David Edward Bernholdt

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Degrees

Ph. D. in Chemistry, with minors in Physics and Mathematics, and Certification in Chemical Physics, 1993, University of Florida, Gainesville, Florida. Thesis: *Triple Excitation Effects in the Fock Space Coupled Cluster Method.* Advisor: R. J. Bartlett.

B. S. in Chemistry *Cum Laude*, with Highest Distinction, 1986, University of Illinois, Urbana, Illinois. Honors thesis: *An* Ab Initio *Study of the H_2-HF Complex.* Advisor: C. E. Dykstra.

Research Experience

Senior Research Scientist and Alex G. Nason Fellow, Northeast Parallel Architectures Center, Syracuse University, September 1995–present.

Additional Affiliations: **Research Assistant Professor, Department of Chemistry, Syracuse University, June 1996–present. Affiliate Staff Scientist, Pacific Northwest Laboratory, August 1995–present.**

Advancement of Chemistry as a Computational Science through research at the interface of chemistry and computer science. Development of novel methods for the treatment of large-scale correlated electronic structure calculations. Development of parallel algorithms for quantum chemistry. Major contributor to the NWChem parallel computational chemistry software package. Applications of quantum chemistry to problems in spectroscopy, atmospheric chemistry, the environment and other areas in collaboration with researchers at Syracuse, Pacific Northwest National Laboratory, and elsewhere.

Activities in other areas of computational science, including distributed computing frameworks, network-based collaboration, distance education. Management of work on computational science research contracts totaling $1.8M/yr.

AWU Postdoctoral Fellow, High Performance Computational Chemistry Group, Environmental Molecular Sciences Laboratory, Pacific Northwest Laboratory, March 1993–August 1995. Advisor: R. J. Harrison.

Development of novel methods for the treatment of large-scale correlated electronic structure calculations. Development of parallel algorithms for novel and traditional methods in quantum chemistry. Major contributor to the NWChem software architecture and associated tools. Applications of quantum chemistry to problems of environmental and materials-related interest in collaboration with other researchers at PNNL.

Graduate Research Assistant, University of Florida, Summer 1987–Spring 1993. Advisor: R. J. Bartlett.

Evaluation of structure, energetics, vibrational spectra, and other properties of small carbon clusters, reaction intermediates, etc., using MBPT and CC methods. Contributed to the development and implementation of new methods to improve the accuracy and broaden the applicability of coupled-cluster-based approaches, especially the Fock-Space Coupled Cluster method. Strongly involved in the development of programs used within the group: GRNFNC, ACES, and ACES II, and other codes.

Undergraduate Research, University of Illinois, Fall 1984–Summer 1986. Advisor: C. E. Dykstra.

Determination of the structure and properties of astrochemical species, and weakly bonded molecular complexes using self-consistent field (SCF) and correlated methods. Helped with porting and performance optimization of computational codes for new computer architectures. Participated in the development of a new code to evaluate electron repulsion integrals.

Chemist, Instrument Services Group, Amoco Corporation, Naperville, Illinois, Summers 1984–1985. Supervisor: E. Watson.

Assisted in the development of techniques for on-line process stream analysis involving UV-Vis and far infrared spectroscopy, mass spectrometry, and other techniques.

Teaching Experience

Florida School on Applied Molecular Orbital Theory, Quantum Theory Project, University of Florida, May 1987–1990.

Physical Chemistry Laboratory (4411L), University of Florida, Spring 1987.

General Chemistry (2041 and 2045L), University of Florida, Fall 1986.

Physical Chemistry Lab II (385), University of Illinois, Spring 1986.

General Chemistry (101), University of Illinois, Fall 1985.

Honors

Alex G. Nason Fellowship, Northeast Parallel Architectures Center, Syracuse University

Shell Fellow, Department of Chemistry, University of Florida

Chemical Physics Fellowship, Center for Chemical Physics, University of Florida

Phi Lambda Upsilon (national chemical sciences honor society)

Phi Kappa Phi (national academic honor society)

Kodak Freshman Fellowship, University of Illinois

Memberships

American Chemical Society. Physical Chemistry Division and Theoretical Chemistry Subdivision.

American Physical Society. Chemical Physics and Computers in Physics Divisions.

Association for Computing Machinery.

Personal information

U. S. citizen, born in Clearfield, Pennsylvania on 26 October 1964.

External Funding

Pacific Northwest National Laboratory, 12/96-present, $258,000. This is an on-going research contract which has supported my research activities in new methods for correlated electronic structure calculations.

Proposals in Preparation

- "Effect of the Solvent on Reactions of $XONO_2$ in Solution and Aerosols", with Theodore S. Dibble, Dept. of Chemistry, SUNY ESF. For submission to NSF.
- "Methods for Large-Scale Correlated Electronic Structure Calculations on Parallel Computers." For submission to NSF, DOE.
- "Chemistry in the Internet Age: A Model for a New Generation of Highly-Interconnected Computational Chemistry Software." For submission to NSF, DOE.
- "Development of Methodologies for Performance Prediction of Scalable Applications on Future MPP Architectures", with researchers at the Pacific Northwest National Laboratory and IBM TJ Watson Research Center. For submission to DOE.

Publications

[1] John B. Nicholas, David E. Bernholdt, and Benjamin P. Hay, On the Conformational Energetics of Tetramethoxycalix[4]arene: RI-MP2 Benchmark Calculations, *J. Am. Chem. Soc.* (submitted).

[2] David E. Bernholdt, Scalability of Correlated Electronic Structure Calculations on Parallel Computers: A Case Study of the RI-MP2 Method, *Parallel Computing* (in press).

[3] David E. Bernholdt and Rodney J. Bartlett, A Critical Assessment of Multireference Fock-Space CCSD and Perturbative Third-Order Triples Approximations for Photoelectron Spectra and Quasidegenerate Potential Energy Surfaces, *Adv. Quantum Chem.* **34**, 271 (1999).

[4] David E. Bernholdt, Geoffrey C. Fox, Roman Markowski, Nancy J. McCracken, Marek Podgorny, Thomas R. Scavo, Debasis Mitra, and Qutaibah Malluhi, Synchronous Learning at a Distance: Experiences with TANGO, in *SC'98 Conference*, Institute of Electrical and Electronics Engineers and Association for Computing Machinery, 1998.

[5] David E. Bernholdt, Object Oriented Methods Without Object Oriented Languages, in Michael E. Henderson, Christopher R. Anderson, and Stephen L. Lyons, editors, *Object Oriented Methods for Inter-operable Scientific and Engineering Computing. Proceedings of the 1998 SIAM Workshop*, volume 99 of *Proceedings in Applied Mathematics*, pages 40–49, Society for Industrial and Applied Mathematics, 1999.

[6] Meenakshi A. Kandaswamy, Mahmut T. Kandemir, Alok N. Choudhary, and David E. Bernholdt, An Experimental Study to Analyze and Optimize Hartree-Fock Application's I/O with PASSION, *Int. J. High Perf. Computing Appl.* **12**, 411 (1998).

[7] Meenakshi A. Kandaswamy, Mahmut T. Kandemir, Alok N. Choudhary, and David E. Bernholdt, Performance Implications of Architectural and Software Techniques on I/O-Intensive Applications, in *1998 International Conference on Parallel Processing (ICPP'98)*, IEEE Computer Society Press, 1998.

[8] David E. Bernholdt and Robert J. Harrison, Fitting Basis Sets for the RI-MP2 Approximate Second-Order Many-Body Perturbation Theory Method, *J. Chem. Phys.* **109**, 1593 (1998).

[9] Meenakshi A. Kandaswamy, Mahmut T. Kandemir, Alok N. Choudhary, and David E. Bernholdt, Optimization and Evaluation of Hartree-Fock Application's I/O with PASSION, in *SC'97 Conference*, Institute of Electrical and Electronics Engineers and Association for Computing Machinery, 1997.

[10] David E. Bernholdt and Geoffrey C. Fox, Internet Resource Discovery for Chemistry – Where are Those Vast Untapped Resources?, *Trends Anal. Chem.* **16**, 230 (1997), available via WWW as http://www.elsevier.nl:80/inca/homepage/saa/trac/resource.htm.

[11] M.F.Guest, E.Apra, D.E.Bernholdt, H.A.Fruchtl, R.J.Harrison, R.A.Kendall, R.A.Kutteh, X.Long, J.B.Nicholas, J.A.Nichols, H.L.Taylor, A.T.Wong, G.I.Fann, R.J.Littlefield, and J.Nieplocha, High-performance Computing in Chemistry; NWChem, *Future Generation Computer Systems* **12**, 273 (1996).

[12] David Feller, Edoardo Aprà, Jeff A. Nichols, and David E. Bernholdt, The Structure and Binding Energy of K^+-Ether Complexes: A Comparison of MP2, RI-MP2 and Density Functional Methods, *J. Chem. Phys.* **105**, 1940 (1996).

[13] David E. Bernholdt and Robert J. Harrison, Large-Scale Correlated Electronic Structure Calculations: The RI-MP2 Method on Parallel Computers, *Chem. Phys. Lett.* **250**, 477 (1996).

[14] M. F. Guest, E. Aprà, D. E. Bernholdt, H. A. Früchtl, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha, Advances in Parallel Distributed Data Software; Computational Chemistry and NWChem, in *Applied Parallel Computing. Computations in Physics, Chemistry and Engineering Science*, volume 1041 of *Lecture Notes in Computer Science*, Springer, Heidelberg, 1996.

[15] D. E. Bernholdt, E. Aprà, H. A. Früchtl, M. F. Guest, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha, Parallel Computational Chemistry Made Easier: The Development of NWChem, *Int. J. Quantum Chemistry: Quantum Chem. Symposium* **29**, 475 (1995).

[16] M. F. Guest, E. Aprà, D. E. Bernholdt, H. A. Früchtl, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha, High Performance Computational Chemistry: NWChem and Fully Distributed Parallel Algorithms, in *High Performance Computing: Technology, Methods, and Applications*, volume 10 of *Advances in Parallel Computing*, pages 395–427, Elsevier, Amsterdam, 1995.

[17] David E. Bernholdt and Robert J. Harrison, Orbital Invariant Second-Order Many-Body Perturbation Theory on Parallel Computers: An Approach for Large Molecules, *J. Chem. Phys.* **102**, 9582 (1995).

[18] M. F. Guest, E. Aprà, D. E. Bernholdt, H. A. Früchtl, R. J. Harrison, R. A. Kendall, R. A. Kutteh, J. B. Nicholas, J. A. Nichols, M. S. Stave, A. T. Wong, R. J. Littlefield, and J. Nieplocha, High Performance Computational Chemistry: Towards Fully Distributed Parallel Algorithms, in A. M. Tentner, editor, *High Performance Computing 1994: Grand Challenges in Computer Simulation*, pages 511–521, San Diego, 1994, Society for Computer Simulation.

[19] Robert J. Harrison, Martyn F. Guest, Rick A. Kendall, David E. Bernholdt, Adrian T. Wong, Mark Stave, James Anchell, Anthony Hess, Rik Littlefield, George I. Fann, Jarek Nieplocha,

Greg S. Thomas, David Elwood, Jeff Tilson, Ron L. Shepard, Albert F. Wagner, Ian T. Foster, Ewing Lusk, and Rick Stevens, High Performance Computational Chemistry. II. A Scalable SCF Program, *J. Computat. Chem.* **17**, 124 (1995).

[20] S. Ajith Perera, David E. Bernholdt, and Rodney J. Bartlett, Localized Hartree Product Orbitals in Correlated Studies of Molecules, *Int. J. Quantum Chem.* **49**, 559 (1994).

[21] Rodney J. Bartlett, Magnus Rittby, John D. Watts, and David E. Bernholdt, Carbon Clusters: The Synergism Between Theory and Experiment, in P. J. Reynolds, editor, *On Clusters and Clustering, From Atoms to Fractals*, pages 23–31, Elsevier, 1993.

[22] John F. Stanton and David E. Bernholdt, An Empirically Adjusted Newton–Raphson Algorithm for Finding Local Minima on Molecular Potential Energy Surfaces, *J. Computat. Chem.* **11**, 58 (1990).

[23] Joseph D. Augspurger, David E. Bernholdt, and Clifford E. Dykstra, Concise, Open–ended Implementation of Rys Polynomial Evaluation of Two–Electron Integrals, *J. Computat. Chem.* **11**, 972 (1990).

[24] Mark S. Gordon, Kim K. Baldridge, David E. Bernholdt, and Rodney J. Bartlett, The Transition State and Barrier Heights for the Reaction $O(^3P) + HCl \longrightarrow OH + Cl$, *Chem. Phys. Lett.* **158**, 189 (1989).

[25] David E. Bernholdt, David H. Magers, and Rodney J. Bartlett, Stability and Properties of C_4 Isomers, *J. Chem. Phys.* **89**, 3612 (1988).

[26] D. E. Bernholdt, J. D. Irwin, J. P. Lacosse, K. J. Mattson, J. B. Miers, K. D. Park, L. K. Tanaka, and C. E. Dykstra, The Structures and Stabilities of $H_4C_2N_2$ Isomers, *J. Mol. Struct. (Theochem)* **153**, 175 (1987).

[27] David E. Bernholdt, Shi-yi Liu, and Clifford E. Dykstra, A Theoretical Study of the Structure, Bonding, and Vibrational Frequency Shifts of the H_2–HF Complex, *J. Chem. Phys.* **85**, 5120 (1986).

[28] L. E. Snyder, C. E. Dykstra, and D. Bernholdt, Calculated Dipole Moments and Resulting Column Densities of Long Carbon Chain Molecules in TMC-1, in A. D. Haschick, editor, *Masers, Molecules, and Mass Outflows in Star Forming Regions*, pages 9–21, Westford, Massachussetts, 1986, Haystack Observatory Meeting, Haystack Observatory.

Significant Software Contributions

[1] J. Anchell, E. Apra, D. Bernholdt, P. Borowski, T. Clark, D. Clerc, H. Dachsel, M. Deegan, M. Dupuis, K. Dyall, G. Fann, H. Früchtl, M. Gutowski, R. Harrison, A. Hess, J. Jaffe, R. Kendall, R. Kobayashi, R. Kutteh, Z. Lin, R. Littlefield, X. Long, B. Meng, J. Nichols, J. Nieplocha, A. Rendell, M. Stave, T. Straatsma, H. Taylor, G. Thomas, K. Wolinski, and A. Wong, *NWChem, A Computational Chemistry Package for Parallel Computers, Version 3.2.1*, Pacific Northwest National Laboratory, Richland, Washington 99325-0999 USA, 1998.

[2] J. F. Stanton, J. Gauss, J. D. Watts, W. J. Lauderdale, and R. J. Bartlett, ACES II, an *ab initio* program system, Quantum Theory Project, University of Florida.

[3] Rodney J. Bartlett, David E. Bernholdt, Samuel J. Cole, George B. Fitzgerald, Robert J. Harrison, William D. Laidig, Yoon S. Lee, David H. Magers, Renee P. Mattie, George D. Purvis III, Magnus Rittby, E. A. Salter, Carlos Sosa, J. F. Stanton, Gary W. Trucks, and John D. Watts, ACES (Advanced Concepts in Electronic Structure) Program System, Quantum Theory Project, University of Florida.

Presentations

[1] David E. Bernholdt, Parallel RI-MP2 Energies and Gradients: Implementation and Applications, talk, 52^{nd} International Symposium on Molecular Spectroscopy, Columbus, Ohio, 1999.

[2] David E. Bernholdt, "Fast" Methods for Correlated Electronic Structure Calculations: The RI-MP2 Approach, seminar, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington, 1999.

[3] David E. Bernholdt, Towards Scalable Quantum Chemistry, seminar, Scalable Computing Laboratory, Ames Lab, Ames, Iowa, 1999.

[4] David E. Bernholdt, Parallel RI-MP2 Energies and Gradients: Implementation and Applications, poster, 39^{th} Sanibel Symposium, St. Augustine, Florida, 1999.

[5] David E. Bernholdt, Object Oriented Methods Without Object Oriented Languages: Can Intermediate Approaches Facilitate the Adoption of Object Oriented Methods in the Research Community?, invited talk, SIAM Workshop on Object Oriented Methods for Inter-operable Scientific and Engineering Computing, Yorktown Heights, New York, 1998.

[6] David E. Bernholdt, The CSIR Web Service – Making it Easier to Find the Software and Information You Need, talk, Chemistry and the Internet, Irvine, California, 1998.

[7] David E. Bernholdt, The RI-MP2 Method for Large-Scale Correlated Electronic Structure Calculations on Parallel Computers, talk, 215^{th} American Chemical Society National Meeting, Dallas, Texas, 1998.

[8] David E. Bernholdt, The CSIR Web Service – Making it Easier to Find the Software and Information You Need, poster, 9^{th} International Congress of Quantum Chemistry, Atlanta, Georgia, 1997.

[9] David E. Bernholdt, The RI-MP2 Method: An Approach for Large-Scale Calculations on Parallel Computers, poster, 9^{th} International Congress of Quantum Chemistry, Atlanta, Georgia, 1997.

[10] David E. Bernholdt, Ask NPAC About Chemistry – An Information Resource for the Chemistry Community, poster, 213^{th} American Chemical Society National Meeting, San Francisco, California, 1997.

[11] David E. Bernholdt, The RI-MP2 Method: An Approach for Large-Scale Calculations on Parallel Computers, talk, 213^{th} American Chemical Society National Meeting, San Francisco, California, 1997.

[12] David E. Bernholdt, Large-Scale Electronic Structure Calculations on Parallel Computers, invited talk, Workshop on High Performance Computational Chemistry, Centre Européen de Calcul Atomique et Moléculaire, Lyon, France, 1996.

[13] David E. Bernholdt and Robert J. Harrison, Large-Scale Correlated Electronic Structure Calculations: The MBPT(2) Method, poster, American Conference on Theoretical Chemistry, Park City, Utah, 1996.

[14] David E. Bernholdt, Parallel Computational Chemistry Made Easier, invited talk, 79^{th} Canadian Society for Chemistry Conference and Exhibition, St. John's, Newfoundland, 1996.

[15] David E. Bernholdt and Robert J. Harrison, Large-Scale Correlated Electronic Structure Calculations: The RI-MP2 Method on Parallel Computers, poster, 36^{th} Sanibel Symposium, St. Augustine, Florida, 1996.

[16] David E. Bernholdt, Parallel Computing and Quantum Chemistry, seminar, Department of Chemistry, Syracuse University, New York, 1996.

[17] David E. Bernholdt, Parallel Computing and Quantum Chemistry, seminar, Department of Chemistry, Binghamton University (SUNY), New York, 1995.

[18] David E. Bernholdt and Robert J. Harrison, Large-Scale Correlated Electronic Structure Calculations: The RI-MP2 Method on Parallel Computers, poster, High Performance Computational Chemistry Workshop, Pleasanton, California, 1995.

[19] David E. Bernholdt, Parallel Quantum Chemistry Made Easier, seminar, Cornell Theory Center, Ithaca, New York, 1995.

[20] David E. Bernholdt, Pushing the Boundaries of Quantum Chemistry with Parallel Computing, seminar, Northeast Parallel Architectures Center, Syracuse University, Syracuse, New York, 1995.

[21] David E. Bernholdt and John B. Nicholas, A Theoretical GIAO Study of NMR Shielding Using Correlation Consistent Basis Sets, poster, 209^{th} American Chemical Society National Meeting, Anaheim, California, 1995.

[22] David E. Bernholdt and Robert J. Harrison, Large-Scale Correlated Electronic Structure Calculations: The MBPT(2) Method, talk, 209^{th} American Chemical Society National Meeting, Anaheim, California, 1995.

[23] David E. Bernholdt and John B. Nicholas, A Theoretical GIAO Study of NMR Shielding Using Correlation Consistent Basis Sets, poster, 35^{th} Sanibel Symposium, St. Augustine, Florida, 1995.

[24] David E. Bernholdt, Parallel Quantum Chemistry Made Easier: The Development of NWCHEM, invited talk, 35^{th} Sanibel Symposium, St. Augustine, Florida, 1995.

[25] David E. Bernholdt, Pushing the Boundaries of Quantum Chemistry with Parallel Computing, seminar, Departments of Physics and Chemistry, Université de Sherbrooke, Quebec, 1994.

[26] David E. Bernholdt, Pushing the Boundaries of Quantum Chemistry with Parallel Computing, seminar, Department of Chemistry, University of Tennessee, Knowville, Tennessee, 1994.

[27] David E. Bernholdt, Robert J. Harrison, and Adrian T. Wong, Scalable Parallel Electronic Structure Algorithms, talk, 15^{th} West Coast Theoretical Chemistry Conference, Sandia National Laboratory, Livermore, California, 1994.

[28] David E. Bernholdt and Robert J. Harrison, Distributed Data Parallel MBPT(2): Implementation and Performance, poster, 34^{th} Sanibel Symposia, Ponte Vedra Beach, Florida, 1994.

[29] David E. Bernholdt and Rodney J. Bartlett, Theoretical Studies of Small Carbon Clusters, seminar, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington, 1992.

[30] David E. Bernholdt and Rodney J. Bartlett, Not All Carbon Clusters Have Sixty Atoms: Recent Results on C_5^+, poster, 32^{th} Sanibel Symposia, St. Augustine, Florida, 1992.

[31] David E. Bernholdt, John D. Watts, Ivan Cernusak, Rodney J. Bartlett, and George F. Adams, Theoretical Studies of Carbon Clusters, poster, 30^{th} Sanibel Symposia, St. Augustine, Florida, 1990.

[32] John F. Stanton and David E. Bernholdt, An Empirically Adjusted Newton-Raphson Algorithm for Finding Local Minima on Molecular Potential Energy Surfaces, poster, 29^{th} Sanibel Symposia, St. Augustine, Florida, 1989.

[33] David E. Bernholdt, David H. Magers, and Rodney J. Bartlett, Stability and Properties of C_4 Isomers, poster, 28^{th} Sanibel Symposia, Marineland, Florida, 1988.

[34] David E. Bernholdt, David H. Magers, and Rodney J. Bartlett, Stability of C_4 Isomers, poster, Gordon Research Conference on Metal and Semiconductor Clusters, Holderness School, Plymouth, New Hampshire, 1987.

[35] David Bernholdt, Shi-yi Liu, and Clifford E. Dykstra, An Ab Initio Study of the HF–H_2 Complex, poster, 19^{th} Midwest Theoretical Chemistry Conference, Bloomington, Indiana, 1986.