Mythreyi Ramesh

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Research Interests

Multi-scale Modelling of Materials ∗ Crystalline Defects in Materials ∗ High Performance Computing ∗ Applied Mathematics

Education

Indian Institute of Technology Madras *2015 – 2020*
Interdisciplinary Dual Degree
B.Tech (Hons.) in Metallurgical and Materials Engineering + M.Tech in Computational Engineering
CGPA: 9.27 (Major CGPA: 9.56), **Topper** B.Tech (MME Department) and **Stream Topper** in M.Tech (across the institute).

Research Experience

- **Computational aspects of the spectral methods for estimation of micromechanical fields in polycrystals**
  (Master's Thesis) *July 2019 – ongoing*
  Advisors: Prof. Anand Krishna Kanjarla, Department of Metallurgical and Materials Engineering, IIT Madras
  Prof. Sivaram Ambikasaran, Department of Mathematics, IIT Madras
  – Using non-uniform grids to perform the Fast Fourier Transform (FFT) to capture large gradients close to interfaces.
  – Will compare and contrast the efficiency and accuracy of non-uniform FFT with Particle-in-Cell methods for evolving grids.

- **Theoretical investigation of stability of High-Entropy Oxides to Lithium intercalation** *January 2018 – January 2019*
  (Undergraduate Research Course)
  Advisor: Prof. Satyesh Kumar Yadav, Department of Metallurgical and Materials Engineering, IIT Madras
  – Generated Special Quasirandom Structures (SQS) for four and five component equimolar high-entropy oxides using the `mcsqs` tool of the Alloy Theoretic Automated Toolkit (ATAT).
  – Performed *ab initio* (DFT+U) calculations using VASP and validated them using experimentally reported lattice parameters.
  – Analysed the interaction of Li atoms in the tetrahedral voids with neighbouring atoms to understand intercalation capabilities.

- **Atomistic simulations of grain boundaries in Fluorite structured oxides** *May 2018 – July 2018*
  (Mitacs Globalink Research Internship, a fully-funded three month internship at Canada awarded to talented students from 10 countries)
  Advisor: Prof. Jerzy Szpunar, Department of Mechanical Engineering, University of Saskatchewan, Canada
  – Computed Coincident Site Lattice (CSL) grain boundary energies in ThO_2 using molecular dynamics simulations.
  – Performed studies on the segregation tendencies of Xe atoms at different distances from the grain boundaries.

- **Thermoelastic analysis of fuel pins** *May 2017 – July 2017*
  Advisor: Prof. Sivasambu Mahesh, Department of Aerospace Engineering, IIT Madras
  – Performed a co-simulation with Abaqus/Standard and Abaqus/CFD to calculate thermal and mechanical stresses.
  – Set up a Fluid-Structure Co-simulation Boundary interaction in the fluid & solid domains to simulate the coolant action.

Academic Projects

- **Parallelising molecular dynamics simulations using MPI** *April 2019*
  Term Project: High Performance Computing for Engineering Applications
  – Wrote a Python script to perform an microcanonical ensemble (NVE) simulation implementing the Velocity-Verlet algorithm for integration and parallelised the NVE simulation using **mpi4py**.

- **Cellular Automata (CA) in solidification modelling** *October 2018 – November 2018*
  Term Presentation: Solidification Phenomena
  – Reviewed all CA rules used to model solidification, including methods to incorporate curvature effects.
  – Compared the most successful models in terms of their treatments of temperature evolution, nucleation and growth kinetics.

- **Analysis of the lid-driven cavity problem using OpenFOAM** *February 2017 – April 2017*
  Term Project: Transport Phenomena in Materials
  – Computed the velocity and pressure distributions in two cases to analyse the impact of cavity geometry on both the fields.
  – Visualised the velocity and pressure fields using ParaView and plotted streamlines to spot dead zones and recirculation loops.

Teaching Experience

- **Computational Materials Engineering Lab (MM3110)** - *Teaching Assistant* *August 2019 – present*
  – Helped undergraduate students to write MATLAB scripts for solving linear, non-linear and differential equations, generating digital microstructures using Voronoi tessellation and performing Principal Component Analysis.

- **Introduction to Scientific Computing (MM2090)** - *Teaching Assistant* *January 2019 – May 2019*
  – Helped undergraduate students to pick up useful skills including Bash scripting, Python, Octave, LaTeX, SageMath and Git.

Communication of Science

- **IMMERSE - IIT Madras Magazine on Research in Science and Engineering** *May 2016 – July 2019*
  - Immerse is an annual magazine that breaks down the research happening in IIT Madras for a general audience.
  - Contributed articles to three editions of Immerse from 2016 to 2019. Editor for three other articles in Immerse 2017-18.
- **Kenyon Review Young Science Writers Workshop** - *Teaching Assistant* *June 2019 – July 2019*
  Kenyon College, Ohio, United States of America
  - Awarded **Fellowship** and was the youngest and the only international instructor for the workshop.
  - The workshop was attended by high school students from the United States, China, Greece and the United Kingdom.
  - Conducted a session on symmetry in crystals and crystallography to explore the parallels between nature and poetry.

Workshops & Conferences

- Volunteered for **ISMANAM** (International Symposium on Metastable, Amorphous and Nanostructured Materials) 2019 conducted at Chennai from July 8 to 12, 2019.
- Attended a Short Term Course on **Foundations of Computational Engineering through Multi-Grid Methods**, instructed by Prof. S. P. Vanka, Professor Emeritus at the University of Illinois (Urbana-Champaign) from September 22 to 23, 2018.
- Attended **PyCon India 2019** conducted at Chennai from October 12 to 13, 2019.

Technical Skills

- **Materials Modelling:** VASP, Quantum ESPRESSO, LAMMPS, Thermo-Calc.
- **Visualisation Tools:** VESTA, ParaView, Ovito.
- **Programming & Scripting Languages:** C, C++, Python, Ruby, Bash.
- **Scientific Computing Tools:** GNU Octave/MATLAB, Mathematica, Jupyter, Open MPI.
- **Continuum Scale Modelling:** Abaqus, OpenFOAM.
- **Web Development:** HTML, CSS, Jekyll, Django, JavaScript.

Relevant Coursework

- **Computational Materials Engineering**: Foundations of Computational Materials Modelling, Atomistic Modelling of Materials, Computational Materials Thermodynamics, Molecular Simulation of Soft Matter.
- **Materials Science and Engineering**: Defects in Materials, Electronic Materials, Devices and Fabrication, Stability of Microstructures, Solidification Phenomena, Electron Diffraction and Microscopy.
- **Mathematics & Computing**: Numerical Linear Algebra, High Performance Computing, Computer Modelling and Simulation, Computational Tools - Data Structures, Algorithms and Programs.

Scholastic Achievements

- Awarded the **Institute Merit Prize** for the best academic performance in the 4^{th} year of the Dual Degree programme. (2020)
- Awarded the **Ratna Award** on Institute Day 2019 for the best academic performance in the 3^{rd} year of B.Tech. (2019)
- Secured District Rank 1 (Coimbatore, Tamil Nadu) with **97.4%** in the All India Senior School Certificate Examination. (2015)
- Selected for Kishore Vaigyanik Protsahan Yojana (**KVPY**) Fellowship with a National Rank of 477 (out of ∼100,000). (2014)
- Awarded National Talent Search Examination (**NTSE**) Scholarship, ranked in top 1000 among 1.5 million candidates. (2013)
- Represented Tamil Nadu state in the **Indian National Mathematical Olympiad** (INMO) 2013. (2012)

Activities and Responsibilities

- **Writing**: Editor-in-Chief of Etch Magazine[1] from 2017 to 2019. Placed second in "Avial," a creative writing competition, in Lit-Soc[2] 2018 & 2017. Awarded first place in the popular science writing competition held during Bhoutics[3] in 2016 & 2017.
- **Social:** Mentored seven freshman during their initiation into IIT Madras as a part of the Student Mentorship Cell (2019).
- **Event Organisation**: Student organiser for Prof. Brahm Prakash Memorial Materials Quiz (BPMMQ) regional rounds conducted by Indian Institute of Metals (IIM) Chennai Chapter every year from 2016 to 2019.
- **Web Development**: Core Member responsible for web operations in the Amalgam[4] 2018 organising team.
- **Performing Arts:** Trained in **Carnatic Music** (Vocal) for 5 years (2007-2011) and **Bharatanatyam** (Classical Dance form of South India) for 5 years (2007-2011). Self-taught **Western Guitar** player since 2008.

References

Anand Krishna Kanjarla,
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Satyesh Kumar Yadav,
Assistant Professor, IIT Madras.
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[1] Bi-annual Magazine of the Department of Metallurgical and Materials Engineering IIT Madras.
[2] Annual series of inter-hostel cultural competitions in IIT Madras
[3] Annual fest, Department of Physics, IIT Madras
[4] Annual fest, Department of Metallurgical and Materials Engineering, IIT Madras