

RAJEEV JAIN

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Quick Facts:

- Lead Developer, UXarray (205+ GitHub stars) • 2× R&D 100 Award Winner (2022, 2023)
- 16+ Years at Argonne National Laboratory • 15+ Peer-Reviewed Publications

Research Interests

High-performance scientific computing, climate modeling, cancer pharmacogenomics, computational physics, mesh generation, parallel I/O optimization, machine learning infrastructure, and reproducible workflows.

Professional Experience

Principal Specialist, Research Software Engineering 2009 – Present
Argonne National Laboratory, Mathematics and Computer Science Division Chicago, IL

- Lead developer for UXarray Python library (205+ GitHub stars), enabling analysis of multi-petabyte unstructured climate datasets for NCAR, DOE labs, and universities worldwide.
- Implemented asynchronous HDF5 I/O for FLASH-X exascale simulations achieving 40-70% reduction in checkpoint times on Summit supercomputer. Integrated SZ3/ZFP compression reducing storage by 50%+.
- Built hyperparameter optimization infrastructure for cancer drug response prediction, running 10,000+ experiments across Summit, Theta, and Cori supercomputers. Framework used by 15+ researchers.
- Led bi-weekly coordination across 4 national labs for DOE Urban ECP project, growing program from \$300k seed funding to \$2.5M. Coupled WRF weather models with Nek5000 CFD simulations achieving 11% improvement in building energy prediction accuracy. Developed parallel reactor core mesh generator (MeshKit/RGG) creating billion-element hex meshes for nuclear simulation. Trained 10+ users at Oak Ridge National Laboratory.
- Recipient of 2× R&D 100 Awards (2022, 2023) for FLASH-X and CANDLE projects.

Staff At-Large 2023 – Present
University of Chicago Chicago, IL

- Joint appointment supporting cancer pharmacogenomics and earth science research projects.
- Mentor graduate students and research associates on software development best practices.

Research and Teaching Assistant 2007 – 2009
Arizona State University, Structural and Computational Mechanics Lab Tempe, AZ

- Conducted research on blast mitigation via FEM-based design optimization.
- Teaching assistant for Structural Analysis and Design courses.

Project Engineer 2006 – 2007
Wipro Technologies Bangalore, India

Engineering Intern Apr – Jul 2005
Tata Motors, Engineering Research Center Pune, India

Education

M.S. in Computer Science 2020
University of Chicago, Chicago, IL

M.S. in Structural Engineering 2009
Arizona State University, Tempe, AZ
Graduate Fellowship Recipient (2007–2009)

B.Tech in Mechanical Engineering 2006
Indian Institute of Technology (IIT), Indian School of Mines, Dhanbad, India

Awards and Honors

R&D 100 Award – CANDLE (Cancer Distributed Learning Environment)	2023
”Oscars of Innovation” for top 100 innovations of the year	
R&D 100 Award – FLASH-X (Multiphysics Simulation Software)	2022
Team contribution for exascale computing software	
Best Paper Award – International Meshing Roundtable	2010
”Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries”	
ATPESC Scholar – Argonne Training Program on Extreme-Scale Computing	2015
Selected for world-class training on HPC and big data	
Graduate Fellowship – Arizona State University	2007–2009

Publications

Refereed Journal Articles

- Partin, A., Vasanthakumari, P., Narykov, O., Wilke, A., Koussa, N., Jones, S., Zhu, Y., Jain, R., et al. (2025). ”Benchmarking community drug response prediction models: datasets, models, tools, and metrics for cross-dataset generalization analysis.” *Briefings in Bioinformatics* (forthcoming). APT #199556.
- Tautges, T. J., Jain, R. (2011). ”Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach.” *Journal of Engineering with Computers*. DOI: 10.1007/s00366-011-0221-4
- Argod, Belegudu, A.D., Aziz, A., Agarwala, V., Rajan, S.D., Jain, R. (2009). ”MPI-enabled Shape Optimization of Panels Subjected to Dynamic Loading.” *Journal of Simulation and Multidisciplinary Design Optimization*, 2, 273-282.

Refereed Conference Proceedings

- 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*, November 17, 2025. APT #198825.
- Jain, R., Tang, H., Dhruv, A., Byna, S. (2024). ”Enabling Data Reduction for Flash-X Simulations.” *Proceedings of 10th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-10)*, SC24, November 2024.
- Jain, R., Wozniak, J.M., Partin, A., Wilke, A., Zhu, Y., Vasanthakumari, P., Narykov, O., Overbeek, J., Weaver, R., Wang, C., Liu, Y., Weil, R., Brettin, T., Stevens, R. (2024). ”Cross-HPO: Optimizing Neural Networks for Cancer Drug Response Using Hyperparameter Tuning on Multiple Pharmacogenomic Datasets.” *Tenth Computational Approaches for Cancer Workshop (CAFCW24)*, SC24.
- Jain, R., Shah Ashka, Mohd-Yosuf, J., Wozniak, J.W., Xia, F., Brettin, T., Stevens, R. (2021). ”Probing Decision Boundaries in Cancer Data Using Noise Injection and Counterfactual Analysis.” *Seventh Computational Approaches for Cancer Workshop (CAFCW21)*, SC21.
- Jain, R., Chawdary, S., Weide, K., Klosterman, T. (2021). ”Checkpoint/Restart for Lagrangian particle mesh with AMR in community code FLASH-X.” *SuperCheck’21, First International Symposium on Checkpointing for Supercomputing*. arXiv:2103.04267
- Jain, R., Tautges, T. J. (2014). ”Generating Unstructured Reactor Core Meshes in Parallel.” *Proceedings of the 23rd International Meshing Roundtable*, October 2014. ANL/MCS-P4092-0713.
- Jain, R., Tautges, T. J. (2013). ”PostBL: Post-Mesh Boundary Layer Generation Tool.” *22nd International Meshing Roundtable* (pp. 445-464), October 2013. ANL/MCS-P4092-0713.
- Jain, R., Tautges, T.J. (2012). ”Parallel Reactor Geometry (and Mesh) Generator.” *International Congress on the Advances in Nuclear Power Plants (ICAPP)*, June 2012.

- Tautges, T. J., Jain, R. (2010). "Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach." *Proceedings of the 19th International Meshing Roundtable*, Springer Berlin Heidelberg, 2010, pp. 351-365. **Best Paper Award**.

Conference Presentations & Posters

- 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 AMS Annual Meeting*.
- Jain, R. (2024). "UXarray: Python Package for Analysis and Visualization of Model Output from Unstructured Climate and Weather Grids." Tutorial, *SC24*, Atlanta, GA, November 2024.
- Jain, R. (2023). "UXarray for unstructured climate data." *Scientific Python Conference 2023*. YouTube Link
- Jain, R. (2023). "Data reduction for FLASH-X simulations." *Hierarchical Data Format User Group 2023*. YouTube Link
- Jain, R. (2024). "UXarray Tutorial." *ESDS Annual Event 2024*. YouTube Link

Technical Reports

- Jain, R., Vanderzee, E., Grindeanu, I., Mahadevan, V. (2016). "Mesh Generation and Algorithm Development for NEAMS." Based on MeshKit v1.42 release, report to Nuclear Energy Advanced Modeling and Simulation program directors, Sept 30, 2016. ANL-P60660916.
- Tautges, T. J., Fischer, P., Grindeanu, I., Jain, R., Mahadevan, V., Obabko, A., Smith, M. A., Hamilton, S., Clarno, K., Baird, M., Berrill, M. (2012). "A Coupled Thermal/Hydraulics – Neutronics – Fuel Performance Analysis of an SFR Fuel Assembly." Report to US DOE, Reactor Campaign, April 30, 2012.
- Tautges, T.J., Jain, R. (2011). "Extensions to MeshKit and RGG." Report to US DOE, Reactors Campaign, ANL/MCS-TM316, October 30, 2011.
- Tautges, T.J., Jain, R. (2010). "Mesh Copy/Move/Merge Tool for Reactor Simulation Applications." Report to US DOE, Reactor Campaign, ANL/MCS-P1773-0610, April 30, 2010.

Software & Open Source Contributions

UXarray – Lead Developer	2022–Present
Python library for unstructured grid analysis. 205+ GitHub stars. https://github.com/UXARRAY/uxarray · https://uxarray.readthedocs.io	
CANDLE/IMPROVE – Core Contributor	2020–2025
Hyperparameter optimization framework and benchmarking tools for cancer drug response models. https://github.com/JDACS4C-IMPROVE	
FLASH-X – I/O & Compression Lead	2019–2024
Multiphysics simulation software for exascale computing. https://github.com/Flash-X/Flash-X	
MeshKit – Principal Investigator	2009–2016
Mesh generation toolkit for reactor core geometries. https://bitbucket.org/fathomteam/meshkit	

Technical Skills

Programming Languages: Python, C++, Fortran, R, Bash, SQL

ML & Data Science: PyTorch, TensorFlow, NumPy, Pandas, Xarray, Scikit-learn, Parsl, Swift/T

HPC & Systems: MPI, OpenMP, HDF5, NetCDF, MOAB, Docker, Singularity, Git, GitHub Actions, Jenkins

Scientific Computing: Finite element methods, computational fluid dynamics, mesh generation, parallel I/O

Domains: Climate modeling, cancer pharmacogenomics, computational physics, nuclear engineering, urban systems

Professional Service

Panelist – "Revolutionizing Public Infrastructure: The Impact of AI and Machine Learning"

5th Infraday Midwest Event, 2024

Program Committee Member – NumGrid 2020

International conference on numerical geometry, grid generation, and scientific computing

Peer Reviewer

Journal of Open Research Software (3 manuscripts, 2024–2025)

NumGrid Conference (2020)

Session Chair – Computational Geometries Session

MC2015, Joint International Conference on Mathematics and Computation

Reviewer – SBIR (Small Business Innovation Research) Funding Proposals

2015

Member – American Nuclear Society

2012–2016

Volunteer – South Side Science Festival, University of Chicago (2023, 2024)

Mentorship

Mentored Research Associates, Graduate Students, and Staff

- Rylie Weaver (Research Aide, 2022–2024) – IMPROVE project, developed novel HPO techniques for cancer drug response prediction across pharmacogenomic datasets
- Aaron Zedwick (Student, 2023–2024) – UXarray development, dual mesh routines and remapping functionality
- Mark Bartoszek (Windows Systems Admin, 2023) – Mentoring on systems administration, Argonne

Funding & Proposals

DOE SEATS (Active, multi-year) – Ongoing participant

Software Ecosystem for Advancing Climate Tools and Services

NSF Raijin (Active, multi-year) – Ongoing collaborator

Collaborative research in climate model analysis

DOE ECP CANDLE (Completed) – Core contributor, 2017–2023

DOE NEAMS (Completed) – Principal Investigator for MeshKit, 2009–2016

Nuclear Energy Advanced Modeling and Simulation