

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

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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

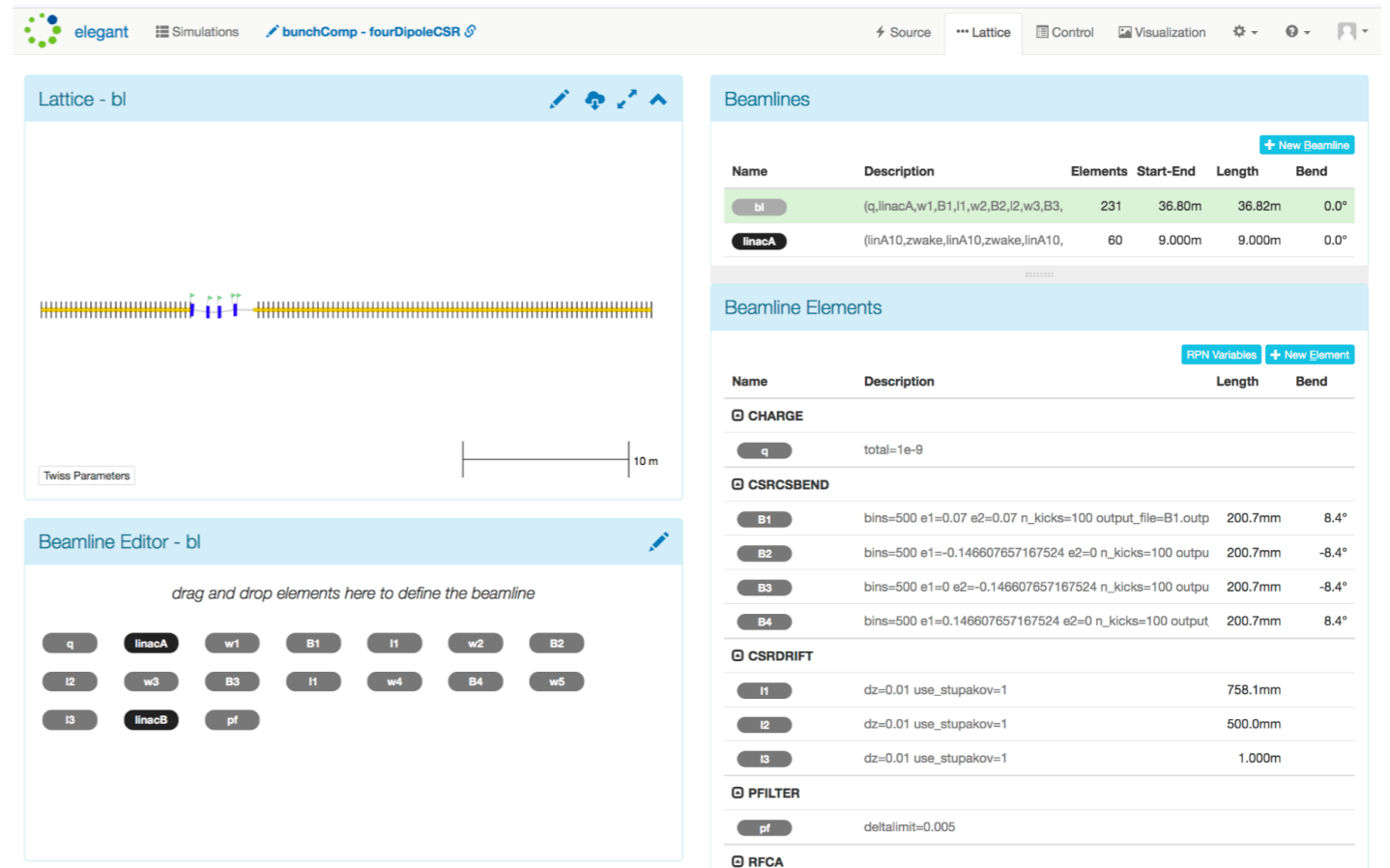
Accomplishments during this project

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



The screenshot displays the Sirepo interface for a beamline named 'bl'. The top navigation bar includes 'elegant', 'Simulations', and 'bunchComp - fourDipoleCSR'. The main area is divided into three panels:

- Lattice - bl:** A visual representation of the beamline lattice, showing a series of elements along a path. A scale bar indicates 10 m.
- Beamline Editor - bl:** A drag-and-drop interface for defining the beamline. It contains buttons for various elements: q, linacA, w1, B1, I1, w2, B2, I2, w3, B3, I1, w4, B4, w5, I3, linacB, and pf.
- Beamlines:** A table listing the beamlines in the simulation.

Name	Description	Elements	Start-End	Length	Bend
bl	(q,linacA,w1,B1,I1,w2,B2,I2,w3,B3,	231	36.80m	36.82m	0.0°
linacA	(linA10,zwake,linA10,zwake,linA10,	60	9.000m	9.000m	0.0°

Below the Beamlines table is the **Beamline Elements** section, which includes a table of individual elements:

Name	Description	Length	Bend
CHARGE			
q	total=1e-9		
CSRCSBEND			
B1	bins=500 e1=0.07 e2=0.07 n_kicks=100 output_file=B1.outp	200.7mm	8.4°
B2	bins=500 e1=-0.146607657167524 e2=0 n_kicks=100 output	200.7mm	-8.4°
B3	bins=500 e1=0 e2=-0.146607657167524 n_kicks=100 output	200.7mm	-8.4°
B4	bins=500 e1=0.146607657167524 e2=0 n_kicks=100 output	200.7mm	8.4°
CSRDRIFT			
I1	dz=0.01 use_stupakov=1	758.1mm	
I2	dz=0.01 use_stupakov=1	500.0mm	
I3	dz=0.01 use_stupakov=1	1.000m	
PFILTER			
pf	deltailimit=0.005		
RFCA			

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>

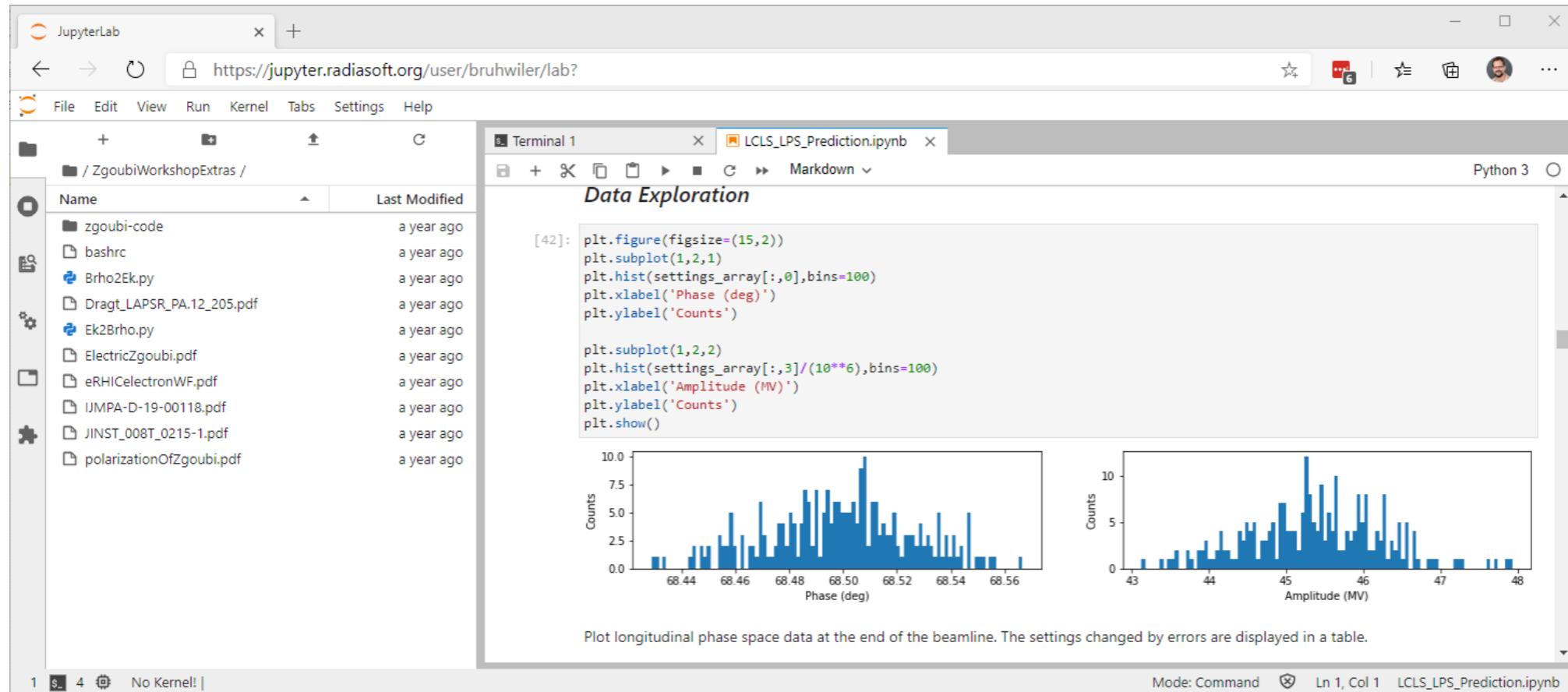
Easy to use: nothing to install, build, or maintain

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

the

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: $\frac{d\vec{p}}{dt} = q(\vec{E} + \vec{v} \times \vec{B})$

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

Then Zgoubi writes the Lorentz force law in the form:

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

$$\implies (B\rho)', \vec{u}', (B\rho)'', \vec{u}'', (B\rho)^{(3)}, \vec{u}^{(3)}, \dots$$

... and the particle update in the form:

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

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

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

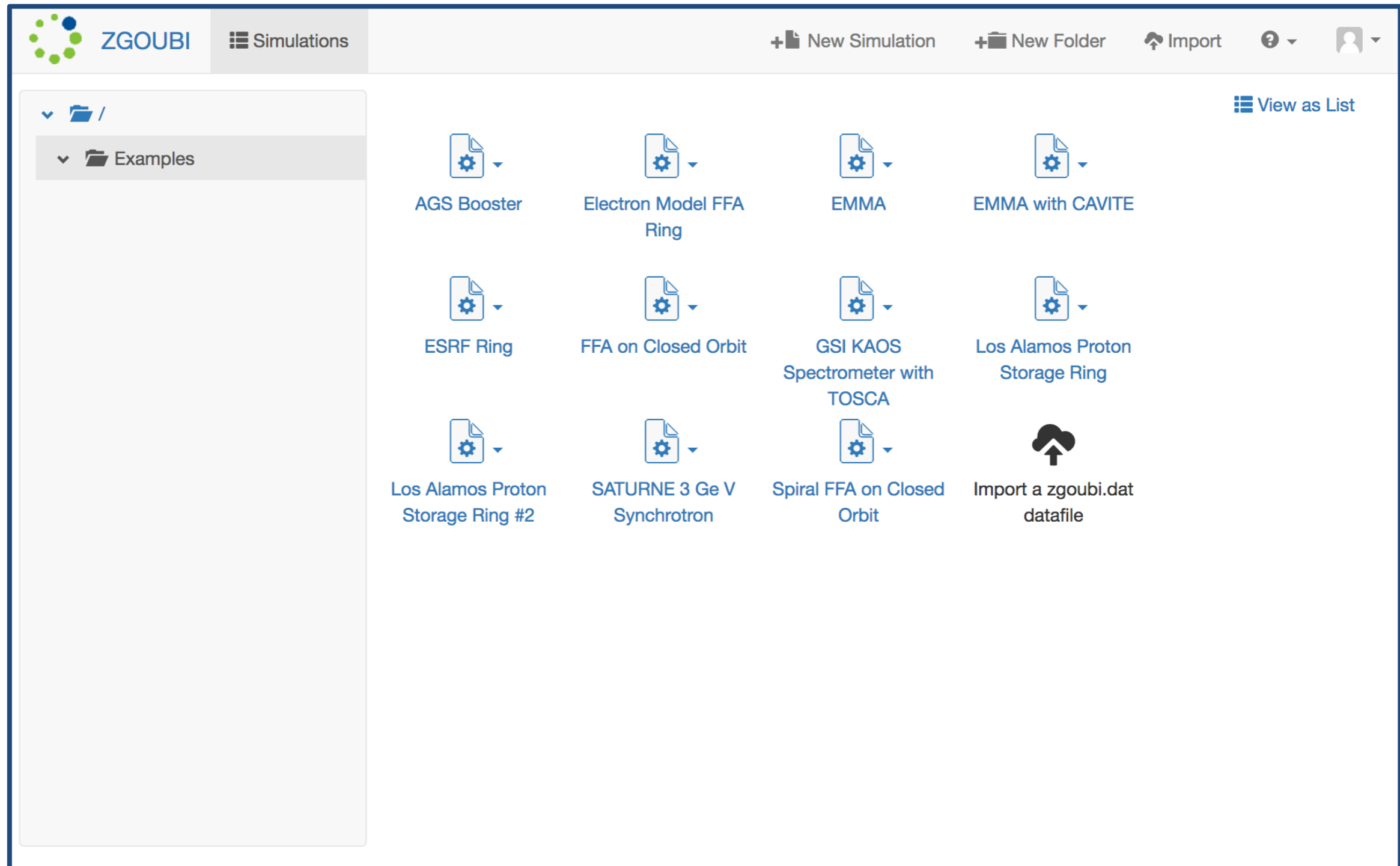
Zgoubi Fortran Development Tools

Zgoubi workshop

Rapid electron depolarization rate

Sirepo Interface for Zgoubi

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



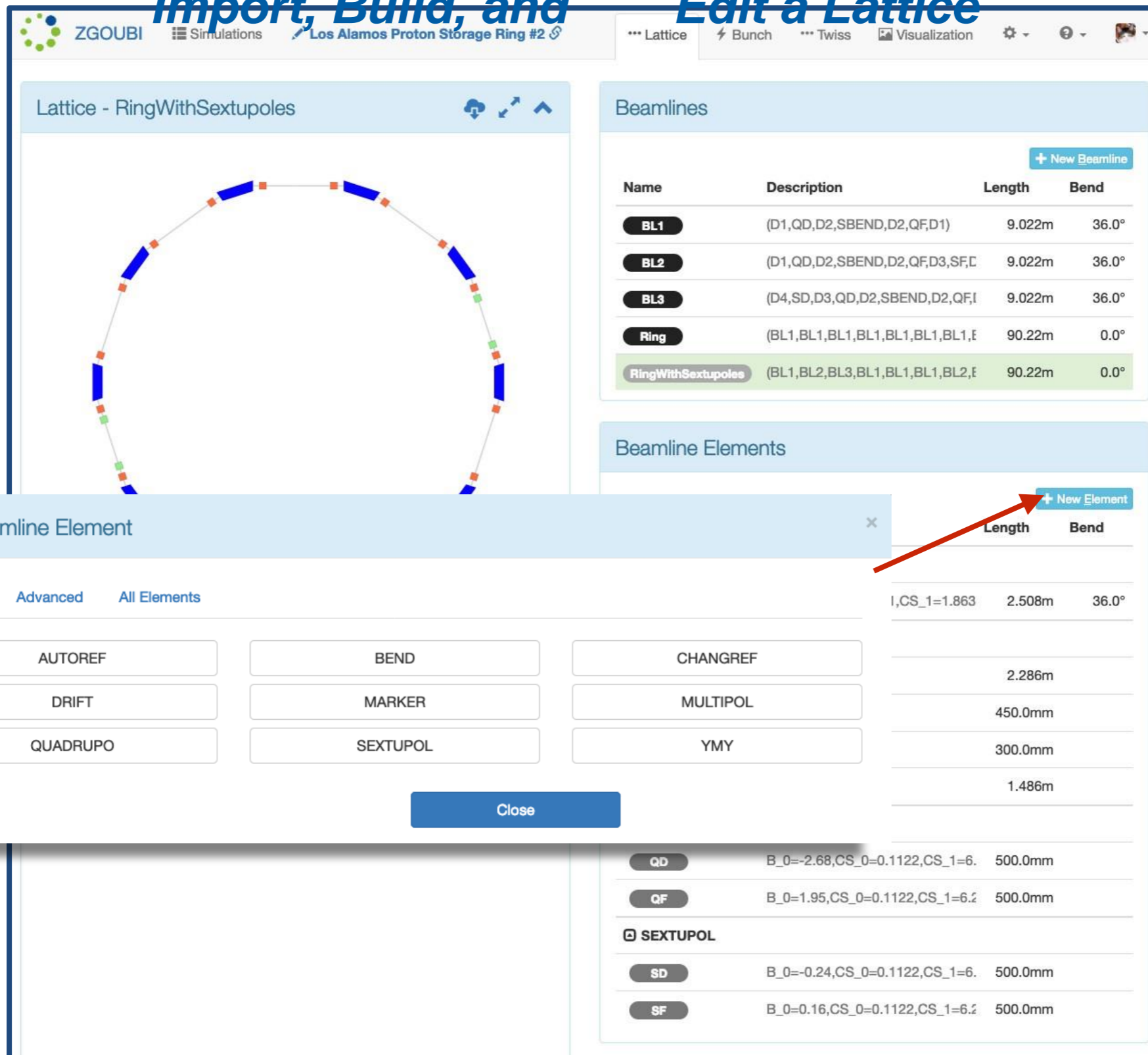
The screenshot displays the Sirepo Zgoubi interface. At the top, there is a navigation bar with the ZGOUBI logo, a 'Simulations' tab, and buttons for 'New Simulation', 'New Folder', and 'Import'. A user profile icon is also visible. Below the navigation bar, a left sidebar shows a file tree with a folder named 'Examples'. The main area displays a grid of simulation examples, each represented by a gear icon and a title. The examples are:

- AGS Booster
- Electron Model FFA Ring
- EMMA
- EMMA with CAVITE
- ESRF Ring
- FFA on Closed Orbit
- GSI KAOS Spectrometer with TOSCA
- Los Alamos Proton Storage Ring
- Los Alamos Proton Storage Ring #2
- SATURNE 3 Ge V Synchrotron
- Spiral FFA on Closed Orbit
- Import a zgoubi.dat datafile

In the top right corner of the main area, there is a 'View as List' button.

Zgoubi:

Import, Build, and Edit a Lattice



The screenshot displays the Sirepo Zgoubi interface. The main window shows a circular lattice diagram titled 'Lattice - RingWithSextupoles'. To the right, there is a 'Beamlines' table and a 'Beamline Elements' section. A 'New Beamline Element' dialog box is open in the foreground, showing a grid of element types and a table of parameters.

Name	Description	Length	Bend
BL1	(D1,QD,D2,SBEND,D2,QF,D1)	9.022m	36.0°
BL2	(D1,QD,D2,SBEND,D2,QF,D3,SF,C	9.022m	36.0°
BL3	(D4,SD,D3,QD,D2,SBEND,D2,QF,I	9.022m	36.0°
Ring	(BL1,BL1,BL1,BL1,BL1,BL1,BL1,F	90.22m	0.0°
RingWithSextupoles	(BL1,BL2,BL3,BL1,BL1,BL1,BL2,F	90.22m	0.0°

Length	Bend
I,CS_1=1.863	2.508m 36.0°
	2.286m
	450.0mm
	300.0mm
	1.486m

QD	B_0=-2.68,CS_0=0.1122,CS_1=6.	500.0mm
QF	B_0=1.95,CS_0=0.1122,CS_1=6.2	500.0mm
SEXTUPOL		
SD	B_0=-0.24,CS_0=0.1122,CS_1=6.	500.0mm
SF	B_0=0.16,CS_0=0.1122,CS_1=6.2	500.0mm

The Sirepo Interface for Zgoubi cont

BNL EIC interaction point, with solenoid spin rotators

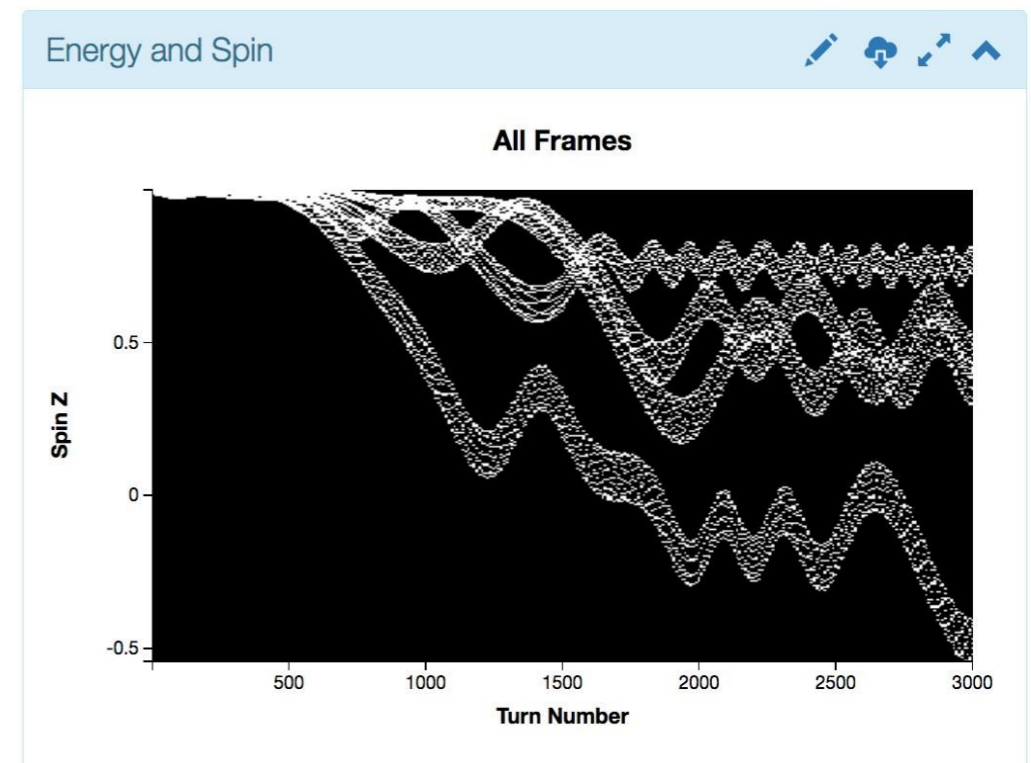
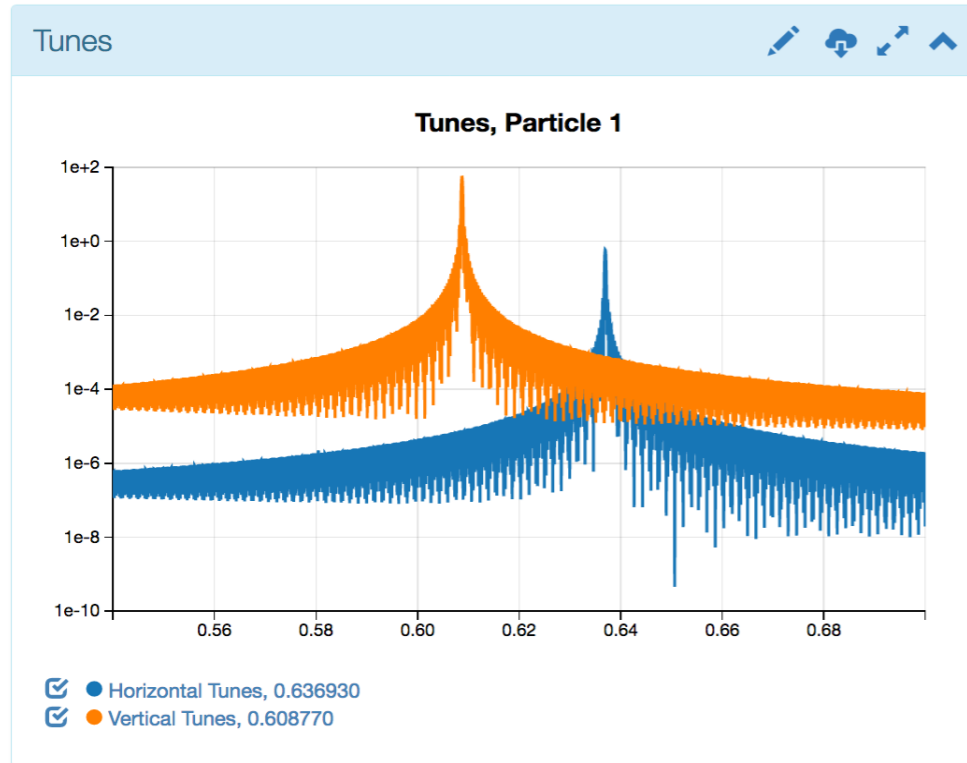


View this simulation at:
<https://www.sirepo.com/zgoubi#/lattice/2SivHeG9>

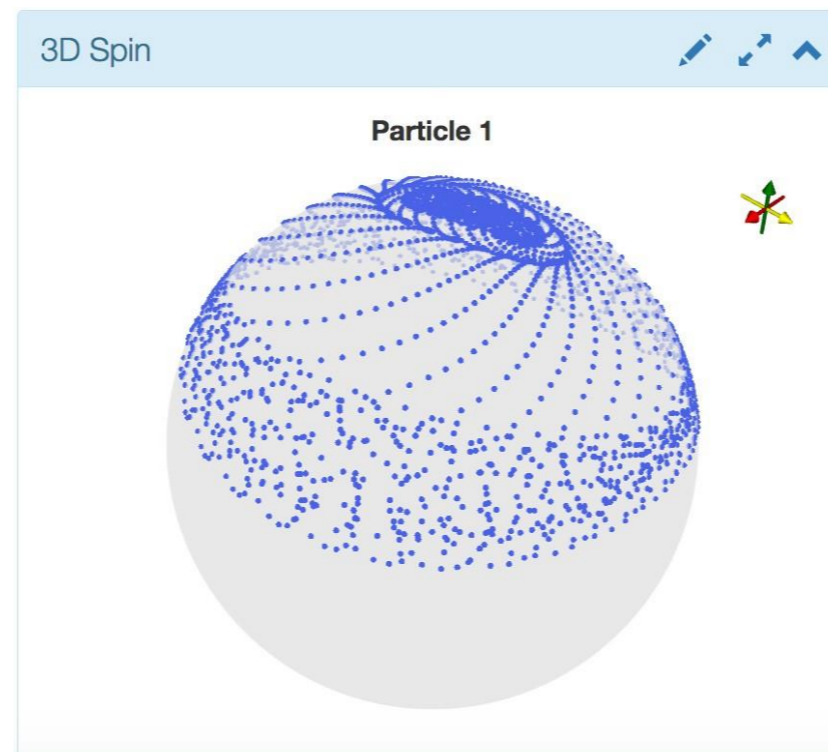
- Read in Zgoubi file for the BNL EIC
- Generate a plot of the Twiss parameters
- Conveniently edit element parameters or insert new elements
- Share updated simulation with collaborators

The Sirepo Visualize

Interface for Zgoubi: the Sirepo Beam



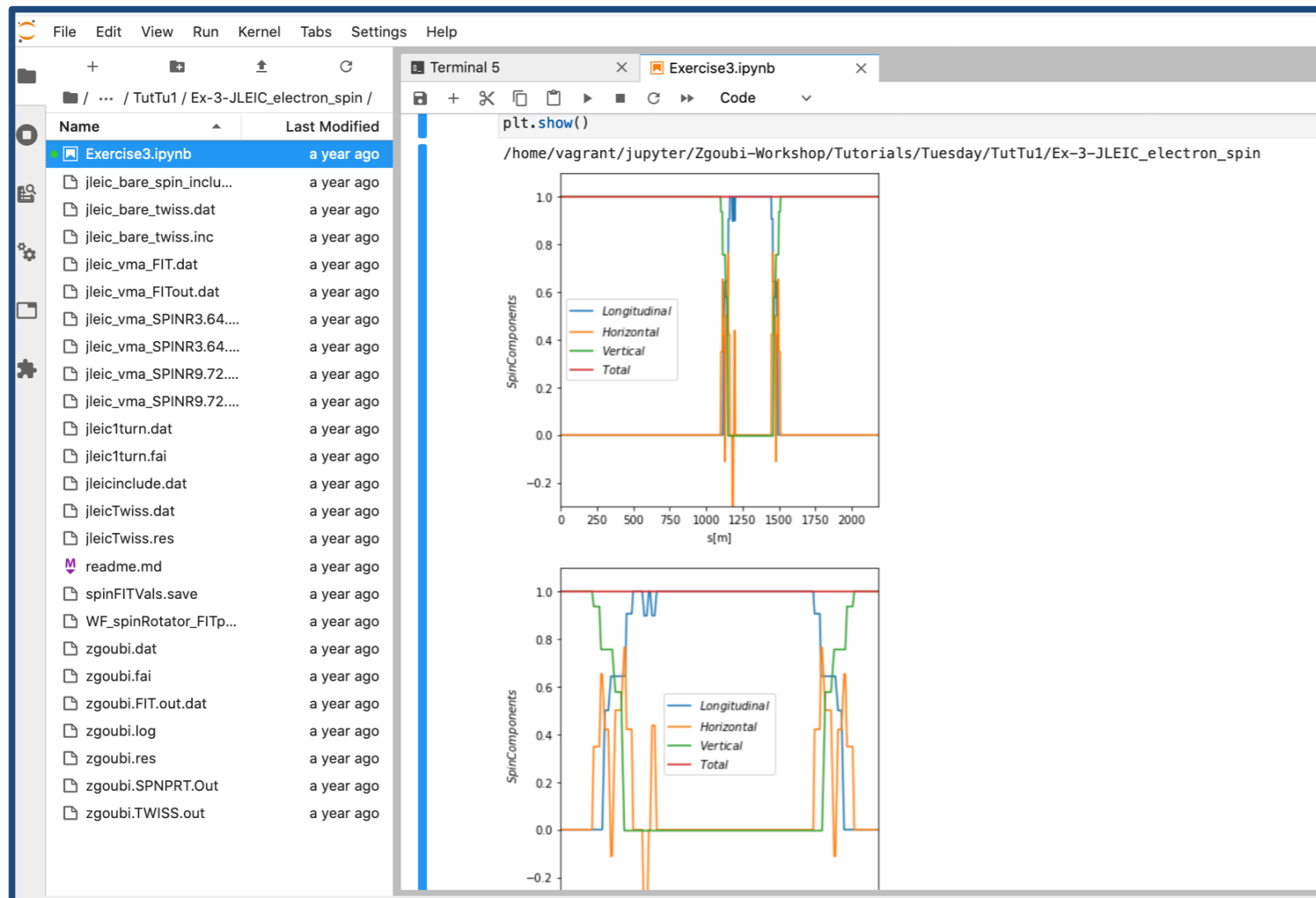
Including
tunes and spin



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



<https://jupyter.radiasoft.org>

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

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

Zgoubi Fortran development tools

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

Testing framework:

ctest is a part of the *cmake* build tools

- 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/>).

Parallel profiling tools:

Fortran *coarrays* used for parallelization

- Applied to achieve for parallel computation.
- In collaboration with Sourcery Institute 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>

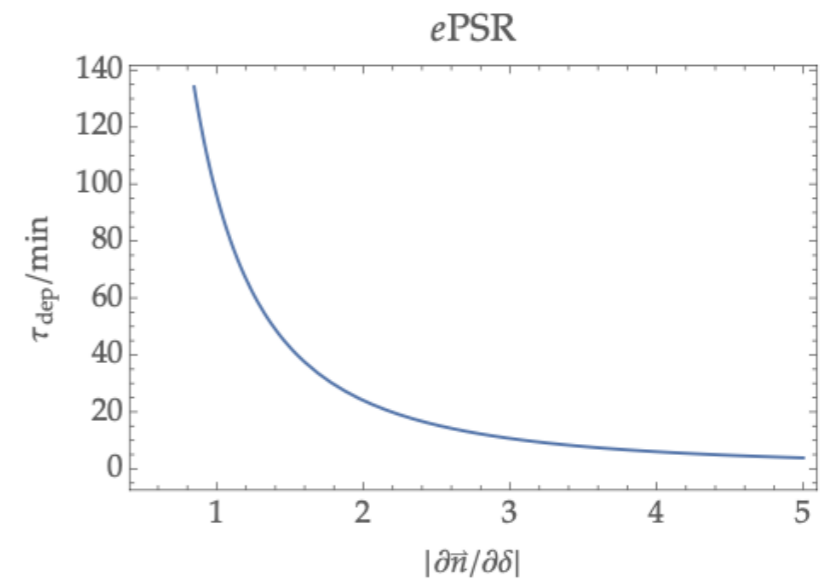
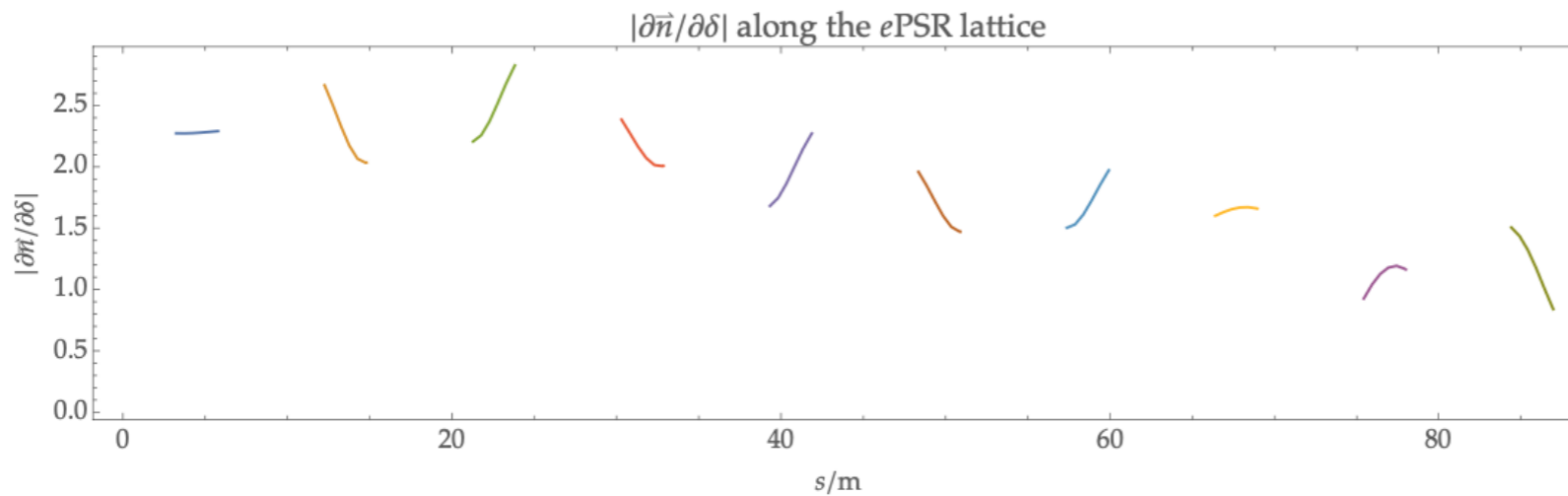
Rapid electron depolarization rate implemented

Electron depolarization comes from stochastic properties of photon emission

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

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

$\frac{d\hat{n}}{d\delta}$ 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!

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<https://radiasoft.net/>



<https://sirepo.com/>