

# Maksim S. Rakitin

## Computer skills

### 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](#)

### 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, Autot3, REXX, SQL, JCL

**Parallelization** MPI, OpenMP, Dask

**IDE/editors** VSCode, PyCharm, Eclipse, vim, emacs

**Writing**  $\LaTeX$ , Bib $\TeX$ , 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