An open source platform for integrated design and control of compact radiation sources

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Sirepo development has been supported by the Department of Energy, Office of Science SBIR program under Award Nos. DE-SC0011237, DE-SC0011340, DE-SC0013855, DE-SC0015212, DE-SC0015897, DE-SC0017162, DE-SC0017057, DE-SC0017181, DE-SC0018556, DE-SC0018571, DE-SC0018719, DE-SC0019682, DE-SC0020593, DE-SC0020931, DE-SC0021553, DE-SC0022386, DE-SC0022799; and also by the US Air Force under Award No. FA864921P1201.

Boulder, Colorado USA | radiasoft.net

19 June 2023

Digital twins for particle accelerators & key subsystems

The words 'digital twin' are becoming more common.
Is this practical for particle accelerator technology?
Papers have recently started appearing; proposals are being written.

It means a lot more than 'an accurate computational model'.
Need high-fidelity modeling at ~kHz rep rates for control systems.

Digital twin

22 languages

Article Talk Read Edit View history Tools

From Wikipedia, the free encyclopedia

A **digital twin** is a digital representation of an intended or actual real-world physical product, system, or process (a *physical twin*) that serves as the effectively indistinguishable digital counterpart of it for practical purposes, such as simulation, integration, testing, monitoring, and maintenance. The digital twin has been intended from its initial introduction to be the underlying premise for Product Lifecycle Management[1] and exists throughout the entire lifecycle (create, build, operate/support, and dispose) of the physical entity it represents. Since information is granular, the digital twin representation is determined by the value-based use cases it is created to implement. The digital twin can and does often exist *before* there is a physical entity. The use of a digital twin in the create phase allows the intended entity's entire lifecycle to be modeled and simulated.[2] A digital twin of an existing entity may be used in real time and regularly synchronized with the corresponding physical system.

Though the concept originated earlier, the first practical definition of a digital twin originated from NASA in an attempt to improve physical-model simulation of spacecraft in 2010.[3] Digital twins are the result of continual improvement in the creation of product design and engineering activities. Product drawings and engineering specifications have progressed from handmade drafting to computer-aided drafting/computer-aided design to model-based systems engineering and strict link to signal from the physical counterpart.

Machine learning has made digital twin technology practical

Journals & Magazines > IEEE Transactions on Nuclear ... > Volume: 63 Issue: 2

Neural Networks for Modeling and Control of Particle Accelerators

Publisher: IEEE

A. L. Edelen ; S. G. Biedron ; B. E. Chase ; D. Edstrom ; S. V. Milton ; P. Stabile All Authors

Abstract:
Particle accelerators are host to myriad nonlinear and complex physical phenomena. They often involve a multitude of interacting systems, are subject to tight performance demands, and should be able to run for extended periods of time with minimal interruptions. Often times, traditional control techniques cannot fully meet these requirements. One promising avenue is to introduce machine learning and sophisticated control techniques inspired by artificial intelligence, particularly in light of recent theoretical and practical advances in these fields. Within machine learning and artificial intelligence, neural networks are particularly well-suited to modeling, control, and diagnostic analysis of complex, nonlinear, and time-varying systems, as well as systems with large parameter spaces. Consequently, the use of neural network-based modeling and control techniques could be of significant benefit to particle accelerators. For the same reasons, particle accelerators are also ideal test-beds for these techniques. Many early attempts to apply neural networks to particle accelerators yielded mixed results due to the

2016 – A.L. Edelen *et al.*,
IEEE Transactions on Nuclear Science **63**, p. 878.
Also on arXiv: https://arxiv.org/abs/1610.06151

- AI/ML makes it possible
  - however, more work to do!
- Standards needed quickly
  - data, file formats
  - physics & engineering codes
  - robustness & validation
- Open source frameworks
  - workflows, collaboration, control system, user interfaces

Building on this work at Fermilab, surrogate models of accelerator components and subsystems are being actively used and deloped at CERN, SLAC, ANL and other labs.

See Auralee's invited talk on Thurs. for recent developments →

Physics and Applications of High Brightness Beams

19-23 June 2023
Europe/Madrid timezone

Overview
Call for Abstracts
Timetable
Contribution List
My Conference
My Contributions
Book of Abstracts

Virtual Diagnostics for High Brightness Accelerators

22 Jun 2023, 17:25
25m

Invited talk | Beam dynamics and c...

Speaker

Auralee Edelen (SLAC)

DOE Office of High Energy Physics: input from GARD/ABP

GARD = General Accelerator R&D; ABP = Accelerator & Beam Physics
Workshop to better define grand challenge problems and plan to address them.

Meeting beam physics grand challenges via HPC

Presenters: Jean-Luc Vay (LBNL) & David Bruhwiler (RadiaSoft)

BERKELEY LAB

radiasoft

GARD ABP Workshop 2 – WG2

April 22-23, 2020 – Organized by FNAL – via Zoom

Other Berkeley Lab contributors: A. Huebl, R. Lehe, C. Mitchell, G. Penn, J. Qiang, R. Ryne, M. Thévenet

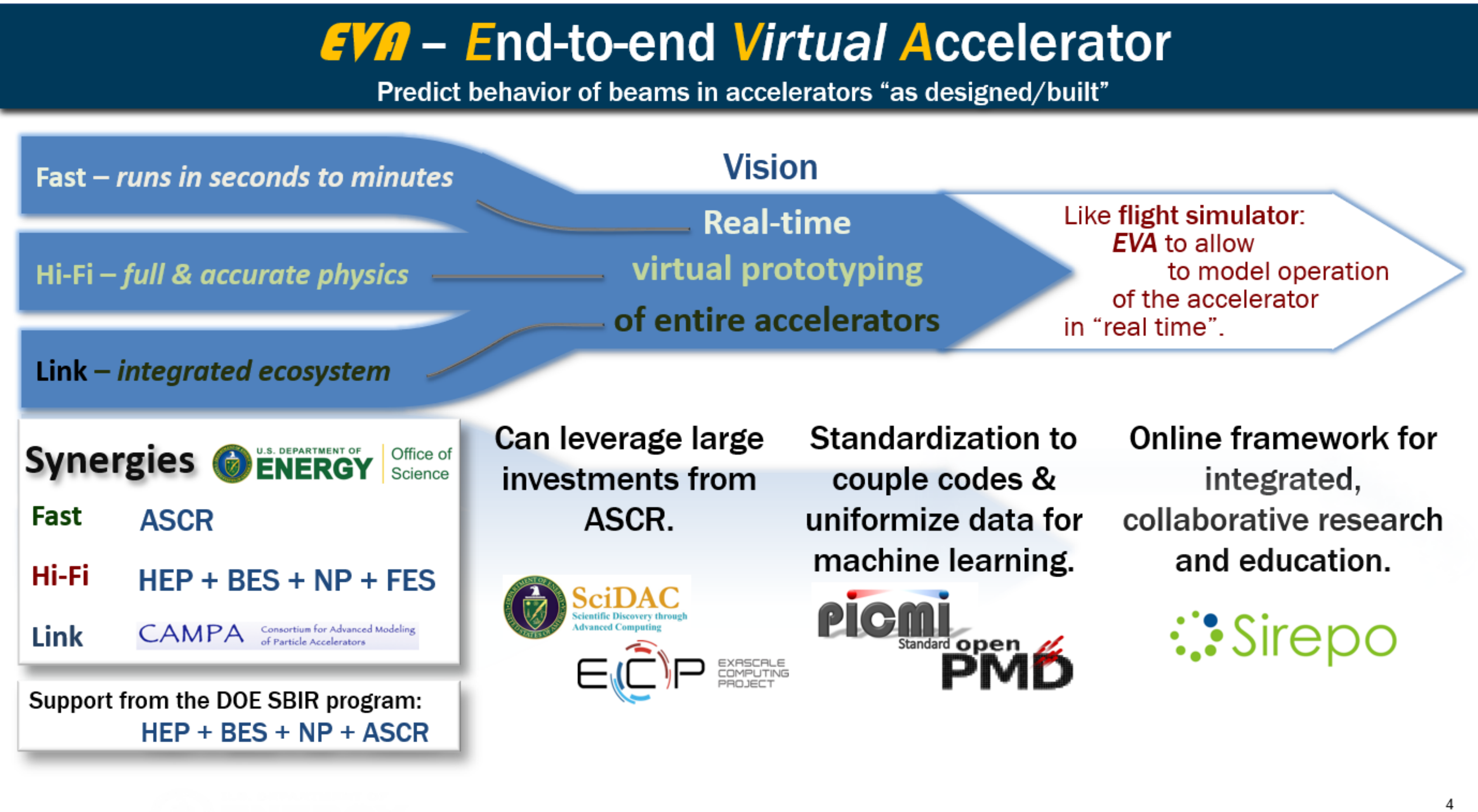
Other RadiaSoft contributors: N. Cook, D.T. Abell, E. Carlin, J. Edelen, C. Hall, M. Keilman, P. Moeller, R. Nagler, B. Nash and S. Webb

This work is supported by the US DOE, Office of Science, Office of High Energy Physics, Office of Nuclear Physics, Office of Basic Energy Sciences and Office of Advanced Scientific Computing Research.

U.S. DEPARTMENT OF ENERGY
Office of Science

DOE/HEP GARD/ABP workshop: slide #2 from Vay/Bruhwiler

In 2020, we were not saying 'digital twin', but most of the ideas were in place.



DOE/HEP GARD/ABP workshop: slide #3 from Vay/Bruhwiler

2020 statement of needs for software / standards / funding / community culture…

Infrastructure required to support "Virtual Accelerators"

- The proposed R&D will enable
  - Code interoperability
    - Rapid benchmarking between many different codes
    - Code coupling (e.g. IMPACT / ELEGANT / MAD-X / MARS)
    - Modular physics – rapid interchange from low-dimensionality / reduced models to full physics
  - Computational reproducibility
    - Archive key simulations (design process) for use years later (e.g. commissioning)
    - Instantaneous collaboration (distributed teams; sharing dynamic results with leadership)
  - Accessibility (cloud computing, documentation, graphical user interfaces)
    - Scientific leaders and experimentalists need direct access to the simulations
    - User Facility approach to computing (assist outsiders with state-of-the-art codes)
    - Integration of codes with facilities, including direct interaction with the control system
- Present state of the art:
  - complicated command-line workflows; each lab or group has its own code(s)

5

Collaboration ideas were developed for Snowmass21

- In Aug. 2020, I organized a Letter of Interest (LOI) for Snowmass
  - LOI received wide-ranging support –

    Industry: RadiaSoft, Kitware

    Universities: NIU, U. Strathclyde, Korea U.

    Laboratories: Fermilab, ANL, SLAC

D.L. Bruhwiler, R. Nagler, P. Moeller, R. O'Bara, D.T. Abell, S. Baturin, E. Carlin, S. Coleman, N.M. Cook, J. Edelen, C. Federer, A.F. Habib, C.C. Hall, T. Heinemann, B. Hidding, A. Huebl, M.V. Keilman, R. Lehe, E. Carlin, P. Messamer, B. Nash, C.-K. Ng, C.S. Park, P. Piot, I. Pogorelov, E. Poore, A. Sauers, P. Scherkl, J. Tourtellott, J.-L. Vay and S.D. Webb, "Collaboration between industry and the HEP community," *Snowmass21 Letter of Interest* (2020); https://www.snowmass21.org/docs/files/summaries/CommF/SNOWMASS21-CommF1_CommF0-AF0_AF1_Bruhwiler-066.pdf

- Some software-specific ideas are described in the IPAC19 proceedings:

D.L. Bruhwiler, D.T. Abell, N.M. Cook, C.C. Hall, M.V. Keilman, P. Moeller, R. Nagler and B. Nash, "Knowledge Exchange within the Particle Accelerator Community via Cloud Computing," *Int. Part. Accel. Conf.*, THPMP046 (2019); http://accelconf.web.cern.ch/ipac2019/papers/thpmp046.pdf

Snowmass21 LOI – data standards & workflows

Develop/integrate data standards & start-to-end workflows for Accelerator Physics

(Letter of Interest to Snowmass21, Computational & Accelerator Frontiers)

A. Huebl*[1], J.-L. Vay[1], R. Lehe[1], M. Thévenet[2], C. Mayes[3], D. Sagan[4], Y.-D. Tsai[5], J. C. E[6], F. Tsung[7], H. Vincenti[8], A. Ferran Pousa[2], N. M. Cook[9], S. J. Gessner[3], F. Poeschel[10], M. Bussmann[11,10], D. P. Grote[12], N. A. Murphy[13], R. Schmitz[14], C. H. Yoon[3], D. L. Bruhwiler[9], K. Cranmer[15], S. R. Yoffe[16], B. Cros[17], A. L. Edelen[3], G. Stark[18]

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Great discussion of data formats and strong workflow technologies.

Snowmass21 LOI – open science

Aspiration for Open Science in Accelerator & Beam Physics Modeling

(Letter of Interest to Snowmass21, Computational & Accelerator Frontiers)

A. Huebl*[1], J.-L. Vay[1], R. Lehe[1], C. Mayes[2], Y.-D. Tsai[3], A. Friedman[4], M. Thévenet[5], H. Vincenti[6], D. L. Bruhwiler[7], A. Sauers[3], N. M. Cook[7], S. J. Gessner[2], M. Bussmann[8,9], D. P. Grote[4], R. Schmitz[10], B. Cros[11], D. Sagan[12], S. R. Yoffe[13], A. L. Edelen[2], A. Ferran Pousa[5], G. Stark[14]

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Great summary of principles with list of some success stories.

DOE/HEP GARD/ABP community developed several 10-year roadmaps

2023 report is available online:
https://science.osti.gov/hep/Community-Resources

Abstract

This document describes a roadmap for the Accelerator and Beam Physics (ABP) thrust of the General Accelerator Research and Development (GARD) program, sponsored by the Department of Energy Office of High Energy Physics (DOE OHEP). Accelerators are a key tool for enabling discoveries in many fields such as particle physics, nuclear physics, and materials sciences and for use-inspired research. The dramatic success of accelerator-based particle physics research has been the result of the development of ever-more powerful accelerators over the past eighty years. Future discoveries in particle physics will similarly require new accelerator capabilities and deeper understanding of beam physics. The roadmap offered here will guide ABP R&D programs and maintain world leadership of U.S. accelerator research for the next decade and beyond.

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Lawrence Berkeley National Laboratory, Berkeley, CA 94720

General Accelerator R&D Program

Accelerator and Beam Physics Roadmap

DOE Accelerator Beam Physics Roadmap Workshop
September 6–8, 2022

10-year roadmap for grand challenge #4 – virtual accelerators

Beam Prediction – Grand Challenge Roadmap – GC4

YEARS 1–2	3–4	5–6	7–8	9–10	GOALS
Virtual Test Stand (VTS)					
HEP community report: specify data & I/O standards	**HEP community report:** specify workflow technologies	Implement ABP **Virtual Test Stand (VTS)** subsystems, with an emphasis on automated workflow, easy access via supercomputers and cloud computing. Simulate new concepts relevant to an HEP experimental test facility.			Production-ready VTS for new ABP science
HEP community report: initial definition of all VTS subsystems					
AI/ML - Controls					
HEP community report: specify AI/ML standards/tools	Develop AI/ML representations of codes and subsystems for test facilities				Realtime model-driven controls for operating facilities
	Validate surrogates via comparison with a test facility		Use VTS subsystem(s) to optimize controls algorithms		
	Batch 1	Batch 2	Batch 3	Batch 4	
High Performance Computing					
Transition ABP codes to hardware-independent programming models, including deployment to serial and parallel platforms via standard tools.					2x to 1000x speedup of >10 codes
Batch 1	Batch 2	Batch 3	Batch 4	Batch 5	
Algorithm R&D					
Advances into advanced mathematical, computational & theoretical methods, including new algorithms, new physics & quantum computing					New science
Review report 1	Review report 2	Review report 3	Review report 4	Review report 5	
V&V and Training					
Software documentation and testing; support and training for both users and developers; workforce development.					Reduce technical risk; increase efficiency
Test Suite v1	Test Suite v2	Test Suite v3	Test Suite v4	Test Suite v5	

Jean-Luc Vay & David Bruhwiler, with input from multiple workshop participants, including A. Edelen
Emphasis on community reports & standards (soon), followed by iterative development.

How do we facilitate collaboration in ML activities?

5th North American Particle Accel. Conf. NAPAC2022, Albuquerque, NM, USA JACoW Publishing
ISBN: 978-3-95450-232-5 ISSN: 2673-7000 doi:10.18429/JACoW-NAPAC2022-MOPA55

FACILITATING MACHINE LEARNING COLLABORATIONS BETWEEN LABS, UNIVERSITIES, AND INDUSTRY

J. P. Edelen, D. T. Abell, D. L. Bruhwiler, S. J. Coleman, N. M. Cook, A. Diaw, J. Einstein-Curtis, C. C. Hall, M. Kilpatrick, B. Nash, I. V. Pogorelov, RadiaSoft LLC, Boulder, CO, USA
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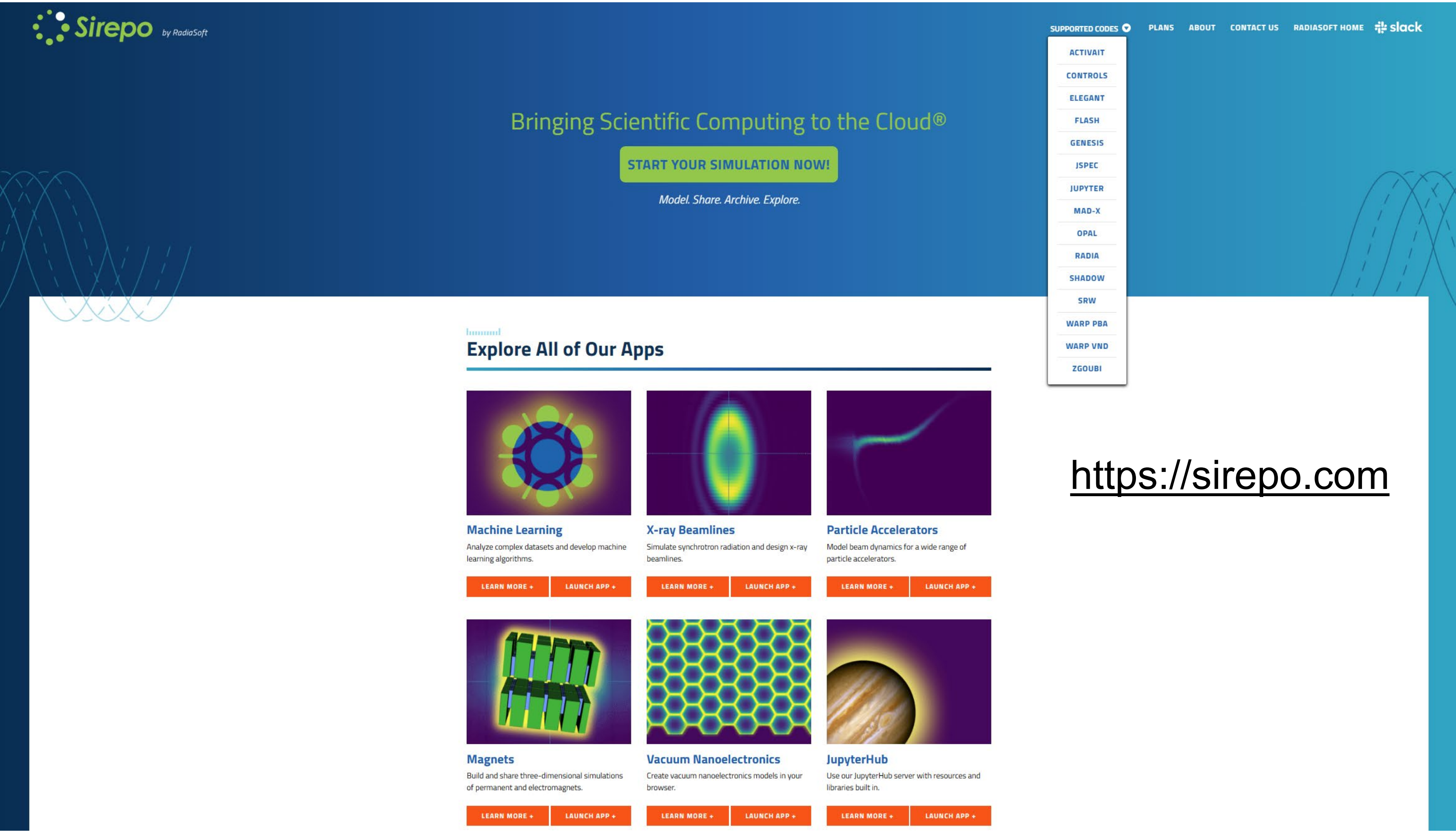
S. Calder, C. Hoffmann, Oak Ridge National Laboratory, Oak Ridge, TN, USA
A. L. Edelen, B. O'Shea, R. Roussel, SLAC, Menlo ParkCA, USA
E.-C. Huang, Los Alamos National Laboratory, Los Alamos, NM, USA

- Funding & publishing realities lead to the wrong incentives
  - Researchers to proof-of-principle, publish and then move on
  - Many ML algorithms are not fully tested
- Important needs to be addressed
  - open-source, portable, extensible software
  - common benchmarks and worked examples
  - investment in personnel to support MLOps and DevOps

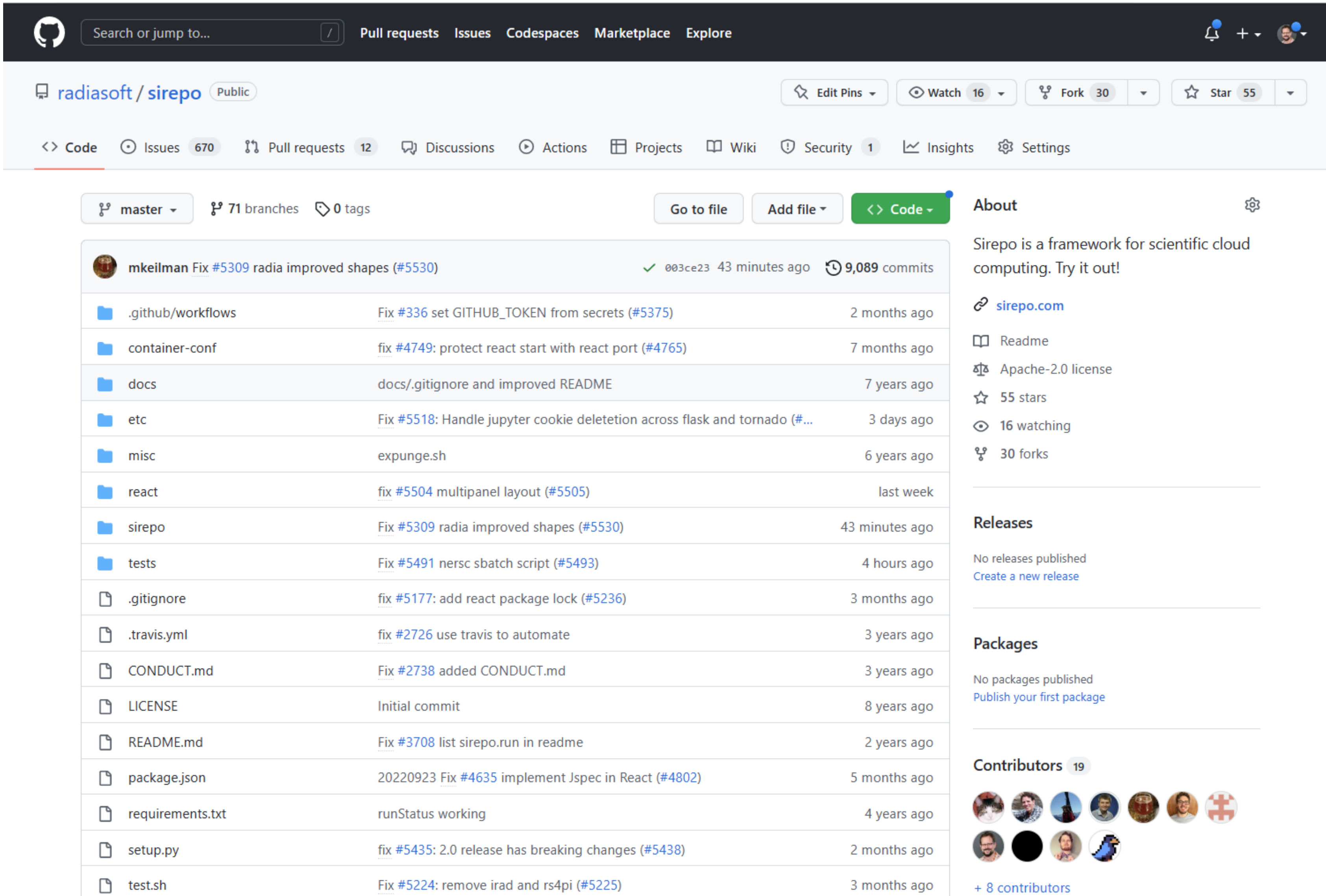
Sirepo – Open Scientific Gateway



https://sirepo.com

Sirepo – an open source framework

https://github.com/radiasoft/sirepo



Sirepo – supported codes and apps

Command line & AI/ML

jupyterhub

Activait

Controls

EPICS

Bluesky

Particle accelerators & adjacent technologies

elegant OPAL MAD-X

Zgoubi Warp (PBA & VND)

Free electron lasers (FEL)

GENESIS

Magnets

Radia

X-ray optics

Shadow

SRW

e- cooling

JSPEC

Plasma (MHD) & hydrodynamics

FLASH

Neutron Transport

OpenMC

USPL - laser pulses

PROMETHEUS

Induction linacs

AMBER

Breakup

NERSC

Powering Scientific Discovery Since 1974

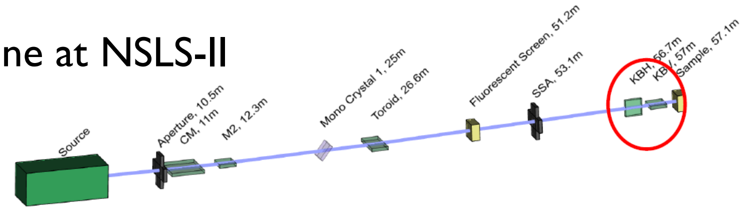
Sirepo – education and training

Clear value proposition for universities and training programs:

- ❖ U.S. Particle Accelerator School (USPAS)
  - Sirepo is used in every session (*2x per year since 2019*)
  - RadiaSoft personnel regularly volunteer to teach
- ❖ Korea University
  - training at multiple levels for planned synchrotron light source
  - graduate students; managers with no physics background
- ❖ Stanford & U. Strathclyde
  - undergraduates

Sirepo – a resource management system

- More than a GUI – the Sirepo server is increasingly powerful
  - integration of Sirepo with Bluesky, EPICS and machine learning (ML) algorithms
  - Aligning an X-ray beamline at the National Synchrotron Light Source (NSLS-II) of Brookhaven National Laboratory (BNL) is now 10x faster & automated
    - Tender Energy X-ray Spectroscopy (TES) beamline at NSLS-II
    - Sirepo-Bluesky made this possible
    - 4 alignment motors used to optimize flux

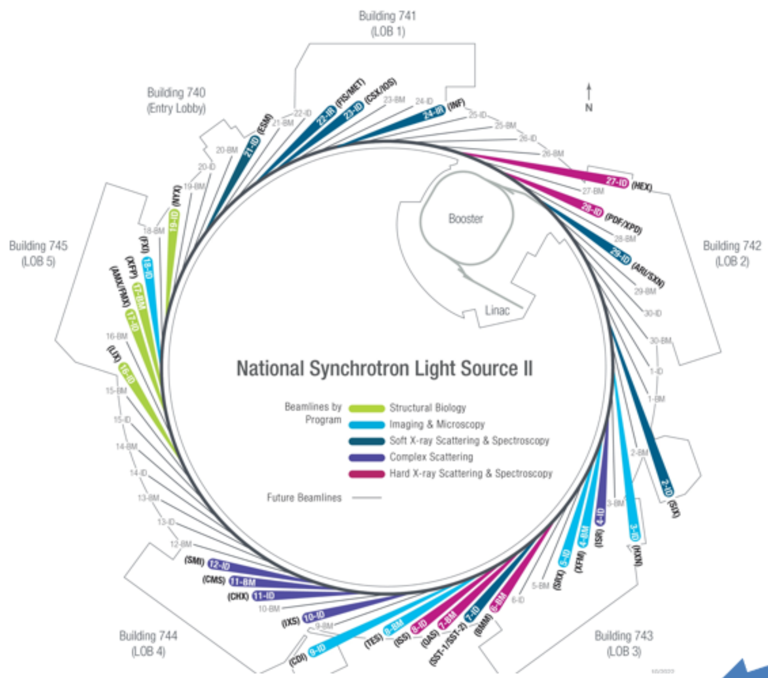


- Sirepo servers can be connected with supercomputing resources
  - SRW simulations can be submitted to NERSC with the push of a button

- Sirepo directly supports command-line workflows
  - Expert users easily move from browser-based GUI to the command line
  - Those who prefer the GUI can easily import command-line files
  - Works directly with the `rsopt` framework for nonlinear optimization & ML

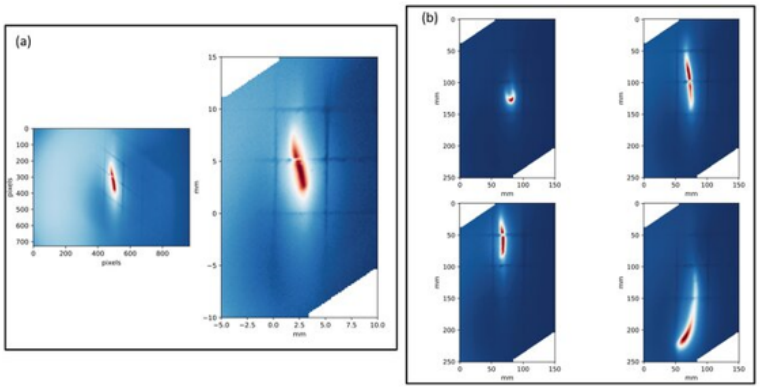
ML-based auto alignment of X-ray beamline, # 1

Online Modeling and Automated Alignment

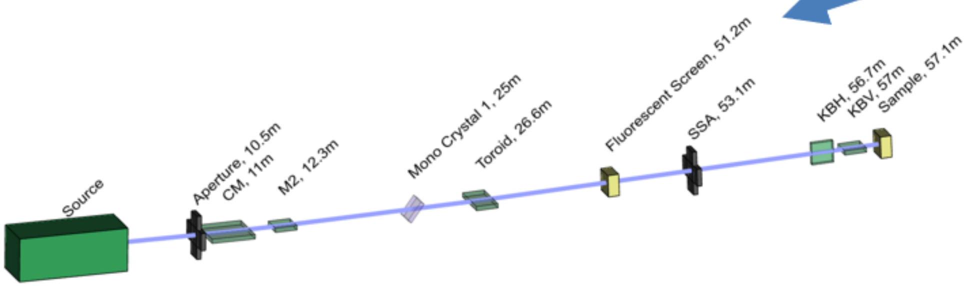


29 Beamlines at NSLS-II (and growing)

How do we know what's going on in a beamline?



Fluorescent screen diagnostic at TES beamline



ML-based auto alignment of X-ray beamline, # 2

RadiaSoft and our collaboration with NSLS-II

RadiaSoft received SBIR funding from the Department of Energy, Office of Basic Energy Sciences to address these questions.

"X-ray Beamline Control with an Online Model for Automated Tuning and Reconfiguration"

This has been a 3 year project, with 1 year for Phase I followed by 2 years for Phase II.

RadiaSoft Team

Boaz Nash (PI)
Dan Abell
Ilya Pogorelov
Nick Goldring (consultant)

Software:
Paul Moeller
Mike Keilman

NSLS-II Team

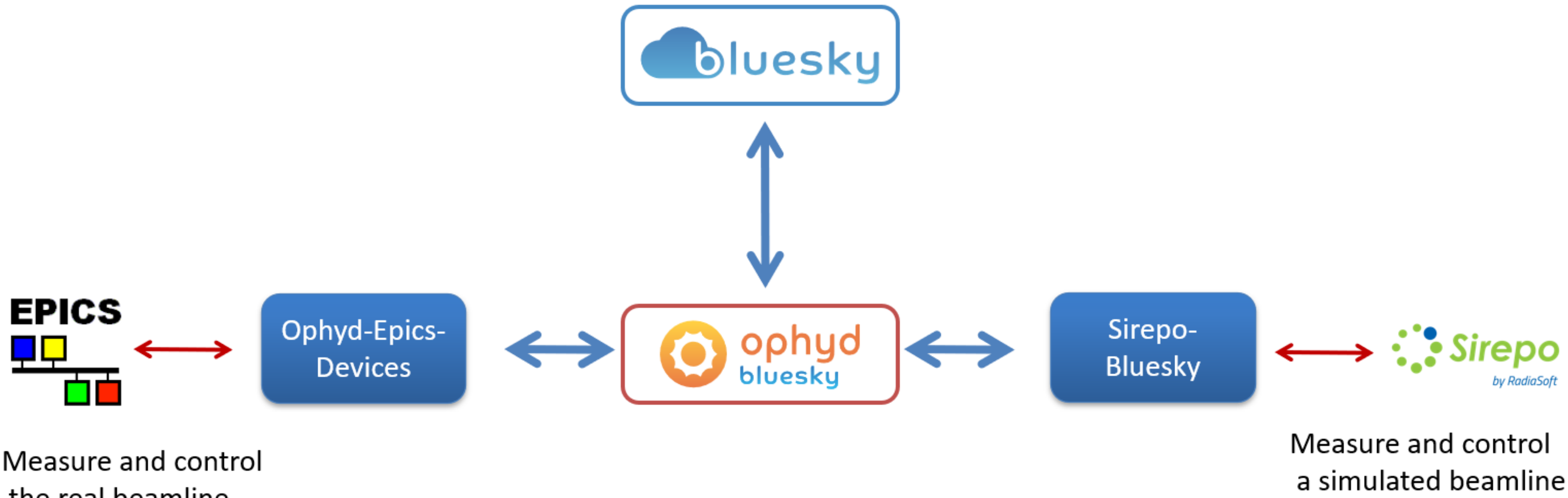
Max Rakitin (PI)

Yonghua Du
Abigail Giles
Joshua Lynch
Thomas Morris
Andrew Walter

ML-based auto alignment of X-ray beamline, # 3

Approach:

We need software that works both in simulation and on the beamline

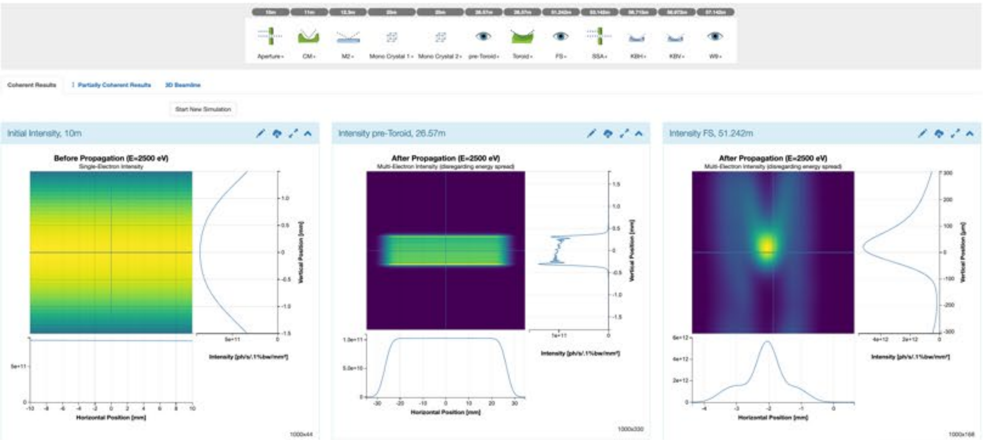


This infrastructure has 2 purposes:

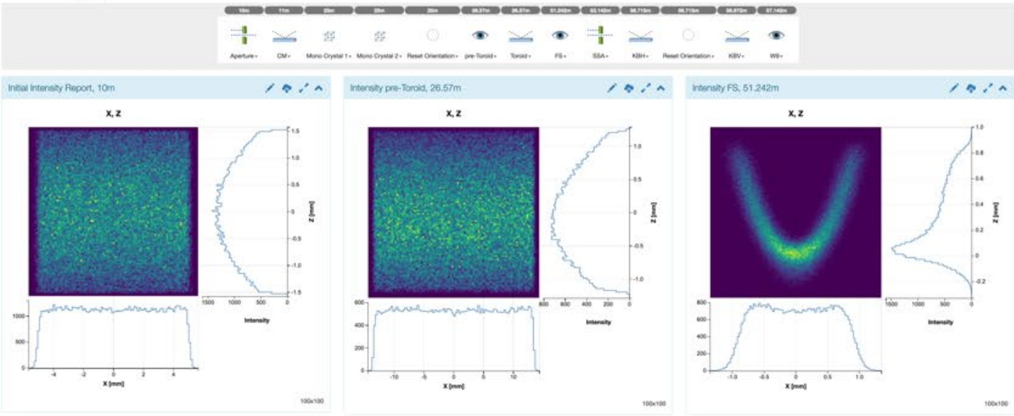
1. Beamline simulations can be used for real beamline control (online model)
2. Make optimal use of expensive beamtime
   Optimization algorithms can be developed and tested in virtual environment before testing and developing on actual beamline.

ML-based auto alignment of X-ray beamline, # 4

Sirepo X-Ray optics simulation



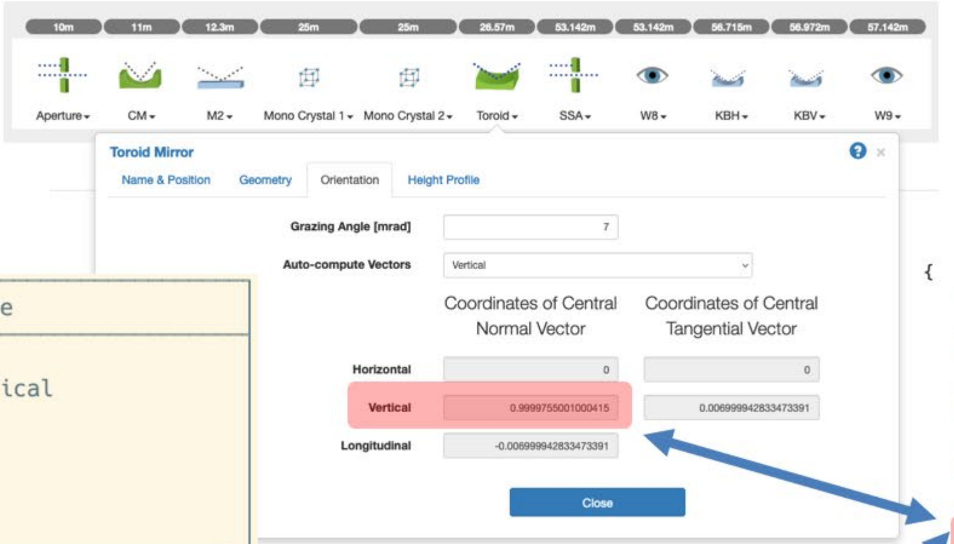
TES simulated in SRW-Sirepo



TES simulated in SHADOW-Sirepo

ML-based auto alignment of X-ray beamline, # 5

Sirepo Widget



Ophyd Device Representation

Ophyd object/component	Value
toroid_apertureShape	r
toroid_autocomputeVectors	vertical
toroid_grazingAngle	7
toroid_heightAmplification	1
toroid_heightProfileFile	
toroid_horizontalPosition	0
toroid_id	6
toroid_normalVectorX	0
toroid_normalVectorY	0.9999755001000415
toroid_normalVectorZ	-0.006999942833473391
toroid_orientation	y
toroid_sagittalRadius	0.186
toroid_sagittalSize	0.08
toroid_tangentialRadius	24500
toroid_tangentialSize	0.96
toroid_tangentialVectorX	0
toroid_tangentialVectorY	0.006999942833473391
toroid_title	Toroid
toroid_type	toroidalMirror
toroid_verticalPosition	0
toroid_element_position	26.57

Sirepo JSON


```
{
  "apertureShape": "r",
  "autocomputeVectors": "vertical",
  "grazingAngle": 7,
  "heightAmplification": 1,
  "heightProfileFile": "",
  "horizontalPosition": 0,
  "id": 6,
  "normalVectorX": 0,
  "normalVectorY": 0.9999755001000415,
  "normalVectorZ": -0.006999942833473391,
  "orientation": "y",
  "position": 26.57,
  "sagittalRadius": 0.186,
  "sagittalSize": 0.08,
  "tangentialRadius": 24500,
  "tangentialSize": 0.96,
  "tangentialVectorX": 0,
  "tangentialVectorY": 0.006999942833473391,
  "title": "Toroid",
  "type": "toroidalMirror",
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},
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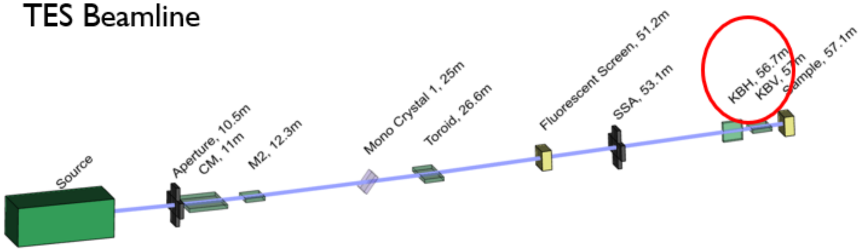
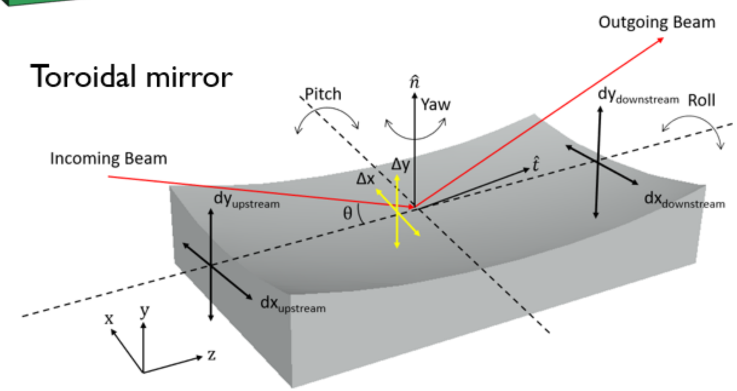
ML-based auto alignment of X-ray beamline, # 6

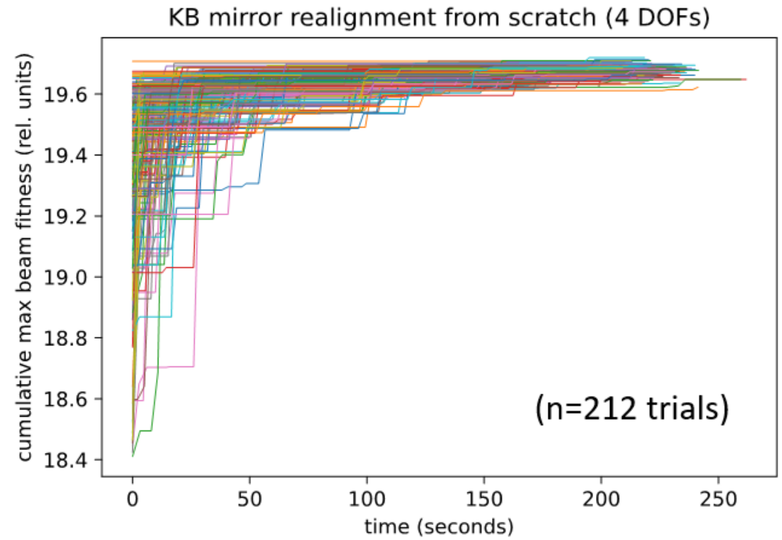
Finally, Automating Beamline alignment with Bayesian Optimization and Gaussian Processes

TES Beamline



Toroidal mirror





Varying 4 alignment motors of KB mirror to optimize flux/(beam area)

The optimization tool was tested and implemented in the Sirepo-Bluesky framework

By hand, this process can take > 1 hour.
Via GPyTorch based optimizer, it takes < 5 min.

The code is a submodule of https://github.com/NSLS-II/bloptools

`rsopt`, slide #1

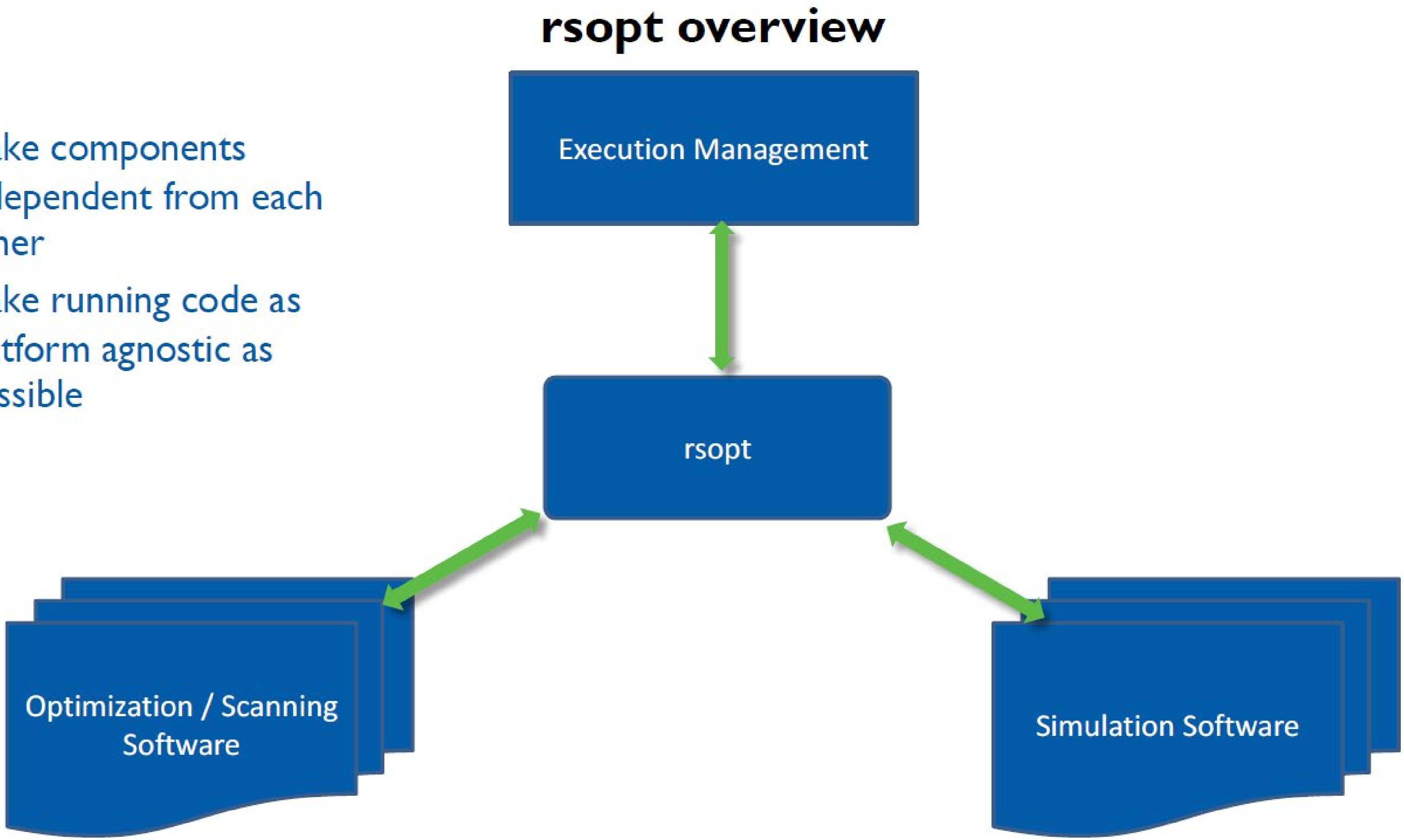
Workflow – pre-rsopt

- Find an optimization library
- Need communication
  - Points to evaluate from the optimizer
  - Evaluation results back in
- Glue code
  - May require dumping and reading data
  - Find and replace in run files
  - Organizing file names / directories
- Code execution
  - Subprocesses to launch executables
  - Manage execution across available resources
- You did all that for your local run environment. Now make it work…
  - On NERSC
  - With a different code
  - A new optimization package

- https://github.com/radiasoft/rsopt
- https://rsopt.readthedocs.io/en/latest/

rsopt, slide #2

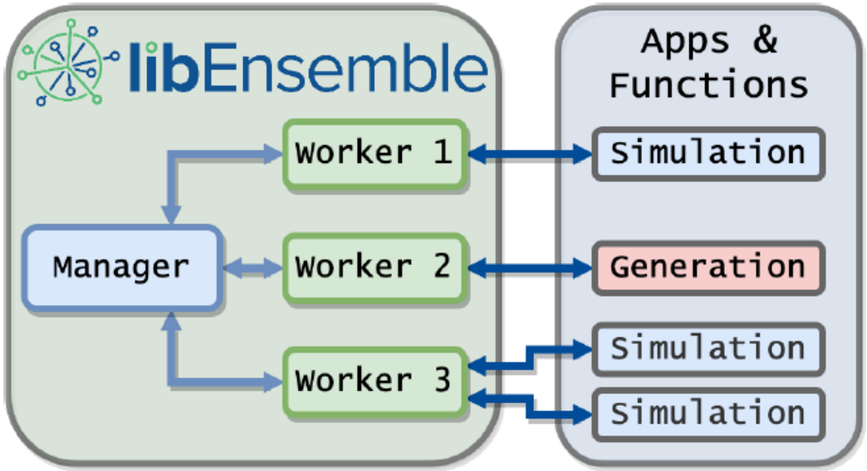
- Make components independent from each other
- Make running code as platform agnostic as possible



rsopt, slide #3

Components I

- libEnsemble
  - Configures workload distribution
  - Runs generators and simulations and handles communication
  - Handles system-dependent simulation execution



libEnsemble

https://github.com/Libensemble/libensemble

rsopt – Sirepo compatibility, slide #1

Currently Supported

- Supported codes
  - elegant
  - OPAL
  - Genesis*
  - Python
  - user supplied executables

- Supported execution methods
  - serial
  - parallel (MPI)
  - Shifter (NERSC)

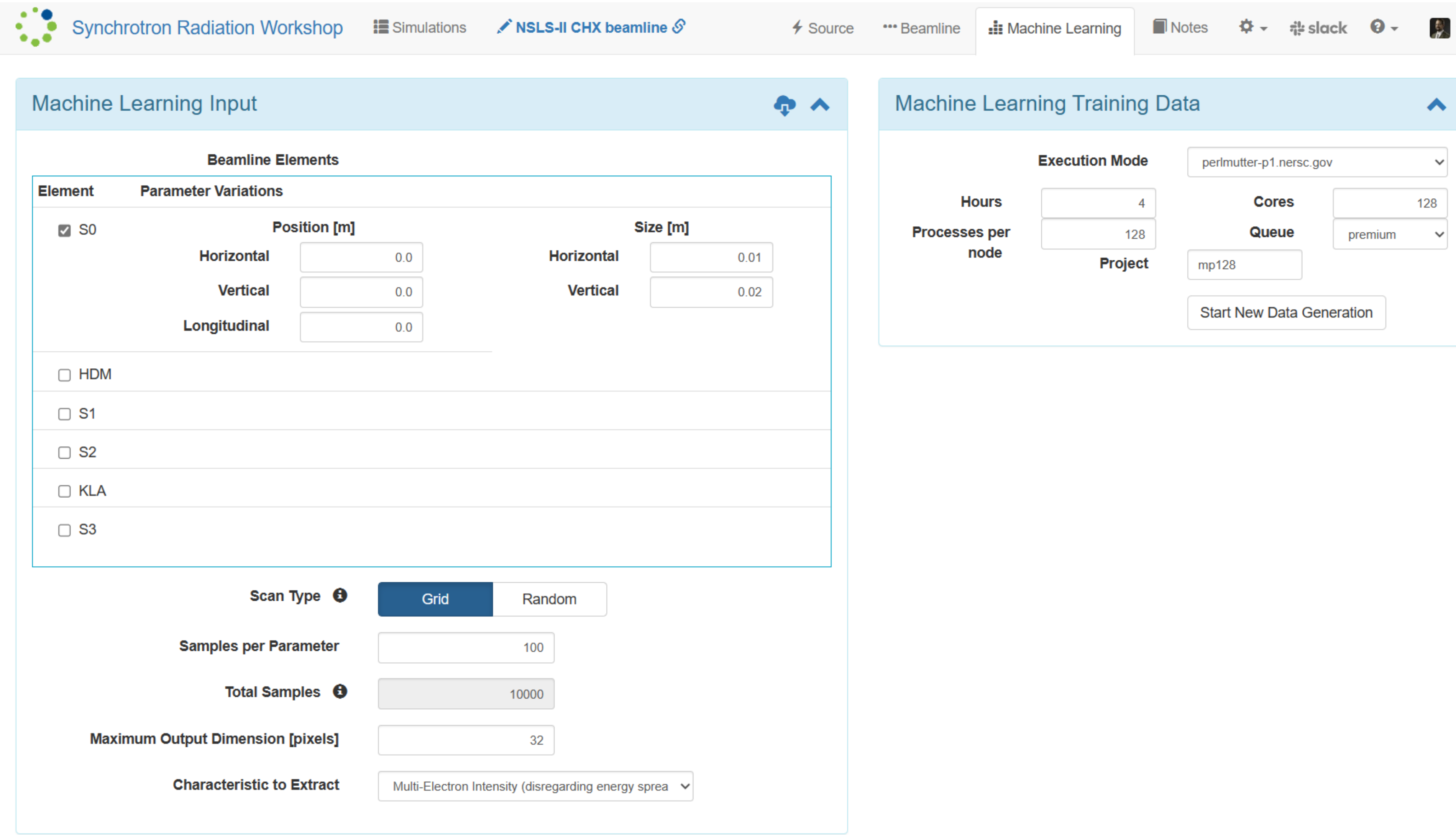
- Optimization libraries / algorithms
  - scipy.optimize †
  - nlopt†
  - DFO-LS
  - APOSMM
  - NSGA-II (through DEAP)

- Parameter Scans
  - Uniform mesh
  - User supplied values
  - Random values
  - Latin hypercube

† Subset of algorithms

*Parsing through forked lume-genesis: https://github.com/slaclab/lume-genesis

rsopt – Sirepo compatibility, slide #2



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Proposal: our community should begin to discuss and adopt standards for the development of digital twins

The Sirepo framework is a good choice for being included, together with other open source technologies:

a) instantaneous collaboration between distributed design teams
b) benchmarking, multiphysics & code chaining for end-to-end sims
c) multi-level support for relevant codes; GUI to supercomputer
d) supports many subsystems, compatible with surrogate models
e) integration with controls for testing, commissioning, operation
f) computational reproducibility

NB: *The Sirepo development team is very strong, with a culture based on open source software, open science, and collaboration.*