Multi-Scale Modeling for Beam-Beam Depolarization

Grant number: DE-SC0013187
PM: Manouchehr Farkhondeh

Benjamin Cowan and Ilya Pogorelov

Tech-X Corporation

Vahid Ranjbar

BNL
Tech-X: high-performance computational science and applications

- Founded in 1994
- ~35 people, 2/3 PHDs, Boulder, Colorado
- Leader of national projects, national lab partner
- Expertise in
  - High-performance computational software for research and engineering simulation and design
  - Enhancing code performance through porting to modern hardware (AVX, GPUs, Phi)
  - High-performance visualization and graphical user interfaces

Only supplier of commercial, high-performance EM and particle simulation tools for wide variety of applications

SIMULATIONS EMPOWERING YOUR INNOVATIONS
VSim: Cutting edge physics and computer science for modeling of interaction of matter with EM fields

- **Accurate**: Utilizing conformal embedded boundaries
  - Superfast surface meshing
  - 2nd order accuracy for metals and dielectrics: more accurate than stairstep, faster than unstructured

- **Proven for Large-Scale Problems**
  - Designed for distributed memory parallelism
  - Efficient scaling results to improve simulation speed
  - Client-server and Cloud ready, supercomputer for large final design runs

- **Wide variety of particle interactions**: Ionization, collisions, secondary emission,…

- **Multiplatform**: from Windows to new supercomputing systems

- **CAD interfaces (STEP and GDS)**

- **FDTD suitable for large simulations**: (many wavelengths per size of the device) and having many wavelengths in one simulation

- **GUI and Python for simulation setup**
Origin of nuclear spin

- Where does nucleon spin come from?
  - ~20% from constituent quarks
  - What about the rest? Gluons?

- Question being studied at RHIC by colliding spin-polarized protons
  - 60–65% polarization at 100 GeV/beam
  - 55% polarization at 250 GeV/beam

- Electron-ion colliders will provide much more precise probes
  - eRHIC at BNL, MEIC at Jlab

- Maintaining polarization of both beams is critical
Accurate spin tracking simulations are essential

• Interaction of colliding beams affects spin
  • Direct effect: EM fields from proton beam alters electron spin
  • Indirect effect: EM fields from one beam alter the other’s orbit, changing spin precession
  • Already observed in e-p collisions at much lower intensities than eRHIC
  • Understanding and mitigating these effects is critical

• Additional effects:
  • Magnet fringe fields
  • Variations in machine optics
Existing spin-tracking capabilities

- State-of-the-art spin tracking code: gpuSpinTrack
  - Grown out of several previous codes, with additional capabilities
  - Orbit tracking from TEAPOT
  - Spin tracking from SPINK
- Full nonlinear orbital motion; full 3D spin motion
- Sensitive to spin-orbit resonances
- Accelerated for GPU
  - Particle tracking is “embarrassingly parallel”
  - Particles are independent (absent space charge and other collective effects)
  - Experience the same computational process
The particle-in-cell (PIC) method

- Beam-beam interactions require more detailed method
- Fully self-consistent modeling of fields and particles
- Using high-performance VSim code

\[ \frac{d\mathbf{u}}{dt} = \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \]
\[ \frac{d\mathbf{x}}{dt} = \mathbf{v} \]

- Interpolate fields to particle positions
  \[ \mathbf{E}_{i,j,k} \rightarrow \mathbf{E}(\mathbf{x}) \]
  \[ \mathbf{B}_{i,j,k} \rightarrow \mathbf{B}(\mathbf{x}) \]

- Advance fields
  \[ \frac{\partial\mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \frac{\mathbf{J}}{\varepsilon_0} \]
  \[ \frac{\partial\mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \]

- Deposit current to grid
  \[ \mathbf{x}, \mathbf{v} \rightarrow \mathbf{J}_{i,j,k} \]
Spin tracking work in Phase II

- New polarized particle species: electrons and positrons
- (Incoherent) synchrotron radiation, including quantum fluctuation effects
- New element type: combined function sector bend (CFSB)
- Using GPU-accelerated random number generation library for modeling of stochastic effects/processes
- Extensive benchmarking and quality assurance work
- Updates to user interface and documentation
Combined Function Sector Bend (CFSB)

- Needed for modeling feed-down multipole field content in bends (due, e.g., to magnet offsets)
- Used in a new RHIC lattice design that aims to minimize polarization loss on the acceleration ramp
- Can also be used in AGS simulations
- Developed a new CUDA kernel and C wrappers, updated the user interface
CFSB element: the Hamiltonian

- Phase space trajectory integration is based on the Hamiltonian in a curvilinear coordinate system written in terms of offset variables and (scaled) conjugate momenta, with $s$ as independent time-like variable:

$$H = -(1 + X/\rho_0)\sqrt{1 + \frac{2}{\beta_0} P_T + P_T^2 - P_X^2 - P_Y^2} - \frac{q}{\rho_0} (1 + X/\rho_0) A_\phi(X,Y) + \frac{1}{\beta_0} P_T$$

- Longitudinal component of the vector potential accurate to 3rd order:

$$(\rho_0 + X) A_\phi = -\frac{B_0}{2} \rho_0^2 - B_0 \rho_0 X - \frac{B_0}{2} X^2 - \frac{b_2 \rho_0}{2} (X^2 - Y^2) + \frac{a_2 \rho_0}{2} (2XY)$$

$$- \frac{b_2}{8} X (X^2 + Y^2) + \frac{a_2}{8} Y (X^2 + Y^2) - \frac{b_3 \rho_0}{3} (X^3 - 3XY^2) + \frac{a_3 \rho_0}{3} (3X^2Y - Y^3)$$

$$+ \frac{b_2}{64 \rho_0} (X^2 + Y^2)^2 - \left( \frac{b_3}{12} - \frac{b_2}{32 \rho_0} \right) (X^4 - Y^4) + \left( \frac{a_3}{6} - \frac{a_2}{16 \rho_0} \right) XY (X^2 + Y^2)$$

$$- \frac{b_4 \rho_0}{4} (X^4 - 6X^2Y^2 + Y^4) + \frac{a_4 \rho_0}{4} (4X^3Y - 4XY^3)$$

where $b_n$ and $a_n$ describe the normal and skew quad, sextupole and octupole ($n = 2, 3, \text{ and } 4$) components of the CFSB field
CFSB: phase space trajectories

- Implemented a split-operator symplectic integrator by separating the Hamiltonian into two parts, $H = H_B + H_K$, $H_B$ corresponding to the “pure” bend and $H_K$ to the “kick” due to the quadrupole and higher-order content of the field.
- Both $H_B$ and $H_K$ admit of an exact solution for the map.
- Bend and kick maps are combined in a time-reversal symmetric manner using the 2nd order accurate symplectic approximation:

$$e^{s:H} \approx e^{(s/2):H_B} e^{s:H_K} e^{(s/2):H_B}$$
For evolving the spin expectation-value variables we use a discretization of the Thomas-BMT equation:

$$\frac{d\vec{S}}{ds} = \vec{\Omega} \times \vec{S}$$

$$\vec{\Omega} = -\frac{1 + X/\rho_0}{(p_0/q)\sqrt{1 + \frac{2}{\beta_0} P_T + P_X^2 + P_Y^2}} \left[ (1 + G\gamma) \vec{B} - G(\gamma - 1)(\hat{u} \cdot \vec{B}) \hat{u} \right] + \frac{\hat{y}}{\rho_0}$$

Spin precession vector of a given particle is stored and manipulated in the quaternion representation.

Romberg integration used to improve accuracy of spin tracking.

The full splitting for a single slice of CFSB is given by (with “spin kick” $S$)

$$(1/2)S \cdot B \cdot K \cdot B \cdot (1/2)S$$

Thoroughly tested and benchmarked.
New capability for tracking $e^-$ and $e^+$

- Enabled trajectory and spin integration in gpuSpinTrack for electrons and positrons
- Required code infrastructure work: Codes from which gpuSpinTrack evolved were designed to model polarized proton beams at RHIC, assumption of protons (charge polarity, rest mass, anomalous magnetic moment) was hard-coded in many places
- Previously implemented element kernels, spin tracking “machinery”, and user interface updated for the new species
- Presently can track $e^-$ and $e^+$ through drifts, sector and rectangular bends, multipoles, CFSBs
- New capability was extensively and rigorously tested
- Necessary for modeling the synchrotron radiation in bend magnets
Developed a new capability for modeling the synchrotron radiation

- Implemented a new element type SRSB, a sector bend with (incoherent) synchrotron radiation, including the quantum fluctuation effect
- Assume instantaneous photon emission in the direction of the electron (or positron) motion
- We model the photon emission as a compound Poisson process with the mean number of photons emitted per unit time

\[
< N > = \int_{0}^{\infty} n(u)du = \frac{5\alpha c\gamma}{2\sqrt{3}\rho} \approx 0.010533 c \frac{\gamma}{\rho}
\]

- Distribution in energy \( u \) given by

\[
n(u) = \frac{\sqrt{3}}{2} \frac{\alpha c\gamma}{\rho} \frac{1}{u_c} \int_{u/u_c}^{\infty} K_{5/3}(y)dy
\]

- where the critical photon energy \( u_c \) is

\[
u_c = h\omega_c = \frac{3hc\gamma}{2\rho}
\]
• Phase space orbital motion and spin rotation are piecewise continuous (between successive photon emissions), but generally speaking discontinuous in traversing the bend due to recoil
• Romberg integration apparatus for spin integration used in other element types cannot be used in SRSB
• Developed and implemented an in-kernel spin tracking approach that can also be used later in other element types with SR (RBend, CFSB)
• SRSB uses an optimized algorithm that only requires 2 RNG calls and a small arithmetic operation count per photon emission
• For efficient parallel generation of uncorrelated random number sequences on device we use pseudorandom number generators from the NVIDIA cuRAND random number generation library with once-per-simulation initialization of the RNG state
• User interface option to choose between a random or user-specified (for reproducibility) RNG seed
Code coupling: consistent beam loading

- For beam-beam interactions, need to transfer particles between gpuSpinTrack and VSim each turn
- Consistent initialization of beam self-fields is necessary when loading particles into PIC simulation
- Otherwise, unphysical transition radiation can occur
- Developing ability to initialize fields as particles are loaded at each step
- Allows beams longer than simulation domain
PIC modeling of particles with spin

- Quantum density matrices added as particle internal variables
- Density matrix evolved according to
  \[
  \frac{d\rho}{dt} = \mathcal{L}[\rho]
  \]
- \(\mathcal{L}\) is a “Lindblad operator” describing the system
- Implemented for Thomas-BMT equation
- Self-consistent spin polarization current added back to field update using dipole moment
  \[
  \mathbf{d} = \text{Tr}(\hat{\rho}\mathbf{d})
  \]
Dual-use application: Active laser media

- Self-consistent modeling of quantum particles also applicable to laser gain media
- Density matrix represents states in relevant metastable transition
- Additional terms in Lindblad operator for homogeneous broadening, transitions to/from additional states in three- and four-level systems
- Implemented Maxwell-Bloch operator
Full GPU capability

- GPUs can provide orders of magnitude more floating-point operations than CPUs
- But requires new programming paradigms
  - SIMD instructions: Must execute the same operations on different data elements
  - Regular memory access patterns required
- Great for particle tracking
- PIC much more difficult, since particles move
- Getting full PIC capabilities on GPU in VSim under DARPA contract
  - Including collisions, materials,…
- Potential for full spin tracking + beam-beam simulation on GPU