

## What is DL\_POLY Classic?

DL\_POLY Classic is a general purpose (parallel and serial) molecular dynamics simulation package derived from the package formerly known as DL\_POLY\_2 (Version 20) which was originally written by W. Smith and T.R. Forester at Daresbury Laboratory to support the CCP5 project 'Computer Simulation of Condensed Phases'.

Please note that DL\_POLY Classic is not the same as DL\_POLY 4 – the performance of the latter will be markedly superior on large core counts and for large system sizes. However, for small to medium sized systems on moderate core counts, DL\_POLY Classic will be competitive and the instructions for using the two codes are very similar, only the performance is different.

## Step 1 - Log in

The example used in this guide is configured to run on the Swansea Sandy Bridge cluster. Connect to `login.hpcwales.co.uk` with your HPC Wales user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal), then `ssh sw-sb-log-001` to connect to the Swansea system.

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

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

More than one DL\_POLY Classic package may be available. Note that in common with most other software packages on the system, these are built with the Intel compiler.

- List preinstalled DL\_POLY Classic versions:  
`module avail dlpoly-classic`
- Load the default version:  
`module load dlpoly-classic`
- Confirm the loaded modules. All dependencies are handled automatically via the module file:  
`module list`

## Step 3 - Create a directory

Create a directory to hold any user data files. For this example, create a directory called DLPOLY-CLASSIC under your home directory:

```
cd ~  
mkdir DLPOLY-CLASSIC
```

## Step 4 - Obtain a test case

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

`/app/chemistry/dlpoly-classic/1.8/intel-11.1/intel-4.0/example`

- Copy the two benchmark files for Bench4 to your user space:

```
cd ~/DLPOLY-CLASSIC
```

```
cp /app/chemistry/dlpoly-classic/1.8/intel-11.1/intel-4.0/example/Bench4.SLURM.q .
```

```
cp /app/chemistry/dlpoly-classic/1.8/intel-11.1/intel-4.0/example/bench4.tar.gz .
```

```
tar xzvf bench4.tar.gz
```

The bench4 subdirectory should contain all required files to run a DL\_POLY Classic 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 27,000 atoms.

## Step 5 - Submit a job

Now you are ready to run this test case with the supplied job script.

- From your working directory, submit the job by:

```
sbatch Bench4.SLURM.q
```

- Check the job queue using:

```
squeue
```

- When completed, output can be found in the file bench4.out.32.<Job\_ID> in the DLPOLY-CLASSIC subdirectory (where <Job\_ID> is the ID assigned by the SLURM queuing system). This can be compared to the reference results in the file

```
/app/chemistry/dlpoly-classic/1.8/intel-11.1/intel-4.0/example/bench4.out.32.
```

## Step 6 - More test cases

More test cases are distributed with DL\_POLY Classic. They can be found at

`/app/chemistry/dlpoly-classic/1.8/intel-11.1/intel-4.0/example`

Run Bench5 and Bench7 – Bench5.SLURM.q and Bench7.SLURM.q – Bench5 is a simulation of Na/K Disilicate Glass with 3 body forces, while Bench7 is a simulation of Gramicidin A with TIP3P Water solvating. The procedure used follows that for Bench4 above.

## References

- Official DL\_POLY Classic home page [http://www.ccp5.ac.uk/DL\\_POLY\\_CLASSIC/](http://www.ccp5.ac.uk/DL_POLY_CLASSIC/)
- CCPForge distribution site [http://ccpforge.cse.rl.ac.uk/gf/project/dl\\_poly\\_classic/](http://ccpforge.cse.rl.ac.uk/gf/project/dl_poly_classic/)
- User manual [http://www.ccp5.ac.uk/DL\\_POLY\\_CLASSIC/MANUALS/USRMAN.pdf](http://www.ccp5.ac.uk/DL_POLY_CLASSIC/MANUALS/USRMAN.pdf)