Spin Tracking in XSuite

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XSuite Introduction

Xsuite is a python-based modular simulation package that integrates tools developed at CERN into one package[1].

Xobjects	infrastructure to manage the memory, compile and execute code on different computing platforms;
Xpart	package to generate and manipulate ensembles of particles;
Xtrack	single-particle tracking library, creation/import of beam line descriptions;
Xcoll	simulation of particle-matter interaction through a native engine and through interfaces with the FLUKA and Geant4 codes;
Xfields	computation of the electromagnetic fields generated by particle ensembles using Particle In Cell (PIC) solvers or analytical distributions,
Xdeps	management of the dependencies, implementation of deferred expressions.

Why is there interest in developing spin tracking?

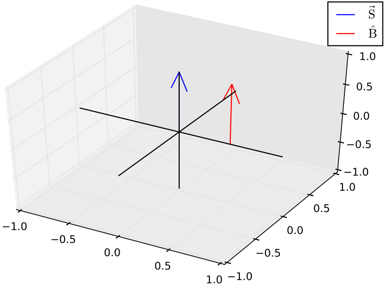
- For the FCC-ee, the intent is to have spin-polarized electron pilot bunches to precisely calibrate the center of mass energy[2].
- See ”Beam Polarization studies: status and challenges” by Yi Wu.

[1] https://xsuite.readthedocs.io/en/latest/
[2] https://inspirehep.net/files/9da23f66d11ee631c044bb4740874a02

Spin Dynamics in Accelerators

Torque on the magnetic moment from a magnetic field: $\vec{\Gamma} \propto \vec{S} \times \vec{B}$

- No torque if the two are parallel
- Maximum if the two are orthogonal



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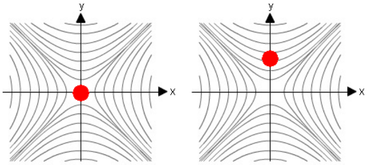
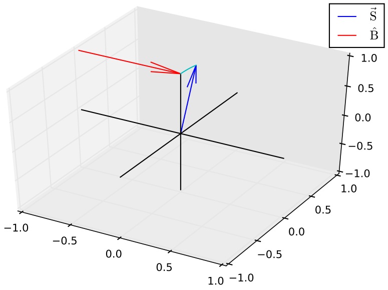
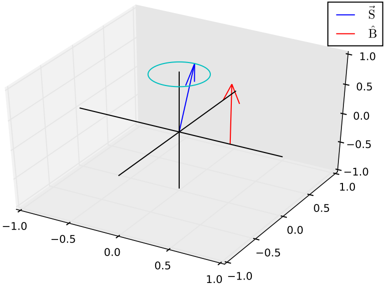




Spin Dynamics in Accelerators

Torque on the magnetic moment from a magnetic field: $\vec{\Gamma} \propto \vec{S} \times \vec{B}$

- No torque if the two are parallel
- Maximum if the two are orthogonal
- Beam now rotates in dipole field since they are no longer parallel.



Number of rotations the spin rotates in one turn is known as the spin tune: $\nu_s = G\gamma$, with G being the anomalous gyromagnetic g-factor ($G_{helions}$=-4.1842, $G_{protons}$=1.7928) and γ being the Lorentz factor.

The Thomas-BMT Equation

The Thomas-BMT equation is the equation of motion for a particle's spin vector, $\vec{S}$, in a synchrotron (neglecting effects of $\vec{E}$)

$$\frac{d\vec{S}}{dt} = \frac{q}{\gamma m}\vec{S} \times \left[(1 + G\gamma)\vec{B_\perp} + (1 + G)\vec{B_\parallel}\right] \tag{1}$$

- Term $\propto \vec{B}_\perp$ is strongest due to presence of strong focusing quadrupoles
- Terms $\propto \vec{B}_\parallel$ is small.

From this, the resonance strength can be calculated with the Fourier transform of spin perturbing fields

$$\epsilon_k = \frac{(1 + G\gamma)}{2\pi} \oint \left[\frac{\partial B_x/\partial y}{B\rho}\right] y e^{iK\theta} ds \tag{2}$$

Eq. 2 is satisfied when $G\gamma = n$ and $G\gamma = nP \pm \nu_y$ which are imperfection and intrinsic resonances.

Spin tracking implementation

The implementation uses the spinor method with calculation at each slice of an element [3]. The real spin vector calculated from spinors is

$$\vec{S} = \begin{pmatrix} S_x \\ S_s \\ S_y \end{pmatrix} = \psi^\dagger \vec{\sigma} \psi = \begin{pmatrix} \psi^\dagger \sigma_x \psi \\ \psi^\dagger \sigma_y \psi \\ \psi^\dagger \sigma_z \psi \end{pmatrix} = \begin{pmatrix} \psi_1 \psi_2^* + \psi_1^* \psi_2 \\ i\psi_1 \psi_2^* - i\psi_z^* \psi_2 \\ |\psi_1|^2 - |\psi_2|^2 \end{pmatrix} \tag{3}$$

where ψ the spinor $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$, $\psi^\dagger$ being its Hermitian transpose, σ are the Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Lastly, we define a rotation vector $\vec{\omega} = \begin{pmatrix} \omega_x \\ \omega_s \\ \omega_y \end{pmatrix}$.

$$\vec{\sigma} \cdot \vec{\omega} = \begin{pmatrix} \omega_y & \omega_x - i\omega_s \\ \omega_x + i\omega_s & -\omega_y \end{pmatrix} \tag{4}$$

[3] As in "Polarized Beam Dynamics and Instrumentation in Particle Accelerators", 2023

Spin tracking implementation

Transporting through an optical element, we will define the spinor transport matrix from i to f as T where

$$\psi_f = T_{f\leftarrow i}\psi_i \tag{5}$$

which rotates the spinor by $\phi\omega$

$$T = e^{\frac{i}{2}(\vec{\omega}\ \cdot\vec{\sigma})} = I\cos\frac{\omega\phi}{2} + i(\frac{\vec{\omega}}{\omega}\dot{\vec{\omega}})\sin\frac{\omega\phi}{2} = \begin{pmatrix} t_o + it_y & t_s + it_x \\ -t_s + it_x & t_o - it_y \end{pmatrix} \tag{6}$$

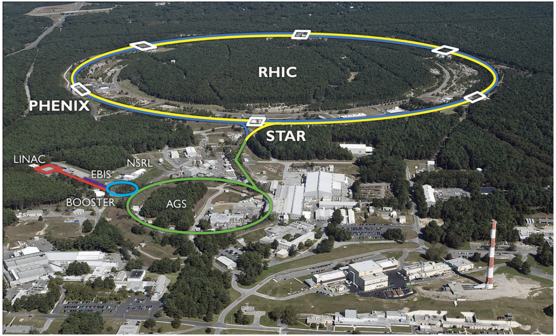
with $t_o = \cos\frac{\omega\phi}{2}$, $t_x = \frac{\omega_x}{\omega}\sin\frac{\omega\phi}{2}$, $t_s = \frac{\omega_s}{\omega}\sin\frac{\omega\phi}{2}$, $t_y = \frac{\omega_y}{\omega}\sin\frac{\omega\phi}{2}$

Bringing this back into the 3D spin vector, we define M where $\vec{S}_f = M_{f\leftarrow i}\vec{S}_i$

$$M = \begin{pmatrix} t_o^2 + t_x^2 - t_s^2 - t_y^2 & 2(t_xt_s + t_ot_y) & 2(t_xt_y - t_ot_s) \\ 2(t_xt_s - t_ot_y) & t_o^2 - t_x^2 + t_s^2 - t_y^2 & 2(t_st_y + t_ot_x) \\ 2(t_xt_y + t_ot_s) & 2(t_st_y - t_ot_x) & t_o^2 - t_x^2 - t_s^2 + t_y^2 \end{pmatrix} \tag{7}$$

The AGS Booster

An aerial view of the RHIC accelerator complex, to be used for the future Electron Ion Collider



The Booster (in blue) is a small synchrotron, 201.78 m in circumference, that serves as the injector to the AGS.

Future benchmarking will be performed in Booster, AGS, and RHIC where there is plentiful data and comparisons with theory.

Benchmarking, Booster

Comparison of one turn of xsuite with zgoubi

$$M_{zgoubi,oneturn} = \begin{pmatrix} 0.309017 & -0.951056 & 0.00000 \\ 0.951056 & 0.309017 & 0.00000 \\ 0.00000 & 0.00000 & 1.00000 \end{pmatrix}$$

(8)

$$M_{xsuite,oneturn,T_{MAT}} = \begin{pmatrix} 0.309017 & -0.951057 & 0. \\ 0.951057 & 0.309017 & 0. \\ 0. & 0. & 1. \end{pmatrix}$$

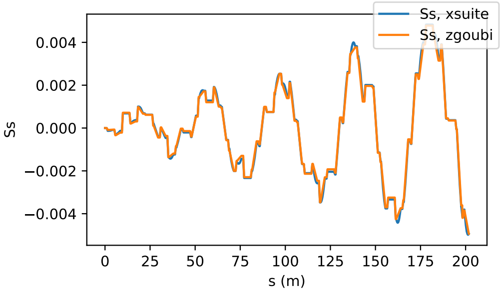
(9)

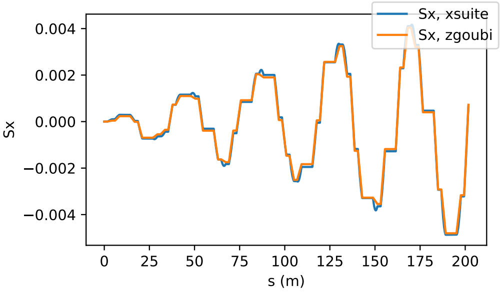
$\mathbf{n}_{o,zgoubi}$=0 0 1

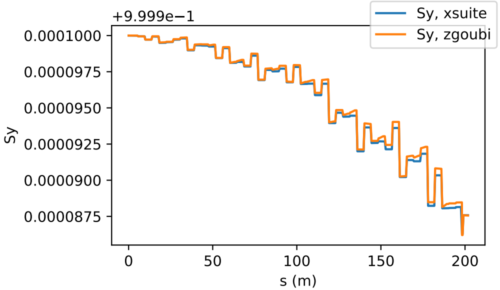
$\mathbf{n}_{o,xsuite}$=0 0 1

- Transport matrix has very good agreement with zgoubi.
- XSuite has been converted to zgoubi units.

Single turn, element by element







- Introduced small vertical orbit error of $\times 10^{-4}$ mrad
- Good agreement between implementation in xsuite and zgoubi.

Multiple turns, crossing $G\gamma = 5$

Froissart-Stora formula for a single particle follows

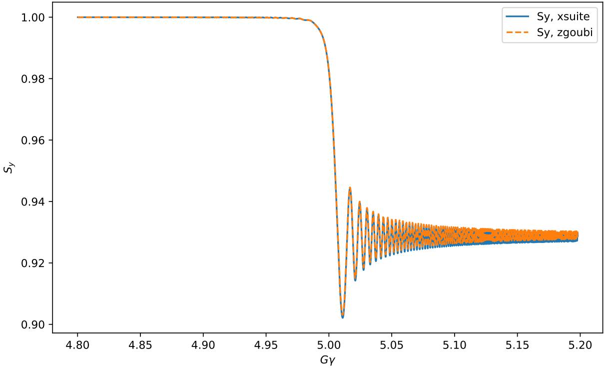
$$\frac{P_f}{P_i} = 2e^{-\frac{\pi|\epsilon|^2}{2\alpha}} - 1 \tag{10}$$

where P_f and P_i are the final and initial polarization, ϵ is the resonance strength, and α is the crossing speed.
The resonance strength calculation follows

$$\epsilon_K = \frac{1 + G\gamma}{2\pi} \oint \frac{\frac{\partial B_y}{\partial x}}{B\rho} y e^{iK\theta} ds \tag{11}$$

where K is the resonance condition (K=$G\gamma = 5$ in this case), θ is the location around the ring. Calculated resonance strength is $\epsilon(theory) = 0.0007491$. With a crossing speed of $\alpha = 2.5331 \times 10^{-5}$, P_f/P_i=0.9316.

Multiple turns, crossing $G\gamma = 5$



- $P_f(xsuite) = 0.9284$, $P_f(zgoubi) = 0.9290$, $P_f(xsuite)/P_f(zgoubi) =$ 0.99932, reminder $P_f(theory)$=0.9316.
- $\epsilon(xsuite)$ =0.0007587, $\epsilon(zgoubi)$=0.0007634, $\epsilon(xsuite)/\epsilon(zgoubi)$ =0.99375.
- $\epsilon(theory)$ =0.0007491, $\epsilon(xsuite)/\epsilon(theory)$ =0.9874, $\epsilon(zgoubi)/\epsilon(theory) = 0.9812$

- $\alpha(xsuite) = 2.5330513779086403e-05$, $\alpha(zgoubi) = 2.533051450608945e-05$, $\alpha(xsuite)/\alpha(zgoubi) = 0.9999999712993178$.
- Very good comparison.

More benchmarking

Spin a dipole around 2π in some discreet step. Verify zgoubi and the current implementation get the same answer. Grabbing the 0°, 10°, 20°, 30° with a rotated 1 cm long, 10.5 T magnet at $B\rho$=79.366 Tm ($G\gamma = 45.5$), spin rotation~3.5 deg.

Zgoubi (0°)

$$\begin{pmatrix} 0.998094 & 0.061715 & 0.00000 \\ -0.061715 & 0.998094 & 0.00000 \\ 0.00000 & 0.00000 & 1.00000 \end{pmatrix}$$

xsuite (0°)

$$\begin{pmatrix} 0.998094 & 0.061714 & 0. \\ -0.061714 & 0.998094 & 0. \\ -0. & 0. & 1. \end{pmatrix}$$

Zgoubi (10°)

$$\begin{pmatrix} 0.998094 & 0.060777 & 0.010717 \\ -0.060777 & 0.998151 & -3.2597\ 10^{-4} \\ -0.010717 & -3.2597\ 10^{-4} & 0.999943 \end{pmatrix}$$

xsuite (10°)

$$\begin{pmatrix} 0.998094 & 0.060777 & 0.010717 \\ -0.060777 & 0.998151 & -3.2597\ 10^{-4} \\ -0.010717 & -3.2597\ 10^{-4} & 0.999942 \end{pmatrix}$$

Zgoubi (30°)

$$\begin{pmatrix} 0.998094 & 0.053446 & 0.030857 \\ -0.053446 & 0.998570 & -8.2539\ 10^{-4} \\ -0.030857 & -8.2539\ 10^{-4} & 0.999523 \end{pmatrix}$$

xsuite (30°)

$$\begin{pmatrix} 0.998094 & 0.053446 & 0.030857 \\ -0.053446 & 0.998570 & -8.2539\ 10^{-4} \\ -0.030857 & -8.2539\ 10^{-4} & 0.999523 \end{pmatrix}$$

- Across all values of $G\gamma\theta$ used, the determinant-1 O10^{-16}

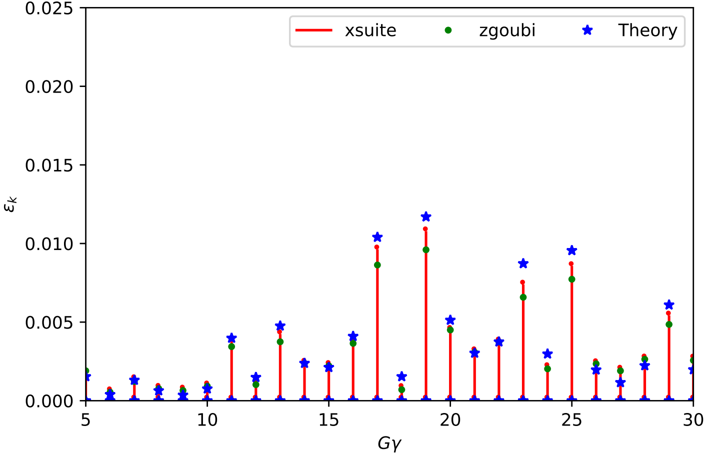
Benchmarking→Computing time and notes on implementation

Currently, the spin tracking implementation is a python layer that is interacting with paramters from xsuite+tracking.

	Zgoubi	Xsuite ($\vec{S}$)	Xsuite ($\vec{\psi}$)
Slices (dipoles)	242	10	10
$G\gamma\theta$/slice	0.2	4.8	4.8
Turns	2500	2500	2500
Particles	4	2	2
Total time	38.7873	354.5727	237.1962
Time per turn per particle (ms)	3.878	70.91	47.44

Implementation into C source code will give significant improvements in computing time.

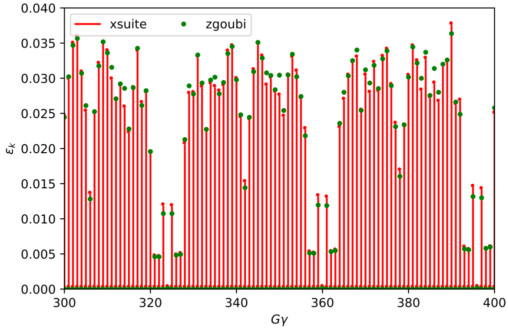
Comparison from $G\gamma$=5 to 30



- Image shows Froissart-Stora
- RMS(xsuite-theory)=2.09%, RMS(xsuite-zgoubi)=0.63%

Comparison up to $G\gamma = 400$

Resonances are too strong with the chosen parameters above $G\gamma = 40$ for comparison with theory $\rightarrow$ P_f saturates at -1.



- Overall, good agreement with RMS difference $\sim$1.3%.
- For good agreement with zgoubi, zgoubi step-size decreased further.
- At $G\gamma = 360$, the precession in a single dipole is $G\gamma\theta = 10$.

Implementation List and Road map

Implementation list

- General T-matrix using Spinor implementation with tracking of
  - 2x2 matrix using $\vec{\psi}$,
  - or 3x3 matrix using $\vec{S}$ (expanded to 9x9 in implementation xsuite).
- Implemented into xsuite [4]. Installation verification ongoing:
  - Repeat benchmarking with the Booster.
  - Check intrinsic resonances.
  - Already nice results with LEP comparisons.
  - Spin integrated with synchrotron radiation.

Road map/benchmarking:

1. Test with RHIC, and HSR, compare with zgoubi and theory.
2. Test with LEP for comparisons with electron spin studies.
3. Test with FCC-ee.

[4] See G. Iadarola, ”Xsuite evolution for FCC studies” FCC week, 2025

Thank you

Questions?