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, GPFlow, Torch
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 2023 - **
- 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 2022 - December 2022*
- Implementations for multi-output multifidelity Gaussian processes.
- Initial work on physics informed Gaussian processes.

Technical University of Munich   *Munich, Germany*
VOLUNTARY TEACHING ASSISTANT   *October 2021 - April 2022*
- Tutorials for Scientific Computing I.

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
Poster Presentation

Amsterdam, Netherlands
March. 2023

- Neural Operators for Fullwaveform inversion.

Projects

SINDY.jl
A julia implementation of the SINDY algorithm

MLCMS at TUM
March. 2022

Non-parametric machine learning potentials
Machine learning potentials using higher order interactions

Masters Thesis at TUM
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
Founding member

Munich, Germany
April 2023-*

Julia SciML community
Contributor

January 2022-*