

RAJEEV JAIN

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EDUCATION

M.S., Computer Science, Computer Science Department, **2020**
University of Chicago, IL, USA

M.S., Structural Engineering (Simulations), School of Sustainable Engineering and Built Environment, **2009**
Arizona State University ([ASU](http://www.asu.edu)), Tempe, AZ, USA

B.Tech, Mechanical Engineering, Department of Mechanical and Mining Machinery Engineering, **2006**
Indian Institute of Technology ([IIT-ISM](http://www.iit-sm.ac.in)), Dhanbad, JH, India

RESEARCH EXPERIENCE

Principal Software Development Specialist	Aug 2018-present
Software Development Specialist	Jan 2011-July-2018
Pre-doctoral Appointee	Aug 2009-Dec 2011

Mathematics and Computer Science Department, **Argonne National Laboratory** (ANL), Chicago

- **Feb2021-present: E3SM: Regression testing for tempestremap and its automation using GitHub actions.**
- **March2020-present:** Research on descriptors machine learning workflows for drug discovery of nCoV19.
- **June 2019-present: FLASH5:** Working on developing and maintaining FLASH5 and adding new functionality for systems exascale and beyond. <http://flash.uchicago.edu/site/>
- **May 2017-present: ECP CANcer Distributed Learning Environment (CANDLE) Project:** Develop hyper-parameter optimization workflows for deep learning cancer benchmarks. Run simulations on compute machines such as Summit, Theta, Cori and Titan.
- **Sept 2016-Sept 2019: Urban Exascale Compute Project:** Conduct bi-weekly meetings with 4 other labs, model and perform coupled urban atmosphere and building energy simulations
- **Oct 2017-present: Kitware SBIR (Phase II):** “DOE Web Based Nuclear Reactor Modeling”, Tailor RGG syntax and workflow for web and develop an algorithm for open-source quadrilateral meshing for reactor assemblies.
- **July 2017-Jan 2019: Radiasoft SBIR (Phase I):** “Multiphysics Design and Optimization of Complex Vacuum Chambers”. Use COMSOL/Matlab livelink to extract stiffness matrix to setup parallel solver and optimization.
- **Dec 2016-June 2019: Urban LDRD:** “An exascale application for simulating urban boundary layers”. Generated meshes and input decks for Nek5000 simulations for a few downtown Chicago city blocks.
- **Sept 2011-Sept 2016: PI-MeshKit:** Created reactor models for coupled-multiphysics simulations and designed/developed Reactor Geometry (& Mesh) Generator ([RGG](#)) tool for the DOE-NEAMS (Department of Energy project Nuclear Energy Advanced Modeling and Simulation (NEAMS) program

- C++ development and mesh generation for various projects in the [SIGMA](#) group, Collaborated with Kitware Inc. for the development of RGG GUI and [CMB](#), Ran large simulation (100k cores) of ALCF machines (Mira/Vesta/Blues etc.) and published the results.

Research Assistant

Jun 2007- Jul 2009

Structural and Computational Mechanics Lab., Arizona State University, Tempe

- **Thesis:** U.S. Army Research Office Project: ‘Blast Mitigation Solutions via FEM-Based Design Optimization’: wrote optimization code and performed parallel simulations for finding optimal shape. Advisor(s): [Dr. S.D. Rajan](#) (chair), [Dr. Gerald Farin](#) and [Dr. A.D. Belegundu](#)

TEACHING EXPERIENCE

Teaching Assistant

Jun 2007- Jul 2009

Structural Analysis and Design, Civil Engineering Department, Arizona State University, Tempe

INDUSTRY EXPERIENCE

Project Engineer

May 2006- May 2007

Wipro Technologies, Bangalore, India

Intern Engineer

Apr 2005-Jul 2005

Engineering Research Center, Tata Motors, Pune, India

HONORS AND AWARDS

- Invited to be a part of the committee for NumGrid 2020 conference 2020
- Session chair, for Computational Geometries session at the at the Joint International Conference on Mathematics and Computation, Supercomputing in Nuclear Application (SNA) and the Monte Carlo (MC) Method, Nashville TN. [MC2015](#) 2015
- [ATPESC](#) scholar world-class training for selected applicants on HPC and big data 2015
- Co-chair, Computer Science, Argonne/CSUI Undergraduate/Graduate Research Symposium 2011
- Best Paper in 2010 International Meshing Roundtable at Chattanooga, TN 2010
- University Graduate Fellowship for Two Consecutive Years at ASU 2007-2009
- Co-chair, Research in Interdisciplinary Science and Engineering (RISE), ASU 2007
- 1st Prize in MindAdvantage Technical Paper Presentation at Minda Ltd., New Delhi 2005
- 1st Prize for Low Budget Car Design Contest, IIT Kharagpur 2005
- Co-char, Society of Automotive Engineering (SAE), ISM Chapter 2003-2005
- Qualified IIT-JEE with All-India-Rank: 3487 out of 150,000 competitors (top 2%) 2002

PROFESSIONAL ACTIVITIES

- Registered mentor to ongoing college kids at <https://www.ustrive.com/> 2020-
- Program Committee Member and Reviewer, NumGrid ([link](#)) 2020
- PI MeshKit NEAMS 2011-2016
- Supervisor – [Evan Vanderzee](#) (25%, ANL, MeshKit, triangle/quad mesh development) 2014-pre
- Supervisor – David Holler (Summer student, Nek5000/MOAB), Penn State University 2015
- Supervisor – Brett Rhodes (Summer student, Reactor meshing), Edinboro University 2003
- Member American Nuclear Society 2012-2016
- Reviewer, SBIR (Small Business Funding Proposals) 2015
- Reviewer, Computational Geometries, SNA and MC conference 2015-pre
- Mentor, School kids with STEM Mentoring Cafe 2015-pre
- Reviewer, International Meshing Roundtable 2012-pre

REFREED JOURNAL ARTICLES

1. Goldring, Nicholas, Bruhwiler, David, Nash, Boaz, Wu, Zhigang, Nagler, Robert, Carter, Jason, Lerch, Jason, Suthar, Kamlesh, Den Hartog, Patric, Jain, Rajeev, and Mahadevan, Vijay. Multiphysics Design and Optimization of Complex Vacuum Chambers. United States: N. p., 2020. Web. doi:10.2172/1635367.
2. R. Jain, X. Luo, G. Sever, T. Hong and C. Catlett. "Representation and Evolution of Urban Microclimate Boundary Conditions in Downtown Chicago," *Journal of Urban Building Energy Modeling*, November 2018 [link](#).
3. J. Wozniak, R. Jain, P. Balaprakash, J. Ozik, N. Collier, J. Bauer, F. Xia, T. Brettin, R. Stevens, J. Yusof, C. Cardona, B. Essen and M. Baughman. "CANDLE/Supervisor: A Workflow Framework for Machine Learning Applied to Cancer Research," Open Access BMC Supplement, Dec 2018. [link](#).
4. V. Mahadevan et al. "High-Resolution Coupled Physics Solvers for Analysing Fine-Scale Nuclear Reactor Design Problems," *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 372(2014), 20130381.
5. T. J. Tautges and R. Jain, "Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach," *Engineering with Computers*, 28 (4) 319-329, 2011.
6. V. Argod et al, "MPI-enabled Shape Optimization of Panels Subjected to Dynamic Loading," *Journal of Simulation and Multidisciplinary Design Optimization*, 2, 273-282, 2009.

7. REFREED CONFERENCE PROCEEDINGS

1. **Jain, R.**, Shah Ashka, Mohd-Yosuf, J., Wozniak, J.W., Xia, F., Brettin, T. and Stevens, R., "Probing Decision Boundaries in Cancer Data Using Noise Injection and Counterfactual Analysis", Submitted to *Seventh Computational Approaches for Cancer Workshop (CAFCW21)*, part of *Super-Computing 2021*.
2. **Jain, R.**, Chawdary, S., Weide, K. and Klosterman, T., "Checkpoint/Restart for Lagrangian particle mesh with AMR in community code FLASH-X. *SuperCheck'21, First International Symposium on Checkpointing for Supercomputing*, 2021. <https://arxiv.org/abs/2103.04267>
3. Harris JA, Chu R, Couch SM, et al. Exascale models of stellar explosions: Quintessential multi-physics simulation. *The International Journal of High Performance Computing Applications*. July 2021. doi:[10.1177/10943420211027937](https://doi.org/10.1177/10943420211027937)
4. Jacob, R. L., Sever, G., Obabko, A., Jain, R., and Catlett, C. E., "CFD simulations of flow in realistic urban geometries initialized from weather models", vol. 2019, Dec 2019.
5. Obabko, A., Sever, G., Jain, R., et al. \ 2019, APS Division of Fluid Dynamics Meeting Abstracts
6. G Sever, A Obabko, R Jacob, R Jain, C Catlett - 18th Conference on Mesoscale Processes, 2019
7. J. Wozniak, R. Jain, P. Balaprakash, J. Ozik, N. Collier, J. Bauer, F. Xia, T. Brettin, R. Stevens, J. Yusof, C. Cardona, B. Essen and M. Baughman. "CANDLE/Supervisor: A Workflow Framework for Machine Learning Applied to Cancer Research," in *SCI7, Computational Approaches for Cancer Workshop*.
8. R. Jain, V. S. Mahadevan, R. O'bara. "Simplifying Workflow for Reactor Assembly and Full-Core Modeling," *Proceedings of Joint International Conference on Mathematics and Computation, Super Computing in Nuclear Applications and the Monte Carlo Method*, ANL/MCS-P5054-1213, Nashville. 2015.
9. R. Jain and T. J. Tautges, "Generating Unstructured Reactor Core Meshes in Parallel," *Proceedings of the 23rd International Meshing Roundtable*. Oct 2014. ANL/MCS-P4092-0713.

10. R. Jain, and T. J. Tautges, "[PostBL](#): Post-Mesh Boundary Layer Generation Tool," *22nd International Meshing Roundtable* (pp. 445-464), Oct 2013. ANL/MCS-P4092-0713.
11. R. Jain and T. J. Tautges, "*Parallel Reactor Geometry (and Mesh) Generator*," International Congress on the Advances in Nuclear Power Plants (ICAPP), June 2012.
12. S. Mohanty, R. Jain, S. Majumdar, T. J. Tautges, and M. Srinivasan, "*Coupled Field-Structural Analysis of HTGR Fuel Brick Using Abaqus*," International Congress on the Advances in Nuclear Power Plants, 2012.
13. T. J. Tautges, Alvaro Caceras, R. Jain, Hong Jun Kim, Jason Kraftcheck and Brandon M Smith, "Coupled Multi-Physics Simulation Frameworks for Reactor Simulation: A Bottom-Up Approach," in *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, May 2011.
14. T. J. Tautges and R. Jain, "Creating Geometry and Mesh Models for Nuclear Reactor Core Geometries Using a Lattice Hierarchy-Based Approach," *Proceedings of the 19th International Meshing Roundtable*, Springer Berlin Heidelberg, 2010, pp. 351-365. [link](#)

REPORTS

1. Nicholas Goldring, David Bruhwiler, Boaz Nash, Zhigang Wu, Robert Nagler, Jason Carter, Jason Lerch, Kamlesh Suthar, Patric Den Hartog, Rajeev Jain, Vijay Mahadevan. "*Multiphysics Design and Optimization of Complex Vacuum Chambers*", June 30th 2020
2. F. Xia, P. Balaprakash, H. Yoon, B. VanEssen, A. Partin, T. Brettin, A. Ramanathan, J. Mohd-Yusof, J. Wozniak, J. Ozik, N. Collier and R. Jain. "*CANDLE version 0.1*", Technical Report to ECP, March. 2019.
3. F. Xia, P. Balaprakash, H. Yoon, B. VanEssen, A. Partin, T. Brettin, A. Ramanathan, J. Mohd-Yusof, J. Wozniak, J. Ozik, N. Collier and R. Jain. "*CANDLE workflow and higher level support library version 0.1*", Technical Report to ECP, Dec. 2018.
4. R. Jain, G. Sever, A. Obabko, and C. Catlett, "*Quantify Data Exchange and Model Performance Impact for simple couplings between EnergyPlus and Nek5000*", June. 2019.
5. G. Sever, R. Jain, C. Catlett, R. Jain, R. Jacob, NVIDIA Corporation: Jeff Adie, Stan Posey, Jeff Larkin "*WRF Benchmarking on Summit*" Technical Report to ECP, Oct. 2019.
6. G. Sever, R. Jain, C. Catlett, R. Jain, R. Jacob, "*Test GPU version of WRF; Test and optimize boundaries and timescale parameters for Nek5000 and evaluate correctness of Nek5000/RANS tests*," Technical Report to ECP, June. 2019.
7. C. Catlett, R. Jain, R. Jacob, R. Muehleisen, T. Hong, X. Luo, B. Bhaduri, J. Sanyal, M. Allen, "*Key Performance Parameters for Urban ECP Applications*," Technical Report to ECP, Mar. 2018.
8. C. Catlett, R. Jain, R. Jacob, R. Muehleisen, T. Hong, X. Luo, B. Bhaduri, J. Sanyal, M. Allen, "*Key Performance Parameters for Urban ECP Applications*," Technical Report to ECP, Mar. 2018.
9. C. Catlett, R. Jain, R. Jacob, R. Muehleisen, T. Hong, X. Luo, B. Bhaduri, J. Sanyal, M. Allen, "*Coupled Model Data Exchange Hub: A Notional Architecture*," Milestone Report to ECP, June 2017.
10. C. Catlett, R. Jain, R. Jacob, R. Muehleisen, T. Hong, X. Luo, B. Bhaduri, J. Sanyal, M. Allen, "*Part 2: Data Flow Characteristics for Coupled Urban Models: Exploring Urban Atmosphere and Building Energy Demand*," Q2-Q3 Report to ECP, Mar. 2017.

11. C. Catlett, R. Jain, R. Jacob, R. Muehleisen, T. Hong, X. Luo, B. Bhaduri, J. Sanyal, M. Allen, “*Part 1: Data Flow Characteristics for Coupled Urban Models: Exploring Urban Atmosphere and Building Energy Demand*,” Q1 Report to ECP, Dec. 2017.
12. R. Jain, E. Vanderzee, I. Grindeanu, V. Mahadevan, “*Mesh Generation and Algorithm Development for NEAMS*,” based on MeshKit v1.42 release, report to Nuclear Energy Advanced Modeling and Simulation program directors, ANL-P60660916. Sept. 2016.
13. E. Merzari, E. Shemon, Y. Yu, J. Thomas, A. Obabko, R. Jain, V. Mahadevan, J. Solberg, R. Ferencz, R. Whitesides, “*Full Core Multiphysics Simulation with Offline Mesh Deformation*,” report to Nuclear Energy Advanced Modeling and Simulation program directors, ANL/NE-15/42. Dec. 2015.
14. R. Jain and Vijay Mahadevan, “*2014 MeshKit Release*,” based on MeshKit v1.2 release, report to Nuclear Energy Advanced Modeling and Simulation program directors, ANL/MCS-TM/344. Sept. 2014.
15. E. Merzari et al, “*Multi-Physics Demonstration Problem with the SHARP Reactor Simulation Toolkit*,” Mar. 2014.
16. R. Jain and T. J. Tautges, “*MeshKit*, based on MeshKit v1.0 release, report to Nuclear Energy Advanced Modeling and Simulation program directors, ANL/MCS-TM/336. Sept. 2013.
17. T. J. Tautges, P. F. Fischer, I. Grindeanu, R. Jain, V. Mahadevan, A. V. Obabko, M. A. Smith, E. Merzari, R. Ferencz, “*SHARP Assembly-Scale Multiphysics Demonstration Simulations*,” Report to Nuclear Energy Advanced Modeling and Simulation program directors, ANL/MCS-NE-13-9. Mar. 2013
18. A. Bingham, J. Ortensi, R. Jain, I. Grindeanu, and T. Tautges. “*SHARP/PRONGHORN*,” INL/EXT-12-27171, June 2012.
19. T. J. Tautges, P. Fischer, I. Grindeanu, R. Jain, V. Mahadevan, A. Obabko, M. A. Smith, S. Hamilton, K. Clarno, M. Baird, M. Berrill, “*A Coupled Thermal/Hydraulics – Neutronics – Fuel Performance Analysis of an SFR Fuel Assembly*,” Report to US DOE, Reactor Campaign, Apr. 2012.
20. T. Tautges and R. Jain, “*Extensions to MeshKit and RGG*,” Report to US DOE, Reactors Campaign, ANL/MCS-TM316, Oct. 2011.
21. T. Tautges and R. Jain, “*Mesh Copy/Move/Merge Tool for Reactor Simulation Applications*,” Report to US DOE, Reactor Campaign, ANL/MCS-P1773-0610, Apr. 2010.

PRESENTATIONS AND POSTERS

1. Jain, R., Mohd-Yosuf, J., Wozniak, J.W., Xia, F., Brettin, T. and Stevens, R., “Training Data Error Impacts on Deep Neural Networks for Classifying RNA-seq Gene Expressions”, Poster SC20
2. Rajeev Jain, “Migrating your DNN to CANDLE”, CANDLE + ExaLearn workshop, Argonne IL, October 19, 2018
3. Jeff Adie, Gökhan Sever, Rajeev Jain, and Stan Posey, GPU performance study for the WRF model on the Summit supercomputer. Podium presentation at the 2019 Joint WRF/MPAS Users’ Workshop, Boulder, CO, June 2019
4. Gökhan Sever, Rob Jacob, Rajeev Jain, Aleks Obabko, Rao Kotamarthi, and Charlie Catlett, Sensitivity experiments of urban canopy parameterizations using ensemble WRF simulations over the Chicago metropolitan. Poster presentation at the 2019 Joint WRF/MPAS Users’ Workshop, Boulder CO, June 2019

5. Aleksandr Obabko, Gökhan Sever, Rajeev Jain, Yu-Hsiang Lan, Paul Fischer, Haomin Yuan, Robert Jacob, Charlie Catlett, Misun Min, “Nek5000 LES of realistic urban geometries initialized from weather models”, Bulletin of the American Physical Society, Aug. 2019
6. MP Silva, A Sharma, M Budhathoki, R Jain, CE Catlett, Neighborhood scale heat mitigation strategies using Array of Things (AoT) data in Chicago, AGU Fall Meeting Abstracts, Dec. 2018.
7. C. Catlett, R. Jain, R. Jacob, A. Obabko, R. Jacob, J. Sanyal, M. Allen, T. Hong and X. Luo, “*Urban ECP Review: Plan for Urban Exascale Simulations 2018 and Beyond*”, at the University of California, Berkeley, Aug. 2018.
8. A. Obabko, R. Jain, R. Jacob, R. Paoli, G. Sever, I. Grindeanu, and P. F. Fischer, “*Nek5000 Wall-Resolved LES for Urban Geometries*” at the 10th International Conference on Urban Climate, New York, NY, Aug. 2018.
9. Gökhan Sever, R. Jacob, R. Jain, A. Obabko, C. Catlett, “*Mesoscale to Microscale Weather Simulations over the Chicago Downtown*”, at the 10th International Conference on Urban Climate, New York, NY, Aug. 2018.
10. Poster: “*Overview of the Urban Exascale Project*”. ECP Annual PI Meeting, Knoxville, TN. Feb. 2018.
11. Poster: “*Components of Urban Exascale Simulations*”. ECP Annual PI Meeting, Knoxville, TN. Feb. 2018.
12. R. Jain, “Urban Coupled Simulations”, CODAR Workshop, at the 2nd Exascale Computing Meeting, Knoxville, TN. Feb. 2018.
13. R. Jain, “*Developing the Metropolitan Systems Energy and Economic Dynamics (Metro-SEED) Modeling Framework*,” at the Workflows Session, 2nd Annual ECP Meeting, Knoxville, TN, Feb. 2018
14. R. Jain, “*Urban Atmosphere Simulations*,” at the Urban ECP Breakout Session, 2nd Annual ECP Meeting, Knoxville, TN, Feb. 2018
15. R. Jain, “*Coupled Urban Systems Hub Design*,” Poster at Exascale Compute Project 2nd Annual Meeting, Knoxville, TX, Feb. 2018.
16. R. Jain, “*Multi-scale Coupled Urban Systems*,” Poster at Exascale Compute Project Annual Meeting, Knoxville, TX, Jan. 2017.
17. R. Jain, “*MeshKit and RGG Training*,” at Nuclear Engineering Div., University of Florida, Feb. 2017.
18. R. Jain, “*Multi-scale Coupled Urban Systems*,” at Argonne ECP Town hall Meeting, Argonne National Lab, Jan. 2017.
19. R. Jain, “*MeshKit Release v 1.3*,” at NEAMS PI Meeting, Washington D.C., Dec. 2015.
20. R. Jain, N. Ray, I. Grindeanu, D. Wu and V. S. Mahadevan, “*Scalable Mesh Generation for HPC Applications*,” Poster in Proceedings of SC15, Austin, TX, Nov. 2015.
21. R. Jain, “*RGG Training*,” at Nuclear Energy Division, Argonne National Lab, June 2014.
22. R. Jain, “*MeshKit Training*,” Oak Ridge National Laboratory, Mar. 2014.
23. Presentation and article by Kitware Inc.: <http://www.kitware.com/source/home/post/146>.
24. R. Jain, “*RGG and MeshKit Progress Report*,” at NEAMS PI Meeting, Washington D.C. Dec. 2013.

25. R. Jain, T. Tautges, I. Grindeanu, C. Verma, S. Cai, and S. Mitchell, “*MeshKit: An Open-Source Library for Mesh Generation and Meshing Algorithm Research*,” In Symposium on Trends in Unstructured Mesh Generation, 12th U.S. National Congress on Computational Mechanics, 2013. Raleigh, NC. July 2013.
26. R. Jain, “*Parallel Reactor Geometry Generator*,” Postdoctoral Research Symposium, Argonne National Lab. Oct. 2013.
27. R. Jain, “*MeshKit and RGG Toolkit*,” invited Presentation at Nuclear Engineering Division, Oak Ridge National Laboratory, Nov. 2011.
28. R. Jain, “*Parallel Reactor Geometry Generator*,” at the Postdoctoral Research Symposium, Argonne National Laboratory, Oct. 2011.
29. R. Jain, “*MeshKit*,” at Annual NEAMS PI Meeting, Argonne National Laboratory, APS Auditorium, Oct. 2011.
30. R. Jain and S. Rajan, “*Blast Mitigation via FEM-Based Design Optimization*,” in Proceedings of 11th US National Congress on Computational Mechanics, July 2011.
31. R. Jain, T. J. Tautges and J. Thomas, “*Tools to Generate Large Reactor Core and Geometry Meshes*,” at Student Poster Competition, 11th US National Congress on Computational Mechanics, July 2011.
32. R. Jain and T. J. Tautges, “*RGG: A Tool for Generating Reactor Core Models*,” Poster at VHTR Technology Development Office 4th Annual Technical Review Meeting 2011, Albuquerque, New-Mexico. April 2011.
33. R. Jain and H. J. Kim, ANL Summer Student Lecture Series, “*Mesh Generation for Scientific Computing*,” June 2010.
34. R. Jain, “*Cubic Bezier Velocity Field for Shape Optimization and Unit-Cell Based Regression Model of Sandwich Honeycomb Panels*,” at the Structural and Computational Mechanics Lab., ASU, July 2008.
35. R. Jain, N. Modi, K. Tawar and S. Malhotra, “Phoenix: Low Budget Car Design,” All-India Technical Festival Presentation for Car Design Contest Sponsored by IBM and Tata Motors at IIT Kharagpur, Sept. 2004.

FUNDING

- E3SM (Feb 2021-present): Role: Developer.
- ECP CANDLE project (2017-present) *Role: Workflow Development and Testing.*
- FLASH-X (2021-present) Role: Developer.
- Urban Exascale Compute Project –(\$300k-\$1.5M) SEED project (2016-present). *Role: Lead – Urban Atmosphere Simulations.* Supporting PI: Charlie Catlett, I was tasked with managing this multi-lab project.
- \$75k (2 years) D. Thompson, P. O'leary, R. O'bara, and R. Jain, ‘*DOE Web Based Nuclear Energy*’, Phase IIB SBIR (Oct 1st, 2017 – present) *Role: Co-PI.*
- NEAMS Integration and Reactor Product Line (Meshing) – 500k+ (2011-2016). *Role: PI: NEAMS-Mesh Generation*
- Urban LDRD: “An Exascale Application for Simulating Urban Boundary Layers” (2017-pre). *Role: Member*

