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 & &, 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 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" &, 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 $oldsymbol{\mathscr{G}},$ Chelyabinsk, Russia
- 2011.10 6th All-Russian scientific-technical conference "Physical properties of metals and alloys" **9**, 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" 🔗 **込**, Moscow, Russia
- 2010.06 International summer school "Computational Materials Science" 🔗 俎, 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,
- 2009.11 9th International conference "High-performance parallel computing on cluster systems" 9, Vladimir, Russia
- 2009.10 $^{12^{ ext{th}}}$ V.A. Fock All-Russian conference on quantum and computational chemistry $oldsymbol{\mathscr{G}}$, Kazan, Russia
- 2007.04 13th All-Russian students conference in physics 🔗 🖺, Rostov-on-Don, Russia