Max Rakitin

Conferences, talks, workshops and schools

About

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

Summary: I am a computational scientist at NSLS-II, BNL. I help beamline staff and users run scientific experiments and perform data analysis. I write code in Python to integrate hardware (motors, cameras, detectors, etc.) and 3rd-party software systems with the Bluesky data acquisition framework. I am developing the Sirepo-Bluesky library that integrates Bluesky and the Sirepo browser-based interface to scientific modeling codes to enable access to "virtual" beamlines. I am a proponent of well-tested, modular, reusable, sustainable, and easily accessible code. I am fluent with modern CI systems (GitHub Actions, MS Azure Pipelines, etc.) I use Docker/Podman (including the creation of images), Linux (RHEL8, CentOS, Ubuntu, etc.), vagrant/VirtualBox on a daily basis. I am maintaining over 100 conda-forge feedstocks (Python, Python with C-extensions, C/C++, Fortran). I lead the continuous integration efforts to deploy and test the conda environments with the Bluesky software stack. I am enthusiastic about new technologies and AI/ML projects. I am a PI on an AI/ML LDRD project and a PI for two SBIR subcontracts with Radiasoft LLC (total funds of \$1M+).

"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: OBNL • SBU • SUSU
```

ORCID: 0000-0003-3685-852X

Conferences, talks, workshops and schools

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

Last updated:

- 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 9, 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
- 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 6, 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 SiO₂ and BeF₂ 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 2^{nd} summer school on computer simulations in modern physics $oldsymbol{\mathscr{O}}$, Chelyabinsk, Russia

NSLS-II - Brookhaven National Laboratory - Upton, NY 11973 Last updated: ☐ mrakitin@bnl.gov • ☐ mrakitin • in mrakitin

- 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" **Tolerance Tolerance** ("Physical properties of metals and alloys" **Tolerance** ("Physical properties of metals and alloys") **Tolerance** ("Physical properties of metals and alloys")
- 2011.09 International conference "Thermodynamics 2011", Athens, Greece
- 2011.05 2nd All-Russian youth school-conference "Modern problems of metal science" **9**, Pitsunda, Abkhazia
- 2010.07 International symposium "Metal-hydrogen systems. Fundamentals and applications" **©** \square , 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" **9**, Vladimir, Russia
- 2009.10 12th V.A. Fock All-Russian conference on quantum and computational chemistry **6**, Kazan, Russia
- 2007.04 13th All-Russian students conference in physics & 🖟, Rostov-on-Don, Russia