Max Rakitin

Curriculum vitae

About

Name: Max Rakitin (a.k.a. Maksim S. Rakitin)

Summary: I am a group leader of the Data Acquisition and Detectors group of the Data Science and Systems Integration Division of NSLS-II, BNL.

News: "Computer, Is My Experiment Finished?" (September 16, 2022)
https://www.bnl.gov/newsroom/news.php?a=220832

"Seeing the Forest Through the Trees: Brookhaven Lab Scientists Develop New Computational Approach to Reduce Noise in X-ray Data." (April 18, 2022)
https://www.bnl.gov/newsroom/news.php?a=219533

Links:
- BNL • SBU • SUSU
- @mrakitin • @mrakitin • Google Scholar • ResearchGate
- ORCID: 0000-0003-3685-852X

Experience

2024.06–present
Computational Scientist (RS-5), **Group Leader**, *Data Science and Systems Integration (DSSI) Division, Data Acquisition and Detectors Group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov, DSSI).
Supervisor: Dr. Stuart Wilkins

2023.01–2024.06
Computational Scientist (RS-5), **Deputy Group Leader**, *Data Science and Systems Integration (DSSI) Program, Data Acquisition and Detectors Group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov, DSSI).
Supervisor: Dr. Thomas Caswell

2021.03–2022.12
Associate Computational Scientist (RS-4), **Supervisor**, *Data Science and Systems Integration (DSSI) Program, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov, DSSI).
Supervisor: Dr. Stuart Campbell

2019.10–2021.03
Associate Computational Scientist, *Data Acquisition, Management and Analysis (DAMA) Group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).
Supervisor: Dr. Stuart Campbell

2017.11–2019.09 Brookhaven National Laboratory

Assistant Computational Scientist, *Data Acquisition, Management and Analysis (DAMA) Group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).
Supervisor: Dr. Stuart Campbell

Software Projects:

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, docs, GitHub.
- **Ophyd** — a device abstraction library, docs, GitHub.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, docs, GitHub.
- **Sirepo-Bluesky** — an interface library between the **Bluesky** data acquisition framework and the **Sirepo** browser-based interface framework to beamline and accelerator simulation codes, docs, GitHub.
- **Blop** — a Bayesian optimization library for autonomous experiment control, docs, GitHub.

Funded Projects (PI roles):

- **LDRD Type B "Simulation-aided Instrument Optimization Using Artificial Intelligence and Machine Learning Methods"** (LDRD #22-031, FY2022–FY2024, Oct. 2021–Sep. 2023) — PI: M. Rakitin, co-PIs: Y. Du, M. Fedurin. BNL Laboratory-Directed Research and Development project, https://www.osti.gov/biblio/1972474.
- **DOE SBIR "X-ray Beamline Control with an Online Model for Automated Tuning and Reconfiguration"** (Award No. DE-SC0020593, 2020–2023) — PI at BNL (subcontract). Lead organization: RadiaSoft, LLC (PI: B. Nash).
- **DOE SBIR "An Integrated Platform for High Performance Data Management and Analysis at X-ray Light Sources"** (Award No. DE-SC0021553, 2021–2024) — PI at BNL (subcontract). Lead organization: RadiaSoft, LLC (PI: N. Cook).

Responsibilities:

- Scientific software development & maintenance.
- Packaging and maintenance of conda packages (`conda-forge`, and formerly `lightsource2-tag` and `nsls2forge` conda channels).
- Deployment of the software with Ansible.
- NSLS-II beamlines and users support.
- Active collaboration with peers at other US DOE National Labs' User Facilities (SLAC — LCLS & SSRL, LBNL — ALS, ANL — APS, ORNL — SNS) and international facilities (DLS, PSI, BESSY-II, CLS, DESY).
- Teaching people to use our software stack.
- Mentor to student interns (summer 2016: 1 intern, summer 2018: 1 intern, summer 2019: 1 intern, spring and summer 2020: 2 interns, summer 2021: 2 interns, summer 2023: 1 intern, summer 2024: co-mentor to 1 intern).

2015.12–2017.10 Brookhaven National Laboratory

Research Associate (Postdoc), *NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).

Supervisor: Dr. Oleg Tchoubar (Chubar)

Software Projects:

- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, GitHub.
- **Sirepo** — a cloud-based framework for SRW, GitHub.
- **Image processing and data visualization**, GitHub and GitHub.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), GitHub.

Responsibilities:

- Adding new functionality to Sirepo (*e.g.*, new optical elements, new reports, implementation of dynamical access of crystal data and optical constants from external servers).
- Adding new functionality to SRW (*e.g.*, new optical elements).
- Creation of new SRW/Sirepo "virtual beamline" scripts/examples.
- Creation and update of Sirepo & SRW wiki documentation.
- SRW & Sirepo users community support via GitHub issues, email communication, *etc.*
- Deployment of SRW & Sirepo to NSLS-II servers for usage by beamline scientists.
- Computational support for NSLS-II beamlines — carrying out required SRW & Sirepo simulations.
- Assistance with scan plans preparation using **Bluesky** data collection framework and **ophyd** package for controlling motors, detectors, *etc.*
- Participation in X-ray experiments (SRX, ESM, SMI, CHX beamlines of NSLS-II) — carrying out measurements and bulk data analysis, processing & visualization using Python (NumPy, SciPy, Matplotlib, PIL, *etc.*; raw data and images, NumPy arrays, HDF5 datasets).
- Implementation and integration of samples simulation code for coherent scattering experiments in SRW and Sirepo (collaborative project with CFN).
- Assisting with development of the Hartmann mask optical element in SRW and its implementation in Sirepo (collaborative project with the Metrology group of NSLS-II).
- Tutorship of summer students.

2013.10–2015.12 **Postdoctoral Associate (Postdoc)**, *Prof. Oganov's lab, Department of Geosciences, Stony Brook University*, Stony Brook, NY (https://stonybrook.edu, https://uspex-team.org/en/uspex).

Supervisor: Prof. Artem R. Oganov

Software Projects:

- Refactoring of USPEX code and porting it from Matlab to Python using modern programming techniques.
- *Ab initio* investigation of BeF_2 and SiO_2 systems in a wide pressures range (paper) using USPEX, VASP, Quantum Espresso, Phonopy.
- Prediction of secondary structures of proteins from knowledge of sequences of amino acids. Development of USPEX interface for Tinker.

Responsibilities:

- Main developer of the project on rewriting USPEX in Python with use of NumPy, SciPy, TkInter, *etc.* Web-based API creation.
- New releases of Matlab/Octave version (USPEX 9.4.1, 9.4.2, 9.4.3, 9.4.4), new features, bug fixes, maintenance.
- Development and maintenance of USPEX continuous integration system (automatic nightly builds + testing).
- Development of tests for USPEX interface with VASP, GULP, LAMMPS, CASTEP, Quantum Espresso, SIESTA, CP2K, QuantumWise ATK, DMACRYS, Tinker, FHI-aims.
- Development and maintenance of online utilities https://uspex-team.org using JavaScript, jQuery, PHP, HTML, JSON, REST API, WebGL, XML, SVN, interfaces to Python, Fortran, Matlab programs, *etc.*
- Installation, configuration, and maintenance of an instance of a Trac system and SVN.
- Creation and maintenance of USPEX manual in LaTeX, PDF, HTML formats.
- USPEX community support.

2008.10–2013.09 **Researcher**, *Department of General and Theoretical Physics, South Ural State University*, Chelyabinsk, Russia (https://www.susu.ru/en).

Supervisor: Prof. Alexander A. Mirzoev

Software Projects:

- Performing research on investigating influence of hydrogen on structure and properties of iron-based alloys using DFT methods (WIEN2k).

Responsibilities:

- Development of bash/Python utilities for monitoring WIEN2k calculations in PBS/Torque and SLURM queues and for processing data of calculations, developing mail notification system for the calculations.
- Installation of WIEN2k on a PC and on the university supercomputers (SKIF Ural, SKIF Aurora, Tornado).
- Teaching and consulting students how to use WIEN2k both on a PC and on supercomputers.

2007.06–2013.10 **QA Engineer, QA Team Leader**, *Applied Technologies Ltd.*, Chelyabinsk, Russia (https://www.appliedtech.ru/en/), a partner of Rocket Software Inc., USA (https://www.rocketsoftware.com)

Supervisor: Valery Ermakov, CEO

Software Projects:

- Tivoli Enterprise Portal (TEP) (August 2011 – October 2013) — QA team leader. Responsibilities: software testing on Windows, Linux, Linux on z, z/OS operating systems, GUI testing automation using IBM Rational Functional Tester, creation of TEP Automated Testing System (TATS) for automatic data verification using Python, REST API, JSON, XML, PHP, HTML, JavaScript, jQuery in six TEP-enabled products:
  - Tivoli Advanced Reporting and Management for DFSMShsm;
  - Tivoli Advanced Audit for DFSMShsm;
  - Tivoli Advanced Catalog Management for z/OS;
  - Tivoli Advanced Backup and Recovery for z/OS;
  - Tivoli Advanced Allocation Management;
  - Tivoli Automated Tape Allocation Manager for z/OS.

  Regular voice and video conversations with colleagues from the US.

- Tivoli Storage Manager for z/OS Media (February 2011 – August 2011) — QA engineer. Responsibilities: software testing on Windows, Linux on z, Solaris, AIX, z/OS operating systems with IBM DB2 databases, testing automation using IBM-developed tools, bash, batch.

- IBM Tivoli Advanced Allocation Management (January 2009 – January 2011) — QA engineer. Responsibilities: software testing on z/OS, testing automation using bash, JCL, REXX. Regular voice and video conversations with colleagues from the US.

- Rocket Servergraph Data Protection Expert (June 2007 – December 2008) — QA engineer. Responsibilities: software testing on Windows, Linux, Solaris, HP-UX, AIX operating systems with PostgreSQL databases, GUI testing automation using AutoIt3, automation of data verification using Perl and SQL. Regular voice and video conversations with colleagues from the US.

2006–2007 **System administrator**, *Department of General and Theoretical Physics, South Ural State University*, Chelyabinsk, Russia (https://www.susu.ru/en)

Administer, secure and support Windows and Linux systems. Support HTTP server (Apache), proxy server (Squid). Help others to troubleshoot operating system, software, hardware and other issues. Also support the testing system for students.

Education

2008.10–2012.09 **Ph.D. in Condensed Matter Physics (defended on September 19, 2012)**

South Ural State University (National Research University), Chelyabinsk, Russia
Thesis: Study of impurities influence on the hydrogen dissolution energy in the bcc iron
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences

2006.09–2008.06 **M.S. in Applied Mathematics and Physics (June 13, 2008)**

South Ural State University (SUSU), Chelyabinsk, Russia
Thesis: Computer simulation of influence of structural relaxation and impurities on dissolution energy of H in Fe
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences
GPA: 3.85 / 4.0

2002.09–2006.06 **B.S. in Applied Mathematics and Physics (June 20, 2006), summa cum laude**

South Ural State University (SUSU), Chelyabinsk, Russia
Thesis: Binding energy of hydrogen in bcc iron lattice
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences
GPA: 3.69 / 4.0

Honors, awards and certificates

2024.09 Spotlight Award in recognition of exceptional job performance (Brookhaven National Lab, Upton, NY)

2022.11 Engineering Award for distinguished contributions to Brookhaven National Laboratory's engineering objectives (a member of a team) — one of Brookhaven Lab's pinnacle awards (Brookhaven National Lab, Upton, NY). news article

2021.02 Certificate of Recognition for scientific contribution to the U.S. Department of Energy National Virtual Biotechnology Laboratory Project "Molecular Design and Analysis to Inform Therapeutics Related to COVID-19" (part of the DOE COVID-19 Pandemic Response in 2020)

2021.01 Certificate of Completion of the course "Scientific & Numeric Computing with Python" (James Powell, DUTC)

2021.01 Certificate of Completion of the course "Expert Level Python" (James Powell, DUTC)

2020 Spotlight Award in recognition of exceptional job performance (Brookhaven National Lab, Upton, NY)

2018 Spotlight Award in recognition of exceptional job performance (Brookhaven National Lab, Upton, NY)

2012 Certificate of summer school on computer simulations and massive calculations in modern physics with invited lectors from the US (Chelyabinsk, Russia)

2010 Certificate of summer school on computational material sciences (San-Sebastian, Spain)

2010 Scholarship of the University President (Chelyabinsk, Russia)

2009 Certificate of courses on high-performance computational systems (Nizhny Novgorod, Russia)

2009–2010 State contract (grant) on Federal Programme "Scientific and pedagogical staff for an innovative Russia" (Moscow, Russia)

2007 Diploma of the 13th All-Russian Physics Students Conference for the talk "Computer simulation of hydrogen atom in bcc iron" (Rostov-on-Don, Russia)

2006 Summa cum laude in Bachelor's studies (Chelyabinsk, Russia)

2006 Scholarship of the President of Russia

Languages

English — Full working proficiency, fluent

Russian — Native language

Computer skills

Data analysis, visualization — Python, NumPy, SciPy, Matplotlib, Bokeh, D3.js, Matlab/Octave, OriginPro, gnuplot, VESTA, XCrysDen, STM4, P4VASP, Molden, VMD, RasTop, *etc.*

Programming — Python (including PyQT, NumPy, SciPy, Matplotlib, PIL), C++, Fortran, Matlab/Octave, JavaScript, jQuery, AngularJS, some React, WebGL, PHP, HTML5, bash, csh/tcsh, make, Perl, AutoIt3, REXX, SQL, JCL

Parallelization — MPI, OpenMP, Dask

IDE/editors — VSCode, PyCharm, Eclipse, vim, some emacs

Writing — LaTeX, BibTeX, TeXlipse/Eclipse, plasTeX, JabRef, MS Word

OS — Linux (CentOS, SuSE, RedHat, Fedora, Ubuntu, Debian, Raspbian, *etc.*), Mac OS X, AIX, Solaris, HP-UX, Windows, DOS, z/OS

Virtualization — Docker, Vagrant, VirtualBox, VMware

VCS — GitHub, Git, SVN, CVS, Bazaar, Trac

Atomistic simulation — VASP, WIEN2k, Quantum Espresso, CASTEP, SIESTA, CP2K, FHI-aims, QuantumWise ATK, Tinker, GULP, LAMMPS, DMACRYS, Phonopy, TB-LMTO-ASA

References

Colleague

Thomas Caswell, Ph.D., Data Acquisition and Detectors Deputy Group Leader,
DSSI, NSLS-II, Brookhaven National Laboratory, Upton, NY 11973
tcaswell@bnl.gov +1 (631) 344–3146

Colleague

Stuart Campbell, Ph.D., Chief Cyber Security Data Scientist,
Information Technology Division, Brookhaven National Laboratory, Upton, NY 11973
scampbell@bnl.gov +1 (631) 344–5578

Additional references available upon request.

Publications

62. Z. Lentz, R. Tang-Kong, M. Rakitin, T. Morris, and S. Miskovich, "ML-assisted beamline optimization at LCLS," in *Proc. 20th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'25)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 20. JACoW Publishing, Geneva, Switzerland, Sep. 2025, paper FRAG001, pp. 1873–1877. https://doi.org/10.18429/JACoW-ICALEPCS2025-FRAG001

61. D. Gavrilov, T. Caswell, A. Sligar, and M. Rakitin, "Bluesky Queue Server for beamline control at NSLS-II," in *Proc. 20th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'25)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 20. JACoW

Publishing, Geneva, Switzerland, Sep. 2025, paper THPD053, pp. 1706–1710. https://doi.org/10.18429/JACoW-ICALEPCS2025-THPD053

60. Y. Hidaka, D. Allan, and M. Rakitin, "A new Python middle layer framework: Particle Accelerator MIddle LAyer (PAMILA)," in *Proc. 6th North American Particle Accel. Conf. (NAPAC2025)*, ser. North American Particle Accelerator Conference, no. 2025. JACoW Publishing, Geneva, Switzerland, Aug. 2025, paper MOP005, pp. 48–51. https://doi.org/10.18429/JACoW-NAPAC2025-MOP005

59. H. Wijesinghe, A. Barbour, L. Wiegart, E. Carlin, J. Einstein-Curtis, P. Moeller, R. Nagler, R. O'Rourke, N. Cook, and M. Rakitin, "Bluesky and Raydata: An Integrated Platform for Adaptive Experiment Orchestration," in *SC24-W: Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis*, 2024, pp. 2162–2167. https://doi.org/10.1109/SCW63240.2024.00271

58. A. Tayal, D. S. Coburn, D. Abel, M. Rakitin, O. Ivashkevych, J. Wlodek, D. Wierzbicki, W. Xu, E. Nazaretski, E. Stavitski, and D. Leshchev, "Five-analyzer Johann spectrometer for hard X-ray photon-in/photon-out spectroscopy at the Inner Shell Spectroscopy beamline at NSLS-II: design, alignment and data acquisition," *Journal of Synchrotron Radiation*, vol. 31, no. 6, pp. 1609–1621, Nov. 2024. https://doi.org/10.1107/S1600577524009342

57. T. W. Morris, M. Rakitin, Y. Du, M. Fedurin, A. C. Giles, D. Leshchev, W. H. Li, B. Romasky, E. Stavitski, A. L. Walter, P. Moeller, B. Nash, and A. Islegen-Wojdyla, "A general Bayesian algorithm for the autonomous alignment of beamlines," *Journal of Synchrotron Radiation*, vol. 31, no. 6, pp. 1446–1456, Nov. 2024. https://doi.org/10.1107/S1600577524008993

56. H. Goel, O. Chubar, R. Li, L. Wiegart, M. Rakitin, and A. Fluerasu, "Efficient end-to-end simulation of time-dependent coherent X-ray scattering experiments," *Journal of Synchrotron Radiation*, vol. 31, no. 3, pp. 517–526, May 2024. https://doi.org/10.1107/S1600577524001267

55. N. M. Cook, A. M. Barbour, E. G. Carlin, J. A. Einstein-Curtis, R. Nagler, R. O'Rourke, M. Rakitin, L. Wiegart, and H. Wijesinghe, "Integrating Online Analysis with Experiments to Improve X-Ray Light Source Operations," in *Proc. 19th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'23)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 19. JACoW Publishing, Geneva, Switzerland, Feb. 2024, paper TUSDSC02, pp. 921–924. https://doi.org/10.18429/JACoW-ICALEPCS2023-TUSDSC02

54. J. A. Einstein-Curtis, D. T. Abell, Y. Du, A. Giles, M. V. Keilman, J. Lynch, P. Moeller, T. Morris, B. Nash, I. V. Pogorelov, M. Rakitin, and A. L. Walter, "Online Models for X-ray Beamlines Using Sirepo-Bluesky," in *Proc. 19th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'23)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 19. JACoW Publishing, Geneva, Switzerland, Feb. 2024, paper MO3BCO05, pp. 165–170. https://doi.org/10.18429/JACoW-ICALEPCS2023-MO3BCO05

53. P. M. Maffettone, D. B. Allan, A. Barbour, T. A. Caswell, D. Gavrilov, M. D. Handwell, T. Morris, D. Olds, M. Rakitin, S. I. Campbell, and B. Ravel, *Book "Methods and*

Applications of Autonomous Experimentation". Chapter 8: "Artificial Intelligence Driven Experiments at User Facilities", 1st ed. Chapman & Hall/CRC Computational Science, 2023, ch. Chapter 8. https://doi.org/10.1201/9781003359593

52. M. Rakitin, R. Bode, T. W. Morris, A. C. Giles, A. L. Walter, J. K. Lynch, J. Maldonado, Y. Du, B. Romasky, M. Fedurin, P. Moeller, and B. Nash, "Recent updates of the Sirepo-Bluesky library for virtual beamline representation," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 126970D. https://doi.org/10.1117/12.2678030

51. T. W. Morris, Y. Du, M. Fedurin, A. C. Giles, P. Moeller, B. Nash, M. Rakitin, B. Romasky, A. L. Walter, N. Wilson, and A. Wojdyla, "Latent Bayesian optimization for the autonomous alignment of synchrotron beamlines," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 126970B. https://doi.org/10.1117/12.2677895

50. B. Nash, M. S. Rakitin, D. T. Abell, M. Keilman, P. Moeller, I. Pogorelov, Y. Du, A. Giles, J. Lynch, T. W. Morris, A. L. Walter, and N. Goldring, "Reduced model representations of synchrotron radiation and a software framework for beamline control," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. PC12697, International Society for Optics and Photonics. SPIE, 2023, p. PC1269703. https://doi.org/10.1117/12.2676921

49. L. Huang, T. Wang, O. Chubar, G. Dovillaire, A. He, M. Rakitin, Y. Yang, A. M. Kiss, and M. Idir, "Investigation of x-ray Hartmann wavefront sensing: from simulation to the initial experiment test," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. PC12697, International Society for Optics and Photonics. SPIE, 2023, p. PC1269705. https://doi.org/10.1117/12.2675754

48. H. Goel, O. Chubar, L. Wiegart, A. Fluerasu, R. Li, A. He, M. Rakitin, M. Lin, P. Moeller, and R. Nagler, "GPU accelerated simulations of time-dependent coherent x-ray scattering experiments," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 1269709. https://doi.org/10.1117/12.2677888

47. N. Cook, E. Carlin, R. Nagler, R. O'Rourke, A. Barbour, M. Rakitin, and L. Wiegart, "An online analysis platform for improving x-ray light source operations," in *Proc. IPAC'23*, ser. IPAC'23 - 14th International Particle Accelerator Conference, no. 14. JACoW Publishing, Geneva, Switzerland, May 2023, paper THPA128, pp. 4266–4268. https://doi.org/10.18429/JACoW-IPAC2023-THPA128

46. M. Rakitin, S. Campbell, D. Allan, T. Caswell, D. Gavrilov, M. Hanwell, and S. Wilkins, "Next generation experimental data access at NSLS-II," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012100, Dec. 2022. https://doi.org/10.1088/1742-6596/2380/1/012100

45. B. Nash, D. Abell, R. Nagler, P. Moeller, M. Keilman, I. Pogorelov, N. Goldring, M. Rakitin, J. Lynch, A. Giles, A. Walter, J. Maldonado, T. Morris, S. Bak, and Y. Du, "Combining diagnostics, modeling, and control systems for automated alignment of the

TES beamline," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012103, Dec. 2022. https://doi.org/10.1088/1742-6596/2380/1/012103

44. H. Goel, O. Chubar, L. Wiegart, A. Fluerasu, R. Li, A. He, M. Rakitin, P. Moeller, and R. Nagler, "Developments in SRW Code and Sirepo Framework Supporting Simulation of Time-Dependent Coherent X-ray Scattering Experiments," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012126, Dec. 2022. https://doi.org/10.1088/1742-6596/2380/1/012126

43. T. W. Morris, M. Rakitin, A. Giles, J. Lynch, A. L. Walter, B. Nash, D. Abell, P. Moeller, I. Pogorelov, and N. Goldring, "On-the-fly optimization of synchrotron beamlines using machine learning," in *Optical System Alignment, Tolerancing, and Verification XIV*, J. Sasián and R. N. Youngworth, Eds., vol. 12222, International Society for Optics and Photonics. SPIE, 2022, p. 122220M. https://doi.org/10.1117/12.2644996

42. L. Huang, T. Wang, O. Chubar, G. Dovillaire, A. He, M. Rakitin, and M. Idir, "Simulation of X-ray Hartmann wavefront sensing with the Synchrotron Radiation Workshop," *Opt. Express*, Oct. 2022. https://doi.org/10.1364/oe.470197

41. T. Konstantinova, L. Wiegart, M. Rakitin, A. M. DeGennaro, and A. M. Barbour, "Machine Learning for analysis of speckle dynamics: quantification and outlier detection," *Phys. Rev. Research*, vol. 4, p. 033228, Sep. 2022. https://doi.org/10.1103/PhysRevResearch.4.033228

40. D. Leshchev, M. Rakitin, B. Luvizotto, R. Kadyrov, B. Ravel, K. Attenkofer, and E. Stavitski, "The Inner Shell Spectroscopy beamline at NSLS-II: a facility for in situ and operando X-ray absorption spectroscopy for materials research," *Journal of Synchrotron Radiation*, vol. 29, no. 4, Jul. 2022. https://doi.org/10.1107/S160057752200460X

39. D. Hidas, A. M. Kiss, M. Rakitin, J. Sinsheimer, T. Tanabe, and M. Musardo, "High precision real-time insertion device and monochromator synchronization at NSLS-II," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, vol. 1031, p. 166505, Mar. 2022. https://doi.org/10.1016/j.nima.2022.166505

38. B. Nash, D. T. Abell, D. L. Bruhwiler, E. G. Carlin, Y. Du, J. P. Edelen, A. Giles, M. V. Keilman, J. Lynch, J. Maldonado, P. Moeller, R. Nagler, I. V. Pogorelov, M. S. Rakitin, A. Walter, and S. D. Webb, "X-Ray Beamline Control with Machine Learning and an Online Model," in *Proc. ICALEPCS'21*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 18. JACoW Publishing, Geneva, Switzerland, Dec. 2021, pp. 695–699. https://doi.org/10.18429/JACoW-ICALEPCS2021-WEPV024

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Conferences, talks, workshops and schools

2024.09 **Invited talk** — *Automated Beamline Alignment and Experiment Steering* 🔗, SSRL/LCLS Users' Meeting, "MFX-HE: Opportunities for High-Throughput Multimodal Structural Studies and Their Computational Challenges" Workshop, Menlo Park, CA

2024.09 **Workshop organizer** — *Bluesky and Bluesky-Queueserver tutorials* 🔗, EPICS Meeting, Oak Ridge National Laboratory, Oak Ridge, TN

2023.11 **Invited talk** — *Bluesky for Multimodal Studies at NSLS-II* 🔗, "Integrating acquisition and AI in tomography" Workshop, Leiden, The Netherlands

2023.08 *Recent updates of the Sirepo-Bluesky library for virtual beamline representation*, SPIE Optics + Photonics, Advances in Computational Methods for X-Ray Optics VI 🔗, San Diego, CA

2023.05 **Invited teacher** at *Beamline and Optics Modeling School*, Advanced Light Source, Berkeley, CA

2023.04 *Ophyd beyond EPICS*, NSLS-II & CFN Users' Meeting, Workshop 4 — "Scientific Python for Data Acquisition, Management, and Analysis", Brookhaven National Laboratory, Upton, NY

2023.03 *AE124: Simulation-aided Instrument Optimization using Artificial Intelligence and Machine Learning Methods*, 25th Annual Accelerator Test Facility (ATF) Users' Meeting, Brookhaven National Laboratory, Upton, NY

2022.08 **Invited talk** — *Automated beamline alignment at NSLS-II*, ALS User Meeting, "Instrumentation and Computation for the Upgraded ALS" Workshop, Virtual Meeting

2022.05 **Invited talk** — *24/7 access to your virtual beamline with Sirepo*, NSLS-II & CFN Users' Meeting, Workshop 6 — "Data Access and Machine Learning at NSLS-II", Brookhaven National Laboratory, Upton, NY

2022.03 **Invited talk** — *Next generation experimental data access at NSLS-II*, SRI2021, Virtual Conference

2020.02 **Invited talk** — *Bluesky Data Collection Framework*, Canadian Light Source, Saskatoon, Canada

2019.10 *Overview of Bluesky*, Imaging Workshop, Oak Ridge National Laboratory, Oak Ridge, TN

2019.07 *Kitware training on vtk.js, girder, tomviz, vtk, paraview, and cmake*, Clifton Park, NY

2019.06 *Jupyter Community Workshop*, LBNL, Berkeley, CA

2019.06 *Ptycho Developer Workshop*, LBNL, Berkeley, CA

2019.01 **Invited talk** — *Bluesky, ophyd, pseudo motors, detectors*, Automation in Beamline Control and Data Acquisition workshop, HZB, BESSY-II, Berlin, Germany

2019.01 **Invited tutorials on Sirepo and Bluesky**, Automation in Beamline Control and Data Acquisition workshop, HZB, BESSY-II, Berlin, Germany

2018.10 *NOBUGS 2018*, Brookhaven National Laboratory, Upton, NY

2018.07 *SciPy 2018*, Austin, TX

2018.06 *EPICS Collaboration meeting*, APS, Argonne National Laboratory, Lemont, IL

2018.05 *2018 NSLS-II & CFN Users' Meeting*: assisting with "Hands-On Data Acquisition and Analysis Tutorial", Brookhaven National Laboratory, Upton, NY

2017.11 *Sirepo — an open-source browser interface for X-ray source and optics simulations*, ORNL Visualization Hackathon, Oak Ridge National Laboratory, Oak Ridge, TN

2017.10 *Sirepo — an open-source cloud-based software interface for X-ray source and optics simulations*, NSLS-II Lunchtime seminar, Brookhaven National Laboratory, Upton, NY

2017.08 **Invited talk** — *Sirepo: a web-based interface for physical optics simulations — its deployment and use at NSLS-II*, SPIE Optical Engineering + Applications, San Diego, CA

2017.05 *2017 NSLS-II & CFN Users' Meeting*, Brookhaven National Laboratory, Upton, NY

2016.12 *Collaboration meeting with RadiaSoft LLC*, Boulder, CO

2016.12 *Early Career Researcher Symposium 2016*, Brookhaven National Laboratory, Upton, NY

2016.10 *Software for Optical Simulations (SOS) Workshop*, ICTP, Trieste, Italy

2016.05 *2016 NSLS-II & CFN Joint Users' Meeting*, Brookhaven National Laboratory, Upton, NY

2015.11 *Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data*, IACS, Stony Brook University, Stony Brook, NY

2015.10 *Collaboration Meeting on "Simulation and Modeling for SR Sources and X-Ray Optics"*, NSLS-II, Brookhaven National Laboratory, Upton, NY

2015.07 **Invited talk** — *Crystal and protein structure modeling, software development and applications*, Brookhaven National Laboratory, Upton, NY

2015.06 *Advances in Functional Materials — Conference 2015*, Stony Brook University, Stony Brook, NY

2015.06 *Recent progress in USPEX development*, Group seminar, Stony Brook University, Stony Brook, NY

2015.04 **Invited talk** — *Crystal structure prediction from first principles*, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany

2015.04 *Oracle R, Advanced & predictive Analytics Workshop*, Stony Brook University, Stony Brook, NY

2015.02 *MATLAB & Simulink for Project-Based Learning using LEGO MINDSTORMS EV3*, Stony Brook University, Stony Brook, NY

2015.01 *IACS workshop "Intro to Python"*, Stony Brook University, Stony Brook, NY

2014.11 *Novel phase of beryllium fluoride at high pressure*, Group seminar, Stony Brook University, Stony Brook, NY

2014.11 **Invited tutor** — *Theory and Computation for Interface Science and Catalysis: Fundamentals, Research and Hands on Engagement using VASP*, Brookhaven National Laboratory, Upton, NY

2014.10 *MATLAB and Simulink Complimentary Technical Sessions at Stony Brook University*, Stony Brook, NY

2014.09 *Proteins structure prediction using USPEX*, Group seminar, Stony Brook University, Stony Brook, NY

2014.09 *USPEX tests for Tinker: Different amino-acids XYZ-20, ALA-40, CASP10, REMD*, Group seminar, Stony Brook University, Stony Brook, NY

2014.07 *Introduction to Python*, Group seminar, Stony Brook University, Stony Brook, NY

2014.04 *SiO_2 and BeF_2 phase transformation under pressure. Proteins simulation with Tinker interface for USPEX*, Group seminar, Stony Brook University, Stony Brook, NY

2014.03 *CECAM workshop "Simulation of biomolecular interactions with inorganic and organic surfaces as a challenge for future nanotechnologies"*, Toulouse, France

2014.03 *USPEX mini-workshop*, Group seminar, Stony Brook University, Stony Brook, NY

2014.02 *SiO_2 and BeF_2 phase transformation under pressure*, Group seminar, Stony Brook University, Stony Brook, NY

2013.11 *Study of impurities influence on the hydrogen dissolution energy in the bcc iron*, Group seminar, Stony Brook University, Stony Brook, NY

2013.08 *2nd summer school on computer simulations in modern physics*, Chelyabinsk, Russia

2012.08 *Summer school on computer simulations and massive calculations in modern physics*, Chelyabinsk, Russia

2011.10 *6th All-Russian scientific-technical conference "Physical properties of metals and alloys"*, Yekaterinburg, Russia

2011.09 *International conference "Thermodynamics 2011"*, Athens, Greece

2011.05 *2nd All-Russian youth school-conference "Modern problems of metal science"*, Pitsunda, Abkhazia

2010.07 *International symposium "Metal-hydrogen systems. Fundamentals and applications"*, Moscow, Russia

2010.06 *International summer school "Computational Materials Science"*, San Sebastian, Spain

2010.03 *All-Russian conference "Parallel computing technologies 2010"*, Ufa, Russia

2010.02 *33rd International conference on theoretical physics "Kourovka-2010"*, Novouralsk, Russia

2009.11 *9th International conference "High-performance parallel computing on cluster systems"*, Vladimir, Russia

2009.10 *12th V.A. Fock All-Russian conference on quantum and computational chemistry*, Kazan, Russia

2007.04 *13th All-Russian students conference in physics*, Rostov-on-Don, Russia