Progress of Space Charge Calculation in the Tracking Code *Orbit*

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Abstract

The code *Orbit* has been designed for PIC tracking of a particle beam in a high intensity circular hadron accelerator. In the code, space charge forces are continuously calculated and applied to the individual macroparticles of the herd as transverse momemtum kicks. Some of the general structure of a recent version of *Orbit* developed at Brookhaven is described. Problems of this type of calculation and solutions are discussed.

PIC Tracking

a particle is represented by a phase space vector

$$\vec{r} = (x, p_x, y, p_y, c\Delta t, \Delta p/p)$$

A "herd" is pushed through a lattice represented by maps (external fields)

At 'space charge nodes' in the lattice, (internal) forces are calculated and applied to the macros as momentum kicks.

Poisson Equation

To calculate space charge kicks:

- bin the heard on a grid according to $(x, y, c\Delta t)$, find ρ
- bin the herd according to $(p_x, p_y, \Delta p/p)$, find $\vec{j}$,
- Solve partial elliptic differential equations

$$\left.\begin{aligned} \nabla^2 \Phi(P) &= -\frac{\rho(Q)}{\epsilon_0} \\ \nabla^2 \vec{A}(P) &= -\frac{\vec{j}(Q)}{\mu_0} \end{aligned}\right\} Q \to P$$

Find scalar electric Φ and the magnetic vector potential $\vec{A}$

- For long bunches in synchrotrons, beam current is parallel to walls, Electric repulsion and magnetic attraction partially compensate: only use Φ (multiplied by a factor $1/\gamma^2$)

Vlasov or Split Operator

- Global approach: **Vlasov Equation**:

Rigorous in principle, but difficult in practice to study beam granularity (halo formation)

- **Split Operator** technique:

Independent treatment of motion through maps and space charge kicks: macros are propagated in a machine element trough maps, and then subjected to momentum kicks

"Leapfrog" procedure as done in symplectic integration.

Orbit uses Split Operator

The Independent Variable

The independent variable to clock propagation can be time t or longitudinal coordinate s

- **Time** is attractive: solve Poisson Equation with all the macros at the same time

- **Space** is convenient in periodic accelerators: particles cyclically pass through the same positions in the lattice

Apply relativistic transformations between space and time.

Orbit uses space as the independent variable and maps from *MAD*

3D Treatment of Space Charge

Transverse grid is terminated at wall boundary, longitudinal grid covers the length of the beam bunch

Long bunches: unpractical to make z grid step as small as the transverse. In practice this is not necessary because:

- z space charge distribution varies smoothly along the beam
- z motion within the beam is much slower than the transverse

Cut the beam in z slices, long enough that the average density and the transverse aspect ratio of the slice, and the wall configuration around the slice can be considered constant

$$\rho(x,y,z) = \rho_{\perp}(x.y)\,\rho_{\|}(z).$$

Only solve the **2D transverse** Poisson problem simultaneously in each slice, best by **parallel** computing

Frozen Be n

- Lattice map sequence controls the propagation.

- Poisson problem must be solved with all macros at the same time t_{SC}

- At a SC node, beam profile must be reconstituted.

Figure

A first herd chosen on the contour of x and y phase space ellipses matched to the (bare) lattice.

The trajectories of these macros are all bounded by the envelope

$$w = \sqrt{\epsilon\beta}.$$

Macros in the second group are also matched and extracted on a Gaussian distribution with the previous ellipses as their r.m.s.

Beam freezing in *Orbit* is as follows.

• The herd "reaches" a SC node at s_{SC} when the synchronous particle reaches SC.

• We know in which lattice element each macro will be or was at t_{SC}.

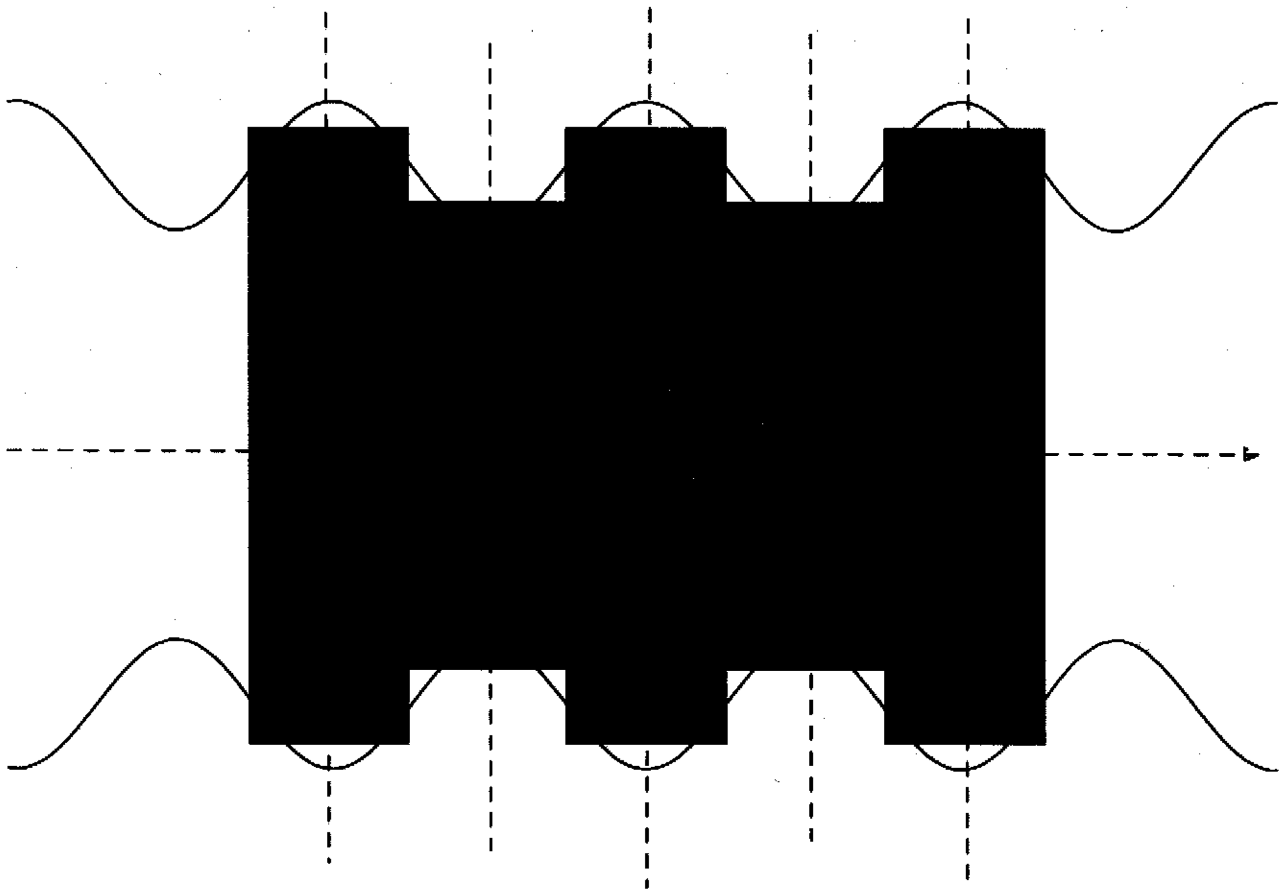
• We can reconstruct the transfer matrix between s and s_{SC} to reconstitute the beam, since Twiss functions at s in that element are known from the integral of the equation

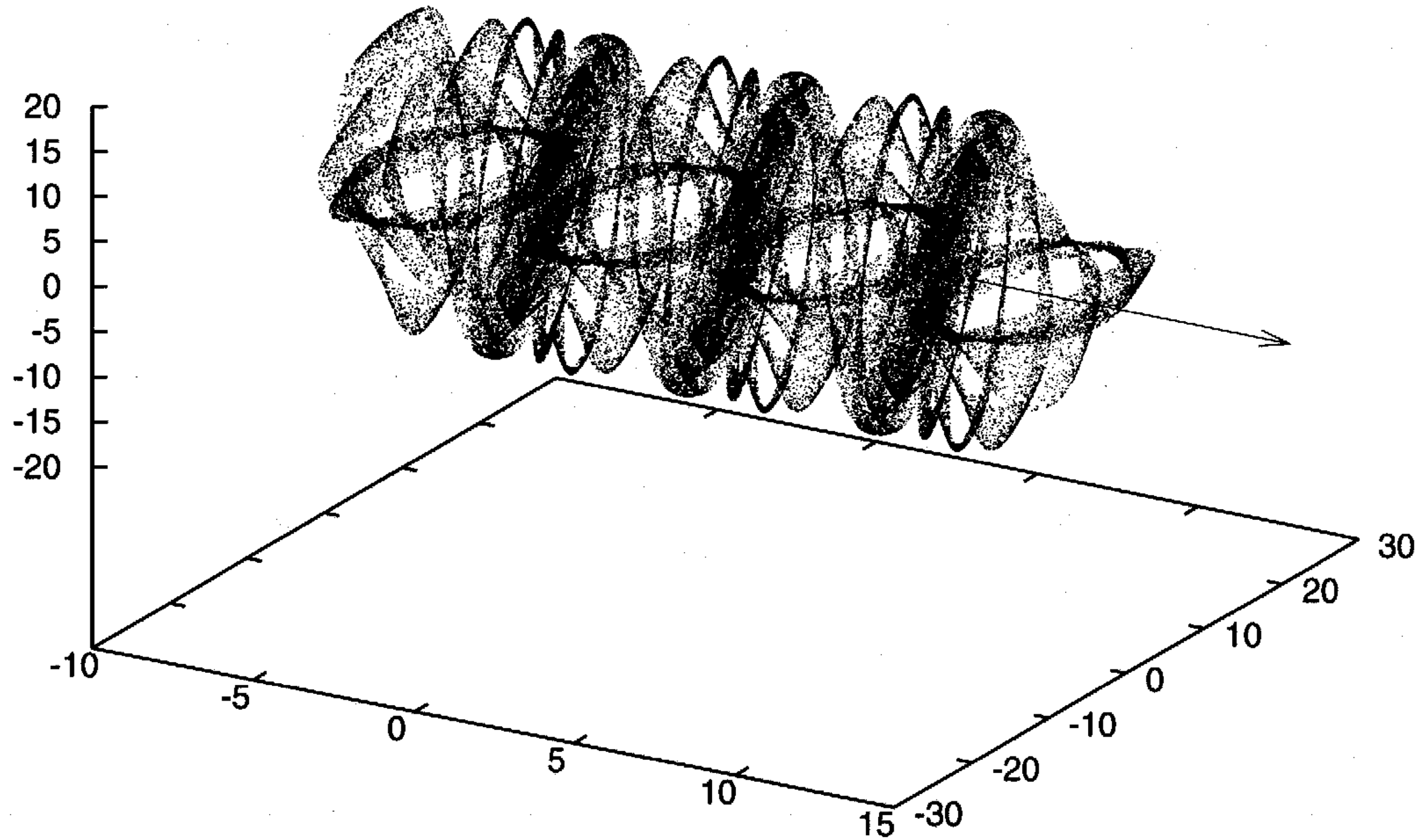
$$\frac{1}{2}\beta\beta'' - \frac{1}{4}\beta'^2 + K\beta^2 = 0,$$

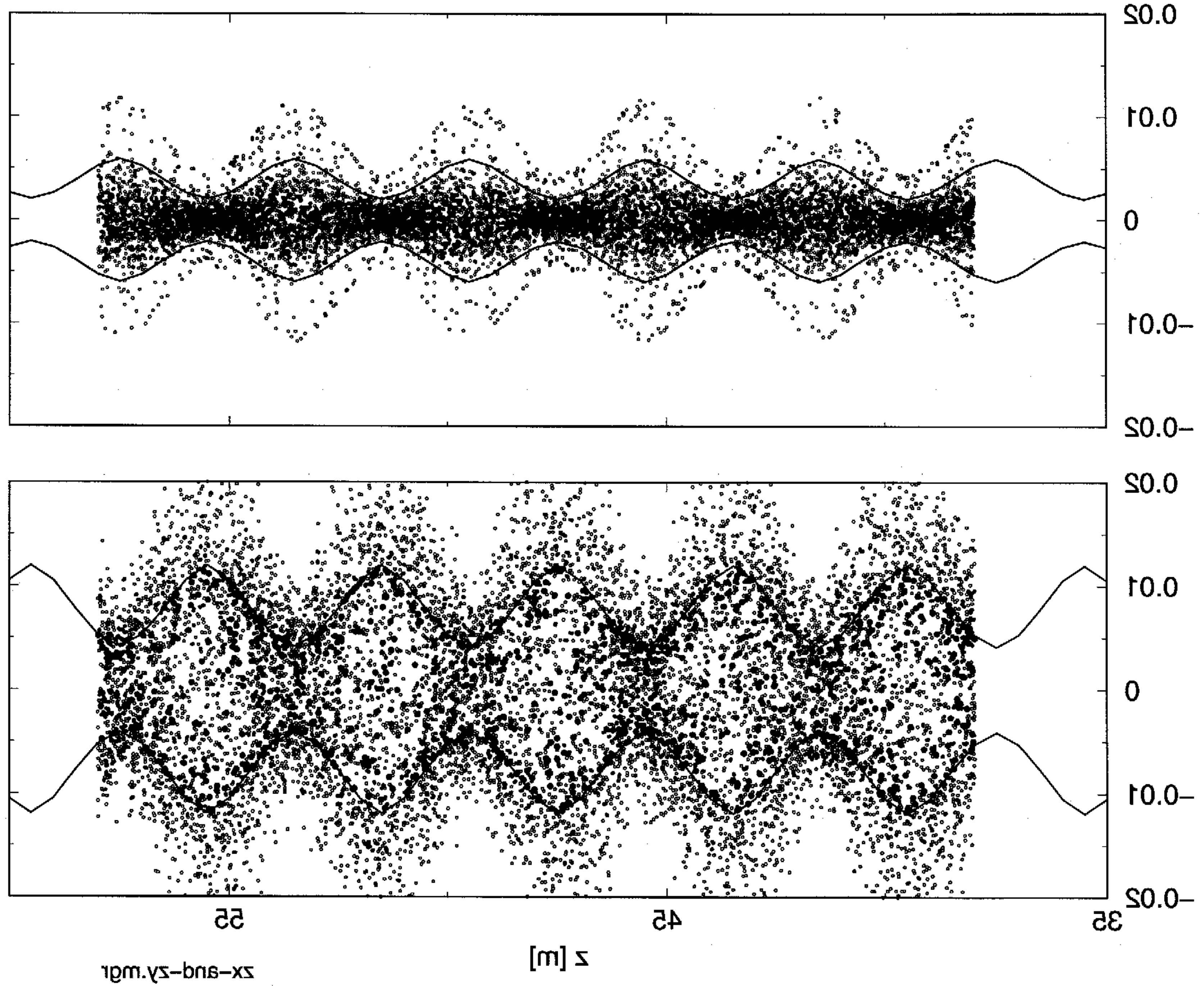
Figure

3D rendition of a frozen beam in a simple FODO lattice.

Beam longitudinal slices




20
15
10
5
0
-5
-10
-15
-20
-10
-5
0
5
10
15
-30
-20
-10
0
10
20
30



x [m]
y [m]
z [m]
0.02
0.01
0
-0.01
-0.02
35
45
55
zx-and-zy.mgr

Table 1: Specifications for the BNL Galaxy Cluster[1].

Nodes:	2 CPU's	512 MB RAM
CPU specs:	Intel Pentium III	
500 MHz	512 kB L2 Cache	
Interconnection:	Cisco Switch	100 MB Ethernet
File System:	NFS	
MPI:	mpich	1.2 compliant

Table 2: Results of Poisson solvers. Two grid sizes

	BF/FFT/LU	
Grid:	33/65/33	65/129/65
	Elapsed Time [s]	
Lu Solver	0.0279	0.1407
FFT	0.0538	0.2558
BruteForce	0.1343	2.1300

Table 3: *Orbit* timing (wall clock) on the Galaxy. 1 Turn.

Nodes	Macros/Turn per Node	With SC time sec	No SC time sec
2	$1.6\ 10^6$	1934	818
9	$0.2\ 10^6$	253	85
17	$0.1\ 10^6$	142	42
33	$0.05\ 10^6$	88	23

Iterative

The discretized Poisson's can be solved by iteration. From

$$\rho_{i,j} = \frac{\Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i+1,j} + \Phi_{i,j-1} - 4\Phi_{i,j}}{h^2}$$

obtain

$$\Phi_{i,j} = \frac{1}{4}\left(\Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i+1,j} + \Phi_{i,j-1} - \rho_{i,j}\right)$$

Solve by iteration, starting with a guess. At iteration k it is

$$\Phi_{i,j}^{k+1} = \frac{1}{4}\left(\Phi_{i-1,j}^{k} + \Phi_{i,j+1}^{k} + \Phi_{i+1,j}^{k} + \Phi_{i,j-1}^{k} - \rho_{i,j}\right).$$

Since the beam density evolves slowly from one space charge node to the next, iterative techniques show **rapid convergence**.

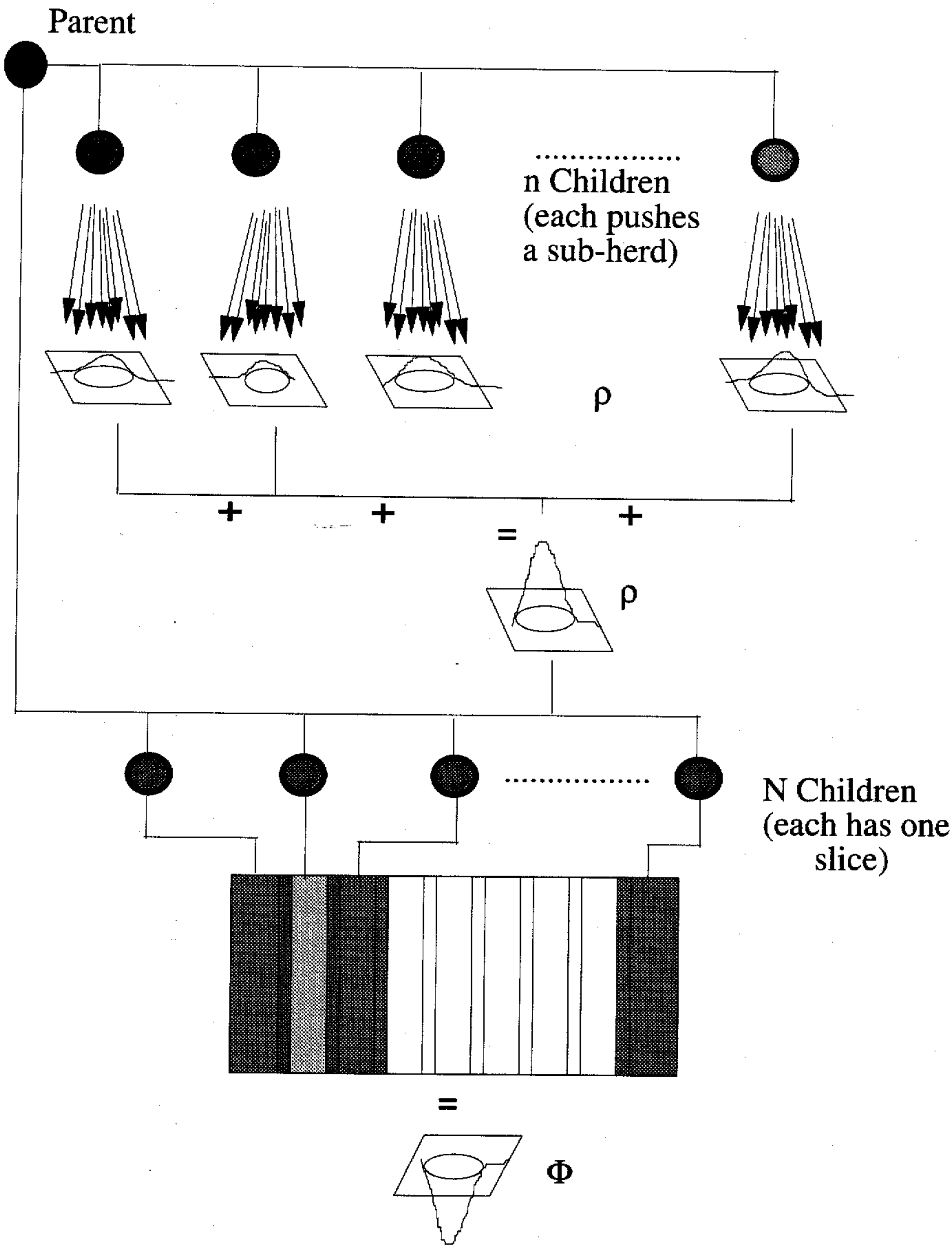
Limitations of this procedure are that maps used to put macros in their appropriate place are for the bare lattice, and not for a **self-consistent** lattice including extra focusing and tune shift due to SC forces.

Consistent with **split operator**

In *Orbit* each slice is comparable in length (equal to or a fraction of) to the length of a machine element.

A slice is surrounded by a given wall configuration. The geometry of the surrounding is stored together with the the transfer maps to completely characterize a machine element.

A similar approach is been used by L.G.Vorobiev *et al* at Michigan


Parent
n Children
(each pushes
a sub-herd)
ρ
+
+
+
=
ρ
N Children
(each has one
slice)
=
Φ

Poisson Solvers

Two basic approaches to find Φ:

- **Differential Poisson** (already shown). and

- **Integral Poisson**:

$$\phi(P) = \frac{1}{4\pi\epsilon_0\gamma^2} \int \frac{\rho(Q)}{r} dQ.$$

$P =$ field point, $Q =$ source point. Green function $=$ the inverse of the distance $r = |P - Q|$

In r we introduce a smoothing parameter to avoid poles that may derive from P coinciding with Q.

In the integral formulation the image charge is part of the **input** -making it more elaborate to include walls in the calculation- Conversely, in a differential formulation the image is part of the **answer**

Integral Poisson Solvers

- **Brute Force**: direct integration.

Method is very transparent. Needs a smoothing parameter. Slow. Good as a check.

- **FFT**: The integral is reduced to a convolution

Differential Poisson Solvers

- Poisson including boundary condition on the walls

$$\begin{cases} \nabla^2\Phi(P) = -\frac{\rho(P)}{\epsilon_0} \\ \Phi(P_{wall}) = 0 \end{cases}$$

There are two distinct classes of numerical algorithms to invert the Laplacian, that makes use of

- finite **differences**: for simple grids say Cartesian
- finite **elements**: adaptive grids -say triangular

Orbit uses finite differences

2-D LU Decomposition

Express the Laplacian operator ∇^2 in discrete form on a $M \times N$ grid that extends to wall

$$-4\pi\rho_{ij} = \mathcal{L}_{ij}^{kl}\Phi_{kl}$$

- Solution

$$\Phi(P) = -\frac{1}{4\pi}\mathcal{L}^{-1}\rho(Q)$$

Second partial derivative (in x, and similarly in y)

$$\frac{\partial^2\Phi}{\partial x^2} = \frac{1}{h^2}\left(\Phi_{i-1,j} - 2\Phi_{i,j} + \Phi_{i+1,j}\right)$$

yields a Laplacian (band-sparse) matrix (δ is Kronecker's)

$$\mathcal{L}_{ij}^{kl} = -4\delta_i^k\delta_j^l + \delta_{i+1}^k\delta_j^l + \delta_{i-1}^k\delta_j^l + \delta_i^k\delta_{j+1}^l + \delta_i^k\delta_{j-1}^l$$

Its inverse is not sparse

Successive Over Relaxation

basic SOR was most efficient for small grids ($N < 128$)

- SOR with **Chebychev acceleration** was most efficient for large grids ($N < 128$). Very dense grids (say, 256×256) are practical.

- **Conjugate Gradient** showed the most rapid convergence, however, the basic algorithm requires more operations

- **Multigrid** methods techniques have the potential of solving systems in N iterations.

Walls -Effects of image charge and current

- Include **boundary conditions** in Poisson Solvers, or
- In a synthetic way use **impedances**, or
- Find an **electrical circuit analog** to the beam-wall interaction.
- Walls are naturally introduced in differential Poisson Solvers,
- Finding images is important as a check, since the balance of charges (real plus image) must be satisfied.

For a perfect conductive walls, the sum of the image charges must be numerically equal to the sum of the beam charges.

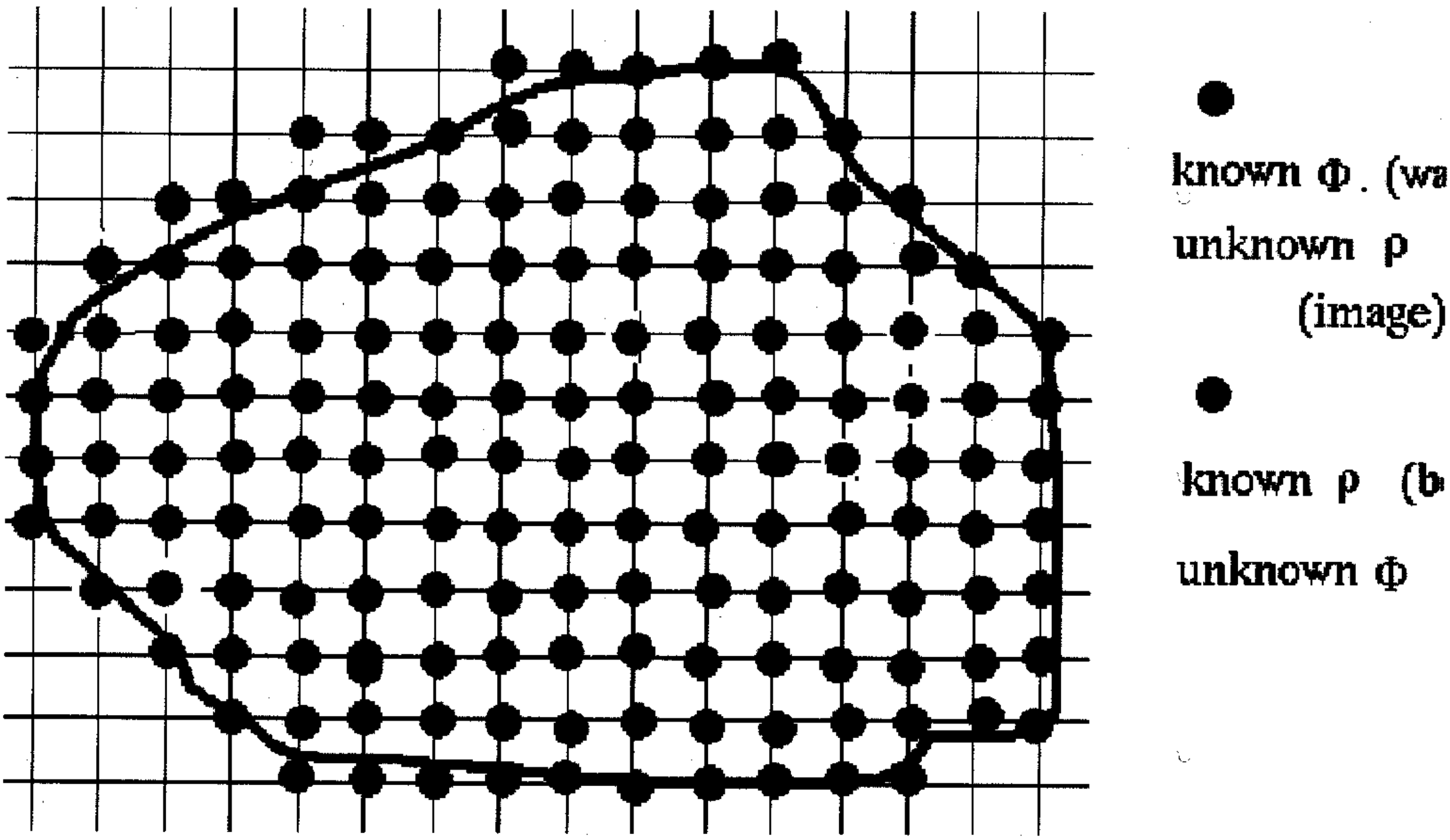
Figure for perfectly conducting walls

Walls are represented by N blue dots. The interior by M red dots

The system of equations is exactly determined.

- $N + M$ **known quantities**: $\Phi = 0$ at the N blue points, ρ at the M red points

- $M + N$ **un-knowns**: M to be calculated as Φ at the red points, ρ_{image} at the N blue points


known Φ. (wa
unknown ρ
(image)
known ρ (b
unknown Φ

Space Charge Momentum Kick

Space charge electric field: $\vec{E} = \vec{\nabla}\phi$, Force: $\vec{F}(P) = \frac{e}{\gamma^2}\vec{\nabla}\phi$

- Momentum kick on each macro: $\frac{\Delta\vec{p}}{p} = \frac{1}{p}\int \vec{F}\,dt$

In a Split Operator sense: $dt = \Delta t = L/\beta c$

- Transverse kick - $L_\perp$ separation between transverse SC kicks

$$\frac{\delta p_\perp}{p} = \wp\frac{\partial\phi}{\partial r}L_\perp$$

- Longitudinal (energy) kick - $L_\|$ separation between longitudinal SC kicks

$$\frac{\delta\Delta E}{E} = \beta^2\wp\frac{\partial\phi}{\partial z}L_\|$$

perveance: $\wp = \frac{4\pi\lambda q h r_0}{\Delta x\beta^2\gamma^3 m_0}$

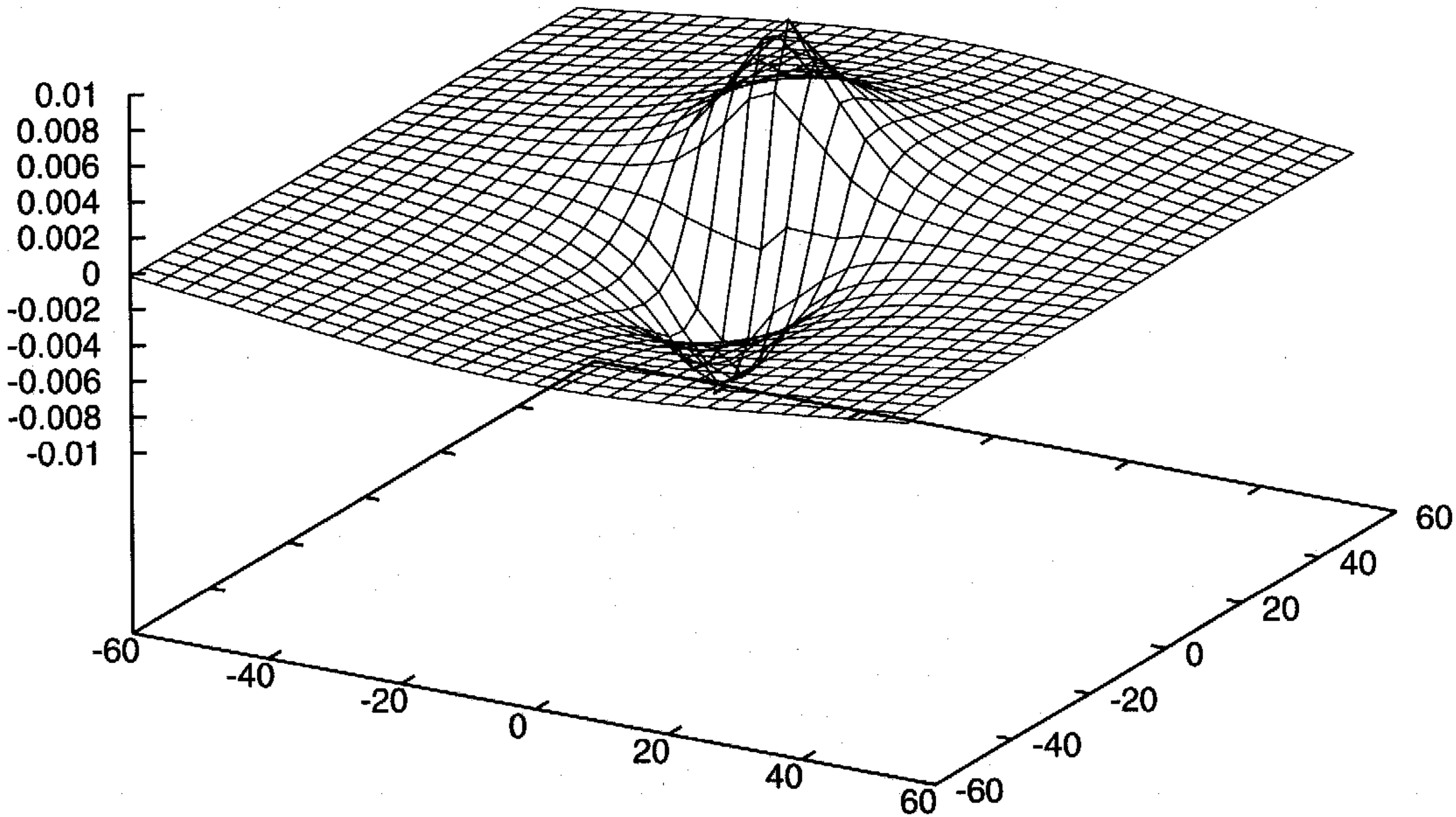
λ: longit. charge per unit length, Δx: size of a grid cell (square)

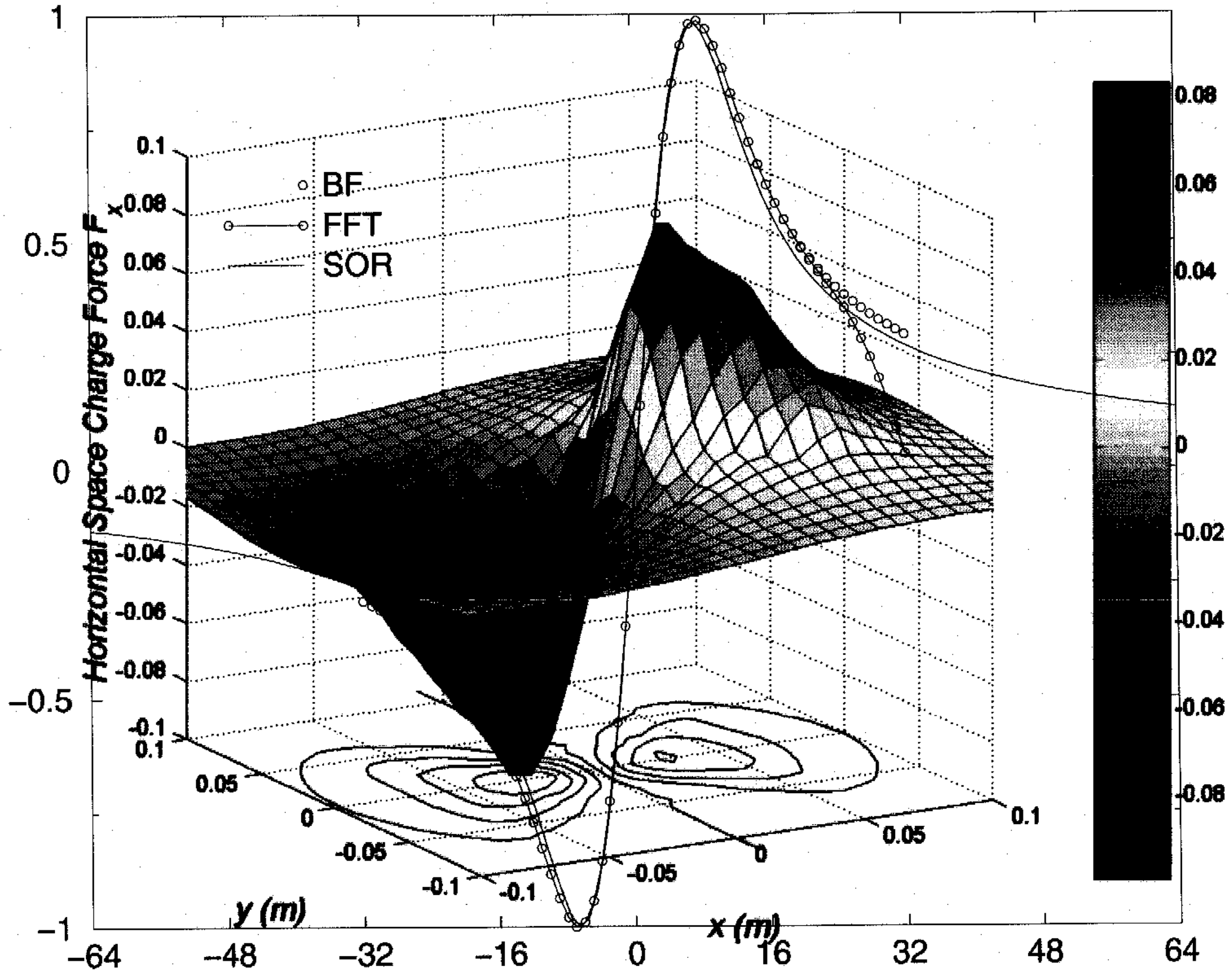
Comparison of Solvers in the Transverse Space-1

- Space Charge field shape calculated with two integral Poisson solvers, i.e. Brute Force and FFT and with a SOR differential solver.

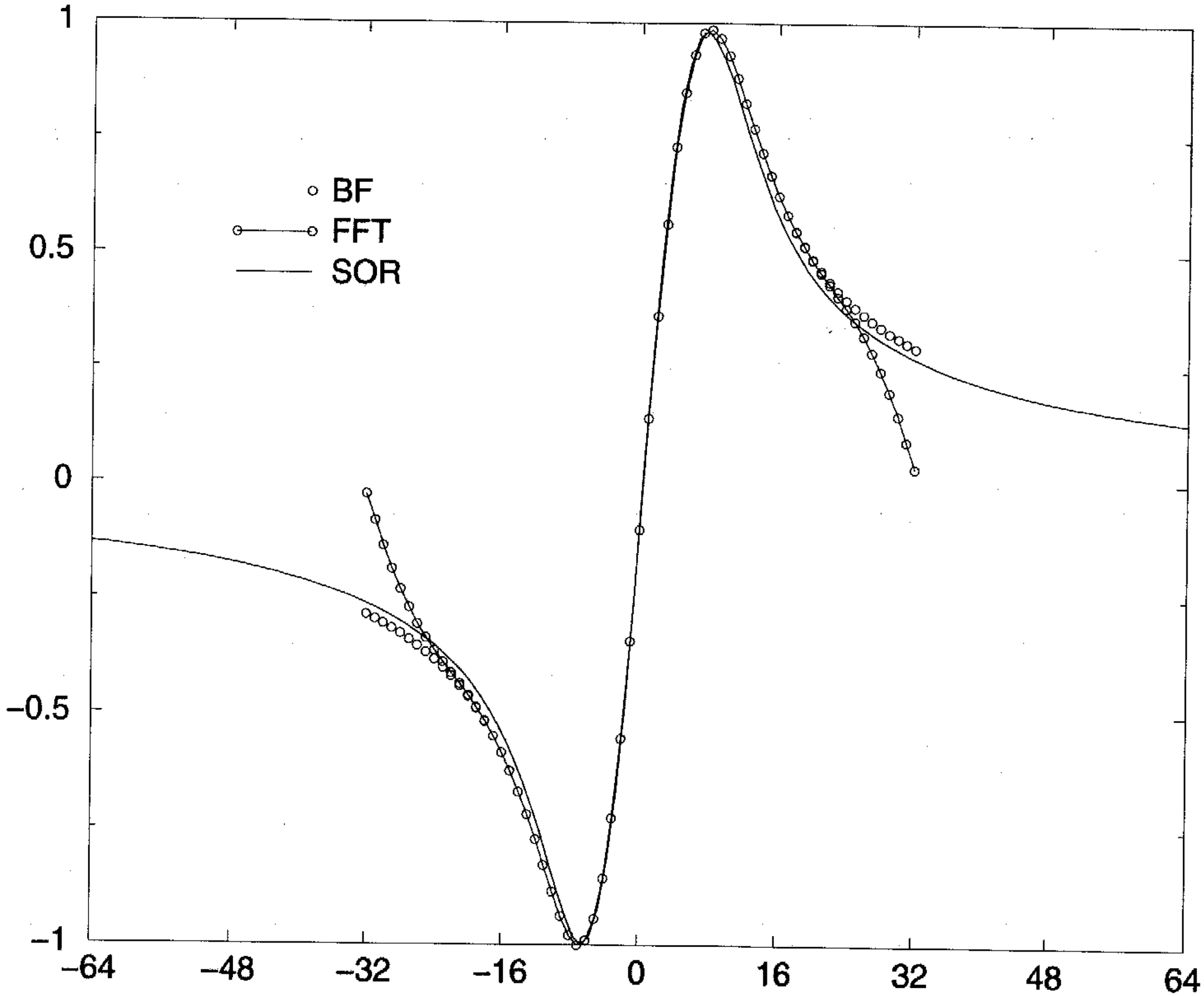
Walls were moved far away, since the two integral methods did not allow their inclusion. For all three cases a gaussian random beam distribution entirely contained in a 64×64 Cartesian grid was used.

The figure clearly shows that the agreement between BF and SOR is good, while the force calculated with FFT vanishes at the edge of the space occupied by the beam, but is in good agreement with the other two methods.


0.01
0.008
0.006
0.004
0.002
0
-0.002
-0.004
-0.006
-0.008
-0.01
-60
-40
-20
0
20
40
60
-60
-40
-20
0
20
40
60


BF
FFT
SOR
Horizontal Space Charge Force F_x
y (m)
x (m)
1
0.5
0
−0.5
−1
−64
−48
−32
−16
0
16
32
48
64
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08

- 18 -



BF
FFT
SOR
1
0.5
0
−0.5
−1
−64
−48
−32
−16
0
16
32
48
64

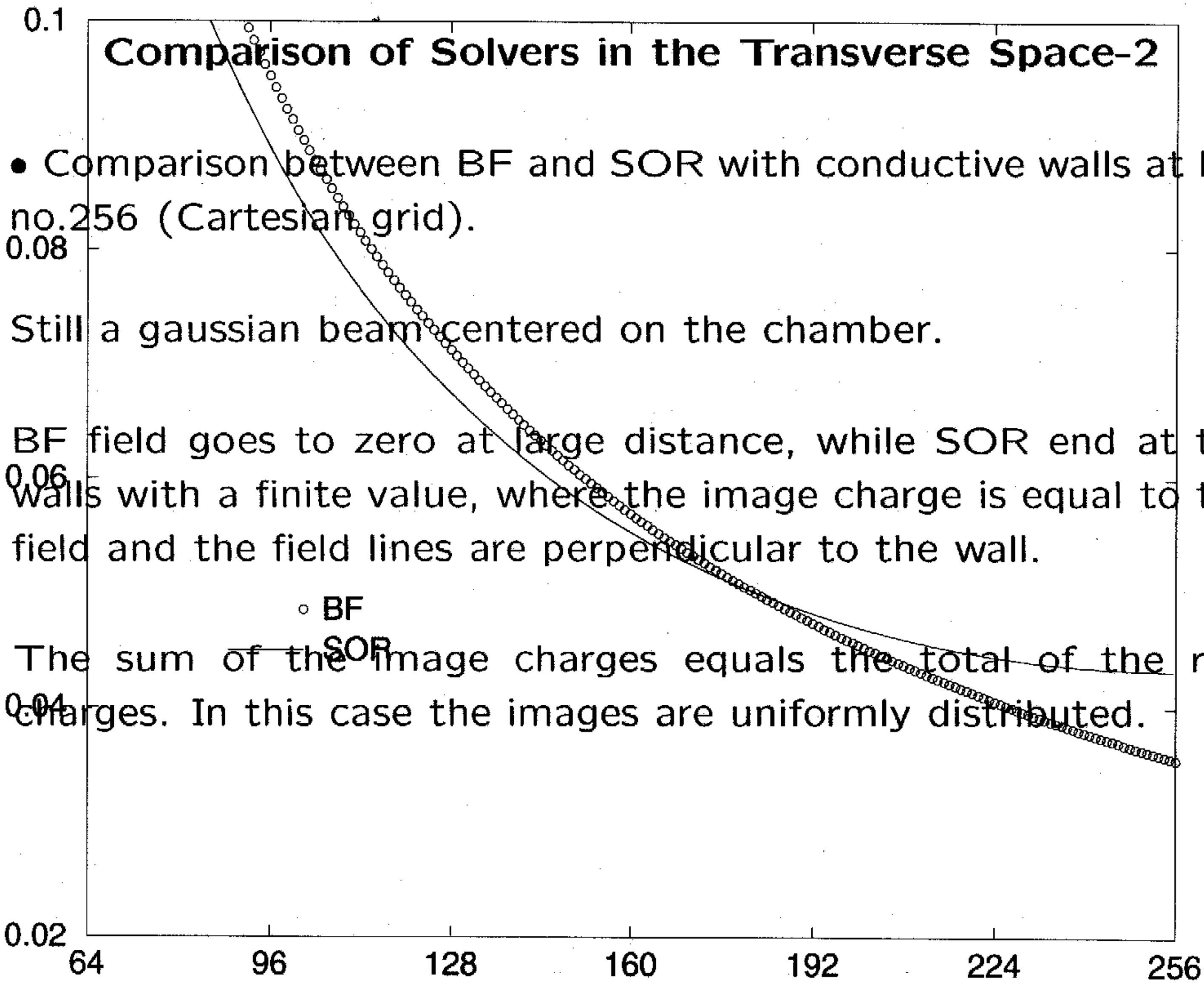
Comparison of Solvers in the Transverse Space-2

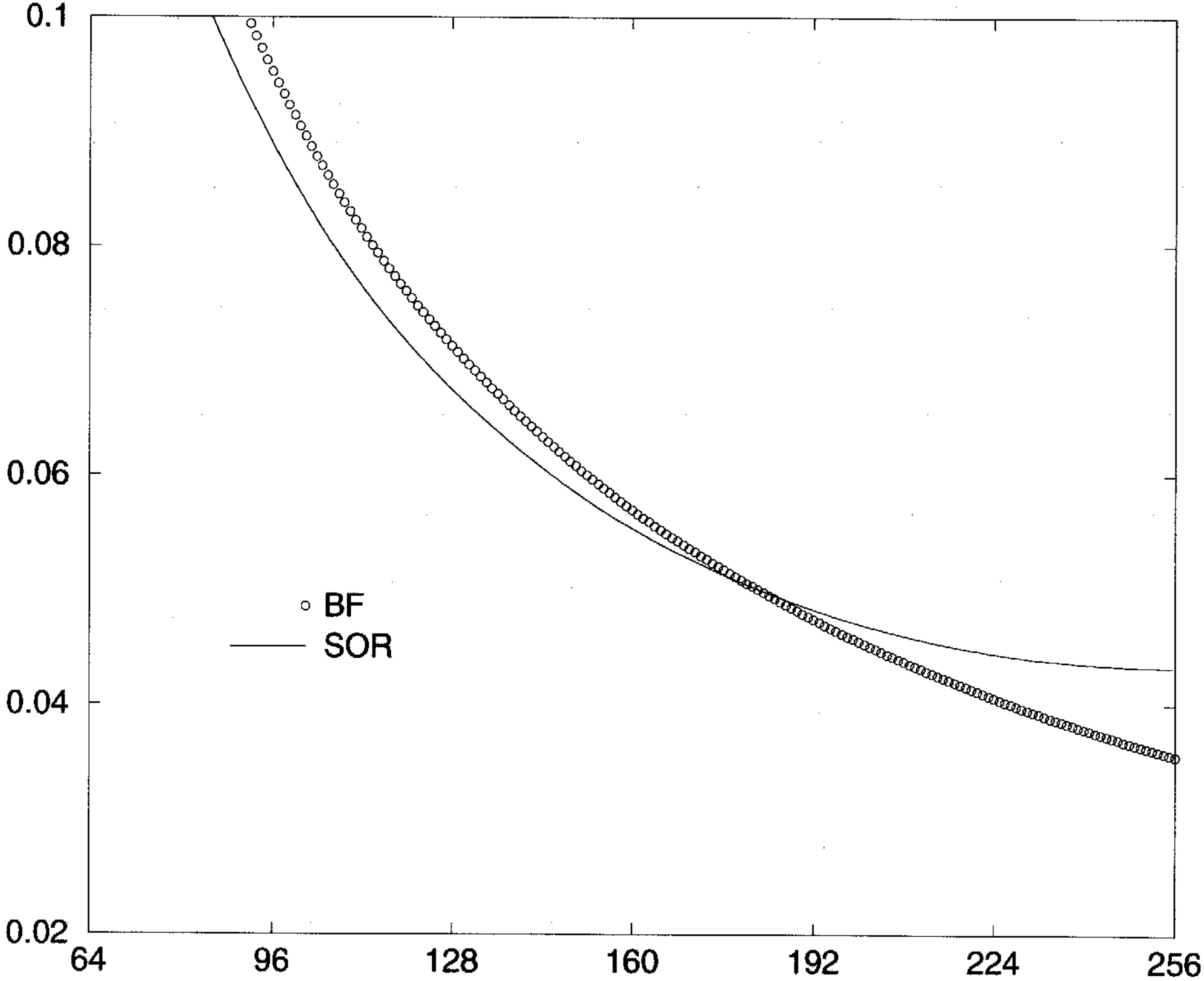
• Comparison between BF and SOR with conductive walls at bin no.256 (Cartesian grid).

Still a gaussian beam centered on the chamber.

BF field goes to zero at large distance, while SOR end at the walls with a finite value, where the image charge is equal to the field and the field lines are perpendicular to the wall.

The sum of the image charges equals the total of the real charges. In this case the images are uniformly distributed.





0.1
0.08
0.06
0.04
0.02
64
96
128
160
192
224
256
BF
SOR

Comparison of Solvers in th Transverse Space-3

- Image charge distribution on the walls

The distribution on the left and botton walls are not identical because the beam is not circular in section.

The integrated image charge is equal to the beam charge, as it should for perfecting conducting walls that don't allow any leaks of the field to the outer world.

- Reference simple case:

Cylindrical symmetric beam in a cylindrical conducting pipe of radius b. Beam is displaced from the center of the pipe by ξ in the direction x. The electric field produced by the image charge at the center of the beam is

$$E_x = \frac{\rho_L}{2\pi\epsilon_0}\frac{1}{(b^2/\xi) - \xi} \tag{1}$$

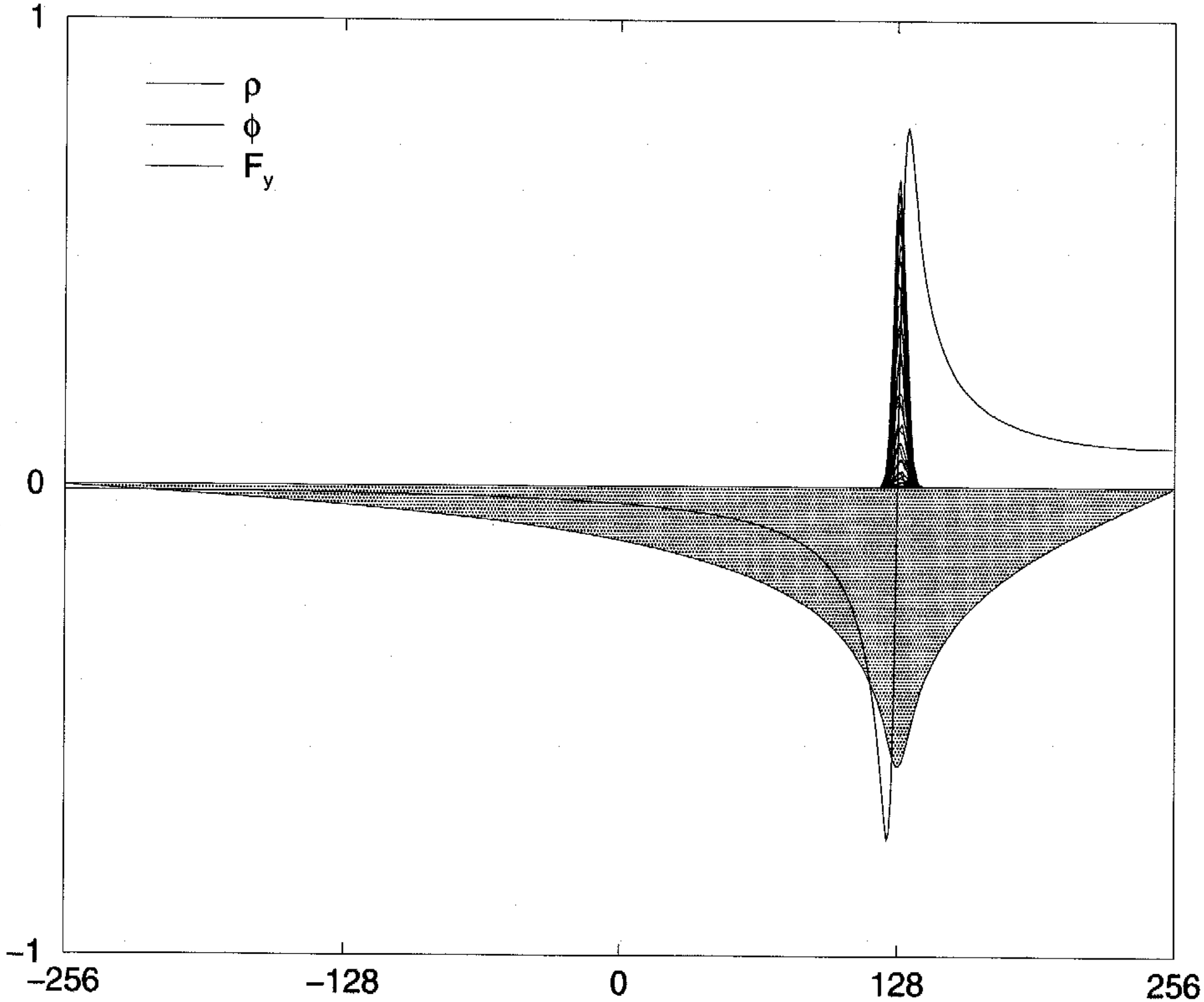
with ρ_L the beam charge per unit length.

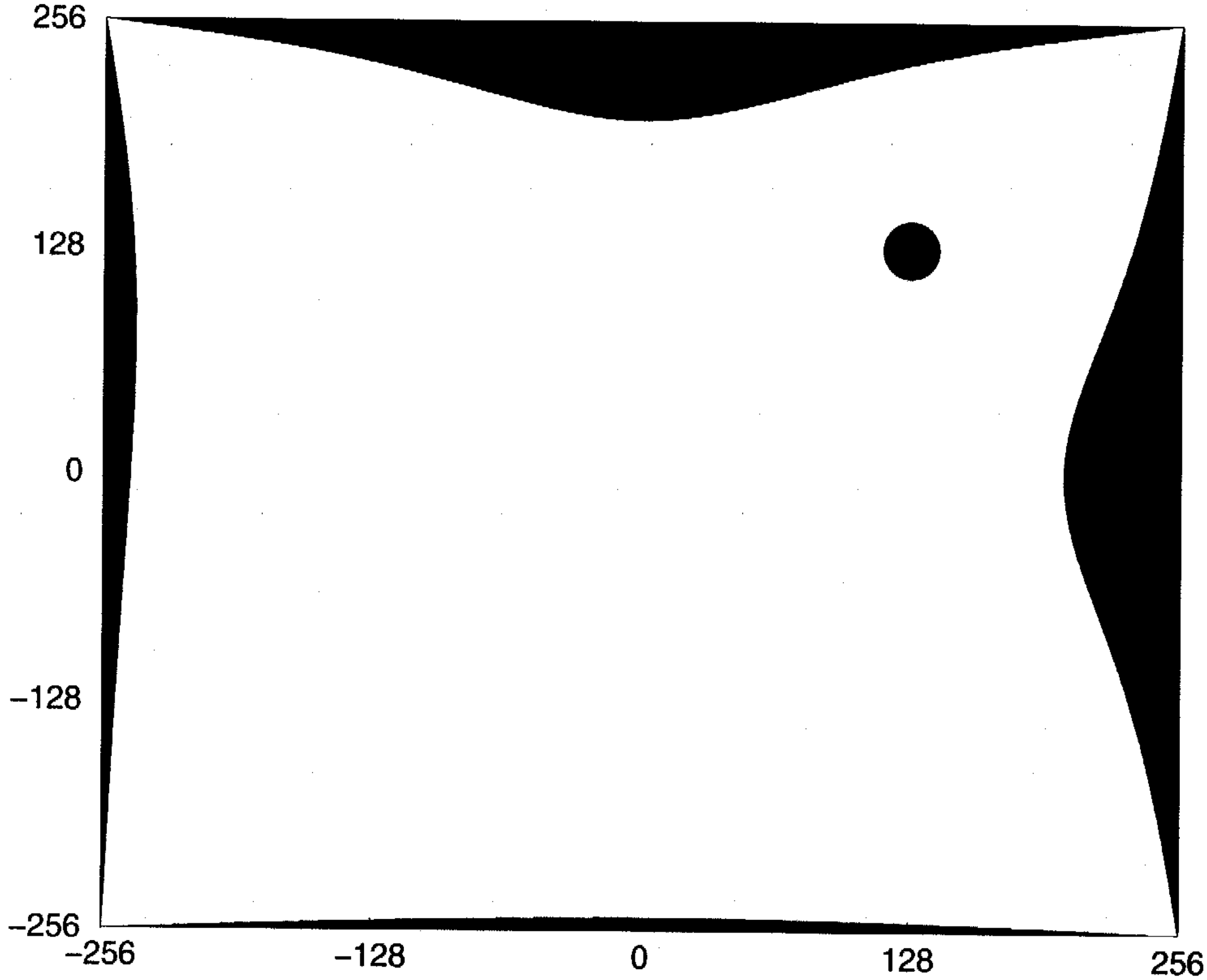
Comparison of Solvers in the Transverse Space-4

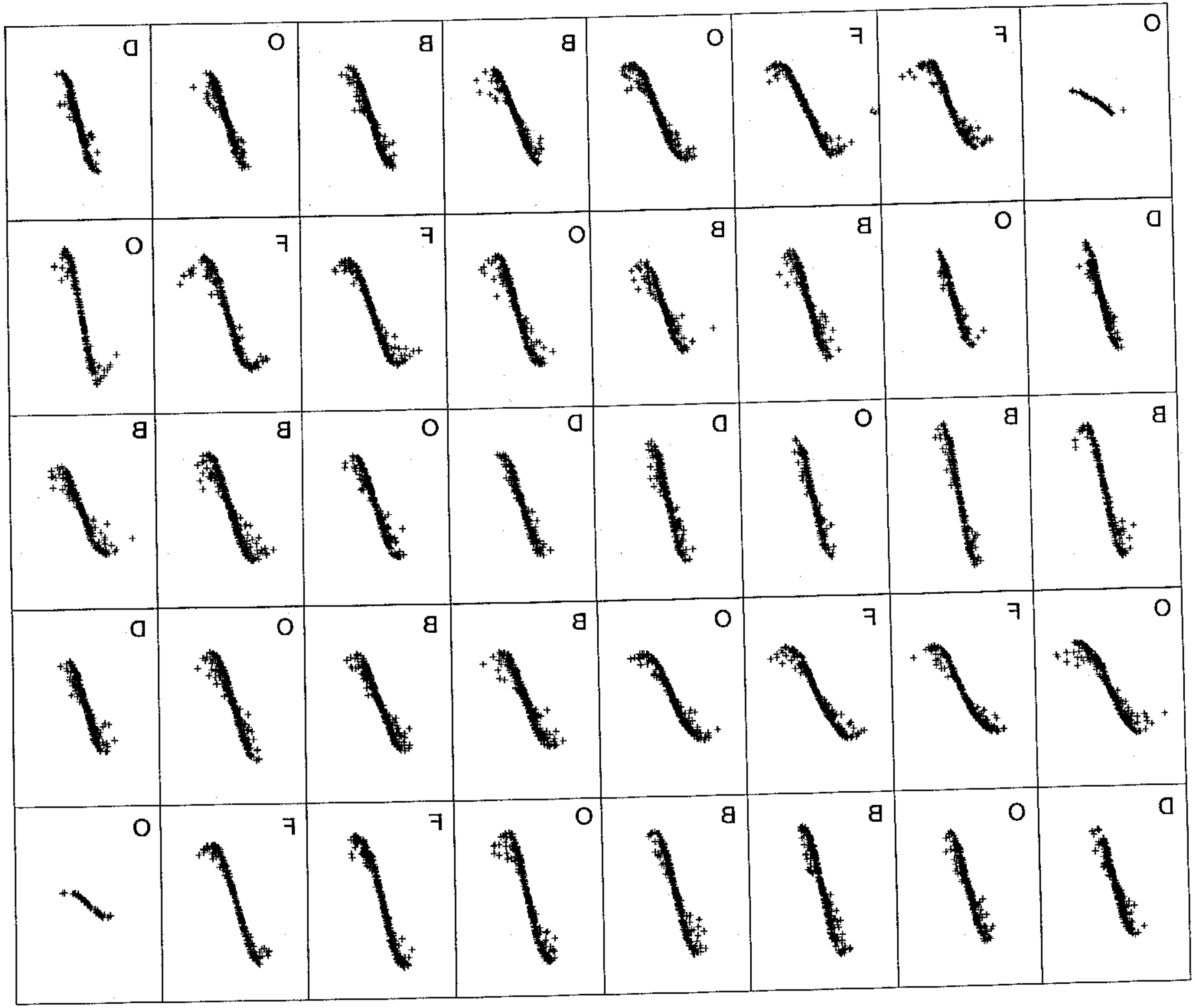
- Charge distribution, potential and one component of the field for a beam offset in x and y in a square conductive chamber.

Grid of 512×512.

Potential goes to zero at the walls, and the field converges at the wall to a finite value numerically equal to the image charge density there

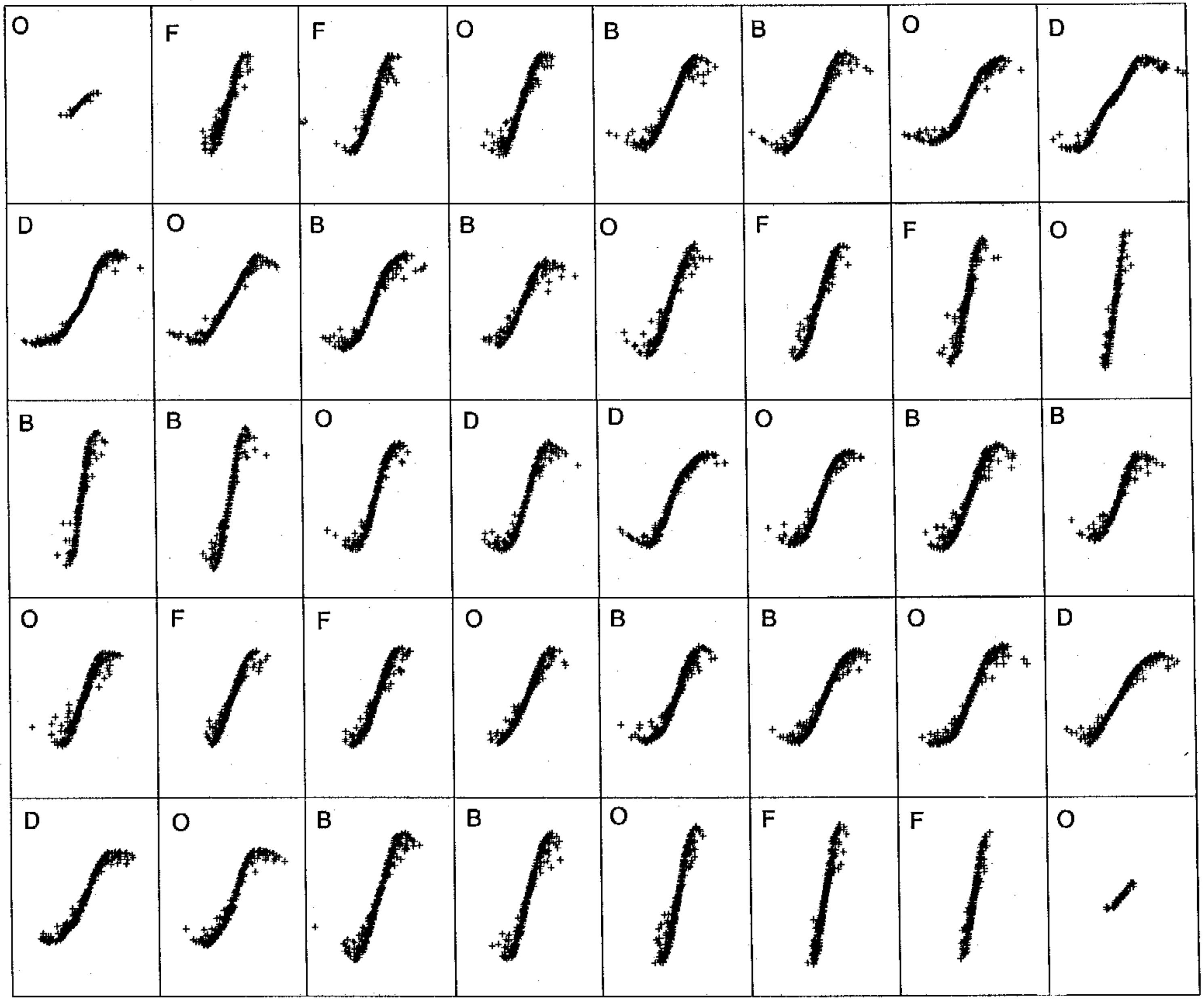

1
0
−1
−256
−128
0
128
256
ρ
φ
F_y


256
128
0
−128
−256
−256
−128
0
128
256



Fx-vs-x.D

Thu Sep 27 10:52:20 2001



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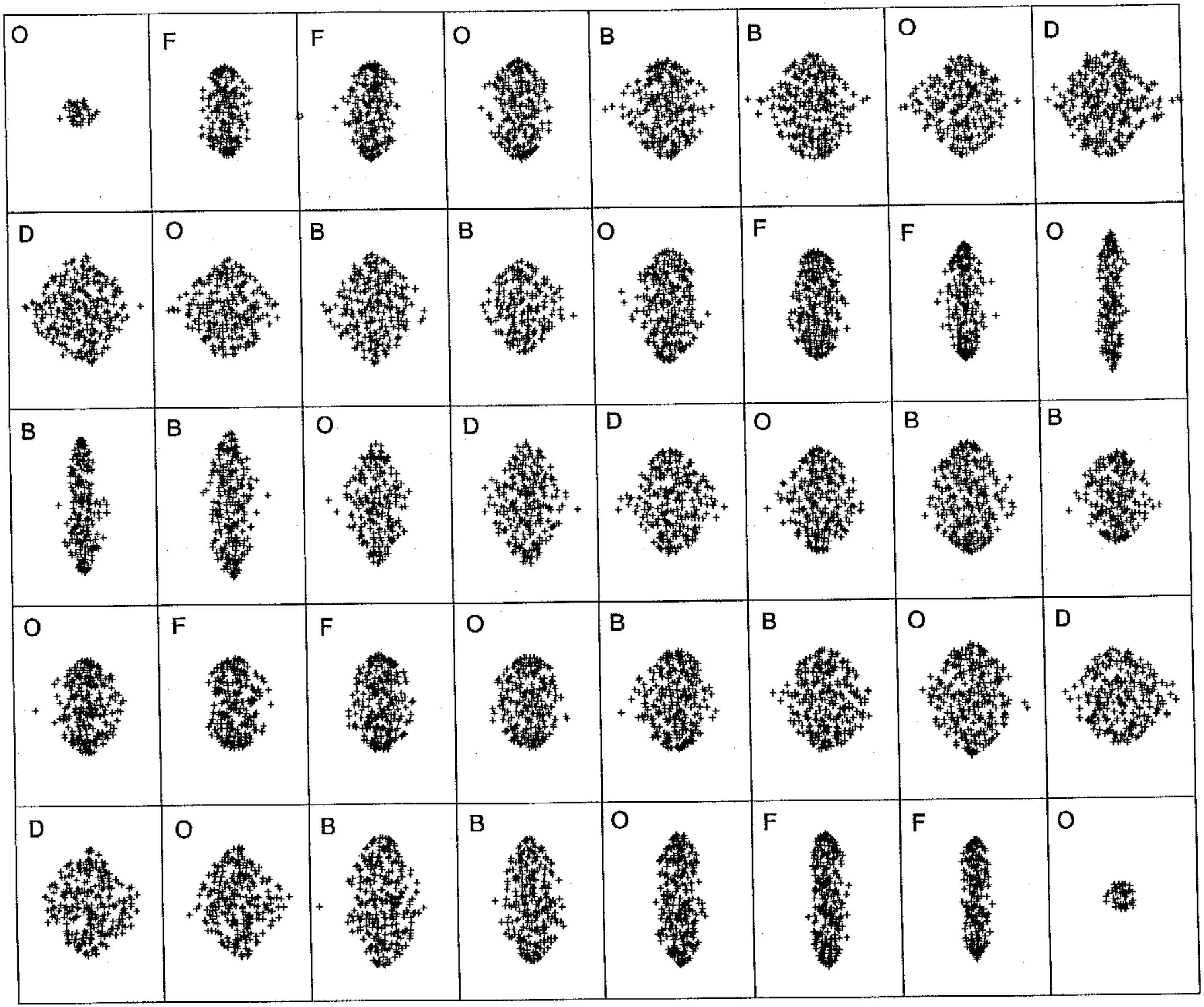
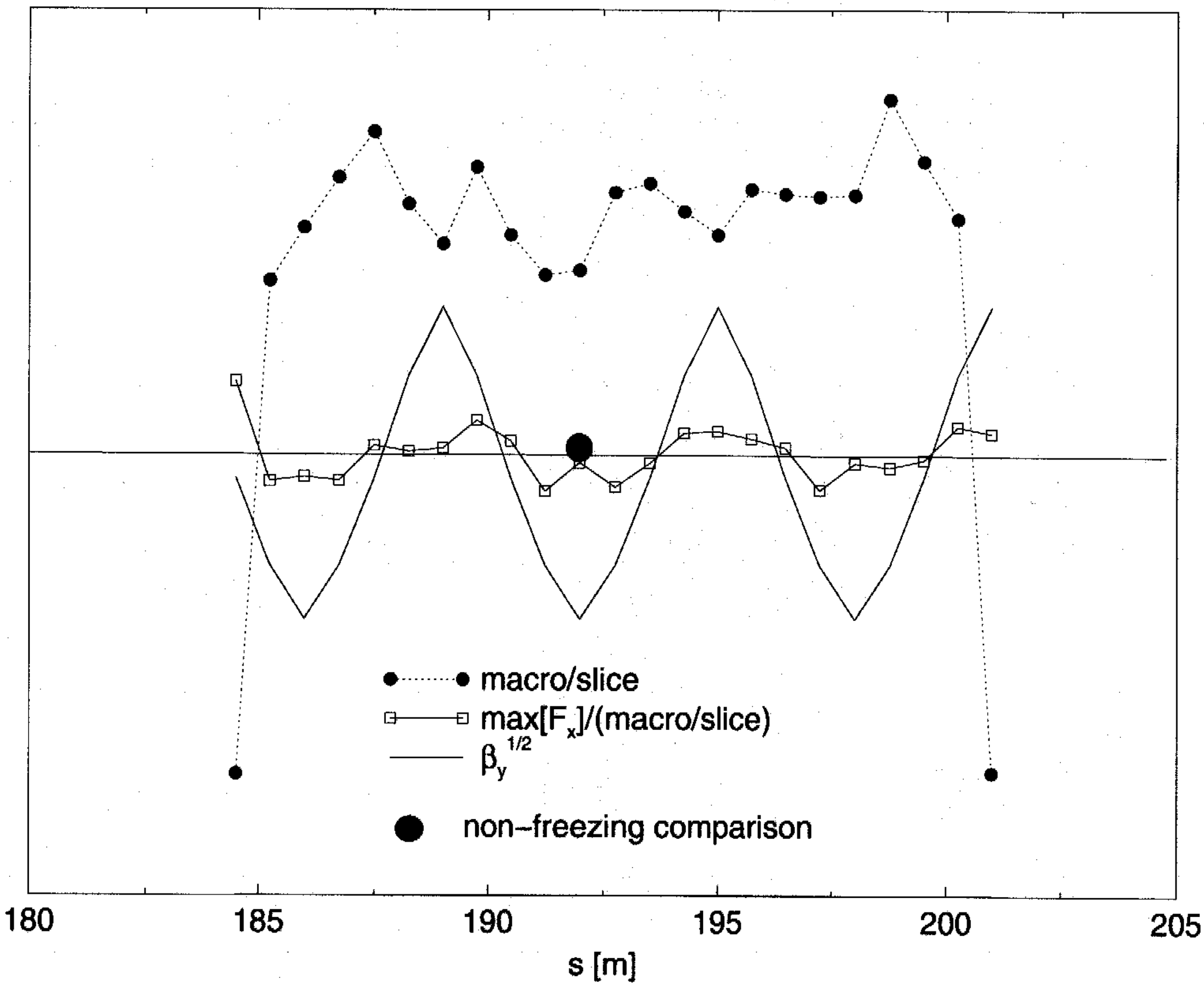
Fy–vs–y.D



Fx–vs–y.D

Thu Sep 27 11:02:53 2001



macro/slice
max[F_x]/(macro/slice)
β_y^1/2
non-freezing comparison
180
185
190
195
200
205
s [m]

Longitudinal Potential in a Frozen Beam-1

The longitudinal potential gradient is calculated as a function of (x, y), as the difference of potential between analogous points in the median transverse plane of successive slices. Actually, we use three slices, say: 1, 2, 3, in a leap-frog fashion

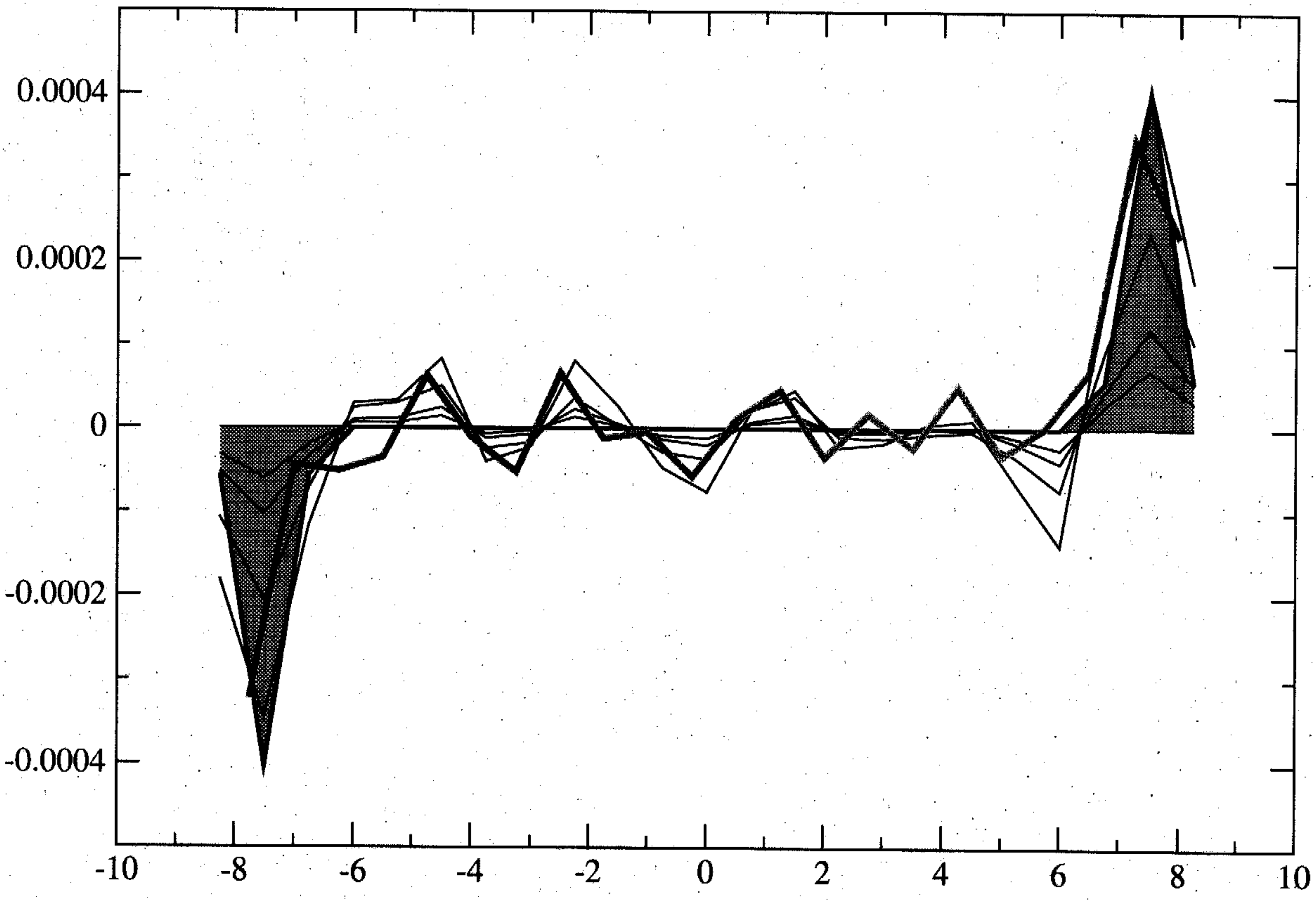
$$\frac{\partial \phi}{\partial z}(x, y)_2 \approx \frac{1}{2L_{slice}} \left[\phi_3 - 2\phi_2 + \phi_1\right](x, y),$$

with L_{slice} is a length of a slice.

A longitudinal SC energy kick is traditionally calculated as

$$(\Delta E)_{SC} \propto Z_0 \frac{\lambda'}{2\gamma^2} \left[1 + 2 \ln \frac{b}{a} + f(r)\right]$$

with λ' the longitudinal gradient of the beam charge, b and a the radius of the accelerating chamber and of the beam, respectively, and f some function of the transverse charge distribution.



Mon Apr 1 19:40 2002

Longitudinal Potential in a Frozen Beam-2

• The advantage of the frozen-sliced beam approach is evident. With this method the longitudinal kick is calculated directly from the configuration of the beam and of the surrounding vacuum walls, that doesn'need necessarily to be a round pipe.