

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)
Mathematics and Computer Science Division, Argonne National Laboratory

Aug 2009 – Present
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
The University of Chicago

Sep 2023 – Present
Chicago, IL

- Joint appointment supporting cancer and earth science research.

Research and Teaching Assistant
Arizona State University

Aug 2007 – Jul 2009
Tempe, AZ

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

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

- Thesis (2009): 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
Bachelor of Technology in Mechanical Engineering

Dhanbad, India
May 2006

Industry Experience

Project Engineer
Wipro Technologies

May 2006 – Jun 2007
Bangalore/Hyderabad, India

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

Intern Engineer <i>Engineering Research Center, Tata Motors</i>	Apr 2005 – Jul 2005 Pune, India
Research and Development Intern <i>Bhilai Steel Plant</i>	Nov 2004 – Jan 2005 Bhilai, India

Research and Technical Contributions

UXarray (Climate Computing)	2021 – Present
<ul style="list-style-type: none"> 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
<ul style="list-style-type: none"> 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
<ul style="list-style-type: none"> 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
<ul style="list-style-type: none"> Coupled urban weather boundary conditions into city-scale building energy workflows. 	
MeshKit and Reactor Geometry Generator (Reactor Modeling)	2009 – 2018
<ul style="list-style-type: none"> 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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. DOI: [10.5194/egusphere-egu25-13873](https://doi.org/10.5194/egusphere-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. ADS.
- 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 Hyper-parameter 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. IEEE.
- 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.