Tutorial Description

This presentation provides a high level overview of techniques for optimizing python code and running code in parallel.

At a cursory level will we cover the following libraries: numpy, scipy, trace, pytables, numba

In detail we will cover: SnakeViz, MPI4PY

In detail we will cover the concept of CPU parallelization with MPI

Instructions and setup:

Expectations

This presentation is an *advanced* python workshop/lecture. You do **not** need to be an expert programmer but you need to have an understanding of the basics of coding. This lecture/workshop does not teach the basics of coding.

You should have a strong understanding of the following:

Simple python programming (for loops, variables, functions/methods etc)
A basic understanding of how to use conda
A basic understanding of how to use the terminal

Understanding the following are helpful but not required

A basic understanding of numpy
A conceptual understanding of DFT/geometry optimization
A basic understanding of the python library matplotlib

Instructions and setup:

Environment/Setup

Coding a long and modifying code can be very helpful for learning. All the code used in the presentation will be provided day of.
In order to make best use of it, you should complete the following setup. Still this is not required if you don't wish to run the code yourself.

Set up a conda environment (conda.io/projects/conda/en/latest/user-guide/getting-started.html or docs.conda.io/projects/miniconda/en/latest/miniconda-install.html)

From in your new conda environment run the following commands

conda install -c conda-forge matplotlib
conda install psi4 python=3.11 -c conda-forge/label/libint_dev -c conda-forge
conda install -c anaconda numpy
conda install -c conda-forge mpi4py
conda install -c anaconda snakeviz