Avik Pal

Ph.D. Candidate · Massachusetts Institute of Technology · AI Compilers · AI for Science

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Education

Massachusetts Institute of Technology   *Cambridge, MA*

S.M. & Ph.D. in Computer Science (Track: AI & Decision Making), GPA: **4.9 / 5.0**   *Sep '21 – Feb '26 (est.)*

- Advisors: Dr. Alan Edelman, & Dr. Chris Rackauckas
- PhD Thesis: *Performance Portability through Composable Compiler Abstractions*
- Masters' Thesis: *On Efficient Training and Inference of Neural Differential Equations*

Indian Institute of Technology Kanpur   *Kanpur, India*

Bachelor of Technology (B.Tech.) in Computer Science and Engineering, GPA: **9.9 / 10.0**   *Jul '17 – May '21*

Work Experience

Google Cloud, XLA TPU Performance Optimization | Student Researcher   *New York City, NY*

Manager: Dr. Mehrdad Khani   *Jun - Aug '25*

- Designed learned cost models as an alternative to expert-designed heuristic cost models typically used in AI compilers.
- Built a Mixture of Experts (MoE) model achieving under **3% runtime prediction error** for fusions. Optimized MoE inference for batched predictions, **reducing runtime to 1s** on mid-tier CPUs.
- Improved **end-to-end TPU model performance by 1%**, realizing **over 70% of available headroom**. Integrated and deployed the learned cost model in the XLA:TPU compiler tool-chain.

MIT CSAIL, Julia Lab | Graduate Research Assistant   *Cambridge, MA*

PI(s): Dr. Alan Edelman & Dr. Chris Rackauckas   *Sep '21 - Present*

- Developed an MLIR-based compiler enabling automatic differentiation and tensor program optimizations for scientific computing and deep learning.
- Deployed the compiler to scale ocean simulation codes from single-node execution to **1700 TPUs** and **6144 A100 CUDA GPUs** with automated parallelization and communication optimizations.
- Introduced a framework for **enforcing physical constraints in neural surrogates of hypersonic flows** (*AIAA SciTech*), made scalable through tensor optimizations. This technology is being transitioned for use inside **US Department of Defense (DoD)**.
- Created a nonlinear root-finding framework (*ACM TOMS*) (with over **10_000 unique monthly downloads**) that **outperforms PETSc and Sundials**, and applied it to training **constrained neural networks** achieving faster runtimes and improved numerical convergence (tolerances up to 10^{-10} vs. 10^{-8} in prior work).

Intel Labs, Parallel Computing Lab | Graduate Research Intern   *Santa Clara, CA*

Manager: Dr. Dipankar Das   *May - Aug '24*

- Explored Kolmogorov–Arnold Networks (KANs) as a **parameter-efficient alternative to MLPs** in scientific ML and vision tasks.
- Developed a systematic evaluation of KANs across Neural ODEs, computer vision, and operator learning benchmarks. Introduced Hessian eigenvalue spectrum analysis to study convergence dynamics.
- Quantified computational trade-offs providing insights into the scalability and practical applicability of KANs.
- Publication: Convergence Dynamics and Eigenvalue Analysis of B-Spline KANs (*NeurIPS 2025 Workshop on Science for Deep Learning*).

Google AI | Student Researcher   *Mountain View, CA*

Manager(s): Dr. Andrey Zhmoginov, & Dr. Lily Hu   *May - Aug '22*

- Proposed a deep learning method to **augment coarse-grained simulations for approximating fine-grained wildfire dynamics**.
- Showed that black-box neural simulators fail to capture stable long-term dynamics in limited-data regimes.
- Developed probabilistic neural simulators that model the full range of possible wildfire outcomes.
- Released open-source wildfire simulator based on percolation models in JAX.

University of Toronto & Vector Institute | Research Intern   *Toronto, CAN*

PI: Dr. Sanja Fidler   *Jan - Dec '20*

- Developed multi-agent reinforcement learning (MARL) environments where **driving rules emerge naturally** from optimizing traffic flow.
- Analyzed how POMDP design factors, such as perception noise and agent density, shape cooperative driving behaviors.
- Demonstrated emergent behaviors including lane following, right of way, fast lanes, communication, and safe distances.
- Released an open-source suite of driving environments to support MARL research in self-driving.
- Publication: Emergent Road Rules in Multi-Agent Driving Environments (*ICLR 2021*).

Selected Publications

550+ citations across all publications and pre-prints. For a complete list of publications check my Google Scholar profile.

Peer-Reviewed Conference Proceedings / Journal Papers

Geometry & Mesh Invariant Neural Surrogates for Hypersonic Flows

Avik Pal, Alan Edelman, Chris Rackauckas, Mathew C. Jones, Steven Spriezer, & Tyler E. Korenyi-Both   *2025*

AIAA SciTech Forum (Accepted, To Appear)

NonlinearSolve. jl: High-Performance and Robust Solvers for Systems of Nonlinear Equations </> 🗎

Avik Pal, Flemming Holtorf, Axel Larsson, Torkel Loman, … , Alan Edelman, & Chris Rackauckas   *2025*

ACM Transactions on Mathematical Software (TOMS)

Locally Regularized Neural Differential Equations: Some Black Boxes Were Meant to Remain Closed! </> 🗎

Avik Pal, Alan Edelman, & Chris Rackauckas   *2023*

International Conference on Machine Learning (ICML)

Continuous Deep Equilibrium Models: Training Neural ODEs Faster by Integrating Them to Infinity </> 🗎

Avik Pal, Alan Edelman, & Chris Rackauckas   *2023*

IEEE High Performance Extreme Computing (HPEC) **(Best Student Paper Award)**

Opening the Blackbox: Accelerating Neural DEs by Regularizing Internal Solver Heuristics </> 🗎

Avik Pal, Yingbo Ma, Viral B. Shah, & Chris Rackauckas   *2021*

International Conference on Machine Learning (ICML)

Pre-prints / Peer-Reviewed Workshop Publications

Making Waves in the Cloud: A Paradigm-Shift for Scientific Computing and Ocean Modeling through Compiler Technology </>

William S. Moses, Mosè Giordano, Avik Pal, … , Albert Cohen, & Oleksandr Zinenko   *2025*

Under Review

Semi-Explicit Neural DAEs: Learning Long-Horizon Dynamical Systems with Algebraic Constraints 🗎

Avik Pal, Alan Edelman, & Chris Rackauckas   *2025*

Under Review

Understanding the Limitations of KANs: Convergence Dynamics and Computational Efficiency 🗎

Avik Pal, & Dipankar Das   *2024*

NeurIPS Workshop on Science for Deep Learning

Differentiable Programming for Differential Equations: A Review </> 🗎

Facundo Sapienza, Jordi Bolibar, … , Avik Pal, … , Per-Olof Persson, & Chris Rackauckas   *2024*

Under Review at SIAM Review

Open Source Software

For a complete list of open source software I have worked on, check my GitHub profile.

</> **Lux.jl,** Elegant and performant deep learning in Julia powered by the XLA compiler.   *Julia*

</> **Enzyme-JAX,** MLIR-based compiler enabling automatic differentiation, sharded-communication optimizations, and various platform-agnostic high-level optimizations.   *C++, MLIR, Jax, XLA*

</> **Reactant.jl,** Optimize Julia functions with MLIR and XLA for execution on heterogeneous hardware.   *Julia, C++*

</> **NonlinearSolve.jl,** High-performance and differentiation-enabled nonlinear solvers with sparsity support.   *Julia*

</> **NeuralPDE.jl & NeuralOperators.jl,** PINN solvers of PDEs for accelerated simulation.   *Julia*

</> **torchgan,** Research framework for easy and efficient training of GANs based on Pytorch.   *Pytorch, Python*

</> **social-driving,** Multi-agent environments and reward functions for social driving behavior emergence.   *Pytorch, Python*

Selected Presentations

2025	**Accelerating Machine Learning in Julia using Lux & Reactant ,** JuliaCon / CSAIL Alliances Workshop	🖥 </>
2025	**Semi-Explicit Neural DAEs: Learning Long Horizon Constrained Dynamical Systems,** SIAM CSE	🖥
2025	**The Tricks Required for Scientific Machine Learning to Work on Real Data,** SIAM CSE	🖥
2025	**Accelerating Physics Informed Machine Learning in Julia using Reactant and Lux,** AAAI	🖥
2022	**Lux.jl: Explicit Parameterization of Neural Networks in Julia,** JuliaCon	🎥
2022	**Mixing Implicit and Explicit Deep Learning with Skip DEQs,** SciMLCon	🎥
2019	**Differentiable Rendering and its Applications in Deep Learning,** JuliaCon	🎥

Professional Activities

'24, '25	**International Conference on Learning Representations (ICLR),** Reviewer for 6 + 3 papers	
'23 - '25	**Neural Information Processing Systems (NeurIPS),** Reviewer for 6 + 6 + 5 papers	
'22	**International Conference on Machine Learning (ICML),** Reviewer for 3 papers	

Honors, Awards & Recognitions

2023	**Best Student Paper Award,** IEEE High Performance Extreme Computing Conference	*USA*
2017-20	**Academic Excellence,** Top 10% students in 3 Consecutive Academic Year	*IIT Kanpur*
2017	**Inspire Scholarship for Higher Education,** Top 1% students in 10+2 board results	*India*