TECH-X
SIMULATIONS EMPOWERING YOUR INNOVATIONS

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

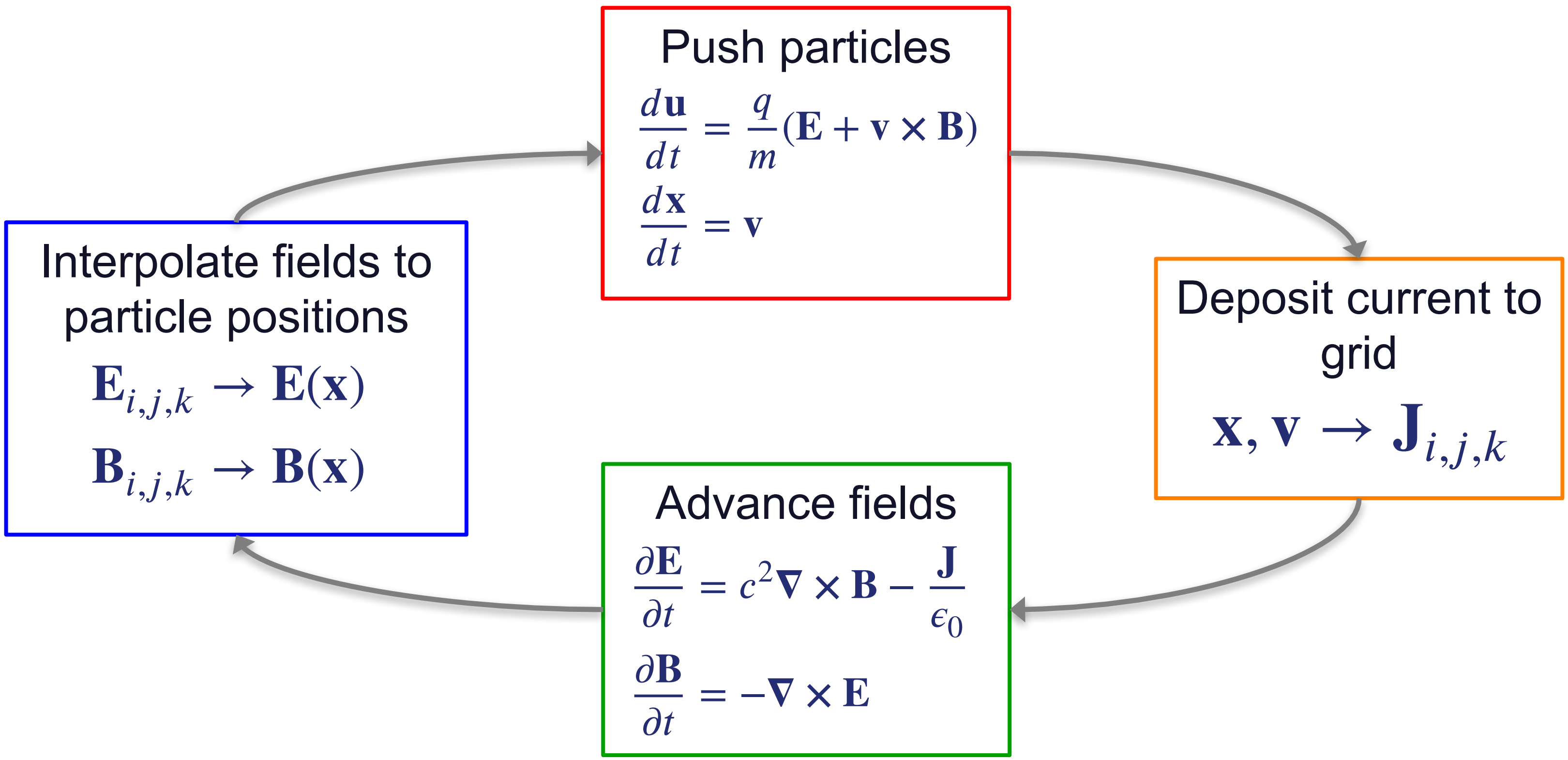
- Interaction of colliding beams affects spin
  - Direct effect: EM fields from proton beam alters electron spin
  - Indirect effect: EM fields from one beam alter the other's orbit, changing spin precession
  - Already observed in e-p collisions at much lower intensities than eRHIC
  - Understanding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



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:

$$H = -(1 + X/\rho_0)\sqrt{1 + \frac{2}{\beta_0}P_T + P_T^2 - P_X^2 - P_Y^2} - \frac{q}{p_0}(1 + X/\rho_0)A_\phi(X,Y) + \frac{1}{\beta_0}P_T$$

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

$$\begin{aligned}(\rho_0 + X)A_\phi = &-\frac{B_0}{2}\rho_0^2 - B_0\rho_0 X - \frac{B_0}{2}X^2 - \frac{b_2\rho_0}{2}(X^2 - Y^2) + \frac{a_2\rho_0}{2}(2XY) \\ &-\frac{b_2}{8}X(X^2+Y^2) + \frac{a_2}{8}Y(X^2+Y^2) - \frac{b_3\rho_0}{3}(X^3 - 3XY^2) + \frac{a_3\rho_0}{3}(3X^2Y - Y^3) \\ &+\frac{b_2}{64\rho_0}(X^2+Y^2)^2 - \left(\frac{b_3}{12} - \frac{b_2}{32\rho_0}\right)(X^4 - Y^4) + \left(\frac{a_3}{6} - \frac{a_2}{16\rho_0}\right)XY(X^2+Y^2) \\ &-\frac{b_4\rho_0}{4}(X^4 - 6X^2Y^2 + Y^4) + \frac{a_4\rho_0}{4}(4X^3Y - 4XY^3)\end{aligned}$$

where b_n and a_n describe the normal and skew quad, sextupole and octupole (n = 2, 3, 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:

$$e^{s:H:} \approx e^{(s/2):H_B:} e^{s:H_K:} e^{(s/2):H_B:}$$

CFSB: spin integration

- For evolving the spin expectation-value variables we use a discretization of the Thomas-BMT equation

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

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

- 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

$$< N > = \int_0^\infty n(u)du = \frac{5\alpha c\gamma}{2\sqrt{3}\rho} \approx .010533c\frac{\gamma}{\rho}$$

- 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

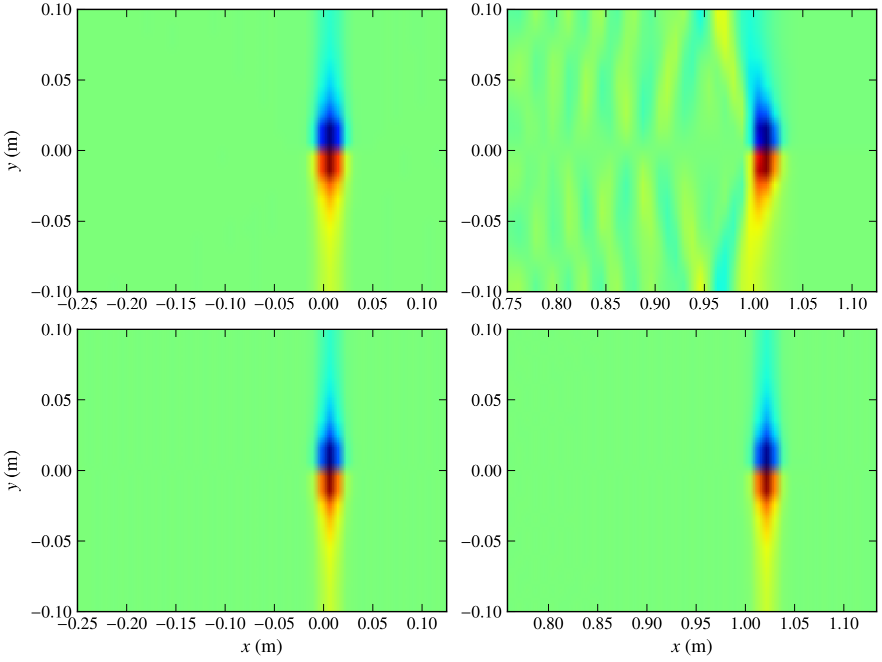
$$u_c = \hbar\omega_c = 3\hbar c\gamma/2\rho$$

Synchrotron radiation bend element

- 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

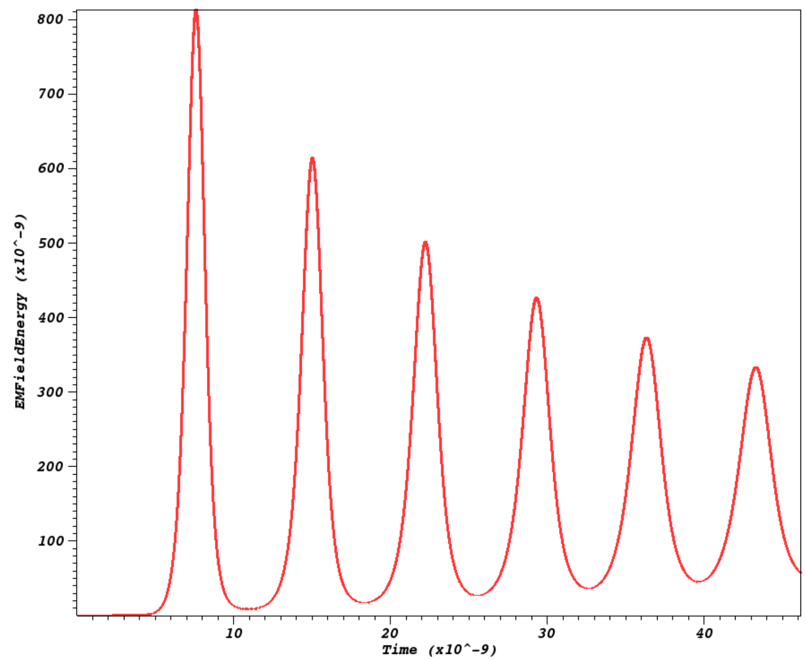
- Quantum density matrices added as particle internal variables
- Density matrix evolved according to

$$\frac{d\rho}{dt} = \mathcal{L}[\rho]$$

- $\mathcal{L}$ 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 $\mathbf{d} = \mathrm{Tr}(\hat{\rho}\hat{\mathbf{d}})$

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