# SRIRAM DEVATA

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## Education

**University of Illinois at Urbana-Champaign (UIUC)**  **Aug. 2024 − Present**
*PhD in Computer Science, Advised by Prof. Sarita Adve*

**International Institute of Information Technology, Hyderabad (IIITH)**  **Aug. 2019 − July 2024**
*Bachelor of Technology (Honours) in Computer Science and*
*MS by Research in Computational Natural Sciences*  *CGPA - 8.99/10*

## Experience

**University of Illinois at Urbana-Champaign (UIUC)**  **Aug. 2024 - Present**
*Graduate Research Assistant*

- Working with Prof. Sarita Adve to develop the software and hardware architecture for datacenters that can efficiently support extended reality workloads.
- Currently focused on devising scheduling methodologies for multi-model machine learning pipelines with complex data and control dependencies.

**STARLab, Carnegie Mellon University**  **Jan. 2022 - June 2024**
*Student Researcher*

- Worked with Prof. Akshitha Sriraman and Dr. Gilles Pokam to identify and leverage hardware design opportunities to enhance efficiency in data centers by optimizing redundant datacenter "tax" operations.
- Developed a methodology that uses perf to profile widely-used open-source microservices to uncover patterns that can guide the development of general hardware accelerators.

**University of Waterloo**  **May 2023 - Aug. 2023**
*MITACS Globalink Research Intern*

- Developed an innovative scoring metric in collaboration with Dr. Aravindhan Ganesan for evaluating and ranking ligand molecules designed by AI-driven generative models.
- Tailored for the SARS-CoV-2 Main Protease's primary binding site, this metric integrates interaction fingerprints and subpocket occupancy maps to offer a holistic approach to assessing molecular efficacy.

**CCNSB, IIIT Hyderabad**  **Apr. 2021 - July 2024**
*Research Assistant*

- Advised by Prof. Deva Priyakumar, I developed a deep reinforcement learning method, akin to AlphaGo, capable of deducing molecular structures from the Infrared and NMR spectra of the molecule.
- Developed a method that predicts structural constraints of RNA using just the RNA sequence as a means to improve the tertiary structure prediction.

**Chaincode Labs**  **Sep. 2021 - Jan 2022**
*Software Developer*

- Continuing on my work from the Summer of Bitcoin program, I spearheaded the development of a '-nomempool' runtime option.
- This feature allows for the operation of a Bitcoin node without a mempool, allowing users to participate in the Bitcoin network without needing to mine blocks.

**Summer of Bitcoin**  **July 2021 - Sep. 2021**
*Student Developer*

- Streamlined the testing operations of Bitcoin Core by replacing the compiled wallet with a more versatile Python mini-wallet.
- Additionally, I also reduced the dependency of a Bitcoin node on its mempool, contributing to the system's overall robustness and performance optimization.

**Paymatrix**  **Feb. - Apr. 2021**
*Software Development Intern*

- Ported numerous features from the web version of Paymatrix to their mobile application, utilizing Flutter.

**Blue Marble Space Institute of Science**  **June - Dec. 2020**
*Research Associate*

- As a participant in the Young Scientist Program at BMSIS, I collaborated with Dr. Henderson James Cleaves and Dr. Markus Meringer to benchmark ML-based Electron Ionization Mass Spectrometry (EI-MS) prediction methods.
- We also formulated and explored various spectral distance metrics that have not been addressed by other works, to help establish a standard for evaluating ML-based EI-MS prediction methods.

**New York University, Abu Dhabi** <span style="float:right">**May - Aug. 2020**</span>

*Summer Research Project*

- In collaboration with Dr. Dimitra Atri, I ran simulations using the Geant4 toolkit for a study focused on understanding the impacts of solar radiation on astronauts.
- I completed the Human Phantom Model within the C++ source code of Geant4 and conducted simulations of solar particle events using this model of astronauts.

## Relevant Coursework

- Compiler Construction (UIUC)
- Distributed Systems (UIUC)
- Advanced Topics in Computer Architecture (UIUC)
- Parallel Computer Architectures (UIUC)
- Computer Systems Organization (IIIT-H)
- Introduction to Software Systems (IIIT-H)
- Data and Applications (IIIT-H)
- Statistical Methods in AI (IIIT-H)
- Topics in Deep Learning (IIIT-H)
- Advanced NLP (IIIT-H)
- ML for Natural Sciences (IIIT-H)
- Data Driven Drug Discovery (IIIT-H)
- Computer Programming (IIIT-H)
- Data Structures and Algorithms (IIIT-H)
- Algorithm Analysis and Design (IIIT-H)
- Automata Theory (IIIT-H)
- Machine, Data, and Learning (IIIT-H)
- Operating Systems and Networks (IIIT-H)
- Compilers (IIIT-H)
- Design and Analysis of Software Systems (IIIT-H)
- Advanced Computer Architecture (IIIT-H)

## Selected Projects

**Meta-Stable State Prediction Using Coarse-Grained Models** <span style="float:right">**Feb - April 2023**</span>

Leveraged the latent space of a coarse-grained auto-encoder for predicting the meta-stable states of a molecular system. The approach involved a conditional exploration of the latentent space to identify various stable states of a system.

**Racket to x86-64 Compiler** <span style="float:right">**Jan - April 2023**</span>

Implemented a compiler that translates a subset of Racket programming language into x86-64 assembly code. The project emphasized on creating a robust and functional compiler, and understanding the intricacies of compiling to x86-64.

**Automation of NMR Spectra Integration Using Machine Learning** <span style="float:right">**June - Sep 2022**</span>

I led a project to understand and automate an existing workflow of a pharmaceutical company. By employing machine learning techniques, we utilized domain-specific knowledge to automate peak identification and integration of NMR spectra to streamline these segments in the company's workflow.

**Inexact Machine Unlearning with Graph Neural Networks** <span style="float:right">**Jan - Apr 2022**</span>

Adapted the IC Test pipeline proposed for image classification to graph and node-level tasks. Produced novel results in graph unlearning about random label memorization and proposed unlearning methodologies for GNNs.

**LeNet-5 from Scratch** <span style="float:right">**Sep - Nov 2021**</span>

We implemented LeNet-5, a renowned convolutional neural network, entirely from scratch without the aid of any automatic differentiation tools. This project demonstrates a deep understanding of neural network mechanics and the underlying mathematical principles.

**Desh: a Custom Linux Shell in C** <span style="float:right">**Oct 2021**</span>

'Desh' is a custom shell designed for Linux-based systems developed from scratch in C, relying exclusively on system calls. This approach required a comprehensive understanding of Linux system architecture and proficient command over C programming, showcasing advanced skills in both system-level programming and operating system concepts.

**ASeniorIsAsking** <span style="float:right">**May 2020**</span>

We developed a web application designed to connect students at IIITH with peers at DLF, a popular fast-food hub. The application was built using ReactJS for an intuitive frontend, Redis as the database, and Flask for a robust backend. This project shows an integrated approach to web development, combining various technologies to create a user-friendly platform.

## Publications

**Generative artificial intelligence for small molecule drug design** <span style="float:right">**August 2024**</span>

*Current Opinion in Biotechnology*

Ganesh Chandan Kanakala*, <u>**Sriram Devata***</u>, Prathit Chatterjee, Deva Priyakumar

**TorRNA - Improved Prediction of Backbone Torsion Angles of RNA by Leveraging Large Language Models** <span style="float:right">**June 2024**</span>

*ChemRxiv*

<u>**Sriram Devata**</u>, Deva Priyakumar

**DeepSPInN - Deep reinforcement learning for molecular Structure Prediction from Infrared and 13C NMR spectra** March 2024

*Digital Discovery, Royal Society of Chemistry*

<u>**Sriram Devata***</u>, Bhuvanesh S.*, Sarvesh M.*, Yashaswi P. , Siddhartha L., Girish V. , Deva Priyakumar

**Comparative Evaluation of Electron Ionization Mass Spectral Prediction Methods** June 2023

*Journal of the American Society for Mass Spectrometry*

<u>**Sriram Devata**</u>, Henderson J. Cleaves, John Dimandja, Christopher A. Heist, Markus Meringer

**Crewed Missions to Mars: Modeling the Impact of Astrophysical Charged Particles on Astronauts and Their Health** Aug 2022

*ArXiv*

Dimitra A., Caitlin M.*, <u>**Sriram Devata***</u>, Konstantin H., Dionysios G., Shireen Mm, Maria V., Giulia C. Bassani, Roberto P., Azza A. Bakr, Tammy W.

## Talks

**Compilers, Architecture, and Parallel Computing (CAP) Seminar, UIUC** April 2025

I presented some literature on problems and solutions on serving ML inference pipeline workloads.

**BlueSciCon II 2020** Aug 2020

I presented a comprehensive talk on NEIMS, one of the state-of-the-art machine learning-based EI-MS prediction methods. The presentation covered the intricate details of NEIMS, its role in the broader context of EI-MS prediction, and its significance in the field of analytical chemistry, demonstrating the potential and impact of machine learning in scientific research and analysis.

**Machine Learning Reading Group, IIITH** Jan - Apr 2021

Within the framework of a paper reading group, I engaged in reading and presenting a series of research papers, each encompassing different domains within Machine Learning. The presentations aimed to foster a deeper understanding of the diverse and evolving landscape of Machine Learning, highlighting its interdisciplinary applications and advancements.

## Teaching Experience

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| **Instructor at Mumbai Workshop on Quantum Chemistry (IIT Bombay)** | **June 2024** |
| **Teaching Assistant for CS1.403 Compilers (IIIT-H)** | **Spring 2024** |
| **Teaching Assistant for CS2.201 Computer Systems Organization (IIIT-H)** | **Spring 2023** |
| **Teaching Assistant for CS7.403 Statistical Methods in AI (IIIT-H)** | **Spring 2022** |
| **Teaching Assistant for CS4.301 Data And Applications (IIIT-H)** | **Monsoon 2021** |
| **Teaching Assistant for ML for Chemistry and Drug Design (IHub-Data, IIIT-H)** | **Spring 2022** |

## Technical Skills

**Languages**: Python, C/C++, SQL
**Frameworks**: PyTorch, PyTorch Lightning, RDKit
**Web Development**: HTML/CSS, JavaScript, Flask, Django, MERN
**Utilies/Technologies**: Linux, Git, Bash, Slurm, Jupyter, Docker

## Awards and Honours

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| W.J. Poppelbaum Memorial Award, *UIUC* | **2025** |
| Student Travel Grant, *MLSys'25* | **2025** |
| Qualcomm Innovation Fellowship Finalist | **2025** |
| Student Travel Grant, *ASPLOS'25* | **2025** |
| CS PhD Fellowship, *UIUC* | **2024** |
| Undergraduate Architecture Mentoring Workshop, *ISCA 2023* | **2023** |
| 1st Place Winner at *ML4Science Conference Hackathon, 2023* | **2023** |
| Recommended for Poster Session, *ACM MICRO 2022 Student Research Competition* | **2022** |
| ISCA 2022 (Virtual) Student Participation Grant, *uArch Workshop* | **2022** |
| Dean's Merit List for Academic Excellence - Monsoon 2021, *IIIT Hyderabad* | **2021** |
| Dean's Merit List for Academic Excellence - Spring 2021, *IIIT Hyderabad* | **2021** |
| Dean's Merit List for Academic Excellence - Monsoon 2020, *IIIT Hyderabad* | **2020** |
| Dean's Merit List for Academic Excellence - Monsoon 2019, *IIIT Hyderabad* | **2019** |
| MEXT Scholarship for Undergraduate Studies (Withheld due to Covid), *Government of Japan* | **2019** |
| UGEE Examination and Interview for CS Research Program - All India Rank 44, *IIIT Hyderabad* | **2019** |

## Professional/Academic Service

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| Operating Systems Design and Implementation (OSDI'25) Artifact Evaluation Committee | **2025** |
| Machine Learning and Systems (MLSys'25) Artifact Evaluation Committee | **2025** |
| Compilers, Architecture, and Parallel Computing (CAP) Seminar Organizing Committee, *UIUC* | **2025-Present** |

## Volunteering/Extracurricular Activities

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| Member of the Apex Student Council, *IIITH* | **2020-2022** |
| Club Coordinator, *The Dance Crew, IIITH* | **2020-2022** |
| Collaborations Team Member, Rotating Head, *Entrepreneurship Cell, IIITH* | **2019-2022** |
| Head of Corporate Team, *Ping! - the student magazine of IIITH* | **2019-2021** |
| Design Team Member, *Pentaprism - the photography club of IIITH* | **2019-2020** |