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 • in @mrakitin • 🎓 Google Scholar • R⁶ ResearchGate
○ ⓘD 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, 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