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AN S-BASED SYMPLECTIC SPACE CHARGE ALGORITHM *

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Abstract

Traditional finite-difference particle-in-cell methods for modeling self-consistent space charge introduce non-Hamiltonian effects that make long-term tracking in storage rings unreliable. Foremost of these is so-called grid heating. Particularly for studies where the Hamiltonian invariants are critical for understanding the beam dynamics, such as nonlinear integrable optics, these spurious effects make interpreting simulation results difficult. To remedy this, we present a symplectic spectral space charge algorithm that is free of non-Hamiltonian numerical effects and, therefore, suitable for long-term tracking studies. We present initial results demonstrating the implementation of the algorithm, using a spectral representation of the fields and macro particles to preserve Hamiltonian structures. We then discuss applications to the Integrable Optics Test Accelerator (IOTA), currently under construction at Fermilab.

INTRODUCTION

High intensity beams are essential for a variety of high energy physics applications, in particular for meeting demands of proton drives for neutrino and neutron production. To meet these requirements, high current proton synchrotrons and accumulator rings are needed, for which particle loss via beam halo is the chief intensity-limiting factor. One novel idea for suppressing these losses is the nonlinear integrable optics proposed by Danilov and Nagaitsev [1]. By meeting a set of conditions, integrability can be maintained even in the presence of large tune spreads, thereby generating regular orbits while suppressing collective instabilities.

The Integrable Optics Test Accelerator (IOTA), currently under construction at Fermi National Laboratory (Fermilab),will provide a testbed for this and other novel concepts in beam dynamics [2]. However, current simulation techniques present challenges to understanding these dynamics for intense beams on long time scales. Accurate modeling of the dynamics of such beams over many turns is susceptible to the non-symplectic nature of traditional PIC codes.

In this paper we outline a novel, symplectic, s-based algorithm for tracking intense beams with self-consistent space charge. This algorithm overcomes the traditional shortcomings of finite-difference codes by neutralizing grid-heating and other noise-driven products central to approximating particle equations of motion. [3] We demonstrate the application of this algorithm using a gridless spectral solver for self-consistent dynamics akin to what was developed in [4]. We present benchmarks against traditional finite-difference codes, and discuss future work for using this algorithm to evaluate nonlinear beam dynamics.

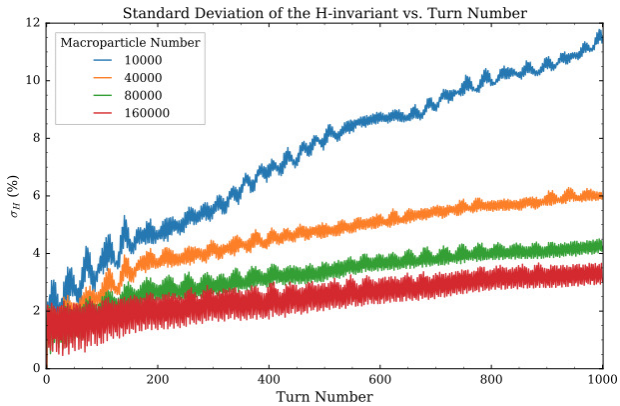

Figure 1: Nonlinear dynamics in the IOTA ring are highly susceptible to noise induced by traditional finite-difference PIC codes. Above, the longterm deviation from integrability scale strongly with particle number.

ALGORITHM

S-based Coordinate System

The first step in generating our algorithm is to define an s-based coordinate system for representing our system, so that we can generate a Hamiltonian describing the system's evolution with the appropriate canonical coordinates. For a s based tracking code we need to transform the independent variable from t to s. We then make the following change of coordinate: $(x, y, s) \rightarrow (x, y, z - \beta_0 ct)$, where $\xi = z - \beta_0 ct$. In most cases, it will be convenient to define β_0 to be the beam beta, but this is not strictly required. We then may define the canonical momentum p_ξ according to $p_\xi = \frac{p_\tau}{\beta_0} = \frac{\gamma mc}{\beta_0}$, where γ is the particle Lorentz factor in the lab frame. Note that p_ξ is related to p_τ in a simple way, and like p_τ it is always greater than mc. We also note that the coordinate transform to ξ is ill-defined at $\beta_0 = 0$, hence there is no concern with the appearance of infinite momenta for a stationary beam.

Key Assumptions

Four critical assumptions have been made in deriving the algorithm, which we outline here for convenience. First, we make the "beam approximation," that $d\xi/ds \ll 1$. Next, we assume that there are no electrostatic elements in our system, and so the only electrostatic scalar potential follows from the beam space charge. Following this, we assume that $d\mathbf{x}_\perp/ds \cdot \mathbf{A}_\perp \approx 0$, which holds if the beam motion is predominantly in the s direction and radiation is neglected. This permits us to ignore the contribution of the self-consistent transverse vector potential components from the beam. Finally, we

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extend this condition to be $A_s = A_{\text{ext}} + \mathcal{A}$, where $\mathcal{A}$ is the self consistent vector potential and A_{ext} arises from external fields. This neglects contributions due to fringe fields.

Hamiltonian and Update Sequence

We begin with the Low Lagrangian [5], devised by Low in 1958 to provide a variational formulation for describing a non-relativistic ionized gas in an electromagnetic field. Note that we work in CGS units throughout the paper.

$$\begin{aligned}\mathcal{L} = &\int \mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{x}_0'\left[-mc^2\sqrt{1-\frac{1}{c^2}\left(\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\right)^2}\right] f(\mathbf{x}_0,\mathbf{x}_0') \\ &+\int \mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{x}_0'\left[-q\phi(\mathbf{x},t)+\frac{q}{c}\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\cdot\mathbf{A}(\mathbf{x},t)\right] f(\mathbf{x}_0,\mathbf{x}_0') \\ &+\frac{1}{8\pi}\int \mathrm{d}\mathbf{x}\left[\left(-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}-\nabla\phi\right)^2-(\nabla\times\mathbf{A})^2\right]. \quad (1)\end{aligned}$$

After changing variables and applying our key assumptions, we arrive at the reduced Lagrangian for the self-consistent fields:

$$\begin{aligned}\mathcal{L}_{\text{em}} = &\int \mathrm{d}\Omega_0\left[-\frac{q}{c}\left(\frac{1}{\beta_0}\phi-\mathcal{A}\right)\right] f(\Omega_0) \\ -\frac{1}{8\pi}&\int \mathrm{d}\mathbf{r}_\perp\times\frac{\mathrm{d}\xi}{\beta_0 c}\left[\left(\beta_0\frac{\partial\mathcal{A}}{\partial\xi}-\frac{\partial\phi}{\partial\xi}\right)^2+(\nabla_\perp\phi)^2-(\nabla_\perp\mathcal{A})^2\right] \quad (2)\end{aligned}$$

The Hamiltonian for our system is defined according to the usual Legendre Transform:

$$\mathcal{H}_{\text{p-c}} = \mathbf{p}\cdot\mathbf{q}' - \mathcal{L}_{\text{p-c}} \quad (3)$$

This is well defined for the particle coordinates, but not for the fields (see next section):

$$\mathcal{H}_{\text{p-c}} = \sum_j -\sqrt{\left(\beta_0 p_j^{(\xi)}\right)^2-\left(\mathbf{p}_j^{(\perp)}\right)^2-(w_j mc)^2}+p_j^{(\xi)}-\frac{w_j q}{\beta_0 c}\psi \quad (4)$$

Self-forces and Spectral Solver

The Lagrangian as defined in Eqn. 2 is degenerate with respect to the fields. As a result, one cannot define canonically conjugate coordinates as needed to perform a Legendre Transform. Therefore, we apply the Euler-Lagrange equations to obtain an auxiliary condition on ψ:

$$\begin{aligned}\partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}-\frac{\partial\mathcal{L}}{\partial\phi} &= 0 \\ \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\mathcal{A})}-\frac{\partial\mathcal{L}}{\partial\mathcal{A}} &= 0\end{aligned}$$

Evaluating these expressions yields the following conditions:

$$\begin{aligned}\beta_0\partial_\xi^2(\beta_0\mathcal{A}-\phi)-\nabla_\perp^2\mathcal{A} &= 4\pi\frac{q}{c}n(\vec{x}) \\ -\partial_\xi^2(\beta_0\mathcal{A}-\phi)-\nabla_\perp^2\phi &= 4\pi\frac{1}{\beta_0}\frac{q}{c}n(\vec{x})\end{aligned}$$

where n describes the particle number density in the new coordinate system (x, y, ξ).

We then define the psuedopotential ψ according to:

$$\psi = \beta_0\mathcal{A}-\phi \quad (5)$$

and we may combine and reduce our two equations to yield the single constraint:

$$\frac{1}{\gamma^2}\partial_\xi^2\psi+\nabla_\perp^2\psi = \frac{1}{\gamma_0^2}4\pi q n(\vec{x}) \quad (6)$$

This equations describes the evolution of our self-consistent psuedopotential, akin to Poisson's equation. We note that this equation has familiar scaling to traditional formulations. In particular the space charge force becomes purely transverse as $\gamma_0 \to \infty$ and the total force scales with$1/\gamma^2$. For the purposes of a 2D algorithm, we can ignore variations in ξ and consider only the evolution described by the $\nabla_\perp^2\psi$ term.

We elect to describe our fields in an orthonormal Fourier basis, according to:

$$\psi = \frac{1}{\sqrt{L_x L_y}}\sum_{k_x,k_y} e^{ik_x x}e^{ik_y y}\sigma_{k_x,k_y} \quad (7)$$

where L_x, L_y are the fundamental length scales of the system, which provide the normalization, and σ_{k_x,k_y} is the matrix of coefficients specifying the relative amplitude of each of mode. Solving equation 6 is therefore equivalent to computing the values of σ_{k_x,k_y} based on the known macroparticle distribution, weights, and shapes.

Macroparticle Discretization

To trace the particles, we introduce macroparticles by decomposing the phase-space density in discrete shapes, treating the particle momenta as delta functions, but permitting shape functions in real space for the positions:

$$\psi(\mathbf{r},\mathbf{p}) = \sum_{j=1}^{N_{\text{macro}}} w_j\Lambda\left(\mathbf{r}-\mathbf{r}^{(j)}\right)\delta\left(\mathbf{p}-\mathbf{p}^{(j)}\right). \quad (8)$$

Here w_j denote the macroparticle weights, δ the Dirac delta function, and Λ the normalized particle shape functions (so that $\int \mathrm{d}\mathbf{x}\,\Lambda = 1$). For this work, we consider two possible particle shapes - delta functions and "tent functions." The use of tent functions permits smooth sampling in Fourier space across a range of wavevectors, corresponding to the macroparticle width and wavevector separation.

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BENCHMARKS AND CONVERGENCE

To test our implementation, we consider the expansion of a KV beam in a drift, and compare our results with analytic predictions. The KV beam is initialized in the zero emittance limit, with zero transverse momentum, and so the resulting envelope expansion is purely a function of the beam's space charge. Figure 2 shows a comparison between the analytic and simulated values for the particle kicks within the distribution, using both tent- and delta-shape functions. We note that for very small radius, the analytic potential approaches 0 and statistical fluctuations in the calculation limit the fidelity of the result. Figure 3 compares the beam envelope expansion against the analytic prediction.

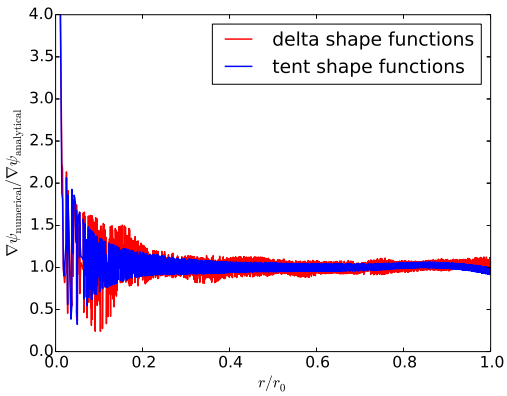

Figure 2: Simulated particle kicks as compared with the analytic result are plotted as a function of particle position for both delta- and tent-shape functions. The tent-shape is superior at resolving the kicks, especially at low radius where the analytic value approaches 0.

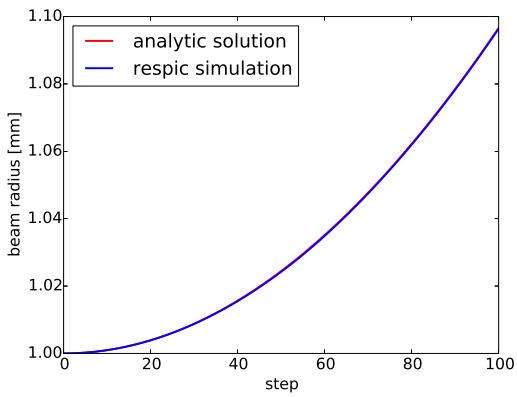

Figure 3: The evolution of the beam envelope is plotted as a function of step number, showing good agreement with the analytic prediction for a KV beam. The beam begins in the zero emittance limit, and so the expected beam growth is quadratic with distance.

Lastly, we evaluated the total momentum of our system. Symplectic integrators preserve phase space structure, and subsequently any derivations from the original values of momenta should remain bounded. This is not true of traditional finite-difference techniques, and we expect to see improved long-term behavior in particle momenta using this algorithm. Figure 4 depicts the total momentum for 1000 steps, which is well conserved.

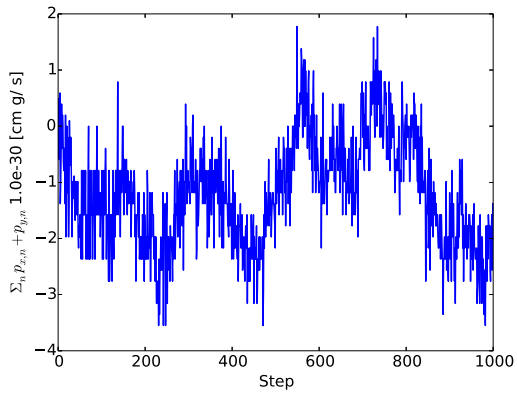

Figure 4: The total transverse momenta of particles in the simulation over 1000 turns is conserved to high precision.

CONCLUSION

The use of symplectic space charge solvers may provide more insight into complex, long-term dynamics in nonlinear systems by significantly reducing numerical noise. We have developed a novel s-based algorithm for symplectic tracking of beams with self-consistent space charge forces in an accelerator. The algorithm makes use a spectral, gridless, representation of the phase space density to reduce numerical noise and permit exact field propagation. The algorithm permits arbitrary particle shapes, with delta- and tent-functions demonstrated for benchmark exercises. Excellent agreement is seen between numerical results and analytic predictions.

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