gpu-Accelerated Spin Tracking

Tech-X
a computational sciences company

Project Motivation & Initial Accomplishments
DOE need; gpuSpinTrack; year 1 accomplishments

Production Phase – Improvements to Usability
spin analysis; build system; interface; documentation; publications

Impact & Future
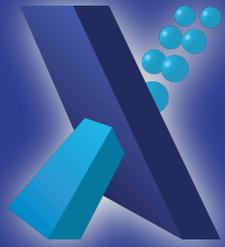gpuSpinTrack at BNL; future work; benefits to Tech-X

SBIR/STTR Exchange Meeting
6–7 November 2013, Gaithersburg, MD

PI: Dan T. Abell
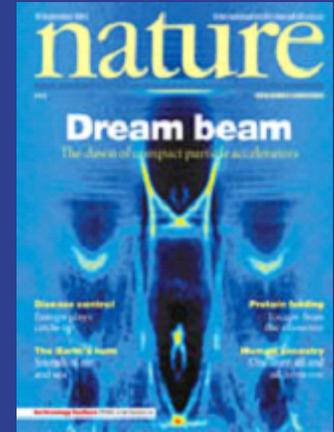Tech-X: Dominic Meiser (physics, GPU), Jacob King (GUI)
BNL Collaborators: Mei Bai, Vahid Ranjbar

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# Tech-X Has a Long History of Addressing DOE Computational Needs

Tech-X has extensive experience with parallel computing, now in both MPI and GPU settings and on a range of platforms, from laptop to LCF.

Tech-X uses its computational expertise for scientific discovery.

Tech-X research covers a broad range: from fusion science to photonics to accelerator physics – including studies of electron cooling and our work on gpuElegant.

Tech-X has been one of the few companies to be included in and to have led SciDAC missions. These efforts include both ComPASS and FACETS.
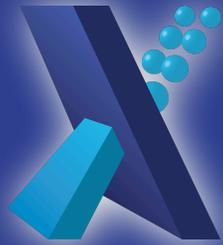
High-quality Spin-polarized Beams Enable Efficient RHIC Operation

The goal of the RHIC spin program is to improve our understanding of the origin of nuclear spin.
This goal is central to nuclear science:

> "*A fundamental challenge for modern nuclear physics is to understand the structure and interactions of nucleons ….*
> *The solution of the spin puzzle … remains incomplete.*"
> Source: *The Frontiers of Nuclear Science*, the Nuclear Science Advisory Committee's December 2007 Long Range Plan

Higher polarization yields better data,
because statistical uncertainties $\sim 1/Polarization^2$.
This means better data for a fixed cost.

Plenty of room for improvement: $P_{source} \approx 70\text{--}80\%$, $P_{final} \approx 50\text{--}55\%$
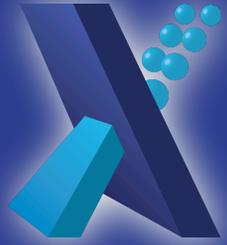
gpuSpinTrack: A Tool for Optimising Beam Polarisation

We are making gpuSpinTrack into a tool that helps scientists optimise beam polarisation more quickly and less expensively than using machine time.

Speed and Usability are critical. We therefore
- build on prior efforts of DOE scientists;
- accelerate spin tracking by porting code to gpus;
- add a build system to make code easier to develop and install;
- develop documentation to make code easier to use;
- implement better algorithms to make code more accurate.
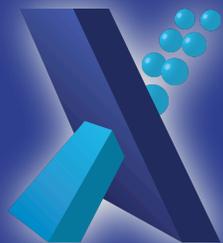
# We Achieved Major Algorithmic Improvements in Year I

Separating the original monolithic gpu kernel into kernels for individual elements simplifies the logic and testing of each kernel, and also our implementation of dynamic lattices.

Implemented improved orbital tracking, which automatically improves spin tracking.

Simple "algorithmic add-on" improves spin convergence by orders of magnitude!

Initial improvements to build system simplify development.

DKD (n_b=8)

DKD (n_b=4, re-tuned)

BK-MK (no Romberg)

BK-MK (n_b=4)
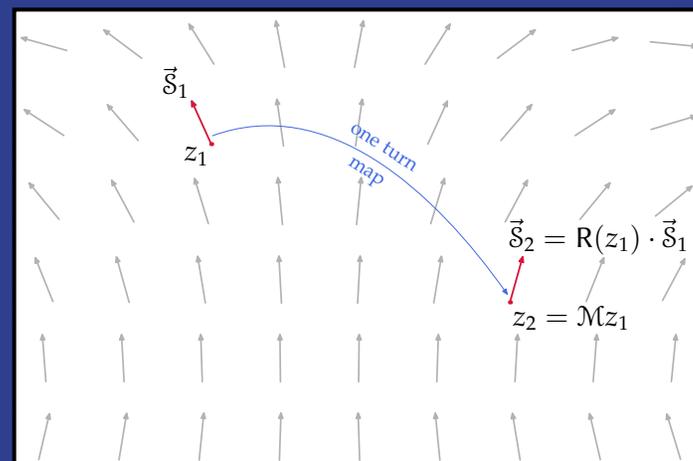
$|S(t)-S^{(ref)}|$

t
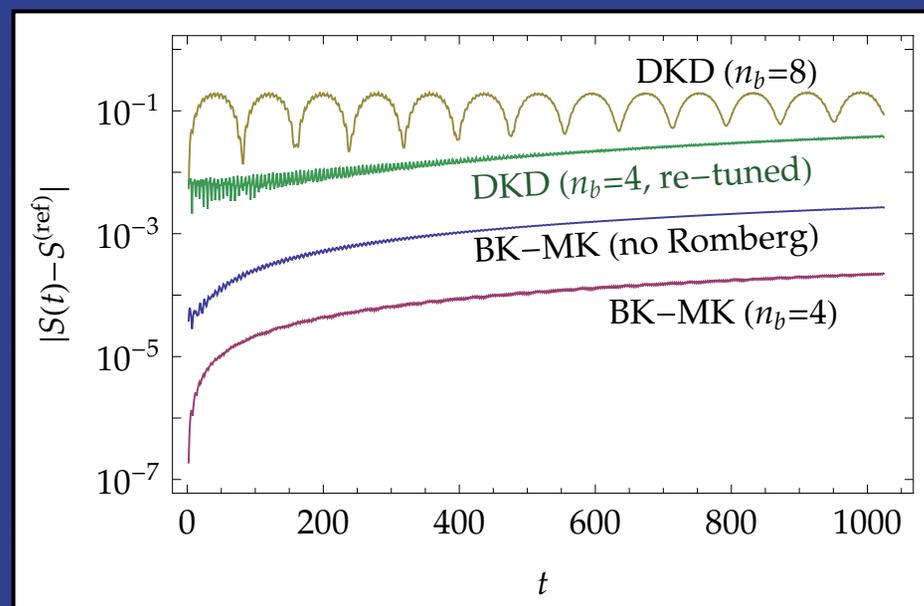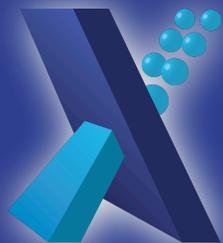
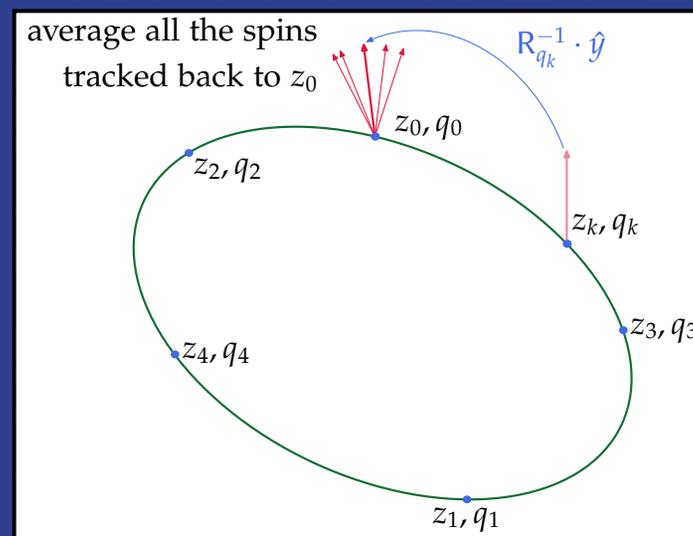# gpuSpinTrack Includes an Essential Tool for Optimising Spin Polarisation

The Invariant Spin Field (ISF) places an important upper limit on the maximum attainable polarisation.

Optimising spin polarisation requires a knowledge of the ISF at a range of optical settings for a given lattice.
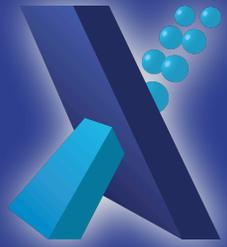
gpuSpinTrack now uses the *best known* algorithm for computing the ISF: on a NERSC gpu node, an ISF computation for RHIC at 10^4 phase-space locations using 10^3 turns takes about an hour.

$\vec{S}_1$

z_1

one turn map

$\vec{S}_2 = R(z_1) \cdot \vec{S}_1$

$z_2 = \mathcal{M} z_1$

Schematic ISF

average all the spins tracked back to z_0

$R_{q_k}^{-1} \cdot \hat{y}$

z_0, q_0

z_2, q_2

z_k, q_k

z_3, q_3

z_4, q_4

z_1, q_1

Computing the ISF

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New Build System Makes gpuSpinTrack Useful on a Variety of Platforms

Tech-X is a leader in cross-platform build systems for scientific software that has complex dependency chains.

gpuSpinTrack now uses `Bilder`, an open-source build system pioneered by Tech-X.

At the beginning of Phase II, gpuSpinTrack was not portable, and it had no real build system. Changes to the code base required rebuilding *everything*.

Installing gpuSpinTrack is now (almost) "turn-key".

Initial install *from scratch* takes ~one hour. Rebuilds during development require at most a few minutes.

gpuSpinTrack now runs on laptops, desktops, and NERSC's gpu cluster, Dirac.
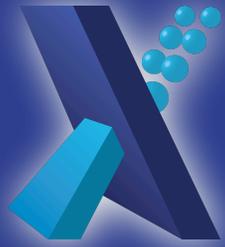
A Simpler Interface Makes gpuSpinTrack Easier to Use

Input files used to have overlapping responsibilities. We have made these as independent as possible.
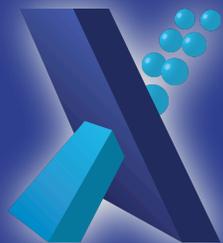
The `.in` file no longer requires a fixed, rigid format. (It actually *reads* parameter names!)

These changes will also simplify our implementation of the dynamic lattice capability.

`.sxf` file describes the lattice – elements, strengths, locations

`.apdf` file describes the integrators

`.in` file describes parameters for a given run of gpuST

Documentation Makes gpuSpinTrack Easier to Learn

The documentation now describes installation, input files, and parameters for all integrators. It also suggests best practices for running gpuSpinTrack.

We continue to update this document as we develop the code.

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gpuSpinTrack: a manual
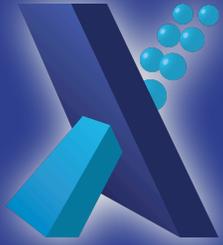
Dominic Meiser
Dan T. Abell

4 November 2013 at 12.45

Abstract

This document describes how to install and run gpuSpinTrack. These instructions discuss specifically how to run gpuSpinTrack on the NERSC GPU cluster DIRAC. Installing and running on other machines—including laptops with GPU cards—will be similar. A companion file, gpuSpinTrack-template.tgz, contains a sample workspace with all required input files, as well as sample shell scripts for queueing and running gpuSpinTrack.

Contents

# gpuSpinTrack Accomplishments Recognised through Publications

"Accurate and efficient spin integration for particle accelerators", D.T. Abell, D. Meiser, and D.P. Barber, submitted to PRST-AB and currently undergoing minor revisions in response to referees.

This reports on an extensive study of the errors associated with our new approach to spin tracking.

"GPU-accelerated spin dynamics and analysis for RHIC", D.T. Abell, D. Meiser, M. Bai, V.H. Ranjbar, and D.P. Barber, IPAC'13 Proceedings.

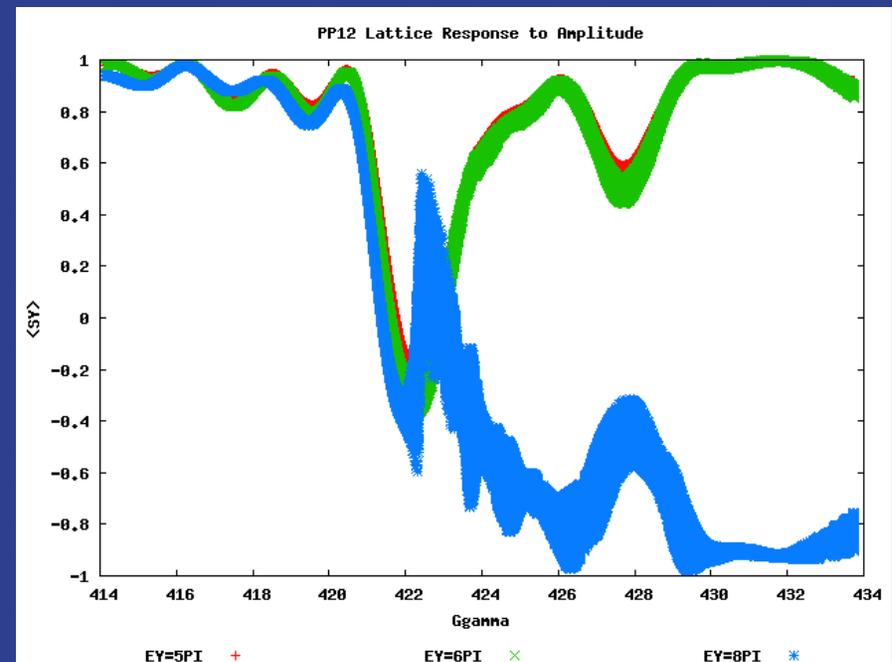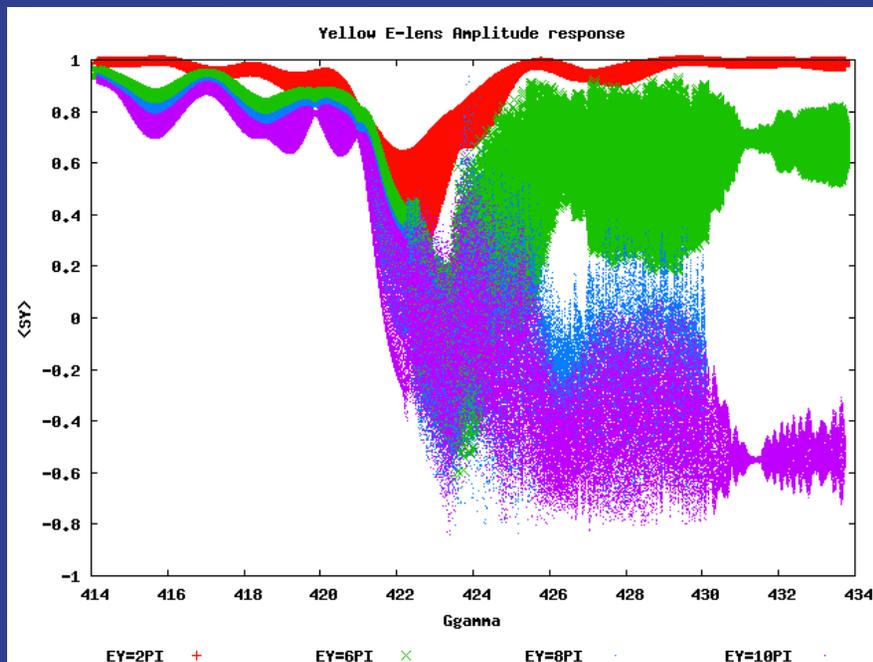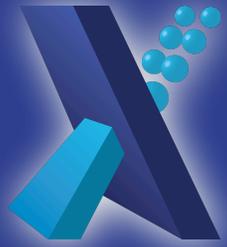Posters presented at IPAC'12 and ICAP'12.
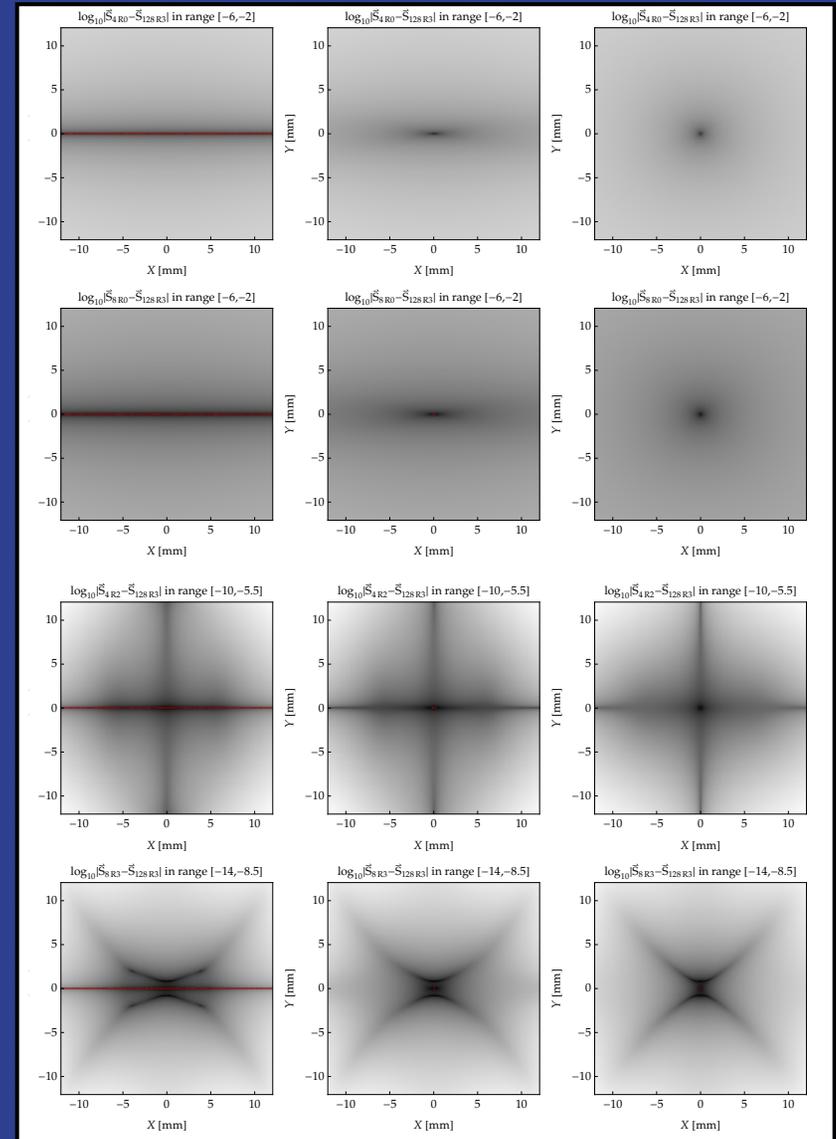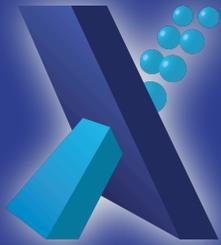
gpuSpinTrack Contributes to RHIC Run Decisions at BNL

A decision made during the last RHIC run to return to using the standard lattice was based, in part, on gpuSpinTrack results.

Our collaborators at BNL are currently using gpuSpinTrack to analyse data from the most recent polarised beam runs at RHIC.
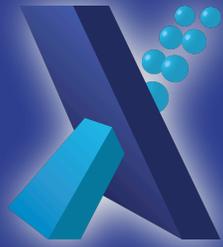
We Are On-track for Finishing Within the Period of Extension

Remaining work:

- implement dynamically changing lattice

- add a few more elements: more realistic snake; elements for EDM lattices

- finish documentation

- complete the Graphical User Interface (GUI)

For Commercialisation, Tech-X Benefits From Its Expertise

Spin tracking is not inherently commercializable.

Our extensive HPC experience and our successful collaborations with DOE labs make us a strong candidate for contributing to an NP-SciDAC.

Our expertise in other areas has proven abilility to attract contract funds from DOE labs: coherent electron cooling.

Our expertise in gpu programming has led to numerous contracts and grants in other areas, mostly in applied math: gpuPETSc is one example.

The work on this project brings us closer to modeling active laser media.