An open source GUI for collaborative cloud-based X-ray optics modeling

D.L. Bruhwiler[&] M. Rakitin[#] P. Moeller^{&,%} R. Nagler[&] O. Chubar[#]



Software for Optical Simulations (SOS) Workshop 4 October 2016 – Trieste

This work is supported in part by the US DOE Office of Science, Office of Basic Energy Sciences under SBIR awards DE-SC0006284 and DE-SC0011237.

Vision

- develop open source software, useful for:
 - X-ray beamline designers & computational physicists
 - full access to capabilities & complexity, with minimal restrictions
 - flexible, publication quality graphics
 - a subset of them require a development environment
 - light source facility users
 - require a graphical user interface (GUI)
 - ease of use, intuitive
 - ability to understand X-ray optics of specific beamline
- software must be sustainable over the long-term
 - all components must be maintainable
 - easy for the X-ray optics community to contribute



Capabilities	Software	Comments
electron beam dynamics	SRW,	more 3D magnetic field sources and elements
synchrotron emission	SRW,	improved solvers
SASE FEL	GENESIS, database	import laser pulse data (2D and 3D)
geometric optics	SHADOW,	interoperability with SRW
physical optics	SRW,	improve reliability, speed
partial coherence	SRW, SHADOW	improve reliability, speed
X-ray optical elements	SRW, SHADOW	increasing diversity & complexity
element imperfections	SRW, SHADOW	benchmark different methods
material properties	database	automated access to community resources
Python scripting	SRW, SHADOW	how much commonality?
file formats	SRW, SHADOW	configuration, binary data – commonality?
GUI	SRW, SHADOW	cloud computing
Jupyter (IPython) notebooks	SRW,	WPG effort at EXFEL
simulate experiments	SRW,	material interactions, diagnostics
optimization & design	SRW,	inverse algorithms, nonlinear optimizers



SOS – 4 Oct 2016 – Trieste # 3

Open Source Cloud Computing for Science

- The browser is the GUI
 - HTML5 technologies, especially JavaScript
 - simulation code runs on a server, supercomputer, etc.
- Seamless legacy
 - export SRW python script, or IPython Notebook from browser
 - GUI will always help users, never restrict what they can do
- Containerized computing
 - open source technology: Docker
 - Docker enables rapid cloud deployment
 - no overhead on Linux
 - headless VMs on Mac OS and Windows with low overhead
 - eliminates pain of code installation, cross-platform development
 - archival, reproducibility, instantaneous collaboration
 - user input files, output files, etc. are saved in the container
 - share the container with a collaborator, students, etc.



SRW in the cloud: https://beta.sirepo.com



BROOKHAVEN A radiasoft SOS – 4 Oct 2016 – Trieste

Sharing your SRW simulation, Part 1:

	C. myladi - Lita	- 44 - 7	-					
)) het -	-	1))		
an fairtige	and the second			O	The second s	M-2		12.20
	Second Sume-	En-			manager as weak	Hattan 1952		1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Bar	and the second second		10.1		Interesty at Barr	ple Paperti 12	81.47%	19-
Rodin of Sorts	in Constant (m)		1948		After Pr	opagation (E+5	06 #W)	
15	ingentia: Star (m)		8.5					Free
	System Sale (m)		10.00					
16 million	(terred) styres (perm)		No. of Concession, Name					- day a
Soontinales o V	of Cerittal Nam Wator	minal .	Coordinates o Tangentiat	f Central Vischor			<	\sim
(Second party)	and all states	-						7- 1
		and a	Vertical	and and an inter-				
S.Longoro	6-000	4.02					1000	- 10.00
			-		- New York	1	(magnetal)	a (Jacobier)
			the second second		See. 1	11		
					-	212	14	
						Normanial Plantines		

https://www.youtube.com/watch?v=Ioa7TZ3PkGc



Sharing your SRW simulation, Part 2:

Committee and a second second					- 0
-> O 8					=
and along a first the second sec	1. ten innite	< > 1	and the second second		
	stag and	the second second	a have to shellow the	Association .	
		-			-
	1 1	100	■: []]) 👘	
	101 - 10 - 10 - 10 - 10 - 10 - 10 - 10	++ ++	(m) (m) (m)	and a manufacture	e
(service and service)	.0		0		
Encircle Holes 3	1.		terrally at Ap	UK Report, 132 (871)	14
Summer Provider Seg			ments of the	ergen Depart, 120-ko	10
Mannas of Software Concession, 202				Par Propagation (Evil)	445
transporting later proj	4.4		50		1
Regular Soc (re)	4-0				
Streams, Argin (mod)	11.00.00				1
Coordination of Central Normal Vector	e Coordinates of	Central Tangersia	(1)		5-1
Verbaut 1	7/2				
Langending Commission	(I)				
	-				
ē	Carlos and a				
			1 mil 1	Charles I.	

https://www.youtube.com/watch?v=DJBCrmB7Kc0

BROOKHAVEN A radiasoft SOS – 4 Oct 2016 – Trieste

Automated access of X0h data server at ANL

Synchroth	ron Had	Sotion Viti	(gonumog)	a second	- A register a	a margane			1.00	-	leaster O
1 Aportase d	CHE.	The		Larra) Etpent Uma	THE MARK] Spharing West	a theory	- Crysta	Hereit .	
					beamline	definition a	10.0				1 march
				NE HOLD	no notice/ elem	enta here, ta	define the tree	15 Genae			
						and the second se					
					•	1					
					•	/					
					1	/ 		0		-	
			that Pa	carrières.	And Andrews	/ 		Ð	3	-	
mai monaty F	teport		Mari Pa	carrière : Eve	Anneget Pratter	/		Ð	3	-	
that internality F	Seport	n (E=900	- Mary Pa	narreporte Elec Norternal F	Anneget Parties	-		Ð		-	
itial interatty F Betave Prog	Seport pagatio	n (E=900	Mary Pa	namenter Bie Northead Of 1	ineget Paster ineget Paster Paster proj he crystal		Miller's indi	9 es		-	
mai manaty P Before Prop	teport pagatio	n (E=900	- Mar Pa	namente Bier Notational P National Of 1	A constraints of the crystal	-	Miller's indi:	9 85		-	
thal interatty F Before Prop	teport pagatio	n (≝=900	Mar Pa	normania Dis Normania Normani of 1	Autor pr)	-	Miller's indi:	85			

https://www.youtube.com/watch?v=r6JEAUXfJoI



Automated access of materials data at LBL



https://www.youtube.com/watch?v=d0Vxj8yYZQA



Experts can download Python script



NATIONAL LABORATORY

SOS – 4 Oct 2016 – Trieste

#

1()

You can export and import JSON files – enables sharing

```
🙈 Sirepo - Radiasoft 🐘 🗙 🔥 myFMX02 - SRW - 💱 🖈 🔥 https://beta.sirepo.c 🗙
     CA
            https://beta.sirepo.com/simulation/srw/znElhQ9a/1
  "models": {
       "beamline": [
               "horizontalOffset": 0,
               "horizontalSize": 1.5,
               "id": 14,
               "position": 20,
               "shape": "r",
               "title": "Aperture",
               "type": "aperture",
               "verticalOffset": 0,
               "verticalSize": 1.5
           },
               "grazingAngle": 13.962599999998195,
               "heightAmplification": 1,
               "heightProfileFile": null,
               "id": 13,
               "normalVectorX": 0.9999025244842406,
               "normalVectorY": 0,
               "normalVectorZ": -0.013962146326506367,
               "orientation": "x",
               "position": 42,
               "radius": 1410,
               "sagittalSize": 0.11,
               "tangentialSize": 0.5,
               "tangentialVectorX": 0.013962146326506367,
               "tangentialVectorY": 0,
               "title": "HFM",
               "type": "sphericalMirror"
           },
               "horizontalOffset": 0,
               "horizontalSize": 0.03,
               "id": 3,
               "position": 55,
               "shape": "r",
               "title": "SSA",
               "type": "aperture",
               "verticalOffset": 0,
               "verticalSize": 10
           },
```

SOS - 4 Oct 2016 - Trieste

11

BROOKHAVEN A radiasoft

Open source: <u>https://github.com/radiasoft</u>

This repository Search Pull requests	Issues Gist	🖍 +- 🕅-
📮 radiasoft / sirepo	O Un	watch ▼ 7 ★ Star 4 % Fork 4
<>Code ① Issues 184 阶 Pull requests 0 Ⅲ Projects 0	Wiki -4~ Pulse <u>III</u> Graphs	Settings
Young's Double Slit Experiment exa Maksim Rakitin edited this page on Mar 28 · 5 revisions	mples	Edit New Page
Young's Double Slit Experiment		▼ Pages 12
The example demonstrates classical Young's interference experiment fi 1801.	rst performed by Young in	Home Backup SRW Sirepo simulations
The optical scheme consists of the following elements:		Dev NewReportExample
 a lens with focal length F=0.5 m located at 1 m from a Gaussian b nm); a double slit (emulated by a 10 by 0.5 mm rectangular aperture ar 	eam source (green laser, 535 Id a 10 by 0.3 mm	Diffraction by an aperture example Dynamical access of crystal data and optical constants from
 a watch point showing the intensity of the beam just after propag a watch point showing the intensity in the far field at 1 m from the 	ation through the aperture; e aperture (Fresnel number	external servers ManualAlphaTest
F=0.3).		SRW CRL
Another example replicates the optical scheme of the above example, removed.	but a focusing lens is	SRW Crystal SRW Electron Beam
		SRW Fiber

Many helpful discussions with and feedback from the following scientists: Gerard Andonian Alexey Buzmakov **Carsten Fortmann-Grote** Mark Glass Jacek Krzywinski Acknowledgments Luca Rebuffi Ruben Reininger Liubov Samoylova Manuel Sanchez del Rio **Timur Shaftan** Xianbo Shi Lin Zhang

Please try our beta implementation of SRW in the cloud: <u>https://beta.sirepo.com</u> Please send all feedback to David Bruhwiler <u>bruhwiler@radiasoft.net</u> YouTube videos can be found here: <u>http://radiasoft.net/youtube</u>

This work is supported by the US DOE Office of Science, Office of Basic Energy Sciences under Award # DE-SC0011237.

