

# Maksim S. Rakitin

## Conferences, talks, workshops and schools

### About

Name: 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+).

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>





















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### Conferences, talks, workshops and schools

- 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<sub>2</sub> and BeF<sub>2</sub> 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<sub>2</sub> and BeF<sub>2</sub> 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<sup>nd</sup> 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 *6<sup>th</sup> All-Russian scientific-technical conference "Physical properties of metals and alloys"* , Yekaterinburg, Russia
- 2011.09 *International conference "Thermodynamics 2011"*, Athens, Greece
- 2011.05 *2<sup>nd</sup> 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 *33<sup>rd</sup> International conference on theoretical physics "Kourovka-2010"*  , Novouralsk, Russia

- 2009.11 9<sup>th</sup> International conference “High-performance parallel computing on cluster systems”  
, Vladimir, Russia
- 2009.10 12<sup>th</sup> V.A. Fock All-Russian conference on quantum and computational chemistry ,  
Kazan, Russia
- 2007.04 13<sup>th</sup> All-Russian students conference in physics  , Rostov-on-Don, Russia