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 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_4 module

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`

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- Load the preferred version (4.07):

```
module load dlpoly/4.07
```

- 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/4.07/examples`

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

```
cd ~/DLPOLY4
cp /app/chemistry/dlpoly/4.07/examples/DLPOLY4.test2.SLURM.q .
cp /app/chemistry/dlpoly/4.07/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 64-core job should complete in less than 30 seconds.

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- Note also that the simulation is ran twice to provide a timing sensitivity analysis.
- If the case runs successfully, the log files - *DLPOLY4.TEST2.sb.out.n64.PPN=16.JobID.0 and DLPOLY4.TEST2.sb.out.n64.PPN=16.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/4.07/examples/DLPOLY4.TEST2.sb.out.n64.PPN=16.617.0***

Step 6 – More test cases

A second test case, Gramicidin A with water solvating (792,960 atoms), is available at **/app/chemistry/dlpoly/4.07/examples:**

/app/chemistry/dlpoly/4.07/examples/TEST8.tar.gz and

/app/chemistry/dlpoly/4.07/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/4.07/doc/USRMAN4.07.pdf

References

[1] Official DL_POLY_4 website at: http://www.stfc.ac.uk/SCD/research/app/ccg/software/DL_POLY/44516.aspx

[2] 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/

[5] DL_POLY_4 FAQ: http://www.stfc.ac.uk/SCD/research/app/ccg/software/DL_POLY/44546.aspx

[6] DL_POLY_4 User Documentation: http://www.ccp5.ac.uk/DL_POLY/MANUALS/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

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