# DIFFERENTIABLE, CPU-/GPU-PARALLELIZED, SYMPLECTIC SPIN-ORBIT TRACKING IN SCIBMAD

J. P. Devlin*[1], G. H. Hoffstaetter[1,2], D. Sagan[1], M. G. Signorelli[2]
[1]CLASSE, Cornell University, Ithaca, New York, USA
[2]Brookhaven National Laboratory, Upton, New York, USA

*Abstract*

SciBmad is a new software library for accelerator simulation and design. Three key pillars which drove the development of SciBmad's tracking code are full differentiability (forwards-, backwards-, and Taylor-mode), high performance, and strict symplecticity. Differentiable integrators enable the trivial extraction of lattice functions and their higher-order generalizations, facilitate the use of machine learning tools, and make optimizations more efficient. The integrators have also been heavily optimized for performance, with SIMD parallelization on the CPU and GPU parallelization for various hardwares. Finally, SciBmad uses Yoshida's symplectic schemes to integrate the fully nonlinear Hamiltonian for magnetic multipoles, RF cavities, and combinations thereof, including implicit symplectic integration where required. All elements allow for spin tracking, which is guaranteed to be orthogonal due to the generality of Yoshida's scheme. Additionally, synchrotron radiation can be turned on in all elements. In this case, the use of a symplectic scheme guarantees that all damping results from the synchrotron radiation and not from numerical errors due to non-symplectic integration.

## INTRODUCTION

Tracking simulations are an extremely important tool in accelerator physics as they provide the most accurate probe of nonlinear spin-orbit motion. Many quantities, such as the dynamic aperture and attainable beam polarization, can only be computed reliably through tracking. As these simulations sometimes require hundreds of thousands or even millions of turns, tracking codes must be as efficient as possible. However, accuracy, at least in the qualitative sense, cannot be sacrificed. Some tracking codes are extremely efficient because they use precomputed Taylor expansions of the motion, but it is easy to find examples where these codes produce qualitatively incorrect results. Other codes use numerical schemes like Runge-Kutta to integrate the full equations of motion, but when the number of steps is reduced to achieve reasonable efficiency, these schemes exhibit problems like artificial damping.

Accelerator physicists have realized that the ideal tracking code, which should be both efficient and accurate, must use symplectic integrators [1]. The canonical example of such a code is the polymorphic tracking code (PTC) [2]. As with Runge-Kutta schemes, the accuracy of a symplectic integrator can always be improved by reducing the step size. However, symplectic integrators do not exhibit the artificial damping seen in other schemes because they produce symplectic maps for any step size. Therefore, the tracking code for our new accelerator simulation program SciBmad is based entirely on symplectic integration [3]. The details of its tracking code, along with some examples, are presented in this paper.

* jpd285@cornell.edu

## HAMILTONIAN MOTION

The motion of charged particles in accelerators is primarily due to external electromagnetic fields. In a canonical coordinate system, this motion can be represented by a Hamiltonian function and is therefore symplectic. The coordinates in SciBmad are the radial offset $x$, the vertical offset $y$, and $z = -\beta c(t_0 - t)$. The subscript 0 indicates "reference" quantities (which may be chosen arbitrarily but should be self-consistent) and the reference time is defined by $s = \beta_0 c t_0$, where $s$ is the distance along the reference trajectory. For a particle with momentum $\vec{P} = m\gamma\vec{v} + q\vec{A}$, where $\vec{A}$ is the vector potential, the momenta conjugate to SciBmad's coordinates are $p_x = P_x/P_0$, $p_y = P_y/P_0$, and $p_z = (P - P_0)/P_0$. In this set of coordinates, the Hamiltonian is

$$H_z = -h\sqrt{(1+p_z)^2 - (p_x - a_x)^2 - (p_y - a_y)^2} - a_s + \frac{\sqrt{(1+p_z)^2 + \widetilde{m}^2}}{\beta_0}, \tag{1}$$

where $\widetilde{m} = (\beta_0\gamma_0)^{-1}$ and $h = 1 + gx$ with the horizontal curvature $g$. The restriction to horizontal curvature is not a problem because the coordinate system can always be rotated to satisfy this constraint.

## SYNCHROTRON RADIATION

The motion of ultrarelativistic particles in electromagnetic fields can be damped significantly by synchrotron radiation. The radiation process leaves the slopes $(x', y')$ invariant and changes the particle energy. The resulting equation of motion is

$$\frac{\mathrm{d}p_z}{\mathrm{d}s} = -\sqrt{h^2 + x'^2 + y'^2}\frac{2}{3}\frac{r_0}{(mc^2)^3}E_0^3(1+p_z)^2 \times \left\| \frac{\vec{\mathscr{E}}_\perp}{c} + \vec{\beta} \times \vec{\mathscr{B}} \right\|^2, \tag{2}$$

where $m$ is the mass and $r_0$ is the classical particle radius [4, 5]. We have defined the "normalized" fields $(\vec{\mathscr{E}}, \vec{\mathscr{B}}) = (q/P_0)(\vec{E}, \vec{B})$ and $\perp$ indicates the component of

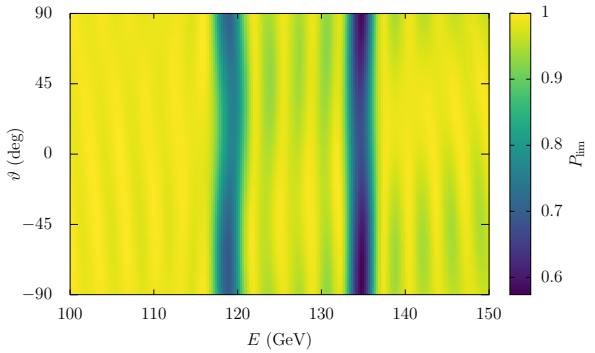


Figure 1: The maximum time-averaged polarization $P_{\mathrm{lim}}$ as a function of the energy $E$ and the Siberian snake angle $\vartheta$.

a vector perpendicular to the normalized velocity $\vec{\beta}$. Equation (2), as with all others in this section, is only accurate when the reference velocity and the particle velocity are both very close to the speed of light.

The radiation process involves emission of photons with random energies and Eq. (2) represents the average effect. We represent the stochastic effect by Gaussian fluctuations in $p_z$ with the correct variance per unit length [5]:

$$\begin{aligned}\Delta p_z &\sim \mathcal{N}(0, \sigma^2),\\ \sigma^2 &= \mathrm{d}s \frac{h}{\sqrt{(1+p_z)^2 - (p_x - a_x)^2 - (p_y - a_y)^2}}\\ &\quad\times \frac{55}{24\sqrt{3}} \frac{\hbar c r_0}{(mc^2)^6} E_0^5 (1+p_z)^5 \left\| \frac{\vec{\mathscr{E}}_\perp}{c} + \vec{\beta} \times \vec{\mathscr{B}} \right\|^3.\end{aligned} \tag{3}$$

In general, the emitted photons do not have momenta parallel to the particle velocity and their emission imparts a transverse kick. The opening angle $\theta$ (out of the plane of instantaneous circular motion) depends on the photon energy. As the transverse kick depends on both the photon energy and the opening angle, these correlations must be taken into account. Our solution is to use independent random numbers and choose the RMS opening angle so that the RMS transverse kick is correct. The appropriate choice is [6]

$$\theta \sim \mathcal{N}\left(0, \frac{13}{55\gamma^2}\right). \tag{4}$$

The angle of emission in the plane of motion could also be taken into account, but this effect is insignificant due to dispersion.

## SPIN MOTION

The semiclassical equation of motion for a spin vector $\vec{S}$ is the Thomas-Bargmann-Michel-Telegdi (T-BMT) equation, which we write as

$$\begin{aligned}\frac{\mathrm{d}\vec{S}}{\mathrm{d}s} &= \vec{\Omega} \times \vec{S},\\ \vec{\Omega} &= g\vec{e}_y - \frac{h}{\sqrt{(1+p_z)^2 - (p_x - a_x)^2 - (p_y - a_y)^2}}\\ &\quad\times \left[ (1 + a\gamma)\vec{\mathscr{B}}_\perp + (1+a)\vec{\mathscr{B}}_\parallel - \left(a\gamma + \frac{\gamma}{1+\gamma}\right)\vec{\beta} \times \frac{\vec{\mathscr{E}}}{c} \right],\end{aligned} \tag{5}$$

where $a = (g-2)/2$ is the anomalous gyromagnetic ratio and $\parallel$ indicates a component parallel to $\vec{\beta}$ [4, 7, 8]. However, we do not solve this equation directly. SciBmad uses quaternions in place of spin vectors because quaternions encode the entire spin rotation very efficiently. The equation of motion for the quaternion $\mathsf{q}$ is

$$\frac{\mathrm{d}\mathsf{q}}{\mathrm{d}s} = -\frac{i}{2}\left(\vec{\Omega} \cdot \vec{\sigma}\right)\mathsf{q}, \tag{6}$$

where $\vec{\sigma}$ is the vector of Pauli matrices [9]. In practice, the quaternions are stored as four-element tuples, not as SU(2) matrices. The connection between the two representations is given by

$$(q_0, \vec{q}) \cong q_0 1 - i\vec{q} \cdot \vec{\sigma}. \tag{7}$$

## EXPLICIT INTEGRATION

The differential equation for the full spin-orbit vector $\vec{\Xi} = (\vec{z}, \mathsf{q})$ can be written as

$$\frac{\mathrm{d}\vec{\Xi}}{\mathrm{d}s} = \vec{F}_{\mathrm{Ham}} + \vec{F}_{\mathrm{rad}} + \vec{F}_{\mathrm{spin}}, \tag{8}$$

with an obvious notation. We solve this equation numerically by splitting, which means that we solve the differential equation corresponding to each term separately and combine these solutions. In SciBmad, we use the second-, fourth-, sixth-, and eighth-order Yoshida schemes [10].

The equation $\vec{\Xi}' = \vec{F}_{\mathrm{rad}}$ is solved by direct integration of Eq. (2) because the electromagnetic fields are constant when the coordinates are unchanged. The same goes for $\vec{\Xi}' = \vec{F}_{\mathrm{spin}}$ and Eq. (6) because $\vec{\Omega}$ is independent of the spin. However, although $\vec{\Xi}' = \vec{F}_{\mathrm{Ham}}$ has an exact solution only in the simplest of cases (namely drifts, solenoids, and dipoles), we can apply this method more generally by splitting $\vec{F}_{\mathrm{Ham}}$ itself. In SciBmad, we combine the aforementioned simple cases with the exact multipole kick and RF cavity kick to produce the solenoid-kick, bend-kick, matrix-kick, cavity-kick, and drift-kick splits of the Hamiltonian [1].

All explicit integration schemes are differentiable in forward mode using ForwardDiff.jl, reverse mode using ReverseDiff.jl, and Taylor mode using GTPSA.jl [11–13]. Taylor-mode differentiation includes derivatives not only with respect to the initial coordinates, but also with respect to lattice parameters. Additionally, tracking is parallelized on both the CPU and the GPU; for more details, see Ref. [3].

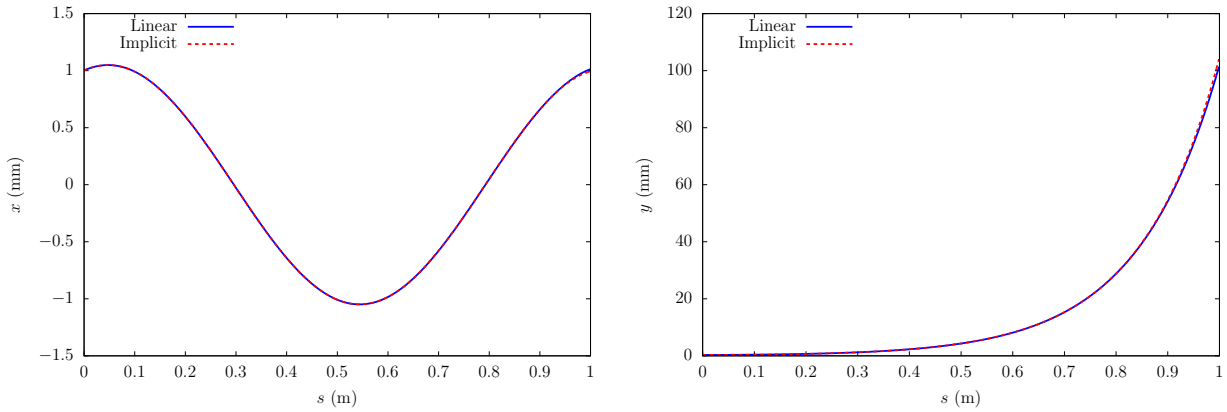


Figure 2: Trajectory through an electrostatic quadrupole. The solid blue line is the solution to the linearized equation of motion and the dashed red line is implicit symplectic integration of the full equation of motion.

## IMPLICIT INTEGRATION

When explicit symplectic integration is not possible, symplectic tracking is still possible using generating functions [14]. In SciBmad, we use the generating functions

$$\begin{aligned} F_3(\vec{q}^f, \vec{p}; \mathrm{d}s) &= -\vec{q}^f \cdot \vec{p} + \mathrm{d}s\, H(\vec{q}^f, \vec{p}), \\ F_2(\vec{q}, \vec{p}^f; \mathrm{d}s) &= \quad \vec{q} \cdot \vec{p}^f + \mathrm{d}s\, H(\vec{q}, \vec{p}^f), \end{aligned} \tag{9}$$

which both provide first-order approximations to the flow of $H$. The corresponding equations are implicit and are solved with a Newton search. With an obvious notation for the individual flows, the combination $\vec{M}_3 \circ \vec{M}_2$ is a second-order, time-reversible approximation to the flow of $H$. It can therefore be used in any of the Yoshida schemes [1]. Radiation damping and spin motion are included just as they were with the explicit schemes. CPU-/GPU-parallelization is supported along with forward-mode and Taylor-mode differentiation.

## EXAMPLES

The first example is spin motion in the Hadron Storage Ring (HSR) of Brookhaven National Laboratory's planned Electron-Ion Collider. The HSR will accelerate polarized protons to high energy, which requires the use of Siberian snakes, magnet structures which rotate the spin by 180° around some axis. Even the most symmetric Siberian snake arrangements, known as Doubly Lee-Courant schemes, have one free angle $\vartheta$ which specifies the axes of the Siberian snakes [15]. The attainable polarization depends on this angle, so it should be chosen carefully. This effect can be quantified using the maximum time-averaged polarization $P_{\mathrm{lim}}$ [9]. In SciBmad, tracking is parallelized on the CPU and GPU not only over particles, but also over lattice parameters using the BatchParam construct [3]. In Fig. 1, $P_{\mathrm{lim}}$ is calculated in the energy range 100-150 GeV for 200 different angles $\vartheta$ in parallel. In other words, in the time that it takes to track one bunch of 200 particles through a single lattice, 200 different lattices are being compared.

The second example is implicit integration through an electrostatic quadrupole with scalar potential $\Phi \propto x^2 - y^2$. When the equations of motion are expanded to first order about the magnet centerline, they match that of a magnetic quadrupole. Therefore, the well-known quadrupole matrix is a good approximation of the motion for small coordinates. However, unlike for a magnetic quadrupole, explicit symplectic integration is not possible. Nonlinear corrections can be derived manually, but the truncation to fixed order generally does not produce a symplectic map and can become quite complicated at higher orders [16]. Implicit integration is thus an appealing tracking method for such elements because the resulting map is exactly symplectic and includes nonlinear terms of all orders. A comparison of the linear calculation and implicit integration is shown in Fig. 2. The agreement is quite good, but some deviation owing to nonlinearities is visible.

## CONCLUSION

The tracking in SciBmad is comprehensive on the single-particle level in the sense that symplectic integration of the classical equations of motion is possible for any external electromagnetic fields with known potentials. Semiclassical spin motion and synchrotron radiation (both damping and diffusion effects) are also included. While these features are often sufficient, there are some cases in accelerator physics where interparticle interactions are of interest. One such example is intrabeam scattering, which has already been implemented in SciBmad for Gaussian beams [17]. Other interactions which are planned for SciBmad but have not yet been implemented include space charge, coherent synchrotron radiation, beam-beam effects, and wakefields.

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