Sikao Guo, Ph.D.

RESEARCH SOFTWARE ENGINEER | SCIENTIFIC COMPUTING | COMPUTATIONAL BIOPHYSICS

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PROFESSIONAL SUMMARY

Research software engineer and computational biophysicist with 6+ years building reliable C++/Python systems for molecular modeling, structural bioinformatics, and high-performance simulation. Strong record translating academic prototypes into tested, documented, reproducible tools for scientific users.

PROFESSIONAL EXPERIENCE

Inria **Jul 2025 - Present**

Research Engineer *Sophia Antipolis, France*

- Architected AutoCLIP, a Python Model-View-Presenter and JSON Schema code-generation system that transforms one application specification into PyMOL/Qt, VMD/Tkinter, Panel/NGL, and Panel/Three.js interfaces; deployed nine applications and replaced separate application-platform implementations with reusable specifications and platform adapters.
- Built the browser deployment stack with FastAPI, Panel/Bokeh, Nginx WebSocket routing, systemd services, authentication, and session isolation, moving local CLI workflows to secure multi-user web access.
- Re-architected GitLab CI/CD and Pixi/Conda packaging for Linux x86-64, macOS Intel, and Apple Silicon; established 232 tests across 22 pytest modules and an 11-file executable reproducibility package.
- Productionized a Hit-and-Run MCMC and tripeptide loop-closure prototype into a modular C++17/Python platform supporting four endpoint modes, multiloop, rigid-secondary-structure, and IDR sampling; added 27 automated test files and deterministic multi-seed execution.
- Engineered expected O(n + K) spatial-hash collision checks, dense/sparse memory backends, and search over 100,000+ loop-closure combinations; corrected SO(3)/SE(3), RNG, indexing, DOVI, and closure defects that caused deadlocks, instability, or zero-output runs, and integrated AttnPacker/OpenMM/PhiSiCal validation.

Johns Hopkins University **Jan 2020 - Jun 2025**

Assistant Research Scientist (2025); Postdoctoral Fellow (2020-2024) *Baltimore, MD*

- Led C++/MPI development of NERDSS using spatial domain decomposition, ghost regions, stable global IDs, and serialized neighbor exchange, achieving near-linear scaling through 96 CPUs and approximately 90x acceleration on 20,000-particle reversible-reaction workloads.
- Designed and validated cross-rank reaction, assembly, dissociation, restart, and event-sampling behavior through seven benchmark models spanning 2D/3D diffusion, membrane reactions, oligomerization, and clathrin lattices; verified results against analytical theory and serial NERDSS.
- Co-developed ioNERDSS, a Python/Biopython structure-to-simulation pipeline using KD-trees, interface geometry, reaction generation, and sequence-alignment fallbacks; benchmarked it on 44,000+ PDB structures and workflows from 3- to 720-subunit assemblies.
- Built end-to-end simulation and restart APIs plus 19 analysis and visualization functions; shipped multiple PyPI releases through v1.2.0 with PyQt6/OVITO interfaces, Docker/Conda/Jupyter environments, pytest/GitHub Actions, and Sphinx documentation.
- Applied the software stack to published clathrin and HIV-1 assembly studies, connecting engineering decisions to experimentally testable models and demonstrating reliability on approximately 3,700-subunit systems.

Institute of Physics, Chinese Academy of Sciences **Sep 2014 - Dec 2019**

Doctoral Researcher *Beijing, China*

- Implemented reusable stochastic Runge-Kutta and Monte Carlo simulation workflows for kinesin ATPase cycling, stepping, run length, and detachment across an approximately 45 pN bidirectional load range, reproducing multiple independent experimental datasets.
- Built nucleotide-state kinesin-microtubule complexes from four PDB structures and automated 200+ ns GROMACS/AMBER99SB simulations with umbrella sampling, PMF, and WHAM analysis.

SELECTED OPEN-SOURCE SOFTWARE

AutoCLIP — cross-platform scientific GUI and deployment framework (GitHub | Docs)
NERDSS-MPI — parallel C++ particle-based reaction-diffusion simulator (GitHub | Guide)
ioNERDSS — automated PDB/mmCIF-to-simulation workflow (GitHub | Docs)

EDUCATION

Ph.D. in Physics | Institute of Physics, Chinese Academy of Sciences | Beijing, China | Sep 2014 - Dec 2019
B.S. in Physics | Nankai University | Tianjin, China | Sep 2010 - Jun 2014

SELECTED PUBLICATIONS

Full publication list: Google Scholar

- **Guo S**, Sarti E, Cazals F. A Unified, Cross-Platform Framework for Automatic GUI and Plugin Generation in Structural Bioinformatics and Beyond. *arXiv preprint, 2026.* arXiv:2602.16047
- **Guo S**, Korolija N, et al. Parallelization of Particle-Based Reaction-Diffusion Simulations Using MPI. *Journal of Computational Chemistry, 2025.* doi:10.1002/jcc.70132
- Ying YM, Sang M, et al., including **Guo S**. Transforming Macromolecular Structures into Simulations of Self-Assembly with ioNERDSS. *bioRxiv preprint, 2026.* doi:10.64898/2026.01.27.702082
- **Guo S**, Saha I, Saffarian S, Johnson ME. Structure of the HIV Immature Lattice Allows for Essential Lattice Remodeling within Budded Virions. *eLife, 2023.* doi:10.7554/eLife.84881
- **Guo S**, Sodt AJ, Johnson ME. Large Self-Assembled Clathrin Lattices Spontaneously Disassemble without Sufficient Adaptor Proteins. *PLOS Computational Biology, 2022.* doi:10.1371/journal.pcbi.1009969

TECHNICAL SKILLS

Languages & HPC: C++, Python, MPI, Bash, Linux, CMake, distributed-memory computing, parallel algorithms
Architecture & Quality: software architecture, API design, JSON Schema, FastAPI, pytest, GitHub Actions/GitLab CI, PyPI, Conda/Pixi, Docker, Sphinx documentation
Scientific Computing: NumPy, SciPy, Biopython, Eigen, CGAL, OpenMM, GROMACS, structural data processing, stochastic simulation, numerical validation
Interfaces & Deployment: PyQt6, Tkinter, Panel/Bokeh, NGL, Three.js, PyMOL, VMD, Nginx, WebSockets, systemd