ZEXI FAN

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Personal Homepage
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PROFILE

I am a Computational Mathematics undergraduate at Peking University focusing on high-dimensional PDE solvers, scientific machine learning (SCiSML), diffusion processes, and quantum Markov dynamics. I develop rigorous simulation-calibrated estimators (theory + large-scale experiments) and prove non-asymptotic guarantees for sampling/estimation algorithms. Seeking PhD opportunities to continue work at the intersection of quantum Markov chains, high-dimensional PDEs, stochastic analysis, and Machine Learning.

EDUCATION

Peking University (PKU) Sep 2022 – Present
B.S. in Computational Mathematics; Major GPA: 3.6/4.0
Selected coursework: High-Dimensional Probability, Stochastic Analysis & Control, Scientific Machine Learning, Optimization Methods, Mathematical Image Processing
GRE: 164(Q) / 169(V) / 4.0(A) Aug 2023

RESEARCH INTERESTS

Quantum Markov dynamics / Markov chain analysis; High-dimensional PDE solvers & multilevel Picard methods; Simulation-calibrated scientific ML (SCaSML); Diffusion processes, transition-path sampling & Schrodinger bridges; Probabilistic ML and concentration inequalities for control / bandits.

PUBLICATIONS & MANUSCRIPTS

Physics-Informed Inference Time Scaling via Simulation-Calibrated Scientific Machine Learning Preprint (arXiv)
Authors: Zexi Fan, Yan Sun, Shihao Yang, Yiping Lu Apr 2025

· Simulation-calibrated estimators for PINNs; theoretical rate improvements via Multilevel Picard and empirical validation on 100d+ PDEs.

Accelerating Non-equilibrium steady state sampling in Quantum Markov Process through Second-order Lifting In preparation
Authors: Zexi Fan, Jianfeng Lu 2025

· Second-order lifting approach for NESS sampling of Lindbladians; analytic bounds on relaxation times via hypocoercivity and flow Poincaré inequalities.

Pessimistic Policy Learning for Continuous-Action Bandit Problem without Uniform Overlap In preparation
Authors: Zexi Fan, Ying Jin 2024–Present

· Pessimism-regularized continuous-action policy estimation; theoretical suboptimality guarantees under relaxed coverage assumptions.

RESEARCH EXPERIENCE

Accelerating Non-equilibrium steady state sampling in Quantum Markov Process through Second-order Lifting Jul 2025 – Present
Advisor: Prof. Jianfeng Lu Duke

· Designed a **second-order lifting** framework to accelerate sampling of non-equilibrium steady states (NESS) for Lindbladian dynamics with Lamb-shift Hamiltonian.

- Applied hypocoercivity theory and flow-Poincaré inequalities to derive **rigorous lower and upper bounds** on relaxation times for lifted dynamics; identified regimes where lifting yields provable spectral-gap improvements.

Continuous-State Contextual Bandit with Pessimism Regularization Aug 2024 – Present
Advisor: Prof. Ying Jin Harvard

- Constructed a novel extension of pessimism regularization to continuous-state, continuous-action contextual bandits, adapting uncertainty-aware penalties to function approximation settings.
- Proved that the estimator's suboptimality guarantee holds **without** the uniform overlap assumption commonly required in prior works; developed concentration analyses tailored to continuous policies.

Simulation-Calibrated Scientific Machine Learning (SCaSML) for High-Dimensional PDEs
Jun 2024 – Apr 2025
Advisors: Prof. Yiping Lu, Dr. Yan Sun Northwestern & Georgia Tech

- Proposed SCaSML: a family of simulation-based estimators that **calibrate PINN surrogates** using randomized Multilevel Monte Carlo and Multilevel Picard (MLP) correction.
- Provided **rigorous rate improvements** by analyzing bias/variance trade-offs under MLP corrections; derived complexity bounds demonstrating superior scaling in dimensionality compared to vanilla PINNs.
- Scaled experiments to multiple **100d+** semilinear/parabolic PDEs verifying accuracy and computational efficiency; open-source implementation: github.com/Francis-Fan-create/SCaSML.

Flow-Calibrated RL for Transition Path Sampling Feb 2024 – Jun 2024
Prof. Yiping Lu, Dr. Dinghuai Zhang NYU Courant& Mila

- Reformulated transition-path sampling as a stochastic schrodinger bridge matching problem; developed continuous Soft Actor-Critic and GFlowNet variants guided by flow calibration. (Slides & notes: link)

Unbiased Square-Root Convergent Estimation for High-Dimensional Semilinear Parabolic Heat Equation Sep 2023 – Feb 2024
Prof. Yiping Lu NYU Courant

- Proposed an unbiased estimator combining Multilevel Picard iteration with randomized MLMC; established unbiasedness and bounded variance properties.

SELECTED COURSEWORK & ACADEMIC ACTIVITIES

Graduate-level: High Dimensional Probability; Applied Stochastic Analysis; Optimization Methods; Mathematical Image Processing; Machine Learning.
Seminars: Stochastic Optimal Control; LLMs & Scientific Computing; Blowup in Fluid Equations.
Summer school: Beauty of Theoretical Computer Science (NJU), Summer 2024.

TECHNICAL SKILLS

Programming	Python, MATLAB, LaTeX, Bash, Markdown
Libraries	PyTorch, JAX, NumPy, SciPy, DeepXDE, WandB
Numerical	Multilevel Picard, MLMC, Gurobi, Mosek
Math Tools	Stochastic analysis, hypocoercivity, concentration inequalities, optimal transport
Languages	Mandarin (native), English (fluent)

SERVICE & LEADERSHIP

Academic & Innovation Dept., SMS Student Union Spring 2023
English Debate Club Summer 2024