Modeling of intense beams

HEP GARD Accelerator and Beam Physics: Workshop #2, WG2

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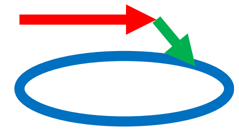
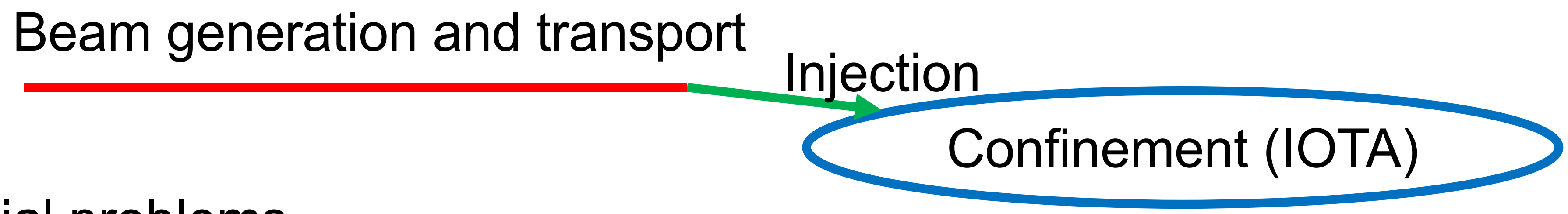
Status of (*Modeling of) Intense Beams*

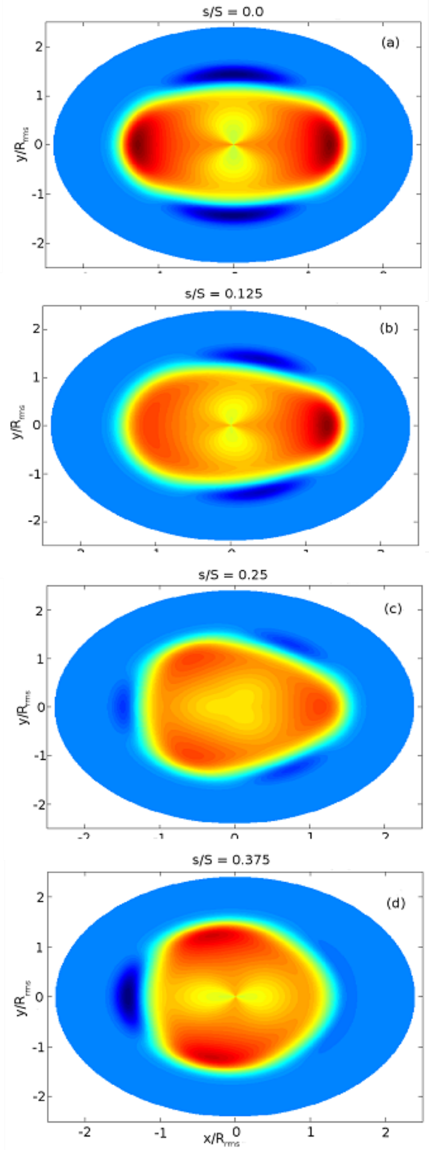




- Potential problems
  - Good (at least halo free) beam equilibria might not exist
  - Might not be able to inject beams without creating halos
  - Might not be able to generate beams that could be injected an not have halos
- To be successful, need results, methods, calculations
  1. Need to have a validated lattice with good beam equilibria
  2. Need to develop and validate an injection system that does not create halos
  3. Need to generate a beam that can be injected successfully and not produce halos

4. <u>Numerical validation</u>, i.e., modeling, critical for validation

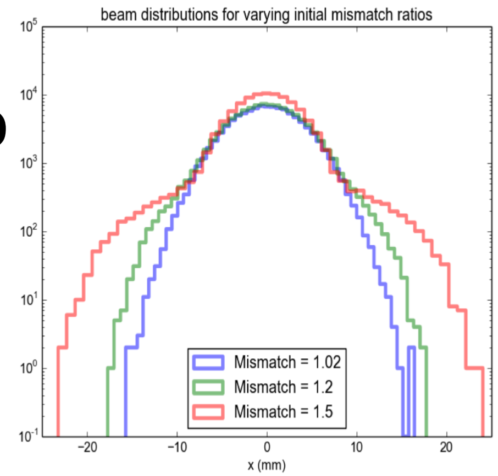
Status of (*Modeling of) Intense Beams*
We have barely scratched the surface



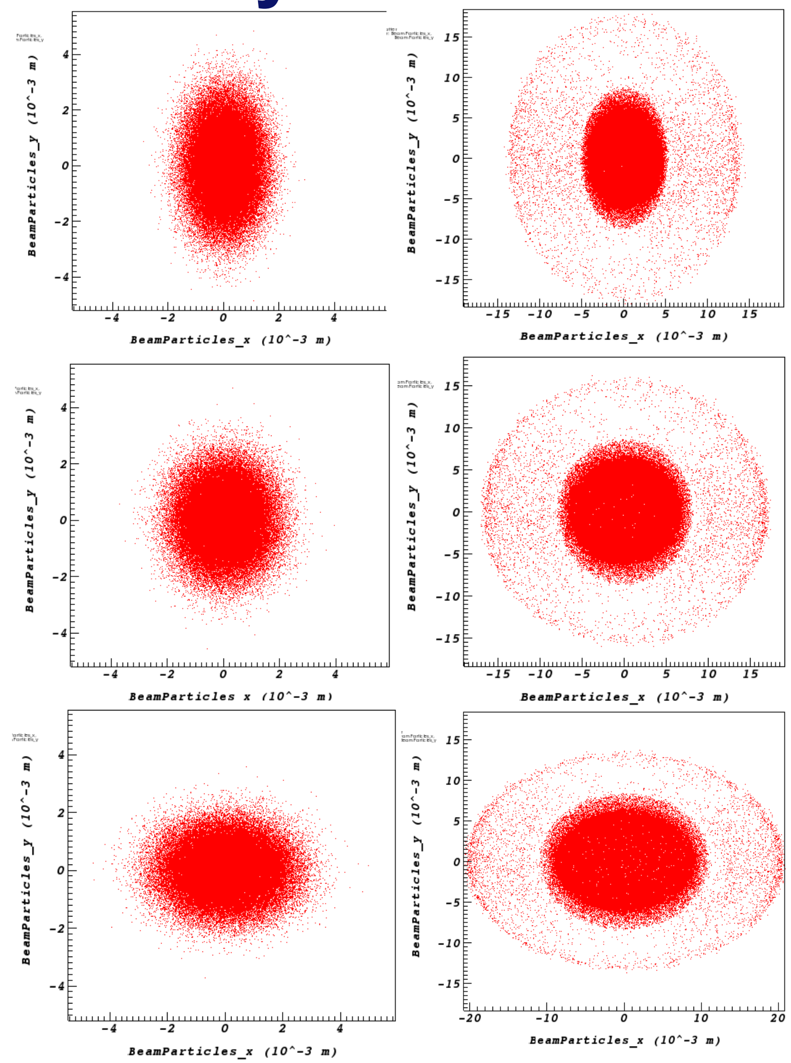
1. Need to have a validated lattice with good beam equilibria
   - Nonlinear lattices found by Sonnad (2004), Danilov (2008)
   - Equilibrium for Sonnad lattice computed by Sonnad (2015)
   - Equilibria for other lattices?
2. Need to develop and validate an injection system that does not create halos
   - Sonnad (2005) indicates that *nonlinear lattices can be robust* to injection
   - Studies?
3. Need to generate a beam that can be injected successfully ?
4. Numerical validation of all concepts needed

Status of (*Modeling of) Intense Beams* Match is key

- Gluckstern halo-core model showed that mismatch causes resonance that drives particles to large amplitudes
- *Sonnad (2005) showed halo formation and mitigation through nonlinear focusing and collimation*.
- Now have 2D simulations showing halo formation in FODO lattices



Tails in constant focusing



FODO, Matched

FODO, Unmatched

Modeling of Intense Beams:
Validated lattice with good beam equilibria

Proposed Research

- Are there other methods for generating integrable lattices? (Antonsen, adjoints)
- How else can we compute the beam equilibrium? (Sonnad, Lie transforms; Lund, principal trajectories)
- Can we make robust software for computing these equilibria?
- What will numerical studies show about the robustness of such lattices and equilibria?

Outcomes

- With a wide variety of methods, explore more configurations, more space for optimization
- Having multiple methods allows comparisons, cross checking, e.g., for accuracy
- Increased productivity through distributable software by allowing explorations by non developers (or builds at major facilities, or easily built, cross-platform software)

Modeling of Intense Beams:
Method for matching in a beam

Proposed Research

- How to design the transport into IOTA?
- Standard idea is adiabatic matching, how will that work with a kicker?
- How to get rapid convergence?
  - Adjoint methods
  - Machine learning

Outcomes

- Ability to match beams into a nonlinear accelerator lattice when space charge is significant
- Ability to test matching methods numerically

Modeling of Intense Beams:
Generation of a matchable beam

<u>Proposed Research</u>

- If no transport system can match the given beam into the lattice, then need to generate different beams
- Cf Antonsen adjoint work on eguns
- Will need detailed beam diagnostics capable of measuring deviations from ellipsoidal, e.g.

<u>Outcomes</u>

- Beams by design applicable far outside of intense beams
- Rapid optimization methods will have wide applicability.

Modeling of Intense Beams:
Numerical simulations outlook

- 3D full PIC simulations needed for intense beams (space charge force ~ magnetic focusing force)
- Eliminates the backwards/forwards transformation from the mapped beam
- 3D full PIC simulations are now within reach
  - 1 turn of IOTA ~ 500 steps
  - Halos show up in ~100 turns, 50k steps
  - 30M particles (1.5 GB), 1500G ptcl-steps
  - 1 Gptcl-steps/GPU-sec (with perf opt.)
  - 1500 sec (25m) on 1 GPU
  - At 1M ptcls/GPU, 30 GPUs make this less than 1m, efficiency good at 100k ptcls/GPU

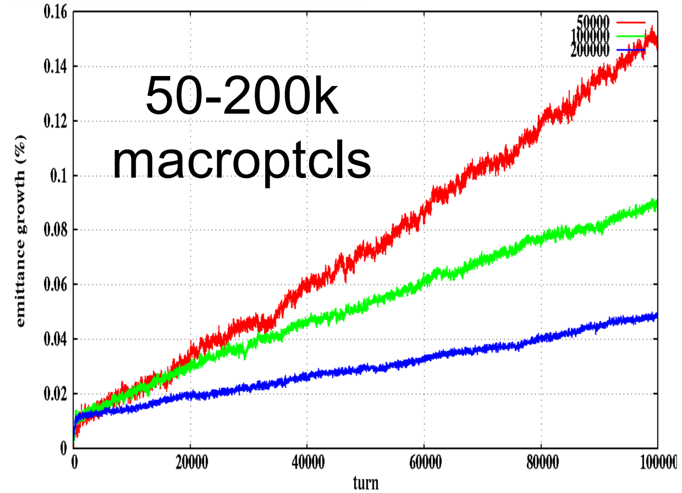
Improved smoothing + symplectic integration reduces noise

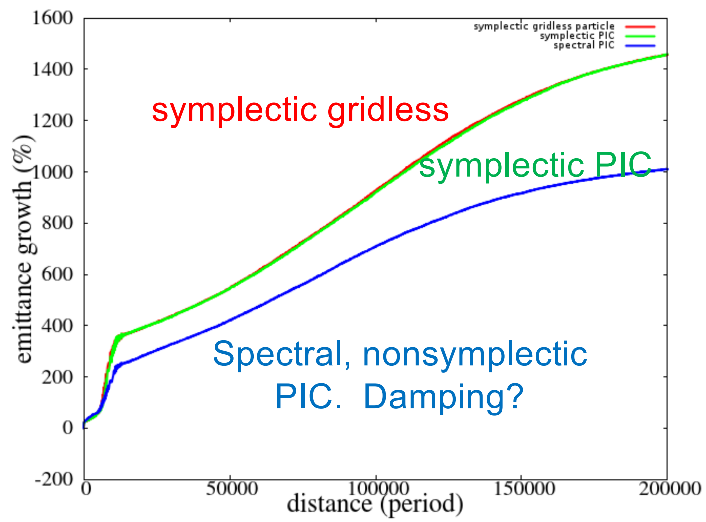
- Using derivatives of shape function for force, is symplectic
- J. Qiang, Phys. Rev. Accel. Beams 21, 054201 (2018) use quadratic shape for accelerator modeling

$$p_{xi}(\tau) = p_{xi}(0) - \tau 4\pi K \sum_I \sum_J \frac{\partial S(x_I - x_i)}{\partial x_i} S(y_J - y_i)\phi(x_I, y_J)$$

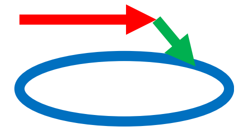
$$p_{yi}(\tau) = p_{yi}(0) - \tau 4\pi K \sum_I \sum_J S(x_I - x_i)\frac{\partial S(y_J - y_i)}{\partial y_i}\phi(x_I, y_J)$$

$$S(x_I - x_i) = \frac{1}{h}\begin{cases} \frac{3}{4} - (\frac{x_i - x_I}{h})^2, & |x_i - x_I| \le h/2 \\ \frac{1}{2}(\frac{3}{2} - \frac{|x_i - x_I|}{h})^2, & h/2 < |x_i - x_I| \le 3/2h \\ 0 & \text{otherwise} \end{cases}$$



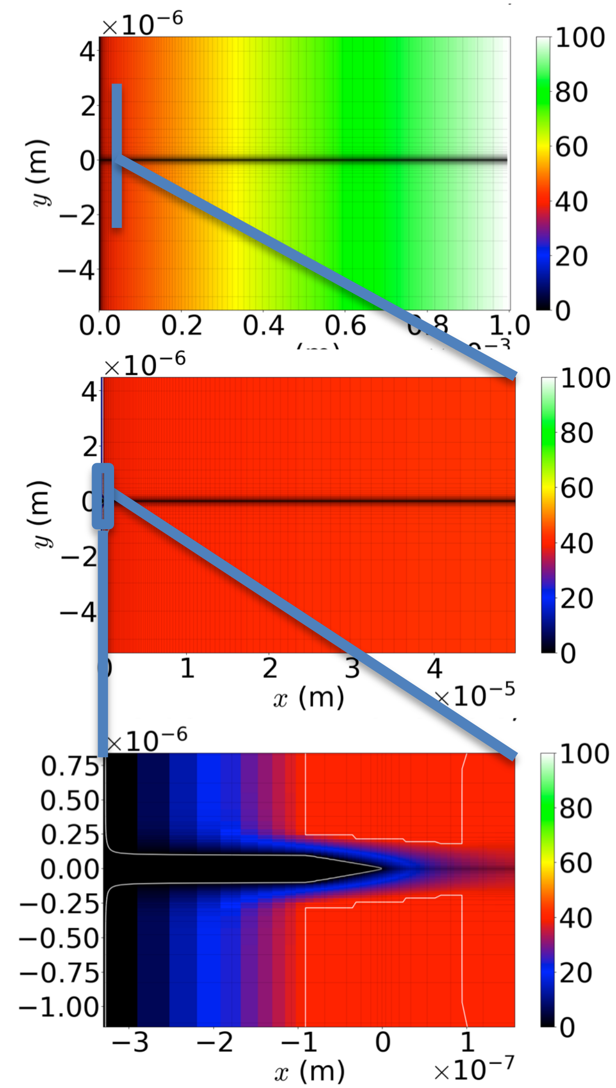


Cf also Birdsall's book, Sec 10.3, Eq. 3



Simulation directions for *Modeling of Intense Beams:* scale disparities and boundaries

- Beams can be small in big pipes
- Pipes change from circular to oval to square, moving window should move shapes
- Want localish (e.g, multigrid) methods for solving for beam fields – not open electrostatic, not Fourier for good HPC performance
- Variable grids applied to nano vacuum channel transistors (AFOSR MURI) transferable to beams in large pipes



V_{src}=0, V_{gate}=40V, V_{drn}=100V.

Modeling of Intense Beams: Higher-order (accuracy, not just smoothing) PIC obtains very low noise levels

- Is symplectic, higher order, C^2.
- Reduced footprint: more cell values, but interpolate from cell only, not neighbors
- Simulated plasmas in the turbulence regime with negligible numerical noise
- Only 1D
- Requires global solve (Fourier)

Numerical observation of turbulence enhanced growth rates

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Center for Integrated Plasma Studies and Department of Physics, University of Colorado, Boulder, Colorado 80309-0390

(Received 13 March 1997; accepted 21 March 1997)

To carry out the present work, we implemented a particle-in-cell (PIC) version of this integrator. The PIC implementation of the integrator follows Cary and Doxas[27] except for the following change. The Hamiltonian (33) is rewritten and then approximated as follows:

$$H_2 = \sqrt{\frac{\eta}{N}} \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{\omega_p^{3/2}}{k_j} \{P_j[\sin(k_j x_i)\cos(\omega_j t) - \cos(k_j x_i)\sin(\omega_j t)] - Q_j[\cos(k_j x_i)\cos(\omega_j t) + \sin(k_j x_i)\sin(\omega_j t)]\}$$

$$\approx \sqrt{\frac{\eta}{N}} \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{\omega_p^{3/2}}{k_j} \{P_j[f_j(x_i)\cos(\omega_j t) - g_j(x_i)\sin(\omega_j t)] - Q_j[g_j(x_i)\cos(\omega_j t) + f_j(x_i)\sin(\omega_j t)]\}. \quad (34)$$

Here the functions $f_j(x_i)$ and $g_j(x_i)$ are interpolations of $\sin(k_j x_i)$ and $\cos(k_j x_i)$ from grid data. Use of interpolation reduces the computational effort scaling from being proportional to the number of particles times the number of waves to being proportional to just the number of particles. However, higher order splines are needed. As the equations of motion involve the derivatives of the functions f and g, in order to use a second-order integrator, f' and g' must have continuous first derivatives. Hence, we use cubic spline interpolation for f and g.

Modeling of Intense Beams: Simulation development needed

<u>Proposed Research</u>

- Algorithms for using new machines
  - GPU: both CUDA and HIP
  - Examine MPI-aware CUDA
  - Migrate to one of the many CUDA friendly data structures and methods? (Kokkos, other)
  - Experiment with sorting, tiling
- Improvements to symplectic algorithms
  - Accuracy
  - Reduced noise
- Improvements to solvers
  - Higher-accuracy Poisson solves?
  - Inclusion of correct boundary conditions (conductors, not open)
- Improvements to particle integrators
  - What's after volume preservation?
  - Symplectic without potential fields
- Moving window for beams
  - Move all elements

<u>Outcomes</u>

- Ability to check ever more complex high-intensity beam systems
- Ability to have fast turnaround, as needed for design codes
- Ability to model for long times with stable results

Contribution of *Modeling of Intense Beams* to the GARD ABP mission

- Developing new *validated* lattices that can confine intense beams is addressing the Intensity Frontier
- Similarly, we need validated methods for computing beam equilibria to show the characteristics of the beams aimed at the interaction locations, and to determine the limits of what is attainable.
- Develop end-to-end modeling, from beam generation through acceleration in a nonlinear, circular lattice, with space charge.
- Extensive simulation capability will provide confidence that our methods and designs will work in practical application
- Training students, interns, and junior scientists at involved institutions (CU, Tech-X, LBNL) develops future accelerator scientists

Testing *Modeling of Intense Beams* to the GARD ABP

Failure modes?

- It's research!
- Needed lattices many not be realizable – difficulty of construction or high cost
- Equilibria may not exist for certain lattices, certain beam intensities
- Practical limitations in obtaining the magnetic fields for nonlinear focusing elements.
- Code development may be too expensive, difficult

Where to test?

- IOTA
- A second facility desirable, but UMER, Paul trap no longer available
- Simulation testing of, e.g., equilibrium codes built into the plan

Grand challenges from *Modeling of Intense Beams*

- Beam intensity, Beam quality, Beam control, Beam prediction
- All but Beam control, with challenging work.
  - Determining (collisionless) equilibria of beams has difficulty matching that of 3D plasma equilibria
  - Significant challenge to developing GPU-performant PIC codes for beams
    - Symplecticity
    - Accuracy (higher order, include boundaries)
    - Scale disparity
    - Scalability (PHC, GPU applicable)
  - Analyzing the large amount of data produced by HPC codes will require new methods

Milestones for *Modeling of Intense Beams*

- See timeline

Importance of *Modeling of Intense Beams*

- Intense beams are needed for the intensity frontier – measuring rare decays, etc.: Main injector
- Advances in general accelerator science, of which HEP is the steward
- Mechanisms might mitigate other accelerator instabilities

Synergies of *Modeling of Intense Beams*

- Synergistic with many other SC offices (BES, NP, QIS, FES), which operate many different accelerators
- FEL injectors (BES)
- Spallation Neutron Sources accumulator rings (BES)
- Nuclear Transmutation of Radioactive Waste (NP),
- Production of Radioisotopes (NP)

Timeline for *Modeling of Intense Beams*

- Year 1
  - Set up simulations of the full ring
  - Explore alternatives ways of getting integrable lattices and equilibria
  - Develop GPU capable modeling (ongoing)
  - Improve integration methods, accuracy, scalability, …
- Year 2
  - Develop and release equilibrium computing code
  - Validate numerical and analytical results
  - Extensive studies of beam halo generation
  - Implement improved integration methods
- Year 3
  - Validate simulation capability against IOTA experiments
  - Propose integrability modifications of IOTA
- Out years
  - Continued modeling/experimental feedback

Collaborations and facilities for *Modeling of Intense Beams*

- Current researchers
  - Ilya Zilberter
  - John Cary
  - Kiran Sonnad (consultant)
  - Ji Qiang
- Potential collaborators
  - Chad Mitchell, JL Vay et al (LBNL)
  - IOTA group (FNAL)
- Primary needs
  - Funding (as usual, is this an HEP priority?)
  - Computational developments
  - Computational resources
  - Experiments (IOTA, other test facility?)