Rajeev Jain

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Summary

- Research software engineer with 16+ years building scientific software across climate, cancer data science, multiphysics simulation, urban systems, and nuclear engineering.
- Focus: parallel I/O, profiling/optimization, reproducibility, and scalable pipelines; strong Python/C++ and HPC background.

Experience

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

- Built and maintained research software across UXarray, FLASH-X, CANDLE/IMPROVE, MeshKit/RGG, and urban simulation workflows.
- Implemented conservative zonal averaging in UXarray (PR #1345) and supported monthly PyPI releases for the package.
- Ran large-scale HPO workflows for CANDLE/IMPROVE; improved reproducibility and benchmarking pipelines.
- Delivered async HDF5 I/O and compression for FLASH-X; reduced I/O time in benchmarks (20%+).
- Work spans exascale-class systems, including the Aurora Accessory system.

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

- Joint appointment supporting computational cancer research.

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

- Researched FEM-based shape optimization for blast-resistant design and supported structural engineering courses.

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

- Developed production software in Java and SAP in large enterprise environments.

Selected Projects

UXarray (Climate Computing) 2021 – Present

- Co-created a Python toolkit for unstructured climate grids; focused on scalable analysis and conservative averaging.

FLASH-X (Multiphysics Simulation) 2016 – 2023

- Built async I/O and verification workflows; contributed to R&D 100 Award (2022).

CANDLE/IMPROVE (Cancer Data Science) 2017 – Present

- Standardized pipelines and HPO workflows for reproducible model evaluation.

MeshKit/RGG (Reactor Modeling) 2009 – 2018

- PI for NEAMS meshing; reduced reactor core modeling time from weeks to hours; SBIR commercialization with Kitware.

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*

Awards

- R&D 100 Awards: CANDLE/Supervisor (2023) and FLASH-X (2022).
- Best Paper, International Meshing Roundtable (2010).
- University Graduate Fellowship, Arizona State University (2007–2009).
- SBIR Phase I and II awards for RGG commercialization with Kitware (2014–2017).

Selected Publications

- UXarray: UXarray presentation and paper.
- FLASH-X: Paper 1 and Paper 2.
- CANDLE: CANDLE/Supervisor and Counterfactuals.
- Urban microclimate: Boundary conditions paper.

Technical Skills

HPC and Programming: Python, C++, Fortran; MPI, OpenMP, HDF5, parallel I/O, performance tuning.
ML and Data Tools: PyTorch, Keras, NumPy, pandas; Git, CI/CD.