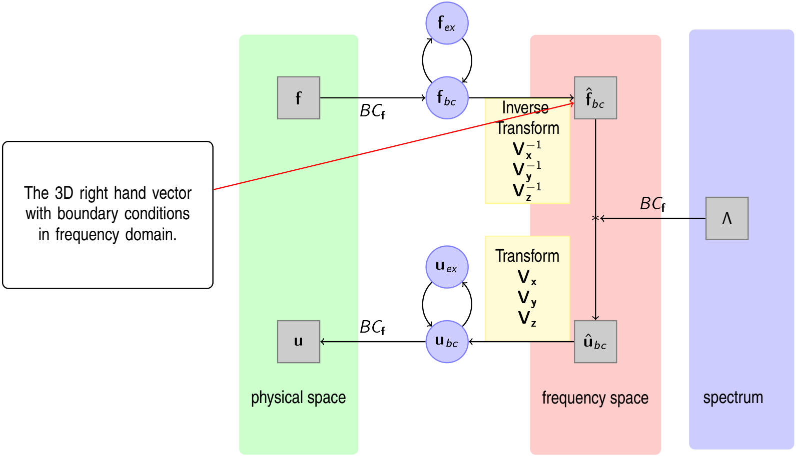

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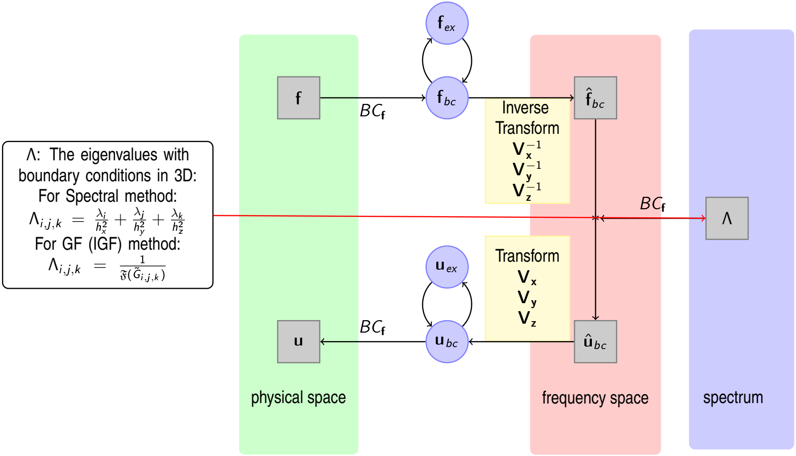

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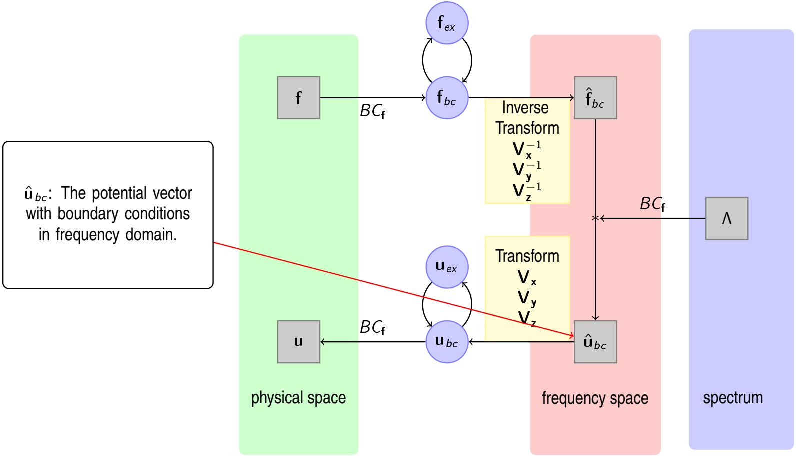

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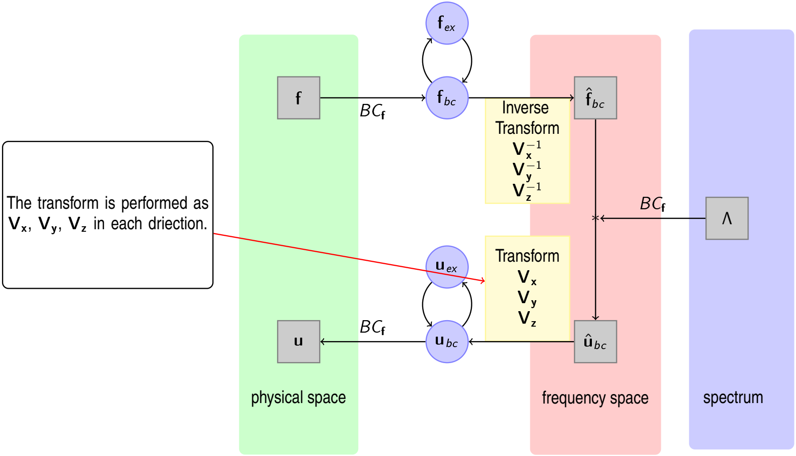

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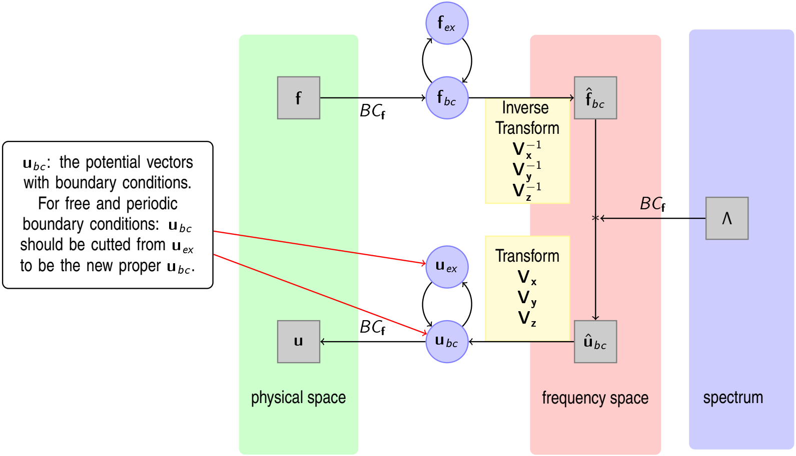

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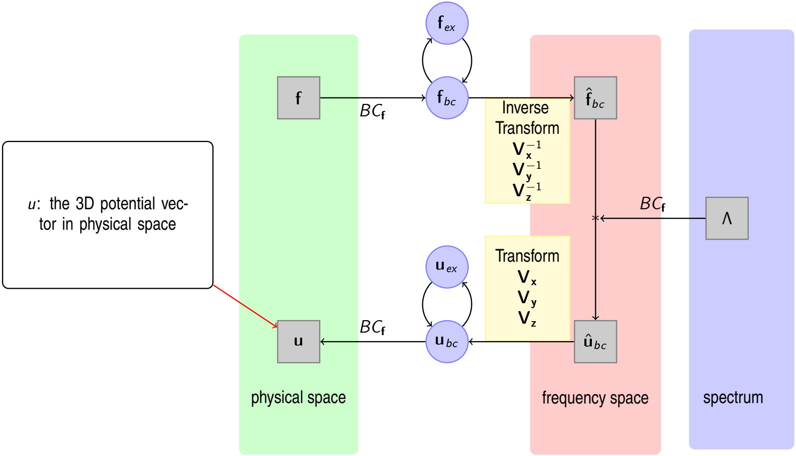
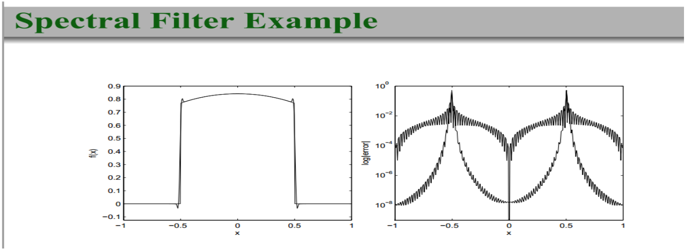


Disadvantages of spectral methods and Green´s function method

- Gibbs phenomenon



- Still time-consuming due to many time step loops.
- High RAM computation

0 www.scottsarra.org

Disadvantages of spectral methods and Green's function method

- Gibbs phenomenon
- Still time-consuming due to many time step loops.

$N_x \times N_y \times N_z$	Spectral Solver	IGF Solver	MG Solver
$33 \times 33 \times 33$	0.035 s	0.115 s	0.077 s
$65 \times 65 \times 65$	0.282 s	1.191	1.087 s
$129 \times 129 \times 129$	2.317 s	11.084 s	9.568 s
$257 \times 257 \times 257$	20.030 s		51.324 s

- High RAM computation

Disadvantages of spectral methods and Green´s function method

- Gibbs phenomenon
- Still time-consuming due to many time step loops.
- High RAM computation

Advantages of spectral methods and Green´s function method

- Together with multigrid methods in MOEVE, the spectral methods can deal with various boundary conditions
- The routine could be efficiently accelerated by parallel technology.
- There are rich theories and tools in spectral theory, that may use to optimize solution
- The spectral methods deal with not too long or short bunches
- The Integrated Green's function method is preferred for too long or short bunches

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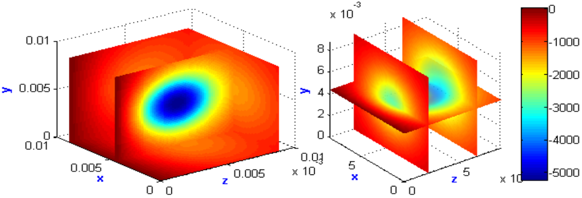
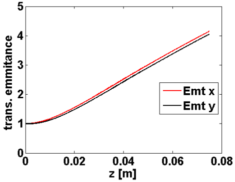
Space charge including image charge

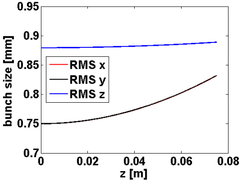
- double sized domain with periodic boundary conditions
- shifted Green's function



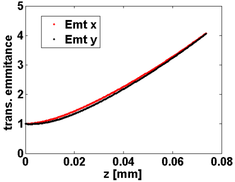
Comparision with ASTRA: First result



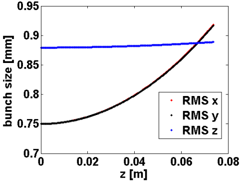
(a) Astra



(b) Astra

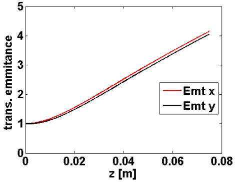


(c) Moeve far bunch

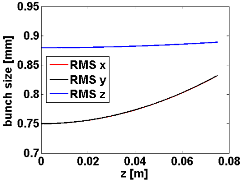


(d) Moeve far bunch

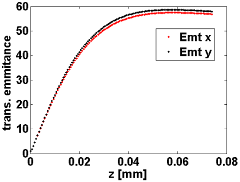
Comparision with ASTRA: First result



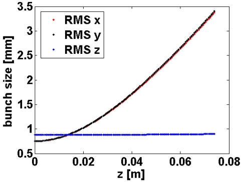
(e) Astra



(f) Astra



(g) Moeve near bunch



(h) Moeve near bunch

Restrictions of the 3D FFT algorithm in ASTRA

- The 3D algorithm does not provide special features for the emission of particles from the cathode in its present form
- Image charge forces cannot be included
- During the emission the complete grid is set up already after the first time step.
- The field description is restricted to the grid; hence the optional use of passive particles, which may travel outside of the grid, is limited

[0] [ASTRA manual V3.0 2011]

Outlook

- More efficient Poisson solver is needed:

  RIGF, CGF and other methods
- Deep study in spectral method
- Parallelization of the FFT-based Poisson solver

  GPU, Open MP
- Check and study the Poisson solver with applications

  Enhance to simulate beam emission.

Thank you !

Real trigonometric transform

The Discrete Sine Transform(DST): $y(1:m-1) = \mathrm{DST}(x(1:m-1))$

$$y_k = \sum_{j=1}^{m-1} \sin(\frac{kj\pi}{m})x_j$$

The Discrete Cosine Transform(DCT): $y(0:m) = \mathrm{DCT}(x(0:m))$

$$y_k = \frac{x_0}{2} + \sum_{j=1}^{m-1} \cos(\frac{kj\pi}{m})x_j + \frac{(-1)^k x_m}{2}$$

The Discrete Sine Transform-II(DST-II): $y(1:m) = \mathrm{DST\text{-}II}(x(1:m))$

$$y_k = \sum_{j=1}^{m} \sin(\frac{k(2j-1)\pi}{2m})x_j$$

The Discrete Cosine Transform-II(DCT-II):$y(0:m-1) = \mathrm{DCT\text{-}II}(x(1:m))$

$$y_k = \sum_{j=0}^{m-1} \cos(\frac{k(2j+1)\pi}{2m})x_j$$