Rajeev Jain

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Experience

CASE Staff At-Large Sep 2023 – Present
The University of Chicago (UChicago) *Chicago, IL*

– Joint appointment supporting computational cancer research initiatives between Argonne National Laboratory (ANL) and UChicago.

Principal Specialist, Research Software Engineering (formerly Research Software Developer) Aug 2009 – Present
Mathematics and Computer Science Division, Argonne National Laboratory (ANL) *Lemont, IL*

– Contributed to five major projects across cancer data science, climate computation, multiphysics simulation, urban coupled simulations, and nuclear reactor modeling.

– Pursued high-performance computing challenges in diverse scientific domains; mentored junior researchers.

Research and Teaching Assistant Aug 2007 – Jul 2009
Structural Engineering, Arizona State University *Tempe, AZ*

– Enhanced blast-resistant structure design for the U.S. Army Research Office using FEM-based shape optimization.

– Graded and supported instruction for structural engineering courses and lab work.

Project Engineer May 2006 – Jun 2007
Wipro Technologies *Bangalore/Hyderabad, India*

– Developed production-ready code in Java and SAP; quickly adapted to large-scale software environments.

Selected Talks

- SciPy: UXarray for Unstructured Grids — YouTube
- HDF5 Annual Meeting: FLASH-X Async I/O — YouTube

Major Projects

IMPROVE/CANDLE (Cancer Data Science - ECP) Jan 2017 – Present

– Lead developer of CANDLE/Supervisor, a scalable deep learning workflow suite on DOE supercomputers; **R&D 100 Award (2023)**.

– Probing decision boundaries in cancer data using noise injection and counterfactual analysis (SC workshop).

Uxarray (Climate Computation/Modeling - DOE) Jun 2021 – Present

– Co-created Uxarray, a performant Python library for unstructured grid analysis; enabled up to 60× speedups via vectorization and parallelization.

FLASH-X (Multiphysics Simulation, Astrophysics - ECP) Jun 2016 – Sep 2023

– Implemented asynchronous HDF5 I/O and SZ3/ZFP compression; **R&D 100 Award (2022)**; ¿20% performance gains on I/O-bound runs.

– Architected a verification framework with nightly testing and baselines.

Urban Coupled Simulations (ECP Seed Funded) Jun 2016 – Sep 2018

– Built coupling and data pipelines integrating high-fidelity weather with building energy models for city-scale analysis.

SIGMA/MeshKit/RGG (Nuclear Reactor Simulations - DOE NEAMS) Aug 2009 – Sep 2018

– Led MeshKit/DAG and RGG tools; advised Kitware during SBIR commercialization; reduced reactor core modeling time from weeks to hours.

Technical Skills

HPC and Programming: Python, Fortran, C++; MPI, OpenMP, HDF5, parallel I/O, performance tuning on supercomputers.

ML and Data Tools: PyTorch, Keras, NumPy, Matplotlib, pandas, Scikit-learn, Jupyter; software engineering with Git, CI/CD.

Education

The University of Chicago Chicago, IL
M.S. in Computer Science *Jun 2020*

Arizona State University Tempe, AZ
M.S. in Structural Engineering (Minor: Computer Science) *Jul 2009*

Indian Institute of Technology (IIT) Dhanbad Dhanbad, India
B.Tech. in Mechanical Engineering *May 2006*

Selected Publications

- **Jain, R.**, Eroglu, O., Chen, H., Chmielowiec, P., Clyne, J., Hannay, C., Jacob, R., Medeiros, B., Ullrich, P., & Zarzycki, C. (2025). UXarray: Extending Xarray for Enhanced Support of Unstructured Grids. *EGU General Assembly 2025*. https://doi.org/10.5194/egusphere-egu25-13873
- Wozniak, J. M., **Jain, R.**, et al. (2018). CANDLE/Supervisor. *BMC Bioinformatics*. https://doi.org/10.1186/s12859-018-2056-3
- Mahadevan, V. S., Merzari, E., Tautges, T., **Jain, R.**, et al. (2014). High-resolution coupled physics solvers. *Phil. Trans. R. Soc. A*. https://doi.org/10.1098/rsta.2013.0381