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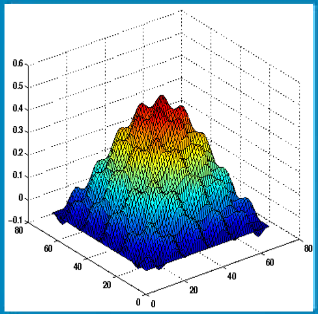
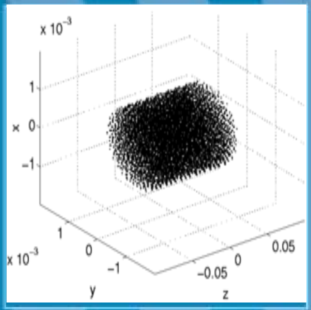
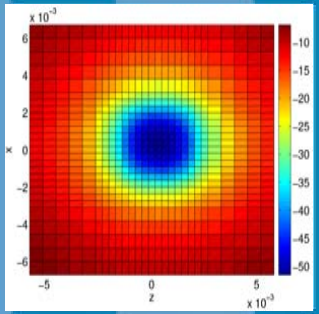
UND ELEKTROTECHNIK
UNIVERSITÄT ROSTOCK

DESY







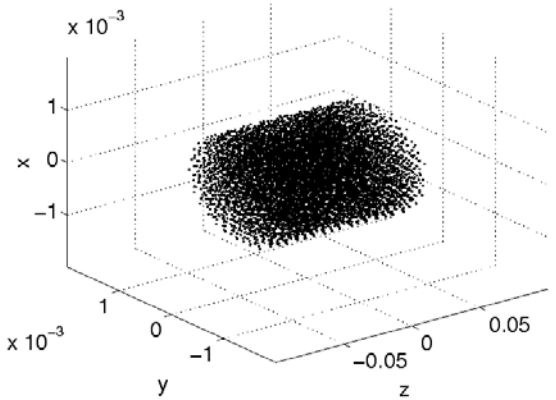
3D Space Charge Routines: The Software Package MOEVE and FFT Compared

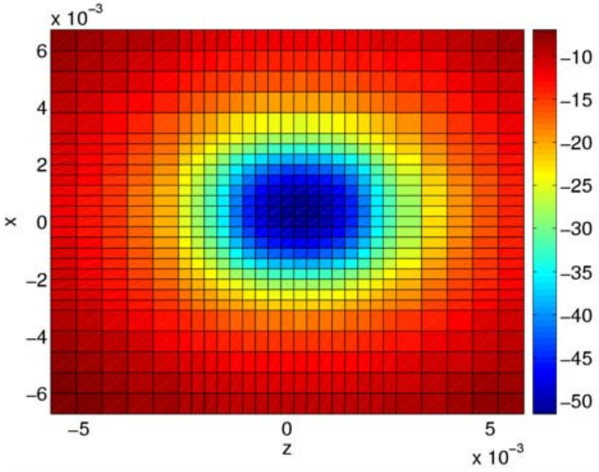
Gisela Pöplau

DESY, Hamburg, December 4, 2007

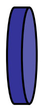
Overview

- Algorithms for 3D space charge calculations
- Properties of FFT and iterative Poisson solvers
- Optimal iterative Poisson solver: multigrid technique
- Numerical investigations:
    - Multigrid performance
    - ASTRA: Tracking example with FFT and multigrid
    - Numerical studies of cylindrical shaped bunches





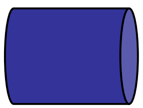
The 3D Space Charge Model



Bunch in laboratory frame

Mesh-based electrostatic solver in rest-frame

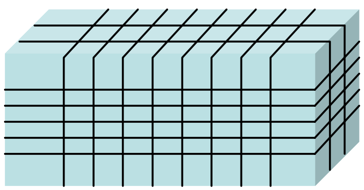
Bunch is tracked in laboratory frame



Bunch in rest frame

Bunch in rest-frame is expanded by γ

$$\gamma = 1/\sqrt{1 - v^2/c^2}$$



Meshlines

meshline positions follow beam density

ρ

Charge density

Trilinear interpolation to obtain charge density

$$-\Delta\varphi = \frac{\rho}{\varepsilon_0}$$

Poisson equation

Solve Poisson's equation

$$E = -\operatorname{grad}\varphi \qquad B = 0$$

Interpolation

2nd order interpolation for the electrostatic field E

$$\{E', B'\} = \mathcal{L}\{E\}$$

Lorentz transformation to laboratory frame

Transform E to E' and B' in laboratory frame

Computation of Space-Charge Fields

Due to Hockney, Eastwood

Particle-Mesh Method

- **Solve Poisson´s equation**

$$-\Delta\varphi = \frac{\rho}{\varepsilon_0}$$

- **Good accuracy for „smooth" particle distributions**
- **Fast with best solver - *O*(*M*): multigrid methods**

Particle-Particle Method

$$E(r) = \frac{1}{4\pi\varepsilon_0} \sum_{\ell=1}^{M_p} q_\ell \frac{r - r_\ell}{\|r - r_\ell\|^3}$$

- **No mesh required**
- **Straightforward summation $O(M_p^2)$**

Particle-Particle Particle-Mesh Method

Particle-Mesh Method

$$-\Delta\varphi = \frac{\rho}{\varepsilon_0}$$

FFT Poisson solvers

$$\varphi_{i,j,k} = \sum_{i',j',k'} G_{i-i',j-j',k-k'} \cdot \rho_{i',j',k'}$$

⇓ Direct solution

$$\hat{\varphi}_{l,m,n} = \hat{G}_{l,m,n}\hat{\rho}_{l,m,n}$$

Boundary conditions

- Free space boundary
- Periodic boundary
- Perfect conducting rectangular box (with Fast Sine Transformation)

G: Green's function

Iterative Poisson solvers

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

⇓ Finite difference discretization

$$Au = f$$

Boundary conditions

- Free space boundary
- Perfect conducting rectangular box
- Perfect conducting pipe with elliptical cross section

Solvers & Properties

$$-\Delta\varphi = \frac{\rho}{\varepsilon_0}$$

FFT Poisson solvers

- FFT
- FFT based algorithms (FST)

Step size: equidistant

Numerical effort: *O(M* log*N)*

Number of grid points (one coordinate): $N+1=2^t+1$

Iterative Poisson solvers

- Multigrid (MG)
- Multigrid Preconditioned Conjugate Gradients (MG-CG)
- Jacobi Preconditioned CG
- Successive overrelaxation (SOR)
- BiCG, BiCGSTAB

Step size: non-equidistant

Numerical effort: *O(M)* (per iteration step)

Convergence:

MG: *O(1)*

CG,SOR: $O(N^2)$ with $h=1/N$

$M \approx N^3$ Total number of unknowns

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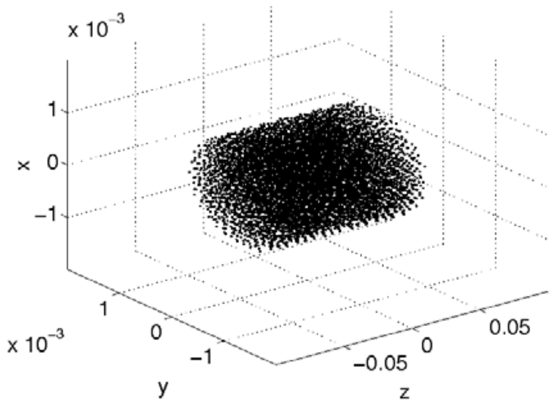
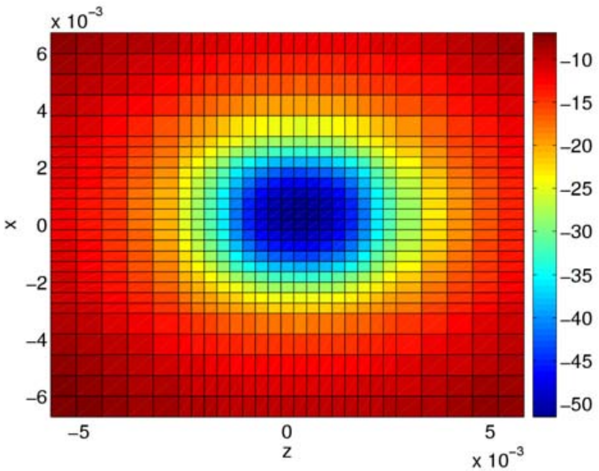
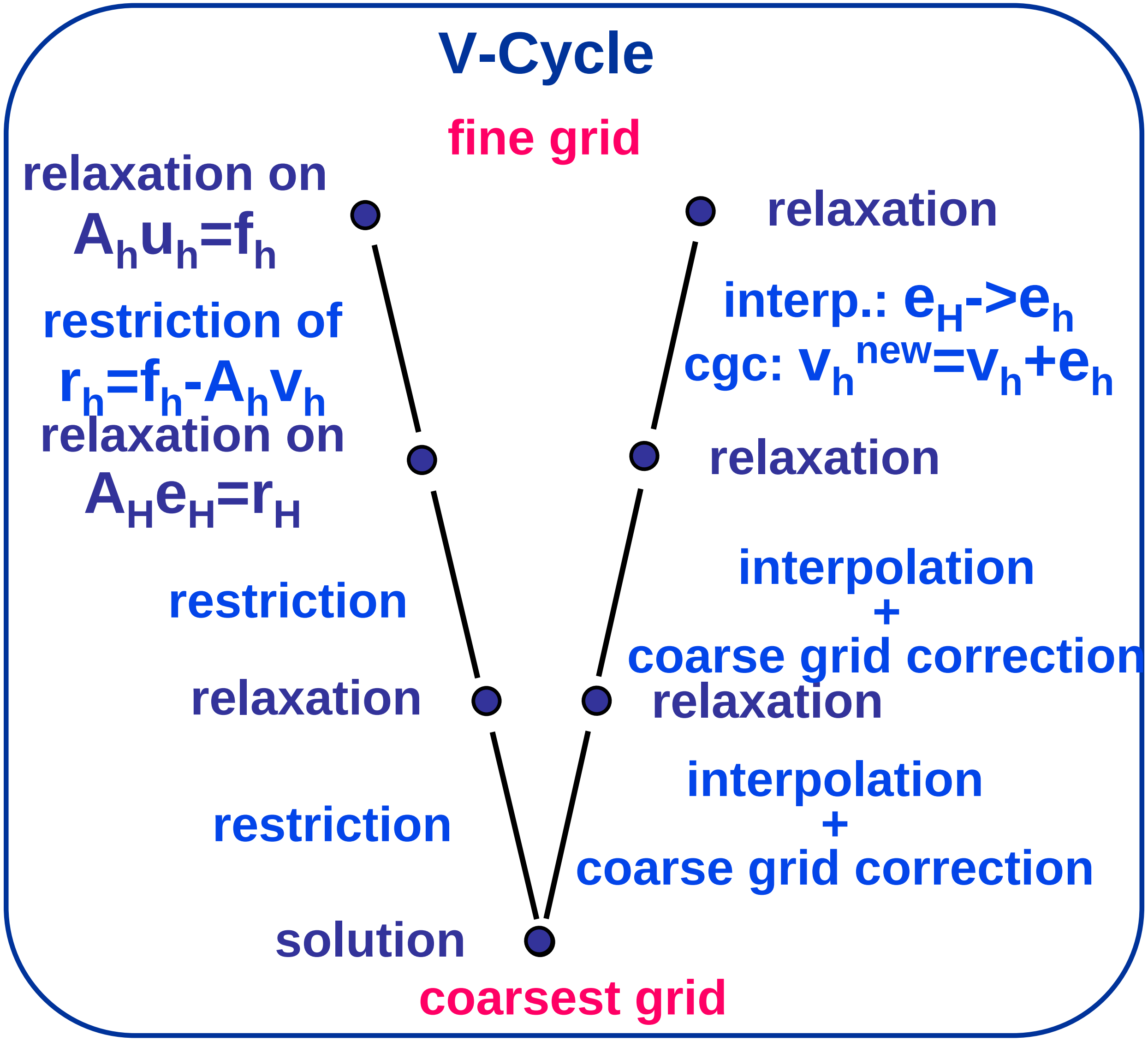
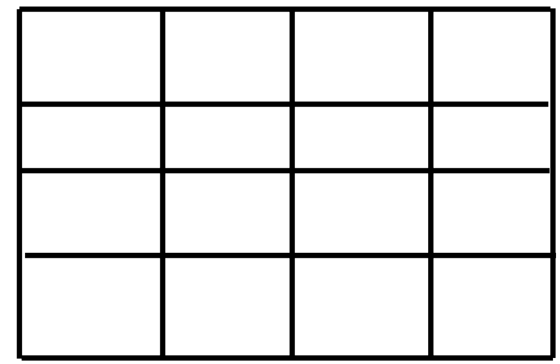


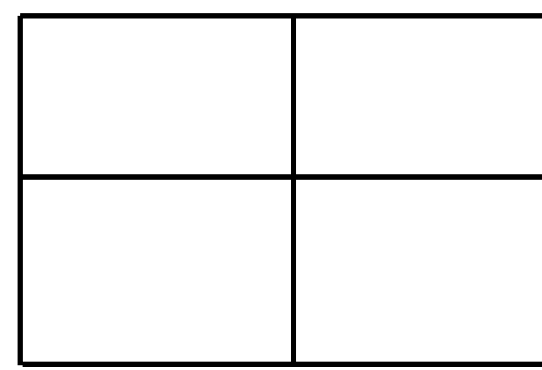


Multigrid Technique





Fine grid



Coarse grid

Gauss-Seidel Relaxtion

Gauss-Seidel relaxation is part of multigrid

↑Simple implementation

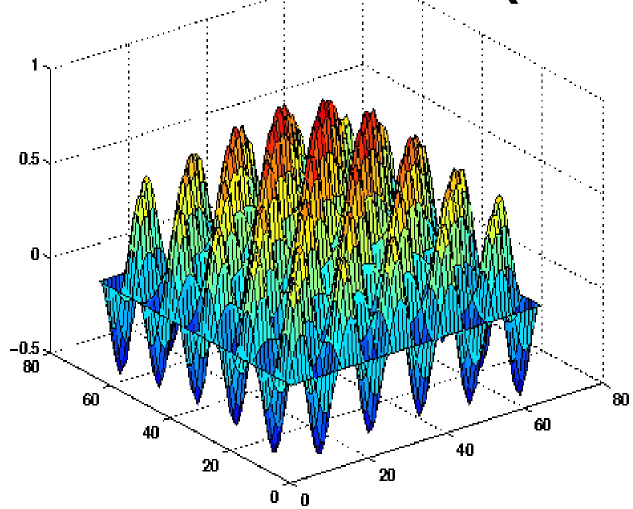
↑Convergence acceptable for

- low number of mesh lines

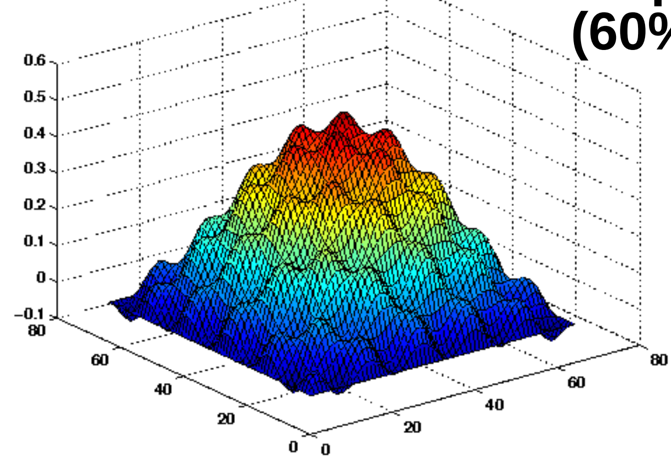
↓Convergence:

- Gauss-Seidel: $O(h^2)$

Initial error (100%)



after 10 Gauss-Seidel steps (60%)

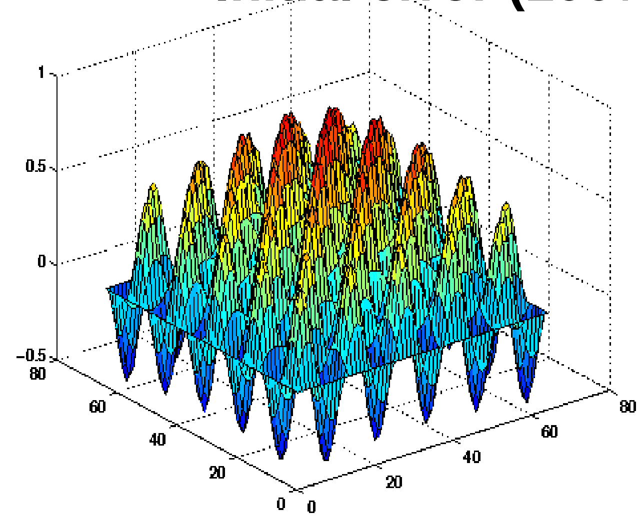


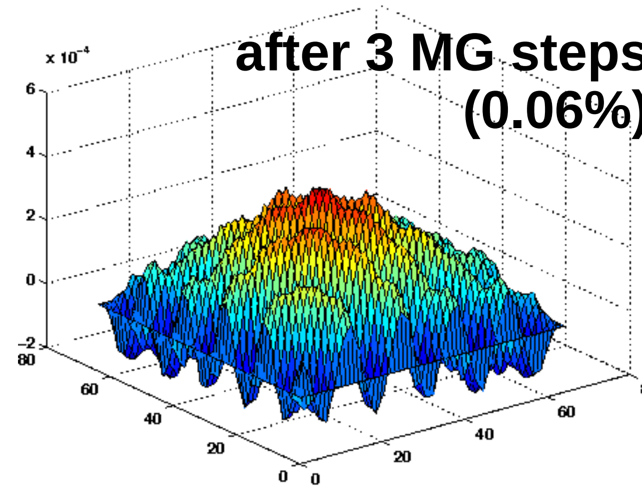
Multigrid & MG-PCG

- ↑ Convergence O(1) on non-equidistant grids
- ↑ Convergence O(1) on grids with high aspect ratios

- ↓ Implementation is more complicated
- ↓ Implementation has always to be adapted to the problem

Initial error (100%)





after 3 MG steps (0.06%)

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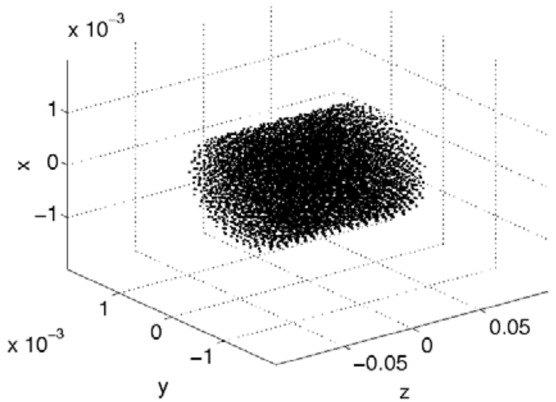
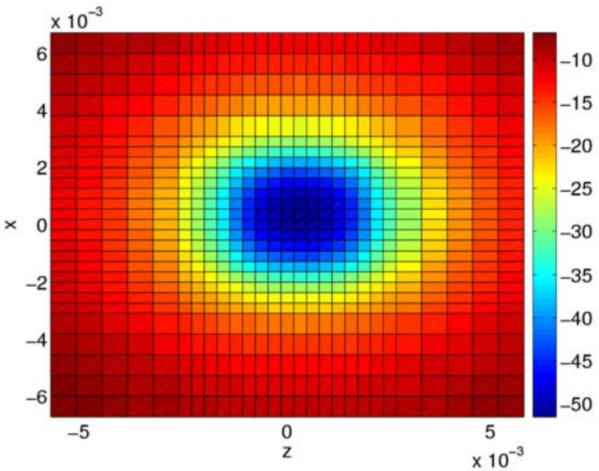
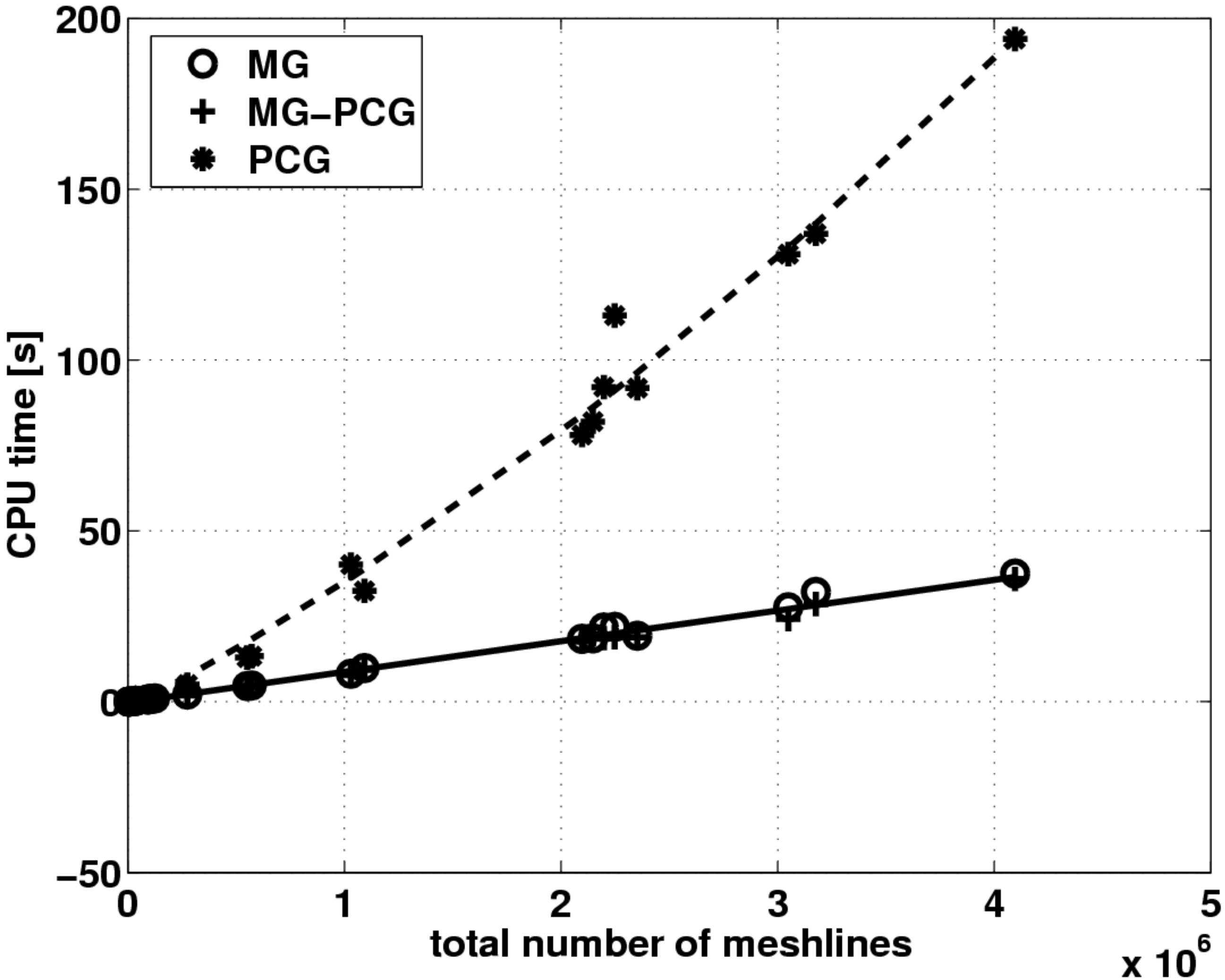




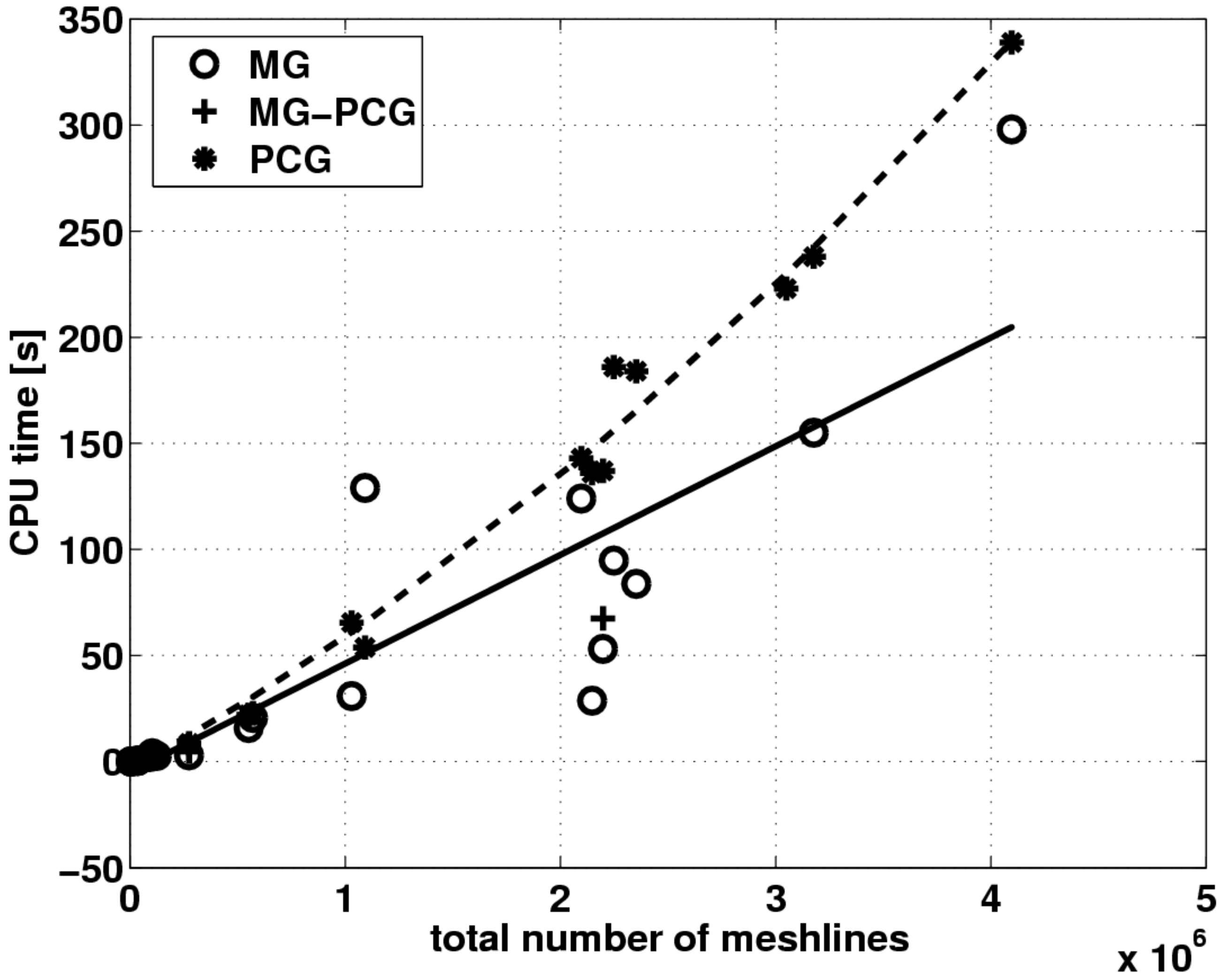
Multigrid Performance (I)

- iterations until rel. residual<10^{-9}
- equidist. mesh
- 8-9 iterations
- Dirichlet bound.



Multigrid Performance (II)

- iterations until rel. residual<10^{-9}
- equidist. mesh
- open boundaries



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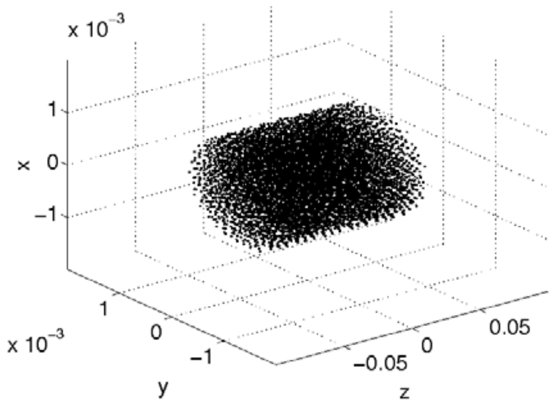
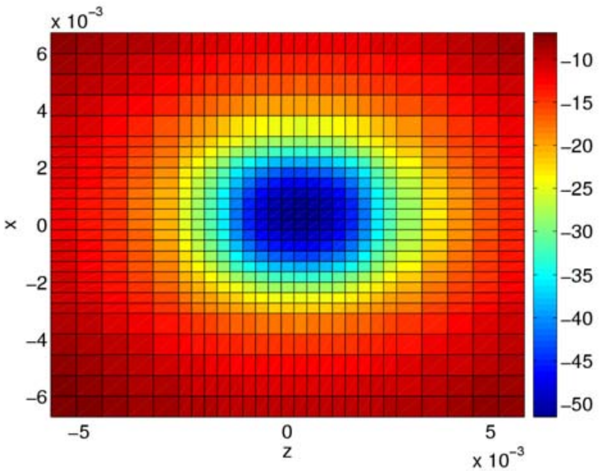


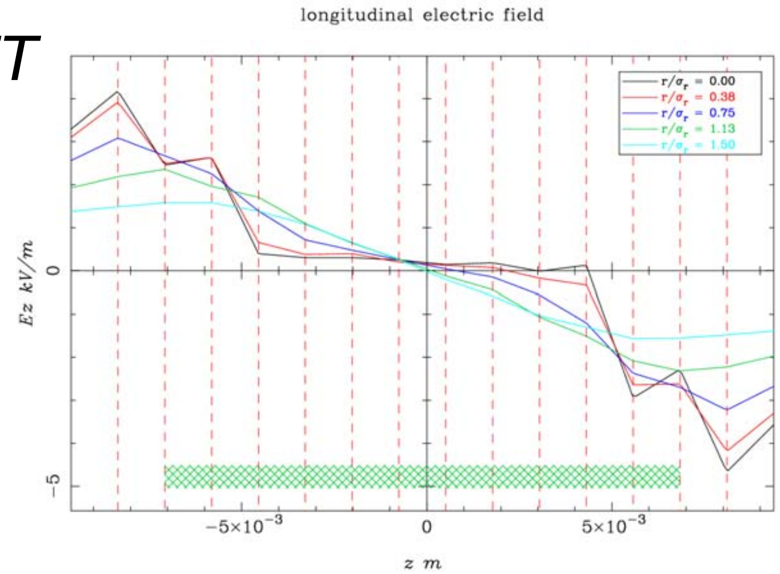


Simulations with ASTRA

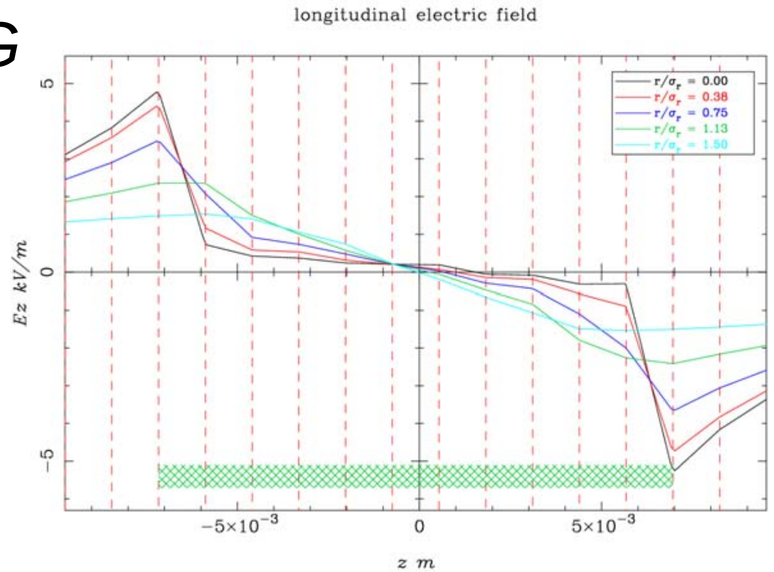
EPAC 2006

- Gaussian particle distribution:
  $\sigma_x=\sigma_y=0.75$ mm , $\sigma_z=1.0$ mm
- 10,000 macro particles
- charge: -1 nC
- energy: 2 MeV
- tracking distance: 3 m
- quadrupol at z=1.2 m
- number of mesh points: 32,768 (Poisson solver): $N_z=32$

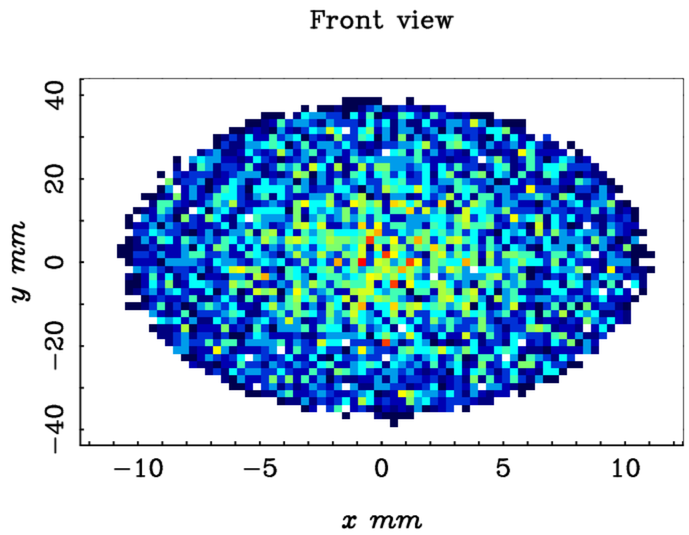
FFT

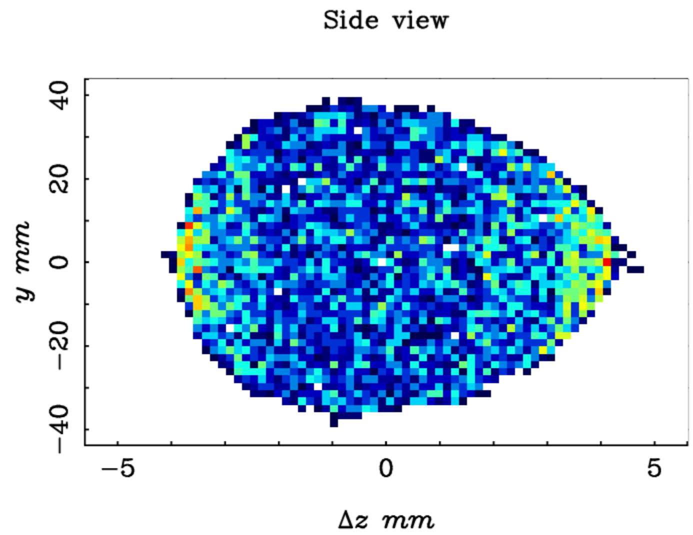


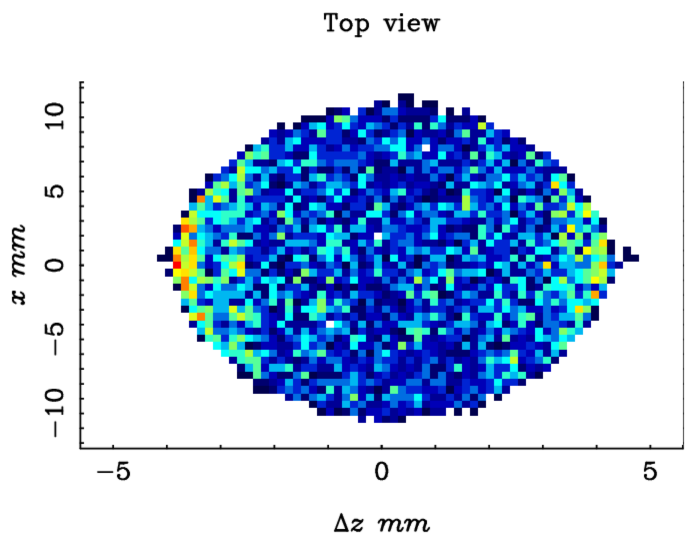
MG



Particle Distribution at z=1.47 m



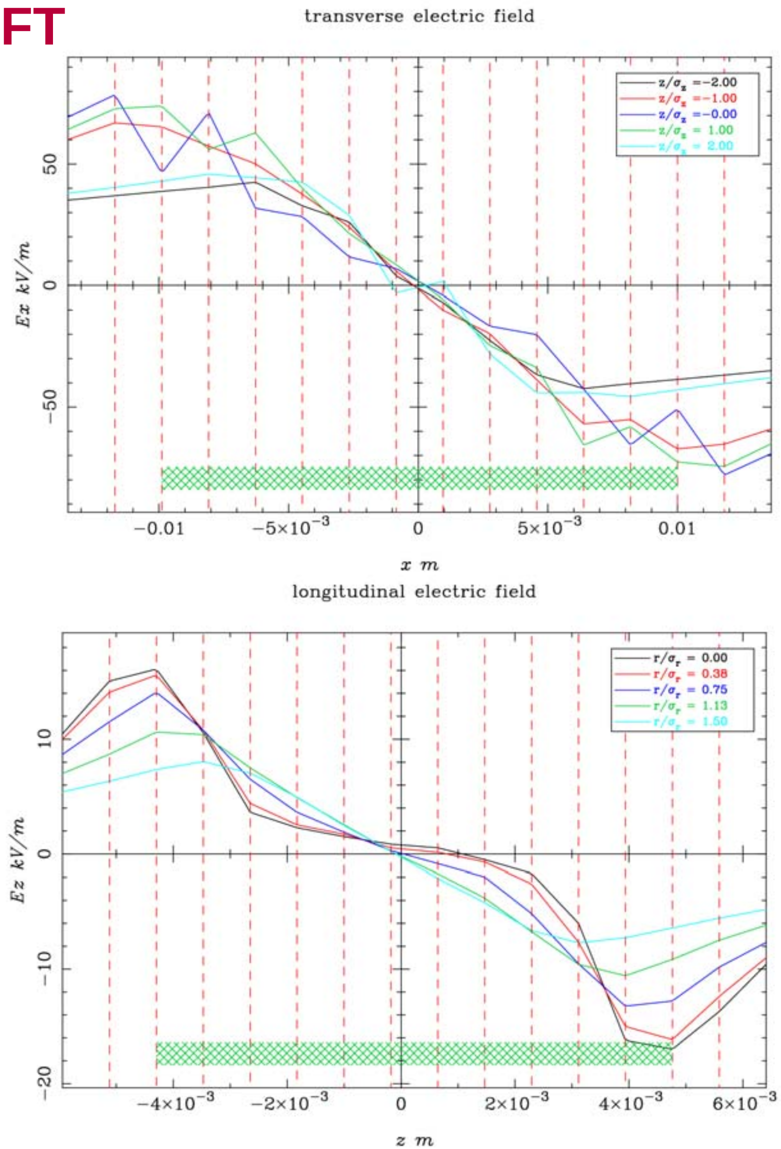




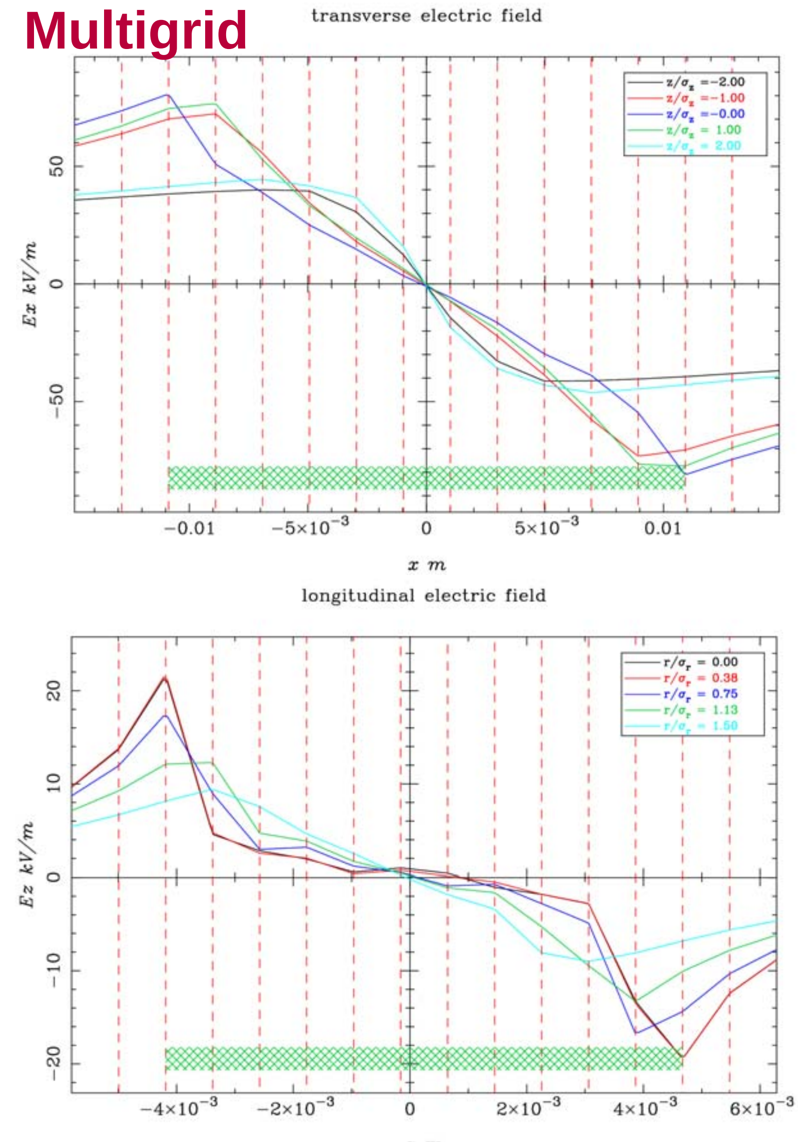
Output of Astra routine: *postpro*

Drift with Quadrupole after 1.47 m

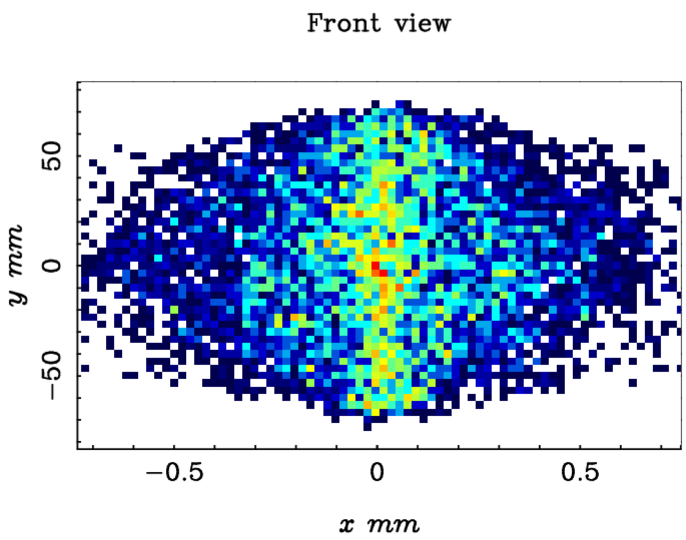
FFT

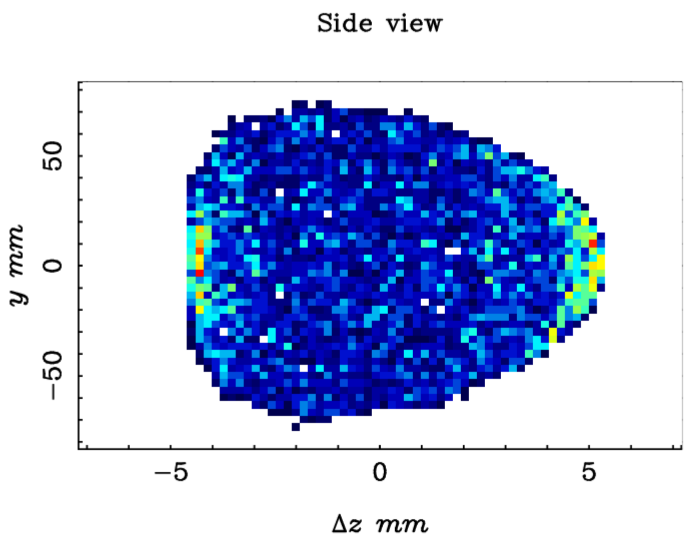


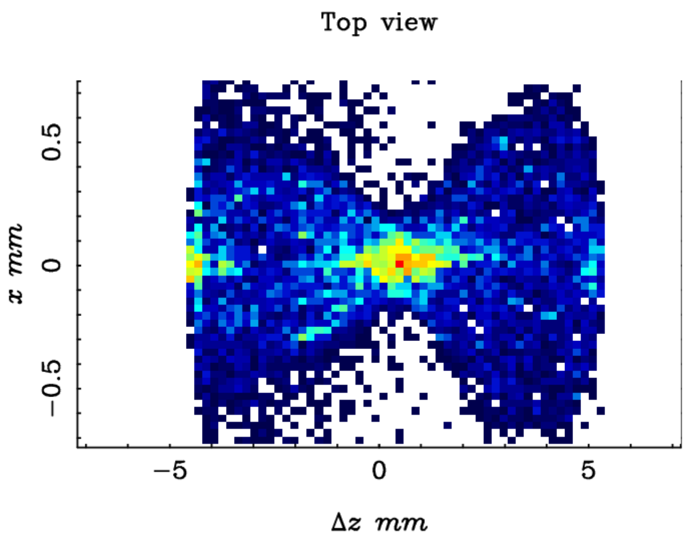
Multigrid



Particle Distribution at z=2.00 m



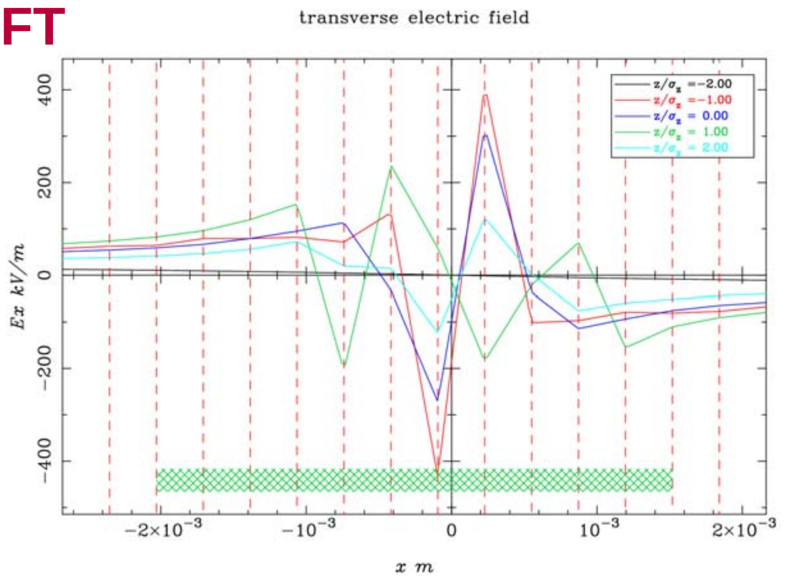




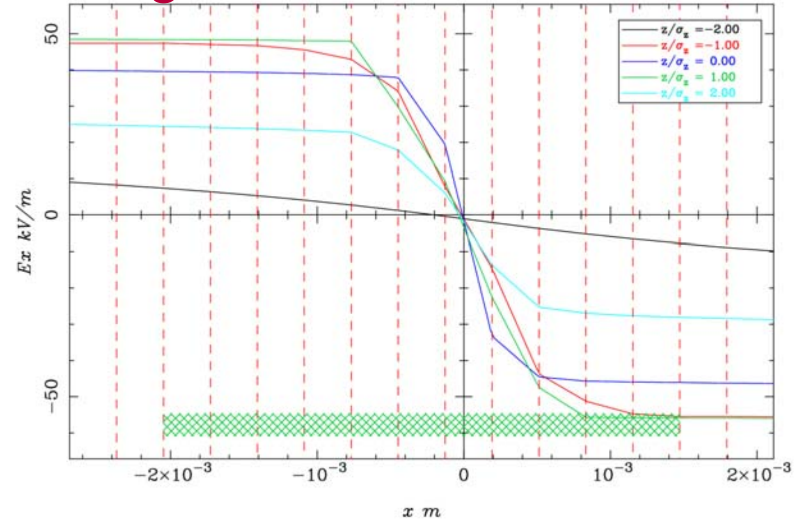
Output of Astra routine: *postpro*

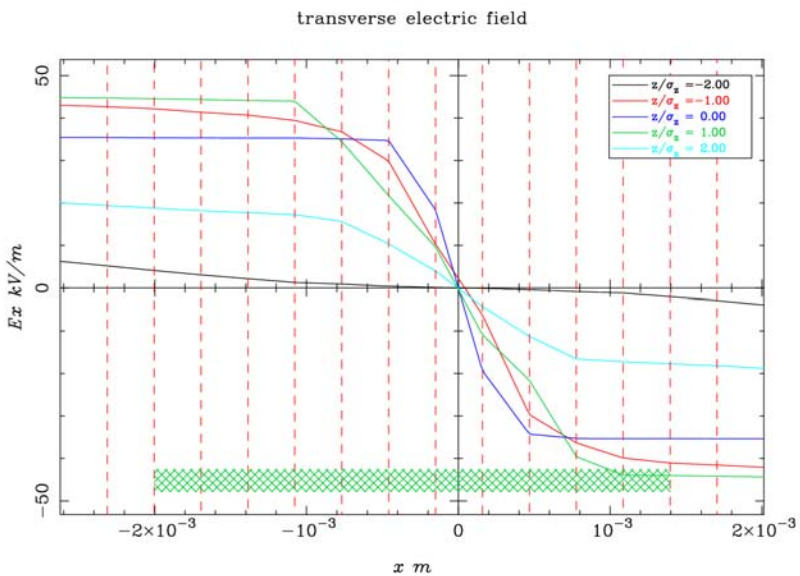
Drift with Quadrupole after 2.0 m

FFT



Multigrid





FFT with integrated Green's function

(Qiang et al, 2006)

Integrated Green‘s Function

Qiang et al, 2006

$$\varphi(x,y,z) = \frac{1}{4\pi\varepsilon_0}\int\int\int G(x,x',y,y',z,z')\rho(x',y',z')\mathrm{d}x\mathrm{d}y\mathrm{d}z$$

Green‘s function

$$G(x,x',y,y',z,z') = \left((x-x')^2+(y-y')^2+(z-z')^2\right)^{-1/2}$$

Integrated Green‘s function

$$\tilde{G}(x_i,x_{i'},y_j,y_{j'},z_k,z_{k'}) =$$

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

$$\varphi_{i,j,k} = \sum_{i',j',k'}\tilde{G}_{i-i',j-j',k-k'}\,\rho_{i',j',k'}$$

Performance time

Poisson solver	N=28	N=32
FFT	--	267 s
FFT, integrated Green‘s function	--	312 s
MG, equi. (initial guess = 0)	247 s	259 s
MG, equi. (initial guess $\neq$ 0)	237 s	240 s
MG, non-equi. (initial guess = 0)	254 s	261 s
MG, non-equi. (initial guess $\neq$ 0)	243 s	241 s
PCG, equi. (initial guess = 0)	261 s	280 s
PCG, equi. (initial guess $\neq$ 0)	246 s	235 s
PCG, non-equi. (initial guess = 0)	266 s	296 s
PCG, non-equi. (initial guess $\neq$ 0)	235 s	235 s

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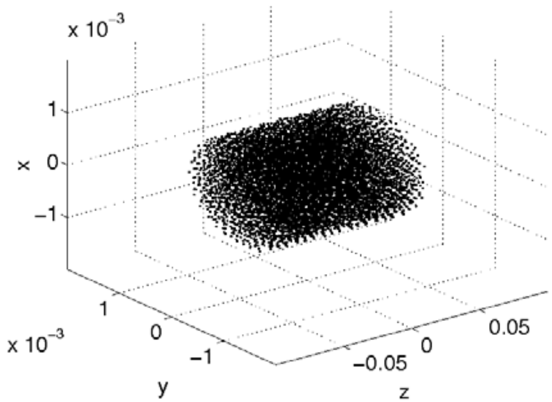
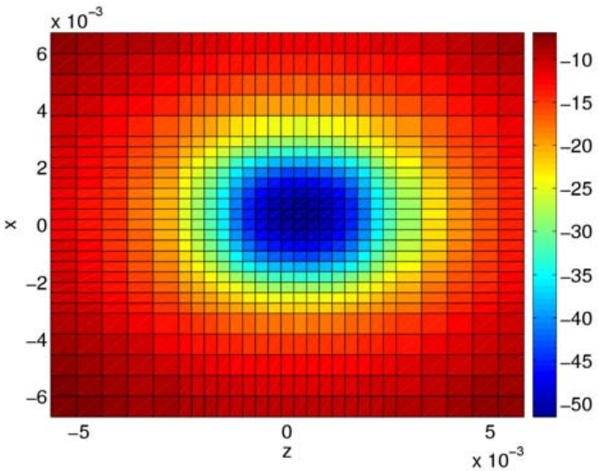
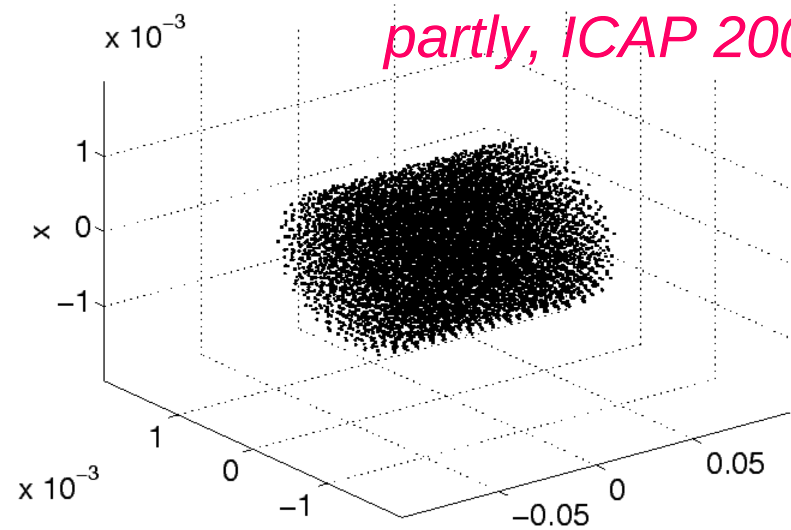




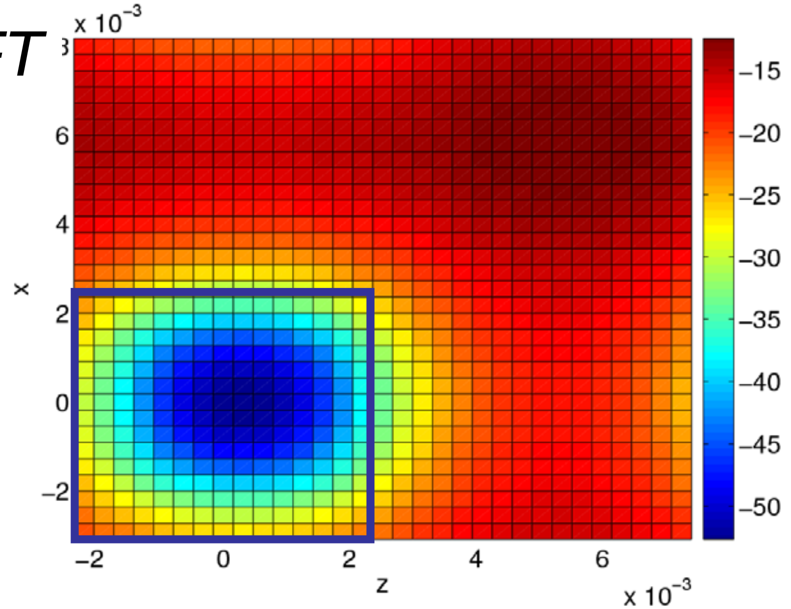
Parameters for simulations

- Cylindrical bunches
- Uniform partical distribution
- 20,000 macro particles
- Charge -1 nC
- Aspect ratio of the bunch σ_x/σ_z

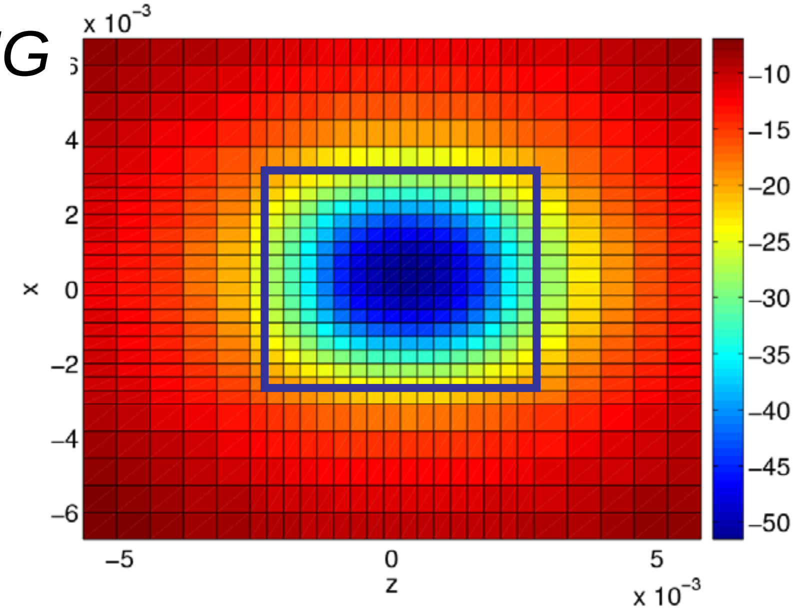
partly, ICAP 2006



FFT

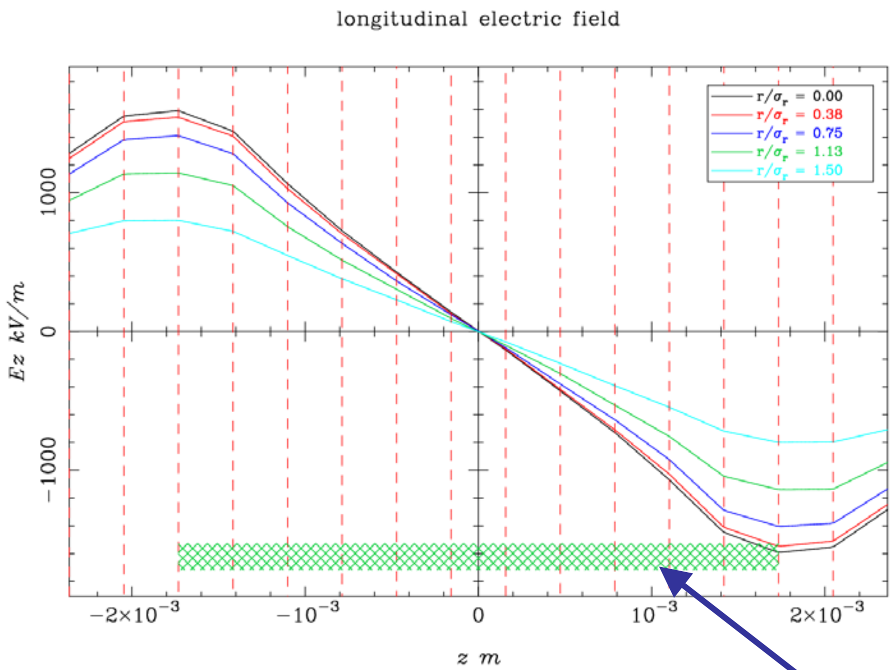


MG

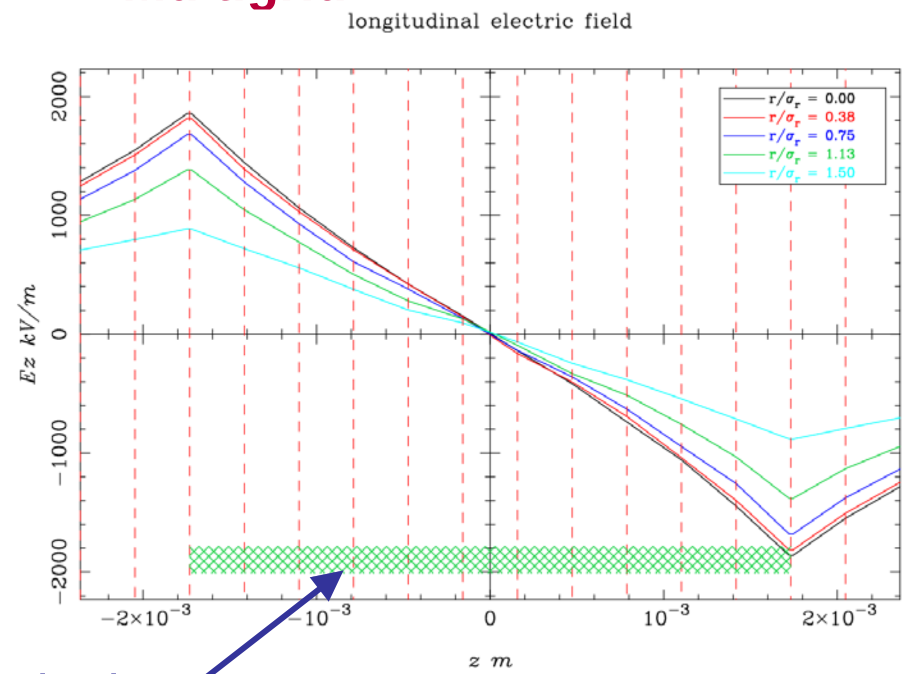


Bunch with Aspect Ratio 1

FFT



Multigrid



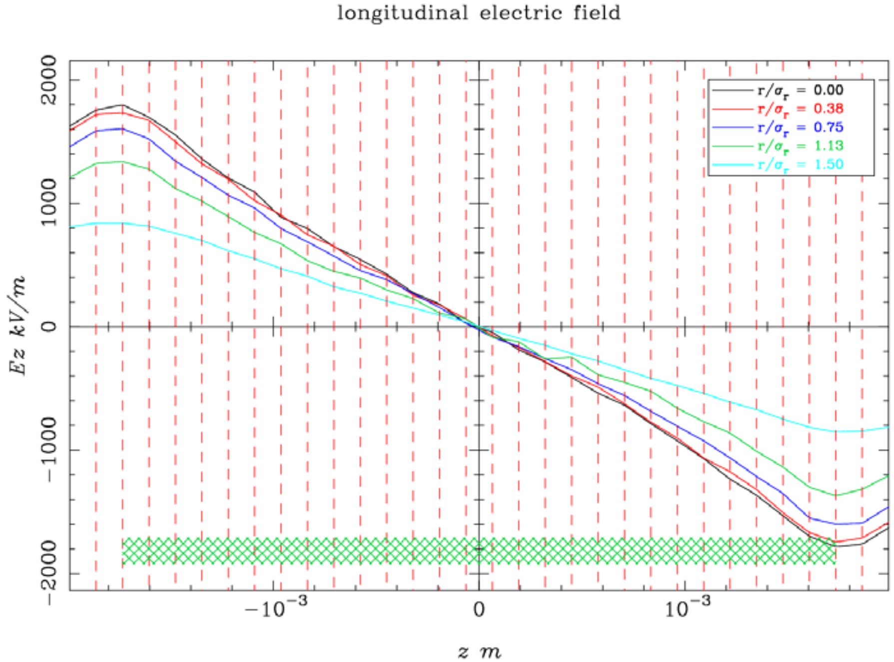
Bunch size

- # of grid points: 32x32x32
- Field at the edges of the bunch is **not** approximated correctly

- # of grid points: 28x28x28

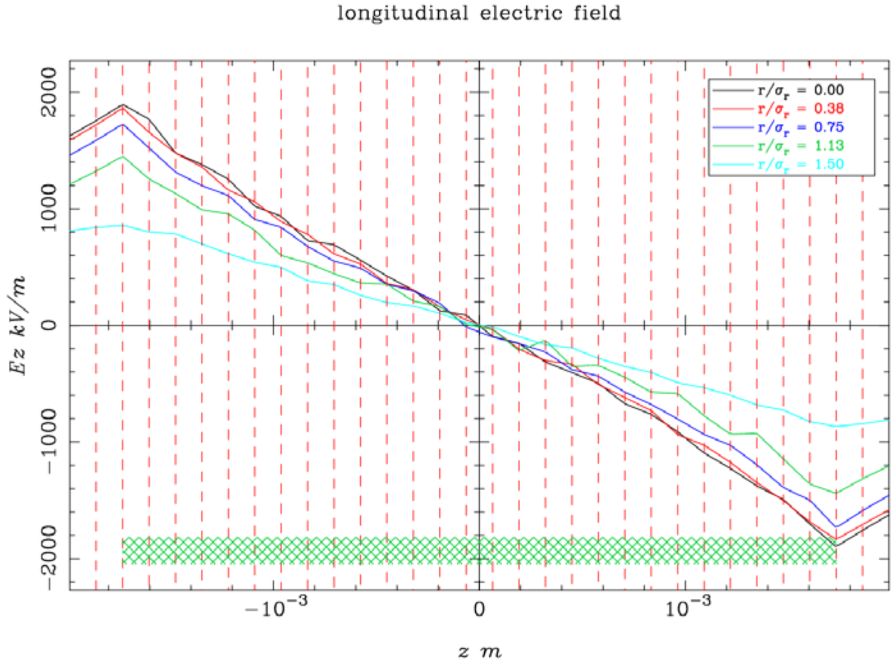
Bunch with Aspect Ratio 1

FFT



- # of grid points: 64x64x64
- Field at the edges of the bunch is better approximated

Multigrid

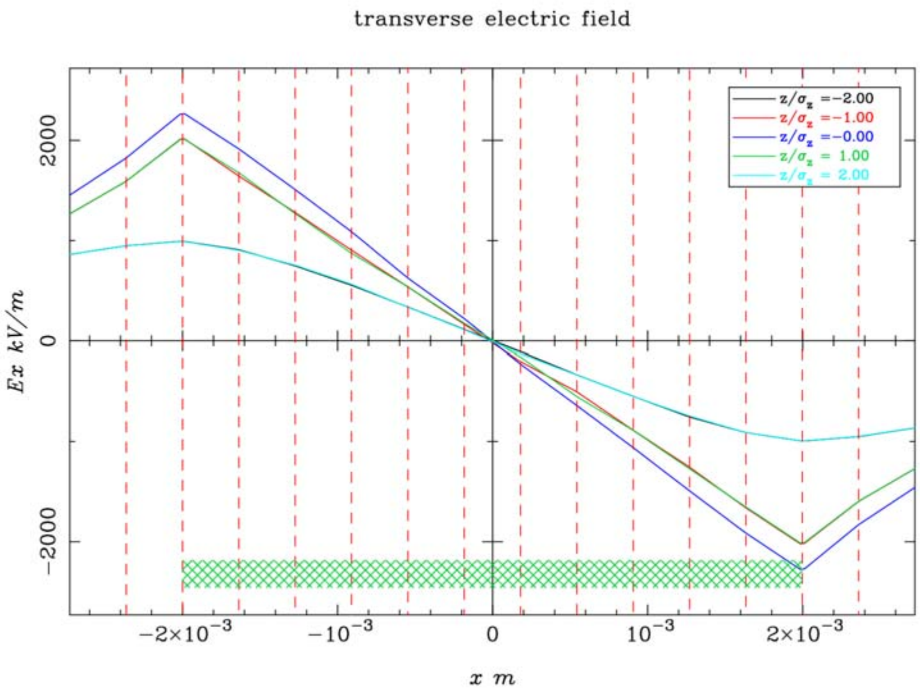


- # of grid points: 60x60x60
- Resolution too high: more particles required for smoother fields

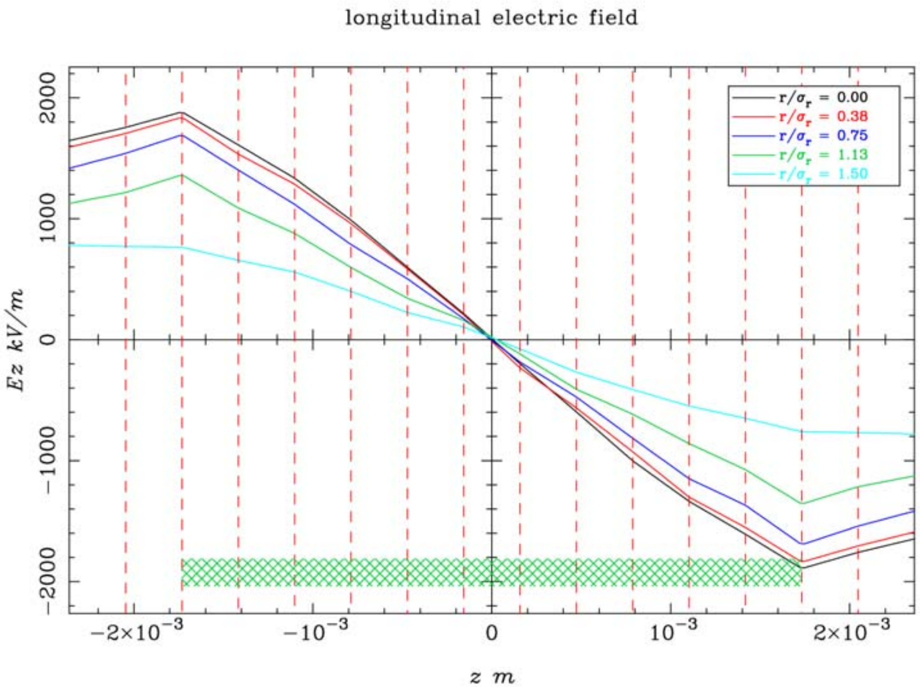
Bunch with Aspect Ratio 1

FFT with integrated Green‘s function

transversal

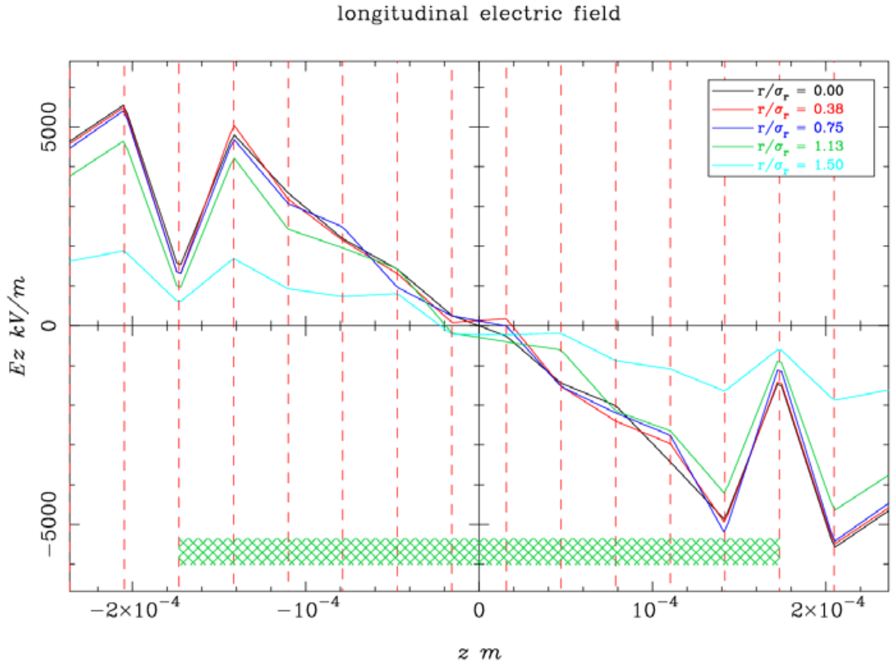


longitudinal



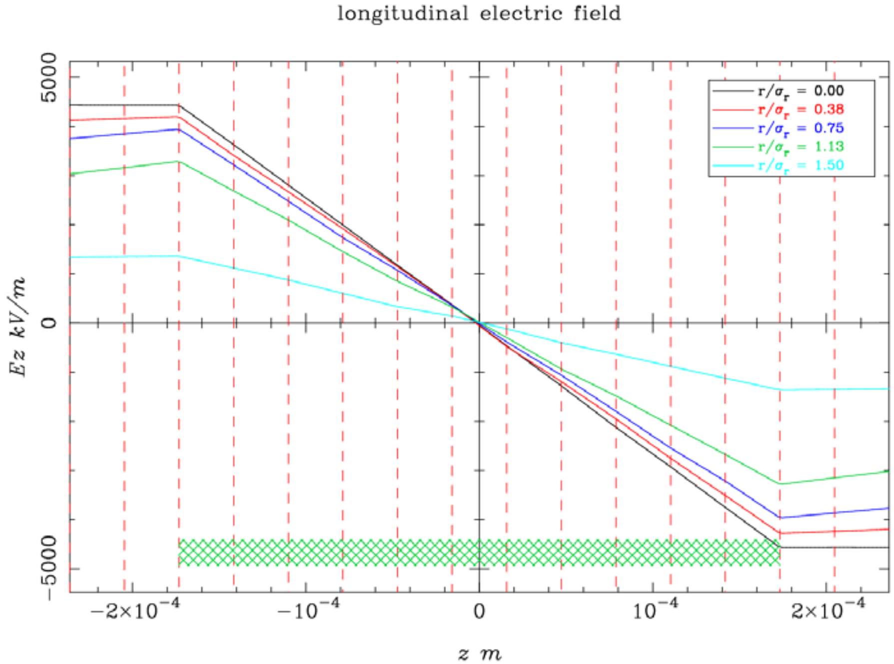
- # of grid points: 32x32x32
- Field at the edges of the bunch is approximated correctly

FFT



- # of grid points: 32x32x32
- Field at the edges of the bunch is **not** approximated correctly

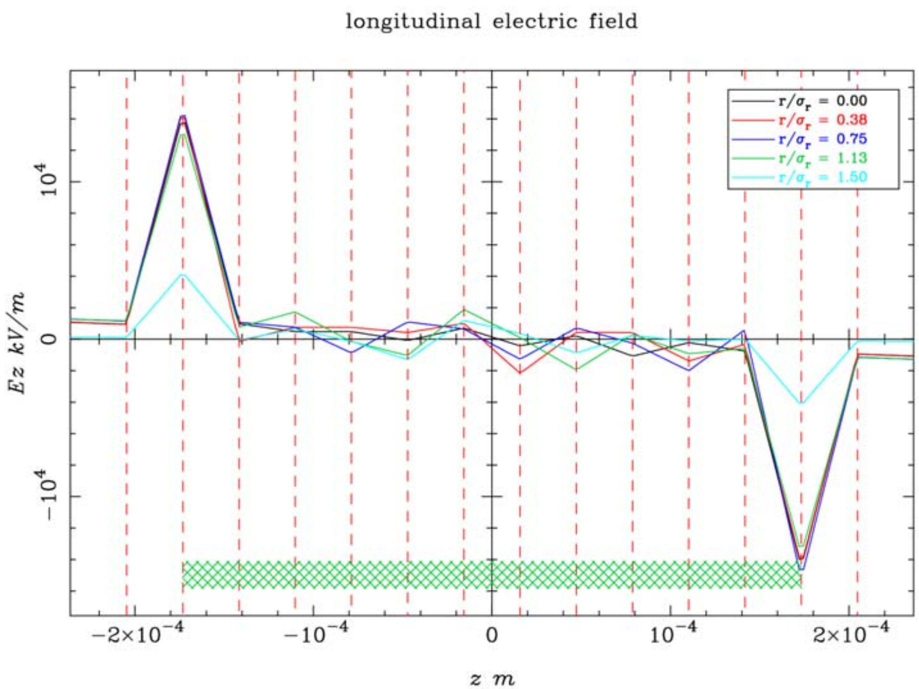
Multigrid



- # of grid points: 32x32x32

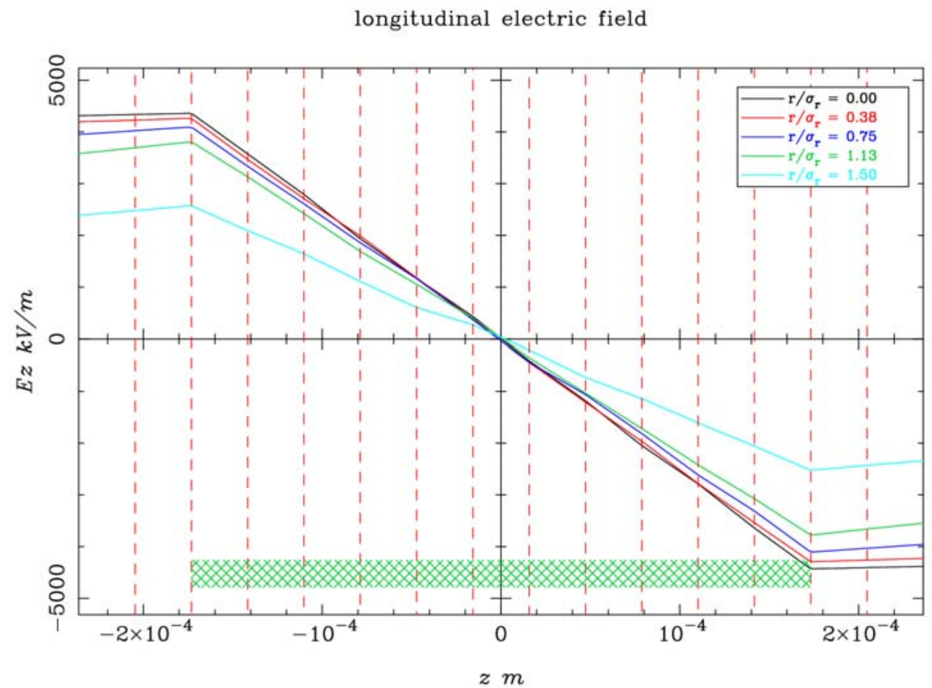
Short Bunch with Aspect Ratio 10

FFT with integrated Green's function



- # of grid points: 32x32x32
- Field of the bunch is **not** approximated correctly

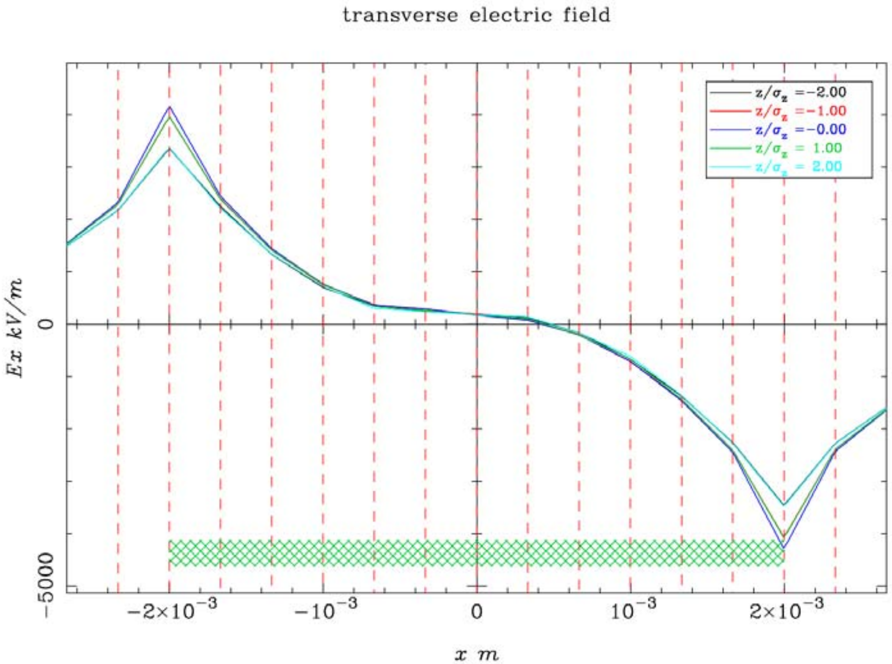
Multigrid



- # of grid points: 32x32x32

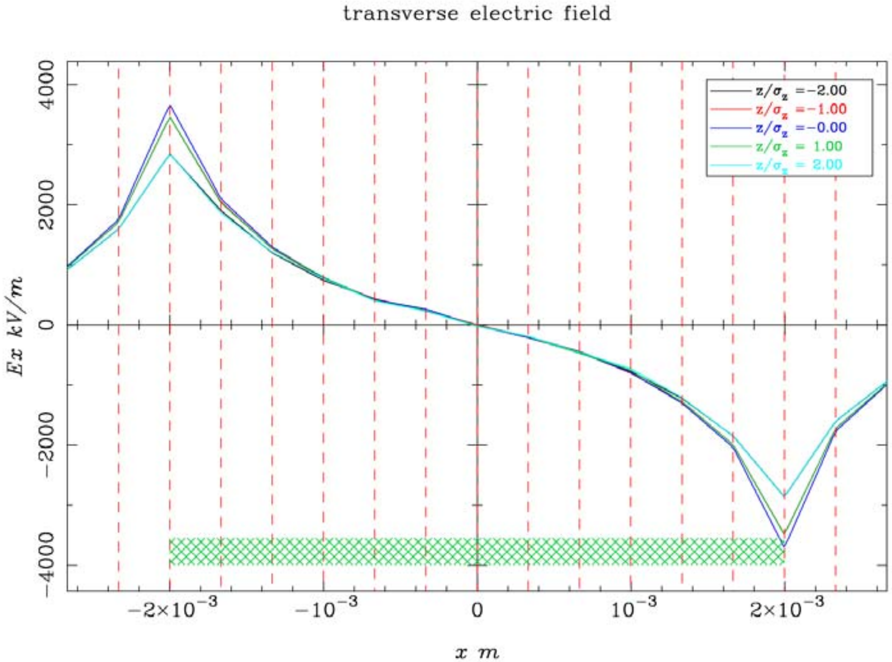
Short Bunch with Aspect Ratio 10

Multigrid, open boundaries "small" computational domain



- # of grid points: 33x33x33
- Field of the bunch around the center is **not** approximated correctly

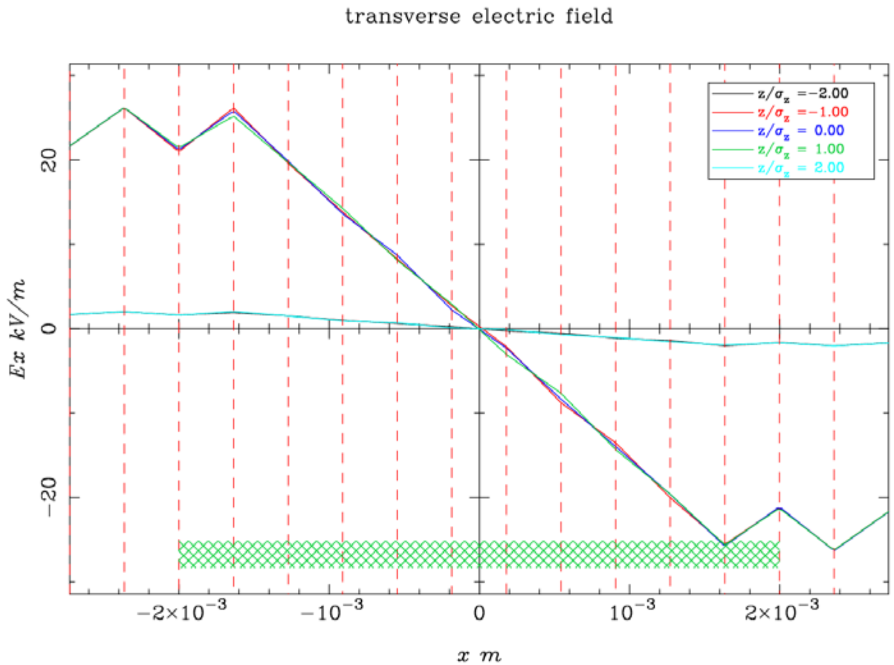
Multigrid, Dirichlet boundaries "large" computational domain



- # of grid points: 51x51x51

Long Bunch with Aspect Ratio 0.01

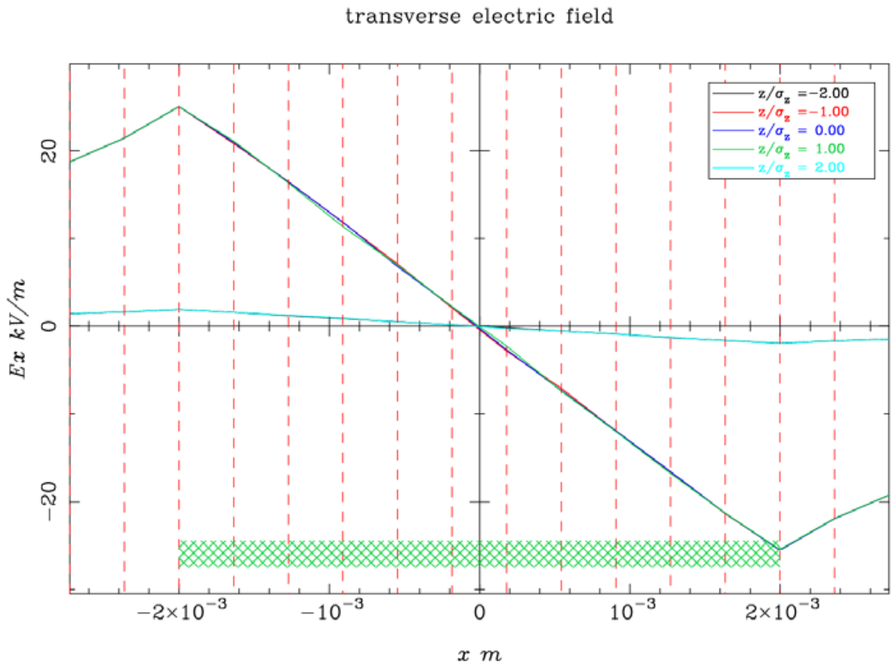
FFT



- # of grid points: 32x32x32
- Transverse field at the edges of the bunch is **not** approximated correctly

Multigrid

FFT with integrated Green's function



- # of grid points: 32x32x32

Summary and Projects

- MG Poisson solvers are much more flexible than FFT Poisson solvers (boundary, discretization)
- MG Poisson solvers enable a better approximation
- Software package MOEVE 2.0 (2.1)
- Part of the tracking codes ASTRA and GPT 2.7
- Projects in Rostock:
  - Simulation of e-clouds (Aleksandar)
  - Adaptive multigrid discretizations for charged particle bunches (DFG-Project, Christian Bahls)