Accurate Spin Tracking on Modern Computer Architectures for Electron-Ion Colliders

Dan T. Abell, Paul Moeller, Boaz Nash, Mike Keilman, Rob Nagler — RadiaSoft LLC, Boulder, CO François Méot, Vahid Ranjbar — BNL C-AD, Upton, NY

Fanglei Lin, Vasiliy Morozov — JLab, Newport News, VA

Damian Rouson — Sourcery Institute, Oakland, CA Izaak Beekman — Paratools, Inc, Eugene, OR

Supported by the US Department of Energy, Office of Science, Office of Nuclear Physics, including Award No. DE-SC0017181.

DOE/NP SBIR/STTR Exchange Meeting

Meeting 13–14 August 2020

Outline

RadiaSoft, Sirepo, and Jupyter server

Spin Dynamics: role in EIC and need for physics/software development

Overview of the Zgoubi code, and value for EIC

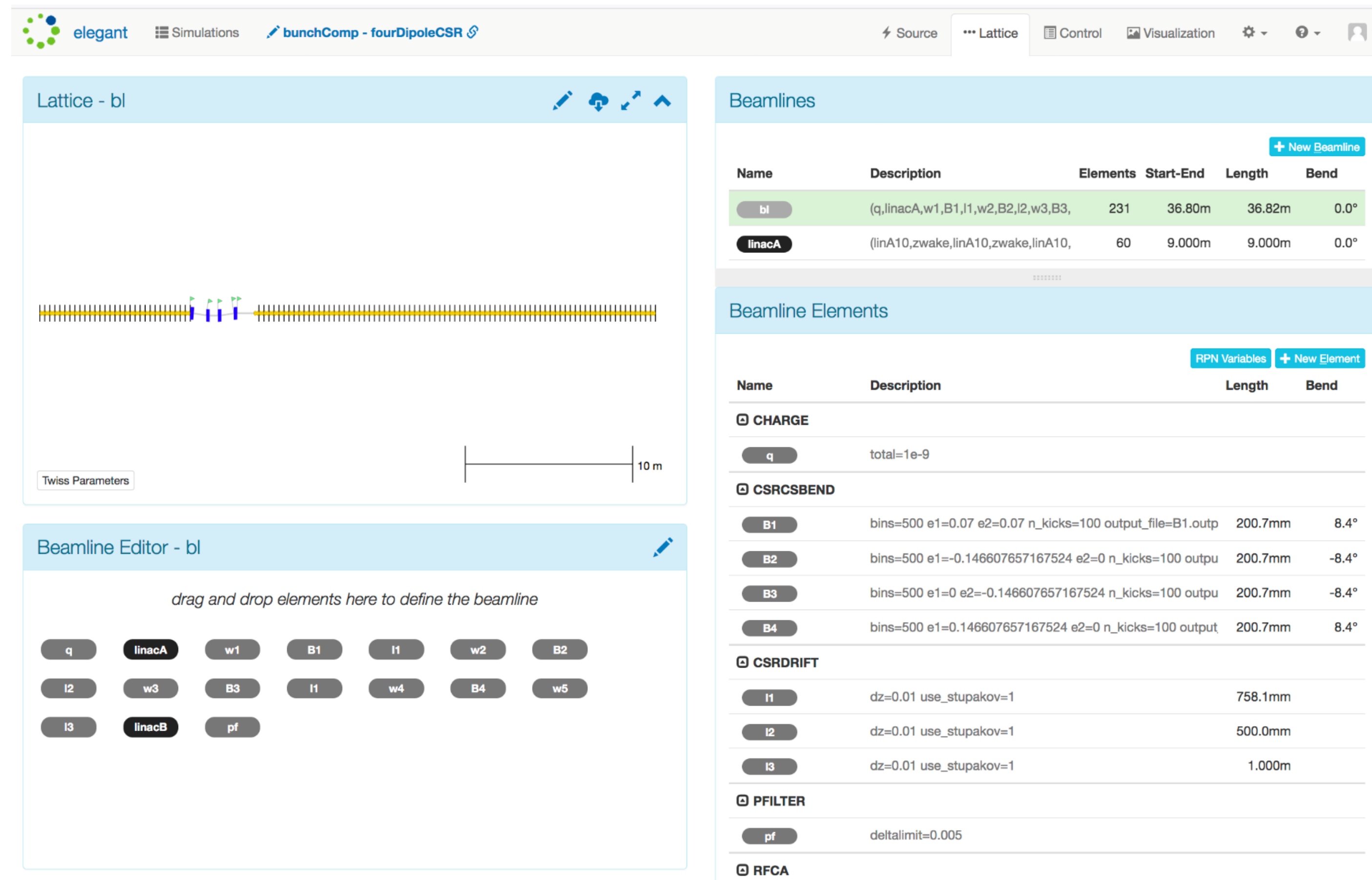
Accomplishments during this project

Summary

Sirepo is a free Scientific Gateway

Supported Codes

JSPEC – *e- cooling, IBS*
Zgoubi – *spin tracking*
MAD-X – *coming soon !!*
Elegant – *e- linacs & rings*
Synergia – *hadron rings*
Warp PBA – *plasma wakes*
Warp VND – *nanoelectronics*
SRW – *SR, X-ray optics*
Shadow – *ray tracing*

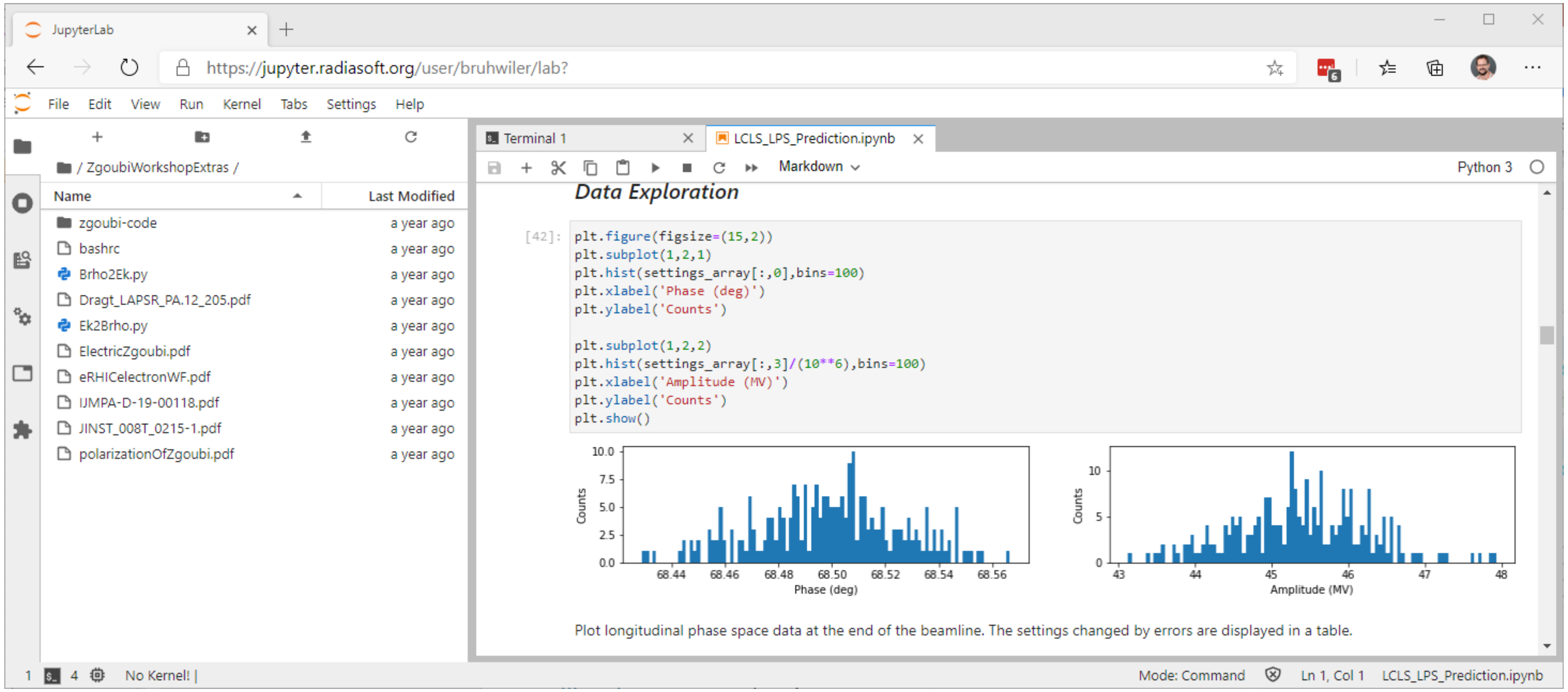


D.L. Bruhwiler *et al.*, “Knowledge Exchange Within the Particle Accelerator Community via Cloud Computing,” in *IPAC* (2019).

The power of Sirepo for users

Access from any browser: https://sirepo.com
Easy to use: nothing to install, build, or maintain
Instantaneous collaboration: share your work with a single link
Archive & save: resume work weeks or months later with zero start-up time
You're not locked in: export files for command-line execution

jupyter.radiasoft.org is also a free Scientific Gateway



Sirepo is a GUI – Jupyter notebooks provide an HPC sandbox

- *All Sirepo codes are pre-installed, together with standard ML tools*
- *Export files with a valid Python script from Sirepo → then run on Jupyter*
- *Work from the command line or from a notebook; use your own workflow*

Actively used by RadiaSoft & the community

- *like Sirepo, it is used in every session of the US Particle Accelerator School*

RadiaSoft Contributes to the Community

RadiaSoft scientists regularly volunteer to teach at the *US Particle Accelerator School.*

USPAS is routinely using Sirepo/elegant for the fundamentals class, and there were plans to use Sirepo/Zgoubi for a spin dynamics class this Summer (unfortunately canceled).

RadiaSoft's Jupyter server is also heavily used.

RadiaSoft is negotiating with USPAS to formalize this relationship with a commercial contract, to begin in a few months.

The MAD-X code will soon be available in Sirepo, with plans to use it during the 2021 Winter session.

USPAS Courses:

2018W: Simulation of Beam and Plasma Systems (D. Bruhwiler co-taught + Sirepo/elegant)
2018S: Classical Mechanics and Electromagnetism (S. Webb taught 2 days)
2019W: Fundamentals of Accelerator Physics and Technology (K. Ruisard used Sirepo/elegant)
2019S: Fundamentals of Accelerator Physics and Technology (N. Neveu used Sirepo/elegant)
*2020S: Spin Dynamics (F. Méot and D. Abell + Sirepo/Zgoubi) (canceled)
*2020S: Measurement and Control of Beams (M. Minty, F. Zimmerman, J. Edelen) (canceled)

RadiaSoft Student Scholars at USPAS:

River Robles, 2019

Jonathan Ang, 2018

Maria Simanovskaia, 2018

Other Education Users:

1st Korea University Accelerator School, 2018 (C. S. Park used Sirepo/Synergia)

NS3 Nuclear Science Summer School
(S. Lund used Sirepo/elegant)

Spin Dynamics Studies Help Reduce Risk in Design for Electron Ion Collider

The origin of nuclear spin remains a significant puzzle in nuclear science.

Because the relevant statistical errors $\propto 1/P^2$, highly polarized beams make the experimental effort more efficient.

Polarization for both electron and ion beams expected to remain > 80%.

Brookhaven National Laboratory was selected on January 9, 2020 as site to build EIC. During this project, both BNL and Jefferson lab designs were supported.

Zgoubi spin tracking software

Zgoubi provides particle tracking capabilities for study of both orbital and spin dynamics in EIC electron and hadron rings.

The initial version of **zgoubi**, dedicated to ray-tracing in magnetic fields, was developed by D. Garreta and J.C. Faivre at CEN-Saclay in the early 1970's. It was perfected for the purpose of studying the four spectrometers SPES I, II, III, IV at the Laboratoire National SATURNE (CEA-Saclay, France), and SPEG at GANIL (Caen, France). It is being used since long in several national and foreign laboratories.

(excerpt from Zgoubi manual)

Zgoubi is a well-trusted particle tracking code, currently maintained by François Mèot of BNL.

Why develop a ~50-year-old Fortran Code?

Zgoubi has unique features for spin tracking studies in the EIC:

- Direct integration of Lorentz Force law (orbit) and BMT equation (spin)
- Arbitrary magnetic field maps can be included
- Accurate stochastic model for synchrotron radiation included
- Many examples included with cross checked results, and multiple publications

Zgoubi Particle Update: ray tracing algorithm

Lorentz force law: $\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = q(\vec{E} + \vec{v} \times \vec{B})$

Zgoubi tracks normalized velocity: $\vec{u} = \frac{1}{v}\vec{v}$ $\qquad \vec{p} = m\gamma\vec{v} = q(B\rho)\vec{u}$

Then Zgoubi writes the Lorentz force law in the form:

$$\frac{\mathrm{d}}{\mathrm{d}s}(B\rho)\vec{u} = (B\rho)'\vec{u} + (B\rho)\vec{u}' = \frac{1}{v}\vec{E} + \vec{u} \times \vec{B}$$

$$\Longrightarrow (B\rho)',\ \vec{u}',\ \ (B\rho)'',\ \vec{u}'',\ \ (B\rho)^{(3)},\ \vec{u}^{(3)},\ \ldots$$

... and the particle update in the form:

$$\vec{r}^{f} \approx \vec{r} + \Delta s\,\vec{u} + \frac{\Delta s^2}{2!}\vec{u}' + \cdots + \frac{\Delta s^6}{6!}\vec{u}^{(5)}$$

$$\vec{u}^{f} \approx \vec{u} + \Delta s\,\vec{u}' + \frac{\Delta s^2}{2!}\vec{u}'' + \cdots + \frac{\Delta s^5}{5!}\vec{u}^{(5)}$$

B field expanded in power series to allow order by order propagation.

Spin transport algorithm has the same structure.

Highlights of RadiaSoft's Zgoubi Development

Sirepo Application

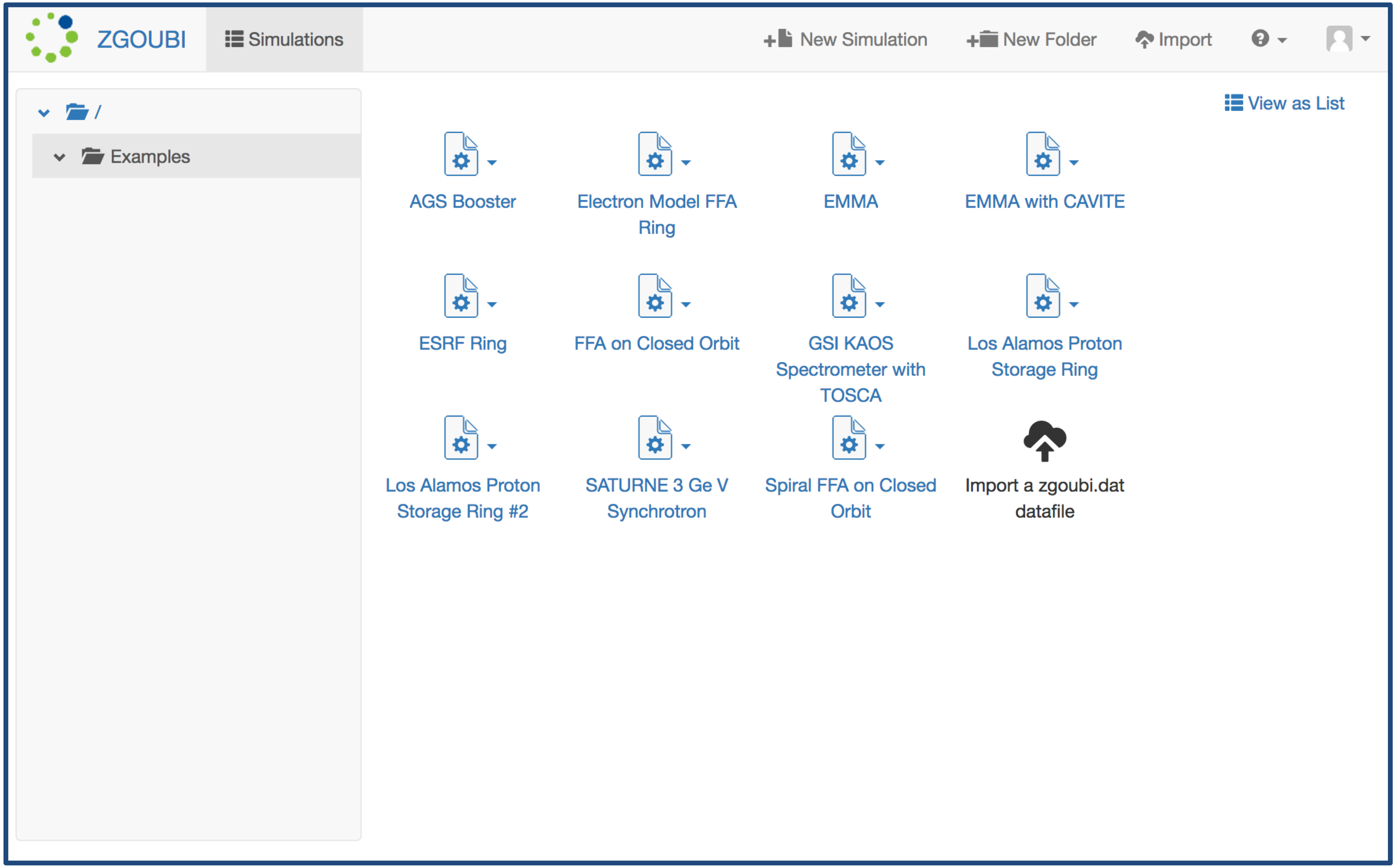
Zgoubi Fortran Development Tools

Zgoubi workshop

Rapid electron depolarization rate

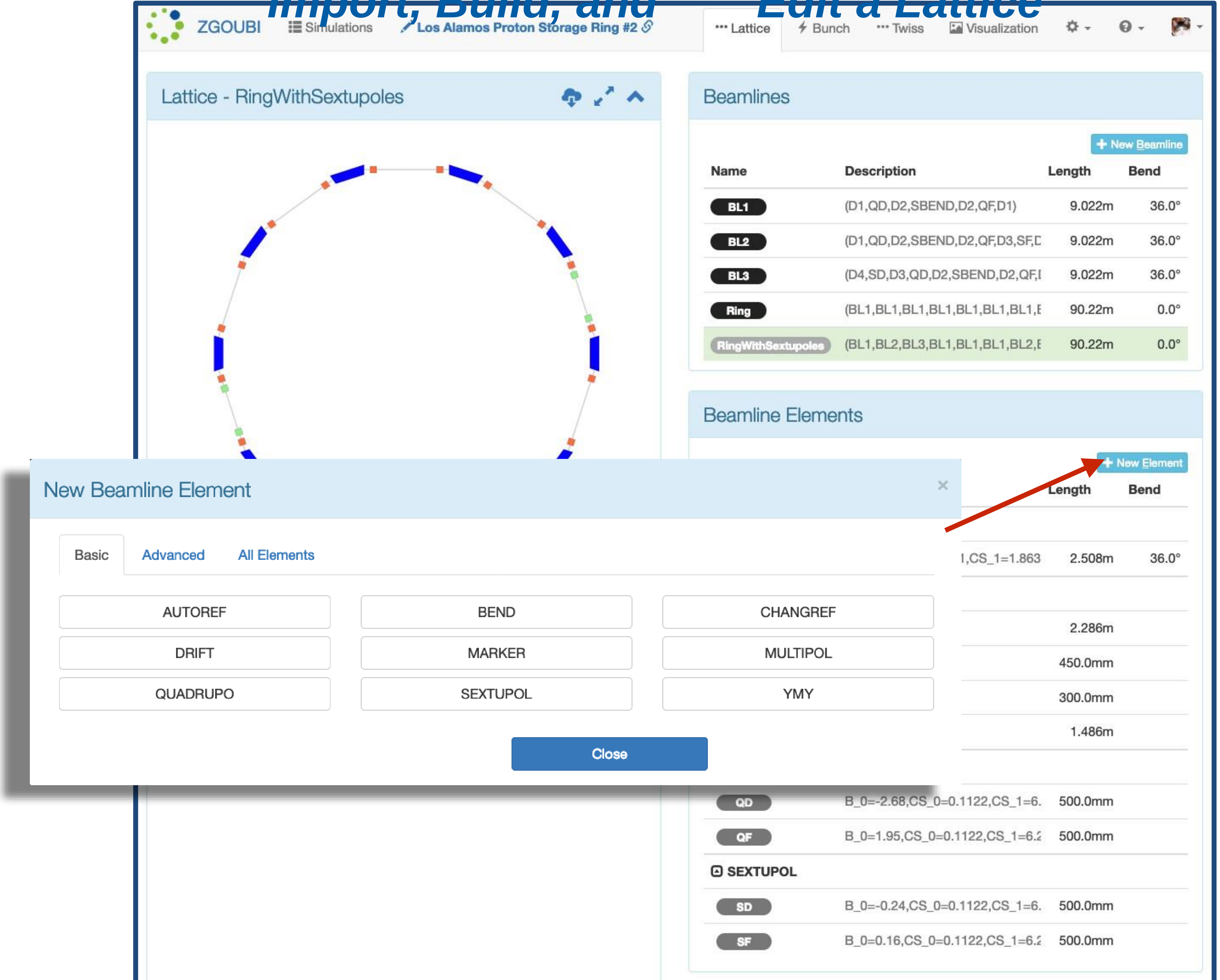
Sirepo Interface for Zgoubi

https://www.sirepo.com/zgoubi#



The Sirepo Interface for Zgoubi:

Import, Build, and Edit a Lattice



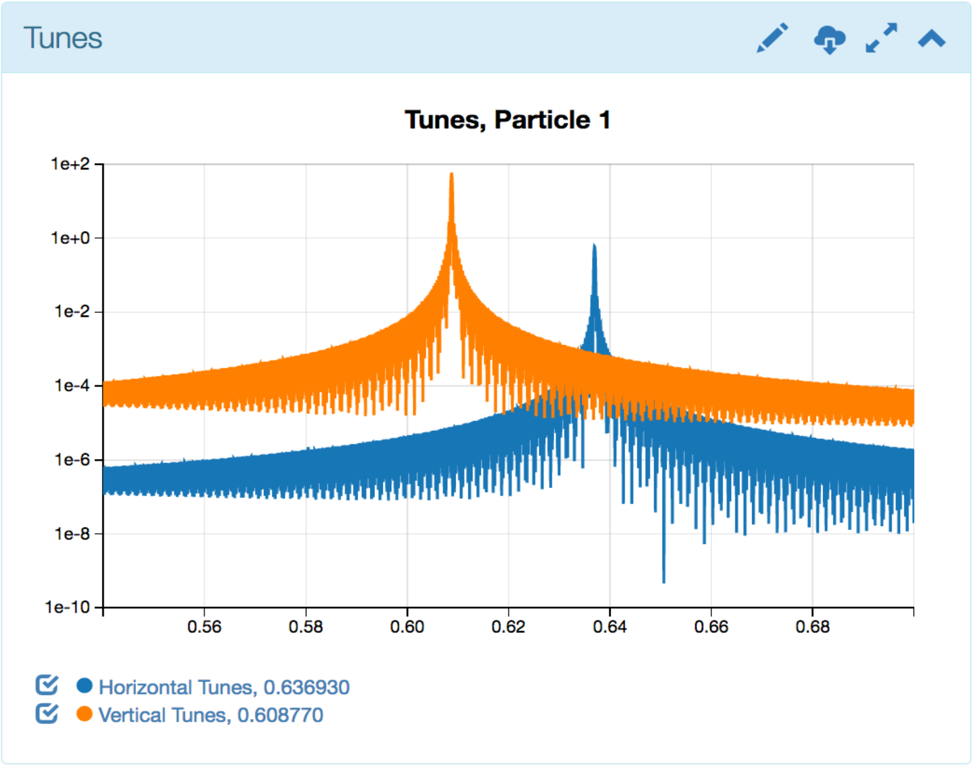
The Sirepo Interface for Zgoubi cont.

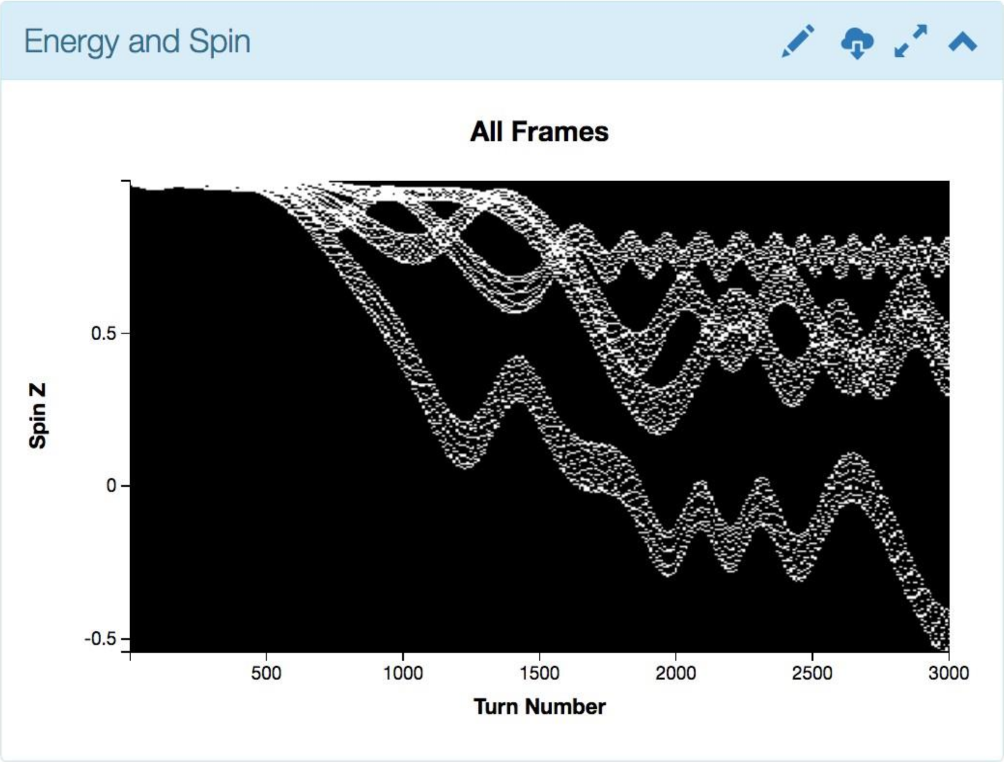
BNL EIC interaction point, with solenoid spin rotators

View this simulation at:
https://www.sirepo.com/zgoubi#/lattice/2SivHeG9

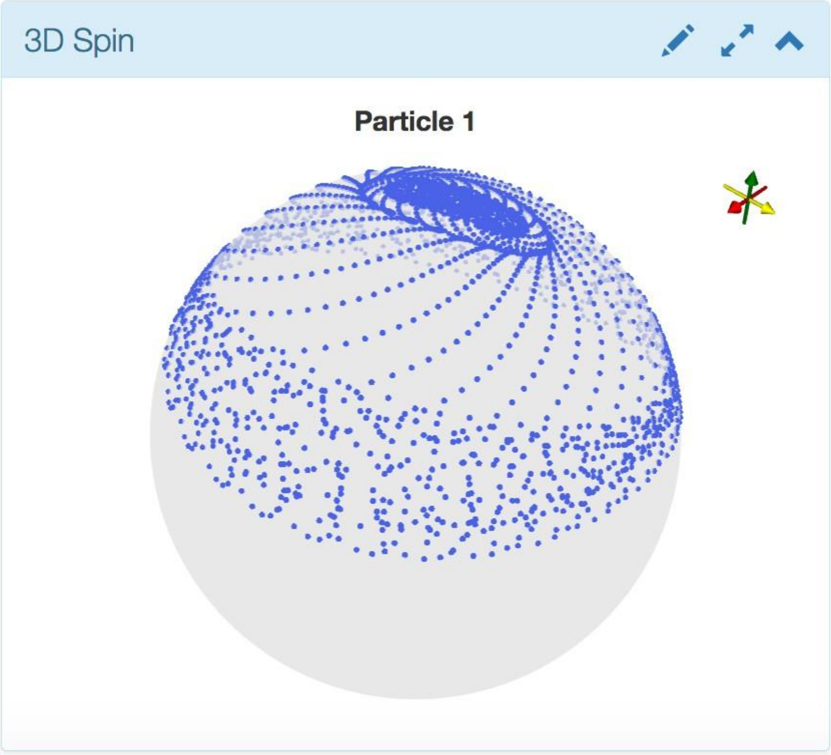
- Read in Zgoubi file for the BNL EIC
- Generate a plot of the Twiss parameters
- Conveniently edit element parameters or insert new elements
- Share updated simulation with collaborators

The Sirepo Interface for Zgoubi: Visualize the Beam





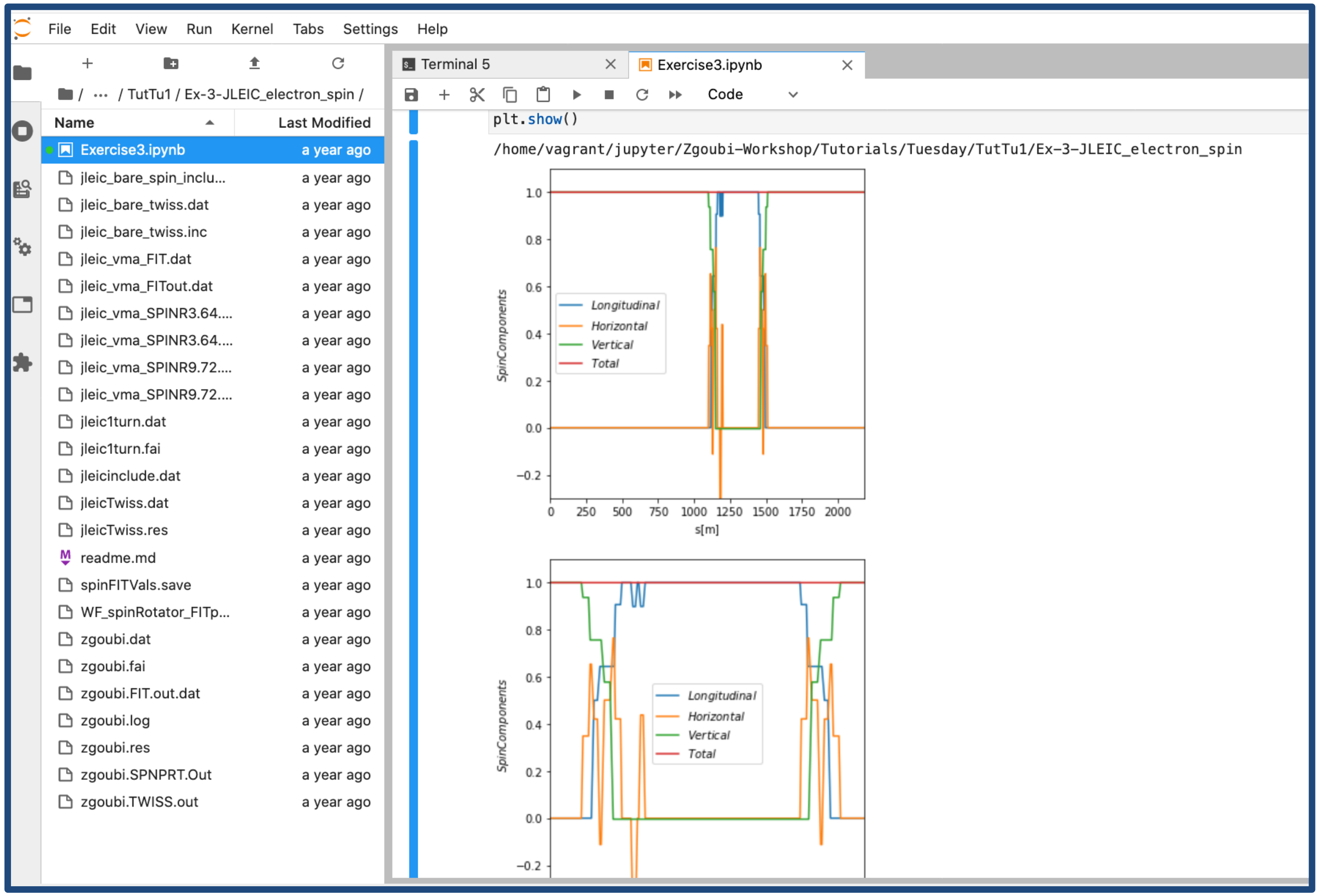
Including
tunes and spin



Transport Sirepo Simulation to Jupyter

Export Zgoubi input file from Sirepo (using PyZgoubi) and imported into a Jupyter session

From here, we continue simulations and visualization with the full suite of Python based tools



Plotting spin components around the ring for the JLEIC lattice in a Jupyter notebook

https://jupyter.radiasoft.org

Up-to-date Zgoubi executable is pre-installed on server

Zgoubi Fortran development tools

Issue: How to modernize a ~50-year-old Fortran code while maintaining accuracy of benchmarked physics?

ctest is a part of the *cmake* build tools

Testing framework:

- Created a ctest based testing framework that ensures that the numerical values of the simulation don't change (to within specified numerical precision) as we develop the code.
- Relies on ndiff (https://www.math.utah.edu/~beebe/software/ndiff/).

Fortran coarrays used for parallelization

Parallel profiling tools:

- Applied to achieve for parallel computation.
- In collaboration with Sourcery Instititue and Paratools (http://taucommander.paratools.com/).
- This allowed us to validate new tracking algorithms and enable parallel processing while ensuring backwards compatibility and consistency of physics results.

Zgoubi workshop

Boulder, Colorado: 26-30 August 2019

Participants from BNL, JLab, Argonne, and abroad: labs from England, Italy, France, and Australia

Machines simulated:

- CBETA at Cornell University,
- additional Fixed Field Accelerators,
- French high-resolution spectrometer HRS-Desir, (part of GANIL)
- Los Alamos PSR
- Accelerators with electrostatic elements including:
  - electrostatic time of flight ring
  - nanoprobe beamline.

Spin dynamics highlighted:

- two days dedicated to simulation of hadron and electron spin tracking in Zgoubi
- examples drawn from both the JLEIC and eRHIC accelerator complexes

Publicly Available
Zgoubi files, Jupyter based tutorial material, and lecture slides:
https://github.com/radiasoft/Zgoubi-Workshop

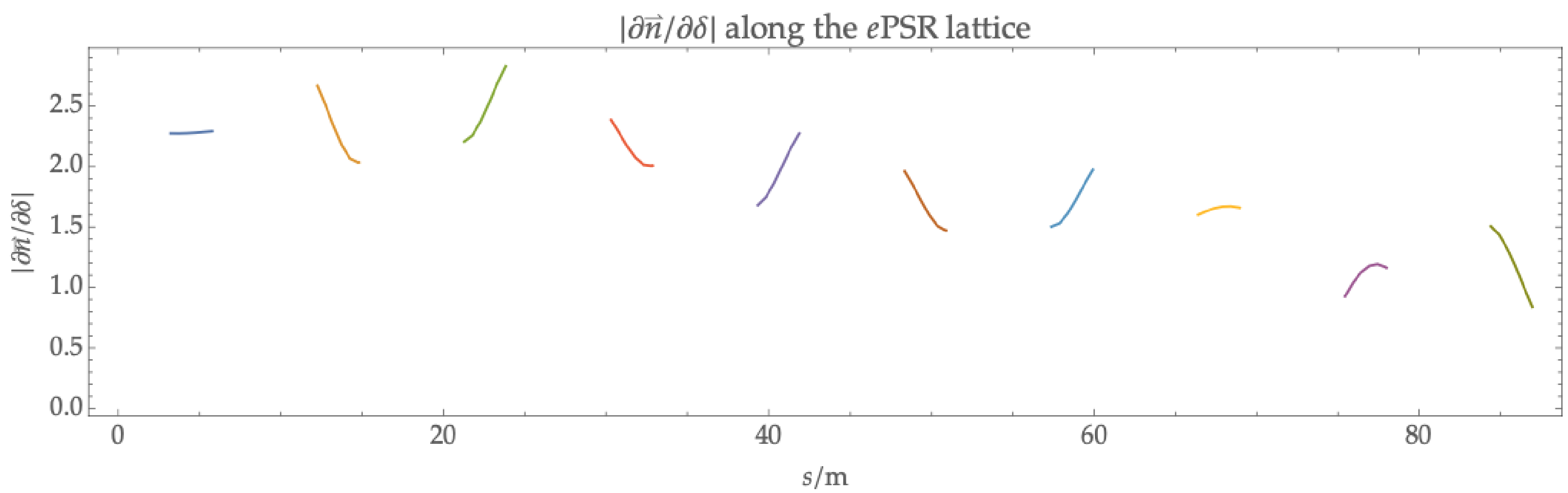
Rapid electron depolarization rate implemented

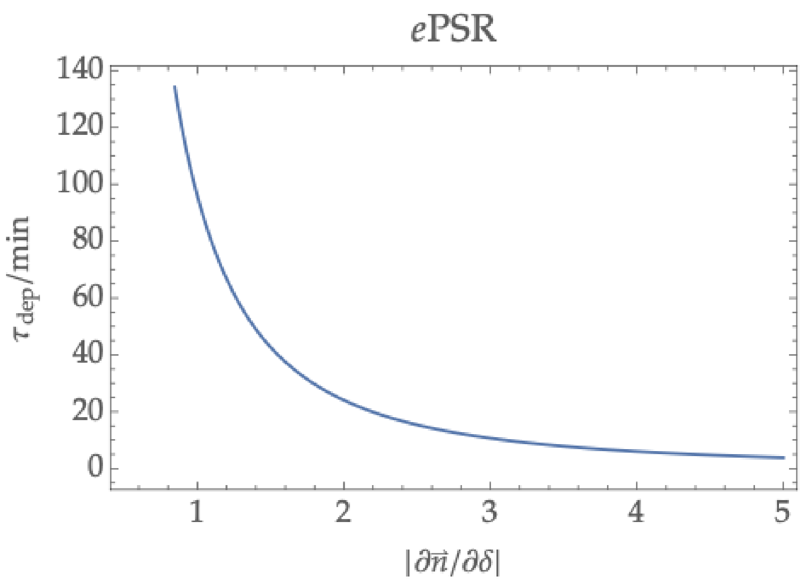
Electron depolarization comes from stochastic properties of photon emission

Analytical expression exists for depolarization rate, called the "Derbenev Kondratenko" equation

$$\tau_{\rm dep}^{-1} = \frac{5\sqrt{3}}{8}\frac{r_e \hbar \gamma^5}{m_e}\frac{1}{C}\oint {\rm d}s \left\langle \frac{\frac{11}{18}\left(\frac{\partial \hat{n}}{\partial \delta}\right)^2}{|\rho(s)|^3} \right\rangle_s$$

$\frac{d\hat{n}}{d\delta}$ computed in Zgoubi around ring using fit routine. One can include realistic effects such as magnet field maps and errors. Implemented for testing in electron version of Los Alamos PSR lattice.





This tool allows a rapid, tracking based estimate of electron depolarization rate.

Summary

RadiaSoft provides an easy-to-use gateway for simulations using a range of well-established scientific codes: https://sirepo.com/

The Zgoubi software with orbital and spin tracking capabilities has been added to the list of available codes: https://sirepo.com/zgoubi. Import/export eases interaction with Jupyter notebook or command line environments.

We organized the Zgoubi Workshop in Boulder, CO; 26–30 August 2019, bringing together experts in spin dynamics and other Zgoubi users.

We used modern development tools to improve the Fortran Zgoubi software, to include new capabilities.

We simulated the spin dynamics of BNL EIC in Zgoubi/Sirepo and implemented a rapid depolarization calculation to understand electron polarization lifetime and help determine machine tolerances during the design process.

Thank you!

Supported in part by the US Department of Energy, Office of Science, Office of Nuclear Physics, including Award No. DE-SC0017181.

https://radiasoft.net/

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