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

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Izaak Beekman — Paratools, Inc, Eugene, OR

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DOE/NP SBIR/STTR Exchange Meeting Meeting
Gaithersburg, MD
13–14 August 2019

RadiaSoft Provides a Gateway to Scientific Computing

Sirepo https://sirepo.com/

Supported Codes

- elegant
- JSPEC (electron cooling)
- Synergia
- SRW (Synchrotron Radiation Workshop)
- Warp VND (Vacuum Nanoelectronic Devices)
- Warp PBA (Plasma-Based Accelerators)
- Zgoubi

Advantages of using Sirepo

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

RadiaSoft Contributes to the Community

At the *US Particle Accelerator School*, RadiaSoft's JupyterHub server provides access to scientific codes for simulating particle accelerators, FELs, and x-ray optics. The codes are preinstalled and can be executed from a browser-based terminal window, or from IPython notebooks.

USPAS:

- 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)
- *2020S: Measurement and Control of Beams (M. Minty, F. Zimmerman, J. Edelen)

RadiaSoft Scholarship Students at USPAS:

- River Robles, 2019
- Jonathan Ang Sixian, 2018
- Maria Simanovskaia, 2018

Other Education:

- 1st Korea University Accelerator School, 2018 (C. S. Park used Sirepo/Synergia)
- NS3 Nuclear Science Summer School (S. Lund used Sirepo/elegant)

DOE/NP Interest: High-fidelity Simulations of Spin Dynamics Help Reduce Risk in Designs for EICs

In the *The 2015 Long Range Plan for Nuclear Science Origin*, the Nuclear Science Advisory Committee (NSAC) recommends "a high-energy high-luminosity polarized electron ion collider (EIC) as the highest priority for new facility construction following the completion of FRIB."

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.

Plans for Zgoubi Include Enhancements to both Performance and Usability

GUI

Implement a Zgoubi graphical interface in Sirepo. *(80%)*

Implement single-click execution of Zgoubi on available linux clusters. *(25%)*

performance

Update the Zgoubi code base to the Fortran 2018. *(80%)*

Re-implement Zgoubi's particle update algorithm. *(65%)*

Parallelize Zgoubi using Fortran 2018. *(35%)*

capabilities

Implement symplectic tracking for field maps. *(30%)*

Add closed-orbit correction to Zgoubi. *(85%), with F. Méot*

science

Assess and improve the spin dynamics in electron and ion rings for the eRHIC design. *(starting this month)*

Benchmark Zgoubi with BMad and other codes used for simulating JLEIC ring designs. *(15%)*

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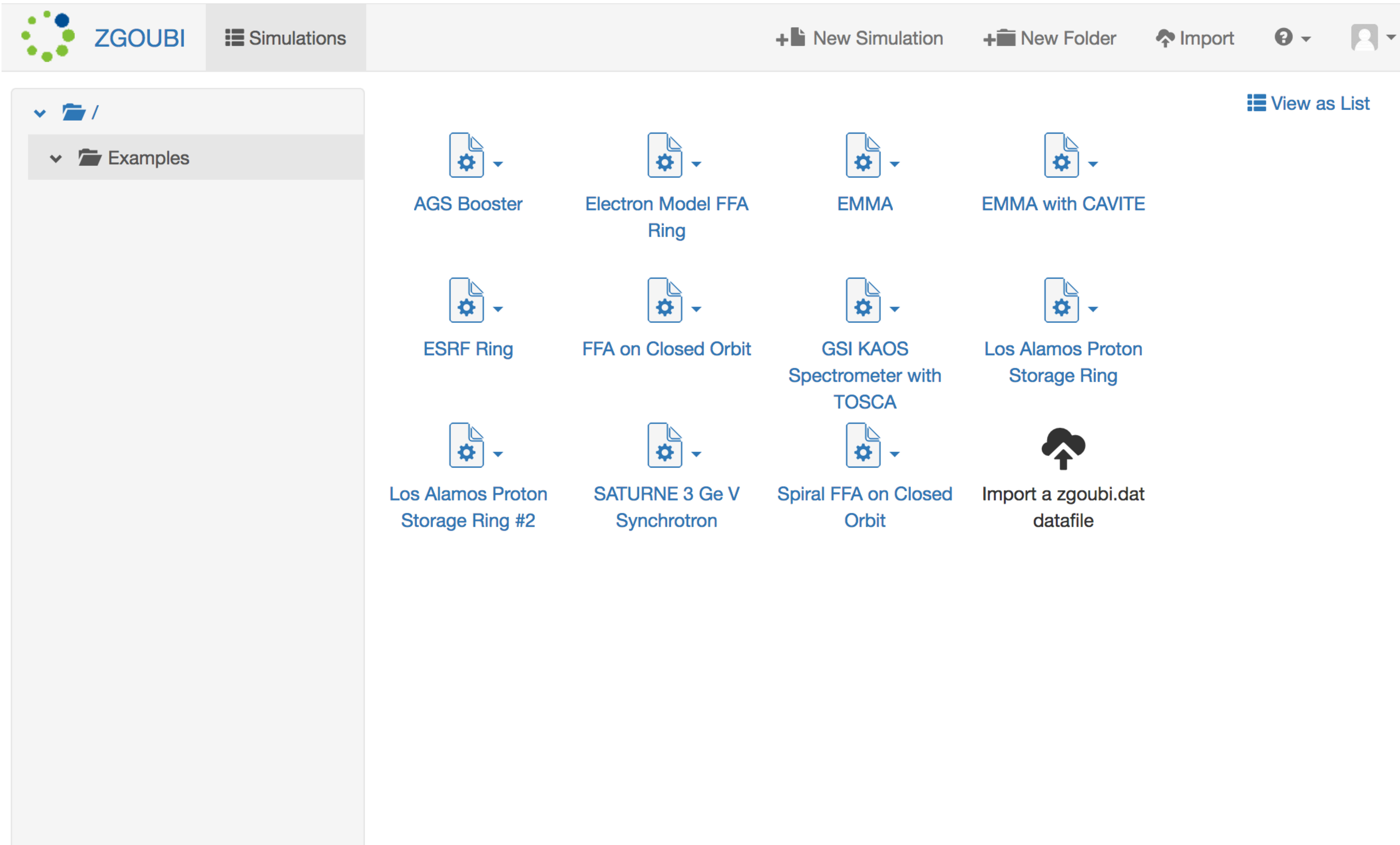
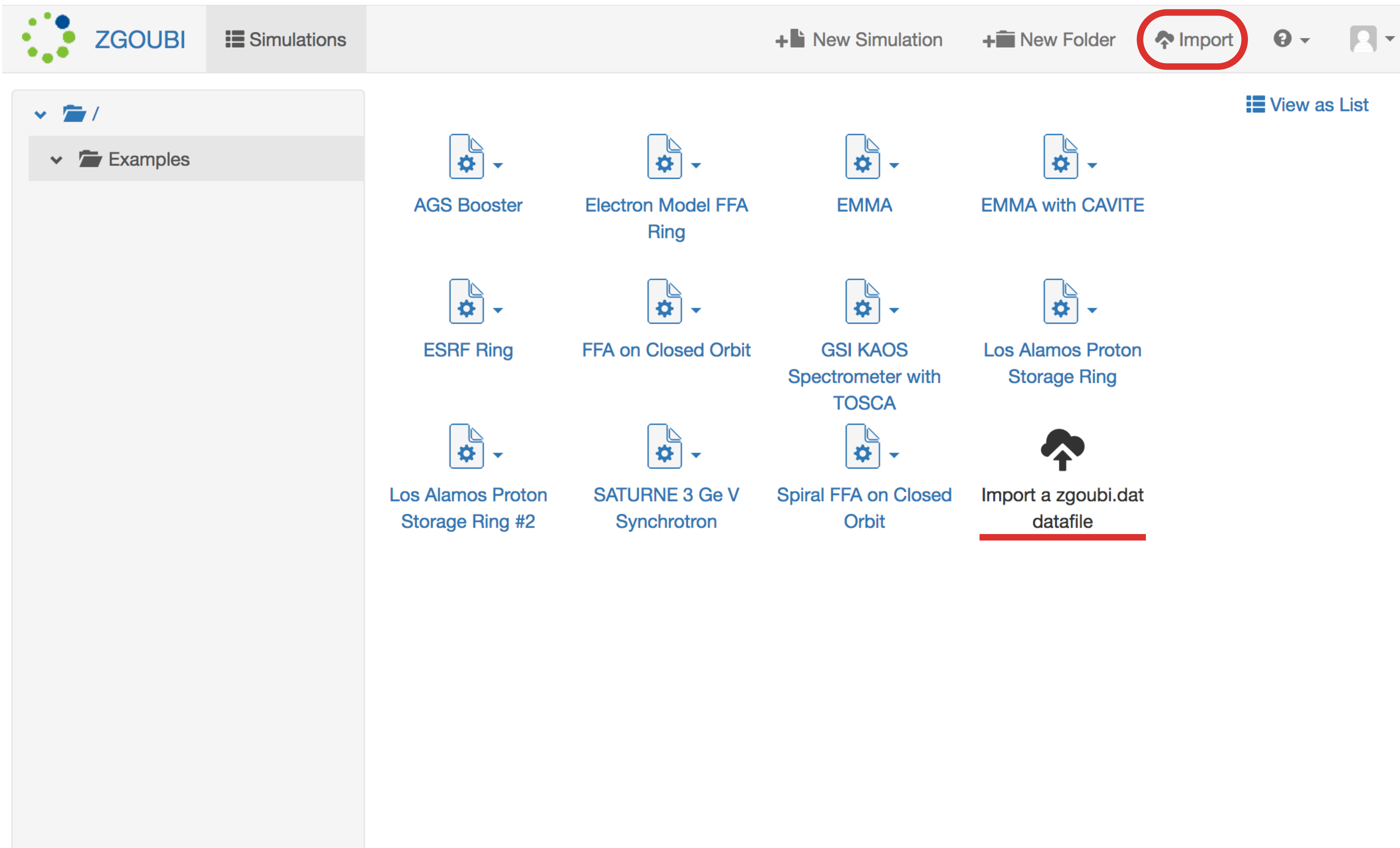
Streamline Zgoubi Simulations: A Sirepo Interface for Zgoubi

Sirepo



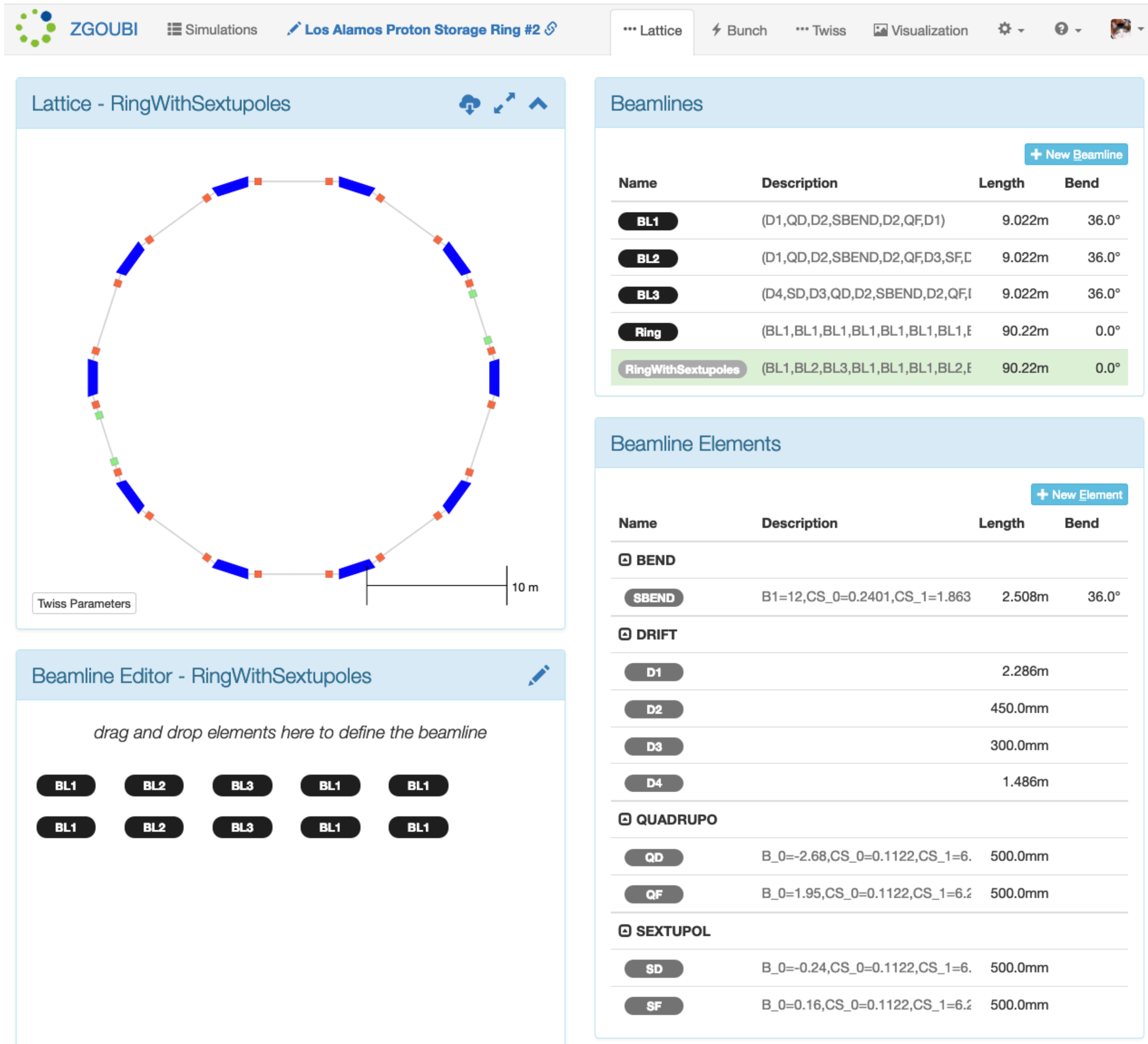
The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice

Sirepo



The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice—cont.

Sirepo

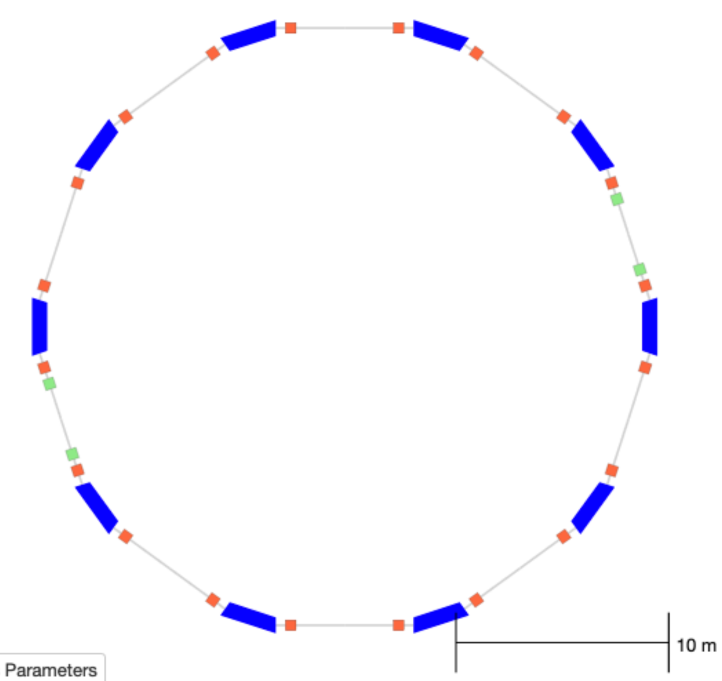


The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice—cont.

Sirepo

ZGOUBI | Simulations | Los Alamos Proton Storage Ring #2 | Lattice | Bunch | Twiss | Visualization

Lattice - RingWithSextupoles



Twiss Parameters

Beamline Editor - RingWithSextupoles

drag and drop elements here to define the beamline

BL1 BL2 BL3 BL1 BL1

BL1 BL2 BL3 BL1 BL1

Beamlines

+ New Beamline

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,D	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,E	90.22m	0.0°
RingWithSextupoles	(BL1,BL2,BL3,BL1,BL1,BL1,BL2,E	90.22m	0.0°

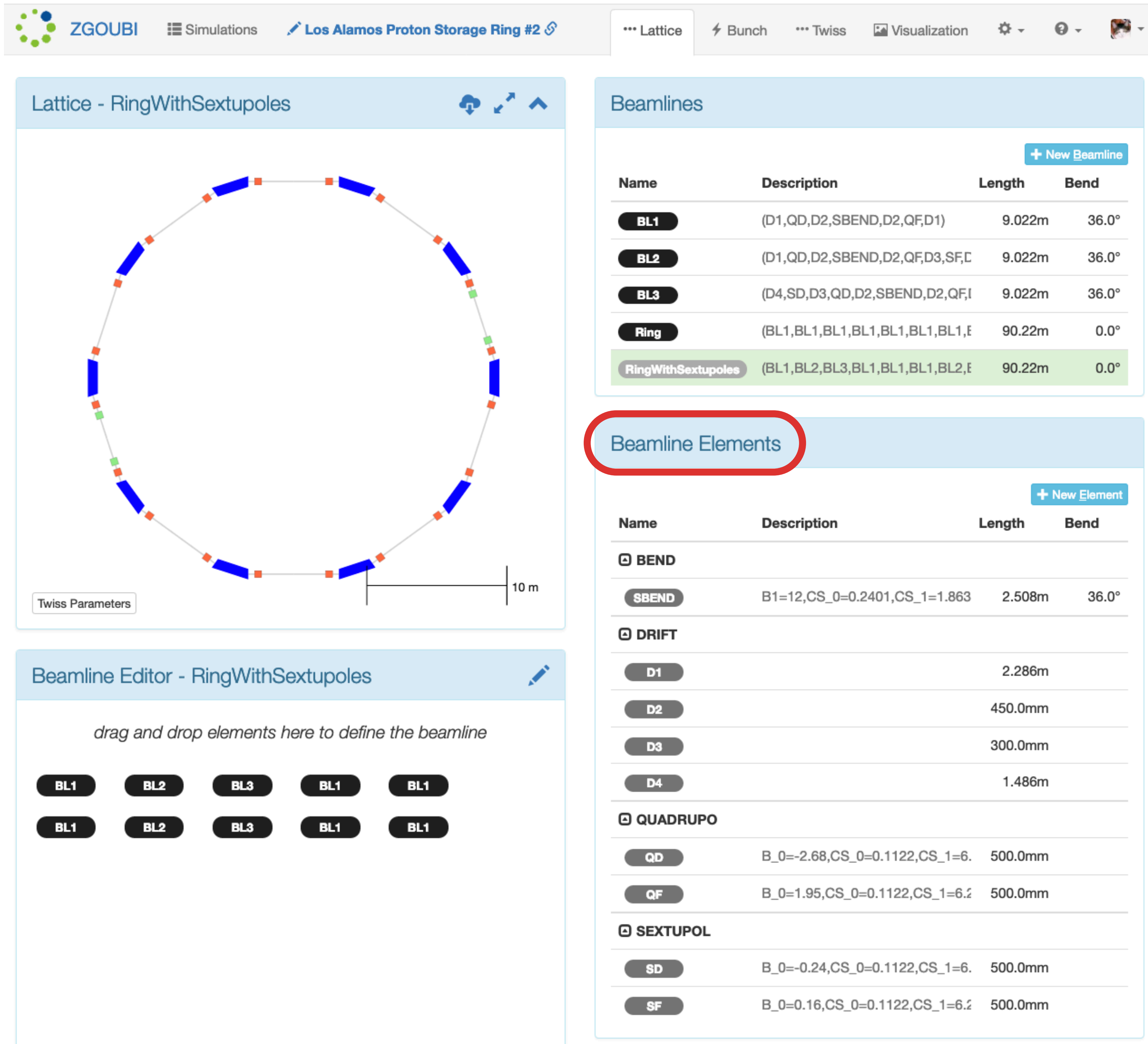
Beamline Elements

+ New Element

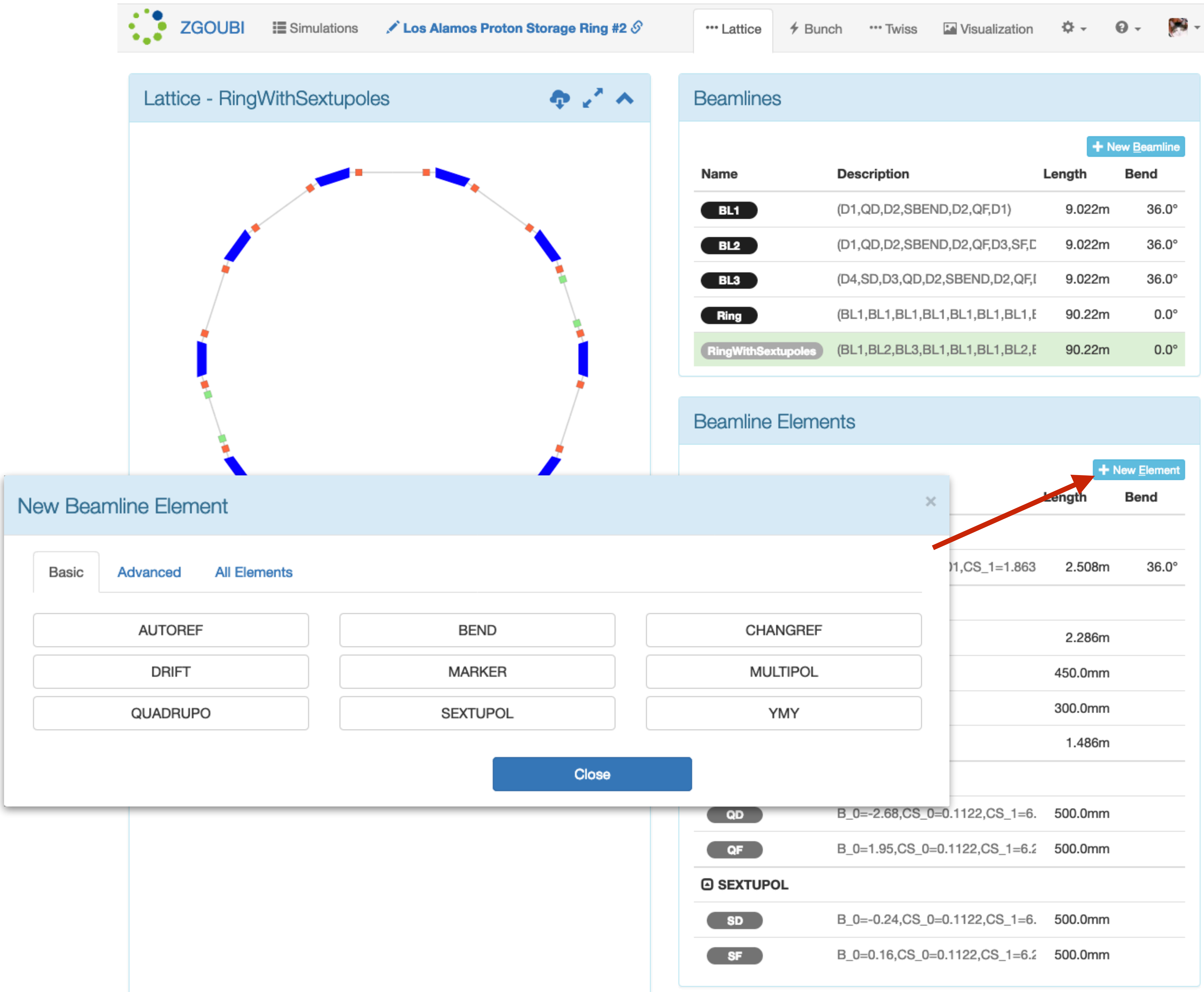
Name	Description	Length	Bend
BEND			
SBEND	B1=12,CS_0=0.2401,CS_1=1.863	2.508m	36.0°
DRIFT			
D1		2.286m	
D2		450.0mm	
D3		300.0mm	
D4		1.486m	
QUADRUPO			
QD	B_0=-2.68,CS_0=0.1122,CS_1=6.	500.0mm	
QF	B_0=1.95,CS_0=0.1122,CS_1=6.2	500.0mm	
SEXTUPOL			
SD	B_0=-0.24,CS_0=0.1122,CS_1=6.	500.0mm	
SF	B_0=0.16,CS_0=0.1122,CS_1=6.2	500.0mm	

The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice—cont.

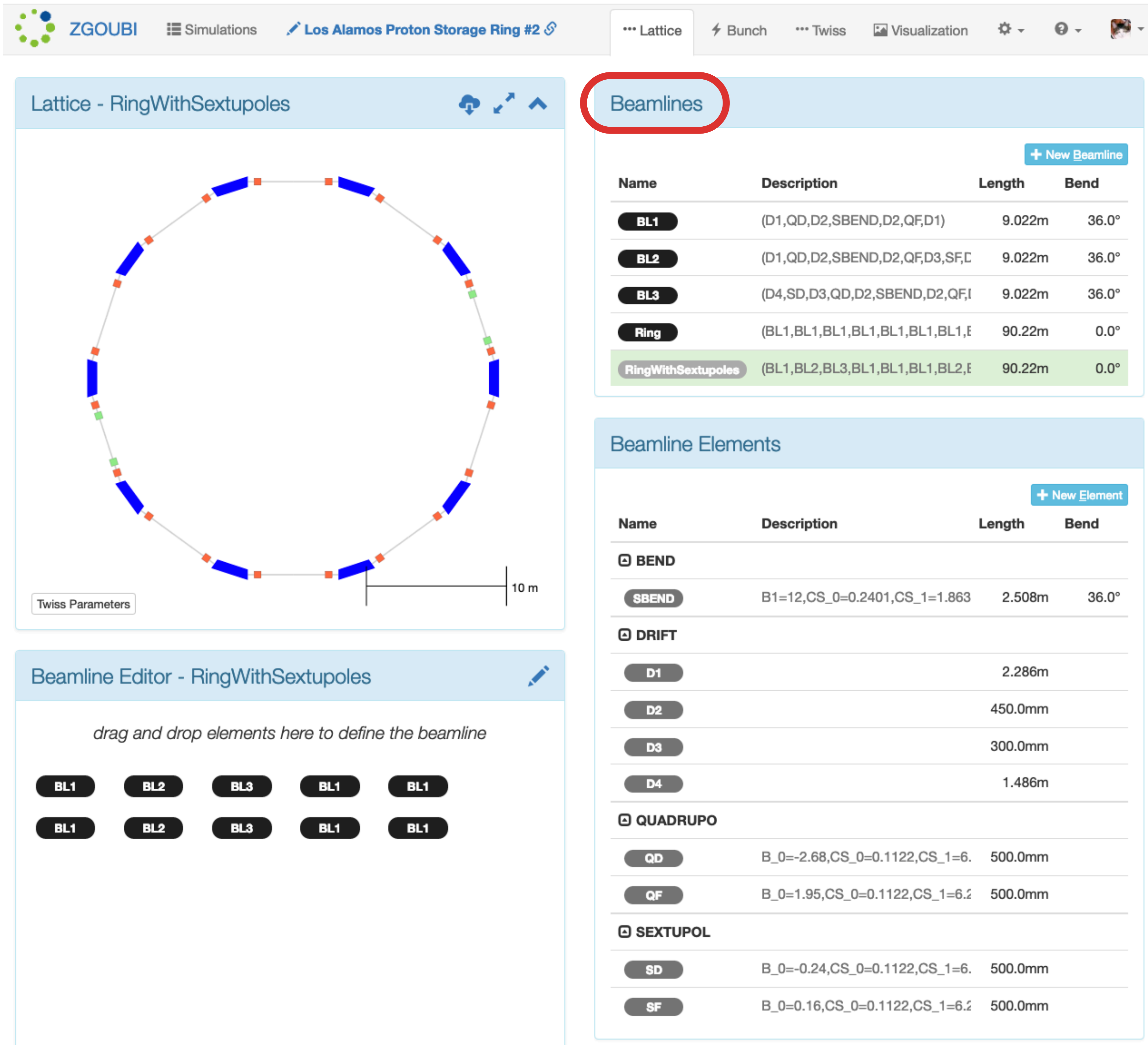
Sirepo



The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice—cont.



The Sirepo Interface for Zgoubi: Import, Build, and Edit a Lattice—cont.



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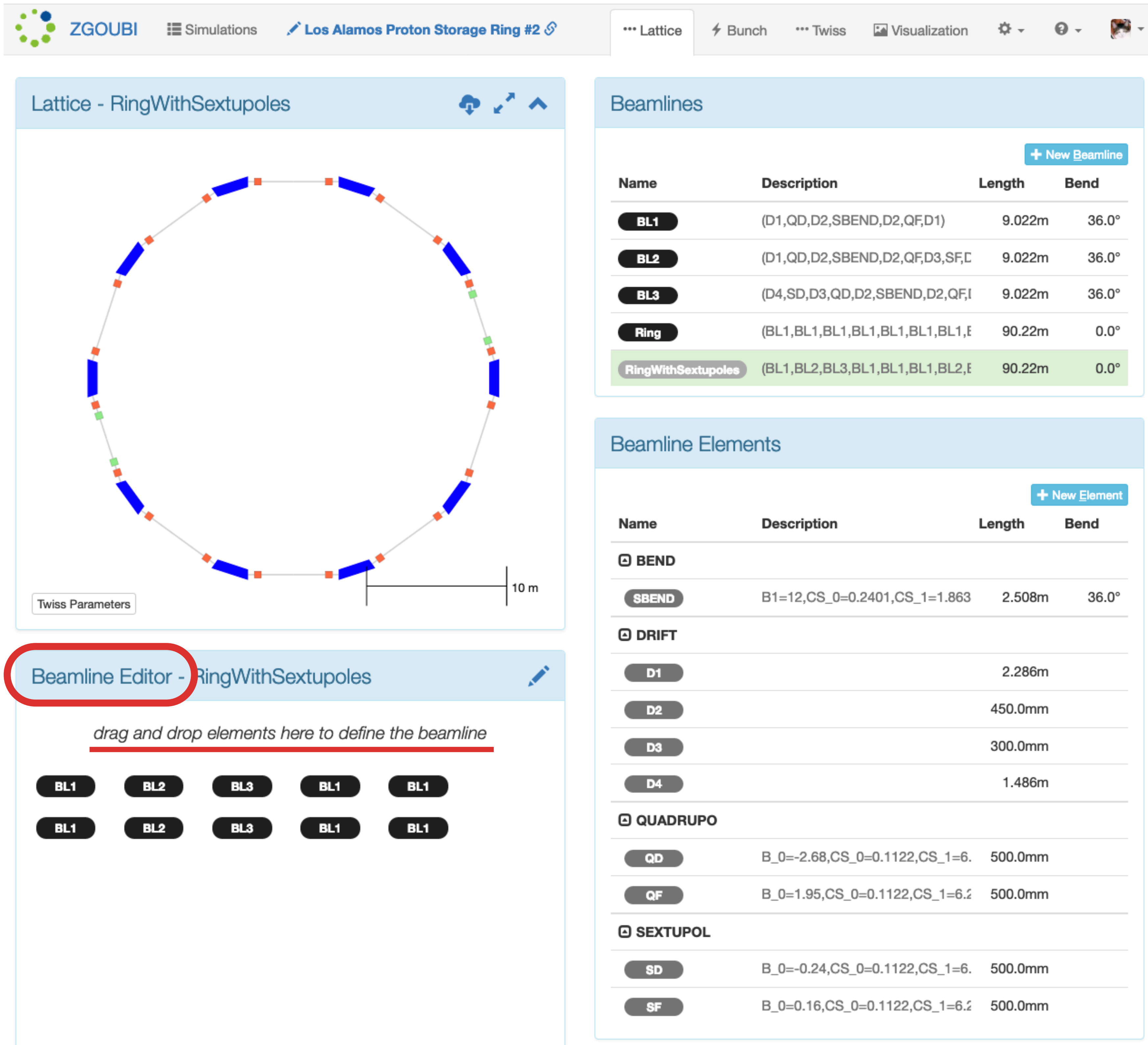
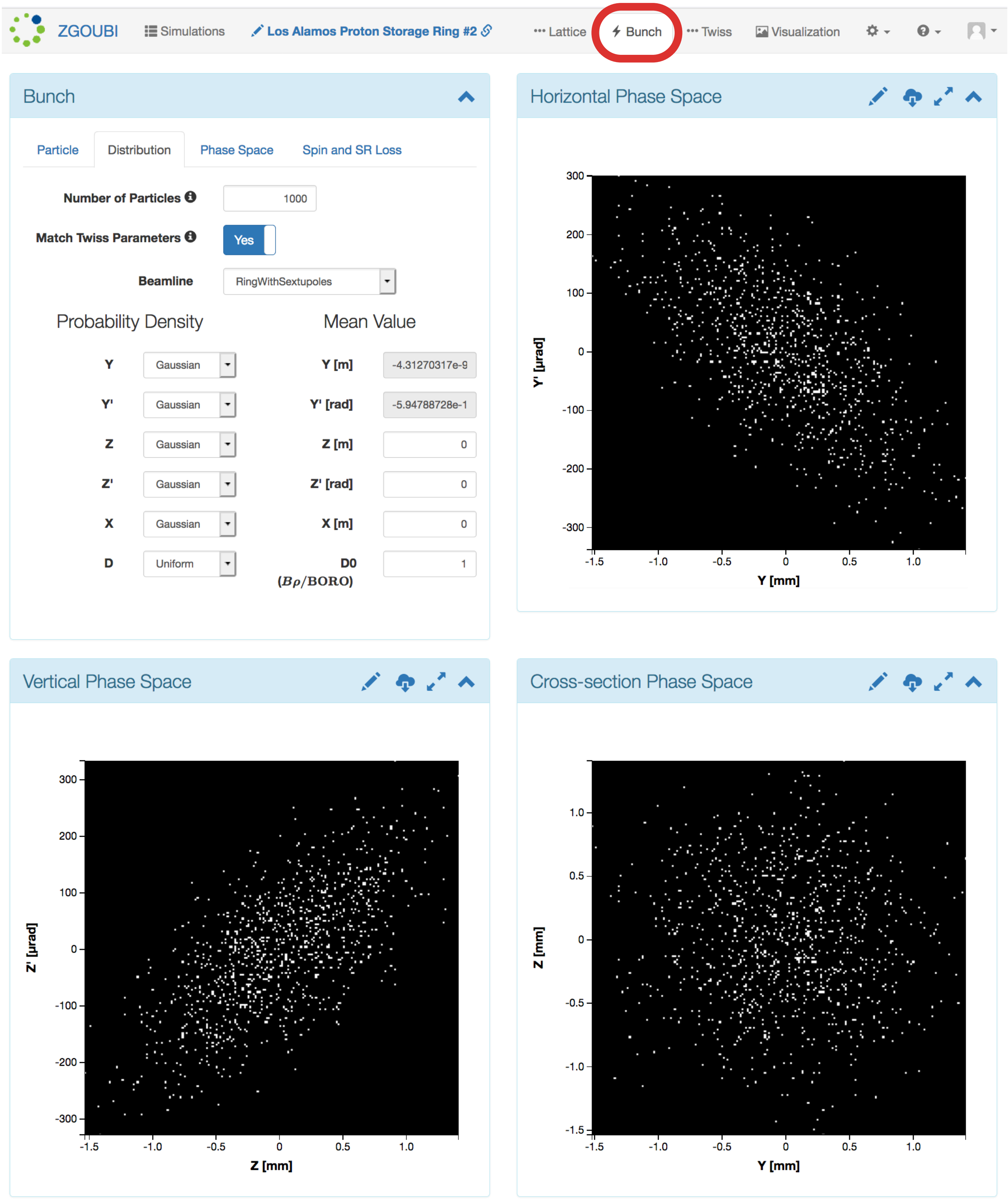
Sirepo

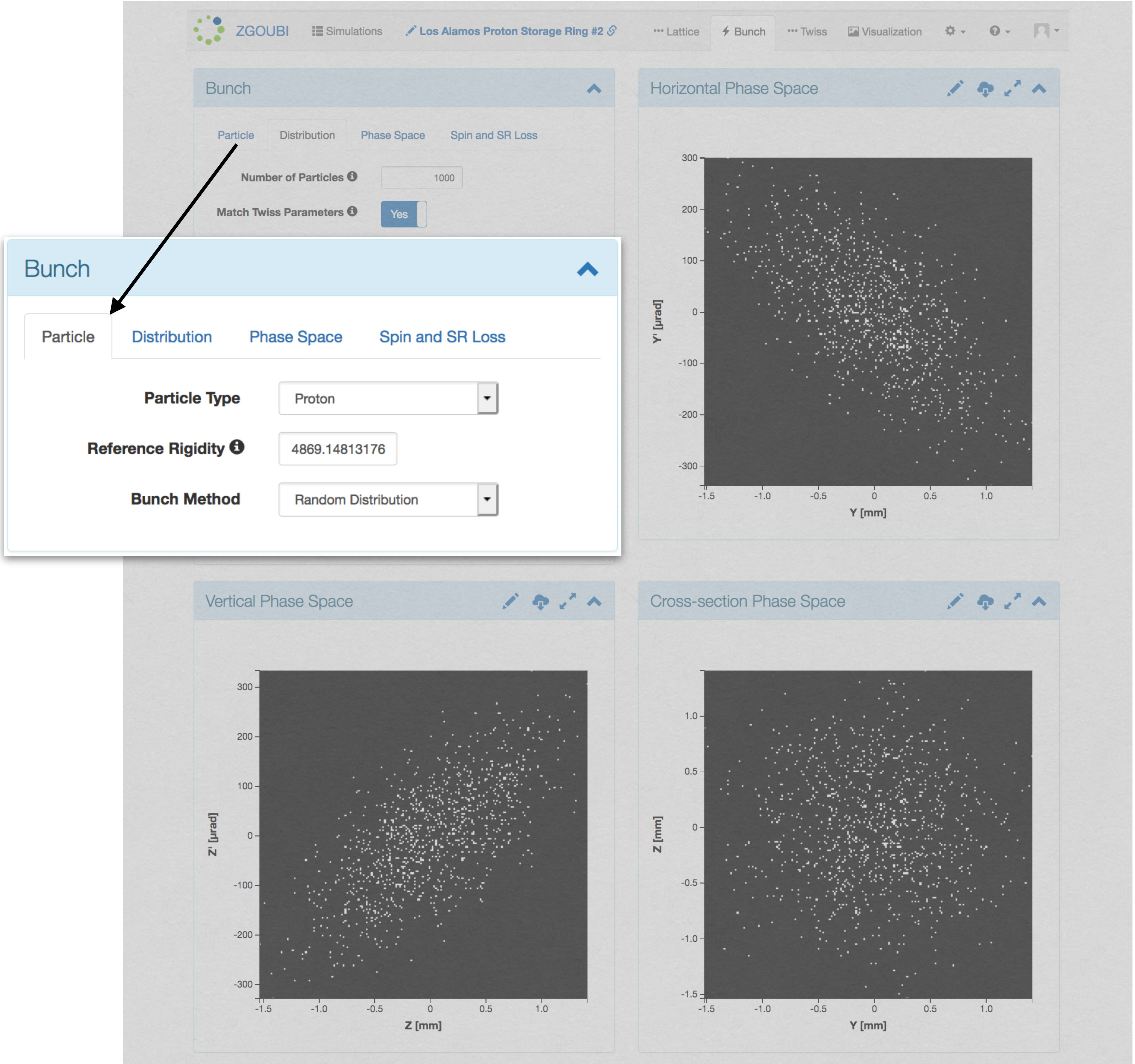


The Sirepo Interface for Zgoubi: Generate a (matched) bunch

Sirepo



The Sirepo Interface for Zgoubi: Generate a (matched) bunch—cont.



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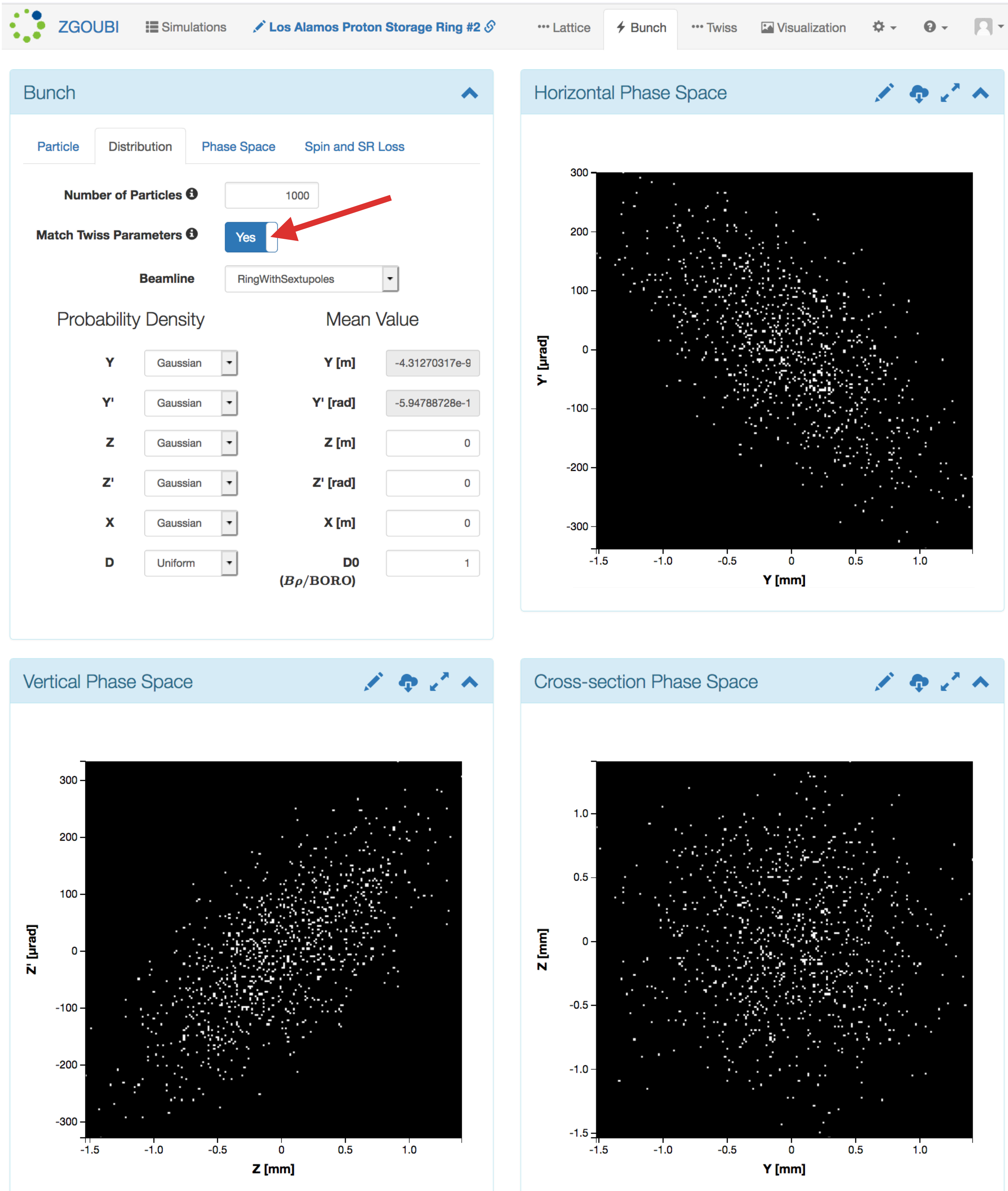
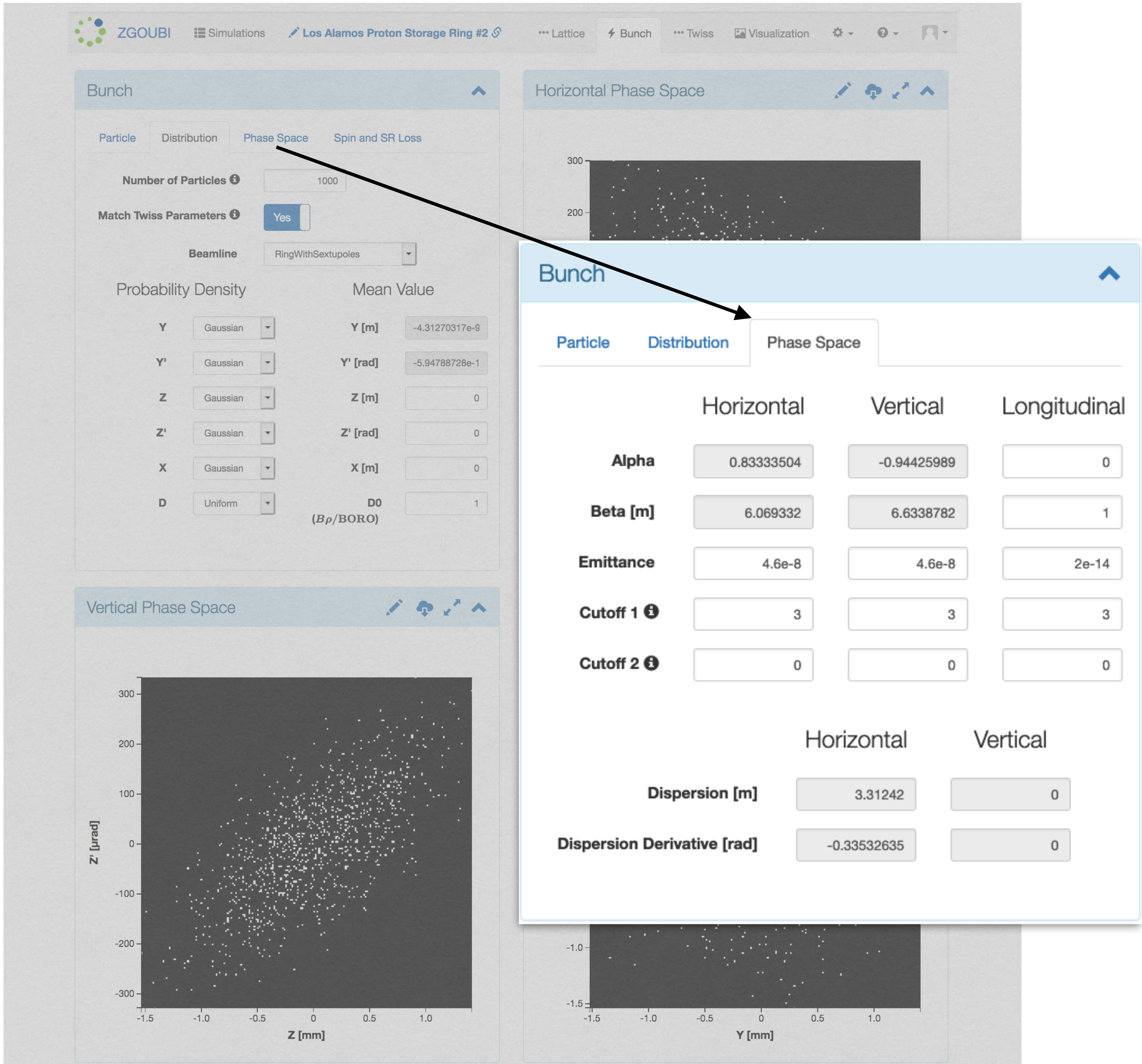


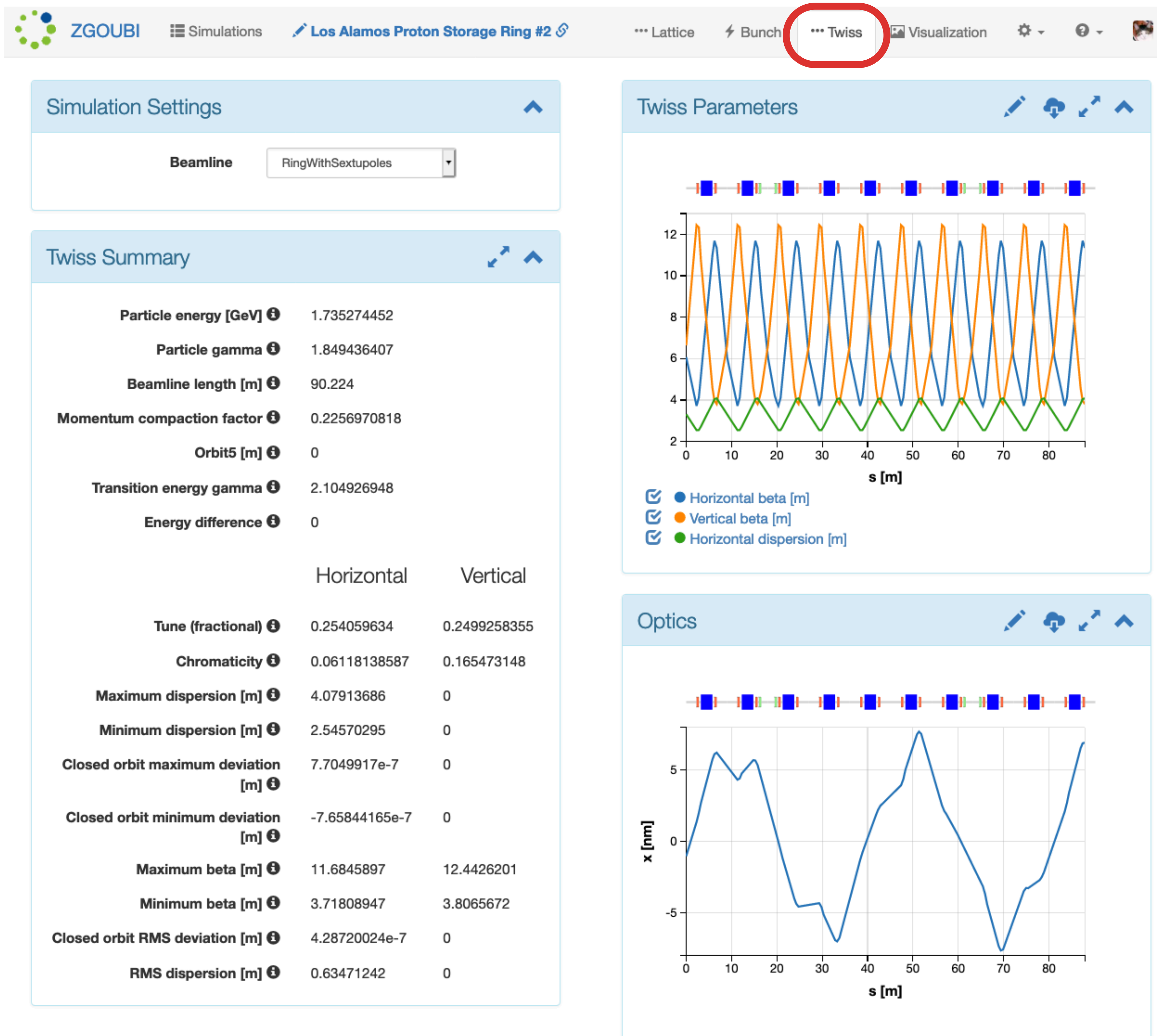
The Sirepo Interface for Zgoubi: Generate a (matched) bunch—cont.

Sirepo

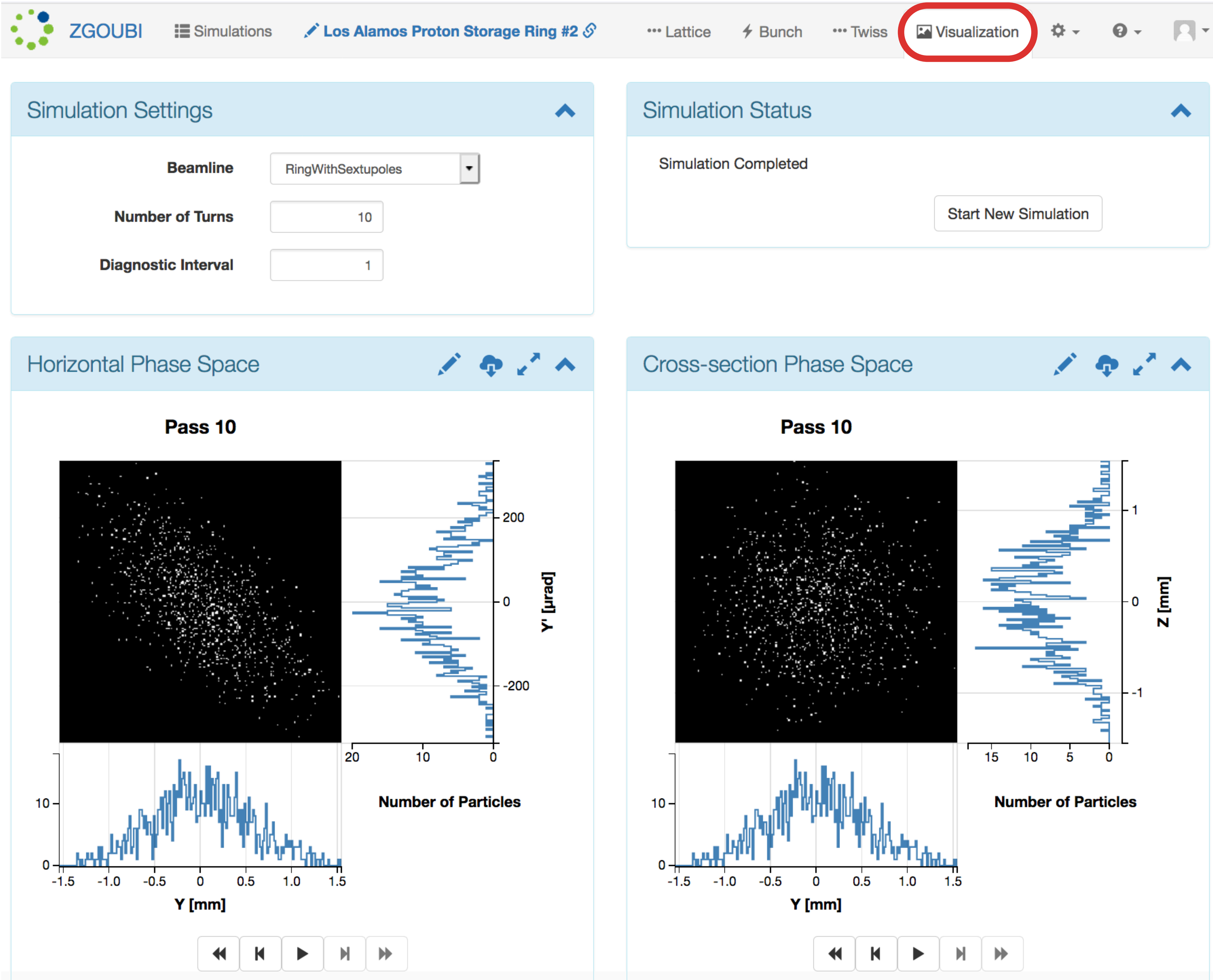


The Sirepo Interface for Zgoubi: View Lattice Parameters

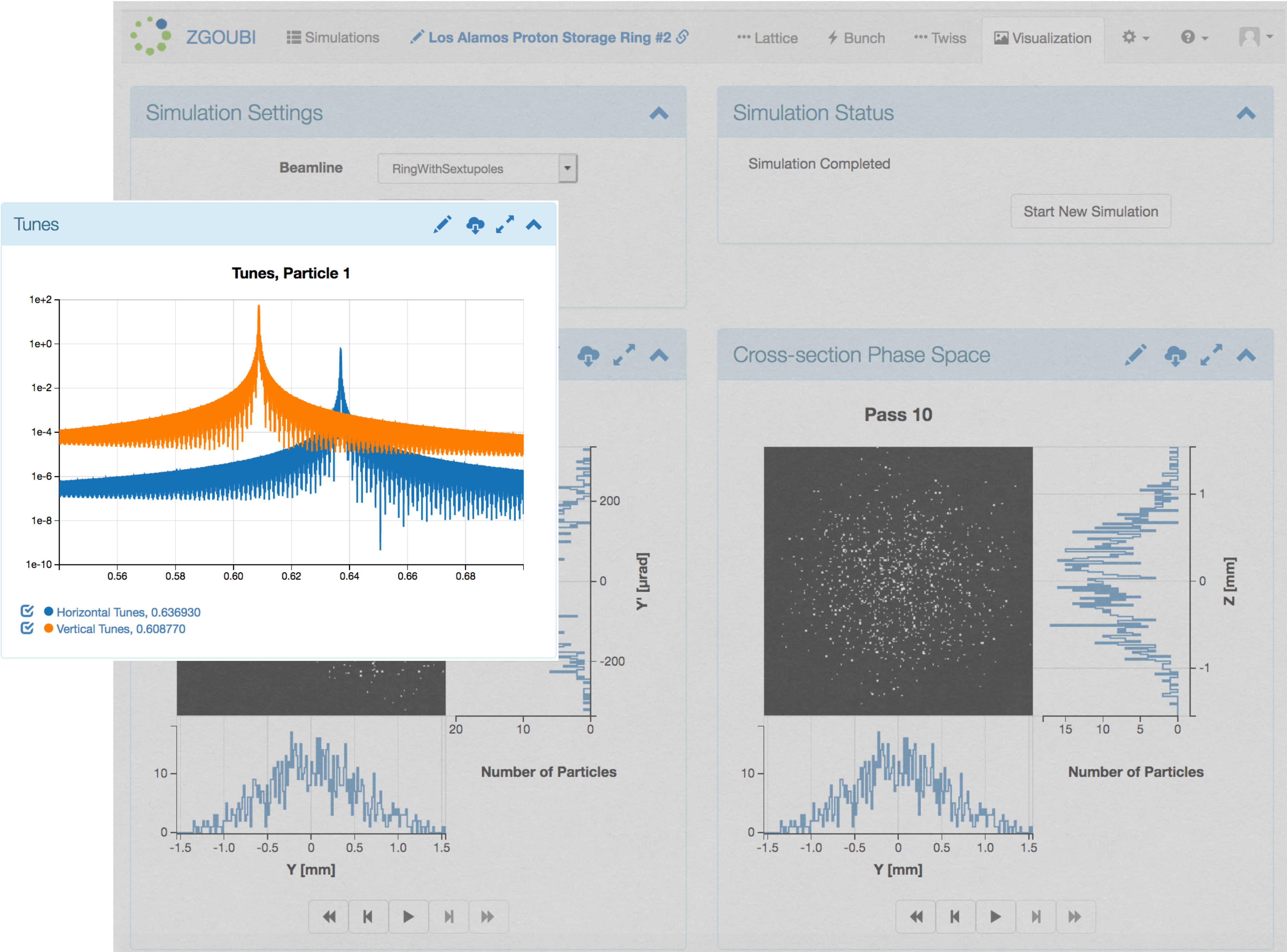
Sirepo



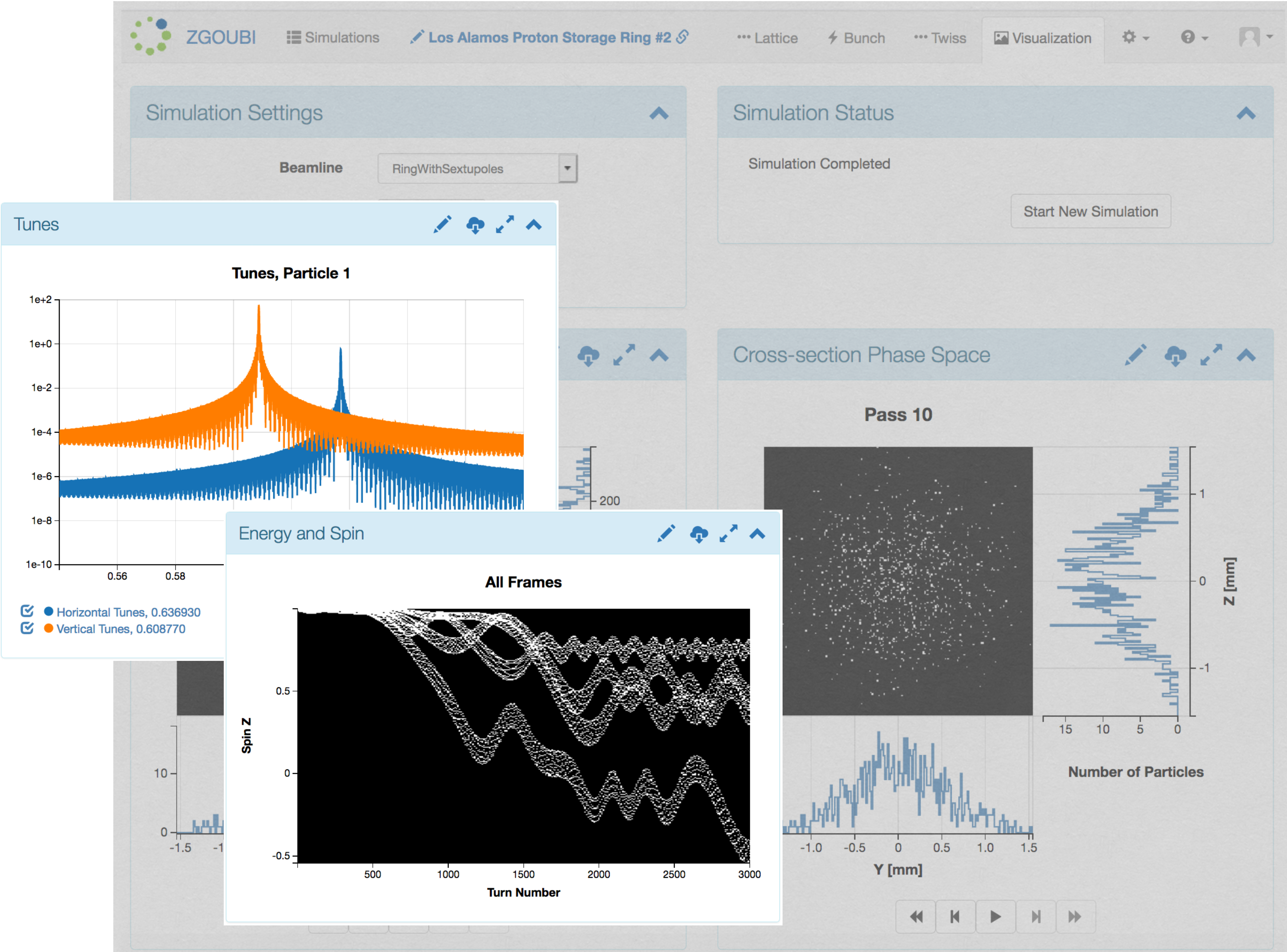
The Sirepo Interface for Zgoubi: Visualize the Beam



The Sirepo Interface for Zgoubi: Visualize the Beam—including tunes



The Sirepo Interface for Zgoubi: Visualize the Beam—including tunes and spin



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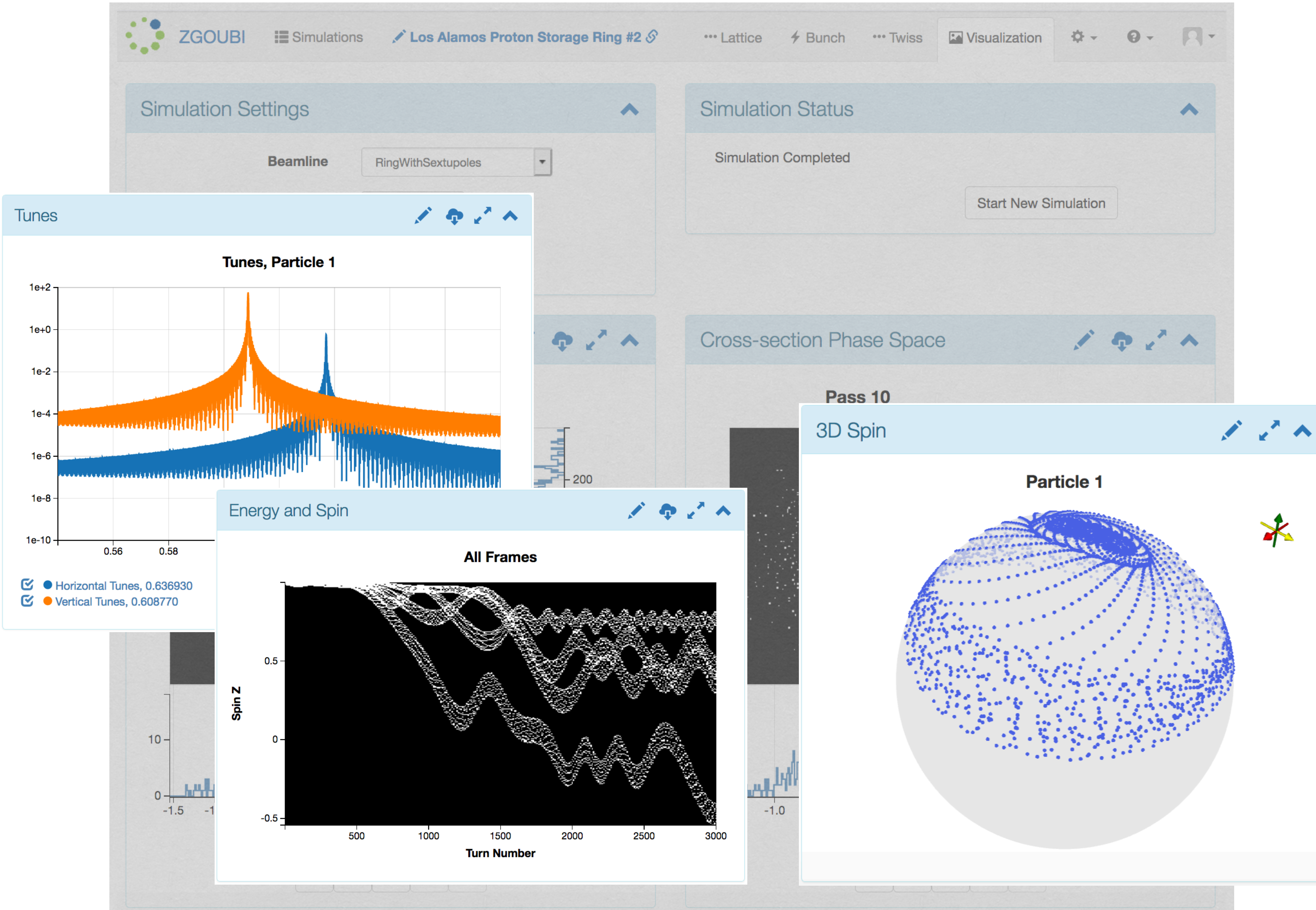
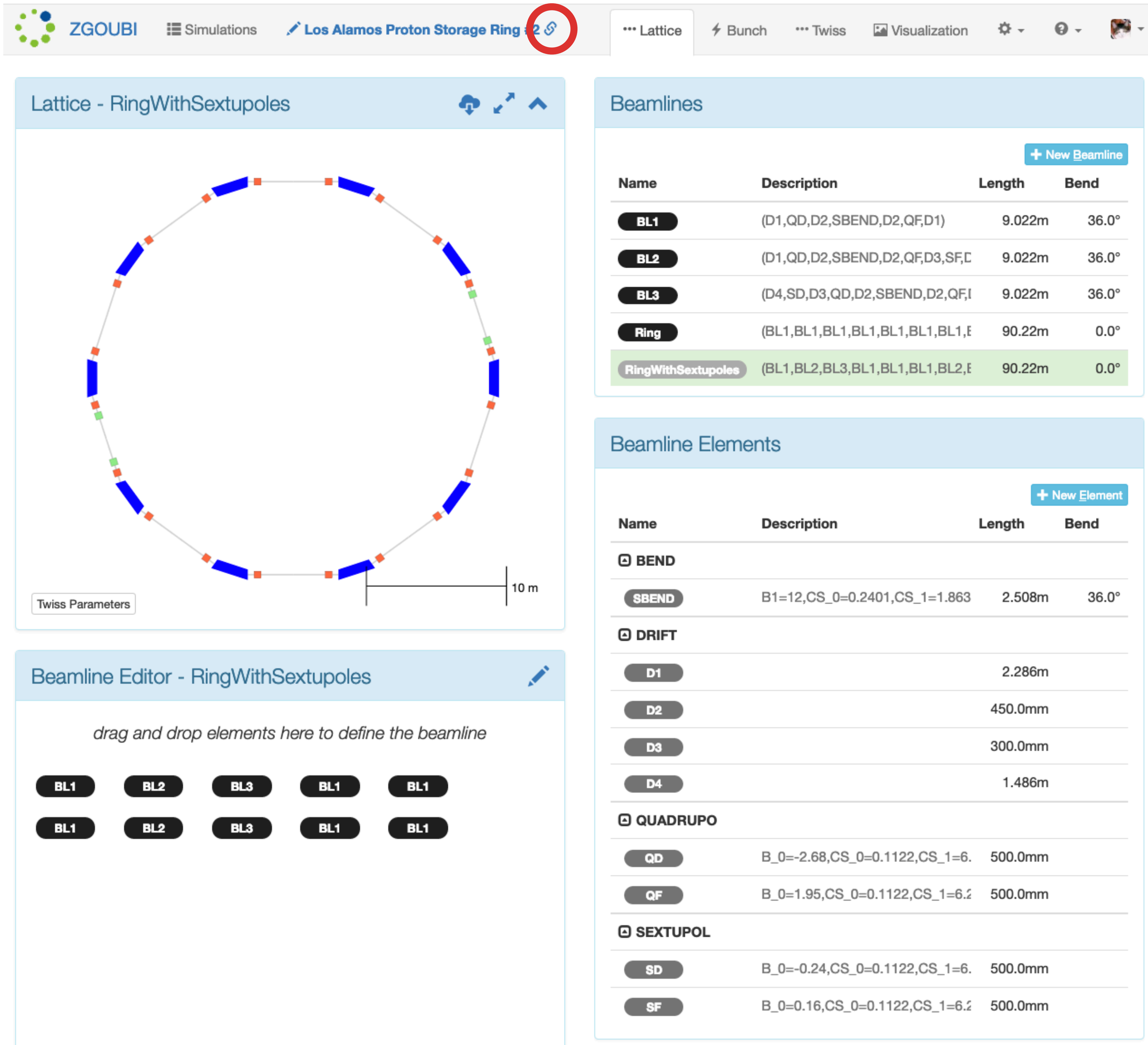


The Sirepo Interface for Zgoubi: Share your Work—Effortlessly!

Sirepo



Improve Performance:
Parallelize Zgoubi using Fortran 2018

Modern Fortran provides facilities for two levels of parallelism:

Fine-grain, at the loop level—requires *pure* functions (no side effects allowed!)

```
do concurrent(iord = 0:nord)
   B(iord+1) = derivB(iord)
end do
```

Coarse-grain, at the processor level—*collective operations*

```
co_min(a)
co_max(a)
co_sum(a)
co_reduce(a, op)
```

and *coarrays*, which "answer the question, 'What is the smallest change required to convert Fortran into a robust and efficient parallel language?'"—John Reid, *ISO/IEC JTC1/SC22/WG5, N1824 (2010)*

Coarray syntax implements a Single Program Multiple Data (SPMD) model. A single program is replicated in units called *images*, and the number of images may be chosen at run time. You must still devise appropriate parallel algorithms, but the case of non-interacting particles is essentially trivial.

```
real :: a[*]   ! scalar coarray
real, dimension(10) :: x[*], y[*]   ! array coarray
real :: m(0:21,6)[*]   ! matrix coarray
type(particle) :: ptcl(128)[*]   ! derived type coarray

x(:) = y(:)[q]   ! access remote data on image q
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A coindex indicates communication.
The programmer must ensure that

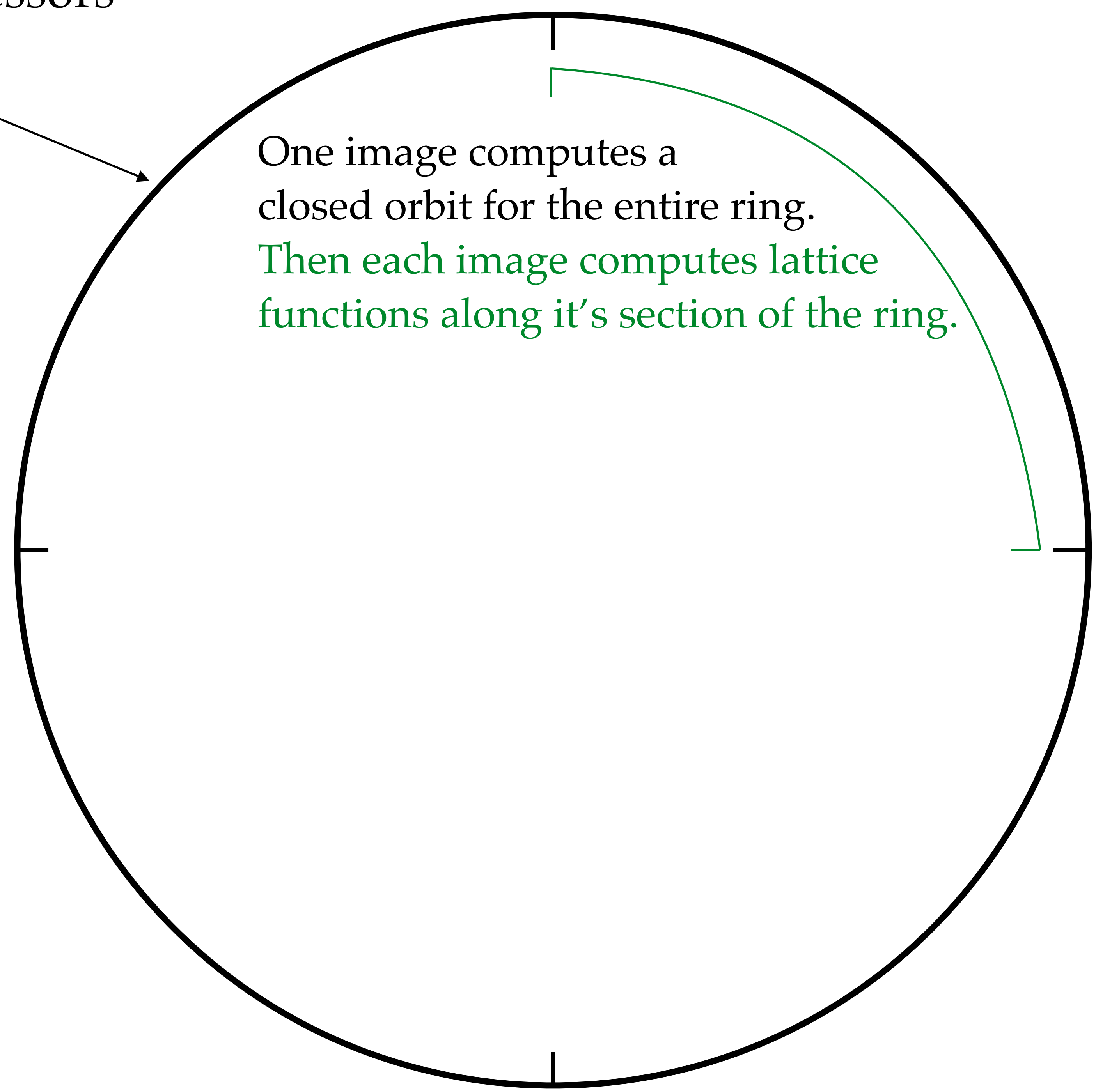
- coarray indices are properly resolved
- synchronization occurs as appropriate.

The new Fortran standard includes new intrinsics that simplify the process, *e.g.* random_init.

Improve Performance: Parallelize Zgoubi using Fortran 2018—cont.

Opportunities for paralellizing Zgoubi:

- Distribute particles on multiple processors
- Distribute lattice computations
- Distribute machine energies
- Distribute misalignments
- Various scans:
  - dynamic aperture
  - polarization studies
  - *etc.*



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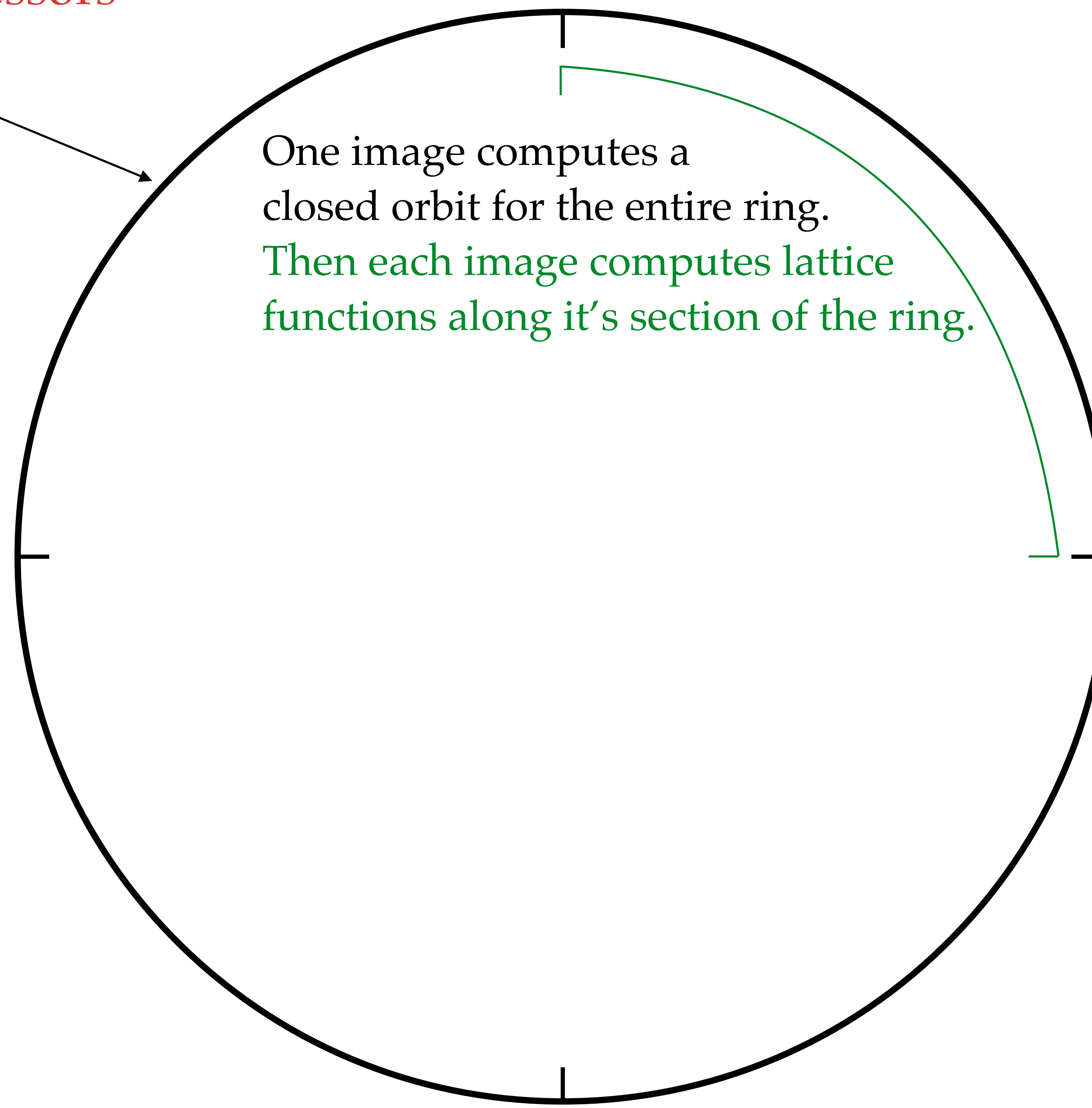

RadiaSoft Revenue Model

Consulting and Contract R&D

- Problem solving across many domains
  - *Accelerator Design*
    - x-ray optics
    - electron linear accelerators
    - free-electron lasers
    - synchrotron radiation
    - high-intensity proton synchrotrons
    - compact ion and accumulator rings
  - *Vacuum Nanoelectronics and Thermionic Converters*
  - *Control Systems*
  - *Machine Learning*
  - *Medical Physics and Treatment Planning*
  - *Theoretical analysis*
  - *Algorithm development*
  - *High-performance computing and computational studies to improve the performance of particle accelerators*
- Custom simulations
  - *Open source codes to eliminate licensing fees*
  - *COMSOL Multiphysics models*
  - *GUIs for customer codes*

Software Design and Development

- Sirepo
  - *Graphical User Interfaces for open-source physics codes*
    - browser-based
    - no installation
    - no maintenance
    - instantaneous collaboration with colleagues
    - high-intensity proton synchrotrons
    - compact ion and accumulator rings
- Sirepo Enterprise
  - *Full instance of Sirepo*
  - *Installed and supported on customer premise*
  - *Protects corporate data and IP*
- HPC Cluster Access On Demand
  - *Pay-as-you-go and subscription access for HPC simulations*
- COMSOL Application Builder
  - *Turn your COMSOL models into apps for increased usage*

Summary and Future Work

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

To share simulations and results with collaborators, simply email the web link.

Responding to feedback as we complete the Sirepo/Zgoubi graphical interface.

Zgoubi Workshop in Boulder, CO; 26–30 August 2019. Participants from BNL, JLab, Argonne, as well as England, Italy, France, and Australia.

Complete the technical work on Zgoubi, with a focus on the needs for our scientific collaboration with BNL on eRHIC, and with JLab on JLEIC.

Summary and Future Work—cont.

Collaborate with BNL to assess and improve the spin dynamics in electron and ion rings for the eRHIC design:

Imperfection resonances are expected to dominate the beam polarization loss during the acceleration ramp. We will extend simulations done so far to use as many as 10^5 particles. This will enable an improved exploration of the full 6-D phase space, including a full range of magnet misalignments, correction settings, and noise in the rf control system.

Collaborate with JLab to benchmark Zgoubi with BMad and other codes used for simulating JLEIC ring designs:

JLab's EIC designs (JLEIC) use a novel figure-8 shape ring possessing a number of beneficial spin dynamics features. New polarization preservation and control techniques have been developed for both ion and electron beams. To improve confidence in the understanding of spin dynamics in the JLEIC designs, we will perform benchmarking simulations between BMAD, SLICK/SLICKTRACK, and Zgoubi.

Thank you!

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

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