# NUMERICAL TOOLS FOR MODELING NONLINEAR INTEGRABLE **OPTICS IN IOTA WITH INTENSE SPACE CHARGE USING** THE CODE IMPACT-Z

C. Mitchell\* and J. Qiang, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

## Abstract

The Integrable Optics Test Accelerator (IOTA) is a novel storage ring under commissioning at Fermi National Accelerator Laboratory designed to investigate the dynamics of beams with large transverse tune spread in the presence of tools have been implemented in the code IMPACT-Z to allow of or high-fidelity modeling of the IOTA ring during Phase II operation with intense proton beams. A primary goal is to ensure symplectic treatment of both single-particle and col-E lective dynamics. We describe these tools and demonstrate

**INTRODUCTION** The Integrable Optics Test Accelerator lattice design [1–3] makes use of a 1.8 m-long nonlinear magnetic insert with an sequence of a sequ s-dependent transverse magnetic field that is shaped to genstribution erate bounded, regular (integrable) motion in the transverse plane for on-momentum particles. The strong dependence ġ; of particle tunes on amplitude leads to a decoherence of f transverse oscillation modes that may help to suppress the particle-core resonances primarily responsible for beam halo 2018). development and particle loss in intense beams [4].

Several challenges are associated with modeling accu-0 a rately the beam dynamics in IOTA, including the strong intrinsic nonlinearity of the system, the complex structure of the fields within the nonlinear magnetic insert, the need for robust long-term tracking with space charge over >1K turns  $\overleftarrow{a}$  (for investigations of beam stability and low-level particle  $\bigcup$  losses), and the sensitivity of the integrability of the system 2 to a variety of perturbative effects.

of A primary goal of this study was to implement tools within the code IMPACT-Z [5] for modeling nonlinear integrable optics (with space charge) in IOTA while avoiding sources d of non-symplectic numerical artifacts, preserving as far as be possible the structure of the rin integrable Hamiltonian system. possible the structure of the ring as an integrable or nearbe used

# STRUCTURE OF THE NONLINEAR **INTEGRABLE POTENTIAL**

from this work may The ideal 2D magnetic field within the nonlinear insert is given by  $\vec{B} = \nabla \times \vec{A} = -\nabla \psi$ , where the magnetic vector potential  $\vec{A}$  and the magnetic scalar potential  $\psi$  at a longitudinal position s are most easily expressed in terms of the

Content THPAK035 3290

dimensionless quantities [6]:

$$F = \frac{A_s + i\psi}{B\rho}, \qquad z = \frac{x + iy}{c\sqrt{\beta(s)}}, \qquad \tilde{t} = \frac{\tau c^2}{\beta(s)}, \qquad (1)$$

using the complex function:

$$F(z) = \left(\frac{\tilde{t}z}{\sqrt{1-z^2}}\right) \arcsin(z).$$

Here  $\beta = \beta_x = \beta_y$  is the betatron amplitude across the drift space that will contain the magnet,  $B\rho$  is the magnetic rigidity,  $\tau$  is a dimensionless parameter characterizing the strength of the magnet, and  $c \neq 0$  [m<sup>1/2</sup>] characterizes the length scale of the potentials in the transverse plane. Fig. 1 illustrates the function F, together with the associated magnetic field lines.



Figure 1: Domain of analyticity of the complex function F, which defines the vector potential of the nonlinear insert in the transverse plane. The curves in blue denote magnetic field lines. The dashed circle denotes the circle of convergence of the multipole series. Singularities occur at the points  $z = \pm 1$ .

Since  $\vec{A}_{\perp} = 0$  in this model, the single-particle Hamiltonian within the nonlinear magnetic insert takes the following form, using the longitudinal coordinate s as the independent variable:

$$H = -\sqrt{1 - \frac{2P_t}{\beta_0} + P_t^2 - |\vec{P}|^2} - \mathcal{A}_s - \frac{1}{\beta_0}P_t, \quad (2)$$

where the transverse momenta  $\vec{P}$  are normalized by the design momentum  $p^0 = mc\beta_0\gamma_0$ , the longitudinal variables are  $T = c\Delta t$  and  $P_t = -\Delta \gamma / (\beta_0 \gamma_0)$ , and  $\mathcal{A}_s = A_s / B\rho$ .

**05 Beam Dynamics and EM Fields** 

ChadMitchell@lbl.gov

In the paraxial approximation  $P_x, P_y \ll 1$ , the Hamiltonian for an on-energy particle ( $P_t = 0$ ) within the nonlinear magnetic insert takes the form:

$$H_{\perp}(X, P_x, Y, P_y; s) = \frac{1}{2}(P_x^2 + P_y^2) - \mathcal{A}_s(X, Y, s).$$
(3)

It can be shown [1, 6] that the Hamiltonian (3) yields integrable transverse motion with the two invariants

$$H_{N} = \frac{1}{2} (P_{xN}^{2} + P_{yN}^{2} + X_{N}^{2} + Y_{N}^{2}) - \tau U (X_{N}, Y_{N}), \qquad (4)$$
$$I_{N} = (X_{N} P_{yN} - Y_{N} P_{xN})^{2} + P_{xN}^{2} + X_{N}^{2} - \tau W (X_{N}, Y_{N}),$$

$$I_N = (X_N P_{yN} - Y_N P_{xN})^2 + P_{xN}^2 + X_N^2 - \tau W(X_N, Y_N)^2$$

where

$$U = \mathcal{R}e\left(\frac{z}{\sqrt{1-z^2}} \arcsin(z)\right), W = \mathcal{R}e\left(\frac{z+z^*}{\sqrt{1-z^2}} \arcsin(z)\right)$$

Here the star \* denotes complex conjugation, and

$$\begin{pmatrix} X_N \\ P_{xN} \end{pmatrix} = \begin{pmatrix} 1/c\sqrt{\beta} & 0 \\ \alpha/c\sqrt{\beta} & \sqrt{\beta}/c \end{pmatrix} \begin{pmatrix} X \\ P_x \end{pmatrix},$$
 (5)

with a corresponding expression for  $(Y_N, P_{\nu N})$ , where  $\alpha(s) = -\beta'(s)/2$ . In IOTA, the transfer map  $\mathcal{R}$  from the exit of the nonlinear insert to its entrance is assumed linear with a phase advance  $n\pi$  for integer *n* (in both planes). It follows that  $H_N$  and  $I_N$  are each invariant under  $\mathcal{R}$ , and are therefore invariant under the one-turn map for the ring.

#### SYMPLECTIC INTEGRATOR

Within the nonlinear magnetic insert, tracking is performed using a second-order symplectic integrator [5,7] via the Hamiltonian splitting:

$$H = H_{drift} + H_{NLL},\tag{6}$$

where  $H_{drift}$  is the Hamiltonian for a drift and  $H_{NLL}$  =  $-\mathcal{A}_s$ . The map for a step of length h is evaluated as:

$$\mathcal{M}(s \to s + h) =$$

$$\mathcal{M}_{drift}\left(\frac{h}{2}\right) \mathcal{M}_{NLL}\left(h, s + \frac{h}{2}\right) \mathcal{M}_{drift}\left(\frac{h}{2}\right) + O(h^3),$$

$$\mathcal{M}_{drift}(h) = e^{-h:H_{drift}}; \quad \mathcal{M}_{NLL}(h, s) = e^{-h:H_{NLL}(s):}.$$

The maps  $\mathcal{M}_{drift}$  and  $\mathcal{M}_{NLL}$  are exactly known. In particular, if we define the quantity  $\mathcal{P} = P_x + iP_y$ , the map

 $\mathcal{M}_{NLL}(h, s)$  acts only on momenta, taking  $\mathcal{P} \to \mathcal{P}_f$  where:

$$\mathcal{P}_f = \mathcal{P} + \frac{h}{c\sqrt{\beta(s)}} \left(\frac{dF(z)}{dz}\right)^*.$$
(8)

Here the derivative in (8) is known, and the map is evaluated numerically using Fortran complex arithmetic. This symplectic integration procedure avoids numerical errors associated with the presence of small denominators that are present in the equations of motion derived from the nonlinear potential in its original form [1].

#### TREATMENT OF SPACE CHARGE

An explicitly symplectic space charge tracking algorithm [8,9] was implemented within the code IMPACT-Z for modeling 2D space charge in an unbunched, coasting beam using a spectral method. For a system of  $N_p$  macroparticles with phase space coordinates  $(\mathbf{r}_i, \mathbf{p}_i), (j = 1, ..., N_p)$ , the collective Hamiltonian of the system is expressed in the form [9]:

$$H = \sum_{j=1}^{N_p} H_{ext}(\mathbf{r}_j, \mathbf{p}_j) + \frac{K}{2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} G(\mathbf{r}_i, \mathbf{r}_j), \quad (9)$$

where  $H_{ext}$  denotes the single-particle Hamiltonian include ing external fields, K is the generalized perveance of the beam, and G is a Green function for the 2D Poisson equation in a rectangular conducting pipe. An approximation for Gis obtained by using a finite number of Fourier modes in xand y as:

$$G(\mathbf{r}_i, \mathbf{r}_j) = 4\pi \frac{4}{ab} \frac{1}{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j)$$
$$\times \sin(\alpha_l x_l) \sin(\beta_m y_l), \qquad (10)$$

where

$$\alpha_l = \frac{l\pi}{a}, \quad \beta_m = \frac{m\pi}{b}, \quad \gamma_{lm}^2 = \alpha_l^2 + \beta_m^2. \tag{11}$$

Here  $N_l$ ,  $N_m$  are the number of Fourier modes and a, b are the aperture sizes in x and y, respectively.

At each longitudinal step, the splitting (9) may be applied to evaluate the map for a second-order symplectic integrator on the collective  $N_p$ -particle phase space. By grouping terms appropriately, the computational complexity of this algorithm scales as  $O(N_{\text{mode}} \times N_p)$ , where  $N_{\text{mode}} = N_l N_m$ is the total number of modes. The algorithm is easily parallelized by distributing particles uniformly among computational cores [9].

#### ADDITIONAL CAPABILITIES

Additional capabilities were implemented that include: numerical diagnostics for statistical characterization of the two invariants (4), a diagnostic for characterizing beam mismatch to the nonlinear integrable lattice, a 2D particle-in-cell solver with free space boundary conditions, and improvements in the quadrupole and dipole models relevant for modeling proton rings at low energy. Dipoles can currently be modeled using symplectic tracking through 3rd order.

### **APPLICATION TO IOTA MODELING**

We studied the effect of space charge on the preservation of the invariants  $H_N$  and  $I_N$  using a version of the IOTA lattice designed for 2.5 MeV protons with a current of 0.411 mA (space charge tune depression  $\Delta Q = -0.03$ ). For propagation in the external fields we use linear tracking for all elements external to the nonlinear magnetic insert (the "arc") to isolate the effect of space charge on the integrability of

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... upole setting , integer tune advance ac ....e of the linearized space charge idistribution with 1.024M particles is initiate to the waterbag-like distribution function:  $f \propto \Theta(H_N - \epsilon_0),$ motion. The lattice quadrupole settings were tuned [10] to restore nearly integer tune advance across the arc in the presence of the linearized space charge fields. A particle distribution with 1.024M particles is initialized according

$$f \propto \Theta(H_N - \epsilon_0), \qquad \Theta(x) = \begin{cases} 1, & x \le 0\\ 0, & x > 0 \end{cases},$$
(12)

where  $\epsilon_0$  is chosen so that  $\langle H_N \rangle c^2 = 4$  mm-mrad. Fig. 2 illustrates the evolution of the moments of the two invariants author( of motion, taken among all particles in the beam. The results g suggests that space charge may induce slow stochastic diffusion due to the breakup of invariant tori [11]. To illustrate 2 attribution the contribution of macroparticle noise, Fig. 3 shows the dependence of the observed diffusion rate on the number of simulation particles in a tracking study with identical beam



(4). Here, we use  $\sqrt{I_N}$  rather than  $I_N$  for practical reasons used related to numerical benchmarking. An initial period of þ rapid phase mixing occurs, followed by slow linear growth.

# CONCLUSIONS

rom this work may A variety of new numerical tools have been implemented in the code IMPACT-Z to facilitate the modeling of nonlinear integrable optics in IOTA with space charge. A treatment of the nonlinear integrable potential of the IOTA magnetic

Content THPAK035 • 8 3292



Figure 3: Convergence of the diffusion rate, evaluated as  $\Delta \sigma_G / \langle G \rangle$  per turn, for the invariants  $G = H_N$  and  $G = \sqrt{I_N}$ with the number of simulation particles for a fixed number of spectral modes ( $64 \times 64$ ). The scaling is not a simple power law, but behaves approximately as ~  $N_p^{-\nu}$ , with  $1 \le \nu \le 2$ .

insert in the complex plane is used as an alternative to [1] for numerical tracking, avoiding a previously problematic numerical instability. This is performed using a second-order symplectic integrator based on Yoshida splitting. Space charge can be treated using either a traditional grid-based Poisson solve (with a variety of possible boundary conditions) or using a new spectral solver that is symplectic (by design) on the N-particle phase space of the macroparticle system [9]. Simulations indicate slow diffusion of the invariants of motion in the presence of space charge, which is well-captured using ~ 1 M particles and 64x64 spectral modes. Studies further exploring the interplay between space charge, numerical noise, and integrability in IOTA are ongoing.

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