CHL Lab

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**Software Installation Instructions for Stampede2:**

If you have not, please read the installation instructions for desktop computers first: Hardwares & Softwares / desktop / 0-software-for-desktop.docx. Reference manuals for software packages, etc. are not repeated in this guide.

To setup your Stampede2 programs, do this:

1. Upload programs-stampede2.tar.gz and bashrc-stampede2.txt onto your stampede2 $HOME directory.

($HOME = ~ )

2. Unzip programs-stampede2.tar.gz. You will get a folder called “programs”. Leave it in your $HOME directory. Remove the tar ball.

3. If you have not worked with stampede2 before / have not modified your .bashrc previously:

mv bashrc-stampede2.txt .bashrc

If you have previous additions in .bashrc: add contents from bashrc-stampede2.txt to the appropriate sections of your .bashrc. Delete bashrc-stampede2.txt.

4. Finally, upload MD/forcefields and put it in your $HOME directory.

Ask Casey if you have any questions regarding the above procedure.

The solefp program is included in the “programs” folder. However, I also have a protocol for manually building solefp on stampede2, if you are interested. See “manually-building-solefp.pdf”.

You might want to take a look at the Stampede2 user guide: <https://portal.tacc.utexas.edu/user-guides/stampede2> and what software are already installed on Stampede2: <https://www.tacc.utexas.edu/systems/software>

Before you proceed, please read the notes on how to work around the Stampede2 platform: “tacc-stampede2.pdf”.