Tools for Modeling Beam Dynamics in Rings Based on Nonlinear Integrable Optics

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Advanced Modeling Program



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Outline

Nonlinear integrable beam optics in rings

Computational and theoretical tools

- single-particle dynamics tracking, analytical methods
- collective effects space charge, matching, relaxation
- numerical diagnostics chaos, filamentation, losses

Optimization for halo suppression

Conclusions







Nonlinear Integrable Beam Optics in Rings •







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The IOTA storage ring : an accelerator R&D test facility with a focus on strategies to mitigate space charge-induced beam halo.

- Possible solutions: electron lenses and columns, nonlinear integrable lattices
- Integrable Optics Test Accelerator (IOTA)
 - Novel accelerator physics: strongly nonlinear design
 - Experimental test bed for space charge mitigation
 - Run first with electrons, then low-energy protons





- Integrability => ensures orbits are regular and remain bounded (no chaos)

S. Danilov, S. Nagaitsev, PRAB 13, 084002 (2010) S. Antipov et al, JINST **12**, T03002 (2017) ¹S. Webb et al, p. 2961, IPAC 2012





Integrability = the single-particle orbits are confined to level sets defined by invariants of motion \implies motion with stable frequencies (tunes)

Liouville-Arnold Theorem

Suppose *H* is a time-independent Hamiltonian for an *n* degree-of-freedom system, invariants and $H = f_1, f_2, ..., f_n$ are *n* smooth functions on the phase space *M* such that: **1**) $\nabla f_1, \ldots, \nabla f_n$ are linearly independent (the f_j are independent) **2)** $\{f_i, f_i\} = 0$ (i, j = 1, ..., n) (the f_i are in involution) level sets \implies The motion is confined to a set $M_z = \{p \in M | f_i(p) = z_i, i = 1, \dots, n\}$ If M_z is compact and connected, then M_z is diffeomorphic to the *n*-torus. **Examples**: - stable linear motion - nonlinear pendulum - 2-body Keplerian motion smooth coordinate action-angle Similar definitions apply original transformation variables to symplectic maps. variables







Fermilab's IOTA Ring: Nonlinear Integrable Optics Lattice Configuration



*S. Danilov and S. Nagaitsev, PRAB 13, 084002 (2010). S. Antipov et al, JINST 12, T03002 (2017)

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- optical stochastic cooling
- single-electron quantum science





R&D Areas: Long-Time Beam Prediction at the Interface Between Nonlinear Dynamics and High Intensity

Advanced Algorithm Development (Goals: improved speed and fidelity of modeling on long time scales.)

- **Fast symplectic tracking** in nonlinear applied fields/fringe fields (non-split Hamiltonians)
- Improved integration of realistic 3D Maxwellian RF and magnet models with tracking tools
- Structure-preserving space charge modeling to ensure phase space preservation
- Improved integration of space charge with s-based tracking (e.g., long, bunched beams, dipoles)
- Efficient space charge modeling at high resolution (adaptive mesh refinement, higher-order particle shapes)
- Addressing computational bottlenecks (eg., fast in-situ numerical phase space diagnostics to reduce I/O)

Mathematical and Theoretical Methods (Goals: validation and physics understanding for effective design.)

- Nonlinear methods (e.g. Lie methods, near-integrable dynamical systems) dynamic aperture
- Self-consistent beam equilibria and stability with nonlinear focusing matching
- Understanding numerical artifacts (particle noise) associated with long-term simulation
- Theoretical models of space-charge-induced beam halo formation with nonlinear focusing
- Theoretical models of collective instabilities and nonlinear decoherence (Landau damping)







IMPACT: Multi-Physics High-Intensity and High Brightness Beam Dynamics Code Suite

Key features include:

- time-dependent and position dependent PICs
- serial and massive parallelization
- detailed 3D RF accelerating and focusing model
- standard elements: dipole, solenoid, multipole, etc.
- multiple charge states, multiple bunches
- 3D space charge effects
- structure and resistive wall wakefields
- coherent synchrotron radiation (CSR)
- incoherent synchrotron radiation (ISR)
- photo-electron emission
- machine errors and steering

The IMPACT code suite is used by > 40

institutes worldwide

- successfully applied to both electron & proton machines:
 - CERN PS2 ring, SNS linac, ...
 - LCLS-II linac
- microbunching simulated using 2B macroparticles

Start-to-end simulation of the Linac Coherent Light Source



J. Qiang et al., Phys. Rev. Accel. Beams 20, 054402 (2017).

https://blast.lbl.gov/



Single-particle dynamics







New algorithms and numerical capabilities a challenges of modeling nonlinear

Implementation of the nonlinear magnetic insert using a symplectic



- Concise, complex representation of the nonlinear integrable potential.
- Uses a 2nd order symplectic integrator to perform s-dependent tracking.
- Avoids instability of previous integrators due to vanishing denominators in equations of motion.
- Additional tools for soft-edge fringe fields.

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Longitudinal variation of quadrupole gradient



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The map for a single numerical step of size *h*:

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

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Longitudinal variation of quadrupole gradient



Nonlinear quadrupole fringe field effects



Other new capabilities implemented in IMPACT-Z

- *Python interface* and postprocessing control using *Jupyter*.
- Implementation of *quadrupole and dipole* nonlinear *fringe field* models relevant for modeling proton rings at low-moderate energy.
- Additional Poisson solvers and diagnostics capabilities (discussed later).



Geometric methods in nonlinear dynamics provide a foundation for the analysis of single-particle optics in integrable accelerator lattices.

Critical initial conditions at

nominal IOTA insert strength

stable

periodic

13

 $p_x = p_v = 0$

fixed boint

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1.0

0.8

0.6

0.4

0.2

0.0

 \mathcal{T}

- Need: To understand the global single-particle dynamics accessible in accelerator designs (such as IOTA) based on nonlinear integrable optics.
- **Problem:** Standard approaches to nonlinear dynamics in the accelerator community are perturbative, neglect fully 4D or 6D coupling, or require a clever choice of coordinates.
- Solution: Geometric methods from the theory of integrable Hamiltonian systems may be applied to locate fixed points, periodic orbits, dynamical bifurcations, and determine frequencies of motion (tunes), using knowledge only of the invariants of motion.

Reveals new operating points for the IOTA ring and guidance for future accelerator designs.

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Science

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Example: Bifurcation diagram for nominal single-particle dynamics in IOTA



$$\begin{split} \underline{Invariants of single_1 particle motion_1} \\ H &= \frac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) - \tau U(x + iy) \\ U(z) &= \mathcal{R}e\left(\frac{z}{\sqrt{1 - z^2}} \arcsin(z)\right) \\ I &= (xp_y - yp_x)^2 + p_x^2 + x^2 - \tau W(x + iy) \\ W(z) &= \mathcal{R}e\left(\frac{z + \overline{z}}{\sqrt{1 - z^2}} \arcsin(z)\right) \end{split}$$

Critical points occur where: $dH \wedge dI = 0$ H

Distinct regions of the diagram correspond to dynamics with qualitatively distinct single-particle orbits.

Curves parameterizing the critical values can be determined exactly using symbolic methods *eg*, *Mathematica*.



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Example: Bifurcation diagram for nominal single-particle dynamics in IOTA



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Examples: level sets (projected onto the x-y plane)





Analytical method for extracting nonlinear tunes of integrable symplectic maps developed and applied to the IOTA ring

- **Need:** To understand *analytically* the frequency content of orbits in accelerator lattices based on nonlinear integrable optics, and to use this information in accelerator design (to control tune spread).
- **Problem:** Traditional method for analysis of integrable systems relies on action-angle coordinates, which are difficult to obtain in explicit form, and which break down near critical phase space structures (*eg*, separatrices).
- **Solution:** A **semi-analytical** method to extract dynamical **tunes** of an integrable symplectic map from its **invariants of motion**, without the need for tracking, using path integrals in the invariant level sets.

Reveals the link between frequencies and geometry of level sets. Can aid in design of future nonlinear integrable lattices.

vector of tunes

 $\nu = R^{-1}S$

$$S = -\int_{\gamma} \left(D\mathcal{F}^{+} \right)^{T} J d\zeta,$$
$$R_{jk} = \left(-\oint_{\gamma_{k}} \left(D\mathcal{F}^{+} \right)^{T} J d\zeta \right)_{j}$$

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Extracting frequencies of the 4D McMillan mapping from its 2 invariants of motion



Extracting tunes for orbits in IOTA for comparison with tracking using NAFF





Collective effects







Implementation of a gridless symplectic space charge solver to enable long-term Hamiltonian tracking of high intensity beams

- Need: Avoid numerical artifacts due to space charge that break the geometric Hamiltonian structure, necessary to ensure reliability on long time scales.
- **Problem:** Most PIC methods result in a particle push that is not symplectic on the phase space due, e.g. due to interpolation and finite differencing.
- Solution: A 2D gridless symplectic space charge solver (J. Qiang, 2017) was implemented in IMPACT-Z to enable robust long-term tracking with space charge. Each step is a map that is symplectic on the collective N-body phase space of the simulated particles.

Avoids the destruction of integrability due to non-symplectic artifacts.



Evolution of the N-particle Hamiltonian









New PDE solver enables the study of intense beam equilibria in strongly nonlinear lattices and relaxation to equilibrium



New PDE solver enables the study of intense beam equilibria in strongly nonlinear lattices and relaxation to equilibrium



General procedure for the generation of an initial beam distribution matched to the periodic nonlinear lattice

Beam is matched to the nonlinear lattice at the NLI midpoint.

-4

-3

-2

-1

0

X (mm)

2



With space charge, adiabatic ramping of beam current

the equilibrium in a CF channel.

I = 0 mA

I = 4 mA

I = 8 mA -

0.5

22

[1] S. Webb et al, p. 3099, IPAC 2013. **III BERKELEY LAB**

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-2

-1

0

X (mm)



Numerical diagnostics







Efficient numerical algorithms reveal the boundary between chaos and integrability in nonlinear integrable lattices with space charge

- **Need:** Accurate tools to distinguish between regular and chaotic motion that do not require long computing times.
- **Problem:** Standard chaos indicators (NAFF) require long time series, and space charge introduces spurious frequency drift and numerical noise.
- Solution: Use symplectic and time-reversible tracking algorithms and an efficient chaos indicator using forward-backward integration. Self-consistent tracking and idealized models of space charge reveal similar structure.

Reveals phase space regions for IOTA that are sensitive to chaos and to be avoided.



Nonlinear resonance lines in IOTA model with space charge tune shift



K. Hwang, C. Mitchell, R. Ryne, Phys. Rev. Accel. Beams 23, 0846021 (2020)







Numerical Tools in IMPACT-Z for Improved Characterization and Visualization of Proton Beam Losses in IOTA

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Characterization and Visualization of Proton Losses in IOTA

- Need: To characterize problematic locations for losses to aid in design of diagnostics for early-stage proton operation, and to aid in selecting location/design of collimation scheme from the RFQ.
- **Problem:** Previous tracking tools available in IMPACT-Z allowed only circular/rectangular aperture, specified by element; only number of lost particles per turn was stored, without phase space information.
- Solution: Symplectic space charge tracking algorithm was updated to allow variable particle number; elliptical and fully s-dependent aperture capability was implemented; phase space information for all lost particles is now stored and visualized via Python interface.
- **Outcome:** Tools for visualizing proton losses were applied to compare methods for truncating the beam distribution in IOTA at the nominal emittance out of the RFQ, studying importance of mismatch, magnetic insert strength, and distribution type.

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from Kilean Hwang



Figure: Aperture and RMS beam size. RMS beam size represent bare lattice optics with the nominal geometric emittance $\varepsilon_{x,y} = 3.3 \mu m$

Visualization of beam loss for an uncollimated beam with mismatch





Numerical diagnostics using statistical distance (distribution "proximity") implemented to characterize a beam's relaxation to a stationary state

- **Need:** To numerically characterize "proximity" and relaxation processes for beams in the presence of high intensity or strong nonlinear focusing.
- **Problem:** Diagnostics using low-order (eg, 2nd) beam moments are insufficient to characterize "proximity" of distributions in the presence of strong nonlinear effects.
- Solution: Implement two-sample measures of statistical distance such as Maximum Mean Discrepancy, effectively embedding each distribution into a linear Hilbert space.

$$k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$
: symmetric positive-definite characteristic kernel
 $\gamma_k(\mathbb{P}, \mathbb{Q}) = \left(\int \int k(X, X') d\Delta(X) d\Delta(X') \right)^{1/2}, \quad \Delta = \mathbb{P} - \mathbb{Q}$

Filamentation of a beam kicked off-axis in a nonlinear focusing system



Distance to equilibirium as characterized by Maximum Mean Discrepancy



Computed with complexity O(n) for translation-invariant kernels (e.g., Gaussian)

n = *number* of *simulated particles*

Provides a quantitative metric for numerical studies of relaxation.

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C. Mitchell et al,

Phys. Rev. E 106,

065302 (2022)

Optimization for halo suppression







High-resolution modeling studies proton beam filamentation, halo, and losses in the IOTA ring and how these can be mitigated.

Impact of magnetic c-parameter on halo



- Halo formation occurs on a time scale of 200-300 turns (at 5-8 mA).
- Due to chaos induced when particles cross a separatrix-like structure in the phase space.
- Increasing *c*-parameter of the nonlinear magnet moves the problematic separatrix farther from the beam.

Design with increased c-parameter is being explored with the vendor.

Shows existing integrable optics designs can be improved!

Intense 8 mA proton beam in IOTA (vertical phase space)



IOTA shows less halo formation than a linear design in this regime, **but** results are sensitive to parameters and to the choice of linear design (mixed).







Conclusions

- Accelerator designs based on nonlinear integrable optics have the potential to provide strong damping of instabilities (decoherence), but require a new toolkit of techniques for analysis and modeling.
- Analytical and semi-analytical methods for dynamical systems play an important role.
- For the case of the IOTA storage ring, theory and modeling reveal an unexpectedly rich single-particle dynamics, with several distinct operating regimes. Modeling reveals a mixture of regular and chaotic orbits at high intensity. Beam halo mechanisms need to be better understood, and room remains for optimization.
- Studies motivated the implementation of new tools in IMPACT-Z, including improved tracking and fringe field models (e.g., for dipoles), nonlinear magnet element types, new space charge models, new beam diagnostics, and a workflow for optimization and postprocessing using Jupyter.
- Exploring the space of possible integrable focusing lattice schemes could have a major impact on beam performance in future high intensity machines.







Backup material







Integrability holds for (single-particle) motion of on-energy particles in the transverse degrees of freedom

• Dynamics inside the nonlinear magnetic insert:

$$H_{\perp} = \frac{1}{2}(P_x^2 + P_y^2) - \frac{\tau c^2}{\beta(s)}U\left(\frac{X}{c\sqrt{\beta(s)}}, \frac{Y}{c\sqrt{\beta(s)}}\right) \implies H_N = \frac{1}{2}(P_{xN}^2 + P_{yN}^2 + X_N^2 + Y_N^2) - \tau U(X_N, Y_N)$$

first invariant

Courant-Snyder transformation, scaling

D&N give in [1] a realizable potential U such that H_N admits a second invariant I_N :

$$\{H_N, I_N\} = 0$$

• Dynamics in the arc external to the nonlinear magnetic insert:

Assumed *linear* with a map R_N given by:

 $R_N=\pm I$ (4x4 identity)

Thus, the phase advance must be $n\pi$.



 H_N , I_N are invariant under the one-turn map.

¹V. Danilov and S. Nagaitsev, Phys Rev Accel Beams **13**, 084002 (2010) BERKELEY LAB APPLIED PHYSICS



Magnetic Vector Potential and Magnetic Field within the IOTA Nonlinear Magnetic Insert

The ideal 2D magnetic field within the nonlinear insert at location s is given by $\vec{B} = \nabla \times \vec{A} = -\nabla \psi$, where the potentials are given in terms of dimensionless quantities:

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

using the complex function:

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

The transverse focusing fields vary longitudinally with s.

$$\frac{\beta(s)}{\beta^*} = 1 + \left(\frac{2s}{L}\right)^2 \tan^2 \pi \mu_0, \qquad \beta^* = \frac{L}{2} \cot \pi \mu_0, \quad 0 < \mu_0 < 1/2$$

L – length of the magnetic insert [m] $2\pi\mu_0$ – phase advance across the magnetic insert β^* - beta function at the longitudinal midpoint



Longitudinal variation of the quadrupole gradient





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Critical and resonance structures in the single-particle phase space (zero current integrable motion)



Critical structures:

- Red curve: primary separatrix-like structure Black curve: I.C.s for unstable periodic orbits
- Separate regions of distinct orbit behavior
- A matched beam at 0 mA with the nominal emittance lies within the primary separatrix

Resonance structures:

- Resonant contour lines $u_y/
 u_x$ are shown
- High density of resonances outside the primary separatrix
 - Color: measure of chaos when phase advance is perturbed (blue = regular)

When the phase advance is depressed, chaos develops first in the region outside the primary separatrix.





Critical and resonance structures in the single-particle phase space (zero current integrable motion)



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Surface Methods Provide a Robust Method for Tracking in the IOTA Nonlinear Magnetic Insert with Realistic 3D Fringe Fields

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- **Need:** Accurate symplectic tracking algorithm for modeling the IOTA nonlinear magnetic insert with realistic fringe fields.
- **Problem:** The standard idealized model of the IOTA insert is non-Maxwellian, and neglects fringe field effects. 3D magnetic field data inherently noisy.
- Solution: Use surface methods to extract a smooth vector potential from 3D magnetic field data.
- **Outcome:** Tracking with quadrupole and octupole fringe field corrections shows evidence of perturbed invariants, with little evidence of enhanced losses (10K turns).

$$C_{m,\alpha}^{[n]}(s) = \frac{i^n}{2^m m!} \int_{-\infty}^{\infty} \frac{k^{n+m-1}}{I'_m(kR)} \tilde{B}^{\alpha}_{\rho}(R,m,k) e^{iks} dk$$

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



C. Mitchell, Proc IPAC2018, Vancouver, THPAK036 (2018).



Effect of the Increasing the c Value on the Matched Beam Distribution in Invariant Space



- Increasing the c value leads the beam footprint to shrink in invariant space.
- The primary separatrix begins at (H,I)=(0.1,0.2) and extends along the ray I = 2H
- For sufficiently large c, the beam can be confined away from the primary separatrix.







Understanding Proton Beam Dynamics at High Space Charge Intensity: An Example of Code Benchmarking (IMPACT-Z & MaryLie/IMPACT)

Goal: Study relaxation of a beam in IOTA to near-equilibrium at high intensity, to compare with halo formation in a standard linear lattice.

- Physical IOTA lattice, 2.5 MeV proton beam with nominal emittance and energy spread.
- 8 mA beam current ($\Delta Q_y \approx -0.6$, $\Delta Q_x \approx -0.9$) near maximum for expected IOTA operation.

Comparing beam after 10 turns



Comparing beam size over turn 10



Reasonable agreement between two codes using different space charge algorithms (spectral, PIC).

Numerical convergence tests: # modes/grid points, # particles, location of Poisson boundary, # sc kicks.







Frequency map analysis of orbits in the total potential (space charge + focusing) for a stationary beam in a nonlinear constant focusing channel.

- Extreme current (space charge tune shift >1 near the origin), shown for illustration purposes only.
- **8K** distinct initial conditions (*x*,0,*y*,0) in a disk.
- Orbits are tracked in the sum of the external potential and the equilibrium space charge potential (using 15x15 modes) for 2048 x 1.8 m distance through the nonlinear constant focusing section.







