Space Charge Models for Particle Tracking on Long Time Scales

J. Holmes, S. Cousineau,

A. Shishlo, and R. Potts

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The Need

- Space charge physics has been successfully incorporated into computational particle tracking studies of linacs, accumulator rings, and rapid cycling synchrotrons.
- Computations for these machines all involve tracking particles on short to moderate time scales.
- With the advent of higher beam intensities, calculations incorporating space charge effects are now being undertaken for storage rings.
- Storage ring calculations require following beams for far longer times than are necessary for linacs, accumulator rings, or rapid cycling synchrotrons.
  - This will place more severe requirements on the speed and accuracy of the physics models.
  - Progress for modeling collective effects, such as space charge, is necessary.
- Problems: Representation and discretization.

Successful Simulations Requiring Space Charge in Accumulator Rings

S. Cousineau, J. A. Holmes, J. Galambos, A. Fedotov, J. Wei, and R. Macek,
Physical Review Special Topics – Accelerators and Beams 6, (2003) 074202 .

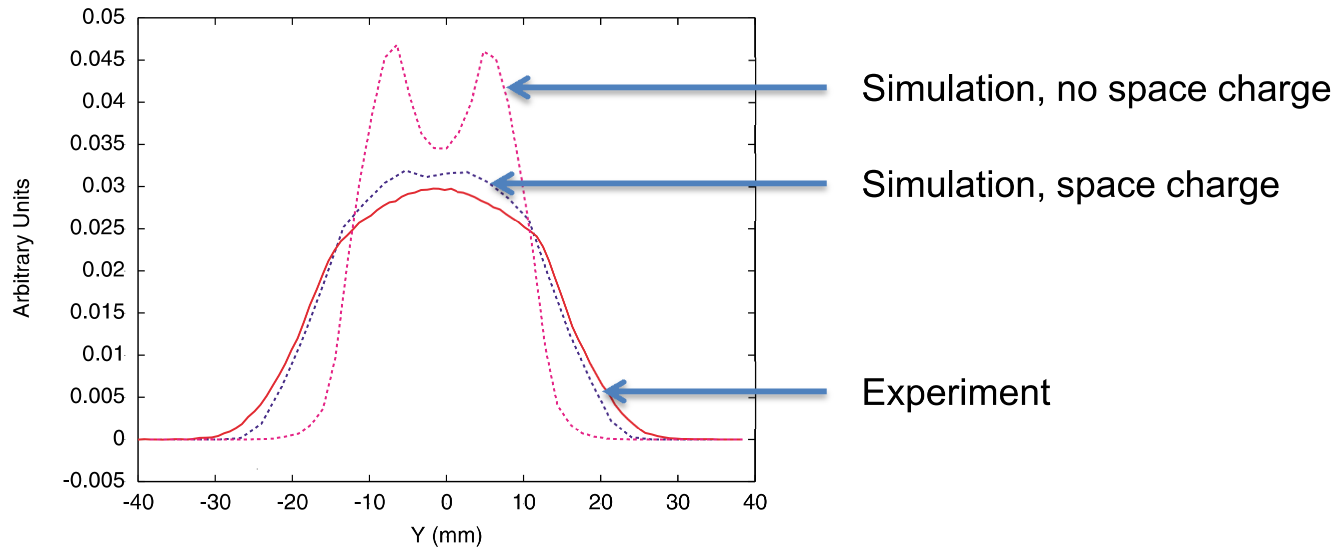


FIG. 1. (Color) Benchmark of vertical experimental profile measurements with PIC simulations. The solid (red) curve is the experimental profile. The dotted (blue) curve is the PIC result with space charge. The (pink) dashed line is the PIC result without space charge.

Transverse profiles: experiment and simulation with and without space charge in PSR ring.

Simplifications We Take for Granted

- A beam consists of many identical indistinguishable particles interacting quantum mechanically with each other and with their surroundings.
- In tracking studies, we simplify to treat the beam as distinguishable particles moving classically. This allows us conceptually to separate the forces acting on the beam into external forces, internal forces, and other beam-induced forces (wake fields, beam loading, …).
- As in plasma physics, we further separate the internal forces into long-range (potential) and short-range (scattering) contributions.
- By space charge, we mean the long range internal electromagnetic forces in the beam.

Further Simplifications

- There are further approximations in arriving at space charge models:
  - Beams consist of bunches.
  - Within each bunch, relative velocities are assumed to be much less than light speed.
  - Intrabunch forces are treated electrostatically.
  - Forces between bunches (beam-beam, electron cloud, etc.) must account for the relative bunch velocities through the full Lorentz force equation.
- These approximations reduce the calculation of space charge effects to the solution of Poisson's equation. To do this numerically, it is necessary to represent the charge/current distribution of the beam and to introduce discretization.

Dimensionality of Model

- 1D Longitudinal
  - Treat as longitudinal impedance. See A. W. Chao, "Physics of Collective Beam Instabilities in High Energy Accelerators", John Wiley and Sons, New York, 1993 for formulation.
  - Can be combined with other longitudinal impedances.
  - Used in 1D longitudinal dynamics or in conjunction with 2D transverse model in 3D tracking.
  - Time between evaluations << (synchrotron frequency)$^{-1}$.
- 2D Transverse
  - Multiply space charge kick by a longitudinal density factor to accommodate bunch factor effects.
  - Fast methods exist to solve for potentials or direct force.
  - Time between evaluations << (betatron frequency)$^{-1}$.
- 2.5D
  - Bin particles to a 3D grid with identical longitudinal slices.
  - Solve for the 2D potential on each slice with conducting wall boundary conditions and use to interpolate the forces at the particle locations in the 3D grid.
  - Needed for transverse impedance calculations or cases where bunch properties change along longitudinal direction.
  - Time between evaluations << (betatron frequency)$^{-1}$ and << (synchrotron frequency)$^{-1}$.
- The models above are all applicable to long bunches, $L_{Bunch} >> r_{BeamPipe}$.
- Full 3D
  - Most general.
  - Necessary for short bunches $L \leq b$: most often used in linac calculations.
- Complexity increases with dimension. Use simplest model containing desired physics.

Representation of the Beam

- Linear envelope and particle core models (in 2D and 3D).
  - Space charge force is linear inside core.
  - Fast and simple evaluation.
  - Used in theoretical studies: halo generation mechanisms, half-integer resonance,...
  - No emittance growth in evolution.
  - Reality?
- Use tracked particles directly to calculate the forces (PIC codes - Multigrid, FFTs, Fast multipoles).
  - Computationally intensive.
  - Discretization due to distribution, and perhaps gridding.
  - Most widely used in simulations.
- Hybrid models: Analytic or smoothed distributions fitted to parameters of tracked particle beam.
  - Track particles and fit to analytic or smoothed distribution.
  - Can be fast.
  - Parameter values evolve with tracked beam distribution.
  - Details of tracked distribution may be lost in force evaluation.

Numerical Discretization

- Time discretization is necessary, regardless of beam representation.
  - Simulations apply space charge forces as impulses, separated by single particle transport.
  - If time between impulses is too large, accuracy is lost.
    - Nearby particles may become anomalously close in single particle transport.
    - Need many space charge evaluations per betatron or synchrotron oscillation.
- Using the tracked particles to provide the charge/current distribution introduces discretization through the bunch.
  - Real accelerator bunches may have 10^8 – 10^{14} particles.
  - Accelerator simulations may use 10^4 – 10^9 macroparticles, with the lower end of this range being typical on workstations or small clusters.
- A further source of discretization relates to the use of spatial meshes.
  - Direct evaluation of forces between N macroparticles requires $O(N^2)$ computational work.
  - Faster methods O(~N) have been developed. Some of these methods involve
    - the distribution of the macroparticle charges to the mesh points,
    - the solution of the potential or forces at the mesh points,
    - and the interpolation of the forces back to the particles.

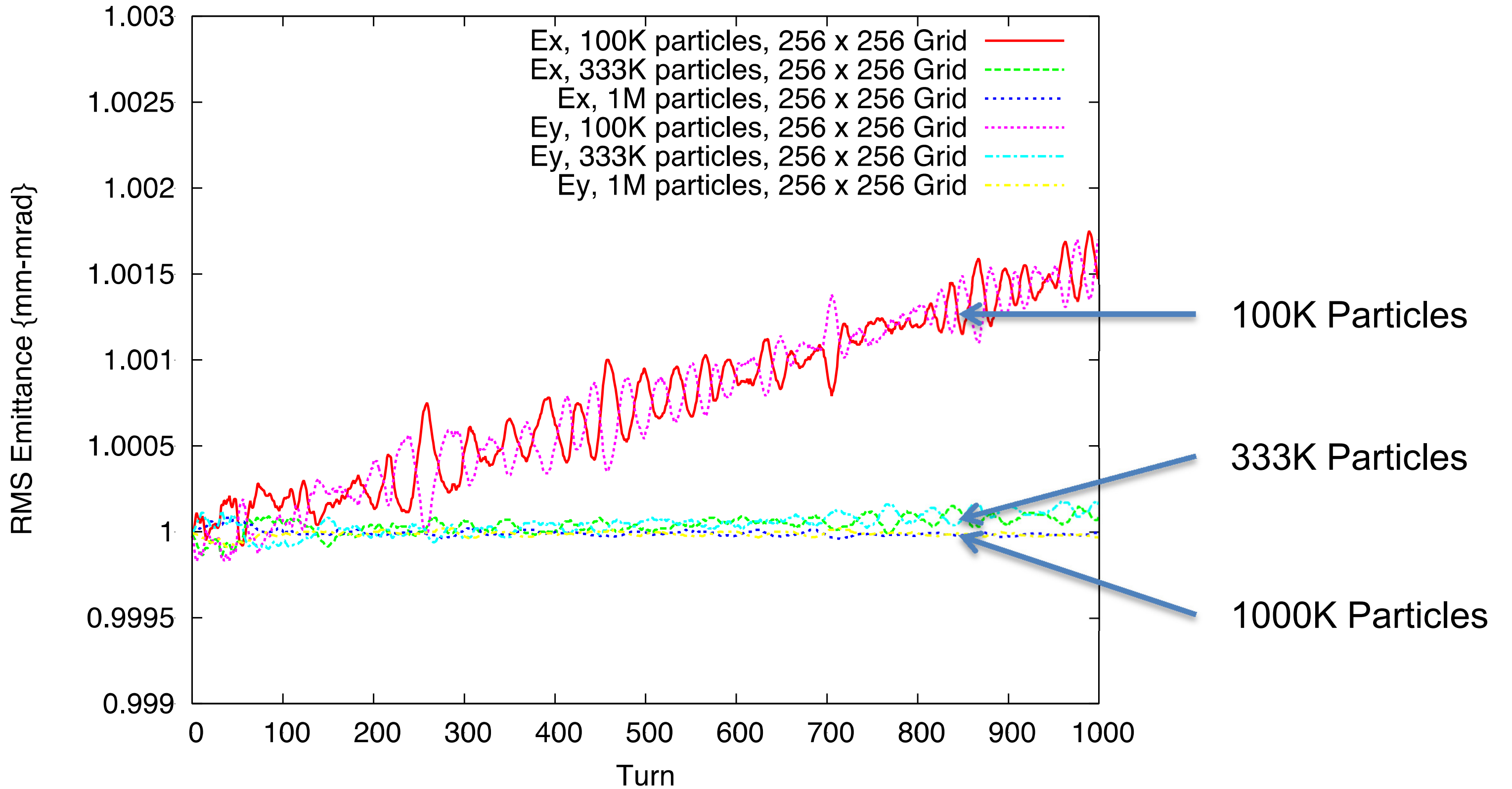
Direct Force From Particle Methods

- A full discussion of numerical methods for solving Poisson's equation is beyond the scope of this talk. Here I mention only three PIC methods with speed of order ~N.
  - Multigrid methods
    - Discretization errors due to gridding.
    - Indirect solution requires iteration to converge.
  - Fast Fourier transforms (FFTs)
    - Discretization errors due to gridding.
    - Direct solution.
  - Fast multipole methods
    - No discretization errors due to gridding, accurate to machine precision.
    - Direct Solution.
- References on numerical solution of Poisson's equation:

  - R. W. Hockney and J. W. Eastwood, "Computer Simulation Using Particles", Institute of Physics Publishing, Bristol, 1988.
  - J. Demmel, NSF-CBMS Short Course on Parallel Numerical Linear Algebra, especially Lectures 24-27, http://www.cs.berkeley.edu/~demmel/cs267-1995/
  - L. Greengard and V. Rokhlin, "A Fast Algorithm for Particle Simulations", Journal of Computational Physics 73, (1987), 325.

Applicability of Model Depends on Information Sought

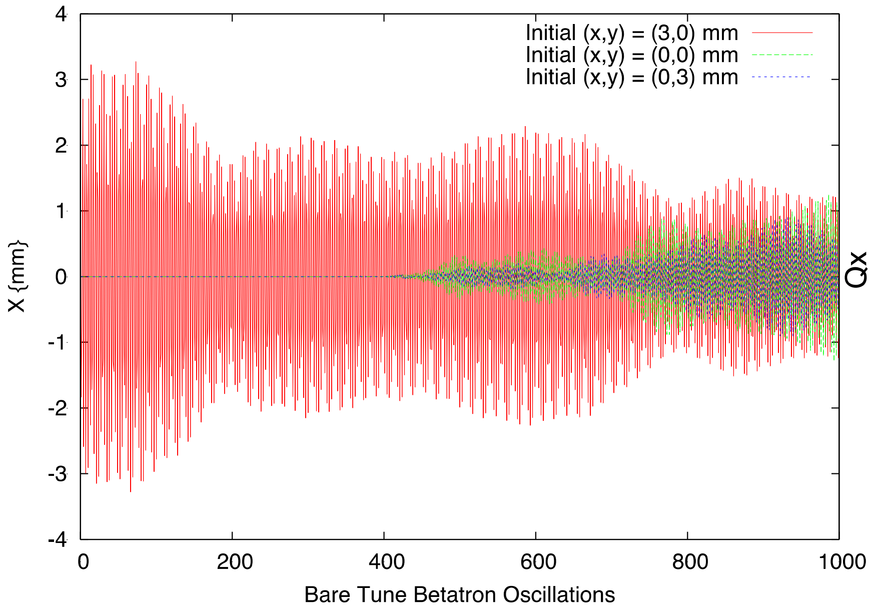
- **Bulk quantities, such as RMS emittances, can be obtained for short to medium time scales with moderate numbers of particles, but numerical diffusion leads to slow growth over long times. Even for short times, it is necessary to be sure the numerics converge.**



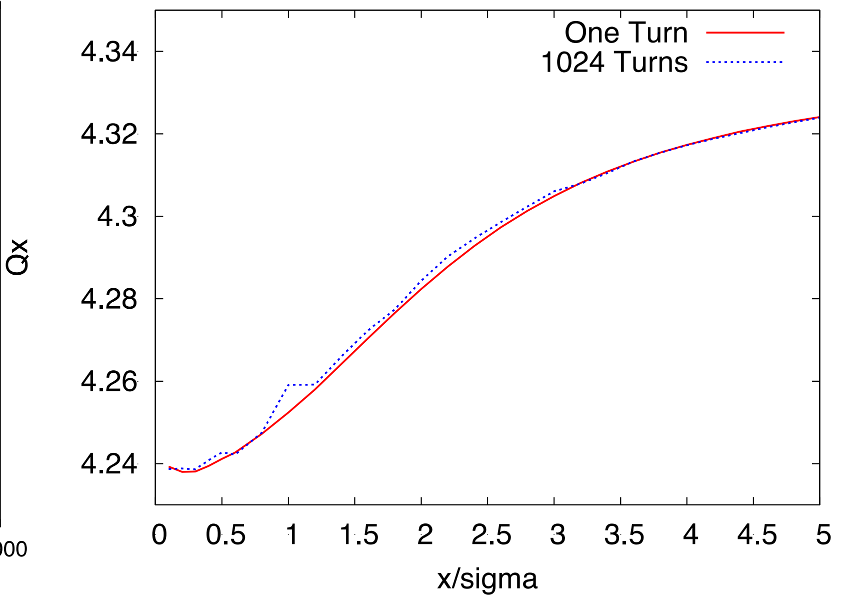
256x256 grid with various numbers of particles.

Goodness of Model Depends on Information Sought

- **Individual particle behavior is much more difficult to converge, due to discretization-induced numerical noise. Discretization arises from time-stepping, numerical distribution, and gridding.**



Individual particle orbits diffuse in time.



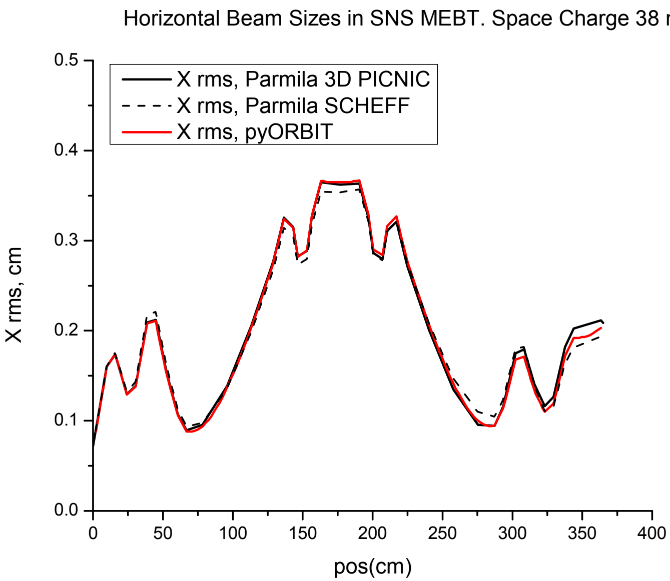
Calculated tunes of individual particles are sensitive to this diffusion.

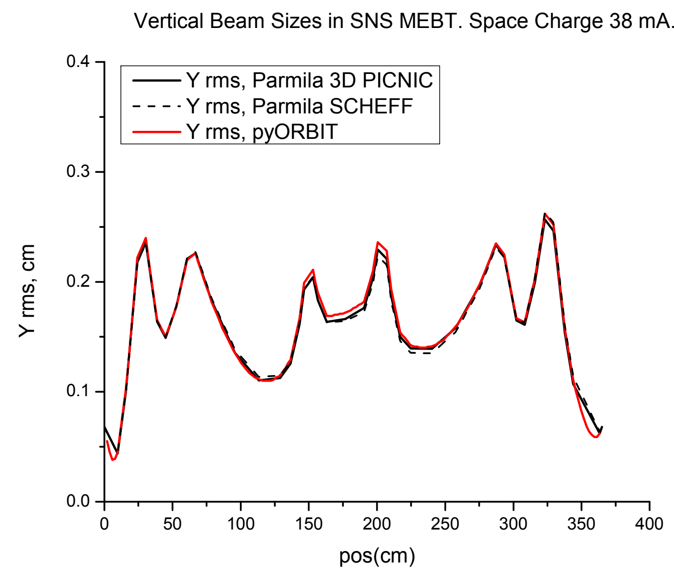
For long times, convergence criteria are hard to satisfy.

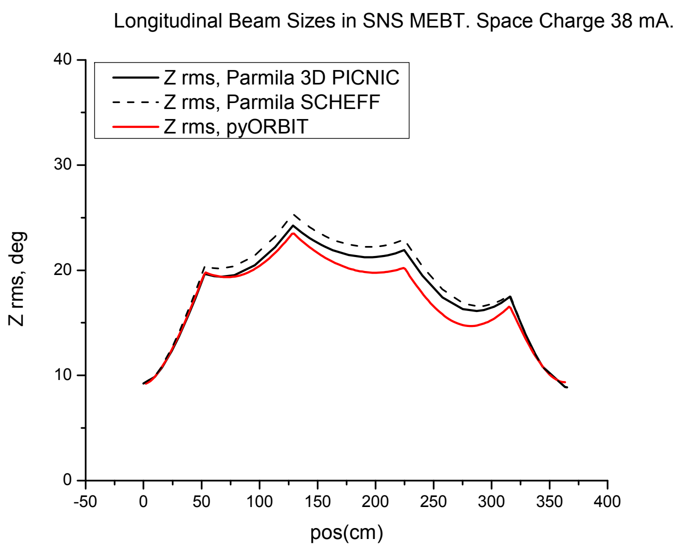
What to do?

- Refinement: More macroparticles, smaller time steps, finer meshes…
  - Feasible to some extent with the help of modern computers: clusters, GPUs, etc.
  - Still expensive and “brute force”.
- Reduce discretization effects
  - Fast multipole methods can alleviate grid discretization errors associated with FFTs. Time and distribution discretization effects are still present.
  - For FFT solvers, try different binning or smoothing algorithms for distributing space charge from the numerical particle distributions to the grid. Like low pass filters, can alleviate grid and distribution discretization effects. One example is the template method of Vorobiev (Leonid Vorobiev, Space Charge 2013, CERN, April, 2013).
  - Simplified or analytic distributions, based on statistically calculated parameters of the macroparticle distribution, provide another type of low pass filter to reduce grid and distribution discretization effects. Such methods can be used to evaluate space charge forces quickly.
  - Questions for the latter approaches: How much physics is lost in the simplification? How important is that physics?
- We are exploring all of these approaches in the ORBIT Code.

MEBT 38 mA. PARMILA vs. pyORBIT







Water Bag 3D, 38 mA
2,000 macro-particles for Ellipse SC
20,000 macro-particles for 3D FFT
32 x 32 x 32 grids
Bunchers RF is on, 90^0 phases

Timing:
Parmila SHEFF – about 4 sec
PARMILA 3D PICNIC – 8 sec
pyORBIT 1 Ellipsoid – 1.6 sec