

# Rajeev Jain

Chicago, IL

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## Summary

- Research software engineer with 16+ years building scientific software across climate, cancer data science, multiphysics simulation, urban systems, and nuclear engineering.
- Focus areas: parallel input/output, profiling and optimization, reproducibility, scalable pipelines, and Python programming.
- Scope includes multi-institution projects, exascale-class systems, and software practices around testing, continuous integration, and releases.

## Appointments

### Research Software Engineering Roles (current: Principal Specialist)

Aug 2009 – Present

*Mathematics and Computer Science Division, Argonne National Laboratory*

*Lemont, IL*

- Research software engineering across UXarray, FLASH-X, Cancer Distributed Learning Environment workflows, MeshKit, Reactor Geometry Generator, and urban simulation workflows.
- Work spans exascale-class systems and large-scale workflows.

### Staff At-Large

Sep 2023 – Present

*The University of Chicago*

*Chicago, IL*

- Joint appointment supporting cancer and earth science research.

### Research and Teaching Assistant

Aug 2007 – Jul 2009

*Arizona State University*

*Tempe, AZ*

- Researched finite element method-based shape optimization for blast-resistant design; supported structural engineering courses.

### Project Engineer

May 2006 – Jun 2007

*Wipro Technologies*

*Bangalore/Hyderabad, India*

- Developed production software in Java and enterprise resource planning systems in large enterprise environments.

## Education

### The University of Chicago

*Master of Science in Computer Science*

Chicago, IL

*Jun 2020*

### Arizona State University

*Master of Science in Structural Engineering (Minor: Computer Science)*

Tempe, AZ

*Jul 2009*

### Indian Institute of Technology Dhanbad

*Bachelor of Technology in Mechanical Engineering*

Dhanbad, India

*May 2006*

## Leadership and Funding

- Principal investigator, Nuclear Energy Advanced Modeling and Simulation Integration (Frameworks) Product Line (Meshing), \$300k+ (2011–2016).

- Principal investigator, MeshKit Nuclear Energy Advanced Modeling and Simulation toolkit development (2012–2016).
- Co-principal investigator and project lead for the Urban Exascale Computing Project effort; contributed to growth from \$300k (fiscal year 2017) to \$1M (fiscal year 2018) with projected \$2.5M (fiscal year 2019).
- Small Business Innovation Research Phase I and II awards for Reactor Geometry Generator commercialization with Kitware (2014–2017).
- Kitware subcontract for web-based nuclear reactor modeling, \$75k (Phase IIB Small Business Innovation Research, 2017).

## Selected Projects and Technical Contributions

### UXarray (Climate Computing)

2021 – Present

- Core contributor to a Python toolkit for unstructured climate grids; pip-installable with monthly releases.
- Implemented conservative zonal averaging (pull request #1345) and accelerated unstructured grid analysis via vectorization.

### FLASH-X (Multiphysics Simulation)

2016 – 2023

- Implemented asynchronous Hierarchical Data Format input/output with compression; reported 20%+ input/output gains in benchmarks.
- Built verification workflows and nightly baselines to stabilize releases.

### Cancer Data Science (Cancer Distributed Learning Environment workflows)

2017 – Present

- Ran large-scale hyperparameter optimization workflows and standardized reproducible pipelines.
- Contributed to counterfactual analysis and benchmarking for drug response modeling.

### Urban Exascale (Urban Microclimate)

2016 – 2018

- Coupled urban weather boundary conditions into city-scale building energy workflows.

### MeshKit and Reactor Geometry Generator (Reactor Modeling)

2009 – 2018

- Led MeshKit and Reactor Geometry Generator development for Nuclear Energy Advanced Modeling and Simulation; reduced reactor core mesh turnaround from weeks to hours.
- Developed PostBL and parallel mesh generation tools for large reactor models.

## Reports to the Department of Energy

- Jain, R. and Tautges, T. J. *MeshKit*, ANL/MCS-TM/336, Sept 30, 2013.
- Jain, R. and Mahadevan, V. *2014 MeshKit Release*, ANL/MCS-TM/344, Sept 30, 2014.
- Jain, R., Vanderzee, E., Grindeanu, I., Mahadevan, V. *Mesh Generation and Algorithm Development for Nuclear Energy Advanced Modeling and Simulation*, ANL-P60660916, Sept 30, 2016.
- Tautges, T. J., Fischer, P. F., Grindeanu, I., Jain, R., et al. *SHARP Assembly-Scale Multiphysics Demonstration Simulations*, ANL/MCS-NE-13-9, Mar 30, 2013.
- Bingham, A., Ortensi, J., Jain, R., Grindeanu, I., Tautges, T. *SHARP/PRONGHORN*, INL/EXT-12-27171, 2012.
- Tautges, T. J., Fischer, P., Grindeanu, I., Jain, R., et al. *Coupled Thermal/Hydraulics – Neutronics – Fuel Performance Analysis of a sodium-cooled fast reactor fuel assembly*, Apr 30, 2012.
- Tautges, T. J. and Jain, R. *Extensions to MeshKit and Reactor Geometry Generator*, ANL/MCS-TM316, Oct 30, 2011.

- Tautges, T. J. and Jain, R. *Mesh Copy/Move/Merge Tool for Reactor Simulation Applications*, ANL/MCS-P1773-0610, Apr 30, 2010.
- Merzari, E., Shemon, E. R., Yu, Y., Thomas, J. W., Obabko, A., Jain, R., Mahadevan, V., et al. *Full Core Multiphysics Simulation with Offline Mesh Deformation*, ANL/NE-15/42, Dec 21, 2015.
- Catlett, C., Jain, R., Jacob, R., Muehleisen, R., Hong, T., Luo, X., et al. *Data Flow Characteristics for Coupled Urban Models*, Exascale Computing Project report, Dec 31, 2017.

## Selected Publications

- UXarray: [UXarray presentation](#) and [paper](#).
- FLASH-X: [Paper 1](#) and [Paper 2](#).
- Cancer Distributed Learning Environment / Supervisor: [BMC Bioinformatics](#).
- Counterfactual analysis in cancer data: [Paper](#).
- Urban microclimate boundary conditions: [Paper](#).
- MeshKit and Reactor Geometry Generator: [Engineering with Computers](#).
- PostBL: *Post-Mesh Boundary Layer Generation Tool*, International Meshing Roundtable 2013.
- MeshKit and Reactor Geometry Generator: *Generating Unstructured Reactor Core Meshes in Parallel*, International Meshing Roundtable 2014.

## Awards and Honors

- Research and Development 100 Award: Cancer Distributed Learning Environment / Supervisor (2023).
- Research and Development 100 Award: FLASH-X (2022).
- Best Paper, International Meshing Roundtable (2010).
- University Graduate Fellowship, Arizona State University (2007–2009).
- Small Business Innovation Research Phase I and II awards for Reactor Geometry Generator commercialization with Kitware (2014–2017).

## Service and Mentoring

- Mentored junior researchers and interns across climate and cancer data science projects.
- Session chair, Computational Geometries, International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (2015).
- Peer reviewer for International Meshing Roundtable papers.
- Judge for Monte Carlo conference submissions.
- Peer reviewer for Journal of Open Research Software (selected manuscripts).

## Professional Memberships (active/inactive)

- American Nuclear Society (ANS).
- Association for Computing Machinery (ACM).
- American Meteorological Society (AMS).

## Technical Skills

**High-performance computing and programming:** Python, C++, Fortran; Message Passing Interface, Open Multi-Processing, Hierarchical Data Format, parallel input/output, performance tuning.

**Machine learning and data tools:** PyTorch, Keras, NumPy, pandas; Git, continuous integration/continuous delivery.