

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 (CAN-DLE) 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.

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

- Thesis: Blast Mitigation Solutions via finite element method (FEM)-based design optimization.
- Advisors: S. D. Rajan (chair), Gerald Farin, A. D. Belegundu.

Indian Institute of Technology Dhanbad Dhanbad, India
Bachelor of Technology in Mechanical Engineering May 2006

Industry Experience

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.

Intern Engineer
Engineering Research Center, Tata Motors
Research and Development Intern
Bhilai Steel Plant

Apr 2005 – Jul 2005
Pune, India
Nov 2004 – Jan 2005
Bhilai, India

Research 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.
- Modernized the test suite and fixtures, added grid validation checks, and expanded grid input/output support.
- Added Earth System Modeling Framework (ESMF) grid writer and improved grid area calculations and temporal grouping behavior.
- Led code reviews and API/documentation updates to stabilize releases.

FLASH-X (Multiphysics Simulation) 2016 – 2023

- Implemented asynchronous Hierarchical Data Format 5 (HDF5) input/output with compression; reported 20%+ input/output gains in benchmarks.
- Added data reduction and compression workflows; results accepted at the 2024 Data Analysis and Reduction for Big Scientific Data workshop.
- 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.
- Maintained the Supervisor repository and benchmarking tools; added continuous integration and packaging automation.
- Contributed to cross-study model evaluation and counterfactual analysis for drug response modeling.

Urban Microclimate and Exascale Workflows 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.

Journal Papers

- Partin, A., Vasanthakumari, P., Narykov, O., Wilke, A., Koussa, N., Jones, S., Zhu, Y., Jain, R., et al. “Benchmarking community drug response prediction models: datasets, models, tools, and metrics for cross-dataset generalization analysis.” *Briefings in Bioinformatics* (forthcoming).
- Dubey, A., et al. (2022). “FLASH-X: A Multiphysics Simulation Software Instrument.” *SoftwareX*. DOI: 10.1016/j.softx.2022.101267.
- Wozniak, J. M., Jain, R., et al. (2018). “CANDLE/Supervisor: A workflow framework for machine learning applied to cancer research.” *BMC Bioinformatics*, 19, 59–69. DOI: 10.1186/s12859-018-2056-3.
- Jain, R., Luo, X., Sever, G., Hong, T., & Catlett, C. (2020). “Representation and evolution of urban weather boundary conditions in downtown Chicago.” *Journal of Building Performance Simulation*, 13(2). DOI: 10.1080/19401493.2020.1739106.

- Mahadevan, V. S., Merzari, E., Tautges, T., Jain, R., Obabko, A., Smith, M., & Fischer, P. (2014). “High-resolution coupled physics solvers for analysing fine-scale nuclear reactor design problems.” *Philosophical Transactions of the Royal Society A*, 372. DOI: 10.1098/rsta.2013.0381.
- Jain, R., & Tautges, T. J. (2012). “Creating geometry and mesh models for nuclear reactor core geometries using a lattice hierarchy-based approach.” *Engineering with Computers*, 28, 319–329. DOI: 10.1007/s00366-011-0221-4.
- Argod, A. D., Belegundu, A., Aziz, A., Agarwala, V., Rajan, S. D., & Jain, R. (2009). “Message Passing Interface (MPI)-enabled shape optimization of panels subjected to dynamic loading.” *Journal of Simulation and Multidisciplinary Design Optimization*, 2, 273–282.

Conference and Workshop Papers

- Gwinn, J., Wozniak, J., Jain, R., Zhu, Y., Partin, A., Brettin, T., & Stevens, R. (2025). “A Workflow for Error Analysis for Drug Response Prediction via Statistical Standardization and Distribution Analysis.” 20th Workshop on Workflows in Support of Large-Scale Science.
- Eroglu, O., Jain, R., Chen, H., Chmielowiec, P., Clyne, J., Hannay, C., Jacob, R., Medeiros, B., Ullrich, P., & Zarzycki, C. (2025). “UXarray: Extending Xarray for Enhanced Support of Unstructured Grids.” European Geosciences Union (EGU) General Assembly 2025, EGU25-13873.
- Eroglu, O., Jain, R., et al. (2025). “UXarray: Python Package for the Analysis and Visualization of Model Output on Unstructured Climate Grids.” 105th American Meteorological Society (AMS) Annual Meeting.
- Chmielowiec, P., Chen, H., DeCiampa, C., Eroglu, O., Hannay, C., Jacob, R., Jain, R., Loft, R., Medeiros, B., & Sun, L. (2024). “UXarray: Extending Xarray with Support for Unstructured Grids.” 104th American Meteorological Society Annual Meeting.
- Jain, R., et al. (2024). “Cross-HPO: Optimizing Neural Networks for Cancer Drug Response Using Hyperparameter Tuning on Multiple Pharmacogenomic Datasets.” Tenth Computational Approaches for Cancer Workshop (CAFCW24), held with Supercomputing 2024.
- Jain, R., Tang, H., Dhruv, A., & Byna, S. (2024). “Enabling Data Reduction for FLASH-X Simulations.” 10th International Workshop on Data Analysis and Reduction for Big Scientific Data, held with Supercomputing 2024.
- Jain, R., et al. (2023). “UXarray: Analysis and Visualization of Unstructured Grid Data in Xarray.” Proceedings of the Python in Science Conference (SciPy 2023).
- Jain, R., & Tautges, T. J. (2013). “PostBL: Post-Mesh Boundary Layer Generation Tool.” 22nd International Meshing Roundtable.
- Jain, R., & Tautges, T. J. (2012). “Parallel Reactor Geometry (and Mesh) Generator.” International Congress on the Advances in Nuclear Power Plants (ICAPP).
- Mohanty, S., Jain, R., Majumdar, S., Tautges, T. J., & Srinivasan, M. (2012). “Coupled Field-Structural Analysis of HTGR Fuel Brick Using Abaqus.” International Congress on the Advances in Nuclear Power Plants (ICAPP).
- Tautges, T. J., Caceras, A., Jain, R., Kim, H. J., Kraftcheck, J., & Smith, B. M. (2011). “Coupled Multi-Physics Simulation Frameworks for Reactor Simulation: A Bottom-Up Approach.” International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C).
- Tautges, T. J., & Jain, R. (2010). “Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach.” 19th International Meshing Roundtable.
- Jain, R., & Rajan, S. D. (2011). “Blast Mitigation via finite element method (FEM)-based design optimization.” 11th US National Congress on Computational Mechanics.

Technical Reports

- 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. and Mahadevan, V. *Documentation for MeshKit – Reactor Geometry Generator*, ANL/MCS-TM/354, 2015.
- 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.

Presentations and Posters

- Tutorial, Earth System Data Science (ESDS) Annual Event: UXarray (2024).
- Tutorial, American Meteorological Society Annual Meeting: UXarray (2024).
- Poster presentation, Earth System Model PI meeting (2024).
- Invited talk, Data Analysis and Reduction for Big Scientific Data workshop: FLASH-X compression methods (2024).
- [UXarray for unstructured climate data](#), Scientific Python Conference (SciPy 2023).
- [Data reduction for FLASH-X simulations](#), Hierarchical Data Format 5 (HDF5) User Group (2023).
- MeshKit Training, Oak Ridge National Laboratory (Mar 2014).
- Reactor Geometry Generator (RGG) and MeshKit Progress Report, Nuclear Energy Advanced Modeling and Simulation (NEAMS) PI meeting, Washington, DC (Dec 2013).
- MeshKit: open-source library for mesh generation and meshing algorithm research, Symposium on Trends in Unstructured Mesh Generation, 12th US National Congress on Computational Mechanics (Jul 2013).
- Parallel Reactor Geometry Generator, Postdoctoral Research Symposium, Argonne National Laboratory (Oct 2013).
- MeshKit and Reactor Geometry Generator toolkit, invited presentation, Oak Ridge National Laboratory (Nov 2011).
- Parallel Reactor Geometry Generator, Postdoctoral Research Symposium, Argonne National Laboratory (Oct 2011).

- MeshKit, Nuclear Energy Advanced Modeling and Simulation (NEAMS) PI meeting, Argonne National Laboratory (Oct 2011).
- Poster: Tools to Generate Large Reactor Core and Geometry Meshes, Student Poster Competition, 11th US National Congress on Computational Mechanics (Jul 2011).
- Poster: Reactor Geometry Generator (RGG): a tool for generating reactor core models, Very High Temperature Reactor (VHTR) Technology Development Office 4th Annual Technical Review Meeting (Apr 2011).
- Argonne National Laboratory (ANL) Summer Student Lecture Series: Mesh Generation for Scientific Computing (Jun 2010).
- Structural and Computational Mechanics Lab, Arizona State University: Cubic Bezier Velocity Field for Shape Optimization and Unit-cell Based Regression Model of Sandwich Honeycomb Panels (Jul 2008).
- Phoenix, All-India Technical Festival Presentation for Car Design Contest Sponsored by IBM and Tata Motors, Indian Institute of Technology (IIT) Kharagpur (Sep 2004).

Awards and Funding

- Research and Development 100 (R&D 100) Award: CANDLE (2023).
- R&D 100 Award: FLASH-X (2022).
- Best Paper, International Meshing Roundtable (2010).
- University Graduate Fellowship, Arizona State University (2007–2009).
- 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 (SBIR) 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 SBIR, 2017).
- Exceeded yearly goals at Argonne National Laboratory (2014).
- MeshKit Reactor Geometry Generator (RGG) training, 5-hour hands-on training to 10+ users (2014).
- Co-chair, Computer Science, Argonne/CSUI Undergraduate/Graduate Research Symposium (2011).
- Co-chair, Research in Interdisciplinary Science and Engineering (RISE), Arizona State University (2007).
- 1st Prize, MindAdvantage Technical Paper Presentation, Minda Ltd., New Delhi (2005).
- 1st Prize, Low Budget Car Design Contest, Indian Institute of Technology (IIT) Kharagpur (2005).
- Co-chair, Society of Automotive Engineers (SAE) ISM Chapter (2003–2005).
- Qualified Indian Institutes of Technology Joint Entrance Examination (IIT-JEE), All-India Rank 3487 of 150,000 (top 2%) (2002).

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).
- Technical program committee member for a Supercomputing-affiliated workshop (2024).
- Panelist, Infraday Midwest Event (2024).
- Volunteer, South Side Science Festival at the University of Chicago (2023, 2024).
- Collaborator, National Science Foundation Raijin project.

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.