Curriculum Vitae

Jaideep Ray, Distinguished Member of the Technical Staff
Quantitative Modeling & Analysis, Sandia National Laboratories
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Education

Ph.D. in Mechanical and Aerospace Engineering, Rutgers, the State University of New Jersey, October 1999.

M.S. in Mechanical and Aerospace Engineering, Rutgers, the State University of New Jersey, January 1997.

B. Tech. in Aerospace Engineering, Indian Institute of Technology, Kharagpur, West Bengal, India. June 1992.

Experience

2013 – present	Distinguished Member of Technical Staff, Sandia National Laboratories.
2004 – 2013	Principal Member of Technical Staff, Sandia National Laboratories.
2000 – 2004	Senior Member of Technical Staff, Sandia National Laboratories.
1999 – 2000	Limited Term Member of Technical Staff, Sandia National Laboratories.
1993 – 1999	Graduate Research Assistant, Rutgers, the State University of New Jersey.
1992 – 1993	Hydraulics Design Engineer, Eicher Tractors, India.

Research Interests

- Bayesian inverse problems, as applied to estimation of multiscale fields.
- Higher-order numerical methods for PDE solutions on adaptively refined meshes.
- Computational and theoretical fluid mechanics, with emphasis on compressible and reactive flows.
- Parallel computing and component-based design of scientific simulation software

Research Projects, Contracts and Grants (as PI)

1. "Conditioning multi-model ensembles for disease forecasting", funded by DoD/Defense Threat Reduction Agency, October 2016 – September 2018.
2. "A scalable multi-chain MCMC method for high-dimensional statistical inverse problems", funded by Office of Science, Advanced Scientific Computing Research, over September 2013 – August 2016.

3. "Evaluating time-series analyses of event-based public health surveillance", US Department of Defense / Defense Intelligence Agency / National Center for Medical Intelligence, over January 2012 – December 2012.

4. "Biosurveillance of Partially Observed Epidemics", funded by US Department of Defense/Defense Threat Reduction Agency. Sandia PI of a joint proposal with Applied Research Associates (PI: Ms. K. Cheng), over June 2009 – May 2012.

5. "Epidemic Evolution Simulations", funded by Department of US Defense/Defense Threat Reduction Agency. Sandia PI of a subcontract from Applied Research Associates (PI: G. McClellan), in 2008.

6. "Online mapping and forecasting of epidemics using open-source data", Laboratory Directed Research & Development, over October 2013 – September 2016.

7. "Kalman-Filtered Compressive Sensing for High Resolution Estimation of Anthropogenic Greenhouse Gas Emissions from Sparse Measurements", Laboratory Directed Research & Development, October 2010 – September 2013.

8. "Bayesian Data Assimilation for Stochastic Multiscale Models of Transport in Porous Media", Laboratory Directed Research & Development, October 2008 – September 2011.

9. "Risk-based decision making for staggered bioterrorist attacks: Resource allocation and risk reduction in reload scenarios", Laboratory Directed Research & Development, over October 2007 – September 2009.

10. "Distributed Micro-releases of Bioterror Pathogens: Threat Characterization and Epidemiology from Uncertain Patient Observables", Laboratory Directed Research & Development, over October 2005 – September 2008.

Research Projects, Contracts and Grants (as a team member)

1. "Climate Science for a Sustainable Energy Future", funded by the US Department of Energy, Biological and Environmental Research Office. PI: Dr. D. C. Bader, Oak Ridge National Laboratory, Oak Ridge, TN, USA. July 2011 – September 2015.

2. "Scalable Methods for Representing, Characterizing and Generating Large Graphs", funded by the US Department of Energy, Advanced Scientific Computing Research Office. PI: Dr. A. Pinar, Sandia National Laboratories, Livermore, CA, USA. October 2009 – September 2012.

3. "Computational Facility for Reacting Flow Science", funded by the US Department of Energy, under the SciDAC (Scientific Discovery through Advanced Computing) program. PI: Dr. H. Najm, Sandia National Laboratories, Livermore, CA, USA. October 2001 – September 2011.

4. "The Center for Component Technology for Terascale Simulation Software", US Department of Energy, under the SciDAC program. PI: Dr. R. Armstrong, Sandia National Laboratories, Livermore, CA, USA. October 2001 – September 2006.

5. "Autonomic Component Framework for Grid Applications", funded by the US National Science Foundation, under the New Generation Software program. PI: Prof. M. Parashar, Rutgers, The State University of New Jersey, Piscataway, NJ, USA. October 2003 – September 2006.

Activities and Awards

- Reviewer, *Phys. Fluids*, *Combustion Theory and Modeling*, *IEEE - Computer Science*, *SIAM Journal on Scientific Computing*, *Epidemiology*, *Public Library of Science* & *Proc. Combust. Inst.*
- Reviewer, *California Energy Commission* & *National Science Foundation.*
- Serving on organizational committees to identify technical needs/gaps in data analytics and develop programs to bridge them.
- Awards for the authorship, release and maintenance of software packages, some of them open-source (http://www.sandia.gov/∼jairay/software.html).
- Best paper award in the "Runtime Systems" category at the 15^{th} IASTED International Conference on Parallel and Distributed Computing and Systems 2003 (PDCS03).
- 2-year Excellence Fellowship awarded by the Dept. of Mech. & Aero. Engg., Rutgers University, NJ, in July 1993 for pursuing an M.S.
- Institute Silver Medal, awarded by the Indian Institute of Technology, Kharagpur, August 1992.

Open-Source Software

- **sparse-msrf: A package for sparse modeling and estimation of fossil-fuel CO2 emission fields**, distributed under BSD license at http://www.sandia.gov/∼jairay. Accompanying theory in Ray et al, Geoscientific Model Development, 7, 1901-1918, 2014.
- **graphMC: A package for testing the independence of graphs**, distributed under BSD license at http://www.sandia.gov/∼jairay. Accompanying theory in Ray et al, Journal of Complex Networks, 2014.
- **HODIF**, a library for **H**igh-**O**rder **D**iscretizations, **I**nterpolations and **F**ilters, distributed under BSD license at http://www.sandia.gov/∼jairay. Accompanying theory in Ray et al, SIAM J. Scientific Computing, 2007, 29(1):139-181.
- **WMDDAC**, a distributed, interactive game for the simulating bioattacks, response and decision support. The package is Sandia-proprietary software. My contribution was in epidemiological modeling.

Books and Journal Publications

A full list of publications, including presentations and technical reports, can be viewed at http://www.sandia.gov/∼jairay. Citation statistics are at http://scholar.google.com/citations?hl=en&user=ojCQQn4AAAAJ

1. V. Yadav, A. M. Michalak, **J. Ray** and Y. P. Shiga, "A statistical approach for isolating fossil fuel emissions in atmospheric inverse problems", *Journal of Geophysical Research - Atmospheres*, 121, 2016.

2. M. Huang, **J. Ray**, Z. Hou, H. Ren, Y Liu and L. Swiler, "On the applicability of surrogate-based MCMC-Bayesian Inversion to the Community Land Model: Case studies at flux tower sites", *Journal of Geophysical Research - Atmospheres*, 121(13), 2016.

3. P. Stradzins, B. Harding, C. Lee, J. R. Mayo, **J. Ray** and R. C. Armstong, "A robust technique to make 2D advection solver tolerant to soft faults", *Procedia Computer Science*, 80:1917-1926, 2016.

4. **J. Ray**, S. Lefantzi, S. Arunajatesan and L. Dechant, "Bayesian parameter estimation of a k-epsilon model for accurate jet-in-crossflow simulations", *American Institute of Aeronautics and Astronautics Journal*, 54(8):2432-2448, 2016.

5. **J. Ray**, J. Lee, V. Yadav, S. Lefantzi, A.M. Michalak, and B. van Bloemen Waanders, "A sparse reconstruction method for the estimation of multi-resolution emission fields via atmospheric inversion", *Geoscientific Model Development*, 8, 1259-1273, doi:10.5194/gmd-8-1259-2015, 2015.

6. K. Carlberg, **J. Ray** and B. van Bloemen Waanders, "Decreasing the temporal complexity for nonlinear, implicit reduced-order models by forecasting", *Computer Methods in Applied Mechanics and Engineering*, 289(0):79-103, 2015.

7. **J. Ray**, Z. Hou, M. Huang, K. Sargsyan and L. Swiler, "Bayesian calibration of the Community Land Model using surrogates", *SIAM Journal on Uncertainty Quantification*, 3(1):199-233, 2015.

8. **J. Ray**, A. Pinar and C. Seshadhri, "A stopping criterion for Markov chains when generating independent random graphs", *Journal of Complex Networks*, 3(2):204-220, 2015.

9. **J. Ray**, V. Yadav, A. M. Michalak, B. van Bloemen Waanders and S. A. McKenna, "A multiresolution spatial parameterization for the estimation of fossil-fuel carbon dioxide emissions via atmospheric inversions", *Geoscientific Model Development*, 7, 1901-1918, 2014.

10. K. Kedia, C. Safta, **J. Ray**, H. N. Najm and A. F. Ghoniem, "A second-order coupled immersed boundary-SAMR construction for chemically reacting flow over heat-conducting Cartesian grid-conforming solid", *Journal of Computational Physics*, 272:408–428, 2014.

11. K. Cheng, D. Crary, **J. Ray** and C. Safta, "Structural models used in real-time biosurveillance: Outbreak detection and outbreak curve isolation from noisy background morbidity levels", accepted September 2012, *Journal of the American Medical Informatics Association*.

12. **J. Ray**, S. A. McKenna, B. van Bloemen Waanders and Y. M. Marzouk, "Bayesian reconstruction of binary media with unresolved fine-scale spatial structures", in *Advances in Water Resources*, 44:1-19, 2012.

13. S. A. McKenna, **J. Ray**, Y. Marzouk and B. van Bloemen Waanders, "Truncated multiGaussian fields and effective conductance of binary media", in *Advances in Water Resources*, 34:617-626, 2011.

14. **J. Ray**, Y. M. Marzouk, and H. N. Najm, "A Bayesian approach for estimating bioterror attacks from patient data", in *Statistics in Medicine*, 30(2):101-126, 2011.

15. **J. Ray**, R. Armstrong, C. Safta, B.J. Debusschere, B. A. Allan and H. N. Najm, "Computational frameworks for advanced combustion simulations", in *Turbulent Combustion Modeling: Advances, New Trends and Perspectives*, T. Echekki and E. Mastorakos, Eds, pgs 407-437, Springer, 2011.

16. C. Safta, **J. Ray** and H. N. Najm, "A high-order low-Mach AMR construction for chemically reacting flows", in *Journal of Computational Physics*, 229:9299-9322, 2010.

17. N. Trebon, A. Morris, **J. Ray**, S. Shende and A. D. Malony, "Performance modeling of component assemblies", *Concurrency and Computation: Practice and Experience*, 2007, 19(5):685-696.

18. **J. Ray**, C. A. Kennedy, S. Lefantzi and H. N. Najm, "Using high-order methods on adaptively refined block-structured meshes - derivatives, interpolations, and filters", *SIAM Journal on Scientific Computing*, 2007, 29(1):139-181.

19. J. C. Lee, H. N. Najm, S. Lefantzi, **J. Ray** and M. Frenklach, M. Valorani and D. Goussis, "A CSP and tabulation based adaptive chemistry model", *Combustion Theory and Modeling*, 2007, 11(1):73-102.

20. David E. Bernholdt, Benjamin A. Allan, Robert Armstrong and Felipe Bertrand, Kenneth Chiu, Tamara L. Dahlgren, Kostadin Damevski, Wael R. Elwasif, Thomas G. W. Epperly, Madhusudhan Govindaraju, Daniel S. Katz, James A. Kohl, Manoj Krishnan, Gary Kumfert, J. Walter Larson, Sophia Lefantzi, Michael J. Lewis Allen D. Malony, Lois C. McInnes, Jarek Nieplocha, Boyana Norris, Steven G. Parker, **Jaideep Ray**, Sameer Shende, Theresa L. Windus, and Shujia Zhou, "A component architecture for high-performance scientific computing", *International Journal of High-Performance Computing Application*, 2006, 20:162-202.

21. J. Steensland and **J. Ray**, "A partitioner-centric model for SAMR partitioning trade-off optimization : Part I", *International Journal of High Performance Computing Applications*, 2005, 19(4):409-422.

22. L. C. McInnes, B. A. Allan, R. Armstrong, S. J. Benson, D. E. Bernholdt, T. L. Dahlgren, L. F. Diachin, M. Krishnan, J. A. Kohl, J. W. Larson, S. Lefantzi, J. Nieplocha, B. Norris, S. G. Parker, **J. Ray** and S. Zhou, "Parallel PDE-based simulations using the Common Component Architecture". Chapter in *Numerical Solution of Partial Differential Equations on Parallel Computers*, 2005. Editors: A. M. Bruaset, P. Bjorstad, and A. Tveito, Lecture Notes in Computational Science and Engg., (51), Springer.

23. S. Lefantzi, **J. Ray**, C.A. Kennedy and H.N. Najm, "A component-based toolkit for simulating reacting flows with high order spatial discretizations on structured adaptively refined meshes". *Progress in Computational Fluid Dynamics: An International Journal*, 2005, 5(6):298-315.

24. **J. Ray** and L. Jameson, "Estimation of shock induced vorticity on irregular gaseous interfaces : A wavelet-based approach". *Shock Waves : An International Journal*, 2005, 14(3):147-160.

25. A. Malony, S. Shende, N. Trebon, **J. Ray**, R. Armstrong, C. Rasmussen and M. Sottile, "Performance technology for parallel and distributed component software". *Concurrency and Computation: Practice and Experience*, 2005, 17(2–4):117-141.

26. C. C. Douglas, J. Hu, **J. Ray**, D. T. Thorn, and R. Tuminaro, "Cache aware multigrid for variable coefficient elliptic problems on adaptive mesh refinement hierarchies", *Numerical Linear Algebra and Applications*, 2004, 11:173-187.

27. B.A. Allan, R.C. Armstrong, A.P. Wolfe, **J. Ray**, D.E. Bernholdt and J.A. Kohl, "The CCA core specification in a distributed memory SPMD framework", *Concurrency: Practice and Experience*, 2002, 14(5):323-345.

28. **J. Ray**, H.N. Najm, R.B. Milne, K.D. Devine and S. Kempka, "Triple flame structure and dynamics at the stabilization point of an unsteady lifted jet diffusion flame", *Proc. Combust. Inst*, 2000, 28(1):219-226.

29. A. D. Kotelnikov, **J. Ray** and N. J. Zabusky, "Vortex morphologies on re-accelerated interfaces: visualization, quantification and modeling of one- and two-mode compressible and incompressible environments", *Phys. Flds*, 2000, 12(12):3245-3264.

30. **J. Ray**, R. Samtaney and N. J. Zabusky, "Shock interaction with heavy gaseous elliptic cylinders: Two leeward side shock competition modes and a heuristic model for interfacial circulation deposition at early times", *Phys. Flds.*, 2000, 12(3):707-716.

31. R. Samtaney, **J. Ray** and N. J. Zabusky, "Baroclinic circulation generation on shock accelerated slow/fast gas interfaces", *Phys. Flds.*, 1998, 10(5):1217-1230.

Refereed Conference Publications

1. **J. Ray**, S. Lefantzi, S. Arunajatesan and L. Dechant, "Bayesian calibration of a RANS model with a complex response surface - A case study with jet-in-crossflow configuration", 45th AIAA Fluid Dynamics Conference, Dallas, TX, June 22-26, 2015. Conference paper: AIAA-2015-2784.

2. **J. Ray**, S. Lefantzi, S. Arunjatesan and L. Dechant, "Bayesian calibration of a k-e turbulence model for predictive jet-in-crossflow simulations", 44th AIAA Fluid Dynamics Conference, Atlanta, GA, June 16-20, 2014.

3. **J. Ray**, Ali Pinar and C. Seshadhri, "Are we there yet? When to stop a Markov chain while generating random graphs", 9th Workshop on Algorithms and Models for the Web Graph, Halifax, Nova Scotia, Canada, June 22-23, 2012. Also, in 9th International Workshop for Algorithms and Models for the Web Graph, A. Bonato and J. Janssen, eds, Lecture Notes in Computer Science (LNCS 7323), 2012.

4. **J. Ray**, S. Lefantzi, S. A. McKenna and B. van Bloemen Waanders, "Bayesian estimation of multiscale structures in a binary medium from sparse observations", 19th International Conference on Water Resources, Urbana-Champaign, IL, June 17-22, 2012.

5. S. A. McKenna, B. van Bloemen Waanders and **J. Ray**, "Low parameter representations of anthropogenic greenhouse gas flux fields for inverse parameter estimation", Ninth International Geostatistics Congress, Oslo, Norway, June 11-15, 2012.

6. C. Safta, **J. Ray** and H. N. Najm, "A high-order AMR algorithm for chemically reacting flows", 23rd International Colloquium on the Dynamics of Explosion and Reactive Systems, UC Irvine, July 24-29, 2011.

7. C. Safta, **J. Ray**, K. Cheng and D. Crary, "Characterization of communicable disease epidemics using Bayesian inference", Proceedings of the International Society for Disease Surveillance, Park City, UT, December 2010.

8. C. Safta, **J. Ray**, K. Cheng and D. Crary, "Statistical methods for classification of partially observed outbreaks", presented at the International Society for Disease Surveillance, Miami, December 2009

9. K. Cheng, D. Crary, G. McClellan, **J. Ray** and C. Safta, "Anomaly detection techniques for biosurveillance application", presented at the International Society for Disease Surveillance, Miami, December 2009.

10. P. T. Boggs, D. M. Gay and **J. Ray**, "Probabilistic attack reconstruction and resource estimation in reload scenarios", IEEE Xplore, Proceedings of the 2009 IEEE Homeland Security Conference , Waltham, MA, May 11-12, 2009. SAND2009-3294C

11. **J. Ray** and Y. M. Marzouk, "Bayesian inference of epidemiological characteristics in a partially observed epidemic", Proceedings of the DTRA Chemical and Biological Technologies Conference, New Orleans, November 17-21, 2008.

12. J. Rodriguez, K. E. Cheng, G. McClellan, D. J. Crary, D. Oldson, B. Adams and **J. Ray**, " Contagious disease module for the Joint Effects Model", Proceedings of the DTRA Chemical and Biological Technologies Conference, New Orleans, November 17-21, 2008.

13. **J. Ray**, Y. M. Marzouk M. Kraus and P. Fast, "Characterizing bioterrorist attacks from a short time series of diagnosed patient data - A Bayesian approach", Proceedings of the Second Conference on Quantitative Methods in Defense and National Security, George Mason University, Fairfax, VA, February 7-8, 2007.

14. S. Chandra, M. Parashar and **Jaideep Ray**, "Analyzing the impact of computational heterogeneity on runtime performance of parallel scientific components", Proceedings of the 15th High Performance Computing Symposium (HPC-07), SCS Spring Simulation Multiconference, Norfolk, VA, USA, March 2007.

15. Sumir Chandra, Manish Parashar and **Jaideep Ray**, "Dynamic structured partitioning of parallel scientific applications with pointwise varying workloads", Proceedings of the International Parallel and Distributed Processing Symposium, April 24-28, 2006. Rhodes, Greece.

16. **J. Ray**, C. Kennedy, J. Steensland and H. Najm, "Advanced algorithms for computations on block-structured adaptively refined meshes," *Journal of Physics: Conference Series,* 2005, 16:113-118.

17. Benjamin A. Allan and **J. Ray**, "The scalability impact of a component-based software engineering framework on a growing SAMR toolkit: a case study," Parallel Computational Fluid Dynamics May 25-27, 2005, College Park, MD.

18. N. Trebon, A. Morris, **J. Ray**, S. Shende and A. Malony, "Performance modeling of component assemblies with TAU," Compframe 2005 June 22-24, 2005, Atlanta, GA.

19. J. C. Lee, H. N. Najm, S. Lefantzi, **J. Ray**, M. Frenklach, M. Valorani and D. A. Goussis, "An adaptive reduced–order chemical model", 20th International Colloquium on the Dynamics of Explosions and Reactive Systems , July 31st to August 5th, 2005, Montreal, Canada.

20. J. C. Lee, H. N. Najm, S. Lefantzi, **J. Ray**, M. Frenklach, M. Valorani and D. A. Goussis, "The role of explosive modes in homogeneous ignition and premixed flames", 20th International Colloquium on the Dynamics of Explosions and Reactive Systems , July 31st to August 5th, 2005, Montreal, Canada.

21. Johan Steensland and **J. Ray**, "A Partitioner-centric model for SAMR partitioning trade-off optimization: Part II", In the proceedings of The 6th International Workshop on High Performance Scientific and Engineering Computing (HPSEC-04), held in conjunction with The 2004 International Conference On Parallel Processing (ICPP-04), in Montreal, Canada, Aug. 15-18, 2004.

22. J.C. Lee, H.N. Najm, S. Lefantzi, **J. Ray**, M. Frenklach, M. Valorani, and D.A. Goussis, "On chain branching and its role in homogeneous ignition and premixed flame propagation", Third MIT Conference on Computational Fluid and Solid Mechanics, June 14-17, 2005, Cambridge, MA.

23. B. Norris, **J. Ray**, R.C. Armstrong, L.C. McInnes, D.E. Bernholdt, W.R. Elwasif, A.D. Malony, S. Shende, " Computational Quality of Service for scientific components", Component-Based Software Engineering, 7^{th} International Symposium, CBSE 2004, Edinburgh, UK, May 24-25, 2004. Also in Lecture Notes in Computer Science, 3054, Pg 264-271. Springer.

24. **J. Ray** and N. Trebon and S. Shende and R. C. Armstrong and A. Malony, "Performance measurement and modeling of component applications in a high performance computing environment: A case study", Proceedings of the 18^{th} International Parallel and Distributed Computing Symposium , April 26–30, 2004, Santa Fe, NM.

25. J. Steensland and **J. Ray**, "A partitioner-centric model for SAMR partitioning trade-off optimization: Part I", Proceedings of the 4^{th} Annual Symposium of the Los Alamos Computer Science Institute (LACSI04).

26. J. Steensland and **J. Ray**, "A heuristic re-mapping algorithm reducing inter-level communication in SAMR applications", Proceedings of the 15^{th} IASTED International Conference on Parallel and Distributed Computing and Systems 2003 (PDCS03). *Best paper award in the "Runtime Systems" category.*

27. S. Lefantzi and **J. Ray**, "A component-based scientific toolkit for reacting flows", Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics, Boston, Mass. 2003.

28. S. Lefantzi, **J. Ray** and H. N. Najm, "Using the Common Component Architecture to design high performance scientific simulation codes", Proceedings of the 17^{th} International Parallel and Distributed Processing Symposium, April 2003, Nice, France.

29. C.C. Douglas, J. Hu, **J. Ray**, D. Thorne and R. Tuminaro, "Fast, adaptively refined computational elements in 3D", presented at 2002 International Conference on Computational Science, Part III, April 21th to 24th, Amsterdam, Netherlands. Also in Lecture Notes in Comput. Sc., 2331, pp 774-783, Springer, Berlin, 2002.

Conference Talks (Unrefereed) and Technical Reports

See the list on my webpage at http://www.sandia.gov/∼jairay

References

Available on request