Alanine dipeptide tutorial help sheet hints.
See http://ambermd.org/tutorials/basic/tutorial0/index.php for the tutorial.

1. Before you start the tutorial connect to the Lethbridge server using ssh or a vnc (see point 7 below). After you connect to the Lethbridge server type *module load amber* and press enter. This will load amber and ambertools, which you need to complete the tutorial.
2. To do this tutorial effectively you need to use vi, vim, or emacs, which are command line text editors (like Microsoft text editor, but much harder to use) that are installed on most linux systems that you can use to create and edit text files on the Lethbridge server. You could also use a text editor on your computer or just download the text files from the tutorial and upload them to your home directory on the Lethbridge server. I would recommend using vim. To use it you simply type vim or vi. To understand how to use it see https://www.tutorialspoint.com/unix/unix-vi-editor.htm

3. In step 13 the tutorial has you create the text file named 03_Prod.in. Reduce nstlim to 50000 in place of the listed 5000000. The production run in step 19 will take forever (~ a month) unless you reduce the number of steps calculated to 50000 in nstlim. 50000 steps took 20 minutes when I ran this on the lethbridge server. If you start the production run with nstlim set to 5000000 please stop the run or let us know so we can help you stop it. After stopping it you can change nstlim to 50000 in 03_Prod.in and then restart the production run.

4. In step 15 you need to run sander. sander is the MD engine that does the calculations that determine all of the atoms movement. The tutorial lists this as $AMBERHOME/bin/sander. This will not work. You can get it to work by doing one of the following two options:
    a. Replace $AMBERHOME/bin/sander with /opt/amber/amber20/bin/sander in the tutorial (starting with step 15).
    b. IF you are comfortable with linux you can change your .bashrc file by adding export AMBERHOME="/opt/amber/amber20" and source "$AMBERHOME/amber.sh" to the .bashrc file in your home directory. If you do this and exit the connection or source your .bashrc file (`source ~/.bashrc`) you can use the tutorial as written as far as references to $AMBERHOME goes. see https://emleddin.github.io/comp-chem-website/AMBERguide-no-AMBERHOME-error.html

5. In step 15 and other steps where you run sander be careful how you copy from the tutorial webpage. The safest way to copy is to copy each line from the tutorial to your terminal window separately. Sometimes if you copy both lines at once it will not work. I have included one line examples of the commands in steps 15, 17, and 19 for your copying convenience below.

```
$AMBERHOME/bin/sander -O -i 01_Min.in -o 01_Min.out -p parm7 -c rst7 -r 01_Min.ncrst -inf 01_Min.mdinfo
$AMBERHOME/bin/sander -O -i 02_Heat.in -o 02_Heat.out -p parm7 -c 01_Min.ncrst -r 02_Heat.ncrst -x 02_Heat.nc -inf 02_Heat.mdinfo
$AMBERHOME/bin/sander -O -i 03_Prod.in -o 03_Prod.out -p parm7 -c 02_Heat.ncrst -r 03_Prod.ncrst -x 03_Prod.nc -inf 03_Prod.info &
```

6. In Step 19 be sure to change pmemd to sander (the Lethbridge server does not have pmemd, which is another MD engine included in amber)
7. In step 23 you visualize your simulation. VMD is loaded on the uleth server; however, you need to set up a vnc connection to use VMD properly on the server (this allows you to have a graphical user interface to operate VMD just as you would on your own computer). To set up the vnc follow the instructions given in steps 1-5 under getting started here: https://www.cch.uleth.ca/computing.php (you likely have already done step 5.