

## **DL\_POLY\_3 I/O Analysis, Alternatives and Future Strategies**

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### **Abstract**

We outline the problems associated with I/O when performing large classical Molecular Dynamics runs, and show that it is necessary to use parallel I/O methods when studying large systems.

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## 1 Introduction

DL\_POLY\_3 is a general purpose molecular dynamics (MD) package developed by I.T. Todorov and W. Smith at STFC Daresbury Laboratory to support researchers in the UK academic community<sup>1</sup>. This software is designed to address the demand for large scale MD simulations on multi-processor platforms, although it is also available in serial mode. DL\_POLY\_3 is fully self-contained and written in Fortran 95 in a modularised manner with communications handled by MPI. The standards conformance of the code has been very rigorously checked using the NAGWare95 and FORCHECK95 analysis tools, so guaranteeing exceptional portability. Parallelisation is achieved by equi-spatial domain decomposition distribution which guarantees excellent load balancing and full memory distribution provided the system's particle density is fairly uniform across space<sup>2</sup>. This parallelisation strategy results in mostly point to point communication with very few global operations, and excellent scaling; one might compare it with the halo exchange algorithms employed in computational fluid dynamics.

However parallelisation of the computation is only part of the story. For DL\_POLY 3 to be an effective tool for researchers all parts of the calculation must scale, and this includes the input and output (I/O) stages of the code. Historically this has most often been performed in an essentially serial manner, not only in DL\_POLY 3 but also many other large scale packages. However with the scale of calculations now possible it is clear that this approach will not scale to the next generation of machines as the time for I/O is becoming prohibitive. In this short technical report we shall describe how DL\_POLY has in the past performed I/O, what problems this has resulted in, and a very first effort to address the problems.

## 2 I/O in DL\_POLY

The main I/O in DL\_POLY 3 is, as is the case for all classical molecular dynamics codes, reading and writing *configurations*. These are simply lists of the coordinates, velocities and forces acting on the particles that comprise the system. In DL\_POLY 3 this has traditionally been performed using formatted I/O for portability; while the MD run itself may be done on the supercomputer the analysis of the results is often done on a workstation at home.

While this is very portable there are a couple of potential problems

1. Formatted I/O is not very efficient
2. For large systems the files can get very big

It is the second point that is causing us to re-evaluate our I/O strategy. With top end machines like HPCx now capable of performing classical MD simulations in millions, or in some cases even billions, of atoms the time taken to write these large files is now beginning to impact on the amount of science that users of DL\_POLY 3 can perform.

As matter of fact it is not the reading of configurations that is the issue. That is typically done only once to define the initial state of the system. It is the writing of

configurations. This need not only be done for the final state of the system, but also many times during the simulation of system so that the time evolution can be studied. Thus it is the writing of configurations that need be parallelised, at least initially. In the remainder of this section we shall describe how the writing of configurations has been performed historically, and also our new parallel method.

## 2.1 *Serial I/O in DL\_POLY 3*

Historically the writing of configurations has been done very simply in DL\_POLY 3, using a master slave method. One processor, the master, receives in turn the coordinates, velocities and forces held by the other processors and writes them to file. While simple, portable and robust this strategy has one obvious drawback, it is inherently serial and so may impact scalability through simple Amdahl's Law effects. For instance on a large Blue Gene system we have observed one run where while a timestep in the MD took around 0.5s to perform, the dumping of a configuration took 450 seconds. Since a configuration is typically dumped every 1,000-10,000 timesteps this is not a very satisfactory situation! We shall call this the *Swrite* algorithm.

Reading of the initial configuration is the reverse of the above. The master reads a chunks of the initial configuration and sends them in turn to the slave processors. As input is not so much of an issue at present all results given here for reading will use this algorithm.

## 2.2 *Parallel I/O in DL\_POLY 3*

The obvious problem with the *Swrite* algorithm is that only one processor ever performs the I/O, and thus all the other processors must wait on it. As an alternative we developed a very simple *Pwrite* algorithm where all processors participate in writing to the file.

Given the simple and regular format of the configuration file it is very simple to calculate where the data for a given atom needs to be written; it depends solely on the global index of that atom. Further given that each item of the data consists of nine real numbers, the components of the position, velocity and force, all the record lengths in the file will be the same. Thus it is very simple to use Fortran direct access files and have each processor writing to the appropriate records for the atoms it holds. So in our *Pwrite* algorithm all the processors write to the file at once, as each processor can calculate where in the direct access file the data need be written.

While this algorithm is simple to implement, it is not robust and will not work on some computers, for instance the Cray T3X series. The reason for this is that it does not conform to the Fortran standard, which essentially assumes that only one process will ever be accessing a file at once. Given the emphasis on standard conformance previously in DL\_POLY this is unacceptable for general release. However it is "good enough" to test the impact of parallel I/O, and much simpler than a full MPI I/O or HDF implementation.

### 3 Results

To test the I/O the system we used was an oxygen deficient pyrochlore  $Gd_2Zr_2O_7$  (zirconite) with a size of 3,773,000 particles, which corresponds to 1.1 GB configuration dump file. It is worth mentioning that no machine was available for exclusive use while benchmarking which could have contributed to the fluctuations of the observed times at low processor counts.

Table 1 shows the results for two IBM systems, the Blue Gene system at Daresbury and HPCx. The times for writing a single configuration are given, as is the time to perform a single timestep. Both systems have a GPFS file system.

CPUs	IBM BG/L			IBM P575		
	PWrite	SWrite	Timestep	PWrite	SWrite	Timestep
32	21.5	228.7	28.22	11.3	98.3	12.02
64	20.8	244.5	13.69	9.7	118.3	5.95
128	16.6	242.1	7.23	9.1	153.5	3.03
256	18.4	238.9	3.86	13.1	120.0	1.58
512	22.5	248.9	2.03	13.3	134.1	0.87
1024	39.5	252.2	1.16	17.1	148.3	0.58
2048	58.8	253.0	0.77			

Table 1

It can be seen that the parallel writing algorithm is markedly superior to performing I/O in serial. Improvements by an order of magnitude can be obtained, and it is clear that if regular writing of configurations is required when studying this system that the parallel strategy will markedly improve the scaling of the whole code, even though the I/O is not scaling especially well itself.

Table 2 contains the timings obtained on a Cray XT3 system. Both single and dual core runs were performed, and again exclusive use was not available.

CPUs	Cray XT3 Single Core			Cray XT3 Dual Core		
	PWrite	SWrite	Timestep	PWrite	SWrite	Timestep
64	16.5	32400	2.93	15.0	32400	3.62
128	16.3	32400	1.61	12.5	32400	2.30
256	14.9	32400	0.87	14.8	32400	1.26
512	17.3	32400	0.48	19.6	32400	0.64
1024				11.5	32400	0.44

Table 2

The improvements here are dramatic, though it probably reflects more a problem in the Lustre I/O system used by the XT3 rather than the code changes we have made. Whatever the number of processors the *Swrite* algorithm took at least 9 hours; remember this is the time to dump **just one configuration!** On the other hand the

*Pwrite* time is comparable to that found on the IBM systems, and show similarly poor scaling. It can also be seen the timestep calculation is appreciably faster on the XT3 compared to the IBM systems.

## 4 Discussion

It is clear from the above that for DL\_POLY to be able to address larger systems we must move to a parallel I/O strategy. However it is also clear that the current strategy, while simple to implement is not optimal as it

1. is not portable
2. does not scale well

To address the second point a simple method would be to use only a subset of the processors to perform the I/O, rather than all of them. For instance on the BG/L system it is clear that 128 processors would be a sensible number to use for this particular simulation, and we suspect that similar considerations will apply whatever the form of parallel I/O is used.

For portability there are two issues, the portability of the implementation and the portability of the resulting file. The current implementation fails the first but passes the second. Unfortunately the most common parallel I/O library, MPI IO, in practice passes the first but fails the second. This is because most current implementations of MPI IO only implement the *native* data representation which is inherently non-portable. As analysis of DL\_POLY runs is often performed on a different machine to that which the code originally executed on, this is not acceptable. We therefore intend to look at other possible solutions, such as HDF, to solve the problem outlined in this report.

[1] Todorov IT and Smith W, 2004, *Phil Trans R Soc Lond, A* **362**, 1835

[2] M.R.S. Pinches, D. Tildesley, W. Smith, 1991, *Mol Simulation*, **6**, 51