Rajeev Jain

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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 (CANDLE) 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 Chicago, IL
Master of Science in Computer Science *Jun 2020*

Arizona State University Tempe, AZ
Master of Science in Structural Engineering (Minor: Computer Science) *Jul 2009*

Indian Institute of Technology Dhanbad Dhanbad, India
Bachelor of Technology in Mechanical Engineering *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 5 (HDF5) input/output with compression; reported 20%+ input/output gains in benchmarks.
- Built verification workflows and nightly baselines to stabilize releases.

Cancer Data Science (CANDLE 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.
- CANDLE / 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 (R&D 100) Award: CANDLE / Supervisor (2023).
- R&D 100 Award: FLASH-X (2022).
- Best Paper, International Meshing Roundtable (2010).
- University Graduate Fellowship, Arizona State University (2007–2009).
- Small Business Innovation Research (SBIR) 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 (MPI), Open Multi-Processing (OpenMP), HDF5, parallel input/output, performance tuning.

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