

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

PROFESSIONAL AND RESEARCH EXPERIENCE

2012-Present

Senior Software Test Engineer

Science Systems and Applications, Inc. (SSAI, Awarded follow-on contract from SAIC)

2009-2012

Senior Scientific Software Engineer

Science Applications International Corporation (SAIC)

Support of the Global Modeling and Assimilation Office at 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, moist, turbulence, and gravity wave drag physics routines. Excluding data transfer, achieved kernel speedups of 25-50x.
- Successfully transitioned the GEOS-5 shortwave radiation kernel for use on the Intel Xeon Phi for use in both Offload and Native modes.
- Experienced with building, setting up, running, and analyzing results from the GEOS-5 Global Circulation Model with various compilers and on various workstations and supercomputers.
- Successfully built and maintained on various clusters and with various compilers the required libraries for the GEOS-5 GCM including HDF5, NetCDF, cURL, and ESMF.

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
- Proficient with CVS, Subversion, and Trac version control software
- Experience in C, C++, Perl, and Ruby
- Experience with NetCDF 4, HDF5, ESMF, cURL, and CDO

Parallel Computing

- Proficient with CUDA C and Fortran including use of PGI Accelerator/OpenACC pragmas
- Proficient with OpenMP 4.0
- Experience with Intel Xeon Phi in Offload and Native modes
- Proficient with PBS queueing system, Global Arrays, and MPI (MPICH, OpenMPI, MVAPICH2, MPT) and MPI-I/O
- Experience in integrating Parallel Python with various 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

System Administration

- Broad experience at both user and administrative level with various distributions of Linux (Red Hat, Fedora, Gentoo, Ubuntu), Compaq Tru64 Alpha, 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

ORGANIZATIONS

- 2012-Present Association for Computing Machinery

TALKS GIVEN

- 2013 Programming Weather, Climate, and Earth-System Models on Heterogeneous Multi-core Platforms Workshop, Boulder, CO
Continued Efforts in Adapting the GEOS-5 AGCM to Accelerators : Successes and Challenges
- 2012 Programming Weather, Climate, and Earth-System Models on Heterogeneous Multi-core Platforms Workshop, Boulder, CO
Progress in Adapting the GEOS-5 GCM to CUDA FORTRAN: Successes and Challenges
- 2011 Programming Weather, Climate, and Earth-System Models on Heterogeneous Multi-core Platforms Workshop, Boulder, CO
Lessons Learned from Adapting GEOS-5 GCM Physics to CUDA Fortran
- 2006 JILA, Boulder, CO
Nonadiabatic MD Simulations of $\text{IBr}^-(\text{CO}_2)_n$ Photodissociation

POSTERS PRESENTED

- 2008 American Conference on Theoretical Chemistry 2008, Evanston, IL
Analytic Density-Functional Theory Optimization with a Parallel Genetic Algorithm
- 2007 American Physical Society, March Meeting, Denver, CO
Nonadiabatic MD Simulations of $\text{IBr}^-(\text{CO}_2)_n$ Photodissociation
- 2006 American Chemical Society, Fall Meeting, San Francisco, CA
Nonadiabatic MD Simulations of $\text{IBr}^-(\text{CO}_2)_n$ Photodissociation

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.