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 (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.