Rajeev Jain

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Experience

CASE Staff At-Large

The University of Chicago (UChicago)

Sep 2023 – Present *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

Structural Engineering, Arizona State University

 ${\rm Aug}\ 2007-{\rm Jul}\ 2009$

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
Wipro Technologies

May 2006 – Jun 2007

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
- SBIR Phase I and II awards for RGG (2014–2017) with Kitware, Inc. [Kitware RGG]
- 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 M.S. in Computer Science

Chicago, IL Jun 2020

Arizona State University

Tempe, AZ

Jul 2009

May 2006

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

Dhanbad, India

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

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.