Rajeev Jain

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Summary

Research software engineer building high-performance tools for climate science, cancer research, and exascale computing. Lead developer of UXarray (205+ GitHub stars), **2× R&D 100 Award winner**, with 16+ years optimizing scientific workflows at Argonne National Laboratory.

Current Appointments

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

- Lead developer for UXarray (205+ stars), enabling analysis of petabyte-scale unstructured climate data.
- Implemented async HDF5 I/O for FLASH-X, reducing checkpoint times by 40-70% on Summit.
- Built hyperparameter optimization infra for cancer drug response (CANDLE), running 10k+ experiments.

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

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

Research Interests

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

Open Source Software

UXarray	Lead Developer · GitHub · Docs Python library for unstructured grid analysis. 205+ GitHub stars.
CANDLE	Core Contributor · GitHub Hyperparameter optimization framework for cancer drug response models.
FLASH-X	I/O & Compression Lead · GitHub Multiphysics simulation software for exascale computing.
MeshKit	Principal Investigator · BitBucket Mesh generation toolkit for reactor core geometries.

Technical Skills

Languages	Python, C++, Fortran, R, Bash, SQL
ML & Data	PyTorch, TensorFlow, NumPy, Pandas, Xarray, Scikit-learn, Parsl, Swift/T
HPC & Systems	MPI, OpenMP, HDF5, NetCDF, MOAB, Docker, Singularity, Git, GitHub Actions
Domains	Climate modeling, cancer pharmacogenomics, computational physics, mesh generation

Education

2020 **University of Chicago**
M.S. in Computer Science

2009 **Arizona State University**
M.S. in Structural Engineering · Graduate Fellowship Recipient

2006 **Indian Institute of Technology (IIT), ISM Dhanbad**
B.Tech in Mechanical Engineering

Honors and Awards

2023 **R&D 100 Award** – CANDLE (Cancer Distributed Learning Environment)
"Oscars of Innovation" for top 100 innovations of the year

2022 **R&D 100 Award** – FLASH-X (Multiphysics Simulation Software)
Team contribution for exascale computing software

2015 **ATPESC Scholar** – Argonne Training Program on Extreme-Scale Computing

2010 **Best Paper Award** – International Meshing Roundtable

Publications

Refereed Journal Articles

2025 J.1 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". *Briefings in Bioinformatics* (forthcoming).

2011 J.2 Tautges, T. J., **Jain, R.** "Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach." *Journal of Engineering with Computers*.

2009 J.3 Argod, Belegudu, A.D., Aziz, A., Agarwala, V., Rajan, S.D., **Jain, R.** "MPI-enabled Shape Optimization of Panels Subjected to Dynamic Loading." *Journal of Simulation and Multidisciplinary Design Optimization*.

Refereed Conference Proceedings

2025 C.4 Gwinn, J., Wozniak, J., **Jain, R.**, et al. "A Workflow for Error Analysis for Drug Response Prediction via Statistical Standardization and Distribution Analysis." *Works Workshop*, SC25.

2024 C.5 **Jain, R.**, Tang, H., Dhruv, A., Byna, S. "Enabling Data Reduction for Flash-X Simulations." *DRBSD-10 Workshop*, SC24.

C.6 **Jain, R.**, Wozniak, J.M., Partin, A., et al. "Cross-HPO: Optimizing Neural Networks for Cancer Drug Response." *CAFCW24 Workshop*, SC24.

2014 C.7 **Jain, R.**, Tautges, T. J. "Generating Unstructured Reactor Core Meshes in Parallel." *23rd International Meshing Roundtable*.

2010 C.8 Tautges, T. J., **Jain, R.** "Creating Geometry and Mesh Models…". *19th International Meshing Roundtable*. **Best Paper Award**.

Selected Presentations

2024 **SC24** · Tutorial: UXarray for Analysis of Unstructured Climate Data
AMS Annual Meeting · UXarray: Extending Xarray with Support for Unstructured Grids

2023 **SciPy 2023** · UXarray for unstructured climate data
HDF User Group · Data reduction for FLASH-X simulations

Funding & Proposals

Active	**DOE SEATS** · Software Ecosystem for Advancing Climate Tools and Services
	NSF Raijin · Collaborative research in climate model analysis
Completed	**DOE ECP CANDLE** · Core contributor (2017–2023)
	DOE NEAMS · Principal Investigator for MeshKit (2009–2016)

Service & Mentorship

Professional Service

Panelist	5th Infraday Midwest Event ("Revolutionizing Public Infrastructure with AI")
Reviewer	Journal of Open Research Software, NumGrid, SBIR Funding Proposals
Committee	NumGrid 2020 Program Committee Member

Mentorship

Rylie Weaver	Research Aide (2022–2024) · IMPROVE project, HPO techniques
Aaron Zedwick	Student (2023–2024) · UXarray development
Mark Bartoszek	Systems Admin (2023) · Mentoring on systems administration