Workshop 1: Monday, July 29, 4:00 - 5:30 pm
Location: Primrose Ballroom

Title: Accelerated DFT Workshop: Accelerating Scientific Discoveries with Microsoft Azure Quantum Elements
Offered by: Microsoft Azure Quantum Elements Technical Staff

Abstract: The ongoing advancements of high-performance, cloud-based supercomputers provide an opportunity to accelerate simulations, increase workflow throughput, and expedite scientific discovery. In this workshop, the Microsoft team will showcase how Accelerated Density Functional Theory (ADFT) accelerates DFT simulations on molecular structures.

Following a presentation on the architecture and performance of the ADFT code, participants will receive hands-on access to learn how to set up and run electronic structure calculations, while also predicting and analyzing the properties of molecular structures.

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Workshop 2: Thursday, August 1,1:30 – 4:00 pm [concurrent]
Location: Primrose Ballroom

Title: Introduction to MoSDEF
Offered by: Clare McCabe, Eric Jankowski, and Peter Cummings
Abstract: This workshop will feature an introduction to MoSDeF. The MoSDeF tools have been designed to facilitate the hierarchical construction of both atomistic and coarse-grained system configurations, the application of classical force fields (i.e., atom-typing), encapsulation of chemical topology information, and the generation of input files for a variety of molecular dynamics and Monte Carlo simulation engines, including LAMMPS, GROMACS, HOOMD-Blue, Cassandra, and GOMC. Participants will follow four specific examples of setting up increasingly complex molecular simulations, including: water in a carbon slitpore, coarse-grained polymers in a box, biomolecules in solution, and coated monolayer surfaces.

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Workshop 3: Thursday, August 1, 1:30 - 4:00 pm [concurrent]
Location: Superior A/B
Title: Simulation Setup and Management with EMC
Offered by: Pieter J. in 't Veld

Abstract: This is a hands-on tutorial for building complex initial structures and management of many simulations using Monte Carlo principles. This workshop will cover both structure generation and simulation management aspects. The Enhanced Monte Carlo (EMC) provides an environment for creating and manipulating input structures for particle simulations using atomistic force fields Born, COMPASS, PCFF, CHARMM, OPLS, and TraPPE, which are typed using straightforward typing rules. Supported coarse-grained force fields DPD, Martini, SDK, and colloidal force fields, are not typed by EMC. To this end, a scripting language designed for this purpose manages access to its functionality. EMC provides manipulation of molecular or coarse-grained structures through SMILES strings, typing these structures – when needed – for selected force fields, and building conformations applying Monte Carlo principles. EMC provides output ports to LAMMPS, PDB, and XYZ data formats. EMC setup scripts allow for the generation of EMC, LAMMPS, and NAMD input scripts in a convenient matter by providing a workflow environment for spawning single or multiple simulations with one script. Besides building, EMC setup scripting allows for several analysis options for analyzing either internal simulations or trajectories include the cavity energetic sizing algorithm (CESA), density, pressure and energy profiles.

If possible, participants should download and install EMC (https://montecarlo.sourceforge.net) and LAMMPS (https://www.lammps.org) on their laptop beforehand, in order to maximize time devoted to working with EMC.