**Jeff R. Hammond**

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## Education and Research Positions

**Intel Corporation - Parallel Computing Lab** (May 2014 - present)
Title: Research Scientist
Supervisors: Drs. Tim Mattson and Pradeep Dubey
Description: Exascale application analysis, programming models and runtime systems.

**Argonne National Laboratory - Leadership Computing Facility** (June 2011 - May 2014)
Title: Assistant Computational Scientist in the Performance Engineering group
Supervisors: Drs. Kalyan Kumaran and Ray Bair
Description: Communication software and programming models for Blue Gene/Q; testing and evaluation of current and next-generation supercomputing technology; development of quantum chemistry methods and software; software and algorithms for enhanced sampling in molecular dynamics; DOE exascale actiities.

**The University of Chicago - Computation Institute** (February 2011 - May 2014)
Title: Fellow (since September 2011)
Description: Collaboration with UChicago faculty and staff on computational science projects; NSF-funded research in computational chemistry and computer science; software development for and performance evaluation of the Beagle Cray XE6 supercomputer.

**Argonne National Laboratory - Leadership Computing Facility** (June 2009 - May 2011)
Title: Argonne Scholar (Director's Postdoctoral Fellowship)
Supervisor: Dr. Ray Bair
Description: Developed quantum chemistry applications and communication software for Blue Gene/P.

**Pacific Northwest National Laboratory** (June 2006 - May 2009)
Title: Alternate Sponsored Fellow (DOE-CSGF practicum)
Supervisors: Drs. Karol Kowalski and Wibe A. de Jong
Description: Developed coupled-cluster molecular property module and other features in NWChem.

**University of Chicago** (September 2003 to May 2009)
PhD in Chemistry, May 2009; MS in Chemistry, August 2004.
Supervisors: Professors Karl F. Freed and L. Ridgway Scott
Thesis: *Coupled-cluster response theory: parallel algorithms and novel applications*

**University of Washington** (January 2001 to August 2003)
BS in Chemistry with Distinction; BA in Mathematics; Minor in Applied Mathematics.
Supervisor: Professor Weston T. Borden
Thesis: *Evaluating the Bishomoaromatic Nature of Diaminodiformylsemibullvalene*

## Honors and Awards

IEEE Technical Committee on Scalable Computing - Young Achiever Award (2013)

Director's Postdoctoral Fellowship, Argonne National Laboratory (2009 - 2011)
Chemical Computing Group Excellence Award, ACS Division of Computers in Chemistry (Spring 2008)
Department of Energy Computational Science Graduate Fellowship (2005 - 2009)
Joan Shiu Award for Student Service, The University of Chicago Chemistry Department (2006)
Freud Departmental Citizenship Award, The University of Chicago Chemistry Department (2005)
McCormick Fellowship, The University of Chicago Physical Sciences Division (2003 - 2005)
Mary Gates Undergraduate Research Training Grant, University of Washington (2003)

## Journal Publications and Book Chapters

25. E. Solomonik, D. Matthews, J. Hammond, J. F. Stanton and J. Demmel. *Journal of Parallel and Distributed Computing* (2014). "A massively parallel tensor contraction framework for coupled-cluster computations." Online

24. R. E. Isele-Holder, W. Mitchell, J. R. Hammond, A. Kohlmeyer, and A. E. Ismail. *J. Chem. Theory Comp.* (2013). "Reconsidering Dispersion Potentials: Reduced Cutoffs in Mesh-Based Ewald Solvers Can Be Faster Than Truncation." Online

23. J. R. Hammond, *ACM XRDS* 19 (3), Spring 2013. "Challenges and methods in large-scale computational chemistry applications." Online

22. Allcock et al. (57 authors). *Contemporary High Performance Computing: From Petascale toward Exascale*, edited by Jeffrey S. Vetter (Chapman & Hall/CRC Computational Science, February 2013). "Blue Gene/Q: Sequoia and Mira."

21. J. Poulson, B. Marker, J. R. Hammond, N. A. Romero and R. A. van de Geijn, *ACM Transactions On Mathematical Software* **39** (2), February 2013, article 13. "Elemental: A New Framework for Distributed Memory Dense Matrix Computations." Online Preprint

20. J. R. Hammond, S. Krishnamoorthy, S. Shende, N. A. Romero and A. D. Malony. *Concurrency and Computation: Practice and Experience* **24** (2), 135-154 (2012). "Performance Characterization of Global Address Space Applications: A Case Study with NWChem." Online Preprint

19. J. Dinan, S. Krishnamoorthy, P. Balaji, J. R. Hammond, M. Krishnan, V. Tipparaju and A. Vishnu. *Recent Advances in the Message Passing Interface* (Lecture Notes in Computer Science, Volume 6960/2011, pp. 282-291), edited by Y. Cotronis, A. Danalis, D. S. Nikolopoulos and J. Dongarra. "Noncollective Communicator Creation in MPI." Online Preprint

18. A. Dickson, M. Maienshein-Cline, A. Tovo-Dwyer, J. R. Hammond and A. R. Dinner. *J. Chem. Theory Comp*. **7**, 2710 (2011). "Flow-dependent unfolding and refolding of an RNA by nonequilibrium umbrella sampling." Online Preprint

17. A. E. DePrince III and J. R. Hammond. *J. Chem. Theory Comp.* **7**, 1287 (2011). "Coupled Cluster Theory on Graphics Processing Units I. The Coupled Cluster Doubles Method." Online

16. K. Kowalski, J. R. Hammond, W. A. de Jong, P.-D. Fan, M. Valiev, D. Wang and N. Govind. *Computational Methods for Large Systems: Electronic Structure Approaches for Biotechnology and Nanotechnology*, edited by J. R. Reimers (Wiley, March 2011, Hoboken). "Coupled Cluster Calculations for Large Molecular and Extended Systems."

15. R. S. Assary, P. C. Redfern, J. R. Hammond, J. Greeley and L. A. Curtiss, *Chem. Phys. Lett.* **497**, 123 (2010). "Predicted Thermochemistry for Chemical Conversion of 5-Hydroxymethyl Furfural." Online

14. R. S. Assary, P. C. Redfern, J. R. Hammond, J. Greeley and L. A. Curtiss. *J. Phys. Chem. B* **114**, 9002 (2010). "Computational Studies of the Thermochemistry for Conversion of Glucose to Levulinic Acid." Online

13. K. Kowalski, S. Krishnamoorthy, O. Villa, J. R. Hammond, and N. Govind. *J. Chem. Phys.* **132**, 154103 (2010). "Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer." Online

12. J. R. Hammond, N. Govind, K. Kowalski, J. Autschbach and S. S. Xantheas. *J. Chem. Phys.* **131**, 214103 (2009). "Accurate dipole polarizabilities for water clusters $N$=2-12 at the coupled-cluster level of theory and benchmarking of various density functionals." Online

11. J. R. Hammond and K. Kowalski. *J. Chem. Phys.* **130**, 194108 (2009). "Parallel computation of coupled-cluster hyperpolarizabilities." Online

10. K. Kowalski, J. R. Hammond, W. A. de Jong and A. J. Sadlej. *J. Chem. Phys.* **129**, 226101 (2008). "Coupled cluster calculations for static and dynamic polarizabilities of $C_{60}$." Online

9. R. K. Chaudhuri, J. R. Hammond, K. F. Freed, S. Chattopadhyay and U. S. Mahapatra. *J. Chem. Phys.* **129**, 064101 (2008). "Reappraisal of *cis* effect in 1,2-dihaloethenes: An improved virtual orbital (IVO) multi-reference approach." Online

8. J. R. Hammond, W. A. de Jong and K. Kowalski. *J. Chem. Phys.* **128**, 224102 (2008). "Coupled cluster dynamic polarizabilities including triple excitations." Online

7. K. Kowalski, J. R. Hammond and W. A. de Jong. *J. Chem. Phys.* **127**, 164105 (2007). "Linear response coupled cluster singles and doubles approach with modified spectral resolution of the similarity transformed Hamiltonian." Online

6. J. R. Hammond, W. A. de Jong and K. Kowalski. *J. Chem. Phys.* **127**, 144105 (2007). "Dynamic polarizabilities of polyaromatic hydrocarbons using coupled-cluster linear response theory." Online

5. J. R. Hammond, M. Valiev, W. A. de Jong and K. Kowalski. *J. Phys. Chem. A* **111**, 5492 (2007). "Calculations of properties using a hybrid coupled-cluster and molecular mechanics approach." Online

4. J. R. Hammond and D. A. Mazziotti. *Phys. Rev. A* **73**, 062505 (2006). "Variational reduced-density-matrix calculation of the one-dimensional Hubbard model." Online

3. J. R. Hammond and D. A. Mazziotti. *Phys. Rev. A* **73**, 012509 (2006). "Variational reduced-density-matrix calculations on small radicals: a new approach to open-shell ab initio quantum chemistry." Online

2. M. Lingwood, J. R. Hammond, D. A. Hrovat, J. M. Mayer, and W. T. Borden. *J. Chem. Theo. Comp.* **2**, 740 (2006). "MPW1K, rather than B3LYP, should be used as the functional for DFT calculations on reactions that proceed by proton-coupled electron transfer (PCET)." Online

1. J. R. Hammond and D. A. Mazziotti. *Phys. Rev. A* **71**, 062503 (2005). "Variational two-electron reduced-density-matrix theory: Partial 3-positivity conditions for $N$-representability." Online

**Conference and Workshop Proceedings (peer-reviewed)**

15. J. R. Hammond, A. Schäfer and R. Latham. Workshop on Exascale MPI (ExaMPI14) at Supercomputing Conference 2014. New Orleans, Louisiana (November 17, 2014). "To INT_MAX... and beyond! Exploring large-count support in MPI." Preprint

14. J. R. Hammond. OpenSHMEM User Group, held in conjunction with PGAS 2014 Eugene, OR (October 7, 2014). "Towards a matrix-oriented strided interface in OpenSHMEM." Preprint

13. David Ozog, Allen Malony, Jeff Hammond and Pavan Balaji. *20th IEEE International Conference on Parallel and Distributed Systems* (ICPADS), Hsinchu, Taiwan, December 16 19, 2014. "WorkQ: A Many-Core Producer/Consumer Execution Model Applied to PGAS Computations."

12. T. M. Smith, R. van de Geijn, M. Smelyanskiy, J. R. Hammond, and F. G. Van Zee. *Proc. 28th Intl. Parallel and Distributed Processing Symp.* (IPDPS), Phoenix, Arizona. May 2014. "Anatomy of High-Performance Many-Threaded Matrix Multiplication." Preprint

11. P. Ghosh, J. R. Hammond, S. Ghosh, and B. Chapman. *4th International Workshop on. Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems* (PMBS13), "Performance analysis of the NWChem TCE for different communication patterns."

10. S. Ghosh, J. R. Hammond, and B. M. Chapman. *First OpenSHMEM Workshop: Experiences, Implementations and Tools*. "Implementing OpenSHMEM using MPI-3 one-sided communication." Preprint

9. D. Ozog, J. R. Hammond, J. Dinan, P. Balaji, S. Shende and A. Malony. *International Conference on Parallel Processing* (ICPP), Lyon, France. October 2013. "Inspector-Executor Load Balancing Algorithms for Block-Sparse Tensor Contractions." Preprint

8. A. Peters Randles, V. Kale, J. Hammond, W. D. Gropp and E. Kaxiras. *Proc. 27th Intl. Parallel and Distributed Processing Symp.* (IPDPS), Boston, Massachusetts. May 2013. "Performance Analysis of the Lattice Boltzmann Model Beyond Navier-Stokes." Online Preprint

7. E. Solomonik, D. Matthews, J. Hammond and J. Demmel. *Proc. 27th Intl. Parallel and Distributed Processing Symp.* (IPDPS), Boston, Massachusetts. May 2013. "Cyclops Tensor Framework: reducing communication and eliminating load imbalance in massively parallel contractions." Online
Preprint

6. V. Morozov, J. Meng, V. Vishwanath, J. Hammond, K. Kumaran and M. Papka. *Proceedings of the P2S2 Workshop*. September 2012. "ALCF MPI Benchmarks: Understanding Machine-Specific Communication Behavior." Online

5. J. R. Hammond, J. Dinan, P. Balaji, I. Kabadshow, S. Potluri, and V. Tipparaju. *The 6th Conference on Partitioned Global Address Space Programming Models* (PGAS), Santa Barbara, CA. October 2012 "OSPRI: An Optimized One-Sided Communication Runtime for Leadership-Class Machines." Preprint

4. S. Hogan, J. R. Hammond and A. A. Chien. *Fault-Tolerance at Extreme Scale* (FTXS), Boston, MA. June, 2012. "An Evaluation of Difference and Threshold Techniques for Efficient Checkpoints." Online
Preprint

3. J. Dinan, P. Balaji, J. R. Hammond, S. Krishnamoorthy and V. Tipparaju. *Proc. 26th Intl. Parallel and Distributed Processing Symp.* (IPDPS), Shanghai, China. May, 2012. "Supporting the Global Arrays PGAS Model Using MPI One-Sided Communication." Online Preprint

2. A. E. DePrince III and J. R. Hammond. Symposium on Application Accelerators in High Performance Computing (SAAHPC), Knoxville, Tennessee. July 2011. "Quantum Chemical Many-Body Theory on Heterogeneous Nodes." Online

1. J. R. Hammond and A. E. DePrince III. Symposium on Application Accelerators in High Performance Computing (SAAHPC), Knoxville, Tennessee. July 2010. "Evaluating One-Sided Programming Models for GPU Cluster Computations." Online

## Preprints and Other Publications (not peer-reviewed or currently under review)

V. Vishwanath, T. Uram, L. Childers, H. Finkel, J. Hammond, K. Kumaran, P. Messina and M. E. Papka. DOE ASCR Workshop on Software Productivity for eXtreme-Scale Science (SWP4XS), Rockville, Maryland, January 13-14, 2014. "Toward improved scientific software productivity on leadership facilities: An Argonne Leadership Computing Facility View." Online

T. M. Smith, R. van de Geijn, M. Smelyanskiy, J. R. Hammond, and F. G. Van Zee. FLAME Working Note #71. The University of Texas at Austin, Department of Computer Science. Technical Report TR-13-20. 2013. "Opportunities for Parallelism in Matrix Multiplication." Online

E. Solomonik, J. Hammond and J. Demmel. Electrical Engineering and Computer Sciences, University of California at Berkeley, Technical Report No. UCB/EECS-2012-29, March 9, 2012. "A preliminary analysis of Cyclops Tensor Framework." Online

A. E. DePrince III, J. R. Hammond and S. K. Gray. Proceedings of SciDAC 2011, Denver, CO, July 10-14, 2011. "Many-body quantum chemistry on graphics processing units." Online

L. R. Scott, P. Brune, J. Hammond, A. Terrel and M. Knepley. Workshop on Automating the Development of Scientific Computing Software, Baton Rouge, Louisiana, March 5-7, 2008. "Software Automation." Online

## Presentations

X. Novel computational methods for quantitative electronic structure calculations, Kobe University & RIKEN AICS, Kobe, Japan, (June 16-20, 2015). *TBD*. (Invited)

69. MVAPICH User Group, Columbus, OH (August 26-27, 2014). *Scaling NWChem with ARMCI-MPI and MPI-3*. (Invited)

68. Future of Computational Chemistry symposium, American Chemical Society national meeting, San Francisco, CA (August 14, 2014). *Evolution and revolution in massively parallel coupled cluster codes*. (Invited)

67. Intel Xeon Phi User Group (IXPug), Texas Advanced Computing Center, Austin, TX (July 8-9, 2014). *NWChem: The Next Generation*. (Invited)

66. Intel Parallel Computing Laboratory, Santa Clara, CA (April 14, 2014). *Quantum Chemistry at Petascale and Beyond*.

65. First OpenSHMEM Workshop: Experiences, Implementations and Tools, Annapolis, MD (March 6, 2014). *Implementing OpenSHMEM using MPI-3 one-sided communication*.

64. NVIDIA Annual Technical Summit for Life and Material Science Developers, Santa Clara, CA (February 13, 2014). *Coupled Cluster Methods and Tensor Contractions*.

X. 22nd Conference on Current Trends in Computational Chemistry (22nd CCTCC), Jackson, MS (November 15-16, 2013). (invited - declined)

63. Argonne Training Program on Extreme Scale Computing, St. Charles, IL (August 8, 2013). *Application Case Studies: NWChem and MADNESS*.

62. Argonne Training Program on Extreme Scale Computing, St. Charles, IL (July 31, 2013). *Combining Performance and Portability*.

61. SIAM Computational Science and Engineering, Boston, MA (March 1, 2013). *NWChem Quantum Many-body Methods on the Intel MIC Architecture*.

60. SIAM Computational Science and Engineering, Boston, MA (February 28, 2013). *Portability Versus Performance: Experiences in Programming Model Compromises*.

59. Advanced Institute for Computational Science, RIKEN, Kobe, Japan (January 30, 2013). *Algorithms and Software for Quantum Chemistry at Petascale and Beyond*.

58. Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki, Japan (January 30, 2013). *Algorithms and Software for Quantum Chemistry at Petascale and Beyond*.

57. Toyohashi University of Technology, Tokyo, Japan (January 29, 2013). *Algorithms and Software for Quantum Chemistry at Petascale and Beyond*. (invited)

56. International Workshop on Massively Parallel Programming Now in Molecular Science; Waseda University, Tokyo, Japan (January 28, 2013). *Algorithms and Software for Quantum Chemistry at Petascale and Beyond*. (invited)

55. Chemistry Department, Northwestern University; Evanston, IL (November 5, 2012). *Verification and validation in quantum many-body methods*.

54. Ineos Technologies; Naperville, IL (October 23, 2012). *Computational chemistry on high-performance computers: What is it good for?*

53. Project Meeting for Computation-Driven Discovery for the Dark Universe (SciDAC-3); Argonne, IL (October 19, 2012). *Hors d'oeuvres for exascale programming*.

52. Validation and Verification in Electronic-Structure calculations: state of the art and perspectives; CECAM-HQ-EPFL, Lausanne, Switzerland (September 6, 2012). *Verification and validation in quantum many-body methods*. (invited)

51. Cavendish Laboratory, University of Cambridge, Cambridge, England (September 3, 2012). *Codesign*

*in action: the hardware and software architecture of Blue Gene/Q and its impact on scientific applications*.

50. Productive Programming Models for Exascale; Pacific Northwest National Laboratory, Portland, OR (August 14-15, 2012). *Algorithms and programming models for coupled-cluster methods*.

49. INRIA Saclay, Paris, France (June 8, 2012). *Programming models and numerical algorithms for quantum chemistry*.

48. Accurate Methods for Accurate Properties - An international conference celebrating the 60th birthday of Peter Taylor, University of Zurich, Zurich, Switzerland (June 4-6, 2012). *Accurate molecular response properties using coupled-cluster methods*. (invited)

47. 10th Annual Workshop on Charm++ and its Applications, University of Illinois at Urbana-Champaign, Urbana, IL (May 7-9, 2012). *Programming models for quantum chemistry applications*. (invited)

46. Department of Computer Science, Illinois Institute of Technology; Chicago, IL (April 16, 2012). *Designing libraries and applications for petascale and beyond*. (invited)

45. Electronic Structure Calculation Methods on Accelerators; ORNL, Oak Ridge, TN (February 7, 2012). *Programming models for quantum many-body methods on multicore and manycore processors*.

44. Synchronization-reducing and Communication-reducing Algorithms and Programming Models for Large-scale Simulations; ICERM, Brown University, Providence, RI (January 11, 2012). *Computational Challenges of Coupled Cluster Theory*.

43. Fault Tolerant and Energy Efficient Algorithms in Molecular Simulations; CECAM-HQ-EPFL, Lausanne, Switzerland (September 5, 2011). *Designing quantum chemistry codes for next-generation supercomputers*. (invited keynote)

42. First International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing (WOLFHPC); Tucson, AZ (May 31, 2011). *Evolving the Tensor Contraction Engine for Next-Generation Multi-petaflop Supercomputers*.

41. National Renewable Energy Laboratory (NREL); Golden, CO (May 4, 2011). *New frontiers in quantum chemistry using supercomputers*. (invited)

40. University of Minnesota; Minneapolis, MN (April 22, 2011). *New frontiers in quantum chemistry using supercomputers*. (invited)

39. Navigating Chemical Compound Space for Materials and Bio Design: Tutorials, Institute for Pure and Applied Mathematics (IPAM), University of California; Los Angeles, CA (March 16, 2011). *Why and how to use high-performance computing for materials and bio design*. (invited)

38. SIAM Conference on Computational Science and Engineering; Reno, NV (March 2, 2011). *OSPRI: A New Communication Runtime System for Global Arrays and Other One-sided Programming Models*.

37. Institute for Computational Engineering and Sciences (ICES), University of Texas; Austin, TX (February 24, 2011). *New frontiers in quantum chemistry using supercomputers*. (invited)

36. Texas Advanced Computer Center (TACC); Austin, TX (February 23, 2011). *Software Architecture of*

*Current and Future High-Performance Computational Chemistry Codes*.

35. Princeton Institute for Computational Science and Engineering (PICSciE), Princeton University; Princeton, NJ (February 21, 2011). *New frontiers in quantum chemistry using supercomputers*. (invited)

34. EU Regional School 2011, Aachen Institute for Computational Engineering Science (AICES), Rheinisch-Westfaelische Technische Hochschule (RWTH); Aachen, Germany (February 8, 2011). *Scientific Programming at Petascale and Beyond*. (invited)

33. EU Regional School 2011, Aachen Institute for Computational Engineering Science (AICES), Rheinisch-Westfaelische Technische Hochschule (RWTH); Aachen, Germany (February 8, 2011). *New Frontiers in Quantum Chemistry Using Supercomputers*. (invited)

32. Jülich Supercomputing Centre; Jülich, Germany (February 7, 2011). *New Frontiers in Quantum Chemistry Using Supercomputers*.

31. Manycore and Accelerator-based High-performance Scientific Computing Workshop, International Center for Computational Sciences, University of California and Lawrence Berkeley National Laboratory; Berkeley, CA (January 26, 2011). *Quantum chemistry many-body methods on GPUs and multicore CPUs*.

30. Argonne Booth Talk, Supercomputing; New Orleans, LA (November 15, 2010). *OSPRI: An Optimized One-Sided Communication Runtime for Leadership-Class Machines*.

29. Advanced Scientific Computing Advisory Committee (ASCAC) Meeting, Argonne National Laboratory; Argonne, IL (November 10, 2010). *Computational Chemistry Beyond Petascale*.

28. Laboratory Computing Resource Center (LCRC) Quantum Chemistry Workshop; Argonne, IL (November 5, 2010). *NWChem Tutorial*.

27. HPC Workshop, Computation Institute, University of Chicago; Chicago, IL (September 14, 2010). *Parallel Programming Models and Scientific Algorithms*.

26. Argonne Postdoc Symposium, Argonne National Laboratory; Argonne, IL (September 8, 2010). *Quantum chemistry at petascale and beyond on Blue Gene/P and Blue Gene/Q*.

25. SciDAC 2010; Chattanooga, TN (July 15, 2010). *The software of the future on the hardware of the future*. (invited; with W. A. Scullin and R. A. Bair)

24. DOE-CSGF HPC Workshop; Washington, DC (June 21, 2010). *The five most important things I've learned about high performance computing*.

23. Student Lecture Series, MCS Division; Argonne, IL (June 8, 2010). *Programming Models for High Performance Scientific Computing*.

22. SIAM Conference on Parallel Processing for Scientific Computing; Seattle, WA (February 24, 2010). *Dense Linear Algebra on GPU Clusters*.

21. Head-Gordon group meeting, Department of Chemistry, University of California; Berkeley, CA (January 22, 2010). *New frontiers in quantum chemistry using supercomputers*.

20. LANS Seminar, MCS Division, Argonne National Laboratory; Argonne, IL (November 24, 2009). *Quantum chemistry for computer scientists*.

19. MPI Forum; Portland, OR (November 12, 2009). *A critical analysis of the MPI-3 RMA interface*.

18. Swiss National Supercomputing Centre Users' Day; Manno, Switzerland (September 11, 2009). *Accurate quantum chemical simulations of large molecules using supercomputers*. (invited)

17. American Chemical Society National Meeting; Washington, DC (August 18, 2009). *The challenging excited states of the membrane-bound fluorophore di-8-ANEPPS*. (with Benoît Roux, Niri Govind and Karol Kowalski)

16. Theory Department, Fritz Haber Institute of the Max Planck Society; Berlin, Germany (July 26, 2009). *Coupled-cluster response theory and accurate electric-field properties for large molecules*. (invited)

15. Aspuru-Guzik group meeting, Department of Chemistry, Harvard University; Cambridge, MA (May 29, 2009). *Untitled*.

14. Rawal group meeting, Department of Chemistry, The University of Chicago; Chicago, IL (May 11, 2009). *Computational approaches for understanding hydrogen-bonding*.

13. SIAM Conference on Computational Science and Engineering; Miami, FL (March 2, 2009). *Accurate Molecular Properties Using a Massively-Parallel Quantum Chemistry Code and Implications for Drug Design*.

12. Computer Science and Mathematics Division, Oak Ridge National Laboratory; Oak Ridge, TN (October 16, 2008). *Accurate molecular property calculations using supercomputers: algorithms and applications*.

11. National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign; Urbana, IL (August 1, 2008). *Accurate molecular property calculations using supercomputers: algorithms and applications*.

10. American Chemical Society National Meeting; New Orleans, LA (April 7, 2008). *Nonlinear optical spectroscopy of conjugated molecules using coupled-cluster theory*. (with K. Kowalski)

9. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 19, 2007). *E Pluribus Duo* (old title, new talk).

8. Department of Chemistry, Cornell University; Ithaca, NY (June 14, 2007). *Quantum many-body theory without so many bodies*.

7. The Twelfth Annual James Franck Institute Symposium, The University of Chicago; Chicago, IL (May 17, 2007). *E Pluribus Duo*.

6. American Chemical Society National Meeting; Chicago, IL (March 27, 2007). *Coupled-cluster property calculations of aromatic molecules*. (with W. A. de Jong and K. Kowalski)

5. American Physical Society National Meeting; Denver, CO (March 7, 2007). *Variational reduced-density-matrix theory applied to the Hubbard model*. (with D. A. Mazziotti)

4. Computer Science and Mathematics Division, Oak Ridge National Laboratory; Oak Ridge, TN (February 8, 2007). *Massively parallel many-body methods for hard systems*.

3. Chemistry Department Tiger Talk, The University of Chicago; Chicago, IL (April 26, 2006). *Solving hard problems with RDM theory: from radical chemistry to ultracold atoms and high-$T_c$ superconductivity*.

2. Mathematics and Computer Science Division, Argonne National Laboratory; Argonne, IL (July 29, 2005). *Quantum chemistry without wavefunctions: the role of semidefinite programming and some new results for radicals*.

1. Mary Gates Undergraduate Research Symposium, The University of Washington; Seattle, WA (May 16, 2003). *Bishomoaromaticity in the Cope rearrangement of semibullvalene*.

**Posters**

14. Supercomputing 2011; Seattle, WA (November 16, 2011). *Fast One-Sided Communication on Supercomputers and Application to Three Scientific Codes*. (with Sreeram Potluri, Zheng (Cynthia) Gu, Alex Dickson, James Dinan, Ivo Kabadshow, Pavan Balaji and Vinod Tipparaju)

13. Supercomputing 2010; New Orleans, LA (November 17, 2010). *Non-equilibrium umbrella sampling on Blue Gene/P using one-sided communication*. (with Alex Dickson and Aaron R. Dinner)

12. SAAHPC 2010; Knoxville, TN (July 13-15, 2010), *Asynchronous Programming Models for GPU Cluster Computing*. (with A. E. DePrince III)

11. Supercomputing 2009; Portland, OR (November 17, 2009). *Scalability of quantum chemistry codes on Blue Gene/P and challenges for sustained petascale performance*.

10. SciDAC 2009; San Diego, CA (June 14, 2009). *Developing polarizable force fields from ab initio calculations and the role of quantum chemical benchmarking in the age of petascale*.

9. American Chemical Society National Meeting; Salt Lake City, UT (March 25, 2009). *Developing polarizable force fields from ab initio calculations: A critical analysis of methods*. (with K. Kowalski and S. Xantheas)

8. American Conference on Theoretical Chemistry, Northwestern University; Evanston, IL (July 21, 2008). *Accurate spectroscopic properties of molecules using coupled-cluster response theory and supercomputers*.

7. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 18, 2008). *Coupled-cluster theory on supercomputers*. (with K. Kowalski)

6. American Chemical Society National Meeting, New Orleans, LA (April 8, 2008). *Coupled-cluster theory on supercomputers*. (with K. Kowalski)

5. NWChem Meeting on Science Driven Petascale Computing and Capability Development, Pacific Northwest National Laboratory; Richland, WA (January 25, 2007). *Coupled-cluster linear response properties for very large systems using new functionality within NWChem*. (with K. Kowalski and W. A. de Jong)

4. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 21, 2006). *New frontiers in quantum many-body theory using state-of-the-art semidefinite programming algorithms*. (with D. A. Mazziotti)

3. American Conference on Theoretical Chemistry, UCLA; Los Angeles, CA (July 18, 2005). *Variational reduced-density-matrix calculations on open-shell systems*. (with D. A. Mazziotti)

2. 30th Reaction Mechanisms Conference, Northwestern University; Evanston, IL (June 25, 2004). *A DFT study of hydrogen transfer in ribonucleotide reductase: mechanisms and the role of mediating water molecules*. (with D. A. Hrovat and W. T. Borden)

1. European Summer School in Quantum Chemistry, Lund University; Lund, Sweden (August 24, 2003). *PCET vs. HAT in ribonucleotide reductase: a DFT study*. (with D. A. Hrovat and W. T. Borden)

## Software

Ohloh (https://www.ohloh.net/accounts/jeff_science) has additional contributions not listed here.

**Applications:**

*NWChem*, ECL-2.
http://www.nwchem-sw.org/.
Contributions:

- Unreleased developments: OpenMP and vectorization of coupled cluster kernels for Intel MIC and other multicore processors; hierarchical dynamic and static partitioning load-balancing algorithms for TCE.
- Version 6.3 (2013): Blue Gene/Q porting.
- Version 6.1 (2011): OpenMP kernels for CCSD(T), vectorization for Blue Gene/P.
- Version 6.0 (2010): CCSD imaginary-frequency dynamic polarizabilities and the associated solvers; double-hybrid DFT functionals (e.g. B2PLYP) with all three MP2 modules, SCS-RI-MP2.
- Version 5.1.1 (2009): Linear response dynamic polarizabilities with CCSDTQ; CCSD quadratic response and hyperpolarizabilities; hybrid out-of-core integral transformation algorithms.
- Version 5.1 (2007): Linear response dynamic polarizabilities with CCSD and CCSDT.

*MADNESS*, GPL v2.
https://code.google.com/p/m-a-d-n-e-s-s/
Contributions: Porting and optimization of the parallel runtime; optimization of the tensor kernel for Blue Gene.

*LAMMPS-Ensembles* (Massively-parallel replica exchange and umbrella sampling in LAMMPS), GPL.
https://github.com/jeffhammond/lammps_ensembles
Contributions: Designed and supervised development of new features for massively parallel ensemble runs for replica-exchange umbrella sampling and related methods.

**One-Sided Communication:**

*ARMCI-MPI* (ARMCI over MPI-RMA), BSD-3.
http://git.mpich.org/armci-mpi.git
Contributions: Assisted in the design of the MPI-2 implementation, which was done by Jim Dinan; lead developer for the MPI-3 RMA implementation.

*OSHMPI* (OpenSHMEM over MPI-3), BSD-3.
https://github.com/jeffhammond/oshmpi

Contributions: Lead developer.

*OSPRI* (One-Sided PRImitives), BSD-3.
https://trac.mcs.anl.gov/projects/ospri/
Contributions: Lead developer.

*A1* (Argonne 1-sided – a completely new implementation of ARMCI for Blue Gene/P), BSD.
https://trac.mcs.anl.gov/projects/a1/
Contributions: I designed and co-authored this library.

*Global Arrays*, BSD.
http://www.emsl.pnl.gov/docs/global/.
Contributions:

- Version 5.0 (2010): Performance optimizations and other improvements.
- Version 4.3 (2009): Performance optimizations in the DCMF (Blue Gene/P) port of ARMCI.

**Other Libraries:**

*Spaghetty* (Self-optimizing Python Automatic Generator of Hierarchically blockEd Tensor Transpose librarY), BSD-2.
https://code.google.com/p/spaghetty/
Contributions: Exclusive developer.

*Elemental*, BSD-3. http://libelemental.org/
Contributions: MPI and threading improvements; Blue Gene/Q maintenance.

**Tutorials:**

*PAMI Examples* (Examples of the IBM PAMI communication API), MIT license.
https://code.google.com/p/pami-examples/
Contributions: Primary author.

*HPCInfo* (Examples of various parallel programming APIs), BSD-3.
https://github.com/jeffhammond/HPCInfo
Contributions: Primary author.

*HPCinChemistryTutorial*, BSD and GPL.
https://code.google.com/p/hpcinchemistrytutorial/ and
https://bitbucket.org/jeffscience/nsf-si2-summer-school-slides/
Contributions: See VCS for attribution.

Students under my supervision have developed some amazing software of which I am at best a minor contributor. Examples:

- Cyclops Tensor Framework (http://ctf.eecs.berkeley.edu/)
- AQUARIUS (https://github.com/devinamatthews/aquarius)
- BLIS (https://code.google.com/p/blis/)

## Mentoring

**PhD Committee Membership**

David Ozog (Computer Science, University of Oregon)
Committee: Allen Malony (chair), Hank Childs, Boyanna Norris, me.

Martin Schatz (Computer Science, The University of Texas at Austin)
Committee: Robert van de Geijn (chair), Don Batory, Keshav Pingali, John Stanton, Tamara G. Kolda, me.

**Postdocs:** (2 total)

Álvaro Vázquez-Mayagoitia (March 2011 - present)
Affiliation: Leadership Computing Facility, Argonne National Laboratory
Project: Blue Gene/Q Early Science Program ("Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC").
Current position: Assistant Computational Scientist, Leadership Computing Facility, Argonne National Laboratory.

A. Eugene DePrince III (January 2010 - August 2010)
Affiliation: Center for Nanoscale Materials, Argonne National Laboratory
Project: Implementation of coupled-cluster theory for massively-parallel processors (e.g. GPUs).
Current position: Assistant Professor, Department of Chemistry, Florida State University.

**Graduate Students:** (16 total)

Yukina Yokoi (Fall 2013)
Affiliation: Department of Computer Science and Engineering, Toyohashi University of Technology
Project: Response theory for molecular DFT in MADNESS.

Tyler Smith (Summer 2013)
Affiliation: Computer Science, University of Texas
Project: Dense linear algebra (BLIS) for Blue Gene/Q.

Scott Rabidoux (Summer 2013)
Affiliation: Computational and Applied Mathematics, University of Texas
Project: Solvers for quasi-symmetric eigenvalue problems in equation-of-motion coupled-cluster theory.

Sayan Ghosh (Summer 2013)
Affiliation: Computer Science, University of Houston
Project: High-performance one-sided communication.

Priyanka Ghosh (Summer 2013)
Affiliation: Computer Science, University of Houston
Project: Reducing communication costs in the NWChem TCE.

David Ozog (Summer and Fall 2012)
Affiliation: Computer Science, University of Oregon
Project: Inspector-executor load-balancing for NWChem TCE.

Kevin Stock (Summer 2012)
Affiliation: Computer Science and Engineering, The Ohio State University

Project: Optimized tensor contraction kernels for MADNESS.

Edgar Solomonik (Summer 2011)
Affiliation: Computer Science, University of California, Berkeley
Project (DOE-CSGF practicum): Parallel tensor contractions for coupled-cluster methods.

Devin Matthews (Summer 2011)
Affiliation: Chemistry, The University of Texas at Austin
Project (DOE-CSGF practicum): Massively-parallel implementation of higher-order coupled-cluster methods.

Zheng (Cynthia) Gu (Summer 2011)
Affiliation: Computer Science, Florida State University
Project: Development of distributed lockless data-structures and one-sided communication optimization for non-equilibrium umbrella sampling.

Martin Schatz (Summer 2011)
Affiliation: Computer Science, The University of Texas at Austin
Project: Arbitrary-order symmetric tensor contraction kernels.

Alex Dickson (January 2010 - July 2011, full-time student with Prof. Aaron Dinner)
Affiliation: Chemistry, University of Chicago
Project: Implementation of non-equilibrium umbrella sampling on supercomputers using Global Arrays and OpenMP.
Current position: Postdoc at the University of Michigan.

Piotr Fidkowski (Summer 2010, primary mentor: Pavan Balaji)
Affiliation: Aerospace Engineering, Massachusetts Institute of Technology
Project (DOE-CSGF practicum): Implementing solid mechanics FEM solver for hybrid GPU-MPI parallelism.
Current position: Google.

Sreeram Potluri (Summer 2010)
Affiliation: Computer Science and Engineering, The Ohio State University
Project: Implementing ARMCI-style one-sided communication for Blue Gene/P.

Jack Poulson (Summer 2010)
Affiliation: Computational and Applied Mathematics, The University of Texas at Austin
Project: Optimizing parallel dense linear algebra (e.g. Cholesky factorization) for Blue Gene/P.
Current position: Assistant Professor, School of Computational Science and Engineering, Georgia Tech.

Kevin Stock (Summer 2010)
Affiliation: Computer Science and Engineering, The Ohio State University
Project: Developing compiler infrastructure for atomic integral generation.

**Undergraduate Students:** (6 total)

Ralf Gunter Correa Carvalho (Fall 2013)
Affiliation: University of Illinois, Urbana-Champaign
Project: Machine learning approaches to force-field development.

Cyrus Karshenas (Summer 2013)
Affiliation: Marquette University (soon to be at UCLA)
Project (SULI): Multithreading and MIC porting of NWChem.

Drew Lewis (Summer 2012)
Affiliation: University of Texas, Austin (now at Virginia Tech)
Project: Evaluation of parallel eigensolvers for quantum chemistry calculations.

Luke Westby (Summer 2012)
Affiliation: University of Notre Dame
Project: Parallelization of enhanced sampling methods.

Mladen Rasic (Summer 2012)
Affiliation: University of Chicago
Project: Parallelization of enhanced sampling methods.

Tyler Bonnen (Summer 2010, co-mentored with Nick Romero)
Affiliation: Chemistry, Columbia University
Project: Studying batteries, specifically lithium-aromatic interactions, using density-functional theory.

## Grants and Other Support

**Funding:**

*Autotuning for Exascale*
Investigators: Mary Hall, Paul Hovland, etc.
Sponsor: DOE-ASCR (X-stack)
Amount: approximately $4M over three years.

*A Linear Algebra Software Infrastructure for Sustainable Innovation in Computational Chemistry and other Sciences*
Investigators: Robert van de Geijn (PI at Texas), John Stanton,... and Jeff Hammond (PI at UChicago).
Sponsor: NSF SI2-SSI (Award #1148485)
Amount: approximately $1.5M over three years.

*Software for enabling ensemble parallelism with application to design of heat transfer fluids for solar thermal power applications*
Investigators: Aaron R. Dinner, Jeff R. Hammond and O. Anatole von Lilienfeld
Sponsor: University of Chicago–Argonne Strategic Collaborative Initiative
Amount: $75,000 for FY2012.

*Parallelization of a novel algorithm for simulating driven biomolecular systems*
Investigators: Aaron R. Dinner and Jeff R. Hammond
Sponsor: University of Chicago–Argonne Strategic Collaborative Initiative
Amount: $75,000 for FY2011.

*Chemistry Exascale Co-design Center (CECC)*
Investigators: R. J. Harrison (PI), E. Aprà, D. Hudson, W. A. de Jong, S. Krishnamoorthy, E. J. Bylaska, R. A. Bair, J. R. Hammond, W. M. Challacombe, R. E. Larsen, K. Kim, C. L. Janssen, J. Nørskov and F. Abild-Pedersen

Sponsor: DOE-ASCR
Amount: $800,000 in planning funds awarded in FY2011.

**Significant Supercomputer Allocations:**

*Computational Actinide Chemistry: Reliable Predictions and New Concepts*
Investigators: David Dixon, Jochen Autschbach, Enrique Batista, Aurora Clark, Wibe de Jong, Laura Gagliardi, Jeff Hammond, Richard Martin, Kirk Peterson, Gustavo Scuseria.
Sponsor/Resource: DOE INCITE program at OLCF and ALCF.
Amount: 250,000,000 hours 2014.

*Dynamic and Adaptive Parallel Programming for Exascale Research*
Investigators: Robert Harrison, George Fann, Jeff Hammond, P. Sadayappan, Eduard Valeev.
Sponsor/Resource: DOE INCITE program at ALCF.
Amount: 20,000,000 hours 2014.

*Development of new parameters for SEMO methods for transition metals and thorium*
Investigators: David Dixon, Al Wagner, Jeff Hammond.
Sponsor/Resource: Great Lakes Consortium for Petascale Computation to use Blue Waters.
Amount: 10,000,000 hours 2014.

*Toward Crystal Engineering From First Principles*
Investigators: James R. Chelikowsky, Noa Marom, Alexandre Tkatchenko, Jeff R. Hammond and O. Anatole von Lilienfeld.
Sponsor/Resource: ASCR Leadership Computing Challenge (ALCC) at ALCF
Amount: 16,000,000 hours FY2011.

*Materials Design From First Principles Calculations*
Investigators: Larry Curtiss, Stephen Gray, Jeffrey Greeley, Jeff Hammond, Nichols Romero and Peter Zapol
Sponsor/Resource: ASCR Leadership Computing Challenge (ALCC) at ALCF
Amount: 20,000,000 hours FY2010.

*Next-Generation Force Fields from Accurate Quantum Chemical Calculations*
Investigators: Karl F. Freed, Jeff R. Hammond, Alex MacKerell and Benoît Roux
Sponsor/Resource: NSF TeraGrid
Amount: 2,100,000 hours for 2009-2010.

*Ultra-high accuracy simulations for large molecular systems: Exploring the Cutting Edge Limits of NWChem*
Investigators: Karol Kowalski, Marat Valiev, Eric Bylaska and Jeff R. Hammond
Sponsor/Resource: Molecular Science Computing Facility, EMSL, Pacific Northwest National Laboratory
Amount: 1,800,000 hours for FY2009

*Development of accurate methods for non-bonded interactions in biological and acqueous environments*
Investigators: Jeff R. Hammond, Karl F. Freed, L. Ridgway Scott, Benoît Roux, Jean-François Truchon, Christopher Bayly, Karol Kowalski, Marat Valiev, Sotiris Xantheas, Jaydeep Bardhan and William A. Farone
Sponsor/Resource: Molecular Science Computing Facility, EMSL, Pacific Northwest National Laboratory
Amount: 6,720,000 hours for FY2008, 8,000,000 hours for FY2009, 8,000,000 hours for FY2010.

**Experimental User-Facility Awards:**

*Hetero-site-specific femtosecond-time-resolved dynamics*
Investigators: Antonio Picón, Steve Southworth, Phay Ho, Gilles Doumy, Elliot Kanter, Bertold Krässig, Anne Marie March, Dipanwita Ray, Linda Young, Steve Pratt, Jeff R. Hammond, Álvaro Vázquez-Mayagoitia, Niri Govind, Artem Rudenko, Christoph Bostedt, Daniel Rolles, Benjamin Erk, and Cedric Bomme.
Sponsor/Resource: SLAC National Accelerator Laboratory - Linac Coherent Light Source (LCLS)

## Computer Skills

Programming Languages (in descending order of skill): C, Fortran 77, LaTeX, Bash, Python, C++, Fortran 90/95/CAF, UPC, CUDA.
Programming Tools: Git, Mercurial, Subversion, Eclipse.
Parallel APIs: MPI-3, OpenSHMEM, OpenMP, Pthreads, Global Arrays, and Cray SHMEM, ARMCI, IBM DCMF and PAMI, Cray DMAPP.
Processor architectures: POWER/PowerPC (esp. Blue Gene), Intel x86 and MIC, NVIDIA Tesla family.
Chemistry Software: NWChem, MPQC, Dalton, PSI, ACES/CFOUR, GAMESS, Gaussian, LAMMPS.

## Professional Memberships

ACM – Association for Computing Machinery (since 2008)
SIAM – Society for Industrial and Applied Mathematics (since 2010)

## Service to the Scientific Community

- MPI Forum since 2009 (Working Groups / Chapter Committees: One-Sided Communication, Hybrid, Datatypes, The Info Object, External Interfaces, Language Bindings, Large-Count); involved in the OpenSHMEM, OpenMP, CPLEX and UPC standardization efforts.
- Associate Editor, *Frontiers in Theoretical and Computational Chemistry*; Technical Program Chair, Conference on Partitioned Global Address Space Programming Models (PGAS) 2014; Co-organizer, The LLVM Compiler Infrastructure in HPC workshop (LLVM-HPC) at SC14; Co-chair for publications, 27th International Conference on Supercomputing (ICS) 2013; Chair, Symposium on Application Accelerators in High Performance Computing (SAAHPC) 2012; Co-chair for computational chemistry, Symposium on Application Accelerators in High Performance Computing (SAAHPC) 2011; Program Committee member for: External Review Committee of ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP) 2015. Extended Review Committee of ACM International Conference on Supercomputing (ICS) 2014; Workshop on Accelerator Programming using Directives (WACCPD), Supercomputing 2014; Third International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing (WOLFHPC) 2013 and 2014; International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS) 2012, 2013, 2014; 26th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD) 2014; Doctoral Showcase Review Committee Member, Supercomputing 2013; ACM SIGPLAN Workshop on Memory Systems Performance and Correctness (MSPC) 2013; 24th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD) 2012; Special Session on Improving MPI User And Developer Interaction (IMUDI) 2012;
- Referee for: *Applied Mathematics and Computation*; *Journal of Chemical Physics*; *Journal of Chemical Theory and Computation*; *Molecular Physics*; *Journal of Physical Chemistry A*; *Journal of Physical Chemistry Letters*; *Physical Chemistry Chemical Physics*; *SIAM Journal on Scientific Computing*

(SISC); *Theoretical Chemistry Accounts*; *Transactions on Parallel and Distributed Systems*; *Computing in Science and Engineering*; The International Conference for High Performance Computing, Networking, Storage, and Analysis (Supercomputing); Parallel Architectures and Compilation Techniques (PACT); Conference on Partitioned Global Address Space Programming Models (PGAS); International Conference on Parallel and Distributed Systems (ICPADS); US Department of Energy INCITE program; US National Science Foundation.

- DOE-CSGF mentor (2009-present); application screening committee member (2011-present); Argonne lab coordinator (2013-present); co-organizer of the CSGF minisymposium at SIAM at PP10 (Miami, FL), CSE11 (Reno, NV), PP12 (Savannah, GA), CSE13 (Boston, MA), PP14 (Portland, OR).

## Argonne Committees and Service

- Committee on Quality Assurance of Science and Technology Information (2013).

## Other Service and Outreach Activities

- UChicago Board of Trustees Externship Program (job shadowing for undergraduates), (March 2012).
- Science fair judge for Chicago Public Schools (annually).
- Panelist, the Univerity of Chicago's Taking the Next Step (01/09/2010).
- Panelist, Miami Dade College Tools for Success Forum (3/04/2009).
- GED tutor at St. Martin De Porres House of Hope women's shelter (Fall 2008 - Fall 2009).
- Member of student committee for the redesign of the University of Chicago home page (Winter 2008).
- Member of student committee for the selection of the Dean of Rockefeller Chapel (Winter 2008).
- Member of panel on Academic Networking event sponsored by UC Grad. Affairs (10/30/2008).