Practical session 4: Run a parallel job

Overview

In **Part A** we are going to:

Copy files supplied in exercise 3 to our *scratch* area.

Run a parallel job using the files [you will need to edit the jobscript].

Run a serial job to create an animation of the simulation results.

Copy files back to the *home* area for safekeeping

In **Part B** we are going to:

Transfer the movie file from the CSF home area to your laptop / PC.

Notes:

So far, we have run jobs from our "home" storage area, because we know they won't create any large files. But for real work, we must use the "scratch" storage, which is faster and has a much larger capacity. It is, however, temporary storage.

This exercise uses the open-source OpenFOAM *Computational Fluid Dynamics* (CFD) app. **Anybody** can have a go at this exercise, even if you are not doing a CFD project. It shows one method of running a parallel job that you might use in your own work. You *do not* need to know anything about CFD!! It will also let you practice downloading a file from the CSF to your laptop / PC.

Part A

1. **Copy to scratch**: You will use the "scratch" storage this time as this is the best place from which to run jobs, in case they create large files. Create a directory (folder) there, then go to that new directory and check where we are:

   ```
   mkdir ~/scratch/mace-course
   cd ~/scratch/mace-course
   pwd
   ls
   ```

   Notice that `pwd` expands the **~** to show your full home directory path.
   The `ls` command also shows no output – there are no files in the directory to begin with!

2. You will need to copy the OpenFOAM files (that you downloaded earlier) to your scratch area. If you didn't complete exercise 3, please ask for help.

   ```
   cp -r ~/mace-course/foam-example/ .
   ```

   (the **.** at the end is important! It means "current directory" - so we are copying

the foam-example folder *from* our home area *to* the current directory – which is in our scratch area. The `-r` flag (recursive) ensures it copies an entire folder.)

3. Now go into the newly copied folder and see what's there:

```
cd foam-example
pwd
ls
```

You should now be in the `foam-example` folder in your scratch area. You should see various OpenFOAM files.

It may not look like it, but the scratch area uses different storage hardware to the home area. The scratch area is much larger, and, because the disks are physically located in the CSF, it is faster, which helps when your jobs read and write large files.

4. **The parallel (multi-core) job**. Now open `foam-solve.sh` with `gedit`.

You should be able to see some differences from the serial script we ran in the earlier exercise. It has a parallel partition line (`#SBATCH -p multicore`) and, further down, the
`mpirun`
commands that it uses to run the various OpenFOAM executables (e.g., named `interFoam`) with the same number of cores, as requested on the pe line.

Notice also that we make sure the batch job can find OpenFOAM executables by including this line in the `foam-solve.sh` file:

```
module purge
module load apps/gcc/openfoam/v2012
```

(the `source $foamDotFile` line is an extra setup step used by OpenFOAM but most apps just require a module to be loaded.)

5. **BUT** the `foam-solve.sh` file contains an **ERROR** – on the `-n` line replace the
`?`
with the number
`4`
so that we request 4 cores on a CSF compute node.

6. Save the jobscript and exit gedit. Then submit the job:

```
sbatch foam-solve.sh
```

If you are trying this outside of a course session, use:

```
sbatch --reservation="" foam-solve.sh
```

7. Monitor with `squeue` and, when it has finished, use the `ls` command to see what files have been created. To see them in date/time order with the newest at the bottom of the output:

   ```
   ls -ltr
   ```

8. You should have some output in `slurm-`*`JobID`*`.out` file and several other output files. Let's have a quick look at the end of the file as this often indicates whether a problem occurred. The Linux `tail` command shows the last few lines of a file:

   ```
   tail slurm-JobID.out
   ```

   The last 3 lines should be something like:

   ```
   ExecutionTime = 29.3 s  ClockTime = 39 s
   End
   Finalising parallel run
   ```

   If you see anything different to the above please ask for help.

9. **The serial job**: We are now going to submit a small serial job to post-process the simulation results and generate an animation of the simulation. Don't worry about the details of how this is done (although if you are an OpenFOAM user you may wish to have a look at the jobscript and so on.) To submit the job:

   ```
   sbatch foam-anim.sh
   ```

   If you are trying this outside of a course session, use:

   ```
   sbatch --reservation="" foam-anim.sh
   ```

10. Again, monitor the job with `squeue` then check the output file:

    ```
    tail slurm-JobID.out
    ```

    If the movie file has been written successfully you should have a new file in your directory (folder):

    ```
    ls -l foam-anim.ogv
    ```

11. Now, remember that *scratch* is **not backed up**, so copy your new movie file to *home* where it will be backed up automatically for you:

    ```
    cp foam-anim.ogv $HOME
    ```

    `$HOME` is a special variable that always maps to your *home* directory. You can also use the `~` symbol (as we saw earlier) as another shorthand for your home directory.

    Caution: the above command will overwrite any existing `foam-anim.ogv` that you might have in your home directory.

    We also modified the jobscript `foam-solve.sh` so we'll copy that back to home for safe keeping:

    ```
    cp foam-solve.sh ~/mace-course/foam-example/
    ```

    (It is always worth keeping important files in the home area – files in scratch that have not been read or written to in the last three months will be deleted by the system.)

PTO for Part B

B. Download the movie file to your laptop / PC

At this point you should have a file named `foam-anim.ogv` in your home directory. Let's check:

```
ls -l ~/foam-anim.ogv
```

If you don't see the file please ask for help.

You should now be able to download the file from the CSF to your laptop / PC, using a similar method to that used in exercise 3:

- **Windows users:** use MobaXterm or WinSCP drag and drop as before.

- **Linux and MacOS Users:** Run the following command in a terminal on your laptop – in a terminal **NOT** logged in to the CSF:

```
scp username@csf3.itservices.manchester.ac.uk:~/foam-anim.ogv .
```

replace ***username*** with your central IT username and enter your ***central IT password*** when asked, then press **1** at the DUO prompt and accept the DUO push on your mobile). Note: There is a **dot at the end of the line above**. This is important, don't forget the **.** because it tells `scp` to put the file in *the current folder* - I.e., wherever you are on your laptop / PC (the file will keep the name `foam-anim.ogv`).

Can you play the animation on your laptop / PC?