Sikao Guo, Ph.D.

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PROFESSIONAL SUMMARY

Research engineer for computational biology and molecular simulation. Develop scalable C++ and Python systems spanning MPI-based high-performance computing, computational geometry, molecular simulation, and scientific workflows, transforming research algorithms into reusable software infrastructure.

EXPERIENCE

Inria | Research Engineer

Jul. 2025 — Present | Sophia Antipolis, France

- Developed a cross-platform GUI code-generation framework that automated interface generation for 9+ computational biology applications across VMD, PyMOL, and Web platforms.
- Engineered a C++ protein backbone sampler that generalized inverse-kinematics loop sampling to backbone and intrinsically disordered region (IDR) conformational sampling using SE(3)-based rigid-body moves.
- Built an automated structural validation pipeline integrating AttnPacker, OpenMM, and PhiSiCal for reproducible evaluation and benchmarking of sampled protein conformations.

Johns Hopkins University | Postdoctoral Researcher, Assistant Research Scientist

Jan. 2020 — Jun. 2025 | Baltimore, MD

- Parallelized the C++ NERDSS reaction-diffusion simulator using MPI domain decomposition, achieving near-linear strong scaling to 96 CPU cores for large-scale biomolecular self-assembly simulations.
- Developed structure-resolved computational models of clathrin-mediated endocytosis and HIV-1 assembly, revealing mechanisms governing critical nucleus formation, adaptor stoichiometry, and Gag-Pol dimerization.
- Developed ioNERDSS, a Python toolkit that automates conversion of PDB/mmCIF structures into simulation-ready coarse-grained reaction–diffusion models, substantially reducing manual model preparation.
- Implemented computational geometry and machine-learning algorithms for interface detection, reaction-network generation, and binding-affinity estimation to automate simulation parameterization.

EDUCATION

Institute of Physics, Chinese Academy of Sciences | Ph.D. Physics

Sept. 2014 — Dec. 2019 | Beijing, China

Nankai University | B.S. Physics

Sept. 2010 — Jun. 2014 | Tianjin, China

SELECTED PUBLICATIONS

Guo, S., Sarti, E., and Cazals, F. “A Unified, Cross-Platform Framework for Automatic GUI and Plugin Generation in Structural Bioinformatics and Beyond”. *arXiv*, 2026. arXiv:2602.16047.

Guo, S., Korolija, N., et al., “Parallelization of Particle-Based Reaction--Diffusion Simulations Using MPI”. *Journal of Computational Chemistry*, 46(14):e70132, 2025. doi:10.1002/jcc.70132.

Ying, Y. M., Sang, M., et al., including **Guo, S.** “Transforming Macromolecular Structures into Simulations of Self-Assembly with ioNERDSS”. *bioRxiv*, 2026. doi:10.64898/2026.01.27.702082.

OPEN-SOURCE SOFTWARE

Scientific GUI Framework (GitHub | Documentation) *Cross-platform scientific GUI generation framework.*
NERDSS-MPI (GitHub | Documentation) *Parallel C++ protein assembly simulator using MPI.*
ioNERDSS (GitHub | Documentation) *Automated construction of coarse-grained reaction--diffusion models.*

SKILLS

Python, C++, Scientific Software Development, High-Performance Computing (MPI), Parallel Computing, Computational Biophysics, Structural Bioinformatics, Protein Modeling, Algorithm Development