

## Jeff R. Hammond

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### Overview

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I develop massively-parallel quantum chemistry programs and the software tools which enable them, focusing on leadership-class supercomputers and accelerator-equipped clusters. In graduate school, I wrote the coupled-cluster linear-response property code in NWChem, the first parallel implementation thereof, and applied it to previously impossible problems. Presently, my research focuses on one-sided and active-message communication on next-generation interconnects, global address and task space models programming models, performance analysis of scientific codes, GPU and multicore software development and the application of high-performance computing to chemistry problems in biology and energy storage/production.

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### Education and Research Positions

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#### **Argonne National Laboratory - Leadership Computing Facility** (June 2011 - present)

Title: Assistant Computational Scientist

Supervisor: Dr. Ray Bair

Description: Development of quantum chemistry algorithms, one-sided communication software and asynchronous programming models for multi-petaflop supercomputers.

#### **The University of Chicago - Computation Institute** (February 2011 - present)

Title: Fellow (since September 2011)

#### **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 one-sided communication software for Blue Gene/P.

#### **Pacific Northwest National Laboratory** (June 2006 - May 2009)

Supervisors: Drs. Wibe A. de Jong and Karol Kowalski

Description: Developed coupled-cluster molecular property module and other features in NWChem.

#### **University of Chicago** (September 2003 to May 2009)

Supervisors: Professors Karl F. Freed and L. Ridgway Scott

Thesis: *Coupled-cluster response theory: parallel algorithms and novel applications*

PhD in chemistry, May 2009

MS in Chemistry, August 2004

#### **University of Washington** (January 2001 to August 2003)

Supervisor: Professor Weston T. Borden

Thesis: *Evaluating the Bishomoaromatic Nature of Diaminodiformylsemibullvalene*

BS in Chemistry with Distinction, Minor in Applied Mathematics

BA in Mathematics

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### Honors and Awards

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Director's Postdoctoral Fellowship, Argonne National Laboratory (2009)

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)

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### Journal Publications and Book Chapters

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X. J. R. Hammond, S. Krishnamoorthy, S. Shende, N. A. Romero and A. D. Malony, accepted to *Concurrency and Computation: Practice and Experience*. "Performance Characterization of Global Address Space Applications: A Case Study with NWChem."

19. J. Dinan, S. Krishnamoorthy, P. Balaji, J. R. Hammond, M. Krishnan, V. Tipparaju and A. Vishnu, in *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."

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."

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."

16. K. Kowalski, J. R. Hammond, W. A. de Jong, P.-D. Fan, M. Valiev, D. Wang and N. Govind, in *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."

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."

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."

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."

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

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  $C_{60}$ ."

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."

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

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."

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."

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."
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."
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."
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)."
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."

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### Conference/Workshop Proceedings and Technical Reports

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8. 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."
7. J. Dinan, S. Krishnamoorthy, P. Balaji, J. R. Hammond, etc., Preprint ANL/MCS-P1914-0711, Mathematics and Computer Science Division, Argonne National Laboratory, July 2011. "Noncollective Communicator Creation in MPI."
6. J. R. Hammond, J. Dinan, P. Balaji, S. Potluri, and V. Tipparaju, Preprint ANL/MCS-P1880-0411, Mathematics and Computer Science Division, Argonne National Laboratory, April 2011. "OSPRI: An Optimized One-Sided Communication Runtime for Leadership-Class Machines."
5. J. Dinan, P. Balaji, J. R. Hammond, V. Tipparaju, Preprint ANL/MCS-P1878-0411, Mathematics and Computer Science Division, Argonne National Laboratory, April 2011. "High-Level, One-Sided Programming Models on MPI: A Case Study with Global Arrays and NWChem."
4. A. Dickson, M. Maienshein-Cline, A. Tovo-Dwyer, J. R. Hammond and A. R. Dinner, arXiv:1104.5180, "Flow-dependent unfolding and refolding of an RNA by nonequilibrium umbrella sampling."
3. J. Poulson, B. Marker, J. R. Hammond, N. A. Romero, and R. van de Geijn. FLAME Working Note #44. The University of Texas at Austin, Department of Computer Science. Technical Report TR-10-20. June, 2010. Revised January 2011. "Elemental: A New Framework for Distributed Memory Dense Matrix Computations."
2. J. R. Hammond and A. E. DePrince III, Symposium on Application Accelerators in High Performance Computing (SAAHPC), Knoxville, Tennessee (July 13-15, 2010). "Evaluating One-Sided Programming Models for GPU Cluster Computations."
1. 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."

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### Presentations

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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 4th, 2011). *New frontiers in quantum chemistry using supercomputers.* (invited)
40. University of Minnesota; Minneapolis, MN (April 22nd, 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 2nd, 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 24th, 2011). *New frontiers in quantum chemistry using supercomputers.* (invited)
36. Texas Advanced Computer Center (TACC); Austin, TX (February 23rd, 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 21st, 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 8th, 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 8th, 2011). *New Frontiers in Quantum Chemistry Using Supercomputers.* (invited)
32. Jülich Supercomputing Centre; Jülich, Germany (February 7th, 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 26th, 2011). *Quantum chemistry many-body methods on GPUs and multicore CPUs.*
30. Argonne Booth Talk, Supercomputing; New Orleans, LA (November 15th, 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 10th, 2010). *Computational Chemistry Beyond Petascale.*
28. Laboratory Computing Resource Center (LCRC) Quantum Chemistry Workshop; Argonne, IL (November 5th, 2010). *NWChem Tutorial.*
27. HPC Workshop, Computation Institute, University of Chicago; Chicago, IL (September 14th, 2010). *Parallel Programming Models and Scientific Algorithms.*
26. Argonne Postdoc Symposium, Argonne National Laboratory; Argonne, IL (September 8th, 2010). *Quantum chemistry at petascale and beyond on Blue Gene/P and Blue Gene/Q.*
25. SciDAC 2010; Chattanooga, TN (July 15th, 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 21st, 2010). *The five most important things I've learned about high performance computing.*
23. Student Lecture Series, MCS Division; Argonne, IL (June 8th, 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 22th, 2010). *New frontiers in quantum chemistry using supercomputers.*
20. LANS Seminar, MCS Division, Argonne National Laboratory; Argonne, IL (November 24th, 2009). *Quantum chemistry for computer scientists.*
19. MPI Forum; Portland, OR (November 12th, 2009). *A critical analysis of the MPI-3 RMA interface.*
18. Swiss National Supercomputing Centre Users' Day; Manno, Switzerland (September 11th, 2009). *Accurate quantum chemical simulations of large molecules using supercomputers.* (invited)
17. American Chemical Society National Meeting; Washington, DC (August 18th, 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 26th, 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 29th, 2009). *Untitled.*
14. Rawal group meeting, Department of Chemistry, The University of Chicago; Chicago, IL (May 11th, 2009). *Computational approaches for understanding hydrogen-bonding.*
13. SIAM Conference on Computational Science and Engineering; Miami, FL (March 2nd, 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 16th, 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 1st, 2008). *Accurate molecular property calculations using supercomputers: algorithms and applications.*
10. American Chemical Society National Meeting; New Orleans, LA (April 7th, 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 19th, 2007). *E Pluribus Duo* (old title, new talk).
8. Department of Chemistry, Cornell University; Ithaca, NY (June 14th, 2007). *Quantum many-body theory without so many bodies.*
7. The Twelfth Annual James Franck Institute Symposium, The University of Chicago; Chicago, IL (May 17th, 2007). *E Pluribus Duo.*
6. American Chemical Society National Meeting; Chicago, IL (March 27th, 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 7th, 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 8th, 2007). *Massively parallel many-body methods for hard systems*.
3. Chemistry Department Tiger Talk, The University of Chicago; Chicago, IL (April 26th, 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 29th, 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 16th, 2003). *Bishomoaromaticity in the Cope rearrangement of semibullvalene*.

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## Posters

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13. Supercomputing 2010; New Orleans, LA (November 17th, 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 17th, 2009). *Scalability of quantum chemistry codes on BlueGene/P and challenges for sustained petascale performance*.
10. SciDAC 2009; San Diego, CA (June 14th, 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 25th, 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 21st, 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 18th, 2008). *Coupled-cluster theory on supercomputers*. (with K. Kowalski)
6. American Chemical Society National Meeting, New Orleans, LA (April 8th, 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 25th, 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 21st, 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 18th, 2005). *Variational reduced-density-matrix calculations on open-shell systems*. (with D. A. Mazziotti)
2. 30th Reaction Mechanisms Conference, Northwestern University; Evanston, IL (June 25th, 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 24th, 2003). *PCET vs. HAT in ribonucleotide reductase: a DFT study*. (with D. A. Hrovat and W. T. Borden)

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## Software

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*OSPRI* (One-Sided PRimitives), Argonne National Laboratory, Argonne, IL 60439, USA. BSD-style License (2010). Contributions: I designed this framework and am the primary developer.

*AI* (Argonne 1-sided – a completely new implementation of ARMCI for Blue Gene/P), Argonne National Laboratory, Argonne, IL 60439, USA. BSD-style License (2010). Contributions: I designed and co-authored this library.

*NWChem, A Computational Chemistry Package for Parallel Computers, Version 6.0* (2010), Pacific Northwest National Laboratory, Richland, WA 99352-0999, USA. Contribution: CCSD imaginary-frequency dynamic polarizabilities and the associated solvers, double-hybrid DFT functionals (i.e. B2PLYP) with all three MP2 modules, SCS-RIMP2.

*NWChem, A Computational Chemistry Package for Parallel Computers, Version 5.1.1* (2009), Pacific Northwest National Laboratory, Richland, WA 99352-0999, USA. Contributions: linear response dynamic polarizabilities at the CCSDTQ levels of theory, hybrid out-of-core integral transformation algorithms, CCSD quadratic response and hyperpolarizabilities.

*NWChem, A Computational Chemistry Package for Parallel Computers, Version 5.1* (2007), Pacific Northwest National Laboratory, Richland, WA 99352-0999, USA. Contributions: linear response dynamic polarizabilities at the CCSD and CCSDT levels of theory.

*Global Arrays 5.0*, Copyright 2010, Battelle Memorial Institute. Contributions: Performance optimizations and other improvements.

*Global Arrays 4.3*, Copyright 2010, Battelle Memorial Institute. Contributions: Performance optimizations in the DCMF (Blue Gene/P) port of ARMCI.

*Spaghetti* (Self-optimizing Python Automatic Generator of Hierarchically blockEd Tensor Transpose librarY), GNU General Public License v3 (2008). Contributions: I am the exclusive author of this program.

I ported MPQC and Dalton to the Blue Gene/P architecture and made changes which enabled their efficient execution on more than 100,000 and 1,000 processors, respectively.

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## Mentoring

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### Postdocs:

Alvaro Vazquez-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”).

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).

### Graduate Students:

Edgar Solomonik (Summer 2011)

Affiliation: Computer Science, University of California, Berkeley

Project (DOE-CSGF practicum): dynamic load-balancing and parallel performance optimization of quantum chemistry codes.

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: optimization of one-sided communication in MPICH2 and development of distributed lockless data-structures for non-equilibrium umbrella sampling.

Martin Schatz (Summer 2011)  
Affiliation: Computer Science, The University of Texas at Austin  
Project: tensor contraction semantics, algorithms and implementations.

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.

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.

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.

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

### **Undergraduate Students:**

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

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## **Grants and Other Support**

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### **Funding:**

*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.

*Open GATS: An Open Unified Framework for Global Address and Task Space Computing in the Exascale Era*  
Investigators: Pavan Balaji, Jeff R. Hammond and Nichols A. Romero  
Sponsor: Argonne LDRD  
Amount: \$300,000 for FY2011.

*Correlated electronic structure simulations of materials: advanced algorithms for Blue Gene/P and Q*  
Investigators: Nichols A. Romero and Jeff R. Hammond

Sponsor: Argonne LDRD  
Amount: \$140,000 for FY2010.

### **Significant Supercomputer Allocations:**

#### *Toward Crystal Engineering From First Principles*

Investigators: James R. Chelikowsky, Noa Marom, Alexandre Tkatchenko, Jeff R. Hammond and O. Anatole von Lilienfeld. Sponsor: ASCR Leadership Computing Challenge  
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: ASCR Leadership Computing Challenge  
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: NSF TeraGrid  
Amount: 2,100,000 hours for 2009-2010.

#### *PArallel Run-Time Systems (PARTS): GA/ARMCI, UPC/GASNet, Charm++, Chapel, X10, etc.*

Investigators: Jeff R. Hammond  
Sponsor: Argonne Leadership Computing Facility (ALCF)  
Amount: 2,000,000+ hours for 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: 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 aqueous 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  
Facility: 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.

#### *Testing and tuning NWChem for BlueGene/P and studies of nonlinear optical properties of conjugated chromophores*

Investigators: Jeff R. Hammond  
Sponsor: Argonne Leadership Computing Facility (ALCF)  
Amount: millions of hours per year for 2008-present.

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### **Computer Skills**

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Programming Languages: C, Fortran 77, Python, Fortran 90/95, C++, CUDA  
Programming Tools: Eclipse, CVS, SVN, Git  
Parallel APIs: MPI, Global Arrays, ARMCI, IBM DCMF, IBM PAMI, Cray DMAPP, OpenMP, Pthreads  
Other Languages: Matlab, Mathematica, L<sup>A</sup>T<sub>E</sub>X, HTML  
Chemistry Software: NWChem, MPQC, Dalton 2, PSI 3, ACES II (MAB), Gaussian, GAMESS

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### **Service to the Scientific Community and Beyond**

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- 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.
- Referee for *Journal of Chemical Physics*; *Journal of Chemical Theory and Computation*; *Theoretical Chemistry Accounts*; *Molecular Physics*; The International Conference for High Performance Computing, Networking,

Storage, and Analysis (Supercomputing); Parallel Architectures and Compilation Techniques (PACT); US Department of Energy INCITE program; US National Science Foundation MRI program.

- Science fair judge for Chicago Public Schools (annually)
- DOE-CSGF mentor (2009-present) and application screening committee (2011-present)
- Co-organizer of the DOE-CSGF symposium at SIAM PP10 (Miami, FL) and CSE11 (Reno, NV).
- The University of Chicago's Taking the Next Step (01/09/2010)
- Career Panelist, Miami Dade College Tools for Success Forum (3/04/2009)
- GED tutor at St. Martin De Porres House of Hope (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)

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## Workshops and Summer Schools

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Frequent attendee of the MPI Forum since 2009.

Global Arrays Technical Meeting (invitee)

Pacific Northwest National Laboratory — Seattle, WA (May 6-7, 2010)

Unconventional Wisdom Workshop (attendee)

Sandia National Laboratory — San Francisco, CA (January 19-21, 2010)

High-Performance Computing in Chemistry Tutorial (organizer)

University of Tennessee — Knoxville, TN (August 3-7, 2009)

NVIDIA Workshop (attendee)

Argonne National Laboratory — Argonne, IL (March 30, 2009)

Numerical Approaches to Quantum Many-Body Systems (attendee)

University of California, Los Angeles — Los Angeles, CA (January 22-30, 2009)

Young Investigators Symposium (invitee)

Oak Ridge National Laboratory — Oak Ridge, TN (October 13-15, 2008)

Accelerators for Science and Engineering Applications: GPUs and Multicores (attendee)

National Center for Supercomputing Applications — Urbana, IL (August 18-22, 2008)

Leap to Petascale BlueGene/P workshop (attendee)

Argonne National Laboratory — Argonne, IL (July 29-31, 2008)

Workshop on Programming Massively Parallel Processors (attendee)

National Center for Supercomputing Applications — Urbana, IL (July 10, 2008)

PSI developer's workshop (attendee)

Virginia Tech — Blacksburg, GA (February 22-23, 2007)

Eighth Workshop on the DOE Advanced Computational Software (ACTS) Collection (attendee)

Lawrence Berkeley National Laboratory — Berkeley, CA (August 21-24, 2007)

NWChem Meeting on Science Driven Petascale Computing and Capability Development (attendee)

Pacific Northwest National Laboratory — Richland, WA (January 24-25, 2007)

European Summer School in Quantum Chemistry (attendee)

Lund University — Lund, Sweden (August 17-30, 2003).

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## **Professional Memberships**

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ACS – American Chemical Society (since 2004)

ACM – Association for Computing Machinery (since 2008)

SIAM – Society for Industrial and Applied Mathematics (since 2010)