

# Introduction to Molecular Dynamics on ARCHER: Running DL\_POLY calculations on ARCHER

## 1 Introduction

This document gives some additional instructions for running DL\_POLY calculations on ARCHER. Detailed instructions on what calculations to run may be found at:

- DL\_POLY Exercises - [http://www.ccp5.ac.uk/DL\\_POLY/TUTORIAL/EXERCISES/index.html](http://www.ccp5.ac.uk/DL_POLY/TUTORIAL/EXERCISES/index.html)
- DL\_POLY Benchmarking - [ftp://ftp.dl.ac.uk/ccp5/DL\\_POLY/DL\\_POLY\\_4.0/DATA/](ftp://ftp.dl.ac.uk/ccp5/DL_POLY/DL_POLY_4.0/DATA/)

**NB: ignore the instructions to download and build DL\_POLY. DL\_POLY is already pre-installed on ARCHER!**

You may wish to refer to the "Instructions for running jobs on ARCHER" handout for details of how to connect and construct batch jobs scripts.

## 2 Running the DL\_POLY Classic GUI

The DL\_POLY Classic GUI is available on ARCHER, and can be launched directly by:

```
ibethune@eslogin006:~>  
  
java -jar /usr/local/packages/cse/dlpoly_classic/1.9-phase1/source/java/GUI.jar
```

## 3 Running jobs

While, most of the provided exercises can be executed within a few seconds on a single core, it is good practice to run jobs using the batch system to avoid impacting other users. To run a DL\_POLY job on the backend of ARCHER, set up a PBS job script with the following entries (to use 2 MPI parallel processes):

```
module load dlpoly/classic-1.9  
  
aprun -n 2 -N 2 DL_POLY.X
```

## 4 DL\_POLY Performance Tests

A large selection of different systems (covering physics, materials, chemistry and biology applications) are available at the FTP site above.

Once extracted, the input files may be run using DL\_POLY 4, using (in a batch script):

```
module load dlpoly
```

```
aprun -n 2 -N 2 DL_POLY.Z
```

DL\_POLY scaling with system size can be tested by scaling up the system using the `nfold x y z` keyword in the CONTROL file. This will dump an additional `CONFIG_x_y_z` and `FIELD_x_y_z`, containing the system enlarged by a corresponding factor in each dimensions. Copy these files in place of the originals and re-run.

DL\_POLY reports the total wallclock time taken at the end of the run, as:

```
time elapsed since job start:      19.322 sec
```