## The Sirepo framework for X-ray optics, linac design, machine learning and controls

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Collaborators -

Sirepo team: R. Nagler, P. Moeller, M. Keilman & E. Carlin (RadiaSoft)

X-ray optics: O. Chubar & M. Rakitin (NSLS-II), B. Nash & N. Goldring (RS)

USPAS: K. Ruisard et al. (ORNL)

ML: J. Edelen, N. Cook, C. Hall, S. Webb (RadiaSoft) K. Brown, P. Dyer (BNL), A. Edelen (SLAC)

#### Seminar – SLAC National Accelerator Laboratory

19 September 2019 – Menlo Park, CA

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DE-SC0011340, DE-SC0013855, DE-SC0015897 and DE-SC0018719 (HEP);
DE-SC0015212 and DE-SC0017181 (NP); DE-SC0017057 and DE-SC0017162 (ASCR).

## Outline

- Brief overview of Sirepo
- Sirepo/SRW undulator SR brightness
- Sirepo/elegant use for education
- Sirepo initiatives for controls & machine learning
- Sirepo developments for submitting to NERSC

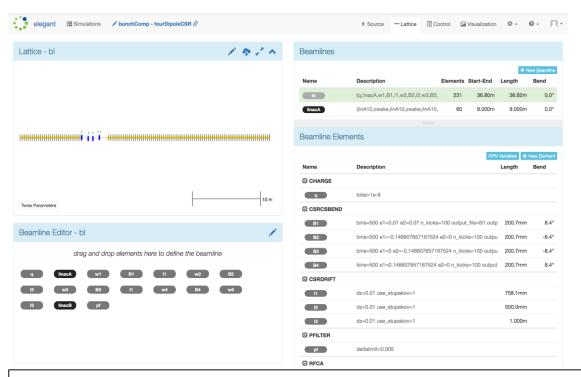


# 2

## https://sirepo.com is a free Scientific Gateway



- Supported Codes
  - SRW
  - elegant
  - Warp VND
  - Warp PBA
  - Synergia
  - Zgoubi
  - JSPEC (e- cooling, IBS)



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

- The power of Sirepo for users
  - 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

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## Sirepo is an open framework for cloud computing

### https://github.com/radiasoft/sirepo

https://github.com/radiasoft/sirepo				110% *** 🛛 1					
Pull requests Issues Marketpla	ice Explore								
📮 radiasoft / <b>sirepo</b>			O Unwatch ▼ 20	★ Star 35 % Fork 20					
Code Issues 406 In P Sirepo is a framework for scienti Manage topics	Pull requests 3 III Project			Edit					
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in etc	Fix #1820 NavController_test commented out			last month					
in misc	expunge.sh			2 years ago					
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<b>A</b> radias	oft	19 Sept	ember 2019 – S	SLAC # 4					

## The Sirepo vision – computational science in the cloud



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- The browser is the Scientific UI
  - via AngularJS, Bootstrap and D3.js
    - 3D graphics via VTK.js
  - share your full simulation via web link
    - ...and many other ways
  - work from tablet, laptop or desktop
  - fast, interactive scientific plotting
- Server is built on Flask & other technologies

M.S. Rakitin, P. Moeller, R. Nagler, B. Nash, D.L. Bruhwiler, D. Smalyuk, M. Zhernenkov and O. Chubar, "Sirepo: an open-source cloud-based software interface for X-ray source and optics simulations," *Journal of Synchrotron Radiation* **25**, 1877 (2018).

Application containers via



- executable, portable; all codes & dependencies
- a single Linux environment for RadiaSoft to maintain

## Online calculations of X-ray photon brightness

- Overview of SRW (Synchrotron Radiation Workshop)
- Brightness formulas

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- Calculating brightness with SRW
- Example calculation for simulated HBB parameters – Trojan Horse; Manahan et al., Nature Comm. (2017)
- Exercise for the audience

   repeat these simulations yourself –

https://sirepo.com/srw#/source/kH9BPjRb

## Synchrotron Radiation Workshop (SRW) -

a physical optics code for SR emission and propagation

First work on Wavefront Propagation applied to SR beamlines (PHASE code): J. Bahrdt, Appl. Opt. 36 (19) 4367 (1997)

 First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); compiled versions are distributed from: <a href="http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW">http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW</a>

Many thanks to Pascal Elleaume.

• SRW was released as Open Source in 2012, thanks to several institutions:

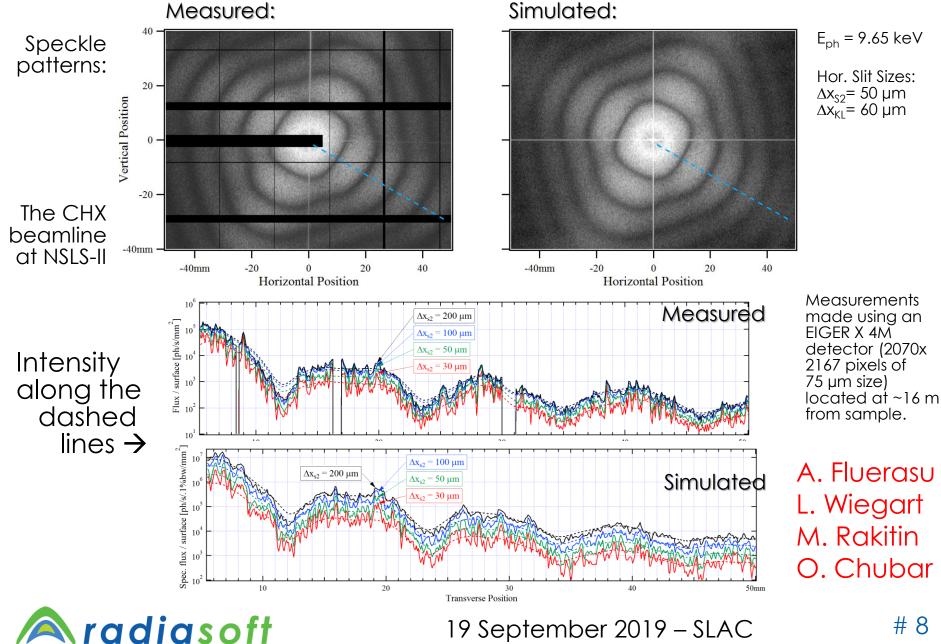


The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: <u>https://github.com/ochubar/SRW</u>

- SRW for Python (2.7.x and 3.x, 32- and 64-bit) was released in 2012
- Sirepo/SRW brings physical optics to the cloud, via support from the US SBIR program of DOE; available from a free Scientific Gateway, hosted by RadiaSoft Sirepo.com

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## SRW validation: coherent scattering exp'ts at NSLS-II

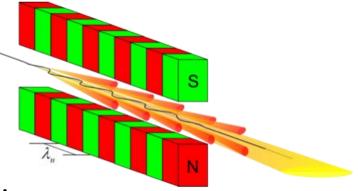


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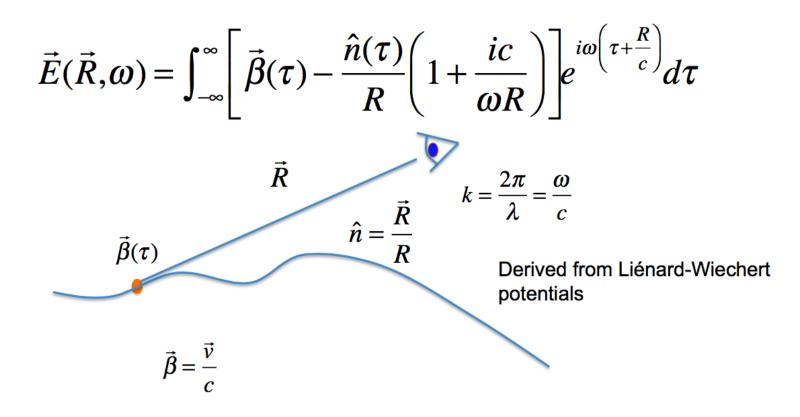
## **Brightness formulas**



## Undulator radiation



Radiation from a single electron trajectory:



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## From radiation wavefronts to "brightness"

Brightness is defined as the phase space density of photon flux:

$$B = W_{me}(0,0) \approx \frac{\Phi}{4\epsilon_x \epsilon_y}$$

$$W_{me}(\vec{x},\vec{p}) = \int W_{se}(\vec{x}-\vec{x}_0,\vec{p}-\vec{p}_0)f_e(\vec{x}_0,\vec{p}_0)d\vec{x}_0d\vec{p}_0 \quad \longleftarrow \text{Multi-electron Wigner func}$$

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## Analytic formulae for undulator SR flux

K.-J. Kim, "Brightness, coherence and propagation characteristics of synchrotron radiation". NIM A **246**, p. 71 (1986).

$$\Phi = \pi C_0 N I_b Q_n(K) \quad \text{photons / s / 0.1\% \delta E/E}_0$$

$$C_0 = \frac{\alpha d\omega/\omega}{q_e} = 4.5546497 \times 10^{13} \text{Coulombs}^{-1} \qquad F_n(K) = \frac{4nq}{1 + \frac{K^2}{2}} J J^2$$

$$Q_n(K) = (1 + \frac{K^2}{2}) \frac{F_n(K)}{n} \qquad JJ = \left[ J_{\frac{1}{2}(n-1)} \left( \frac{nK^2}{4 + 2K^2} \right) - J_{\frac{1}{2}(n+1)} \left( \frac{nK^2}{4 + 2K^2} \right) \right]$$

- We have generalized Kim's result in 3 ways:
  - allow elliptical undulators

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- include effects of e- beam dp/p (also done by Tanaka et al.)
- include off-resonance effects

## Calculating brightness with SRW



## Generalization of the total flux calculation (1)

This is previous, unpublished work by O. Chubar (BNL), which has been implemented in the "Igor Pro" interface to SRW, <u>https://github.com/ochubar/SRW</u>

Recently ported to the SRW Python API, and to the Sirepo/SRW web app.

$$\Phi = C_0 N_u I_b \frac{nk_1^2}{1 + \frac{K^2}{2}} \overline{JJ}^2(qq) F_f(\Delta, \epsilon) G(\Delta, k_1, k_2)$$
allows for elliptical undulators
$$\overline{JJ}^2(n, k_1^2, k_2^2) = \left[J_{\frac{n-1}{2}}(qq) - J_{\frac{n+1}{2}}(qq)\right]^2 + \frac{k_2^2}{k_1^2} \left[J_{\frac{n-1}{2}}(qq) + J_{\frac{n+1}{2}}(qq)\right]^2$$

$$k_1^2 = k_y^2 \cos^2(\phi_x - \phi_0) + k_x^2 \cos^2(\phi_y - \phi_0)$$

$$k_2^2 = k_y^2 \sin^2(\phi_x - \phi_0) + k_x^2 \sin^2(\phi_y - \phi_0)$$

$$qq = \frac{n}{4} \frac{k_1^2 - k_2^2}{1 + \frac{1}{2}(k_1^2 + k_2^2)}$$

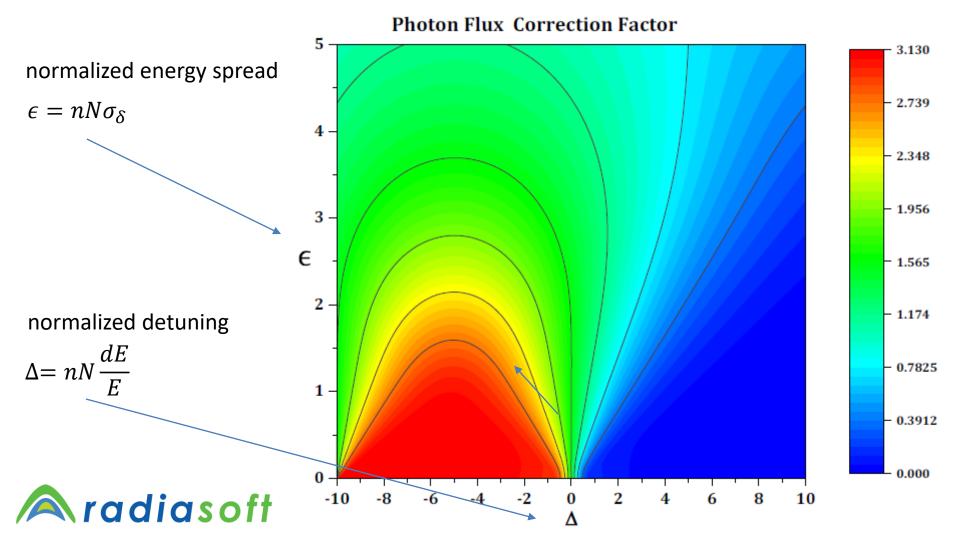
 $F_f(\Delta, \epsilon) \rightarrow$  tabulated "universal function"  $G(\Delta, k_1, k_2) \rightarrow$  analytic function

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B. Nash *et al*, "Detailed X-ray Brightness Calculations in the Sirepo GUI for SRW," AIP Conf. Proc. **2054**, 060080 (2019), <u>https://aip.scitation.org/doi/10.1063/1.5084711</u>

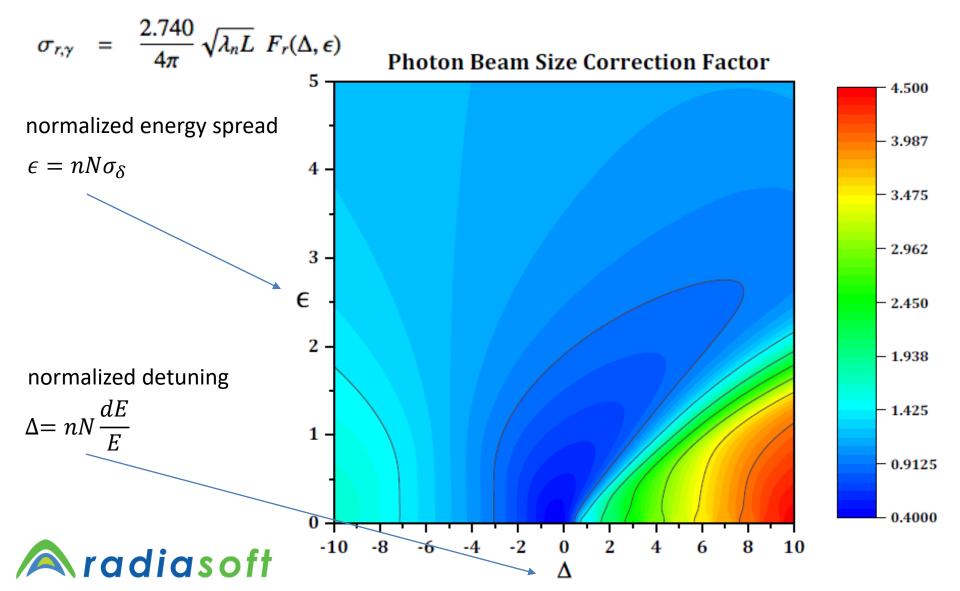
Generalization of the total flux calculation (2)

- A pre-calculated "universal function" is used to:
  - include effects of e- beam dE/E
  - include detuning from resonance

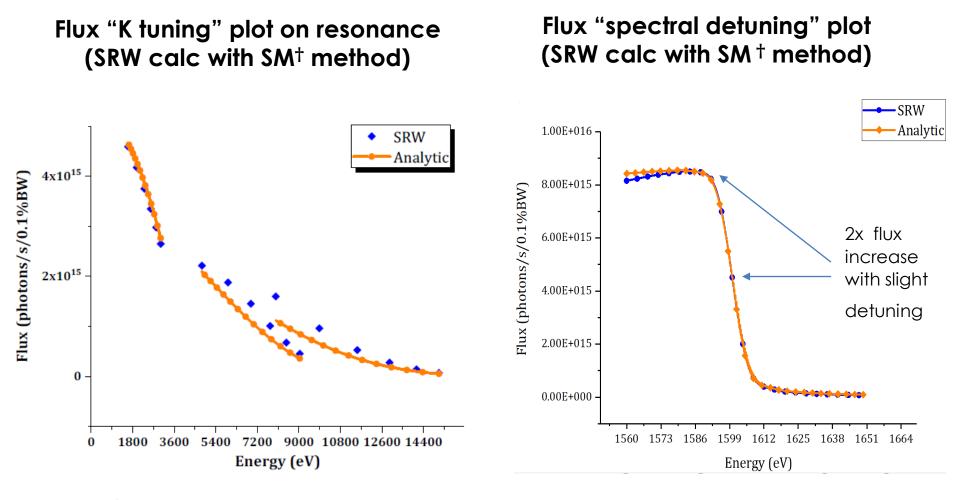


## Generalization of the photon beam source size

This is previous, unpublished work by O. Chubar (BNL), which has been implemented in the "Igor Pro" interface to SRW, <u>https://github.com/ochubar/SRW</u>



## SRW benchmarking results



<sup>†</sup>SM method includes e- beam emittance and energy spread using a finite collection aperture. These calculations executed with an 8 mm x 8 mm aperture.

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## Consideration of Trojan Horse e- beam param's

E = 770 MeV  $\tau$  = 2.5 fs Q = 5 pC  $x_{rms} \sim 5 \mu m$ dE/E  $\sim 5\%$  (uncorrected) dE/E  $\sim 0.3\%$  (via Manahan *et al.*) Article | OPEN | Published: 05 June 2017

Single-stage plasma-based correlated energy spread compensation for ultrahigh 6D brightness electron beams

G. G. Manahan ⊠, A. F. Habib, P. Scherkl, P. Delinikolas, A. Beaton, A. Knetsch, O. Karger, G. Wittig, T. Heinemann, Z. M. Sheng, J. R. Cary, D. L. Bruhwiler, J. B. Rosenzweig & B. Hidding ⊠

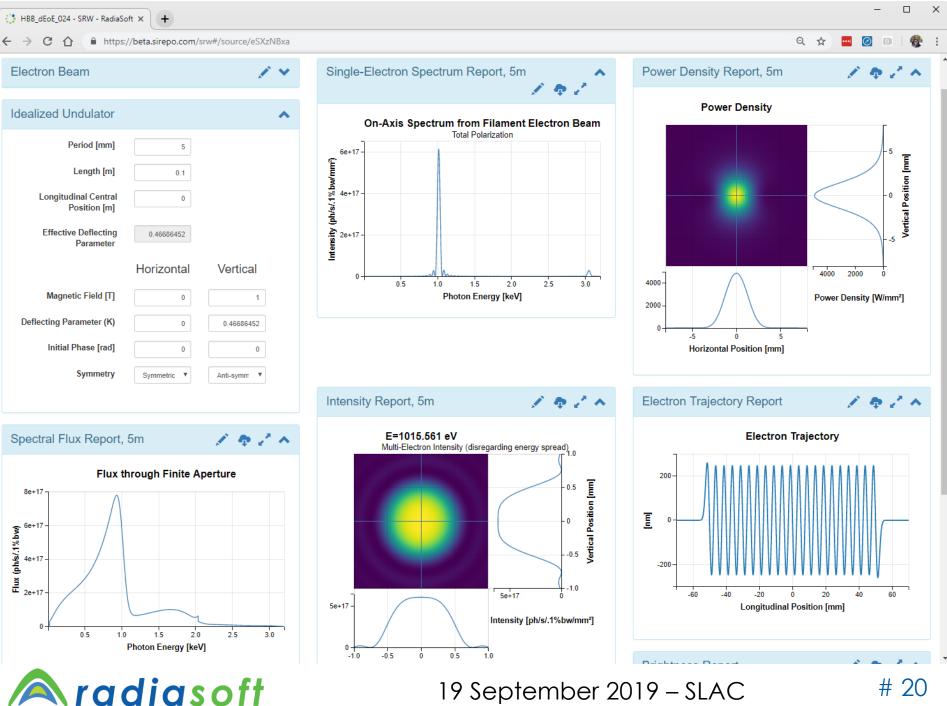
Nature Communications 8, Article number: 15705 (2017) 🔰 Download Citation 🛓

1 KeV can be achieved: requires a micro-undulator,  $\lambda_u = 5$  mm requires strong quadrupole focusing  $L_u$  is kept short here: 10 cm = 20 periods

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## Browser-based simulations of X-ray brightness

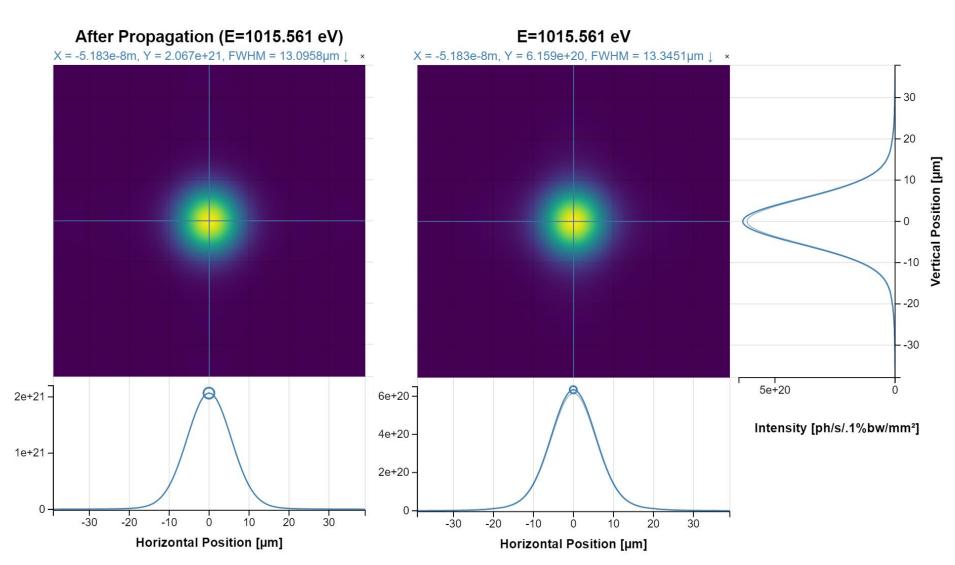




## Energy spread reduces flux

• e-beam energy spread of 0.3% to 4.8%

- photon flux decreases by 3x



## X-ray optics & brightness – conclusions

Classic formula for brightness by K.-J. Kim is a starting point.

This formula needs to be generalized to include energy spread, detuning effects, and to allow for elliptical undulators.

Partially coherent Sirepo/SRW wavefront simulations agree with the generalized brightness formulae

Sirepo provides a convenient GUI for SRW calculations.

Analytic formulae in Sirepo provide rapid feedback for source parameters allowing a starting point for more detailed coherent and partially coherent calculations for realistic x-ray beamlines.

Repeat our calculations yourself:

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https://sirepo.com/srw#/source/kH9BPjRb

## US Particle Accelerator School – <u>http://uspas.fnal.gov</u>

Home

The 2019 USPAS Achievement

 The 2019 International Accelerator School on "Ion Colliders" will be held

Nov 7. Information is available

Find us on **f** 

here

in Dubna, Russia from October 28 to

Prize winners have been announced. Read more here.

- intensive 1 & 2 week courses
  - Sirepo has been used 4 times
    - used elegant
- other examples of Sirepo use:
  - Korea particle accelerator school
    - Used Synergia
  - La Trobe University
    - X-ray optics
    - used SRW

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#### 



#### Accelerator Tutorials

#### LHC Superconducting Magnets

Watch this first video, in a sequence of three, explain the role of superconducting magnets in the Large Hadron Collider and also explain how they work and are constructed. Used with permission: CERN

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See more Accelerator Tutorials.

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## Simulation of Beam and Plasma Systems

https://people.nscl.msu.edu/~lund/uspas/sbp\_2018

- S. Lund, J.-L. Vay, R. Lehe, D. Winklehner
  - expanded 1 week course to 2 weeks
  - invited me to contribute
- Sirepo/elegant used to discuss CSR
  - principles of bunch compression
  - CSR models and the physical effects
- RadiaSoft now routinely supports schools and workshops with a 400 core cluster
  - JupyterHub and/or Sirepo
  - rapid reconfiguration as needed to support specified number of students
  - other nodes reserved for internal computing
  - nodes are routinely made available to customers or collaborators

US Particle Accelerator School Winter Session, 2018 15-26 January Sponsored by Old Dominion University Hampton, VA 2 Week Course (3 units)

#### Lecturers:

Prof. Steven M. Lund Michigan State University Physics and Astronomy Department Facility for Rare Isotope Beams (FRIB) 510-459-4045 (mobile) Lund@frib.msu.edu

Dr. David Bruhwiler Radiasoft, LLC Boulder, CO 720-502-3928 (Office) Bruhwiler@Radiasoft.net

Dr. Rémi Lehe Lawrence Berkeley National Laboratory (LBNL) 510-486-6785 (LBNL Office) RLehe@lbl.gov

Dr. Jean-Luc Vay Lawrence Berkeley National Laboratory (LBNL) 510-486-4934 (LBNL Office) JLVay@lbl.gov

Dr. Daniel Winklehner Massachusetts Institute of Technology (MIT) 510-479-6501 (mobile) winklehn@mit.edu



## Sample from the final exam –

## Problem 4 - Sirepo/elegant

- a) Create a copy of an existing Sirepo/elegant simulation, by pasting this URL into your browser: https://uspas-sirepo.radiasoft.org/elegant#/source/o7oYeBDe
  - 1 Modify the 4<sup>th</sup> dipole of your chicane by enabling the OUTPUT FILE parameter, on page 5 of the parameter input window.
    - Make sure that N Kicks = 16 for the dipole.
    - Make sure you have steady-state CSR turned on by setting value = 1 for the alter\_elements command with item = STEADY\_STATE, name = BEND?.
  - 2 Go to the Visualization tab and click "Start new simulation".
    - You may see an error message: "elegant Errors: warning: 7 elements had no matrix", but you can ignore it.
    - In the window for BEND4, plot DeltaGamma vs. s.
    - This is a plot of the CSR wakefield along the bunch with the field plotted in units of  $\Delta \gamma/m$ .
    - Each plot is at one of the 16 steps through the dipole.
    - Rewind the movie to the beginning, then step through the images one by one.
    - Observe how the wake evolves as the beam enters the dipole.
    - Go back to the beginning again, then step one by one through the first 5 images, saving each of them to a file.
    - The first image should look like Figure 1.

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# Sirepo/Elegant classroom example: USPAS fundamentals of accelerator physics

Kiersten Ruisard

Sirepo User Workshop, Sept. 3, 2019

On behalf of Jan 2019 teaching team: Jeff Holmes, Sarah Cousineau, Nick Evans, Martin Kay

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

# Sirepo/elegant used for a lab in the January & June 2019 "Fundamentals" course

#### Jan 2019 teaching team:

Jeff Holmes, Sarah Cousineau, Nick Evans, Kiersten Ruisard & Martin Kay

June 2019 teaching team:

Linda Spentzouris, Pavel Snopok, Nicole Neveu, Josiah Kunz, Tanaz Mohayai, Elvin Harms and Bob Zwaska Jan 2019 Fundamentals Course

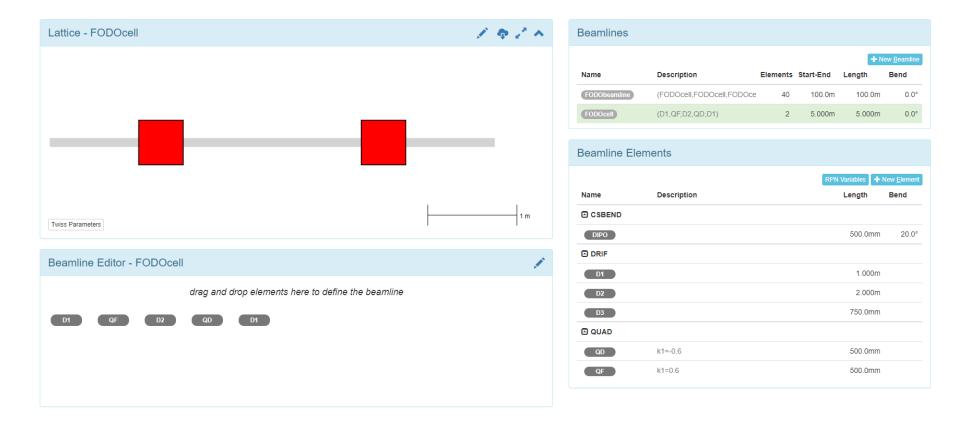


Photo by Irina

The Sirepo lab is comprised of 3 exercises:

- 1. Matched/mis-matched beam in FODO line
- 2. Dispersion and chromaticity
- 3. Build your own beamline (offered as optional/extra credit)

# Exercise 1: Matched/mismatched beam propagation in FODO line

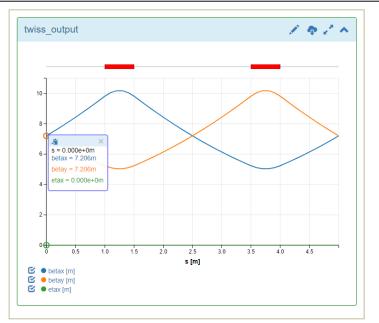


#### D. Propagation of mismatched beam

We will initialize our beam with a 10% mismatch and examine the effect this has on transport. In the periodic solution,  $\beta_x = \beta_y = 7.206$  meters and  $\alpha_x = -\alpha_y = 1.122$ . (You can verify this by interacting with the twiss\_output plot or downloading the data in CSV format).

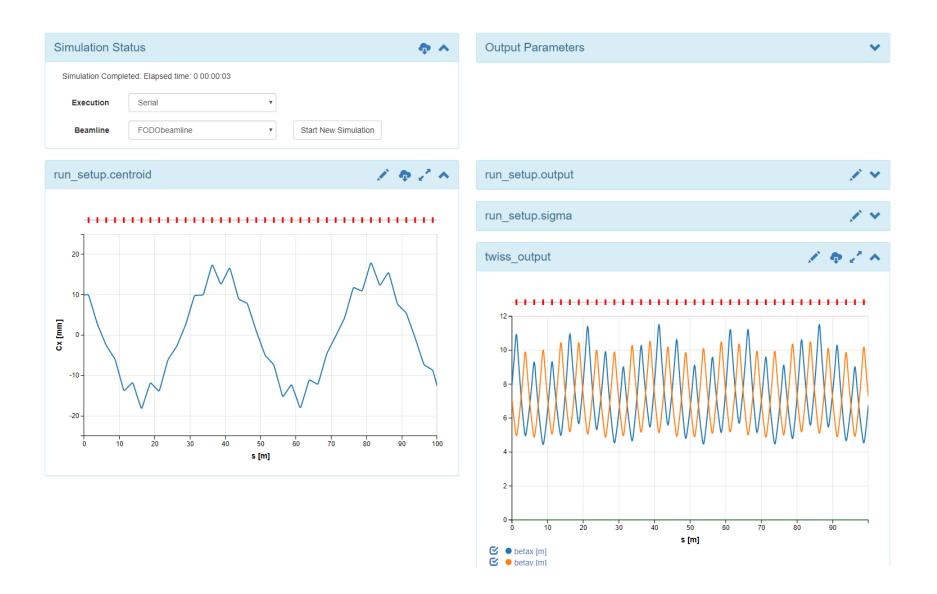
To initialize a mismatched beam, under the "Control" Tab and "twiss\_output" module, set the following fields:

Parameter	Value
Matched	No
Beta X (pg 2)	7.206 * 1.1
Alpha X (pg 2)	-1.178
Beta Y (pg 3)	7.206 * 1.1
Alpha Y (pg 3)	1.178





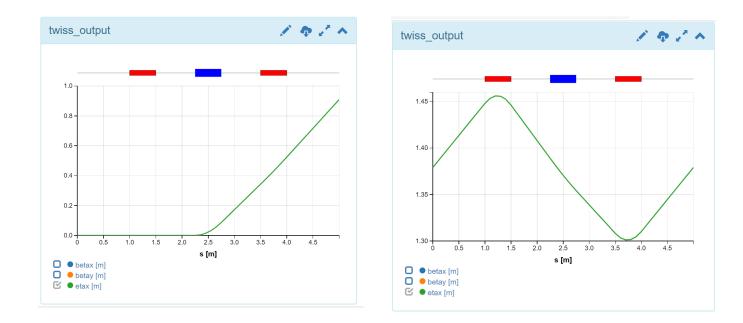
twiss_output		<b>()</b> ×
compute and output uncoupled Twiss parameters, or set up to	do so.	
Page 1 Page 2 Page 3 Page 4		
Filename 🕄	twiss_output_tangme.sdds	
Matched 🕄	No VS	
Output At Each Step 🕄	No Yes	
Output Before Tune Correction 😫	No <b>v</b>	
Final Values Only 🕄	No <b>v</b>	
Statistics	No <b>v</b>	
Radiation Integrals	No	
Concat Order 🕄	3	
twiss_output		<b>?</b> ×
compute and output uncoupled Twiss parameters, or set up to	do so.	
Page 1 Page 2 Page 3 Page 4		
Higher Order Chromaticity 🕄	No	
Higher Order Chromaticity Points	5	
Higher Order Chromaticity Range	4e-4	
Chromatic Tune Spread Half Range 🚯	0.0	
Quick Higher Order Chromaticity	No	
Beta X 🤂	7.206*1.1	7.9266
Alpha X	-1.178	
Eta X	0.0	
(ORNL)	ave Changes Cancel	



# **Exercise 2: Dispersion and Chromaticity**

elegant 🔚 Simulations 🖍 FODObeamline 🔗			✤ Source	••• Lattice	Contro	ol 🍱	Visualization	¢ -	0 · []
Lattice - FODOcell	1. 4. 2. 4	Beamlines							
		Name	Description					Length	New <u>B</u> eamline Bend
		FODObeamline FODOcell	(FODOcell,FODC		II,FODO	40 2	100.0m 5.000m	100.0m	
		Beamline Elen	nents						
		Name	Description				RPN	Variables + Length	- New <u>E</u> lement Bend
Twiss Parameters	1 m							500.0mm	n 20.0°
Beamline Editor - FODOcell	1	DRIF						1.000m	1
drag and drop elements here to define	the beamline	D2 D3						2.000m 750.0mm	
D1 QF D2 QD D1	Saved to this PC		k1=-0.2					500.0mm	1
		QF	k1=0.2					500.0mm	1
		(DAD) <b>A</b>							0.000-114
	ANGLE	[RAD] 🖯							20*pi/1

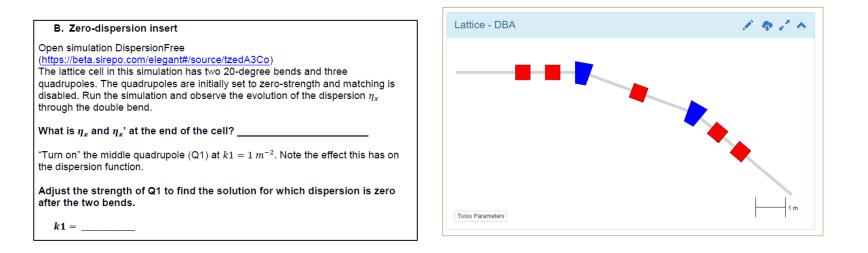
## https://beta.sirepo.com/elegant#/source/tzedA3Co

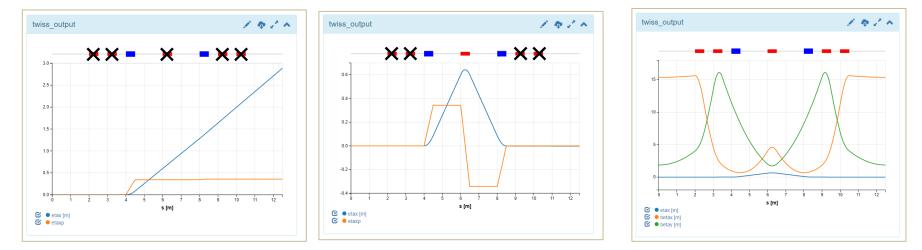


Assuming a 0.1% energy spread in the beam, what is the horizontal beam size we expect in the focusing quadrupole QF? How does this compare to our beam size without energy spread?  $\frac{\Delta p}{p_0}$ 

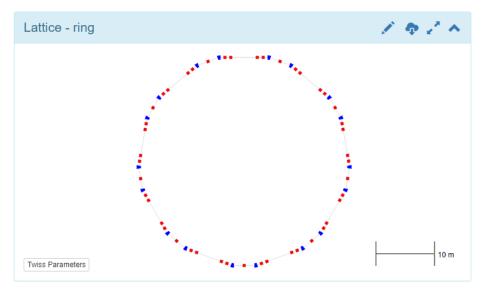
$$\sigma_x^2 = \epsilon_x \beta_x + \eta^2 \frac{\Delta}{\mu}$$

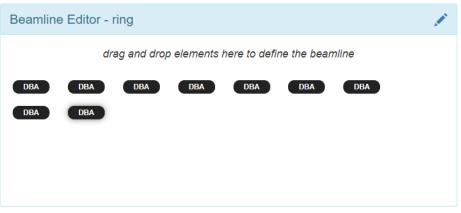
 $\sigma_x =$ 





C. Tune in a ring
Repeat your cell 9 times to create a ring; propagate particles; Record x and y tunes (to 3 significant figures):
$v_x = $ $v_y = $
Note that this lattice still has chromaticity; that is, although off-momentum particles will not increase the beam size in the dispersion-free drifts, they will still feel different focusing strength and have a tune different from the on-momentum particles. For a 0.1% energy spread in the beam, what is the spread of tunes due to chromaticity? $\Delta v_x = C_x \frac{\Delta p}{p_0}$ hint: in Elegant Twiss output, look for dnux/dp and dnuy/dp for chromaticity values
$\Delta v_x = \_$ $\Delta v_y = \_$





## Summary of USPAS experience

- One of the established "Fundamentals" labs has recently been replaced with a Sirepo/elegant lab
- Sirepo/elegant lab focuses on beamline design, lattice functions
- Generally positive student feedback

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- Portability and GUI are great for instructional use
- Recent interest at USPAS in "modernizing" computer labs → continued use of Sirepo

Machine Learning @ RadiaSoft: An overview of recent developments and projects

Jonathan Edelen, Nathan Cook, Christopher Hall and S. Webb with the Sirepo team Kevin Brown, Philip Dyer Auralee Edelen



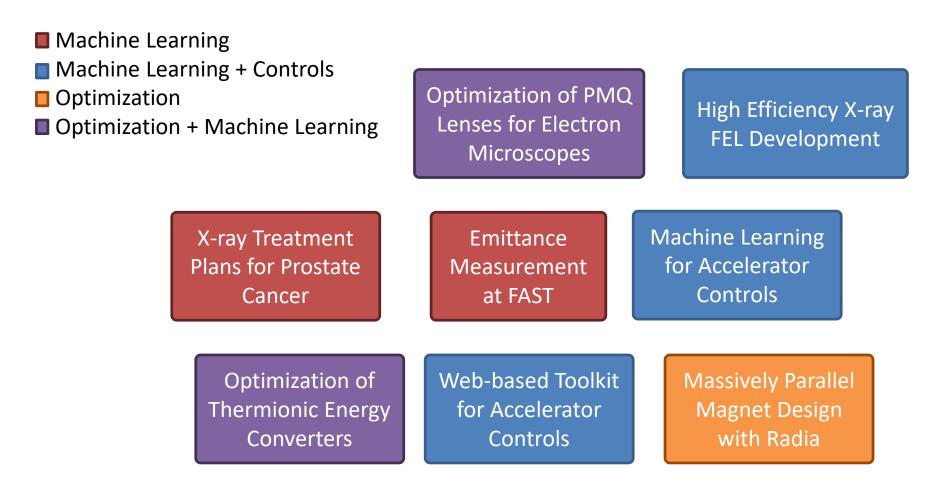




Adapted from a recent presentation for:

Advanced Control Methods for Particle Accelerators Santa Fe, New Mexico – 21 Aug 2019

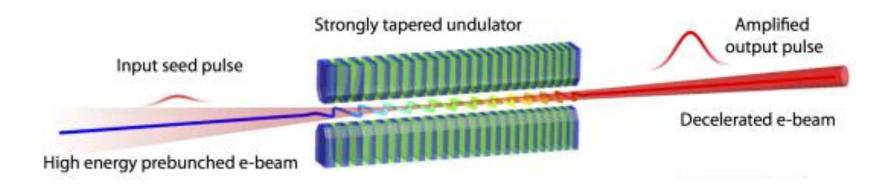
## RadiaSoft projects involving ML/Controls/Optimization





## The TESSA-266 proof-of-principle experiment a high-efficiency FEL

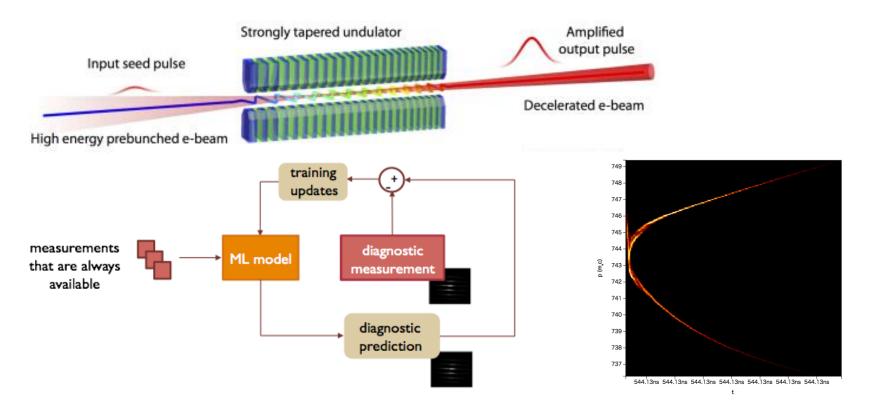
A collaboration between ANL, UCLA, RadiaBeam and RadiaSoft



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J. Duris et al. "Tapering enhanced stimulated superradiant amplification", New J. Phys. (2015).

# **TESSA-266:** plans for virtual (non-intercepting) phase space diagnostics

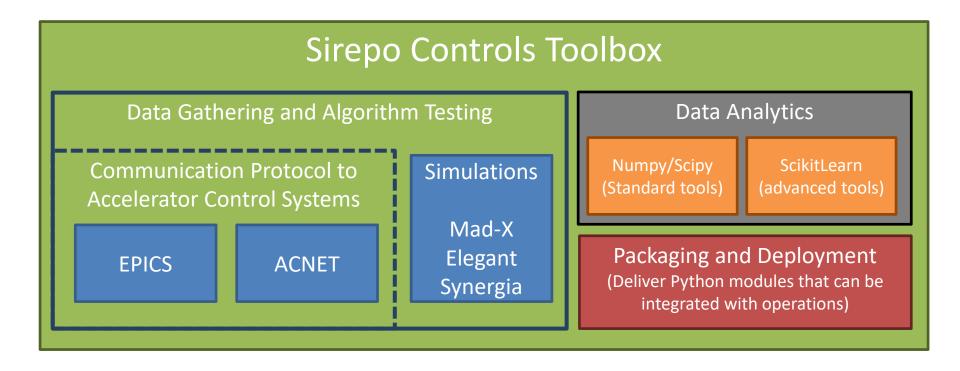


- We want to know the shot-to-shot longitudinal phase space going into the tapered TESSA undulator, which is an intercepting diagnostic
- LEA beamline has CSR, wake fields, and longitudinal space charge, which can cause shot to shot variation in the LPS that we need to understand to analyze TESSA performance

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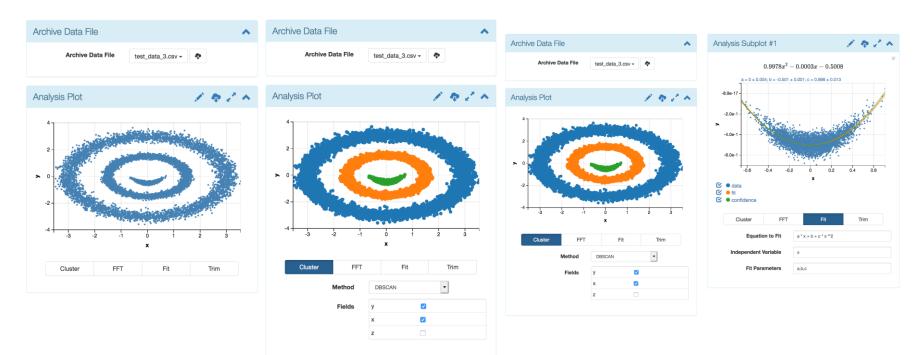
## A web-based toolkit for accelerator controls

 Develop an easy to use framework using Sirepo for developing and testing control algorithms and improving operations



## Prototype web interface for data analysis

- Develop interface and connect with analytics toolboxes
- Currently implemented features:
  - Curve fitting, clustering, frequency analysis, plotting and datasplitting
- Features to be implemented in Ph-1
  - 2-D histograms , 2-D frequency analysis



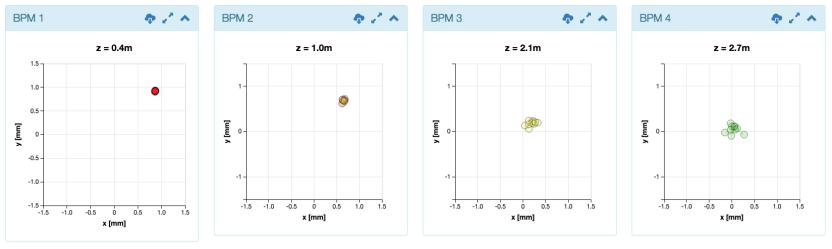
## Prototype web interface for control development

					E Analysis	Controls	\$~	0 -	1.
▲ Beam Steering									
Connect to EPICS Yes Use Steering Yes									
Running Nelder-Mead									
			-						
HV KICKER 2	•	HV KICKER 3		•	HV KICKER	4			^
H. Kick [rad]	-2.54501e-4	H. Kick [rad]		1.76276e-4	H. Kick [ra	d]		2.2933e	<del>≽</del> -4
V. Kick [rad]	-7.96997e-5	V. Kick [rad]		2.62518e-4	V. Kick [ra	d]		2.303276	-4
D QUAD 1	*	F QUAD 2		~	D QUAD 2				~
Strength [1/m <sup>2</sup> ]	5	Strength [1/m <sup>2</sup> ]		-5	Strength [1/m	n²]			5
	HV KICKER 2 H. Kick [rad V. Kick [rad	Use Steering Yes Running Nelder-Mead HV KICKER 2 H. Kick [rad] -2.54501e-4 V. Kick [rad] -7.96997e-5 D QUAD 1	Use Steering Yes Running Nelder-Mead HV KICKER 2 HV KICKER 2 HV KICKER 3 H. Kick [rad] -2.54501e-4 V. Kick [rad] -2.54501e-4 V. Kick [rad] X. Kick [rad] V. Kick [rad] F QUAD 2	Use Steering         Yes           Running Nelder-Mead           HV KICKER 2         HV KICKER 3           H. Kick [rad]         -2.54501e-4           V. Kick [rad]         -7.96997e-5           D QUAD 1         F QUAD 2	Use Steering Yes Running Nelder-Mead HV KICKER 2 H. Kick [rad] -2.54501e-4 V. Kick [rad] -7.96997e-5 H. Kick [rad] 2.62518e-4 V. Kick [rad] 2.62518e-4 Kick [rad] 2.62518e-4	Beam Steering   Use Steering   Running Neider-Mead     HV KICKER 2   H. Kick (rad)   -2.54501e-4   V. Kick (rad)   -7.96997e-5     HV KICKER 3   H. Kick (rad)   -2.54501e-4   V. Kick (rad)   -2.62518e-4   D QUAD 1     F QUAD 2	Beam Steering   Use Steering   Yes   Running Nelder-Mead     HV KICKER 2   H. Kick (rad)   -2.54501e4   V. Kick (rad)   -2.5251e4   D QUAD 1     F QUAD 2	Beam Steering   Use Steering   Running Nelder-Mead     HV KICKER 2   H. Kick (rad)   -2.54501e4   V. Kick (rad)   -7.96997e5     HV KICKER 3   H. Kick (rad)   -2.54501e4   V. Kick (rad)   -2.54501e4   D. QUAD 1     F. QUAD 2	Beam Steering   Use Steering   Running Neider-Mead     HV KICKER 2   HV KICKER 3   HV KICKER 4   H. Kick (rad)   -2.54501e4   V. Kick (rad)   -2.54501e4   D QUAD 1     F QUAD 2

 Interface connects to EPICS database currently running an elegant simulation of a simple beam-line

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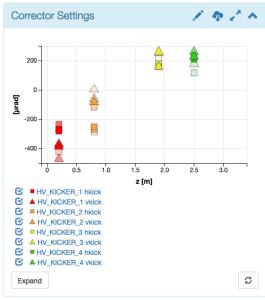
## Prototype web interface for control development





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**A**radiasoft

Present initiative: single-click supercomputing

- Sirepo web server does not require HPC resources
  - simulation requests are submitted to other nodes
  - available servers are configured when Sirepo server is started
  - typically a moderately sized cluster
  - MPI-based codes are typically executed on a single node
- How do you increase the resolution or particle number?
   it would be convenient and powerful to submit jobs at NERSC
- Present server-side technology is being refactored
  - Celery provides an asynchronous job queue for executing longrunning simulations and provides cluster management
  - It uses RabbitMQ as a message broker for communication between the web server and the execution nodes.

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Present initiative: single-click supercomputing

- We need to support Torque, SLURM, PBS, etc.
  - Sirepo's job management system is being redesigned
  - implementing a Docker-based job execution environment
    - more efficient, robust and secure than Celery/RabbitMQ
- The new implementation will rely on Tornado
  - highly concurrent web server/framework
  - provides a microservice called the "Job Supervisor"
    - manages the Sirepo job queue
    - can start "Job Agents" on remote clusters and supercomputers
    - also for local use development & single-node deployments
  - Agents create a WebSocket to communicate with Supervisor
    - enables fast, asynchronous inter-process communication
    - will go through common firewalls
  - Agents will start jobs, cancel jobs, extract in situ visualizations, report job progress, etc.

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Present initiative: single-click supercomputing

- Sirepo will be enhanced to support single-click execution on supercomputers and remote clusters
  - Users will be asked for a token or other credentials
  - The Sirepo NERSC interface will use multifactor authentication,
    - create a token that Supervisor uses to login via NERSC Web Toolkit (NEWT) interface
    - will invoke an Agent running inside NERSC's SHIFTER environment
    - departmental clusters may require users supply SSH keys
- implementation should be completed in 2019



## Thanks!

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