Lijie Ding

Contact: (401)-410-4049, ljding.jobs@gmail.com
For more: Github, LinkedIn, Google Scholar, CV

Skills

Scientific Computing: Monte Carlo (MC), Molecular Dynamics (MD), LAMMPS, HOOMD-blue, HPC, Slurm
Programming: Python (PyTorch, CrewAI, LangChain, NumPy, Pandas, Scikit-learn), C/C++, CUDA, SQL
Domain Knowledge: Agentic AI, Large Language Models (LLMs), Deep Learning (DL), Machine Learning (ML), Physics-informed ML, Computational Physics, Small-Angle Scattering (SAS), Quantitative Finance

Experience

Oak Ridge National Laboratory (ORNL) — Oak Ridge, TN
Postdoctoral Research Associate — May 2024 – Present

Agentic AI for Science: Engineered multi-agent systems (CrewAI, LangChain, and OpenCode) to orchestrate complex scientific workflows such as SAS data analysis, MD (LAMMPS) and MC (HOOMD-blue) simulations.
LLM Application: Architected an LLM-driven proposal review pipeline using pairwise preference and AI-as-a-judge, achieved 800× cost reduction while maintaining review performance for Spallation Neutron Source.
AI for Characterization: Developed and trained physics-informed ML/DL models (e.g., Gaussian process regression, Bayesian inference, VAEs, CNNs) to extract hidden information from SAS, applied to colloids, polymers, lamellae, and polydisperse systems.
Scientific Computing: Developed MD/MC simulations using C++, Python, LAMMPS, and HOOMD-blue for colloids, polymers, active fluid and rheology systems.

Goldman Sachs — New York, NY
Quantitative Strategist, Vice President (Jan24-May24), Associate (Jun22-Dec 23) — Jan 2024 – May 2024

Model Development: Owned the full lifecycle development of proprietary production valuation models, ensuring high reliability and performance for interest rate (IR) derivative pricing. Executed the SOFR transition for IR products and conducted statistical validation for SOFR-based pricing.
Large-Scale Attribution Analysis: Built analysis pipelines to explain price variance vs. market consensus and decompose moves into key risk factors for multi-billion-dollar inventory instruments.

Brown University — Providence, RI
Ph.D. Research Assistant — Sep 2017 – Jun 2022

Scientific Computing: Developed high-performance MC simulations for colloidal membranes in C++. Performed mathematical modeling and numerical studies in Python.
Scientific Data Analysis: Developed OpenCV-based image analysis tools for DNA Brownian motion and performed time series analysis.

Publications

Lijie Ding, Jan Michael Y. Carrillo, and Changwoo Do. ToPolyAgent: AI agents for coarse-grained bead-spring topological polymer simulations. *Digital Discovery*, 2026. DOI: 10.1039/D5DD00471C
Lijie Ding, Janell Thomson, Jon Taylor, and Changwoo Do. LLMs can assist with proposal selection at large user facilities. *arXiv preprint arXiv:2512.10895*, 2025. arXiv: 2512.10895
Lijie Ding and Changwoo Do. Deciphering the small-angle scattering of polydisperse hard spheres using deep learning. *APL Machine Learning*, 3(3):036112, 08 2025. DOI: 10.1063/5.0290589
More: full list can be found at Google Scholar, or CV

Education

Brown University — Providence, RI
Ph.D. in Physics (Dissertation: Chiral Liquid Crystals on Deformable Surfaces) — 2022
University of Science and Technology of China (USTC) — Hefei, China
B.Sc. in Applied Physics — 2017