Ruichen Xu

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Objective

Ph.D. candidate in Applied Mathematics & Statistics (Stony Brook University) seeking an **internship** focused on applying **large language models (LLMs)** and **diffusion models** to real-world applications. Interests include agentic LLM workflows (tool use, structured generation, retrieval), multimodal/diffusion modeling for generation and inverse problems, and rigorous evaluation. I aim to build reliable, reproducible ML systems—from rapid prototyping to scalable training/inference—and collaborate to turn research into usable products and tools.

Experience

- **Stony Brook University — Department of Applied Mathematics & Statistics (AMS)** *Aug 2022 – Present*
  Graduate Researcher, Teaching Assistant & Instructor (Advisor: Prof. Yuefan Deng) Stony Brook, NY, USA
  - Research in **neural operators**, **AI for PDEs**, **simulated annealing**; large-scale runs on **Seawulf/NVwulf** (SLURM, CUDA, job arrays, logging).
  - **Teaching Assistant:** AMS 310 (F'22, S'23), AMS 326 (S'24), AMS 510 (F'24; led recitations), AMS 595 (F'24), AMS 528 (S'25), AMS 502 (S'25); ran discussions, grading, office hours.
  - **Instructor:** AMS 394 (W'23, W'24, Su'24, Su'25); AMS 326 (Su'25)— designed/delivered lectures, created/graded assessments, mentored students.
  - Lightning Speaker, **IACS Annual Meeting** (2025, 2024).
- **Courant Institute of Mathematical Sciences, New York University (NYU)** *Jan 2021 – May 2022*
  Recitation Leader New York, NY, USA
  - Courses: Mathematics for Economics II (Sp'21, Sp'22); Probability, Statistics & Decision Making (Fa'21, Sp'22). Led recitations, graded, held office hours.
- **Courant Institute of Mathematical Sciences, New York University (NYU)** *Fall 2020, Fall 2021*
  Grader New York, NY, USA
  - Courses: Analysis (Fa'20); Special Topics (Fa'21).

Education

- **Stony Brook University (The State University of New York)** *Aug. 2022 – May. 2027 (Expected)*
  Ph.D., Computational Applied Mathematics (GPA 4.00/4.00) Stony Brook, NY, USA
- **Courant Institute of Mathematical Sciences, New York University (NYU)** *Sept. 2020 – May. 2022*
  M.S., Mathematics (GPA 4.00/4.00) New York, NY, USA
- **University of California, Davis** *Sept. 2019 – Jun. 2020*
  M.S., Statistics (GPA 3.94/4.00) Davis, CA, USA
- **Beijing University of Chemical Technology (BUCT)** *Sept. 2015 – Jun. 2019*
  Bachelor, Financial Mathematics (89.33/100); Minor: Commercial Management Beijing, China

Projects

- **ORACLE: LLM-Guided Edits + Simulated Annealing for SBDD (ongoing)** *2025 – Present*
  Tools: Python, PyTorch; Topics: structure-based design, multi-objective optimization (docking, QED, SA-Score) [🌐]
  - Couples contact-aware, LLM-driven molecular edits with SA under a unified score to improve pocket interaction quality *and* drug-likeness while preserving pocket fidelity.
  - Builds a reproducible pipeline for scoring/selection and ablation across objectives; emphasizes careful control of docking/QED/SA-Score trade-offs.
- **RL-Guided Simulated Annealing (QESA) (ongoing)** *2024 – Present*
  *Tools: Python, PyTorch; HPC: **Seawulf** & **NVwulf**; Topic: adaptive temperature control via quasi-equilibrium* [🌐]
  - Learns a temperature-adjustment policy that maintains near-equilibrium sampling, stabilizing exploration and reducing schedule hand-tuning.
  - End-to-end sweeps and logging on Seawulf/NVwulf (job arrays, checkpoints, metrics), with comparisons to classical SA schedules and move schemes.
- **Physics-Informed Active Learning for Neural Operators (ongoing)** *2025 – Present*
  Tools: PyTorch; Topics: operator learning, physics-aware acquisition [🌐]
  - Designs a physics-aware query strategy over parameters/initial conditions to cut training data while maintaining operator accuracy.
  - Targets robust generalization under limited sensing; integrates uncertainty and PDE residuals into acquisition.
- **PartialObs–PDEBench: Benchmarking PDE Solvers with Partial Observations (ongoing)** *2025 – Present*
  Tools: Python; Topics: standardized sparse sensing, MAP recovery interface [🌐]
  - Standardizes sensing protocols (random/uniform/subdomain/FFT masks) and a MAP-recovery API for fair, reproducible comparison under partial observations.
  - Provides loaders/format and leaderboard hooks to evaluate solvers consistently across PDE families.

PUBLICATIONS

Peer-Reviewed — Conferences

[c.1] Discretization-invariance? On the Discretization Mismatch Errors in Neural Operators.
Wenhan Gao, **Ruichen Xu**, Yuefan Deng, Yi Liu. *International Conference on Learning Representations (ICLR), 2025.* (OpenReview) (ICLR Page)
Contribution: formalizes discretization-mismatch errors and introduces CROP for robust cross-resolution operator learning.

[c.2] Kolmogorov–Arnold Representation for Symplectic Learning: Advancing Hamiltonian Neural Networks.
Z. Wu, **R. Xu**†, L. Chen, G. Kementzidis, S. Wang, Y. Deng. *International Joint Conference on Neural Networks (IJCNN), 2025.* (IEEE / IJCNN)
Role: †*co-first author; project lead*.
Contribution: Kolmogorov–Arnold–based parameterization for symplectic HNNs preserving energy and long-horizon phase-space structure.

[c.3] Boundary-Informed Method of Lines for Physics-Informed Neural Networks.
Maximilian Cederholm, Siyao Wang, Haochun Wang, **Ruichen Xu**, Yuefan Deng.
New York Scientific Data Summit (NYSDS) 2025, SIAM Proceedings, 2025. (SIAM DOI: 10.1137/1.9781611978933.12)
Contribution: hybrid MOL–PINN solver fusing classical method-of-lines with PINNs to achieve high-accuracy PDE solutions using far fewer collocation points. *Role: project lead and co-corresponding author (with Y. Deng).*

[c.4] Velocity-Inferred Hamiltonian Networks: Symplectic Dynamics from Position-Only Observations.
Ruichen Xu, Claire Yu, Zongyu Wu, Siyao Wang, Luoyao Chen, Georgios Kementzidis, Haochun Wang, Yuefan Deng.
New York Scientific Data Summit (NYSDS) 2025, SIAM Proceedings, 2025. (SIAM DOI: 10.1137/1.9781611978933.13)
Contribution: introduces velocity-inferred Hamiltonian networks that reconstruct latent velocities from position-only trajectories while preserving symplectic structure and long-horizon energy. *Role: project lead and co-corresponding author (with Y. Deng).*

[c.5] Physics-Informed Active Learning via Functional Simulated Annealing for Neural Operator.
Albert Ding, Siyao Wang, Haochun Wang, **Ruichen Xu**, Yuefan Deng.
New York Scientific Data Summit (NYSDS) 2025, SIAM Proceedings, 2025. (SIAM DOI: 10.1137/1.9781611978933.14)
Contribution: proposes a physics-informed active-learning scheme using functional simulated annealing to select informative neural-operator training queries under PDE constraints. *Role: project lead and co-corresponding author (with Y. Deng).*

Peer-Reviewed — Journals

[j.1] Dynamic Schwartz–Fourier Neural Operator for Enhanced Expressive Power.
Wenhan Gao, Jian Luo, **Ruichen Xu**, Yi Liu. *Transactions on Machine Learning Research (TMLR), 2025.* (OpenReview)
Contribution: augments FNOs with dynamic Schwartz operators for adaptive cross-frequency interactions on physics tasks.

[j.2] Coordinate Transform Fourier Neural Operators for Symmetries in Physical Modeling.
Wenhan Gao, **Ruichen Xu**, **Haochun Wang**, Yi Liu. *TMLR*, 2024. (OpenReview)
Contribution: enforces coordinate-transform consistency in FNOs to respect domain symmetries and improve cross-frame generalization.

Peer-Reviewed Workshops

[w.1] APOD: Adaptive PDE-observation diffusion for physics-constrained sampling.
Ruichen Xu, Haochun Wang, Georgios Kementzidis, Chenhao Si, Yuefan Deng. *ICML 2025 Workshop on Assessing World Models (Poster).* (OpenReview)
Contribution: couples diffusion sampling with PDE constraints to generate fields consistent with sparse observations and physics.

[w.2] RL-QESA: Reinforcement-Learning Quasi-Equilibrium Simulated Annealing.
Ruichen Xu, Kai Li, Haochun Wang, Georgios Kementzidis, Wei Zhu, Yuefan Deng. *2nd AI for Math Workshop @ ICML 2025 (Poster).* (OpenReview)
Contribution: learns temperature adjustments that keep SA near quasi-equilibrium for steadier exploration.

[w.3] An Iterative Framework for Generative Backmapping of Coarse-Grained Proteins.
Georgios Kementzidis, Erin Wong, John Nicholson, **Ruichen Xu**, Yuefan Deng. *ICML 2025 GenBio Workshop (Poster).* (OpenReview)
Contribution: iterative generative pipeline reconstructing atomistic detail from coarse-grained structures.

[w.4] SP: Learning Physics from Sparse Observations — Three Pitfalls of PDE-Constrained Diffusion Models.
Ruichen Xu, Haochun Wang, Georgios Kementzidis, Chenhao Si, Yuefan Deng. *ICML 2025 Workshop on Assessing World Models (Poster).*
Contribution: identifies noise-phase futility, grid-locking, and scale mismatch; outlines APOD to mitigate them.

Preprints

[s.1] **Velocity-Inferred Hamiltonian Neural Networks: Learning Energy-Conserving Dynamics from Position-Only Data.**
R. Xu, Z. Wu, L. Chen, G. Kementzidis, S. Wang, H. Wang, Y. Shi, Y. Deng. *arXiv preprint, 2025.* (arXiv)
Contribution: infers latent velocities from position-only trajectories to train energy-preserving HNNs with reduced sensing needs.

[s.2] **The Impact of Move Schemes on Simulated Annealing Performance.**
R. Xu, H. Wang, Y. Deng. *arXiv preprint, 2025.* (arXiv)
Contribution: systematic study of SA move strategies, identifying regimes where single-coordinate and other proposals converge fastest.

[s.3] **An Iterative Framework for Generative Backmapping of Coarse-Grained Proteins.**
G. Kementzidis, E. Wong, J. Nicholson, **R. Xu**, Y. Deng. *arXiv preprint, 2025.* (arXiv)
Contribution: iterative generative pipeline reconstructing atomistic detail from coarse-grained structures with improved fidelity.

Talks & Presentations

- **Lightning Talk — Diffusion4PDE** *2025*
  IACS Annual Meeting, Institute for Advanced Computational Science (Stony Brook University) [🌐]
  ◦ Topic: diffusion-based sampling under PDE constraints.
- **Lightning Talk — Active Learning for Neural Operators** *2024*
  IACS Annual Meeting, Institute for Advanced Computational Science (Stony Brook University) [🌐]
  ◦ Topic: physics-aware acquisition strategies for neural operators.
- **Student Seminar Speaker — AI for PDEs** *2025*
  IACS Student Seminar (Stony Brook University) [🌐]
  ◦ Overview: neural operators and optimization; current projects.

Professional Service

- Reviewer, *International Joint Conference on Neural Networks (IJCNN)*, 2025.
- Reviewer, *IEEE Transactions on Neural Networks and Learning Systems (TNNLS)*.
- Reviewer, *International Conference on Learning Representations (ICLR)*, 2026.

Skills

- **Programming Languages:** Python, C/C++, MATLAB, R
- **Web Technologies:** Basic HTML/CSS for docs & sites
- **Database Systems:** HDF5
- **Data Science & Machine Learning:** PyTorch, PyTorch Lightning, scikit-learn; diffusion models; neural operators (FNO/PINO variants)
- **High-Performance Computing:** **Seawulf** & **NVwulf** clusters (SLURM, CUDA, job arrays, logging); Linux servers
- **DevOps & Version Control:** Git/GitHub, Docker, experiment tracking
- **Specialized Area:** Scientific ML for PDEs, Simulated Annealing, Reinforcement Learning (policy-guided optimization)
- **Mathematical & Statistical Tools:** Numerical PDEs, optimization, spectral/FFT methods, uncertainty evaluation
- **Other Tools & Technologies:** LaTeX, Markdown, shell scripting
- **Research Skills:** Reproducible pipelines, dataset preparation, benchmarking, paper writing

References

1. **Prof. Yuefan Deng**
   Professor, Department of Applied Mathematics & Statistics
   Stony Brook University
   Email: yuefan.deng@stonybrook.edu
   Relationship: Ph.D. Advisor
2. **Prof. Bertal H. Aktas**
   Assistant Professor of Medicine, Department of Medicine
   Brigham and Women's Hospital; Harvard Medical School
   Email: huseyin_aktas@hms.harvard.edu
   Relationship: Key Collaborator