



## Guide to Running DL\_POLY\_4

### What is DL\_POLY\_4?

DL\_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith.

DL\_POLY\_4 [1] general design provides scalable performance from a single processor workstation to a high performance parallel computer. DL\_POLY\_4 offers fully parallel I/O as well as a netCDF alternative (HDF5 library dependence) to the default ASCII trajectory file.

DL\_POLY\_4 is the direct successor of DL\_POLY\_3 (I.T. Todorov and W. Smith) which also incorporates concepts and functionality from DL\_POLY\_2 (W. Smith, T.R. Forester and I.T. Todorov). Like DL\_POLY\_3, DL\_POLY\_4 parallelisation is based on the static/equi-spatial Domain Decomposition (DD) model. It enables an excellent load-balancing and parallel performance provided that:

- The particle density of the modelled system is close to uniform in space and time (ensuring load balancing)
- The system dimensions per processor/domain are no smaller than the largest system cutoff, preferably no smaller than three times (ensuring good parallel performance).

Future plans include a hybridisation from purely MPI mapped DD to usage of OpenMP threading within the MPI framework for better per core performance and improved load balance (LB) of the DD strategy.

Note that the former DL\_POLY\_2 version (authored by W. Smith, T.R. Forester and I.T. Todorov) is now transformed into DL\_POLY\_CLASSIC [2] and available as open source under the BSD [3] at CCPForge [4].

### Step 1 - Log in

The example used in this guide is configured to run on the Cardiff Skylake *Hawk* cluster. Connect to *hawklogin.cf.ac.uk* with your Supercomputing user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal), thus

```
ssh -l your_username hawklogin.cf.ac.uk
```

The steps below involve typing commands (**in bold font**) in the terminal window.

### Step 2 - Load a DL\_POLY\_4 module

In common with most of the application guides in this series, we assume at the outset that the module of choice would be selected from those originally available on HPC Wales. Thus a necessary first step would be to gain access to that module set by issuing the commands

```
module purge  
module load hpcw
```

Note that the “module purge” command is required to prevent any unintentional collision with pre-existing modules. Subsequently issuing the module command

```
module avail
```

will provide visibility of and access to the entire set of HPCW modules.

A number of DL\_POLY\_4 binary packages are available. Note that in common with most other software packages on the system, these are built with the Intel compiler.

- List pre-installed DL\_POLY\_4 versions:

```
module avail dlpoly
```

- Load the preferred version (4.08):

```
module load dlpoly/4.08
```

- Confirm the loaded modules. Note that this is currently the latest version of the code. All dependencies are handled automatically via the module file:

```
module list
```

### Step 3 - Create a directory

From your home directory, create a directory to hold the DL\_POLY4 data:

```
cd ~
```

```
mkdir DLPOLY4
```

### Step 4 - Obtain a test case

A number of benchmark test cases are provided with the installation at

```
/app/chemistry/dlpoly/4.08/examples
```

- Copy the two benchmark files for Test2 to your user space:

```
cd ~/DLPOLY4
```

```
cp /app/chemistry/dlpoly/4.08/examples/DLPOLY4.test2.SLURM.q .
```

```
cp /app/chemistry/dlpoly/4.08/examples/TEST2.tar.gz .
```

```
tar xzvf TEST2.tar.gz
```

The TEST2 subdirectory should contain all required files to run a DL\_POLY\_4 job:

- CONFIG contains the initial positions and velocities for the ions,
- FIELD defines the force-field and,
- CONTROL holds the control parameters for the job (e.g. number of steps, temperature, etc.).

The directory also contains sample output files and a batch script.

This particular benchmark is a simulation of a sodium chloride melt with Ewald sum electrostatics. The system is comprised of 216,000 atoms.

## Step 5 - Submit a job

You are now ready to run this test case with the supplied job script *DLPOLY4.test2.SLURM.q*

- From your working directory, submit the job using: **sbatch DLPOLY4.test2.SLURM.q**
- Check the job queue using: **squeue**
- Note that the majority of the files created during the job are routed to the user's scratch directory, */scratch/\$USER*, and may be deleted on job termination. The 120-core job should complete in less than 15 seconds.
- Note also that the simulation is ran twice to provide a timing sensitivity analysis.
  - If the case runs successfully, the log files -  
*DLPOLY4.TEST2.Hawk.out.n120.PPN=40.JobID.0* and  
*DLPOLY4.TEST2.Hawk.out.n120.PPN=40.JobID.1* –  
routed to the DLPOLY4 directory should contain all the output and the message “Thank you for using the DL\_POLY\_4 package in your work”. Inspect the log files for more information.
  - Compare your job output with the reference output file

*/app/chemistry/dlpoly/4.08/examples/DLPOLY4.TEST2.Hawk.out.n120.PPN=40.24485.0*

## Step 6 – More test cases

A second test case, Gramicidin A with water solvating (792,960 atoms), is available at */app/chemistry/dlpoly/4.08/examples*:

*/app/chemistry/dlpoly/4.08/examples/TEST8.tar.gz* and

*/app/chemistry/dlpoly/4.08/examples/DLPOLY4.test8.SLURM.q*

Copy the file and job script and run as in TEST2 above. To create a new case, refer to the section on Input Examples of the DL\_POLY\_4 Manual, a PDF version of which is available at: [/app/chemistry/dlpoly/4.08/doc/DL\\_POLY4.User\\_Manual\\_4.08.pdf](http://app/chemistry/dlpoly/4.08/doc/DL_POLY4.User_Manual_4.08.pdf)

## References

[1] Official DL\_POLY\_4 website at: [https://www.scd.stfc.ac.uk/Pages/DL\\_POLY.aspx](https://www.scd.stfc.ac.uk/Pages/DL_POLY.aspx)

[2] [http://www.ccp5.ac.uk/DL\\_POLY\\_CLASSIC/](http://www.ccp5.ac.uk/DL_POLY_CLASSIC/)

[3] <http://www.opensource.org/licenses/bsd-license.php>

[4] [http://ccpforge.cse.rl.ac.uk/gf/project/dl\\_poly\\_classic/](http://ccpforge.cse.rl.ac.uk/gf/project/dl_poly_classic/)

[5] DL\_POLY\_4 FAQ:

[http://www.stfc.ac.uk/SCD/research/app/ccg/software/DL\\_POLY/44546.aspx](http://www.stfc.ac.uk/SCD/research/app/ccg/software/DL_POLY/44546.aspx)

[6] DL\_POLY\_4 User Documentation:

[ftp://ftp.dl.ac.uk/ccp5/DL\\_POLY/DL\\_POLY\\_4.0/DOCUMENTS/USRMAN4.pdf](ftp://ftp.dl.ac.uk/ccp5/DL_POLY/DL_POLY_4.0/DOCUMENTS/USRMAN4.pdf)

[7] “DL\_POLY\_3: new dimensions in molecular dynamics simulations via massive parallelism”, Ilian T. Todorov, William Smith, Kostya Trachenkob and Martin T. Dove, J. Mater. Chem., 2006, **16**, pp. 1911-1918, [DOI: 10.1039/B517931A](https://doi.org/10.1039/B517931A)