# 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, and molecule design.

## AREAS OF EXPERTISE

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|---|---|---|---|
| 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 |
| quantum field and string th | mathematics | carbohydrates, proteins | machine learning |
| numerical algorithms | | | |

## 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 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)**

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

UNIVERSITY OF GEORGIA (UGA), COMPLEX CARBOHYDRATE RESEARCH CENTER (CCRC) **2021**
**Visiting Scholar**
- Research in molecule design.

RENSSALAER POLYTECHNIC INSTITUTE (RPI), CENTER FOR BIOTECHNOLOGY AND INTERDISCIPLINARY STUDIES (CBIS) **2020-2021**
**Staff Research Scientist**, Montelione Lab
- Research and calculations of proteins in the areas of computational chemistry, NMR, machine learning, generating software including data mining. Supported group computer usage including software, sys-admin.
- 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. Collaborative and independent research.
- 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.
- Continued research in theoretical particle physics.

ARGONNE NATIONAL LABORATORY – Chicago, IL **1998-2001**
**Postdoctoral Associate**
- Conducted research in the theoretical particle physics. Collaborative and independent research.
- 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. Collaborative and independent research.
- Refereed journal articles.

## RELATED EXPERIENCE

RAYTHEON AEROSPACE – El Segundo, CA **2002-2004**
**Engineer IV**
- Algorithm and software development pertaining to AESA radars.
- 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***: CCDC GOLD, AM-MN Corina, Amber, Cyana, Cpptraj, VMD, Chimera, Glylib, PpmOne, ShiftX2, Cyrange, PdbStat, AutoDock, VinaCarb, Oculus Nanome, 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:***

Gordon Chalmers. Ligand GA: a genetic algorithm for automated protein design, submitted to J. Comp. Chem. bioRxiv: doi: 10.1101/2021.10.11.463970.

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, Structure 2021 Aug 5, 29(8):886-898. bioRxiv 2020.09.21.306696. doi: 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 3, 431(12):2369-2382. doi: 10.1016/j.jmb.2019.04.029. 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. O2 sensing associated glycosylation exposes the F-box combining site of the Dictyostelium Skp1 subunit in E3 ubiquitin ligases, Journal of Biological Chemistry 2017 Nov 17, 292(46):18897-18915. doi:10.1074/jbc.M117.809160. PMID: 28928219. PMCID: PMC5704474.

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. 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 April, 67:283–294. doi: 10.1007/s10858-017-0101-1.

G. Chalmers, J.N. Glushka, Bethany Foley, R.J. Woods, J.H. Prestegard. Direct NOE simulation from long MD trajectories. Journal of Magnetic Resonance, 2016 Jan 21, 265:1-9. doi: 10.1016/j.jmr.2016.01.006. PMID: 26826977. PMCID: PMC4818662.

>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.