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 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 (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
- **R&D 100 Award (2022):** FLASH-X — RDWorld
- University Graduate Fellowship, Arizona State University (2007–2009)

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.

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.

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.

– SBIR Phase I and II awards for RGG (2014–2017) with Kitware, Inc. — [Kitware RGG].

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, Talks & Media

- Wozniak, J. M., **Jain, R.**, et al. (2018). CANDLE/Supervisor. *BMC Bioinformatics*. [DOI]
- Mahadevan, V. S., Merzari, E., Tautges, T., **Jain, R.**, et al. (2014). High-resolution coupled physics solvers. *Phil. Trans. R. Soc. A*. [DOI]
- **Jain, R.**, Luo, X., Sever, G., Hong, T., & Catlett, C. (2020). Urban weather boundary conditions. *Journal of Building Performance Simulation*. [DOI]
- **Jain, R.**, & Tautges, T. J. (2012). Geometry and mesh models for reactor cores using a lattice hierarchy. *Engineering with Computers*. [DOI]
- Dhruv, A., **Jain, R.**, et al. (2023). Verification of Flash-X. *ICSE Companion*. [DOI]
- **Jain, R.**, et al. (2025). UXarray: Extending Xarray for Unstructured Grids. *EGU General Assembly*. [DOI] — [Video]
- HDF5 Annual Meeting: FLASH-X Async I/O — [Video]

Teaching & Mentoring

- TA/RA at Arizona State University (2007–2009): blast mitigation research (U.S. Army Research Office) and structural engineering instruction.
- Mentored summer interns: Rylie Weaver (2023); Aaron Zedwick (2023–2025); Brett Rhodes (2014).

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.