
# Multi-Scale Modeling for Beam-Beam Depolarization

Grant number: DE-SC0013187
PM: Manouchehr Farkhondeh

Ilya Zilberter, Benjamin Cowan
*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

# 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.
- Over $1M commercial revenue for FY 2018
- Tech-X has spun out products to the oil exploration, plasma processing, and defense industries
- 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

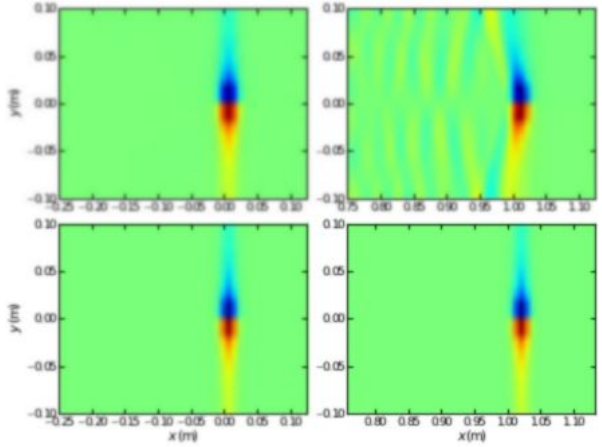
- Interaction of colliding beams affects spin
  - Direct effect: EM fields from proton beam alters electron spin
  - Indirect effect: EM fields from one beam alter the other's orbit, changing spin precession
  - Already observed in e-p collisions at much lower intensities than eRHIC
  - Understanding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

# Status of project

- In last year, ending April 2020
- Implemented infrastructure for tracking / PIC code coupling to simulate space charge, other effects in future efforts
- Goal is to leave BNL, broader DOE/NP community with quality spin tracking code
  - Thoroughly tested and benchmarked
  - Easy to build and run

# Phase II work towards PIC/Tracking integration

- **Initialization of self-consistent fields as particles are loaded into VSim**
  - Allows simulation of bunches larger than computational domain



- **Implementation of quantum states to particles**
  - Density matrix evolved using Lindblad operator $\frac{d\rho}{dt} = \mathcal{L}[\rho]$
  - Applicable to two-level laser modeling

# 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

# 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
- **Build system cleanup**
- **In progress**: Detailed eRHIC simulation

# Emphasis on DoE Priorities

- **Ensure accuracy and usability** of gpuSpinTrack for eRHIC design
  - Needed to benchmark against, eg, Zgoubi
- **Eliminate unused features and libraries**
  - ~50% reduction in code base
- **Ensure code works out of the box**
  - Tech-X “bilder” system installs dependencies, but is not widely used outside of Tech-X and difficult for outside users to develop
  - Requires pre-installed CUDA and specific gcc compiler versions
  - Ideally, move to SPACK or similar

# Moving to Spack build system

- http://spack.io
- Spack is an open-source build system for supercomputers, Linux, and macOS
- Can customize all package dependencies on install
  - Eg, to install hdf5 and link it with specific versions of openmpi and hwloc:
  - $ spack install hdf5@1.10.1 %gcc@4.7.3 ^openmpi+cuda ^hwloc+gl
- Packages with different dependencies can coexist, installation can be local to user. Can bootstrap by installing required C++ and CUDA compilers
- Preliminary Spack package for gpuSpinTrack has been written and tested
- Development tasks:
  - Create infrastructure for local installation of gpuSpinTrack
  - Ensure that CUDA version is appropriate for installed NVIDIA drivers

# Progress of eRHIC Simulation

- 4096 element SXF lattice developed for Rapid Cycling Synchrotron
- Necessary elements ported to GPU
- Some issues tracking high energy electrons
  - RF cavity at full power causes particle loss
  - Stability / sensitivity to high emittance
- Developing battery of eRHIC-specific unit tests
- Benchmarking against Zgoubi
- Removing hard-coded, RHIC-specific parameters

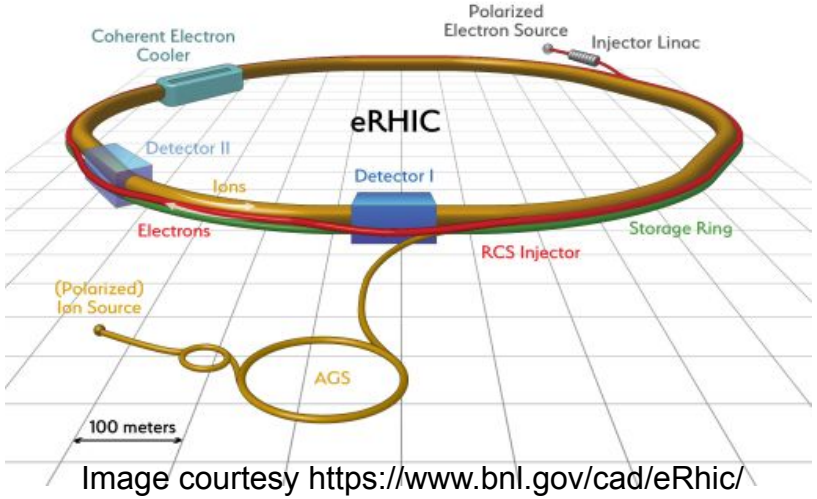
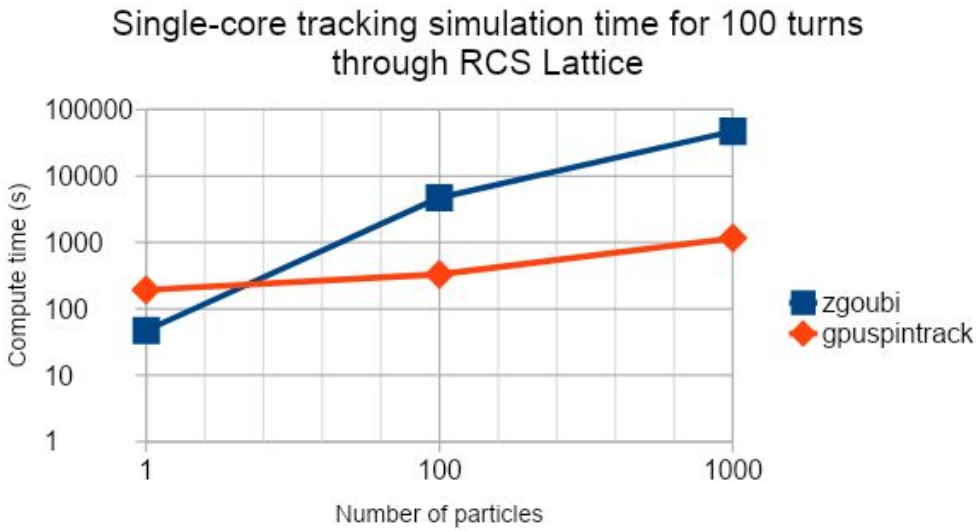


Image courtesy https://www.bnl.gov/cad/eRhic/



# Summary

- **Implemented code coupling infrastructure** to allow simulation of spin-polarized bunch dynamics in VSim
- **Developed accurate, GPU-accelerated electron spin tracking code**
  - Added CFSB, synchrotron radiation
  - Simultaneous tracking of 1000s of particles on single card
- **Ongoing eRHIC simulation**
  - Final benchmarking and QC of gpuSpinTrack
  - Quality of life improvements before handoff to BNL / DoE