SYLLABUS
Summer Theoretical and Computational Chemistry (STACC) Workshop

The objective of this workshop is to introduce younger undergraduate students with no prior experience in theoretical and computational chemistry to this diverse research area through lectures and hands-on training.

Main point of contact:
Dr. Joshua Kretchmer jkretchmer@gatech.edu

You should e-mail Dr. Kretchmer if you run into any technical issues logging on to the virtual meetings or accessing the computational resources.

Participating Professors:
Dr. JC Gumbart jcgumbart@gatech.edu
Dr. Jesse McDaniel jesse.mcdaniel@chemistry.gatech.edu
Dr. David Sherrill sherrill@gatech.edu

Graduate Student Assistants:
Jordan Hale
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Learning Objectives:
- Obtain a sufficient level of understanding of the various areas of theoretical chemistry to make informed decisions about future classes and research opportunities
- Working knowledge of how to navigate and utilize a high-performance computing cluster to perform calculations
- Training in the utilization of several computational chemistry software packages

Daily Schedule:

10 am – 11 am EDT	Practical lecture on the daily assignment
11 am – 12 pm EDT	Open work time on the daily assignment
12 pm – 1 pm EDT	Break for lunch
1 pm – 2 pm EDT	General lecture

The STACC workshop is being held completely virtually. Both the practical lecture and general lecture will occur via BlueJeans at this link:

https://gatech.bluejeans.com/5598553443

The open work time will occur via Gather at this link:

https://app.gather.town/invite?token=VjCCXw_0WQrk96gYkpoIl6t3-KhXZYe-

Both links will be used for the entirety of the workshop.

Computational Resources:
The STACC workshop will utilize the educational computer cluster at Georgia Tech known as PACE ICE. To access this resource you will need to first:

1) Be logged on to the Georgia Tech VPN. You can download the GlobalProtect VPN client here:
   mac
   windows
   ubuntu

2) Have access to an SSH client (terminal). Mac and linux machines come already with a terminal application, which can be found most easily by simply searching for the application called "terminal" on the computer. On a mac, it is located under Applications/Utilities and on a linux machine a new terminal window can be opened by using the short key Ctrl+Alt+T. For a windows machine you need to download a separate client. We recommend using MobaXterm, which can be obtained here:
   download MobaXterm

3) Once you are on the Georgia Tech VPN (see step 1 above) you can log on to the cluster using SSH. To do so open up a new terminal window or MobaXterm and type the following command:

   ssh username@pace-ice.pace.gatech.edu

   where you should replace username with either your Georgia Tech username, if you're a Georgia Tech student, or the username you should have received via e-mail. Then provide your Georgia Tech or corresponding password at the prompt. No asterisks nor text will appear when you type, so enter your password then <Enter>. More information about logging on to the cluster can be found here:
   ICE User Guide

4) To log off the cluster type exit followed by <Enter> or simply close the terminal window.

Workshop Schedule:

Date	Topic of workshop assignment	Code for workshop assignment	Topic of general lecture
Monday, May 23	Introduction to Linux and the cluster	N/A	Introduction to areas of theoretical chemistry – Dr. Kretchmer
Tuesday, May 24	Potential energy surface of H_2 dissociation	Psi4	Introduction to electronic structure theory - Dr. Sherrill
Wednesday, May 25	Geometry and vibrational frequencies of water	Psi4	More about molecular orbital theory and example applications - Dr. Sherrill
Thursday, May 26	Molecular dynamics of mixing of two Lennard-Jones fluids	LAMMPS / VMD	Molecular dynamics of biological systems - Dr. Gumbart
Friday, May 27	Solvation energy of methane in water	LAMMPS / VMD	Quantum effects in biology - Dr. Gumbart
Monday, May 30	Memorial Day – No Workshop		
Tuesday, May 31	Rare-event sampling of barrier crossing	LAMMPS / VMD	Introduction to molecular dynamics simulations – Dr. McDaniel
Wednesday, June 1	Ab-initio MD simulation of water	CP2K	Electrostatics in chemistry – Dr. McDaniel
Thursday, June 2	Real-time DFT of charge transfer between a dimer	NWChem	Marcus theory of electron transfer – Dr. Kretchmer
Friday, June 3	Photoisomerization reaction with surface hopping	In-house code	Conclusion and Q & A with graduate students – Dr. Kretchmer