Jeff R. Hammond

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Education and Research Positions

Intel Corporation - Data Center Group (September 2016 - present)
Title: Senior System Architect
Description: Hardware-software co-design for high-performance computing.

Intel Corporation - Parallel Computing Lab (May 2014 - August 2016)
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; DOE exascale activities.

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.

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)

Professional Memberships

ACM – Association for Computing Machinery (since 2008)

Journal Publications and Book Chapters

39. A. Amer, H. Lu, P. Balaji, Y. Wei, J. Hammond and S. Matsuoka. *ACM Transactions on Parallel Computing*. "Lock Contention Management in Multithreaded MPI." Online Preprint

38. M. Si, A. J. Peña, J. Hammond, P. Balaji, M. Takagi and Y. Ishikawa, *IEEE Transactions on Parallel and Distributed Systems* (2018). "Dynamic Adaptable Asynchronous Progress Model for MPI RMA Multiphase Applications." Online

37. Eric J. Bylaska, Edoardo Aprà, Karol Kowalski, Mathias Jacquelin, Wibe A. de Jong, Abhinav Vishnu, Bruce Palmer, Jeff Daily, Tjerk P. Straatsma, Jeff R. Hammond, Michael Klemm. In T. Straatsma, K. Antypas, T. Williams, (eds), *Exascale Scientific Applications.* New York: Chapman and Hall/CRC (2018). "Transitioning NWChem to the Next Generation of Manycore Machines." Online

36. A. Chien, P. Balaji, N. Dun, A. Fang, H. Fujita, K. Iskra, Z. Rubenstein, Z. Zheng, J. Hammond, I. Laguna, D. Richards, A. Dubey, B. van Straalen, M. Hoemmen, M. Heroux, K. Teranishi, and A. Siegel. *The International Journal of High Performance Computing Applications* **31** 6, 564-590 (2017). "Exploring versioned distributed arrays for resilience in scientific applications: global view resilience." Online

35. P. Springer, J. R. Hammond, P. Bientinesi. *ACM Transactions on Mathematical Software* (TOMS) **44**, 2 (2017). "TTC: A high-performance Compiler for Tensor Transpositions." Online Preprint

34. B. Peng, N. Govind, E. Apra, M. Klemm, J. R. Hammond, and K. Kowalski. *The Journal of Physical Chemistry A* (2017). "Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single Walled Carbon Nanotubes." Online

33. Robert J. Harrison, Gregory Beylkin, Florian A. Bischoff, Justus A. Calvin, George I. Fann, Jacob Fosso-Tande, Diego Galindo, Jeff R. Hammond, Rebecca Hartman-Baker, Judith C. Hill, Jun Jia, Jakob S. Kottmann, M-J. Yvonne Ou, Laura E. Ratcliff, Matthew G. Reuter, Adam C. Richie-Halford, Nichols A. Romero, Hideo Sekino, William A. Shelton, Bryan E. Sundahl, W. Scott Thornton, Edward F. Valeev, Álvaro Vázquez-Mayagoitia, Nicholas Vence, Yukina Yokoi. *SIAM Journal on Scientific Computing* **38** (5), S123-S142. "MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation." Online Preprint

32. A. E. DePrince III, J. R. Hammond, and C. D. Sherrill, in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, edited by Ross Walker and Andreas Goetz (Wiley, 2016). "Iterative Coupled-Cluster Methods on Graphics Processing Units"

31. H. Hu, Y.-F. Zhao, J. Hammond, E. Bylaska, E. Apra, H.J.J. van Dam, J. Li, N. Govind, and K. Kowalski. *Chem. Phys. Lett.* **644**, 235242 (2016). "Theoretical studies of the global minima and polarizabilities of small lithium clusters." Online

30. Sameer Varma, Mohsen Botlani, Jeff R. Hammond, H. Larry Scott, Joseph P.R.O. Orgel, Jay D. Schieber. *Proteins: Structure, Function, and Bioinformatics* (2015). "Effect of Intrinsic and Extrinsic Factors on the Simulated D-band Length of Type I Collagen." Online

29. A. Chien, P. Balaji, P. Beckman, N. Dun, A. Fang, H. Fujita, K. Iskra, Z. Rubenstein, Z. Zheng, R. Schreiber, J. Hammond, J. Dinan, I. Laguna, D. Richards, A. Dubey, B. van Straalen, M. Hoemmen, M. Heroux, K. Teranishi, and A. Siegel. *Procedia Computer Science* **51**, 29-38 (2015). "Versioned Distributed Arrays for Resilience in Scientific Applications: Global View Resilience." Online Preprint

28. E. Chow, X. Liu, S. Misra, M. Dukhan, M. Smelyanskiy, J. R. Hammond, Y. Du, X.-K. Liao and P. Dubey. *Int. J. High Perf. Com. Appl.* (2015). "Scaling up Hartree-Fock Calculations on Tianhe-2." Online Preprint

27. E. Chow, X. Liu, M. Smelyanskiy, and J. R. Hammond. *J. Chem. Phys.*, **142**, 104103 (2015). "Parallel scalability of Hartree-Fock calculations." Online Preprint

26. E. Apra, K. Kowalski, J. R. Hammond, and M. Klemm. *High Performance Parallelism Pearls*, edited by James Reinders and James Jeffers (Morgan Kaufmann, 3 Nov. 2014). "NWChem: Quantum Chemistry Simulations at Scale."

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

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Conference and Workshop Proceedings (peer-reviewed)

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26. Vishakha Agrawal, Michael J. Voss, Pablo Reble, Vasanth Tovinkere, Jeff Hammond, and Michael Klemm. *International Workshop on OpenMP* (IWOMP). Barcelona, Spain, Sept. 2018. "Visualization of OpenMP Task Dependencies Using Intel Advisor - Flow Graph Analyzer."

25. Eric J. Bylaska, Mathias Jacquelin, Wibe A. de Jong, Jeff R. Hammond, and Michael Klemm. In J. Kunkel, R. Yokota, M. Taufer, J. Shalf (eds), *High Performance Computing. ISC High Performance 2017. Lecture Notes in Computer Science*, vol 10524. "Performance Evaluation of NWChem Ab-Initio Molecular Dynamics (AIMD) Simulations on the Intel Xeon Phi Processor." Online **Best Paper Award at the IXPUG 2017 workshop.**

24. Y. Yan, J. R. Hammond, A. Alqazzaz, C. Liao. *International Workshop on OpenMP* (IWOMP). Nara, Japan, Oct. 2016. "A Proposal to OpenMP for Addressing the CPU Oversubscription Challenge." Online

23. A. Fanfarillo and J. R. Hammond. *EuroMPI*. Edinburgh, Scotland, Sept. 2016. "CAF Events Implementation Using MPI-3 Capabilities." Online

22. S. Ghosh, J. Hammond, A. J. Peña, P. Balaji, A. Gebremedhin and B. Chapman. *International Conference on Parallel Processing* (ICPP). Philadelphia, PA, August 16-19, 2016. "One-Sided Interface for Matrix Operations using MPI-3 RMA: A Case Study with Elemental." Online

21. R. Van der Wijngaart, A. Kayi, J. Hammond, G. Jost, T. St. John, S. Sridharan, T. Mattson, J. Nelson, and J. Abercrombie. *International Supercomputing Conference* (ISC). Frankfurt, Germany (June 20-22, 2016). "Comparing runtime systems with exascale ambitions using the parallel research kernels." Online

20. D. Ozog, A. Kamil, Y. Zheng, P. Hargrove, J. R. Hammond, A. Malony, W. de Jong, and K. Yelick. Proc. 30th Intl. Parallel and Distributed Processing Symp (IPDPS). Chicago, IL (May 23-27, 2016). "A Hartree-Fock Application using UPC++ and the New DArray Library." Online

19. K. Vaidyanathan, D. Kalamkar, K. Pamnany, J. Hammond, P. Balaji, D. Das, J. Park, and B. Joo. *The International Conference for High Performance Computing, Networking, Storage, and Analysis* (Supercomputing). Austin, TX (November 15-20, 2015). "Improving concurrency and asynchrony in multithreaded MPI applications using software offloading." Online

18. R. Van der Wijngaart, S. Sridharan, A. Kayi, G. Jost, J. Hammond, T. Mattson, and J. Nelson. *The 9th International Conference on Partitioned Global Address Space Programming Models* (PGAS). September 17-18, 2015. Washington, D.C. "Using the Parallel Research Kernels to study PGAS models." Online

17. M. Si, A. J. Peña, J. R. Hammond, P. Balaji, and Y. Ishikawa. *IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing* (CCGrid). May 4-7, 2015, Shenzhen, China. **Scalable Computing Challenge Finalist.** "Scaling NWChem with Efficient and Portable Asynchronous Communication in MPI RMA." Online Preprint

16. M. Si, A. J. Peña, J. Hammond, P. Balaji, M. Takagi, Y. Ishikawa. Proc. 29th Intl. Parallel and Distributed Processing Symp (IPDPS). Hyderabad, India, May 2015. "Casper: An Asynchronous Progress Model for MPI RMA on Many-Core Architectures." Online Preprint

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." Online 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." Online Preprint

13. D. Ozog, A. Malony, J. Hammond and P. 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." Online

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." Online 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." Online

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." Online 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." Online 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

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

C. Cantalupo, V. Venkatesan, J. R. Hammond, K. Czurylo, and S. Hammond *User Extensible Heap Manager for Heterogeneous Memory Platforms and Mixed Memory Policies*. March 18, 2015. Online

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

Internal Intel presentations are excluded from this list.

91. Eleventh International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2). Eugene, Oregon (August 13th, 2018). *All programming models are wrong but some are useful: Identifying productive abstractions for exascale simulation*. (Invited keynote)

90. Los Alamos National Laboratory (July 25, 2018). *Evaluating modern programming models using the Parallel Research Kernels*.

89. Intel eXtreme Performance User Group (IXPUG). King Abdullah University of Science and Technology, Thuwal, Saudi Arabia (April 23, 2018). *Evaluating data parallelism in C++ programming models using the Parallel Research Kernels*. (Invited)

88. Lawrence Livermore National Lab (February 15, 2017). *Exploring the exascale software design space using the Parallel Research Kernels and mini-apps*.

87. Department of Mechanical Engineering and Material Science (seminar). Duke University, Durham, NC (February 1, 2017). *Hardware and software technology for computational atomistic simulation*. (Invited)

86. Australian Symposium on Computational Chemistry. University of Western Australia, Perth, Australia (December 2, 2017). *Hardware and software technology for coupled-cluster theory*. (Invited - Pawsey Plenary Lecture)

85. ELSI meeting University of California, Berkeley, CA (August 2017). *Hardware and software technology for computational atomistic simulation.* (Invited)

84. Third Scalable Hierarchical Algorithms for eXtreme Computing (SHAXC-3) workshop. King Abdullah University of Science and Technology, Thuwal, Saudi Arabia (May 9-11, 2016). *Comparing Runtime Systems With Exascale Ambitions Using The Parallel Research Kernels*. (Invited)

83. Third Scalable Hierarchical Algorithms for eXtreme Computing (SHAXC-3) workshop. King Abdullah University of Science and Technology, Thuwal, Saudi Arabia (May 9-11, 2016). *MPI: As easy as 2, 3, 4 - Why most of what you think you know about MPI is wrong*.

82. To Thread or Not To Thread minisymposium, SIAM Conference on Parallel Processing, Paris, France (April 12-15, 2016). *Threads: the Wrong Abstraction and the Wrong Semantic*. (Invited)

81. Preparing for the Real World: Challenges Faced by Young Investigators symposium, American Chemical Society national meeting, San Diego, CA (March 13, 2016). *Down the rabbit hole: from B3LYP to x86*. (Invited)

80. Scientific Software Days, University of Texas, Austin, TX (February 25-26, 2016). *MPI: As easy as 2, 3, 4 - Why most of what you think you know about MPI is wrong*. (Invited)

79. Challenges and Opportunities for Exascale Computational Chemistry symposium, Pacifichem conference, Honolulu, HI (Dec 15-20, 2015). *Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers*. (Invited)

78. The 9th International Conference on Partitioned Global Address Space Programming Models (PGAS), Washington, D.C. (September 17-18, 2015). *Lessons learned from Using MPI-3 as a PGAS Runtime System*. (Invited)

77. ALCF Theta Early Science Program: Training Session, Argonne National Laboratory (September 9, 2015). *Usage models and APIs for Intel Knights Landing In-Package Memory*.

76. Electronic Structure Theory for Large Systems symposium, American Chemical Society national meeting, Boston, MA (August 16-20, 2015). *Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers*. (Invited)

75. Novel computational methods for quantitative electronic structure calculations, Kobe University & RIKEN AICS, Kobe, Japan, (June 16-20, 2015). *Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers*. (Invited)

74. Florida (American Chemical Society) Annual Meeting and Exhibition (FAME), Tampa, FL, May 8, 2014. *Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers*.

73. Sarkar/Mellor-Crummey groups, Department of Computer Science, Rice University, Houston, TX, January 21, 2015. *All programming models are wrong, but some are useful - what we really need to survive exascale*.

72. Workshop on Exascale MPI at Supercomputing Conference 2014 (ExaMPI14), New Orleans, LA, November 17, 2014. *To INT_MAX... and beyond! Exploring large-count support in MPI*.

71. The 27th annual Pacific Northwest Numerical Analysis Seminar (PNWNAS), Portland State University, Portland, Oregon (October 18, 2014). *High-performance tensor computations in quantum chemistry*.(Invited)

70. 8th International Conference on Partitioned Global Address Space Programming Models (PGAS14), Eugene, Oregon, USA (October 10, 2014). *All programming models are wrong, but some are useful - what we really need to survive exascale*. (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*.

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: OpenMP in semidirect CCSD(T) and TCE; TCE coupled-cluster response properties; porting to HPC architectures; other performance and functional improvements.

One-Sided Communication:

ARMCI-MPI (ARMCI over MPI-RMA), BSD-3.
https://github.com/jeffhammond/armci-mpi
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.

Global Arrays, BSD.
http://www.emsl.pnl.gov/docs/global/.
Contributions: Thread-safety; Blue Gene support.

Other Libraries:

BigMPI (Implementation of MPI that supports large counts), BSD-3.
https://github.com/jeffhammond/bigmpi
Contributions: Lead developer.

Tutorials:

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

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://github.com/flame/blis)
- Elemental (http://libelemental.org/)

Computer Skills

Please do not trust my assessement - you can verify and make your own evaluation using my open-source projects on Github, etc.

Programming Languages (in descending order of skill): C11, Fortran 77/90/95/03/08 (incl. coarrays), C++17, Bash, LaTeX, Python, CUDA.
Programming Tools: Git (primary), Subversion, Mercurial; VI (primary), Eclipse; GNU Make, Autotools, CMake; Travis Continuous Integration (CI); TAU, gprof, Vtune.
Parallel APIs: MPI 3.1, OpenMP 4.5, OpenCL 1.2, C++17 parallel STL and things like it (Boost.Compute, RAJA, Kokkos), Intel Threading Building Blocks (TBB), POSIX threads, OpenSHMEM and Cray SHMEM, Global Arrays and ARMCI, IBM DCMF and PAMI, Cray DMAPP.
Processor architectures: Intel Xeon and Xeon Phi, POWER/PowerPC (esp. Blue Gene), NVIDIA Tesla and Fermi, ARM (32-bit).

Service to the Scientific Community

Standardization efforts

- MPI Forum (2009-present): Working Groups / Chapter Committees: One-Sided Communication, Hybrid, Datatypes, The Info Object, External Interfaces, Language Bindings, Large-Count (chair).
- ISO C++ (2017-present): SG1 (parallelism), SG14 (performance), heterogeneity WG.
- OpenMP (2014-present)
- OpenSHMEM (2012-present)
- UPC (2013-2014)

Program Committees

- 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
- Co-chair for PhD Forum, International Conference on Parallel Processing (ICPP) 2018
- 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:
  - The International Conference for High Performance Computing, Networking, Storage, and Analysis (Supercomputing): Doctoral Showcase (2013), Tutorials (2015), Performance Measurement, Modeling, and Tools (2016), State of the Practice (2017), Programming Systems (2017), Clouds & Distributed Computing (2018)
  - IEEE International Parallel & Distributed Processing Symposium, 2017
  - 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

- International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS) 2012, 2013, 2014, 2015, 2016, 2017
- Workshop on Accelerator Programming using Directives (WACCPD), Supercomputing 2014, 2015, 2016, 2017
- The LLVM Compiler Infrastructure in HPC workshop (LLVM-HPC) (part of Supercomputing) 2015, 2016, 2017
- Workshop on Memory Centric Programming for HPC (MCHPC) 2017
- Third International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing (WOLFHPC) 2013 and 2014
- International European Conference on Parallel and Distributed Computing (Euro-Par) 2016
- International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD) 2012, 2014
- International Conference On Computational Science (ICCS) 2015, 2016, 2017
- Conference on Partitioned Global Address Space Programming Models (PGAS) 2015
- IEEE International Conference on Computational Science and Engineering (CSE) 2015
- International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS) 2018
- International Workshop on Accelerators and Hybrid Exascale Systems (AsHES) 2015, 2016, 2017, 2018
- Chapel Implementers and Users Workshop (CHIUW) 2015, 2016, 2017, 2018
- International Workshop on Extreme Scale Programming Models and Middleware (ESPM) 2016, 2017
- PGAS Applications Workshop (PAW) 2016, 2017
- Workshop on Exascale MPI (ExaMPI) 2016
- Workshop on Representative Applications (WRAp) 2017, 2018
- Workshop on OpenSHMEM and Related Technologies 2015, 2016
- Programming Models, Languages and Compilers for Manycore and Heterogeneous Architectures (PLC) (part of IPDPS) 2015
- ACM SIGPLAN Workshop on Memory Systems Performance and Correctness (MSPC) 2013
- Special Session on Improving MPI User And Developer Interaction (IMUDI) 2012

Journal Refereeing

- *Applied Mathematics and Computation*
- *Computing in Science and Engineering*
- *Computer Physics Communications* (CPC)
- *Concurrency and Computation: Practice and Experience* (CCPE)
- *International Journal of High Performance Computing Applications* (IJHPCA)
- *Journal of Chemical Physics* (JChP)
- *Journal of Chemical Theory and Computation* (JCTC)
- *Journal of Physical Chemistry A* (JPCA)
- *Journal of Physical Chemistry Letters*
- *Molecular Physics*
- *Physical Chemistry Chemical Physics* (PCCP)
- *SIAM Journal on Scientific Computing* (SISC)
- *Theoretical Chemistry Accounts* (TCA)
- ACM *Transactions on Mathematical Software* (TOMS)
- IEEE *Transactions on Architecture and Code Optimization* (TACO)
- IEEE *Transactions on Parallel and Distributed Systems* (TPDS)

Other Refereeing

- EU Partnership for Advanced Computing in Europe (PRACE) program
- US Department of Energy INCITE program
- US Department of Energy Exascale Computing Project (ECP)
- US Department of Energy Office of Advanced Scientific Computing Research (ASCR)
- US National Science Foundation
- US Department of Energy Computational Science Graduate Fellowship (CSGF) application screening committee member (2011-2014, 2016-2018)