Multi-Scale Modeling for Beam-Beam Depolarization

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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

Tech-X philosophy and success

- The Tech-X plan is to develop computations for DOE needs, continuously converting IP to commercial grade software with a significant addressable market.
- Commercial revenue for 1H 2018 exceeded all of 2017
- Tech-X has spun out products to the oil exploration, plasma processing, and defense industries
- Computational workshops in US and EU. TWSS in 2 weeks will have participants from DOE labs including JLab, LANL, and industry including HPE, Schlumberger
- Perform service to community: USPAS, APS DPB, IEEE, AAC
- Tech-X software has been purchased by many DOE labs including FNAL, LANL, SLAC.
- Tech-X is a subcontractor for DOE labs, including Sandia.
- Tech-X software is in use by multiple EU labs (members of ELI, TU-Darmstadt) as well as labs in China and Japan.

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

Push particles

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

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

Deposit current to grid

$$\mathbf{x}, \mathbf{v} \rightarrow \mathbf{J}_{i,j,k}$$

Advance fields

$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \frac{\mathbf{J}}{\epsilon_0}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

Interpolate fields to particle positions

$$\mathbf{E}_{i,j,k} \rightarrow \mathbf{E}(\mathbf{x})$$

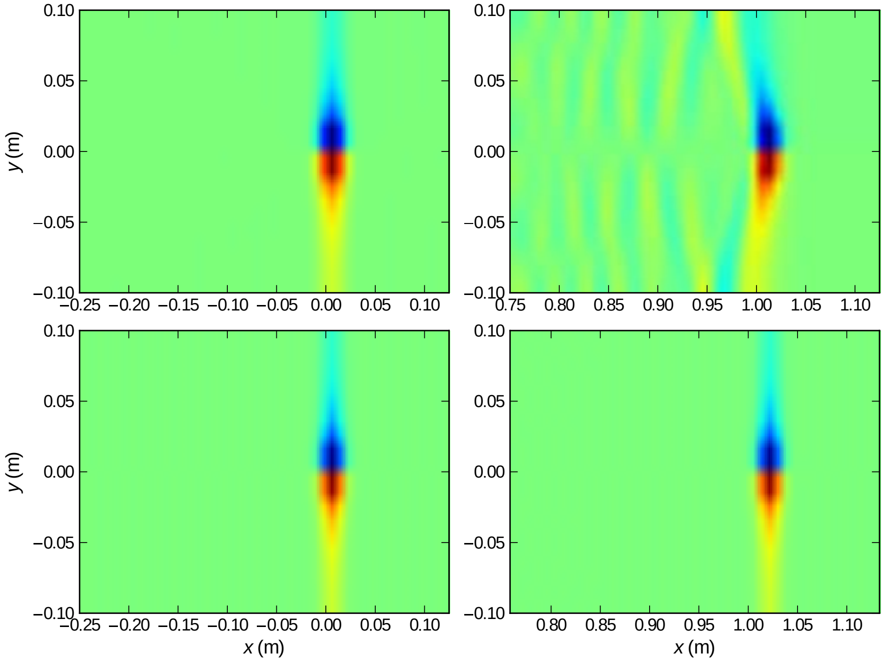
$$\mathbf{B}_{i,j,k} \rightarrow \mathbf{B}(\mathbf{x})$$

Spin tracking work in Phase II

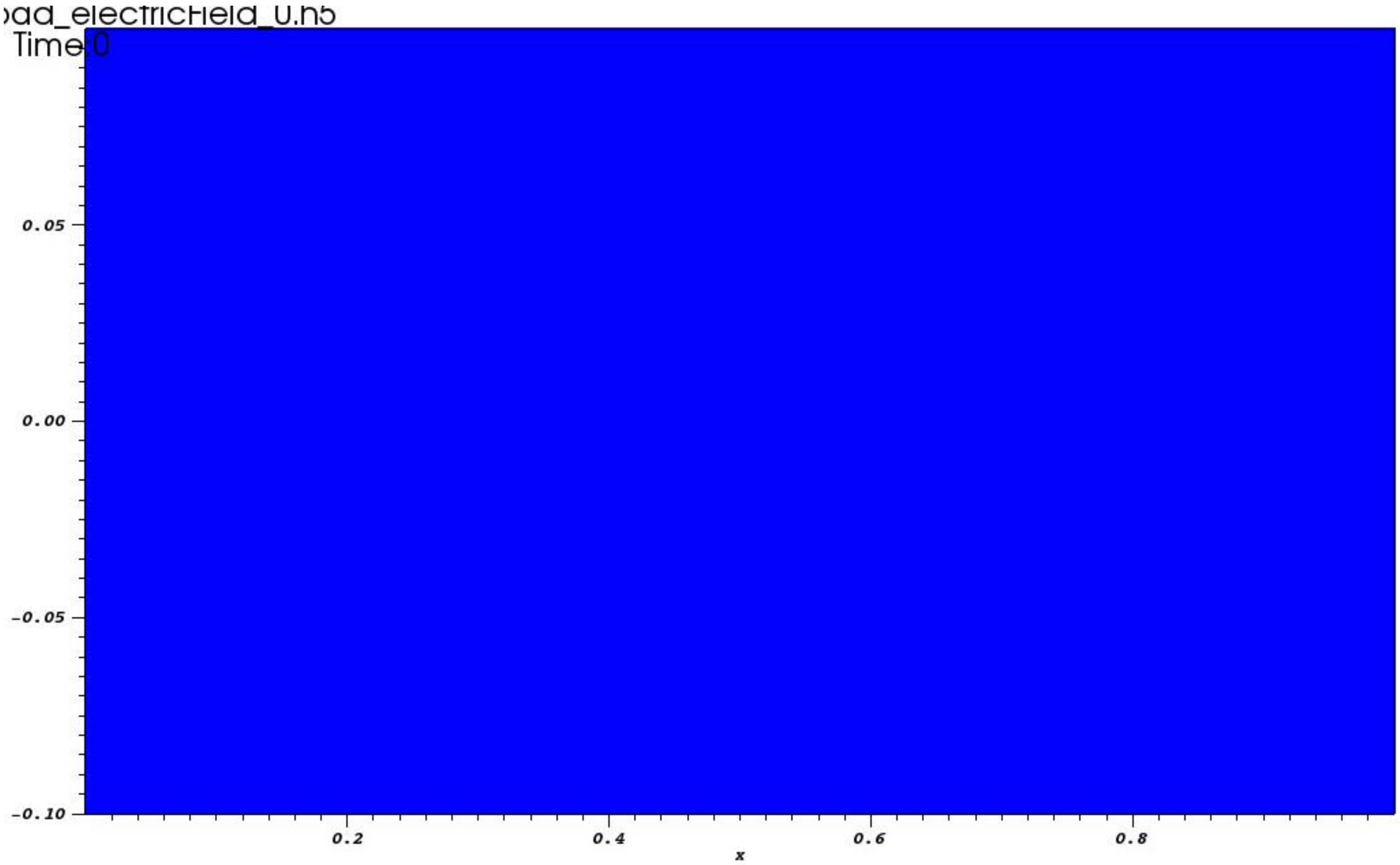
- New polarized particle species: electrons and positrons
- (Incoherent) synchrotron radiation, including quantum fluctuation effects
- New element type: combined function sector bend (CFSB)
- Using GPU-accelerated random number generation library for modeling of stochastic effects/processes
- Extensive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

Code coupling: consistent beam initialization

- 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



Consistent beam initialization example



PIC modeling of particles with spin

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

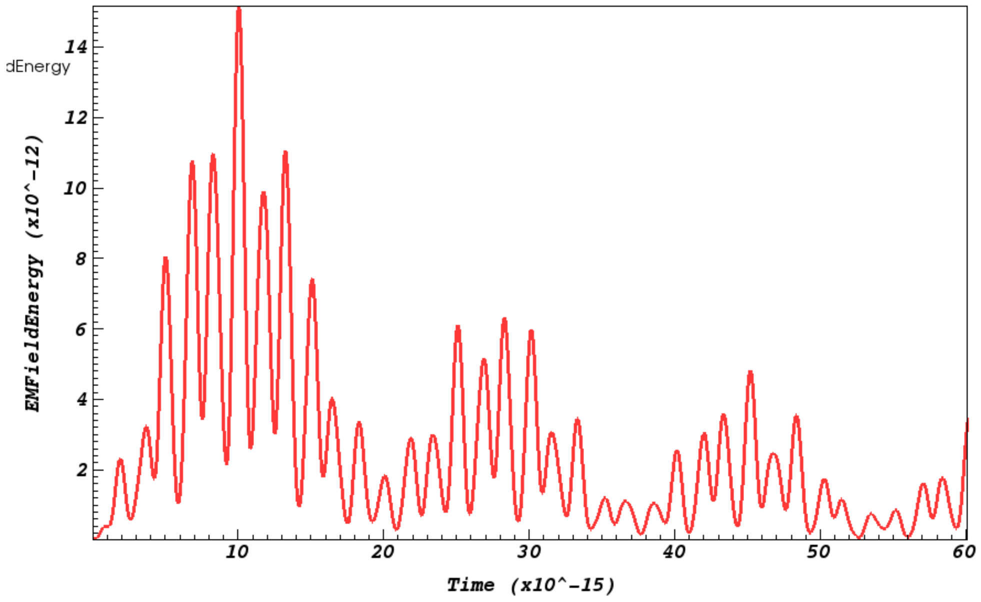
$$\frac{d\rho}{dt} = \mathcal{L}[\rho]$$

- $\mathcal{L}$ 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

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

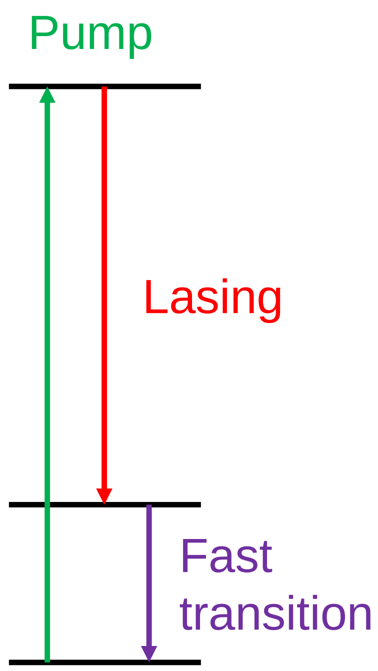
Dual-use application: Active laser media

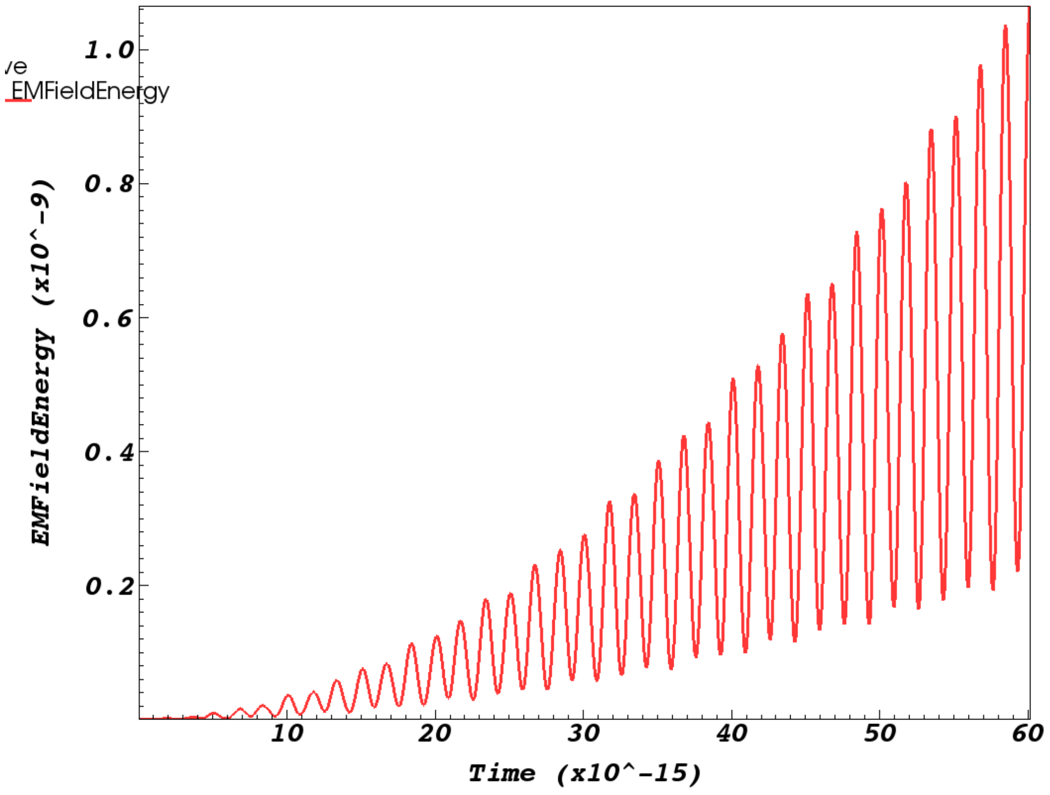
- Self-consistent modeling of quantum particles also applicable to laser gain media
- Density matrix represents states in relevant metastable transition
- Implemented Maxwell-Bloch operator
- 2-state systems are represented
- PIC features to allow Doppler broadening



Three (and four) level systems

- Real lasers have at least 3 levels
- But additional states have fast interactions, so can be handled through decays
- Additional terms in Lindblad operator for decaying states; also homogeneous broadening





Full GPU capability

- GPUs can provide orders of magnitude more floating-point operations than CPUs
- But requires new programming paradigms
- Great for particle tracking
- PIC much more difficult, since particles move
- Getting full PIC capabilities on GPU in VSim under DARPA contract
- GPU EM capabilities now competitive with state of the art
- Potential for full spin tracking + beam-beam simulation on GPU
    - Or laser modeling