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Education

Ph.D. in Chemistry, minors in Physics and Mathematics, and Certification in Chemical Physics, Univ. of Florida, Gainesville, FL, 1993.

B.S. in Chemistry *Cum Laude* with Highest Distinction, Univ. of Illinois, Urbana, IL, 1986

Professional Experience

1996– Research Assistant Professor, Department of Chemistry, Syracuse University, Syracuse, NY. **1995**– Alex G. Nason Fellow and Research Scientist, Northeast Parallel Architectures Center, Syracuse University, Syracuse, NY. **1995**– Affiliate Staff Scientist, Pacific Northwest National Laboratory, Richland, WA. **1993–1995** AWU Postdoctoral Fellow, High Performance Computational Chemistry Group, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA. **1986–1993** Teaching or Research Assistant, University of Florida, Gainesville, FL. **1985–1986** Teaching Assistant, University of Illinois, Urbana, IL.

Related and Significant Publications

- [1] J. Anchell, E. Apra, D. Bernholdt, P. Borowski, T. Clark, D. Clerc, H. Dachsel, M. Deegan, M. Dupuis, K. Dyll, 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 3.1*. Pacific Northwest National Laboratory, Richland, Washington 99325-0999 USA, 1997.
- [2] 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*, 29:475–483, 1995.
- [3] 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(24):9582–9589, 22 June 1995.
- [4] David E. Bernholdt and Robert J. Harrison. Large-scale correlated electronic structure calculations: The RI-MP2 method on parallel computers. *Chem. Phys. Lett.*, 250:477–484, 8 March 1996.

- [5] 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.*, submitted.
- [6] 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(5):1940–1950, 1 August 1996.
- [7] 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.
- [8] 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.
- [9] 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. Supercomputer Appl.*, in press.
- [10] M.F.Guest, E.Apra, D.E.Bernholdt, H.A.Frucht1, 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(4):273–289, December 1996.

Recent Collaborators

JL Anchell,¹ E Apra,² RJ Bartlett,³ RR Birge,⁴ AN Choudhary,⁵ PD Ellis,⁶ D Elwood,⁶ GI Fann,⁶ DF Feller,⁶ IT Foster,⁷ GC Fox,⁴ HA Früchtl,⁸ MF Guest,⁹ RJ Harrison,⁶ AC Hess,⁶ MA Kandaswamy,⁴ MT Kandemir,⁴ RA Kendall,⁶ RA Kutteh,⁶ RJ Littlefield,⁶ X Long,⁶ E Lusk,⁷ JB Nicholas,⁶ JA Nichols,⁶ J Nieplocha,⁶ SA Perera,³ RL Shepard,⁷ MS Stave,¹⁰ R Stevens,⁷ HL Taylor,⁶ GS Thomas,⁶ JL Tilson,⁷ AF Wagner,⁷ AT Wong.¹¹

Institutional Affiliations: ¹Schrödinger, Inc., ²Center for Study of the Relations between Structure and Chemical Reactivity, Nat'l Research Council of Italy, ⁴Syracuse Univ., ⁵Northwestern Univ., ⁶Pacific Northwest Nat'l Lab., ⁷Argonne Nat'l Lab., ⁸Fujitsu European Centre for Information Technology, ⁹Daresbury Lab., UK, ³Univ. of Florida, ¹⁰Oxford Molecular, Inc., ¹¹Nat'l Energy Research Supercomputer Center.

Students and Postdoctoral Scholars

None

Advisors

Graduate: Rodney J. Bartlett, University of Florida

Postgraduate: Robert J. Harrison, Pacific Northwest National Laboratory