

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. 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

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) "Oscars of Innovation" for top 100 innovations of the year	2023
R&D 100 Award – FLASH-X (Multiphysics Simulation Software) Team contribution for exascale computing software	2022
Best Paper Award – International Meshing Roundtable "Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries"	2010
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

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 Rajjin (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