Jorge Luis Gálvez Vallejo

Graduate Student

+52 833 155 0304
https://github.com/JorgeG94
jg4@iastate.edu

Software proficiency

GAMESS
Git
CUDA
C++
Julia
Python
MPI
OpenMP
Mathematica
Fortran
QChem

(*)[The skill scale is from 0 (Fundamental Awareness) to 6 (Expert).]

Education

Since 2017	Iowa State University Advisor: Mark S. Gordon.	PhD Program
2013-2017	Universidad de las Americas Puebla *Magna cum laude*, graduated with honors	Bs. Chemistry

Research Experience:

- Current lead developer of the LibCChem library for GAMESS
- Porting of CUDA code to the HIP programming model for AMD execution on the Frontier supercomputer
- Helped develop a novel electronic structure package written entirely in the Julia programming language. Project led by Dr. David Poole as a graduate student in the Gordon group
- Development of a Graphics Processing Unit accelerated resolution of the identity MP2 program. Project done in collaboration with Assistant Professor Giuseppe Barca at the Australian National University
- Development of a Graphics Processing Unit accelerated self-consistent field program. Project done in collaboration with Assistant Professor Giuseppe Barca at the Australian National University
- Development of a Graphics Processing Unit accelerated electron repulsion integral code using the Head-Gordon-Pople algorithm. Project done in collaboration with Dr. Giuseppe Barca at the Australian National University
- Analyzing the thermochemical properties and possible degradation pathways of solid rocket fuels upon long storage
- Analysis of using heteropolyacids as heterogeneous catalysts for endothermic fuels applications for hypersonic jet cooling
- Bonding analysis of sigma and hydrogen bonds in different sized small water clusters using *ab initio* quantum chemistry

Mentoring Experience:

2021	Advised a first year PhD student in Assistant Professor Giuseppe Barca's research group working on implementing the Fragment Molecular Orbital method using GPU acceleration
Summer 2021	Co-supervised an undergraduate student in Professor Mark Gordon's research group working on heterogeneous catalysis and integral evaluation software development
Summer 2020	Co-supervised an undergraduate student in Professor Mark Gordon's research group working on bonding analysis of short lived carbon based intermediates

Awards

2021	American Association of Hispanics in Higher Education - Fellow
2021	Klaus Ruedenberg Theoretical Chemistry Award
2020	Joseph F. Nelson Scholar Iowa State University

Service

2016	Founder - President ACS Student Chapter UDLAP
2019-2021	Treasurer - Graduate Student Liason Committee
2020	Panel member MU3C Conference
2021	Member - Organizing Committee Midwest Retreat for Diversity in Chemistry

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Publications

9 D Poole, JL Galvez Vallejo, Mark S. Gordon.
A Task-Based Approach to Parallel Restricted Hartree-Fock Calculations
Submitted JCTC

8 G. Barca, M. Alkan, JL Galvez Vallejo, D. Poole, A. Rendell, M. Gordon.
High-Performance, Faster SCF Calculations on GPU clusters
Submitted JCTC

7 JL Galvez Vallejo, J. Duchimaza-Heredia, Mark S Gordon.
Bonding Analysis of water clusters using Quasi Atomic Orbitals
Phys. Chem. Chem. Phys., 2021, Advance Article

6 G. Barca, JL Galvez Vallejo, M. Alkan, D. Poole, A. Rendell, M. Gordon.
Scaling the RI-MP2 method on Summit
Accepted SC21 conference

5 GMJ Barca, JL Galvez Vallejo, DL Poole, AP Rendell, MS Gordon
High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm
J. Chem. Theory Comput. 2020, 16, 12, 7232–7238

4 G Barca, D Poole, JL Galvez Vallejo, M Alkan, C Bertoni, A Rendell, M Gordon
Scaling the Fock build on Summit
Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis DOI: 10.5555/3433701.3433808

3 D Poole, JL Galvez Vallejo, Mark S. Gordon
A New Kid on the Block: Application of Julia to Hartree–Fock Calculations
J. Chem. Theory Comput. 2020, 16, 8, 5006–5013

2 Giuseppe MJ Barca, Colleen Bertoni, Laura Carrington, Dipayan Datta, Nuwan De Silva, J Emiliano Deustua, Dmitri G Fedorov, Jeffrey R Gour, Anastasia O Gunina, Emilie Guidez, Taylor Harville, Stephan Irle, Joe Ivanic, Karol Kowalski, Sarom S Leang, Hui Li, Wei Li, Jesse J Lutz, Ilias Magoulas, Joani Mato, Vladimir Mironov, Hiroya Nakata, Buu Q Pham, Piotr Piecuch, David Poole, Spencer R Pruitt, Alistair P Rendell, Luke B Roskop, Klaus Ruedenberg, Tosaporn Sattasathuchana, Michael W Schmidt, Jun Shen, Lyudmila Slipchenko, Masha Sosonkina, Vaibhav Sundriyal, Ananta Tiwari, JL Galvez Vallejo, Bryce Westheimer, Marta Włoch, Peng Xu, Federico Zahariev, Mark S Gordon
Recent developments in the general atomic and molecular electronic structure system
J. Chem. Phys. 152, 154102 (2020)

1 Mark S Gordon, Giuseppe Barca, Sarom S Leang, David Poole, Alistair P Rendell, JL Galvez Vallejo, Bryce Westheimer
Novel Computer Architectures and Quantum Chemistry.
J. Phys. Chem. A 2020, 124, 23, 4557–4582

Publications - in preparation

1 JL Galvez Vallejo, G. Barca, Mark. S Gordon.
Hydrocarbon Cracking on Heteropolyacids for Endothermic Fuels Applications
In preparation

2 Daniel del Angel, JL Galvez Vallejo, Mark S. Gordon.
QUAO study of tetrahedranes
In preparation

3 G. Barca, JL Galvez Vallejo, M. Alkan, D. Poole, A. Rendell, M. Gordon.
A new GPU accelerated RI-MP2 method.
In preparation

4 JL Galvez Vallejo, Garrett Tow, Edward Maginn, Mark S. Gordon.
Ab initio study of aging fuels - thermochemistry
In preparation

5 JL Galvez Vallejo, G. Barca, Mark. S Gordon.
High-Performance, GPU Accelerated evaluation of two electron integrals - HGP
In preparation

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Presentations

Oral

2018	Midwest Regional Meeting American Chemical Society QUAO Bonding Analysis of small water clusters
2017	XLVI Meeting in Statistical Physics Spinodal decomposition of dipolar colloids under a Smoluchowski equation approach

Poster

2021	Pacifichem A Graphics Processing Unit optimized Head-Gordon-Pople algorithm
2021	Pacifichem Aging fuels: thermochemistry and degradation paths
2021	Airforce Office for Scientific Research Thermochemistry of aging fuels
2020	LatinXChem Accelerating 2 electron integral evaluation on graphical processing units
2016	51st Meeting of the Mexican Chemical Society Bonding analysis of small water clusters
2015	50th Meeting of the Mexican Chemical Society Synthesis of a Arsenic trapping molecule

Teaching Experience:

Spring 2018	Thermodynamics Teaching Assistant
Fall 2017	General Chemistry Teaching Assistant - Laboratory
Fall 2017	General Chemistry Teaching Assistant - Recitation

Affiliations:

Since 2014	American Chemical Society

Languages spoken:

Native	Spanish
Fluent	English
Fluent	German
Basic	French

Workshops

2021	Frontier COE Workshop
2020	Performance, Portability, and Productivity in HPC Forum
2020	Argonne Training Program in Extreme Scale Computing
2020	NVIDIA Hackathon - Princeton
2020	Aurora COE Workshop 2
2019	Aurora COE Workshop 1
2019	NVIDIA Hackathon - MIT
2018	OpenMP Workshop - Supercomputing Conference 2018