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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] 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.
- [2] D. Bernholdt, G. C. Fox, W. Furmanski, B. Natarajan, H. T. Ozdemir, Z. Odcikin Ozdemir, and T. Pulikal, WebHLA – An Interactive Programming and Training Environment for High Performance Modeling and Simulation, in *8th DoD HPC User Group Conference*, Department of Defense High Performance Computing Modernization Program, 1998, in press.
- [3] David E. Bernholdt, Object Oriented Methods Without Object Oriented Languages: Can Intermediate Approaches Facilitate the Adoption of Object Oriented Methods in the Research Community?, in Michael E. Henderson, Christopher R. Anderson, and Stephen L. Lyons, editors, *SIAM Workshop on Object Oriented Methods for Inter-operable Scientific and Engineering Computing*, volume 99 of *Proceedings in Applied Mathematics*, pages 41–50, Society for Industrial and Applied Mathematics, 1998.
- [4] 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).
- [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.* **109**, 1593 (1998).

- [6] 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>.
- [7] 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).
- [8] 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).
- [9] 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).
- [10] 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.

Recent Collaborators

JL Anchell,¹³ E Apra,³ RJ Bartlett,¹⁷ RR Birge,¹⁶ AN Choudhary,¹¹ MJO Deegan,⁴ DA Dixon,¹⁴ M Dupuis,¹⁴ KG Dyall,⁶ RA Eades,¹⁴ PD Ellis,¹⁴ D Elwood,¹⁴ W Ermler,¹⁵ GI Fann,¹⁴ DF Feller,¹⁴ IT Foster,¹ GC Fox,¹⁶ HA Früchtl,⁷ W Furmanski,¹⁶ MF Guest,⁵ RJ Harrison,¹⁴ B Hay,¹⁴ AC Hess,¹⁴ Y Hsu,⁸ MA Kandaswamy,¹⁶ MT Kandemir,¹⁶ RA Kendall,¹⁴ RA Kutteh,¹⁴ RJ Littlefield,¹⁴ X Long,¹⁴ E Lusk,¹ JM Malard,¹⁴ Q Malluhi,⁹ R Markowski,¹⁶ NJ McCracken,¹⁶ M Minkoff,¹ D Mitra,¹ B Natarajan,¹⁶ JB Nicholas,¹⁴ JA Nichols,¹⁴ J Nieplocha,¹⁴ JS Olivera,¹⁴ HT Ozdemir,¹⁶ O Ozdemir,¹⁶ SA Perera,¹⁷ RM Pitzer,¹² M Podgorny,¹⁶ T Pulikal,¹⁶ X Qin,⁸ TR Scavo,² RL Shepard,¹ M Snir,⁸ MS Stave,¹³ R Stevens,¹ HL Taylor,¹⁴ GS Thomas,¹⁴ JL Tilson,¹ AF Wagner,¹ AT Wong.¹⁰

Institutional Affiliations: ¹Argonne Nat'l Lab., ²Bowling Green State Univ. ³Center for Study of the Relations between Structure and Chemical Reactivity, Nat'l Research Council of Italy, ⁴Digital Equipment Corp., ⁵Daresbury Lab., UK, ⁶Eloret Institute, ⁷Fujitsu European Centre for Information Technology, ⁸IBM Corp., ⁹Jackson State Univ., ¹⁰Nat'l Energy Research Super-computer Center. ¹¹Northwestern Univ., ¹²Ohio State Univ., ¹³Oxford Molecular, Inc., ¹⁴Pacific Northwest Nat'l Lab., ¹⁵Stevens Inst. of Tech., ¹⁶Syracuse Univ., ¹⁷Univ. of Florida,

Students and Postdoctoral Scholars

None

Advisors

Graduate: Rodney J. Bartlett, University of Florida

Postgraduate: Robert J. Harrison, Pacific Northwest National Laboratory