

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.

Professional Experience

- 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.
- 2007 - 2009 **Arizona State University**, Research and Teaching Assistant
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.
- 2006 - 2007 **Wipro Technologies**, Project Engineer
Bangalore, India
- 2005 **Tata Motors**, Engineering Intern
Pune, India

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

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| 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

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| 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

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| 2020 | University of Chicago M.S. in Computer Science |
| 2009 | Arizona State University M.S. in Structural Engineering |
| 2006 | Indian Institute of Technology (IIT), ISM Dhanbad B.Tech in Mechanical Engineering |

Honors and Awards

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| 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 |
| 2007 | Graduate Fellowship – Arizona State University |

Publications

Refereed Journal Articles

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| 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". <i>Briefings in Bioinformatics</i> (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." <i>Journal of Engineering with Computers</i> . |
| 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." <i>Journal of Simulation and Multi-disciplinary Design Optimization</i> . |

Refereed Conference Proceedings

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| 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." <i>Works Workshop</i> , SC25. |
| 2024 | C.5 | Jain, R. , Tang, H., Dhruv, A., Byna, S. "Enabling Data Reduction for Flash-X Simulations." <i>DRBSD-10 Workshop</i> , SC24. |
| | C.6 | Jain, R. , Wozniak, J.M., Partin, A., et al. "Cross-HPO: Optimizing Neural Networks for Cancer Drug Response." <i>CAFCW24 Workshop</i> , SC24. |
| 2014 | C.7 | Jain, R. , Tautges, T. J. "Generating Unstructured Reactor Core Meshes in Parallel." <i>23rd International Meshing Roundtable</i> . |
| 2010 | C.8 | Tautges, T. J., Jain, R. "Creating Geometry and Mesh Models...". <i>19th International Meshing Roundtable</i> . Best Paper Award . |

Selected Presentations

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| 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

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| 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

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| 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

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| 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 |