Anoop A. Nair

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About me

I'm a doctoral researcher at the University of Iceland looking to transition into industry. I have seven years of research, data analysis and programming expertise in the topics of software development, FOSS, machine learning, optimization and statistics. I'm enthusiastic to work on both research and non-research oriented problems and find efficient answers to them. I can also communicate research effectively, as proven by my several research articles, and I've worked with four research groups.

Education

2021– PRESENT (2024) **Doctoral studies (Ph.D): Specialization: Software engineering**, *University of Iceland*, Reykjavík, *Iceland*

2016-2021 **M.Sc, Physics, Specialization: Machine learning**, *Indian Institute of Science Education and Research*, Thiruvananthapuram, *Iceland*

Work Experience

2023– PRESENT **Science Institute**, *University of Iceland*, Eimskip grant fellow
Team lead for developing a C++/pybind11 code for simulating solvent systems which resulted in winning a research grant for 16 million ISK for the research group.

2021–2023 **Faculty of Physical Sciences**, *University of Iceland*, Doctoral Researcher
Developed a C++ code with a python interface (via pybind11) for simulating quantum chemistry systems.This was done to simulate an aqueous/non-aqueous solvent environments.

2020–2021 **Department of Physics**, *Indian Institute of Science Education and Research, Thiruvananthapuram*, Masters thesis
Developed an efficient computer vision algorithm based on Haar cascades in conjunction with convolutional neural networks to automate identifcation of hexagonal structures in images obtained from an electron microscope. This increased the analysis speed by 5 times. The ML model was build using TensorFlow, with the analysis done using sklearn. The model and methodology followed was published in this research article.

2019–2020	**Material Science and Technology division**, *Council of Scientific and Industrial Research , Thiruvananthapuram*, Research intern

  ○ Simulation and detection of curie temperature for core-shell systems using the C++ package Vampire which reduced the need for expensive experimental prototyping: <u>article</u>
  ○ Prediction of thermo-electric material properties in $BaVSe_3$ and magneto-electric properties in Sr_2FeNbO_6 using the Fortran based code "Quantum ESPRESSO" which enabled more streamlined experimental prototyping. The software was run in a parallel paradigm on a high performance computing cluster using OpenMP. Research articles : <u>article 1</u>,<u>article 2</u>

2019–2020	**Department of Chemistry**, *Indian Institute of Science Education and Research, Thiruvananthapuram*, Research Intern

  ○ Developed a python package for the statistical analysis of time series data obtained from quantum dot blinking which enabled the group to override expensive experimental prototyping. The result of this venture were two research articles: <u>article 1</u>, <u>article 2</u> and a <u>pip module</u>.
  ○ The construction of a deep convolutional neural network (Deep-CNN) used for identifying the presence of trace amounts of pesticides in produce by infereing the same from its raman spectra. This enabled us to developed a hand-held cost-effective device to detect adulterants in real-time. The publication is still under preparation.

Technical Skills

Programming Languages

EXPERIENCED	C++, Python, R, FORTRAN, Shell (zsh, bash), OpenMP, OpenMPI, CSS, JavaScript, HTML, C, Matlab	FAMILIAR	Kotlin

Modules

EXPERIENCED	Pybind11, TensorFlow, Pytorch, keras, numpy, sklearn, pandas, matplotlib, BLAS, LAPACK, SCME(A C++ package to simulate solvents), PySCF(A quantum chemistry package in python and C++), QuantumBlink (A python package for analyzing quantum dot data)	FAMILIAR	LAMMPS (A C++ program to do molecular dynamics)

Simulation Projects

EXPERIENCED	LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), OVITO, Quantum Espresso, PySCF, GPAW	FAMILIAR	Gaussian16, VMD (Visual Molecular Dynamics)

Tools

EXPERIENCED	Git (version control), ssh, Vim, Sublime Text Editor 3, gnuplot, MATLAB (matrix laboratory), Visual Studio Code, SQL(Database management)

FAMILIAR	Continuous Integration Services (Wercker, Travis CI, Semaphore CI)

Opensource Contributions

SCME QM/MM Project, QuantumBlink Project, GPAW, PySCF

Opensource Projects Created

SCME QMMM PROJECT
A FOSS project created using C++ and python3, with python bindings to enable communication between C++ and python3. The software package is used to simulate a solvent enviroment consisting of 100 thousand molecules efficiently.: Gitlab Link

QUANTUM BLINK PROJECT
FOSS python module developed by me, under the supervison of Vishnu E K,Ph.D [@ K.G.T. Labs]. It helps in the analysis of flouresence intermittency data obtained from the MT-300 single photon detector. The module when provided with the Intensity vs Time trace derives the ON/OFF event PDFs and the correlations in data indicating the memory effect: Pip module Link

ICEWAY PROJECT
IceWay is a project birthed during the Gagnaþon Ríkiskaupa Datathon, aimed at leveraging AI to forecast road conditions in Reykjavik and across Iceland. Github Link

Awards

OCTOBER 2023
Gagnaþon Ríkiskaupa Hackathon winner, *Reykjavik University, Iceland*, 400 thousand ISK
TITLE: Developed an eco-friendly solution for ice-free roads in Iceland.

2023–2026
Eimskip Doctoral Grant, *University of Iceland*, 15.5 million ISK, Doctoral Fellowship
TITLE: H_2O reactivity in nanoconfined highly concentrated electrolytes studied using QM/MM simulations with polarizable models.

2016–2021
INSPIRE Scholarship, *IISER-TVM, India*, 300 thousand INR, Integrated Masters Scholarship
TITLE: Detection of hexagonal structures in confocal microscope images via machine learning