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 areas: parallel input/output, profiling and optimization, reproducibility, scalable pipelines, and Python programming.
- Scope includes multi-institution projects, exascale-class systems, and software practices around testing, continuous integration, and releases.

Experience

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

- Built and maintained research software across UXarray, FLASH-X, Cancer Distributed Learning Environment (CANDLE) workflows, MeshKit, Reactor Geometry Generator, and urban simulation workflows.
- Implemented conservative zonal averaging in UXarray (pull request #1345) and contributed to regular Python Package Index releases.
- Ran large-scale hyperparameter optimization workflows for cancer data science projects; standardized reproducibility and benchmarking pipelines.
- Implemented asynchronous Hierarchical Data Format 5 (HDF5) input/output and compression for FLASH-X; reduced input/output time in benchmarks (20%+).
- Work spans exascale-class systems and large-scale workflows.

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

- Joint appointment supporting cancer and earth science research.

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

- Researched finite element method-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 enterprise resource planning systems in large enterprise environments.

Selected Projects

UXarray (Climate Computing) 2021 – Present

- Core contributor to a Python toolkit for unstructured climate grids; focused on scalable analysis and conservative averaging.

FLASH-X (Multiphysics Simulation) 2016 – 2023

- Built async input/output and verification workflows; contributed to Research and Development 100 Award (2022).

Cancer Data Science (CANDLE workflows) 2017 – Present

- Standardized pipelines and hyperparameter optimization workflows for reproducible model evaluation.

MeshKit and Reactor Geometry Generator (Reactor Modeling) 2009 – 2018

- Principal investigator for Nuclear Energy Advanced Modeling and Simulation meshing; reduced reactor core modeling time from weeks to hours; Small Business Innovation Research commercialization with Kitware.

Education

The University of Chicago Chicago, IL
Master of Science in Computer Science *Jun 2020*

Arizona State University Tempe, AZ
Master of Science in Structural Engineering (Minor: Computer Science) *Jul 2009*

Indian Institute of Technology Dhanbad Dhanbad, India
Bachelor of Technology in Mechanical Engineering *May 2006*

Awards

- Research and Development 100 (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).
- Small Business Innovation Research (SBIR) Phase I and II awards for Reactor Geometry Generator commercialization with Kitware (2014–2017).

Selected Publications

- UXarray: UXarray presentation and paper.
- FLASH-X: Paper 1 and Paper 2.
- CANDLE: Supervisor workflow and Counterfactual analysis.
- Urban microclimate: Boundary conditions paper.

Technical Skills

High-performance computing and programming: Python, C++, Fortran; Message Passing Interface (MPI), Open Multi-Processing (OpenMP), HDF5, parallel input/output, performance tuning.

Machine learning and data tools: PyTorch, Keras, NumPy, pandas; Git, continuous integration/continuous delivery.