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+).

Links: OBNL • SBU • SUSU

○ 🕤 @mrakitin • 🛅 @mrakitin • 🕿 Google Scholar • 🗷 ResearchGate • 📵 ORCID

Conferences, talks, workshops and schools

- 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,
- 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 & S, Brookhaven National Laboratory, Upton, NY
- 2018.07 SciPy 2018 6, 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 **9**, 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 **6**, 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 SiO₂ and BeF₂ 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" **O**, 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 2^{nd} summer school on computer simulations in modern physics \mathfrak{G} , 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" **Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Tolerance Toleran**
- 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" &
- 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