Rajeev Jain

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Experience

CASE Staff At-Large Sep 2023 – Present
The University of Chicago (UChicago) *Chicago, IL*

– Joint appointment supporting computational cancer research initiatives between Argonne National Laboratory (ANL) and UChicago.

Principal Specialist, Research Software Engineering (formerly Research Software Developer) Aug 2009 – Present
Mathematics and Computer Science Division, Argonne National Laboratory (ANL) *Lemont, IL*

– Contributed to five major projects across cancer data science, climate computation, multiphysics simulation, urban coupled simulations, and nuclear reactor modeling.

– Pursued high-performance computing challenges in diverse scientific domains; mentored junior researchers.

Research and Teaching Assistant Aug 2007 – Jul 2009
Structural Engineering, Arizona State University *Tempe, AZ*

– Enhanced blast-resistant structure design for the U.S. Army Research Office using FEM-based shape optimization.

Project Engineer May 2006 – Jun 2007
Wipro Technologies *Bangalore/Hyderabad, India*

– Developed production-ready code in Java and SAP; quickly adapted to large-scale software environments.

Major Projects

IMPROVE/CANDLE (Cancer Data Science - ECP) Jan 2017 – Present

– Lead developer of CANDLE/Supervisor, a scalable deep learning workflow suite on DOE supercomputers; awarded R&D 100 Award in 2023.

– Pioneered gene discovery method using noise injection and counterfactual analysis.

Uxarray (Climate Computation/Modeling - DOE) Jun 2021 – Present

– Co-created Uxarray, a performant Python library for unstructured grid analysis; enabled 60× speedups via vectorization and parallelization.

FLASH-X (Multiphysics Simulation, Astrophysics - ECP) Jun 2016 – Sep 2023

– Improved FLASH-X with HDF5 async I/O and SZ3/ZFP compression, achieving ¿20% performance gains; R&D 100 Award 2022.

– Architected a test and verification framework for composable physics solvers.

Urban Coupled Simulations (ECP Seed Funded) Jun 2016 – Sep 2018

– Led a cross-disciplinary team to build an urban climate simulation framework.

SIGMA/MeshKit/RGG (Nuclear Reactor Simulations - DOE NEAMS) Aug 2009 – Sep 2018

– Principal investigator for RGG/MeshKit, a toolkit for reactor mesh generation; commercialized via SBIR (Kitware, 2014–2017).

– Enabled parallel mesh generation for large-scale multiphysics simulations.

Technical Skills

HPC and Programming: Python, Fortran, C++; MPI, OpenMP, HDF5, parallel I/O, performance tuning on supercomputers.

ML and Data Tools: PyTorch, Keras, NumPy, Matplotlib, pandas, Scikit-learn, Jupyter; software engineering with Git, CI/CD.

Education

The University of Chicago — Chicago, IL
M.S. in Computer Science — *Jun 2020*

Arizona State University — Tempe, AZ
M.S. in Structural Engineering (Minor: Computer Science) — *Jul 2009*

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

Selected Publications

- **Jain, R.**, Eroglu, O., 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. *EGU General Assembly 2025*, Vienna, Austria, 27 Apr–2 May 2025, EGU25-13873. https://doi.org/10.5194/egusphere-egu25-13873
- Wozniak, J. M., **Jain, R.**, Balaprakash, P., Ozik, J., Collier, N. T., Bauer, J., Xia, F., Brettin, T., Stevens, R., & Mohd-Yusof, J. (2018). CANDLE/Supervisor: A workflow framework for machine learning applied to cancer research. *BMC Bioinformatics*, 19, 59–69. (Cited by 107). https://doi.org/10.1186/s12859-018-2056-3
- 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(2021), 20130381. (Cited by 79). https://doi.org/10.1098/rsta.2013.0381
- **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), 182–194. (Cited by 23). https://doi.org/10.1080/19401493.2020.1739106
- **Jain, R.**, Shah, A., Mohd-Yusof, J., Wozniak, J., Brettin, T., Xia, F., & Stevens, R. (2021). Probing decision boundaries in cancer data using noise injection and counterfactual analysis. *Computational Approaches for Cancer Workshop@ SC*. (Cited by 2). https://doi.org/10.1145/3489146.3492790
- **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. (Cited by 35).
  https://doi.org/10.1007/s00366-011-0221-4