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VALIDATING pyORBIT FOR MODELING BEAM DYNAMICS IN THE IOTA RING*

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Abstract

The Integrable Optics Test Accelerator (IOTA) ring is a new Fermilab facility dedicated to beam physics experiments, currently operating with 150 MeV electrons. Space charge effects are expected to be significant when it operates with 2.5 MeV protons. In this contribution, we present results of a suite of validation tests of PyORBIT, a PIC-style space charge code. Single particle dynamics of quasi-integrable optics using an octupole string in IOTA is compared with MADX, and shown to be in good agreement. Requirements for the convergence of space charge computations are systematically established and when possible, tests involving space charge are compared with theoretical predictions.

INTRODUCTION

The Fermilab Integrable Optics Test Accelerator (IOTA) is a storage ring for beam physics research. It will be used to explore the potential of integrable optics to mitigate deleterious effect of space charge in high intensity proton synchrotrons. In theory, integrable single particle dynamics eliminates resonances, providing stable motion over a wide tune range. The resulting large betatron tune spread is known to be effective at suppressing instabilities. Details about IOTA can be found in [1]. The main parameters are shown in Table 1.

Table 1: Machine and Beam Parameters of the IOTA Proton Ring

IOTA proton parameters	
Circumference	39.97 [m]
Kinetic Energy	2.5 [MeV]
Maximum bunch intensity /current	9×10^{10} / 8 mA
Transverse normalized rms emittance	(0.3, 0.3) mm-mrad
Betatron tunes	(5.3, 5.3)
Average transverse beam sizes (rms)	(2.22, 2.22) [mm]
Kinematic γ / Transition γ_T	1.003 / 3.75
Rf voltage	400 V
Rf frequency / harmonic number	2.2 MHz / 4
Bucket wavelength	~ 10 m
Bucket half height in $\Delta p/p$	3.72×10^{-3}
rms bunch length	1.7 m
rms energy /momentum spread	1.05×10^{-5} / 1.99×10^{-3}

Experiments are planned with protons at a kinetic energy of 2.5 MeV and space charge is expected to impact beam stability. As in any other low energy proton synchrotron, both incoherent and coherent space charge effects will play a role; furthermore, the impact of space charge on integrability needs to be understood. In this context, it is important to assess the capability and suitability of existing simulation codes. We report here on a variety of relevant validation tests that were performed using pyORBIT [2], a PIC code developed and maintained at ORNL and motivated by the need to simulate certain aspects of SNS.

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VALIDATION OF pyORBIT SINGLE PARTICLE TRACKING

In this section, we aim to validate single-particle tracking in pyORBIT against MADX, an extensively tested code. To minimize discrepancies possibly introduced by subtle differences in the way distributed nonlinearities are modeled by the two codes, all nonlinear elements in IOTA are removed, except for an optional octupole insert region. All residual nonlinearities in the pyORBIT dipole and quadrupole elements are turned off (but not in MADX). Symplecticity tests, dynamic aperture tests, and tune footprint tests show excellent agreement between the codes. This provides confirmation that pyORBIT 1 - interprets the element sequence correctly and 2 - models basic single particle motion correctly.

Symplecticity Test

We test the symplectic condition $J^T S J = S$ and its corollary $\det J = 1$ for 4D transverse motion. Here J is the Jacobian matrix of the transformation, and S is the symplectic matrix. The entries $J_{kl} = \frac{\partial X_k(s_f)}{\partial X_l(s_0)}$ of the Jacobian matrix are obtained numerically using centered differences of canonical Floquet phase space coordinates X_k.

Detailed results of the symplecticity tests can be found in reference [3]. In summary, for the IOTA lattice without the octupole insert, we find that $\det J$ deviation from from unity is on the order of 10^{-7} with MADX while in pyORBIT the deviation is much smaller, typically 10^{-11}. Similarly, $\|J^T S J - S\| \sim 10^{-8}$) with MADX ~ 10^{-12} with pyORBIT For IOTA with octupoles, up to amplitudes of 4σ, the largest deviation of $\det J$ from unity is ~ 10^{-4} in both codes. This conclusion is reinforced by the second test $\|J^T S J - S\|$ where the same pattern is observed.

Dynamic Aperture

The 4D, 5D and 6D dynamic apertures were calculated for the IOTA lattice with octupoles using both MADX and pyORBIT. Circular physical apertures with radius 25 mm are assigned to all elements. 5000 particles are initialized

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depending on the phase space dimension. The rf cavity is turned off for both 4D and 5D calculations and turned on for the 6D calculation. The particles are tracked for 10000 turns, and the initial coordinates in the x-y plane of all surviving particles are recorded. The largest excursions of the surviving particles yield an upper bound for the dynamic aperture. As shown in Fig. 1, results from pyORBIT and MADX are in good agreement.

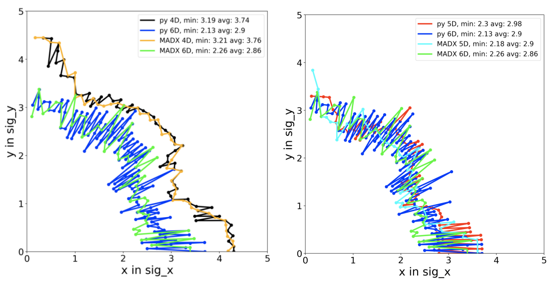

Figure 1: 4D, 5D, and 6D dynamic apertures (expressed in units of the rms beam sizes) for IOTA with octupoles from pyORBIT and MADX. Comparison of 5D and 6D apertures, they are nearly the same.

Tune Footprint

This test compares the tune footprint plots obtained from pyORBIT and MADX. In both codes, test particles are initialized uniformly from nearly zero amplitude to 5σ in the x-y plane. They are then tracked for 5000 turns and the transverse positions of every particle are recorded for each turn. For each particle, the fractional part of the tunes Q_x and Q_y are then obtained by performing a Fast Fourier Transform (FFT) of the transverse coordinates. The tunes obtained from both codes are shown in Fig. 2.

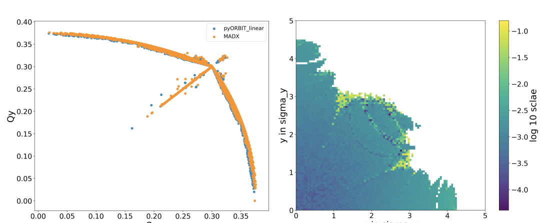

Figure 2: Left: Tune footprint of the IOTA lattice with octupoles, obtained with pyORBIT and MADX. Right: Difference in tune shifts (on a log scale) between pyORBIT and MADX as functions of the initial positions of the test particles.

The right plot in Fig. 2 shows the tune difference dQ for all test particles as a function of their initial coordinates. In most cases the difference between the tunes predicted by MADX and pyORBIT falls within the range 10^{-4} to 10^{-3}, which is comparable to the resolution of the FFT sampling. This result confirms the correctness of single particle tracking in pyORBIT. Particles exhibiting the largest discrepancies are located close to the dynamic aperture boundary, which is likely due to increasingly unstable motion. Beyond this boundary, the particles are lost and $\log dQ$ is undefined.

VALIDATION OF PYORBIT SPACE CHARGE MODEL

pyORBIT is a particle-in-cell code. A finite number of macro-particles represent all charged particles in a bunch. The charge is deposited on a grid and a smoothed density is extracted by interpolation between the grid points. The electric potential is found by numerically solving Poisson's equation in the beam rest frame which thereby allows evaluation of the space charge forces on the macro-particles. In this report, only transverse space charge forces are considered. The particle distribution are Gaussian in the transverse planes and waterbag in the longitudinal plane. Space charge is the only source of nonlinearity. All lattice non-linearities are turned off.

Slow Initialization

Slow initialization is used to allow the beam to reach a steady state in a numerically efficient manner. Rather than injecting with the full charge, the charge per macro-particle is linearly increased from zero to full value at turn T_{init} (the initialization time). Provided the process is sufficiently adiabatic, one expects the beam to remain in near equilibrium at every step as it has time to adjust to a slowly changing space charge force. A 100 mm transverse physical aperture is used in order to contain the halo growth. Figure 3 shows emittance growth and particle loss after 500 turns using different T_{init}.

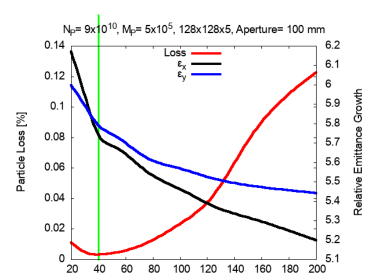

Figure 3: Loss and emittance growth as a function of the slow initialization time T_{init}.

Referring to Fig. 3, the losses are minimum at $T_{init} = 40$, and this value is used in all following tests. While emittance growth decreases monotonically by about 15% as the initialization time is increased, losses exhibits a 40-fold reduction over this range. This suggests that the particle halo is strongly affected by the charge on the macro-particle while the growth of the core is less affected.

Convergence Tests

There are three sets of parameters in pyORBIT that influence the accuracy of space charge simulation: the number of macro-particles (M_p), the number of space charge kicks per betatron wavelength (N_{sc}), and the number of spatial grid

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points ($N_x \times N_y \times N_z$) used to solve Poisson's equation. The convergence value for one parameter is found b varying it while holding the rest two constant. We use particle loss and relative emittance growth after 1000 turns of tracking as figures of merit to check for convergence. Based on the results presented in Fig. 4, $M_p = 5 \times 10^5$, grid size $128 \times 128 \times 5$, and $N_{sc} = 63$ are used as default parameters in all following tests.

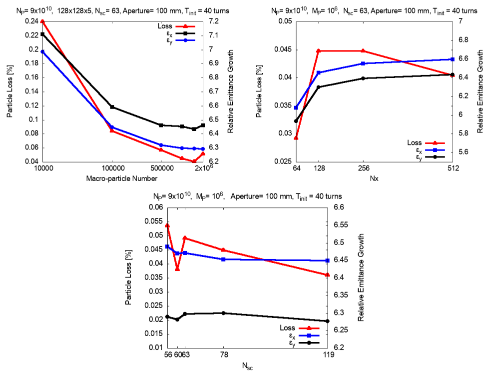

Figure 4: Particle loss (red) , relative emittance growth (black, blue) after 1000 turns as a function of the macro-particle number (top left), the number of grid points $Nx = Ny$ (top right), and the number of space charge kicks N_{sc} per betatron wavelength (bottom). Data is shown for three step sizes are shown, the deviations decrease with decreasing step size.

Symplecticity Test

Following a procedure similar as previously described, symplecticity tests are performed in the presence of space charge. The results are presented in Fig. 5. The deviation of $detJ$ from 1 is 0.02. This is at least two orders of magnitude larger than what is observed with octupoles present but without space charge.

Deviation from symplecticity is expected in a PIC code such as pyORBIT. While it implies that such codes should not be used for long term tracking, they still remain useful for predictions on a short time scale [4].

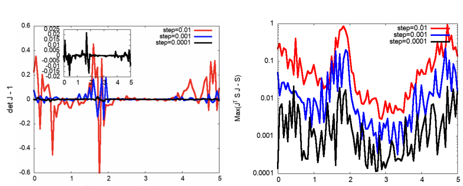

Figure 5: Symplecticity tests with space charge. $\det J - 1$ (left) and $\|J^T SJ - S\|$ (right) as functions of the transverse amplitude in units of the rms beam size.

Tune Shifts and Footprint

This test validates the accuracy of pyORBIT space charge model by comparing tune shifts obtained by tracking to analytical predictions. For Gaussian transverse distributions, the analytical zero- amplitude tune shift is $\Delta Q_{0,sc} = \frac{r_p}{\beta_k \gamma^2 \epsilon_N} \bar{\lambda}_L N_p R$, where r_p is the classical proton radius, β and γ are Lorentz factors, R the effective machine radius, ϵ_N the normalized transverse emittance and N_p is the number of protons per bunch. The amplitude-dependent tunes for a transverse Gaussian distribution can be calculated analogously to those from a head-on beam-beam interaction between two Gaussian beams [5].

After slow initialization, 100 particles are injected at small amplitudes around 0.01σ. It has been pointed out [4] that chaotic motion is observed at very small betatron amplitude in PIC codes due to numerical noise, so the FFT tunes for 100 test particles are averaged. The computed zero-amplitude tune shift at 4 different bunch intensity levels is presented in Table 2 together with analytical predictions.

Table 2: Analytical and Simulated Zero Amplitude Tune Shift at Different Intensity Levels

Intensity	**Zero amplitude tune shifts**	
	Theory	Simulation
0	(0.0, 0.0)	(0.0, 0.001)
10^9	(-0.0371, -0.0372)	(-0.03, -0.034)
10^{10}	(-0.29, -0.29)	(-0.262, -0.266)
10^{10}	(-0.514, -0.514)	(-0.50, -0.536)

The tune footprints in Fig. 6 are obtained using the same method as in Fig. 2, with linear IOTA lattice under space charge effect at two intensity levels. At intensity 10^{10}, the simulated footprint matches the theoretical footprint quite well but is wider. However, a larger discrepancy exists at intensity 9×10^{10}. Such result could be due to the numerical noise in PIC codes, since here the scatter plot represents the tune of individual test particles without averaging. In addition, there are differences between the analytical and simulation models.

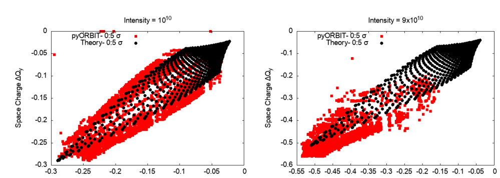

Figure 6: Tune shifts with amplitude due to space charge from pyORBIT and theory at intensity 10^{10} (left) intensity 9×10^{10} (right).

CONCLUSION

We validated the PIC code pyORBIT to model transverse space charge effects in IOTA. We first validated single particle tracking by performing tests of symplecticity, tune footprint, and dynamic aperture and compared results with MADX. Using a slow initialization procedure and parameters that ensures convergence of the space charge solver, we tested symplecticity and compared simulated tune shifts and footprints against theory and observed good agreement.

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