Maksim S. Rakitin

Curriculum vitae

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:
- BNL • SBU • SUSU
- @mrakitin • @mrakitin • Google Scholar • ResearchGate • ORCID

Experience

2021.03–present
Associate Computational Scientist and Supervisor, *Data Science and Systems Integration (DSSI) program, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).
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
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

Projects:

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, https://blueskyproject.io/bluesky.

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- **Ophyd** — a device abstraction library, https://blueskyproject.io/ophyd.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, https://blueskyproject.io/databroker.
- **Sirepo-Bluesky** — an interface library between the **Bluesky** data acquisition framework and the **Sirepo** browser-based interface framework to beamline and accelerator simulation codes, https://github.com/NSLS-II/sirepo-bluesky.
- Many other related software projects.

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 (SLAC, APS, ALS).
- 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 intern), summer 2021 (2 interns)).

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)

Projects:

- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, https://github.com/ochubar/SRW.
- **Sirepo** — a cloud-based framework for SRW, https://github.com/radiasoft/sirepo.
- **Image processing and data visualization**, https://github.com/mrakitin/plotting and https://github.com/mrakitin/experiments.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.

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

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 http://han.ess.sunysb.edu and 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 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://susu.ac.ru).

Supervisor: Prof. Alexander A. Mirzoev

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 (http://www.appliedtech.ru), a partner of Rocket Software Inc., USA (https://www.rocketsoftware.com)

Supervisor: Valery Ermakov, CEO

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://susu.ac.ru)
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

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 cources 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, WebGL, PHP, HTML5, bash, csh/tcsh, make, Perl, AutoIt3, REXX, SQL, JCL

Parallelization MPI, OpenMP, Dask

IDE/editors VSCode, PyCharm, Eclipse, vim, 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

Supervisor

Brookhaven National Laboratory

Stuart Campbell, Ph.D., Chief Data Scientist and Deputy Program Manager for DSSI
NSLS-II/Photon Science Division, Brookhaven National Laboratory, Upton, NY 11973
scampbell@bnl.gov +1 (631) 344–5578

Additional references available upon request.

Publications

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38. 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

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Eds., vol. 11493, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 78–87. https://doi.org/10.1117/12.2567448

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3. A. A. Mirzoev, D. A. Mirzaev, and M. S. Rakitin, "Impurities influence on dissolution of hydrogen in bcc iron," *Bulletin of the South Ural State University: Math., Mech. and Phys.*, vol. 4, no. 10, pp. 77–83, 2011, Original Russian Text. https://vestnik.susu.ru/mmph/issue/viewFile/46/22#page=77

2. M. S. Rakitin, A. A. Mirzoev, and D. A. Mirzaev, "Change of electronic structure in iron containing interstitial atoms of hydrogen," *Bulletin of the South Ural State University: Metallurgy*, vol. 14, no. 13, pp. 67–71, 2010, Original Russian Text. https://vestnik.susu.ru/metallurgy/issue/archive

1. A. A. Mirzoev, M. M. Yalalov, and M. S. Rakitin, "Dependence of TB-LMTO calculations accuracy on k-points number: effect of iterations mixing parameter using Broyden scheme," *Bulletin of the South Ural State University: Math., Phys. and Chem.*, vol. 6, no. 6, pp. 103–105, 2005, Original Russian Text. https://vestnik.susu.ru/mmph/issue/viewFile/36/12#page=103

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, 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 *2^{nd} 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^{th} All-Russian scientific-technical conference "Physical properties of metals and alloys"*, Yekaterinburg, Russia

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

2011.05 *2^{nd} 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

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