SIDDHARTH PRABHU

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AREAS OF EXPERTISE

• Optimal Control • Optimization • Parameter Estimation • Automatic Differentiation • Machine Learning

EDUCATION

Ph.D., Lehigh University, USA | **GPA** 3.81 2020 - 2025 (Expected)
Thesis Title : Data-Driven Methods for Discovering Dynamical Equations
Advisor : Dr. Srinivas Rangarajan, Dr. Mayuresh Kothare

M.S., Rutgers University, USA | **GPA** 3.94 2016 - 2018
Thesis Title : Practical Application of Simulation and Campaign Scheduling of Manufacturing Process Based on MAB
Advisor : Dr. Marianthi Ierapetritou

B.E., Institute of Chemical Technology, India 2012 - 2016
Thesis Title : Techno-Economic Feasibility Report of Continuous Manufacturing of Potassium Sulphate

PUBLICATIONS

1. **S Prabhu**, S Rangarajan, and M Kothare. A condensing approach to multiple shooting neural ordinary differential equation, 2025
    - Developed an optimization method to incorporate equality constraints from multiple shooting into the training of Neural Ordinary Differential Equation (NODE).
    - Demonstrated that the proposed approach achieves better performance on highly nonlinear, complex and oscillatory dynamics using fewer parameters compared to single shooting NODE.
2. **S Prabhu**, S Rangarajan, and M Kothare. Bi-level optimization for parameter estimation of differential equations using interpolation, 2025
    - Designed a bilevel optimization framework for parameter estimation that leverages the convexity of linear parameters in dynamical systems.
    - Demonstrated superior performance of the proposed method over shooting-based techniques across multiple complex dynamical systems.
3. **S Prabhu**, S Haque, D Gurr, L Coley, J Beilstein, S Rangarajan, and M Kothare. An event-based neural partial differential equation model of heat and mass transport in an industrial drying oven. *Computers & Chemical Engineering*, page 109171, 2025
    - Developed a fully differentiable physics-based simulator for Universal Partial Differential Equations (UPDE) to model noisy, partially observed dynamical systems with events.
    - Demonstrated that incorporating physics-based priors enables effective learning from partially observed states and improves generalization to unobserved regions.
4. **S Prabhu**, S Rangarajan, and M Kothare. Differential dynamic programming with stagewise equality and inequality constraints using interior point method. *arXiv preprint arXiv:2409.12048*, 2024
    - Developed and Interior Point Differential Dynamic Programming algorithm to incorporate stagewise arbitrary equality and inequality constraints in an optimal control problem.
    - The algorithm outperforms nonlinear programming based methods on several benchmark problems such as car parking, obstacle avoidance, quadcopter, robot arm, quadcopter, continuously stirred tank reactor.
5. **S Prabhu**, N Kosir, M V Kothare, and S Rangarajan. Derivative-free domain-informed data-driven discovery of sparse kinetic models. *Industrial & Engineering Chemistry Research*, 2025
    - Developed an integration-based technique for sparse identification of dynamical equations compatible with domain knowledge such as mass balance and chemical constraints.
    - Demonstrated that the proposed method achieves lower error rates and accurately recovers kinetic models for complex reaction networks across varying noise levels, sampling frequencies, and numbers of experiments.

6. **S Prabhu**, S Rangarajan, and M Kothare. Data-driven discovery of sparse dynamical model of cardiovascular system for model predictive control. *Computers in biology and medicine*, 166:107513, 2023
    - Developed a data-driven, physics-constrained symbolic reduced-order model for model predictive control (MPC) of the cardiovascular system.
7. O Yang, **S Prabhu**, and Marianthi Ierapetritou. Comparison between batch and continuous monoclonal antibody production and economic analysis. *Industrial & Engineering Chemistry Research*, 58(15):5851–5863, 2019

PROFESSIONAL EXPERIENCE

Research Assistant *at* **Lehigh University & Owens Corning, USA** 01/2023 - Present

- Developed data-driven neural partial differential models to study the transition of moisture and temperature inside an industrial oven. Energy optimization efforts led to a 15 % reduction in energy consumption.
- Designed algorithms and optimization procedures for efficient parameter estimation and discovery of differential equations in physical systems such as reaction engineering, physics, biological systems.
- Developed a reinforcement learning framework for discovering symbolic equations using policy gradient methods. RL provides a gradient-based approach to efficiently navigate the constraint search space.

Process Engineer *at* **Dishman Carbogen Amcis, India** 08/2019 - 08/2020

- Introduced CFD simulations for targeted experiments, and performed simulations using OpenFOAM to evaluate mixing performance across various impeller–reactor configurations.
- Simulated the drying process in the formulation of soft gelatin capsules using material and energy balance equations, and proposed optimized temperature and airflow profiles over time.

Research Assistant *at* **Rutgers University & Eli Lilly, USA** 01/2017 - 04/2019

- Developed a flowsheet simulation model of the upstream and downstream operations of monoclonal antibody. The model incorporates material balances, scheduling, capacity and variability analysis, facility fit, and economic evaluation.
- Identified bottlenecks and proposed alternatives, resulting in a 30 % reduction in takt time.

Industrial Intern *at* **Reliance Industries, India** 05/2015 - 06/2015

- Modeled crude oil processing in ASPEN to obtain intermediate stream flow rates for heat optimization. Successfully calculated heat losses and proposed ways for heat recovery. Also designed equipment for the same.

ADDITIONAL PROJECTS

Control of High-dimensional Partial Differential Equation

- Implemented a Proper Orthogonal Decomposition (POD)-based reduced-order modeling technique combined with a dynamic programming-based iterative Linear Quadratic Regulator (iLQR) for controlling high-dimensional PDE systems.
- Achieved over $50\times$ computational speedup in convergence to the optimal solution, thereby enabling potential applications in online control.

Reinforcement Learning based Symbolic Regression

- Designed and implemented an RNN-based symbolic regression policy to uncover dynamic expressions from time series data, leveraging domain constraints to reduce the search space and enhance model interpretability
- Demonstrated its applicability for system identification, scientific model discovery, and model predictive control, enabling interpretable and data-driven modeling of complex dynamic systems.

Algorithmic Improvements for Scientific Machine Learning

- Developed and optimized scalable algorithms for parameter estimation by leveraging structural sparsity of Jacobians, significantly reducing computational complexity and memory overhead.
- Developed a parallel event-aware PDE solver with full support for forward- and reverse-mode automatic differentiation in JAX, achieving a 25 % reduction in simulation time over off-the-shelf solvers.

- Derived and implemented efficient forward and reverse-mode automatic differentiation algorithms for sensitivities of differential equations and bilevel optimization, reducing computational costs.
- Implemented forward- and reverse-mode automatic differentiation of SciPy ODE solvers in JAX, using both optimize-then-discretize (integrate the differential equations) and discretize-then-optimize (differentiate through the solver) approaches to enable gradient-based learning of dynamic systems.
- Implemented decomposition methods such as Cholesky, LU, used in linear system solve, for sparse matrices.

Gradient Based Hyperparameter Optimization

- Developed and implemented efficient forward- and reverse-mode automatic differentiation algorithms for hyperparameter optimization in training Physics-Informed Neural Networks (PINNs), enabling dynamic model tuning.

TALKS AND POSTER PRESENTATIONS

- **S Prabhu**, S Rangarajan, and M Kothare. Data-Driven Methods for Discovery and Parameter Estimation of Dynamical Systems. AIChE Annual Meeting, Boston, MA, 2025.
- **S Prabhu**, S Rangarajan, and M Kothare. An Event-Based Neural Partial Differential Equation Model of Heat and Mass Transport in an Industrial Drying Oven.. AIChE Annual Meeting, Boston, MA, 2025.
- **S Prabhu**, S Rangarajan, and M Kothare. Differential Dynamic Programming with Stagewise Equality and Inequality Constraints Using Interior Point Method. ACC, Denver, CO, 2025.
- **S Prabhu**, M Kothare.Learning, and S Rangarajan. Data-Driven Discovery of Sparse Kinetic Models Using Domain Information and Derivative-Free Techniques. Lehigh Symposium, Bethlehem, PA, 2024.
- **S Prabhu**, S Rangarajan, and M Kothare. Learning Dynamical Process Models Using Plant Data: A Real-World Case Study in the Sustainable Manufacturing of Insulation Products. AIChE Annual Meeting, Orlando, FL, 2023.
- **S Prabhu**, M Kothare.Learning, and S Rangarajan. Kinetic Models from Data Using a Derivative-Free Sparse Identification Method and Domain Information. AIChE Annual Meeting, Orlando, FL, 2023.
- **S Prabhu**, S Rangarajan, and M Kothare. Data-Driven Discovery of Sparse Dynamical Model of Cardiac System for Model Predictive Control. AIChE Annual Meeting, Phoenix, AZ, 2022.

RESEARCH MENTORSHIP

- CS and ECE Engg Undergraduate: Interactive Visualizing of the Dynamics of Industrial Drying Oven
- ME and CHE Engg Undergraduate: Adding Constraints to Sparse Identification of Nonlinear Dynamics

TEACHING EXPERIENCE

- **Teaching Assistant:** Separation Processes
- **Teaching Assistant:** Renewable Energy
- **Tutorial:** Data Manipulation in Pandas
- **Tutorial:** Automatic Differentiation in Python
- **Tutorial:** Calculating Sensitivities of Ordinary Differential Equations
- **Tutorial:** Forward and Reverse Gradient-Based Hyperparameter Optimization
- **Tutorial:** Reinforcement Learning for Discovering Symbolic Dynamic Equations
- **Tutorial:** Interactive Plotting in Bokeh

SKILLS

Relevant Courses : Non-linear Optimization, Machine Learning, Optimal Control, Algorithms and Datastructures, Natural Language Processing (NLP), Reinforcement Learning, Deep Learning, GPU Programming, Automatic Differentiation, Deep Generative Models, Sparse Linear Algebra
Software : Python, C++, JAX, Cyipopt, CasADi, Diffrax, Pandas, PyTorch, NumPy, SciPy, Linux, CVX, High-Performance Computing, CUDA, MATLAB