Gordon Chalmers

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Results-oriented and passionate computational scientist with a background in molecular chemistry, physics and computer science. Adept in continuing work in computational chemistry, molecular modeling and analysis with strong background in NMR (nuclear magnetic resonance) data. Possessing excellent analytical skills in math, physics, and science. General work areas span molecular chemistry (computational, modeling, and NMR related data), computer science, and physics. Much work has been in machine learning and within this area in particular, genetic algorithms.

In addition to other activities, participates in research projects innovating, applying intellectual ability and in-depth knowledge of the application of molecular modeling as well as investigation of conformational changes relevant to the function of proteins and carbohydrates, calculating NMR observables from molecular models.

AREAS OF EXPERTISE

computational chemistry	nuclear magnetic resonance	complexity theory	genetic algorithms
molecular dynamics	NP-Hard, NP-complete	real-time systems	optimization algorithms
theoretical particle physics	databases	software dev.	system administration
numerical algorithms	mathematics	carbohydrates, proteins	machine learning

SEVERAL HIGHLIGHTS

- My contributed software: at the Glycam site (glycam.org) has been uniquely downloaded more than 2400x. Not tallied at the Prestegard lab site (tesla.ccrc.uga.edu). National Institute of Health (NIH) funded projects.
- Programming work involved the use of many specialty scientific programming software, primarily in molecular dynamics simulations, modeling, and analysis.
- Funded by the Department of Education fellowship, research assistantships, and teaching assistants during the 1st PhD, and from a Graduate Research Assistantship during the 2nd PhD from the Complex Carbohydrate Research Center.
- Some of the C++ and Matlab software that was written and used in published work can be seen by downloading from the Robert J. Woods group site at http://glycam.org/docs/othertoolsservice/downloads/downloads-software/, the James H. Prestegard group site http://tesla.ccrc.uga.edu/software/and, and Gaetano T. Montelione group site, http://montelionelab.chem.rpi.edu
- Work with Prestegard generated an awarded R01 NIH grant, 2019.
- Extensive use of computer science, molecular chemistry, machine learning, mathematics, physics in work.

EDUCATION & CREDENTIALS

UNIVERSITY OF GEORGIA **2019**
PhD Computer Science: *Genetic Algorithms in Different Areas of Science*
(Doctoral Minor in Statistics)

- Demonstrating expertise in real-time systems and scheduling, including multi-processors.
- Performing all tasks related to computational complexity as one of focal topics as well as in computational chemistry using molecular models with experimental NMR to improve both the modeling and experimental techniques. Proficient in collaborative research.
- Applying in-depth knowledge in pure computer science.

UNIVERSITY OF CALIFORNIA, LOS ANGELES [UCLA] – Los Angeles, CA **1991 & 1995**
PhD Physics – *1995* • **M.S. Physics** & **B.S. Physics** – *1991 – Outstanding Graduate Student Award 1995*

ACADEMIC EXPERIENCE

RENSSALAER POLYTECHNIC INSTITUTE (RPI), CENTER FOR BIOTECHNOLOGY AND INTERDISCIPLINARY STUDIES (CBIS) **2020-2021**
Staff Research Scientist, Montelione Lab

- Conducted research and calculations of proteins in the areas of computational chemistry, NMR, generating software including data mining and machine learning, supporting group computer usage including software, sys-admin.
- Refereed journal articles.
- Remote work mostly.

UNIVERSITY OF GEORGIA (UGA), COMPLEX CARBOHYDRATE RESEARCH CENTER (CCRC) **2013-2019**
Research Assistant, Prestegard Lab, Woods Lab

- Research and calculations with proteins and carbohydrates in the areas of computational chemistry, NMR, and various.
- Software development in both labs.
- Completed graduate work in computer science, computational chemistry, and statistics.

UNIVERSITY OF CALIFORNIA – LOS ANGELES (UCLA) – Los Angeles, CA **2001-2009**
Lecturer – *2001-2002* • **Postdoctoral Associate** – *2006-2009*

- Research and teaching, undergraduate and graduate level in physics.
- Supervised undergraduate students. Graded examination scripts to identify area of challenges. Prepared students' score sheets and approved final scores.
- Continued research in theoretical particle physics.

ARGONNE NATIONAL LABORATORY – Chicago, IL **1998-2001**
Postdoctoral Associate

- Conducted research in the theoretical particle physics field while performing other duties. Collaborative research.
- Manuscript writing for publication in scientific journals and/or presentations.
- Refereed journal articles.

STATE UNIVERSITY OF NEW YORK – Stony Brook, NY **1995-1998**
C.N. YANG INSTITUTE FOR THEORETICAL PHYSICS
Postdoctoral Associate

- Conducted theoretical particle physics research.
- Used demonstrated scientific creativity, collaborated with others, and independent thought to expand technical capabilities and identify new research opportunities.
- Refereed journal articles.

RELATED EXPERIENCE

RAYTHEON AEROSPACE – El Segundo, CA **2002-2004**
Engineer IV

- Worked with research groups to help identify, implement and improve their computational and data workflow; assisted in facilitating computing and data infrastructure solutions specific to researchers
- Assisted in optimizing researchers' codes for maximum performance.
- Received Patent for: Instantaneous 3—D target location resolution utilizing only bistatic range measurement in a multistatic system.

MEMBERSHIP

GLYCAM SOFTWARE DEVELOPER TEAM in the WOODS GROUP • **Member**

Compiled languages: C++, C, Java, Fortran, and others as needed
Non-compiled languages: Matlab, R, Html, Javascript, Python, Bash,... ***Operating sys***: Linux, Windows, VMs
Specialty software for computational chemistry: Amber, Cpptraj, VMD, Chimera, Glylib, PpmOne, ShiftX2, Cyana, Cyrange, PdbStat, AutoDock, VinaCarb, Oculus Nanome, CCDC GOLD, AM-MN Corina, Open Babel, and many others
Web design: Wordpress, Drupal ***Parallel processing***: Pmemd, Posix threads, CUDA
Database management: MySql, Apache **Collaboration**: Git (proficient)

PUBLICATIONS

Papers in physics: 88 found at https://scholar.google.com/citations?user=LOyh-tYAAAAJ&hl=en

Papers in computational chemistry:

Sriram Aiyer, G.V.T. Swapna, Li-Chung Ma, Gaohua Liu, Jingzhou Hao, Gordon Chalmers, Brian C. Jacobs, Gaetano T. Montelione, Monica J. Roth, A common binding motif in the ET domain of BRD3 forms polymorphic structural interfaces with host and viral proteins, accepted to Structure, bioRxiv 2020.09.21.306696; doi: https://doi.org/10.1101/2020.09.21.306696

Gordon Chalmers, Shelby H. Funk, Genetic Algorithms in Real-Time Systems, submitted to the Journal of Real-Time Systems, 2020.

Gordon Chalmers, Alexander Eletsky, Laura Morris, Jeong-Yeh Yang, Fang Tian, Robert J. Woods, Kelley W. Moremen and James H. Prestegard, NMR resonance assignment methodology: characterizing large sparsely labeled glycoproteins, J Mol Biol. 2019 May 31;431(12):2369-2382. doi: 10.1016/j.jmb.2019.04.029. Epub 2019 Apr 26. PMID: 31034888; PMCID: PMC6554063

Gordon Chalmers, Shelby H. Funk, Adjusting Real-Time Mode Transitions via Genetic Algorithms, 2017 16th IEEE International Conference on Machine Learning and Applications. (presented at conference)

Sheikh, Mohammed, Thieker, David, Chalmers, Gordon, Schafer, Christopher, Ishihara, Mayumi, Azadi, Parastoo, J. Woods, Robert, N. Glushka, John, Bendiak, Brad, H. Prestegard, James, M. West, Christopher. (2017). O2 sensing associated glycosylation exposes the F-box combining site of the Dictyostelium Skp1 subunit in E3 ubiquitin ligases. Journal of Biological Chemistry. 292. jbc.M117.809160. 10.1074/jbc.M117.809160.

Kari Pederson, Gordon R. Chalmers, Qi Gao, Daniel Elnatan, Theresa A. Ramelot, Li-Chung Ma, Gaetano T. Montelione, Michael A. Kennedy, David A. Agard, James H. Prestegard, NMR characterization of HtpG, the E. coli Hsp90, using sparse labeling with 13C-methyl alanine, J Biomol NMR. 2017 Jul;68(3):225-236. doi: 10.1007/s10858-017-0123-8. Epub 2017 Jun 26. PMID: 28653216; PMCID: PMC5546222.

Qi Gao,Gordon R. Chalmers, Kelley W. Moremen, James H. Prestegard, NMR assignments of sparsely labeled proteins using a genetic algorithm, Journal of Biomolecular NMR (2017) 67:283–294

G. Chalmers, J.N. Glushka, Bethany Foley, R.J. Woods, J.H. Prestegard. Direct NOE simulation from long MD trajectories. Journal of Magnetic Resonance. 265. 10.1016/j.jmr.2016.01.006.

Additional papers in preparation with 2 of these completely written.

>30 presentations, seminars about topics regarding my work at the CCRC (UGA) and CBIS (RPI) are available at https://github.com/gordonchalmers/GRC_Presentations or upon request.

REFERENCES

Professor James H. Prestegard, Eminent Scholar, University of Georgia, Departments of Chemistry, Biochemistry and Molecular Biology, jpresteg@uga.edu

Professor Robert J. Woods, University of Georgia, Departments of Chemistry, Biochemistry and Molecular Biology, rwoods@ccrc.uga.edu or rwoods.glycam@gmail.com

Professor Shelby H. Funk, University of Georgia, Department of Computer Science, shelby@cs.uga.edu

Professor Christopher West, University of Georgia, Department of Biochemistry and Molecular Biology, Department Head, westcm@uga.edu

Dr. Lachele Foley, Research Scientist, University of Georgia, Complex Carbohydrate Research Center, lfoley@ccrc.uga.edu

Additional upon request.