Rahul **Manavalan**

Student Researcher · Masters Student

rahul.manavalan@tum.de | https://dynamic-queries.github.io/ | dynamic-queries | @dynamicqueries

Education

Technical University of Munich — *Munich, Germany*

MS in Computational Science and Engineering — *October. 2020 - **

- Scientific Computing and Numerical Analysis.
- Dynamical Systems and Machine Learning.
- Quantum Information and Tensor Networks.

Sorbonne Université — *Paris, France*

Summer School in Density Functional Theory — *August. 2022*

- Numerical Methods in DFT.
- Convergence and error bounds.
- Differentiable and scalable softwares.

Government College of Technology — *Coimbatore, India*

BS in Mechanical Engineering — *June. 2015 - April. 2019*

- Metallurgical Physics.
- Continuum Mechanics.
- Design of Machine Elements and Product Design.

Tools/Skills

Machine Learning	Tensorflow, Flux.jl, Zygote.jl, JAX
Programming Languages	Julia, Python, C++
High Performance Computing	OpenMP, MPI, CUDA, Slurm, Docker, PAPI

Research Stays

Juelich Supercomputing Center — *Juelich, Germany*

Student Researcher — *May 2021 - July 2021*

- Identifying recurring tensor contractions in Tensor Network algorithms.
- Implementing such sub-routines using the Tensor contraction library and Juelich's legacy TN code.
- Benchmarking results.

Experience

Technical University of Munich — *Munich, Germany*

Student Researcher — *February 2021 - **

- Fourier Neural Operators for forward wave propagation problems in non-destructive testing.
- Fullwaveform inversion with developed surrogate.

Technical University of Munich — *Munich, Germany*

Student Researcher — *May 2021 - December 2022*

- Implementations for multi-output multifidelity Gaussian processes.
- Initial work on physics informed Gaussian processes.

Robert Bosch Engineering and Business solutions — *Coimbatore, India*

Associate Software Engineer — *Aug 2019 - Sept 2020*

- System simulation.
- Computer Aided Design, Failure Mode Effective Analysis

Talks and Presentations

SIAM conference on Computational Science and Engineering — *Amsterdam, Netherlands*

Poster Presentation — *March. 2023*

- Neural Operators for Fullwaveform inversion.

Projects

SINDY.jl — *MLCMS at TUM*

A Julia implementation of the SINDY algorithm — *March. 2022*

Non-parameteric machine learning potentials — *Masters Thesis at TUM*

Machine learning potentials using higher order interactions — *May. 2023 - **

Academic Interests

Scientific Computing

- Function approximation
- Outer-loop applications
- Surrogates for partial differential equations
- Non-linear model order reduction

Computational Chemistry

- Machine learning potentials
- Deep learning methods in DFT
- Coarse grained modeling

Data Science

- Generative models
- Temporal graph neural networks
- Higher order graph neural networks
- Dynamical systemic theory of Deep Learning

Open Source Software

OrdinaryDiffEq.jl

- High performance ordinary differential equation (ODE) and differential-algebraic equation (DAE) solvers, including neural ordinary differential equations (neural ODEs) and scientific machine learning (SciML)

ModelOrderReduction.jl

- High-level model-order reduction to automate the acceleration of large-scale simulations

LinearPDEs

- An aggregation of linear PDEs for scientific machine learning.

Communities

SIAM Munich student chapter — *Munich, Germany*

Founding member — *April 2023- **

Julia SciML community

Contributor — *January 2022- **