Contribution ID: **3** Type: **Workshop**

Windows Subsystem for Linux with GPU support for molecular dynamics simulations

Sunday, 1 December 2024 13:30 (1h 30m)

Windows Subsystem for Linux (WSL) is a feature of the Windows operating system that enables you to run a Linux file system, along with Linux command-line tools and graphical user interface (GUI) applications, directly on Windows. Unlike conventional virtual machines such as those run with Oracle Virtualbox or VMWare, WSL requires fewer resources (CPU, memory and storage) and can access all the hardware components of your machine (including the graphical processing unit (GPU)) that Windows has access to.

There are several Centre for High Performance Computing (CHPC) users that still make use of the compute resources for both testing and production, especially when it comes to molecular dynamics codes such as AMBER. This is not an ideal situation for testing purposes as it would mean that individuals need to queue, sometimes for long periods of time, before discovering something might be wrong with their setup. Recently, AMBER has become opensource for non-commercial use, which means that users no longer need to do their testing on the CHPC as they can test on their local laptop/desktop prior to submitting simulations to the queuing system at the CHPC.

In this workshop we will:
• Setup WSL on a Windows machine.
• Install a version of Ubuntu using WSL.
• Install essential libraries needed to compile AMBER in Ubuntu.
• Install CUDA Toolkit in Ubuntu for GPU support.
• Compile the serial, parallel and GPU versions of AMBER.
• Export the above WSL instance so that it can be deployed onto other laptops/desktops.

This workshop will be ideal for researchers, scientists and students that make use of the CHPC resources for their computational chemistry research.

Prerequisite:
Laptop with Windows 10 or 11 (If you have Linux, you will still be able to learn how to compile the software package/s).
Preferably 8GB RAM or more (not a must, but things can be slow with less RAM).
Nvidia GPU (not a must as you can still get the CPU version of the code compiled and running).

Note: We can consider other applications should there be time as it is possible to install opensource electronic structure codes within WSL.

Student or Postdoc?

Email address

Co-Authors

CHPC User

CHPC Research Programme

Workshop Duration

Full day

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