Prajval K

Undergraduate Student

DST-INSPIRE SHE Scholar (2022-2027)

Indian Institute of Science and Education Research (IISER), Thiruvananthapuram

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RESEARCH INTERESTS

- Computational Modelling of Physical Systems
- Numerical solutions of ODE systems
- Classical Computational Chemistry

PROGRAMMING SKILLS

Languages: C++, Java, Python, Bash/Scripting, HTML/CSS

Technologies: Git, MATLAB, openFOAM, AutoDock, Qt, cxxplot & Eigen (C++), numpy & scipy (Python), JNI (Java)

EDUCATION

Aug 2022 - Present — **Indian Institute of Science and Education Research (IISER), Thiruvananthapuram** — **University**
2nd Year, Integrated BS-MS Program, Aspiring Chemistry Major
CGPA: 9.05/10

May 2020 - June 2022 — **Swamy Vivekananda Rural Pre-University College (SVRPUC), Chandapura** — **College**
Grade 11-12, Karnataka State Board (96%)

Apr 2010 - May 2020 — **Nazareth School, Chandapura** — **School**
Grade 1-10, CICSE Board (96%)

INTERNSHIPS

Feb 2023 - Present — **Noble Gas Dimers | IISER TVM**
Involved in a computational modelling internship about studying noble gas dimer interaction under the supervision of Prof. R S Swathi (IISER TVM) and her research group.

WORKSHOPS

Feb 2024 — **High Performance Computing in Bioinformatics | IIT Kharagpur**
Attended a workshop organized at IIT Kharagpur under the aegis of National Supercomputing Mission (NSM), focused on molecular dynamics, protein folding and design, and protein docking, with hands-on training on GROMACS and Autodock Vina

Dec 2023 — **High Performance Computing in Complex and Moving Geometries | Jadavpur University**
Attended a workshop organized by IIT Kharagpur at Jadavpur University, Kolkata under the aegis of National Supercomputing Mission (NSM), with hands-on training on large-scale computational techniques for compressible and incompressible fluid flow using openFOAM.

RESEARCH PROJECTS

Feb 2023 – Apr 2023 — **Advancements in Theoretical Chemistry Presentation** — **Reading Project under Prof. R S Swathi, IISER TVM**

- Reading about the academic research of frontier people in the field of Theoretical Chemistry to understand the scope of the subject.
- This included the works of older scientists, such as Pauling, and Prigogine as well as recent well-recognized results, such as the conception and development of Density Functional Theory (DFT) by Kohn-Pople and multiscale modelling approaches of Karplus-Levitt-Warshell.
- This was presented to the research group of Prof. R S Swathi in Apr. 2023.

Apr 2023 – Present — **Study of Noble Gas Dimers** — **Project under Prof. R S Swathi, IISER TVM**

- Developed a program in Python for analysis into Lennard-Jones (LJ) and Improved Lennard-Jones (ILJ) schemes for noble gas dimer molecules.
- Worked with Gauss-Newton and Simplex algorithms in Python for curve-fitting and non-linear root finding.
- We are also looking into nobel gas dimer-dimer interactions and multi-dimensional configurations.

Mar 2023 – Present **Water Rocket Analysis** **Orbiton Labs, Independent Student Group Study**

- Developed a simulation program in C++ (GitHub: @orbitonlabs/fastsim) for the design and analysis of a simple model of water rockets.
- For completeness, the program includes a from-scratch implementation of simpler Euler ODE solvers and more complex Runge-Kutta (RK) methods, including implicit and Diagonally Implicit RK methods using a custom linear algebra system.
- Our student research group is interested in finding physical or statistical models that resemble experimental and fluid dynamics results for water rockets at high-pressure limits. We have presented our results in Anvesha 2023, our flagship annual student exhibition.
- Additionally, we are also looking into developing a novel propulsion system based on Liquid Nitrogen water rocket engines and low-latency flight correction in the future. We are also working on a parallelized version of the simulation using openMPI and openACC libraries.

VOLUNTEERING

Feb 2023	**Frontier Symposium in Mathematics (FS-MATH), 2023**	**Core Organizer**
Sep 2023	**International Genetic Engineering Machine (iGEM) 2023, IISER TVM**	**Wiki Team Volunteer**
Dec 2023	**Inter-IISER Sports Meet (IISM) 2023**	**Website Team**
Nov 2023 – Present	**TEDxIISERTVM 2024**	**Tech Team**
Feb 2023 – Present	**Club Mathematics of IISER TVM (CMIT)**	**Club Coordinator**
Aug 2023 – Present	**Chemical Society of IISER TVM (CSIT)**	**Club Coordinator**
Oct 2023 – Present	**Physics Society of IISER TVM (PSIT)**	**Website Volunteer**
Apr 2023 – Present	**Ether Magazine**	**Website Volunteer**
Feb 2023 – Present	**Orbiton Labs : Student Rocket Research Group**	**Team Lead, Numeric Computation**
Jan 2021 – Jan 2023	**openAOD : Open Source Developer Group**	**Core Contributor**

LANGUAGES

English, Kannada, Telugu, Hindi