Maksim S. Rakitin

Experience

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

Links:
- BNL • SBU • SUSU
- @mrakitin • @mrakitin • Google Scholar • ResearchGate
- ORCID: 0000-0003-3685-852X

Experience

2021.03–present
Brookhaven National Laboratory
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
Brookhaven National Laboratory
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

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2017.11–2019.09 Brookhaven National Laboratory

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.
- **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.