New Spin Tracking Software Developed For General Particle Tracer

Examples of Existing Software

Motivation for Development and Current Applications Particle Tracking and Spin Dynamics GPT: Element and Programs GPT: Versatility and Customizability GDFMGO (Multi-objective genetic global optimizer) GDFSolve

Mark Stefani & S.B. van der Geer

October 21, SPIN2021



Particle Spin Tracking







- BMAD
 - Runge–Kutta integration, FFTs, interpolation and extrapolation
 - software toolkit for the simulation of charged particles and X-rays
 - Provides a simple mechanism for lattice function calculations from within control system programs.

Use Examples:

Lattice design, X-ray simulations, Spin tracking, Wakefields and HOMs, Beam breakup simulations in ERLs, Intrabeam scattering (IBS) simulations, Coherent Synchrotron Radiation (CSR)

- Zgoubi
- NEW: General Particle Tracer Spin



- BMAD
- Zgoubi
 - Dynamics calculated by integrating the Lorentz equation, based on Taylor series expansion,
 - closed orbits in periodic machines, computation of optical functions and parameters, tune scans, dynamic aperture scans, spin dynamics data treatment, graphic scripts, FFA and cyclotron design, AGS and RHIC studies, synchrotron radiation losses.
 - Unique Reference frame and coordinates

Use Examples:

- Neutrino Factory simulations, lepton and hadron colliders, spin dynamics investigations at SuperB, RHIC, etc.
- NEW: General Particle Tracer Spin





- BMAD
- Zgoubi
- NEW: General Particle Tracer Spin
 - Fifth order Runge-Kutta driver with adaptive stepsize control
 - Fully relativistic 3D charged-particle dynamics
 - Most standard beam-line components are represented in GPT. Users of GPT can easily extend the code to perform highly specialized calculations for specific applications.
 - Hierarchical data analysis, automatic parameter scans and graphical output allow for fast and detailed interpretation of simulation results.

Use Examples:

Ultrahigh spectral brightness femtosecond XUV and X-ray sources, Coherent Synchrotron Radiation (CSR), laser plasma wakefield accelerator design, space-charge induced distortions of ultrafast electron diffraction, high power proton drivers

Now polarized positron collection and injector design. Many more potential uses.



Motivation for Development and Current Applications

- GPT has been the principle software used in countless studies. There are at least 81 publications on GPT specific applications alone.
- Expansion of applications with spin tracking capabilities are numerous.

This expansion of GPT capabilities was part of a Laboratory Directed Research & Development project at Jefferson National Laboratory focused on the conceptual design of a polarized positron sources as an upgrade to the existing CEBAF Machine.

An efficient, robust, and versatile simulation software would be necessary to fully capture the physics of particle dynamics, spin dynamics, space charge, 3D fields and particle particle interactions to successfully design a polarized positron collection and injection scheme. Sophisticated analysis and optimization codes would also be necessary.





Motivation for Development and Current Applications

 Particles distributions from GEANT4, poisson/SF Adiobatic Matching Device field maps and build in accelerator elements



• Investigating E-field bending element for longitudinal to horizontal spin.







Particle Position and Momentum tracking in GPT

• The position x and the momentum $p = \gamma m v$ are used as the coordinates of a particle. The equations of motion for particle i are given by:

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i \qquad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i = \frac{\mathbf{p}_i c}{\sqrt{\mathbf{p}_i^2 + m_i^2 c^2}}$$

- The force on particle i is calculated using: $\mathbf{F}_i = q(\mathbf{E}_i + \mathbf{v}_i \times \mathbf{B}_i)$
- Due to the spacecharge, the force on each particle depends on the position of all other particles. vector y(t) containing the six coordinates of all the particles.

$$\frac{d\mathbf{y}(t)}{dt} = \mathbf{f}(t, \mathbf{y}(t))$$

- The only boundary conditions are the initial particle coordinates at a specified time.
- GPT solves all particles variables simultaneously, the results are always self-consistent





Particle Position and Momentum tracking in GPT

• fifth-order Runge-Kutta advances y(t) to y(t+h) by performing the following steps:

$$\mathbf{k}_{1} = h\mathbf{f}(t, \mathbf{y}) \\ \mathbf{k}_{2} = h\mathbf{f}(t + a_{2}h, \mathbf{y} + b_{21}\mathbf{k}_{1}) \\ \vdots \\ \mathbf{k}_{6} = h\mathbf{f}(t + a_{6}h, \mathbf{y} + b_{61}\mathbf{k}_{1} + \dots + b_{65}\mathbf{k}_{5}) \\ \mathbf{y}(t + h) = \mathbf{y}(t) + c_{1}\mathbf{k}_{1} + c_{2}\mathbf{k}_{2} + c_{3}\mathbf{k}_{3} + c_{4}\mathbf{k}_{4} + c_{5}\mathbf{k}_{5} + c_{6}\mathbf{k}_{6} + \mathcal{O}(h^{6})$$

 To monitor the accuracy of y(t+h) each step is calculated again using an embedded fourth-order formula:

$$\mathbf{y}^{*}(t+h) = \mathbf{y}(t) + \mathbf{c}_{1}^{*}\mathbf{k}_{1} + \mathbf{c}_{2}^{*}\mathbf{k}_{2} + \mathbf{c}_{3}^{*}\mathbf{k}_{3} + \mathbf{c}_{4}^{*}\mathbf{k}_{4} + \mathbf{c}_{5}^{*}\mathbf{k}_{5} + \mathbf{c}_{6}^{*}\mathbf{k}_{6} + \mathcal{O}(h^{5})$$

- The error estimate is given by: $\Delta \equiv \mathbf{y}(t+h) \mathbf{y}^*(t+h) = \sum_{i=1}^{6} (c_i c_i^*) \mathbf{k}_i$
- Keeping specified accuracy is done by adjusting the stepsize h.



Particle Spin tracking in GPT

With spin-tracking, additional differential equations are solved for each particle ٠

$$\frac{d\mathbf{s}_i}{dt} = \mathbf{\Omega}_i \times \mathbf{s}_i \qquad \mathbf{\Omega}_i = -\frac{q_i}{m_i} \left[\left(a_i + \frac{1}{\gamma_i} \right) \mathbf{B}_i - \frac{a_i \left(\gamma_i \boldsymbol{\beta}_i \cdot \mathbf{B}_i \right)}{\gamma_i + 1} \boldsymbol{\beta}_i - \left(a_i + \frac{1}{\gamma_i + 1} \right) \frac{\boldsymbol{\beta}_i \times \mathbf{E}_i}{c} \right]$$

- Generalized Thomas-BMT equation
- In Lab Frame
- s is the particle spin coordinate
- $a_i = \frac{g}{2} 1$
- g is the particle's magnetic moment.





Benchmark Simulations

- Simple Example: Wien Filter, Solenoid, and Dipole Pair Beamline
 - Total spin processions in lab frame; not relative to momentum.
 - Theoretical values make approximations of field integration and time of flight.

Solenoid:
$$\theta = \frac{180}{\pi} \frac{e}{m} T \left[\frac{1}{\gamma}(a+1)\overrightarrow{B_{\parallel}}\right]$$

Dipole:
$$\theta = \frac{180}{\pi} \frac{e}{m} T \left[\left(a + \frac{1}{\gamma} \right) \overrightarrow{B_{\perp}} \right] \qquad T \cong \frac{L}{\beta c}$$

Wein filter:
$$\theta = \frac{180}{\pi} \frac{e}{m} T \left[a \frac{E}{\beta c} + \left(\frac{1}{\gamma^2 - 1} - a \right) \frac{\beta E}{c} \right]$$



Theory: $S_0 = (0,0,1) \rightarrow S = (0,1,0) \rightarrow S = (-1,0,0) \rightarrow S = (-0.707,0,0.707) \rightarrow S = (-1,0,0)$





Theory: $S_0 = (0,0,1) \rightarrow S = (0,1,0) \rightarrow S = (-1,0,0) \rightarrow S = (-0.707,0,0.707) \rightarrow S = (-1,0,0)$







Theory: $S_0 = (0,0,1) \rightarrow S = (0,1,0) \rightarrow S = (-1,0,0) \rightarrow S = (-0.707,0,0.707) \rightarrow S = (-1,0,0)$





0.8286

Theory: $S_0 = (0,0,1) \rightarrow S = (0,1,0) \rightarrow S = (-1,0,0) \rightarrow S = (-0.707,0,0.707) \rightarrow S = (-1,0,0)$





Theory: $S_0 = (0,0,1) \rightarrow S = (0,1,0) \rightarrow S = (-1,0,0) \rightarrow S = (-0.707,0,0.707) \rightarrow S = (-1,0,0)$





Generalized Particle Properties and Distributions

- Arbitrary particle properties and can be specified
 - Particle: mass, magnetic moment, charge, magnitude of spin
- Simultaneous simulation of multiple particles species
 - Electrons and Positrons
 - simultaneous propagation and spin tracking
 - recombination and scattering can be implemented
- Arbitrary particle distributions
 - Spin tracking Minimally requires:

x, y, z, px, py, pz, spinx, spiny, spinz, g, q

Momentum, p, can be defined by $\gamma\beta$ or simply β of the associated vector

 Built in functions can be used to generate arbitration distributions or input files can be used to import distributions from software such as GEANT4.



e-&e+



GPT elements and programs

- Sandbox approach
- GDFAs are build in features of GPT that include components of the simulation itself as well as post-processing analysis.
 - Avgs
 - Stds
 - Bstatic
 - Setspinx
 - Ect...
- Custom elements and programs can be compiled (GPT's super power).
 - WriteGBall()
 - UncorEmit()
 - Bunchfactor()
 - Whatever you want to code...
- Programs (progs): post-processing features used to analyze simulation results. These are the features that can be used for optimization.





GDFMGO and **GDFSolve**

- Built in Optimization features GDFsolve and GDFMGO
- GDFSolve used as a root-finder or as optimizer, assumes that the target objective(s) are smooth with respect to the variables.
- Both allow a non-equal number of variables and constraints as well as external boundary conditions for all variables. The objectives are all calculated by standard GDFA data-analysis, allowing both built-in and custom GDFA programs to be used.
- In theory GDFMGO is the best algorithm. It can solve, optimize, and it is not very sensitive to local minima. GDFMGO is intrinsically slow, but there is an MPI version that can launch thousands of GPT runs simultaneously
- Multi-Objective Genetic Global Optimizer
 - Less likely to be trapped by local max or mins
 - .mgo file used to set optimization condition for separate simulation file
 - Convenient optimization analysis and quickly alternate optimization and standard simulation
 - Optimization time can be improved by specifying accuracy and number of cores used.





GDFMGO example output





GDFMGO example output



New Spin Tracking Software Developed For General Particle Tracer

Jefferson Lab

References

- S.B. van der Geer, M.J. de Loos. User Manual, http://www.pulsar.nl/gpt
- S.B. van der Geer, M.J. de Loos. *Custom Elements,* <u>http://www.pulsar.nl/gpt</u>
- S.B. van der Geer, M.J. de Loos, Mark Stefani. GPT-Spin, http://www.pulsar.nl/gpt
- F. Meot. ZGOUBI USERS' GUIDE, Note C-AD/AP/470 BNL 2012, https://www.bnl.gov/isd/documents/79375.pdf
- David Sagan. The BMAD Reference Manual, <u>https://www.classe.cornell.edu/bmad/bmad-manual-2021-09-24.pdf</u>
- William H. Press, Brian P. Flannery, Saul A. Teukolsky and William T. Vetterling, *Numerical Recipes*, The Art of Scientific Computing, Cambridge University Press, 2nd edition, 1992
- Jackson J D. *Classical Electrodynamics*, 3rd ed (New York:Wiley) 1998
- Bargmann V, Michel L and Telegdi V L. Phys. Rev. Lett.2435–6 1959
- S.B. van der Geer, O.J. Luiten, M.J. de Loos, G. Pöplau, U. van Rienen, 3D space-charge model for GPT simulations of high brightness electron bunches, Institute of Physics Conference Series, No. 175, p. 101. 2005
- Gisela Pöplau, Ursula van Rienen, Bas van der Geer, and Marieke de Loos, Multigrid algorithms for the fast calculation of space-charge effects in accelerator design, IEEE Transactions on magnetics, Vol 40, No. 2, p. 714. 2004





Thank you





