Multithreaded Optimisation

Exercise Notes

Download and extract the exercise files

Firstly, change directory to make sure you are on the /work filesystem on ARCHER.

```
guestXX@archer:~> cd /work/y14/y14/guestXX/
```

/work is a high performance parallel file system that can be accessed by both the frontend and compute nodes. All jobs on ARCHER should be run from the **/work** filesystem. ARCHER compute nodes cannot access the **/home** filesystem at all: any jobs attempting to use **/home** will fail with an error.

Copy the exercise files archive on ARCHER from **/home/z01/shared** and unpack it with the commands

```
cp /home/z01/shared/tpo.tar .
tar xvf tpo.tar
```

Exercise

The **TPO/*/MolDyn/** directory contains a not very efficient parallel version of the molecular dynamics code. First load the performance tools modules with

```
module load perftools-base
module load perftools
```

Build the code using the supplied Makefile. Instrument the executable for OpenMP profiling using

```
pat_build -g omp md
```

This will produce a new binary called **md+pat** . Run this using 4 threads by submitting the batch file **md.pbs** . This will produce a file with a **.xf** extension. Generate the profile using

```
pat_report md+pat+???????.xf
```

Now modify the code so that it uses a better loop schedule and/or atomic updates instead of CRITICAL — does the performance improve? Redo the profiling.