

MATTHEW ALAN THOMPSON, PHD

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EDUCATION

1999-2007

University of Colorado at Boulder, Boulder, CO, USA

PhD, Chemistry

From Femtoseconds to Nanoseconds: Simulation of IBr^- Photodissociation Dynamics in CO_2 Clusters

1995-1999

The Colorado College, Colorado Springs, CO, USA

Otis A. and Margaret T. Barnes Chemistry Scholar

BA, *summa cum laude*, Chemistry

RESEARCH AND TEACHING EXPERIENCE

2009-Present

Senior Scientific Software Engineer

Science Applications International Corporation

Support of the Global Modeling and Assimilation Office at the NASA/Goddard Space Flight Center

- Successfully adapted the GEOS-5 global atmospheric model for use with NVIDIA GPUs by converting the existing Fortran code into CUDA Fortran.
- Demonstrated speedups of 10-15x within the full model with radiation and moist process routines. Excluding data transfer, achieved kernel speedups of 25-50x.
- Gained experience building, setting up, running, and analyzing results from the GEOS-5 Global Circulation Model with various compilers and on varying workstations and supercomputers.

2007-2009

National Research Council Postdoctoral Fellowship

Naval Research Laboratory (Advisor: Brett Dunlap)

Investigation on the use of genetic algorithms for optimization of analytic density functional theory (DFT)

- Constructed and integrated a genetic algorithm in Python with existing analytic DFT code leading to better results than previous efforts.
- Leveraged Parallel Python and MPI to rapidly parallelize genetic algorithm on a per-node and per-core basis for use on workstations and clusters.

2000-2007

Graduate Research Assistant

University of Colorado at Boulder (Advisor: Robert Parson)

Nonadiabatic molecular dynamics and high-level (MRCI and CR-CCSD(T)) electronic structure calculations of IBr^- (CO_2)_n and ICl^- (CO_2)_n

- Predicted the later confirmed appearance and disappearance of a long-time absorption recovery process in near-infrared photodissociation of intermediate-size clusters.
- Mentored fellow students and researchers in installation and use of Linux and quantum chemistry programs on local workstations and clusters.

COMPUTING SKILLS

Programming

Proficient in FORTRAN 77 and Fortran 95/2003/2008 including Intel and PGI Compilers

Proficient in Python, Parallel Python, and iPython

Proficient with sed/awk, bash, tcsh, and zsh shell scripts

Experience in C, C++, Perl, and Ruby

Experience with CVS, Subversion, and Trac version control software

COMPUTING SKILLS CONT.

Parallel Computing	Proficient with CUDA including use of PGI Accelerator/OpenACC pragmas for Fortran 95/2003 Proficient with PBS queueing system, OpenMP, and MPI (MPICH, OpenMPI) and MPI-I/O Experience in integrating Parallel Python with varying multi-core workstation and multi-node cluster architectures
Quantum Chemistry	Proficient with GAMESS-US and Molpro including modification of source code Experience with Gaussian 98 and Gaussian 03
Administration	Broad experience at both user and administrative level with Compaq Tru64 Alpha, various distributions of Linux (Red Hat, Fedora, Gentoo, Ubuntu), OS X, and Windows XP/Vista Proficient with PC, Apple, and printer hardware installation and troubleshooting
General	Proficient with Microsoft Office and OpenOffice products Proficient with TeX, LaTeX, and BibTeX Experience with HTML, XHTML, MathML and CSS

AWARDS AND SCHOLARSHIPS

2007	National Research Council Postdoctoral Fellowship
1999	Phi Beta Kappa
1999	Alpha Lambda Delta Book Award
1999	Merck Award in Chemistry
1996	CRC Press Freshman Chemistry Achievement Award
1996	Alpha Lambda Delta
1995-1999	Otis A. and Margaret T. Barnes Chemistry Scholar
1995-1999	Hach Scientific Foundation Scholar
1995-1999	First Bank System Foundation Scholar

TALKS GIVEN

2011	Programming Weather, Climate, and Earth-System Models on Heterogeneous Multi-core Platforms Workshop, Boulder, CO <i>Lessons Learned from Adapting GEOS-5 GCM Physics to CUDA Fortran</i>
2006	JILA, Boulder, CO <i>Nonadiabatic MD Simulations of $IBr^-(CO_2)_n$ Photodissociation</i>

POSTERS PRESENTED

2008	American Conference on Theoretical Chemistry 2008, Evanston, IL <i>Analytic Density-Functional Theory Optimization with a Parallel Genetic Algorithm</i>
2007	American Physical Society, March Meeting, Denver, CO <i>Nonadiabatic MD Simulations of $IBr^-(CO_2)_n$ Photodissociation</i>
2006	American Chemical Society, Fall Meeting, San Francisco, CA <i>Nonadiabatic MD Simulations of $IBr^-(CO_2)_n$ Photodissociation</i>

PUBLICATIONS

L. Sheps, E. M. Miller, S. Horvath, M. A. Thompson, R. Parson, A. B. McCoy, and W. C. Lineberger.
Solvent-mediated charge redistribution in photodissociation of IBr^- and $\text{IBr}^-(\text{CO}_2)$.
J. Chem. Phys., 134(18):184311, 2011

L. Sheps, E. M. Miller, S. Horvath, M. A. Thompson, R. Parson, A. B. McCoy, and W. C. Lineberger.
Solvent-mediated electron hopping: Long-range charge transfer in $\text{IBr}^-(\text{CO}_2)$ photodissociation.
Science, 328(5975):220–224, 2010

M. A. Thompson, J. P. Martin, J. P. Darr, W. C. Lineberger, and R. Parson.
A combined experimental/theoretical investigation of the near-infrared photodissociation of $\text{IBr}^-(\text{CO}_2)_n$.
J. Chem. Phys., 129:224304, 2008

M. A. Thompson and B. I. Dunlap.
Optimization of analytic density functionals by parallel genetic algorithm.
Chem. Phys. Lett., 463:278–282, 2008

V. Dribinski, J. Barbera, J. P. Martin, A. Svendsen, M. A. Thompson, R. Parson, and W. C. Lineberger.
Time-resolved study of the solvent induced recombination in size-selected $\text{IBr}^-(\text{CO}_2)_n$ clusters.
J. Chem. Phys., 125:133405, 2006

T. Sanford, S.-Y. Han, M. A. Thompson, R. Parson, and W. C. Lineberger.
Photodissociation dynamics of $\text{IBr}^-(\text{CO}_2)_n$, $n < 15$.
J. Chem. Phys., 122:054307, 2005

T. Sanford, D. Andrews, J. Rathbone, M. Taylor, F. Muntean, M. Thompson, A. B. McCoy, R. Parson, and W. C. Lineberger.
Time resolved solvent rearrangement dynamics.
Faraday Discuss., 127:383–394, 2004

References available upon request.