

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

- Delivered reliable research software across cancer data science, climate computation, multiphysics simulation, urban systems, and reactor modeling.
- Partnered with domain scientists and engineers to turn prototypes into maintainable, tested tools used at DOE facilities.
- Mentored junior researchers; emphasized performance, reproducibility, and clear engineering practices.

Research and Teaching Assistant

Aug 2007 – Jul 2009

Structural Engineering, Arizona State University

Tempe, AZ

- Researched FEM-based shape optimization for blast-resistant structural design sponsored by the U.S. Army Research Office; supported structural engineering courses and labs.

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.

Awards

- **R&D 100 Award (2023):** CANDLE/Supervisor — [RDWorld](#); coverage: [NVIDIA News](#), [CACM](#)
- **R&D 100 Award (2022):** FLASH-X — [RDWorld](#)

Major Projects

IMPROVE/CANDLE (Cancer Data Science - ECP)

Jan 2017 – Present

- Led CANDLE/Supervisor across DOE supercomputers; standardized experiments and HPO; **R&D 100 (2023)**.
- Improved reproducibility and fair model comparisons; widely cited and covered by NVIDIA News and CACM.

Uxarray (Climate Computation/Modeling - DOE)

Jun 2021 – Present

- Co-created a Python toolkit for unstructured climate grids; enabled up to 60x speed-ups via vectorization and parallelization; adopted by DOE climate users.

FLASH-X (Multiphysics Simulation, Astrophysics - ECP)

Jun 2016 – Sep 2023

- Implemented asynchronous HDF5 I/O with compression; **R&D 100 (2022)**; improved I/O-bound runs by more than 20%.
- Architected a verification framework with nightly testing and baselines to stabilize releases.

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.

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

Open-Source Contributions

- **UXarray:** github.com/UXARRAY/uxarray — unstructured climate grids toolkit (Python)
- **FLASH-X:** Asynchronous I/O and verification contributions — flash-x.org
- **CANDLE/Supervisor:** Workflow framework for ML — github.com/ECP-CANDLE/Supervisor

Selected Publications

- Wozniak, J. M., **Jain, R.**, et al. (2018). CANDLE/Supervisor. *BMC Bioinformatics*. doi: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*. doi:10.1098/rsta.2013.0381
- **Jain, R.**, Luo, X., Sever, G., Hong, T., & Catlett, C. (2020). Urban weather boundary conditions. *Journal of Building Performance Simulation*. doi:10.1080/19401493.2020.1739106
- **Jain, R.**, & Tautges, T. J. (2012). Geometry and mesh models for reactor cores using a lattice hierarchy. *Engineering with Computers*. doi:10.1007/s00366-011-0221-4
- Dhruv, A., **Jain, R.**, et al. (2023). Verification of Flash-X. *ICSE Companion*. doi:10.1109/ICSE-Companion60176.2023.00107
- **Jain, R.**, et al. (2025). UXarray: Extending Xarray for Unstructured Grids. *EGU General Assembly*. doi:10.5194/egusphere-egu25-13873

Teaching & Mentoring

- TA/RA at Arizona State University (2007–2009): blast mitigation research (U.S. Army Research Office) and structural engineering instruction.

Talks & Media

- SciPy: UXarray for Unstructured Grids — [YouTube](#)
- HDF5 Annual Meeting: FLASH-X Async I/O — [YouTube](#)

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
M.S. in Computer Science

Chicago, IL
Jun 2020

Arizona State University
M.S. in Structural Engineering (Minor: Computer Science)

Tempe, AZ
Jul 2009

Indian Institute of Technology (IIT) Dhanbad
B.Tech. in Mechanical Engineering

Dhanbad, India
May 2006