Max Rakitin

Bio

Personal details

Name: Max Rakitin (a.k.a. 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:
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Education and training

2008.10–2012.09 **Ph.D. in Condensed Matter Physics (defended on September 19, 2012)**
South Ural State University (National Research University), Chelyabinsk, Russia

2006.09–2008.06 **M.S. in Applied Mathematics and Physics (June 13, 2008)**
South Ural State University (SUSU), Chelyabinsk, Russia

2002.09–2006.06 **B.S. in Applied Mathematics and Physics (June 20, 2006), summa cum laude**
South Ural State University (SUSU), Chelyabinsk, Russia

Research and professional expertise

2017.11–present **Associate Computational Scientist**, *DAMA group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2015.12–2017.10 **Research Associate (Postdoc)**, *NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2013.10–2015.12 **Postdoctoral Associate (Postdoc)**, *Department of Geosciences, Stony Brook University*, Stony Brook, NY (https://stonybrook.edu, https://uspex-team.org/en)

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2007.06–2013.10 **QA Engineer, QA Team Leader**, *Applied Technologies Ltd.*, Chelyabinsk, Russia (https://www.appliedtech.ru/en/), a partner of Rocket Software Inc., USA (https://www.rocketsoftware.com)

Software 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.
- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, https://github.com/mrakitin/SRW.
- **Sirepo** — a cloud-based framework for SRW, https://github.com/radiasoft/sirepo.
- **Databroker extractor** — image processing and data visualization, https://github.com/mrakitin/databroker-extractor.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.
- **USPEX** — a code for evolutionary crystal structure prediction, https://uspex-team.org/en.
- **USPEX online utilities** — a set of pre- and post-processing tools for crystal structure simulations, https://uspex-team.org/en/uspex/tools.
- **USPEX manual** — https://uspex-team.org/en/uspex/documentation.
- Utilities for DFT simulations
- IBM Mainframe software projects

Publications

52. M. Rakitin, R. Bode, T. W. Morris, A. C. Giles, A. L. Walter, J. K. Lynch, J. Maldonado, Y. Du, B. Romasky, M. Fedurin, P. Moeller, and B. Nash, "Recent updates of the Sirepo-Bluesky library for virtual beamline representation," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 126970D. https://doi.org/10.1117/12.2678030

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automated alignment of the TES beamline," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012103, Dec. 2022. https://doi.org/10.1088/1742-6596/2380/1/012103

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20. O. Chubar, C. Kitegi, Y.-C. K. Chen-Wiegart, D. Hidas, Y. Hidaka, T. Tanabe, G. Williams, J. Thieme, T. Caswell, M. Rakitin, L. Wiegart, A. Fluerasu, L. Yang, S. Chodankar, and M. Zhernenkov, "Spectrum-Based Alignment of In-Vacuum Undulators in a Low-Emittance Storage Ring," *Synchrotron Radiation News*, vol. 31, no. 3, pp. 4–8, 2018. https://doi.org/10.1080/08940886.2018.1460173

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18. M. S. Rakitin, O. Chubar, P. Moeller, R. Nagler, and D. L. Bruhwiler, "Sirepo: a web-based interface for physical optics simulations - its deployment and use at NSLS-II **(invited paper)**," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 103880R. https://doi.org/10.1117/12.2274031

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