A DaFT (Mixed Radix) FFT for DL_POLY_4

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1 Introduction and Background

DL_POLY_4[i] and its predecessor, DL_POLY_3, is a general purpose classical molecular dynamics (MD) simulation software package which has been developed at Daresbury Laboratory by I.T. Todorov and W. Smith. The package is used to model the atomistic evolution of the full spectrum of models commonly employed in the materials science, solid state chemistry, biological simulation and soft condensed-matter communities. It has been developed under the auspices of CCP5[ii] and is widely used throughout the UK as well as world-wide. It is a fully data distributed code, employing methodologies such as spatial domain decomposition (DD), link-cells (LC) built Verlet neighbourlist (VN)[iii] and 3D Daresbury Fourier Transform (DaFT)[iv]. The code demonstrates excellent performance and has been shown to scale to large numbers of processors.

As stated above the linked cells algorithm[v] is the basis upon which DL_POLY_4 is parallelised, which it achieves by using an equispatial domain decomposition. The simulation cell is divided into a number of equal volume, isomorphic, parallelipiped domains, and each domain is assigned to an MPI process. As most inter-atomic interactions become negligible beyond a finite distance, the "cutoff", only position data for atoms near the edges of each domain need communicating to neighbouring cores for the atomic interactions to be calculated, provided the cutoff is much smaller than the length of the edge of the domains. The LC method thus has much in common with the halo exchange methods used in solving differential equations on grids, except that it is generalised to allow for the "grid points", i.e. the atoms, to be disordered in space, and for them to move from time step to time step.

However the key phrase in the above paragraph is "most inter-atomic interactions become negligible beyond a finite distance," and in particular the word "most." An extremely important exception is the Coulomb potential, which decays as 1/r, where r is the inter-atomic separation. This is therefore an extremely long ranged interaction and in fact it strictly can not be cut off at all. It therefore appears that it can not be used at all within a periodic system, which is the kind DL_POLY is most often used to study, as the sums involved to evaluate the inter-atomic interactions will run over all periodic images of the particles, an infinite number of operations! However this problem can be circumvented by using the Ewald Summation[vi], which is essentially a summation acceleration method that exploits the translational symmetry of the periodic system. The traditional method for performing this scales as $N^{3/2}$[vii] [viii], where N is the number of particles in the system being studied. However more modern variants, such as the Smooth Particle Mesh Ewald method (SPME) due to Darden *et al.*[ix], employ fast Fourier transforms (FFTs)[x] to reduce this scaling to N*log(N), and it is the SPME method that DL_POLY_4 employs.

In the remainder of this report I shall briefly describe the steps in the SPME method and how DL_POLY_4 employs it within the LC method. Then I shall describe the original implementation in DL_POLY which employed a radix-2 parallel FFT written by myself, and discuss the limitations that a single radix transform results in. After that I shall describe the current work, namely how the FFT has been generalised to a mixed radix parallel transform and how this

has impacted the rest of the code. Finally I shall report some performance figures for the current code, and also its current status.

2 The Ewald Summation and SPME

In this section I shall outline the steps in the SPME method so as to provide a better understanding of the work required. A much more comprehensive discussion, including error analyses, is given in the references above

The main steps of the SPME method are as follows:

1. Form Q. This is defined on a grid within the unit cell and given by

$$Q(k_{1,}k_{2,}k_3)=\sum_{i=1}^{N}\sum_{n_{1,}n_{2,}n_3=-\infty}^{\infty} q_i$$
$$M_n(u_{1i}-k_1-n\,\mathrm{K}_1)\,M_n(u_{2i}-k_2-n\,\mathrm{K}_2)\,M_n(u_{3i}-k_3-n\,\mathrm{K}_3)$$

   In this q_i is the charge on atom i, $u_{\mu i}=K_\mu r_{\mu i}$ is the scaled position of atom i, $K_{1,2,3}$ are the dimensions of the grid, $0\le k_\mu<K_\mu$ and M_n is a cardinal b-spline[xi] of order n

2. Forward Fourier transform Q(**k**) to Q(**m**)
3. Form V(**m**) $V(\boldsymbol{m})=\dfrac{e^{\frac{-\pi^2 m^2}{\beta^2}}}{m^2}Q(\boldsymbol{m})$
4. Form G(**m**) $G(\boldsymbol{m})=\prod_{\mu=1}^{3}\left|b_\mu(m_\mu)\right|^2 V(\boldsymbol{m})$ where

$$b_\mu(m_\mu)=e^{(2\pi i(n-1)m_\mu/\mathrm{K}_\mu)}\left[\sum_{k=0}^{n-2}M_n(k+1)\,e^{\frac{2\pi i m_\mu k}{\mathrm{K}_\mu}}\right]^{-1}$$

5. Inverse Fourier Transform G(**m**) to G(**k**)
6. From G(**k**) it is straightforward to calculate both the total energy of the system and the forces on the ions comprising it.

This scheme has 2 important properties which allow it to be used easily within a the data distribution used by DL_POLY_4

1. First a very important property of the cardinal b-splines, $M_n(u)$, is that they are non-zero **only** in the range $0<u<n$. Thus in the calculation of the contribution due to atom i to Q(**m**) it is necessary to consider only points near the atom. This is effectively a short range interaction with a cutoff, precisely the kind at which that the link cell algorithm excels
2. In Fourier space all operations are local, i.e. all that is required to evaluate the quantities at a given point in space are values at that point, there is no coupling of different points in the grid.

3 DaFT

Thus the main steps in the evaluation of the quantities of interest are the calculation of Q(**k**) which exploits the link cell decomposition of the problem, and then a forward and back Fourier transform. Unfortunately standard parallel three dimensional FFTs such as FFTW[xii] require data decomposed in planes, not the equispatial domain decomposed form that DL_POLY_4 uses. Thus a large scale data redistribution would be required to use FFTW or similar, a process that is notoriously inefficient on distributed data parallel machines.

Instead a number of years ago I wrote DaFT, the Daresbury Fourier Transform, which can perform the 3D FFT using the DL_POLY_4 data distribution directly. The core idea is to perform each of the 1D FFTs in parallel and the original version of DaFT used the radix 2 Sande-Tukey[xiii] algorithm for the forward transform. This is a decimation in frequency (DIF) algorithm; given a Fourier transform

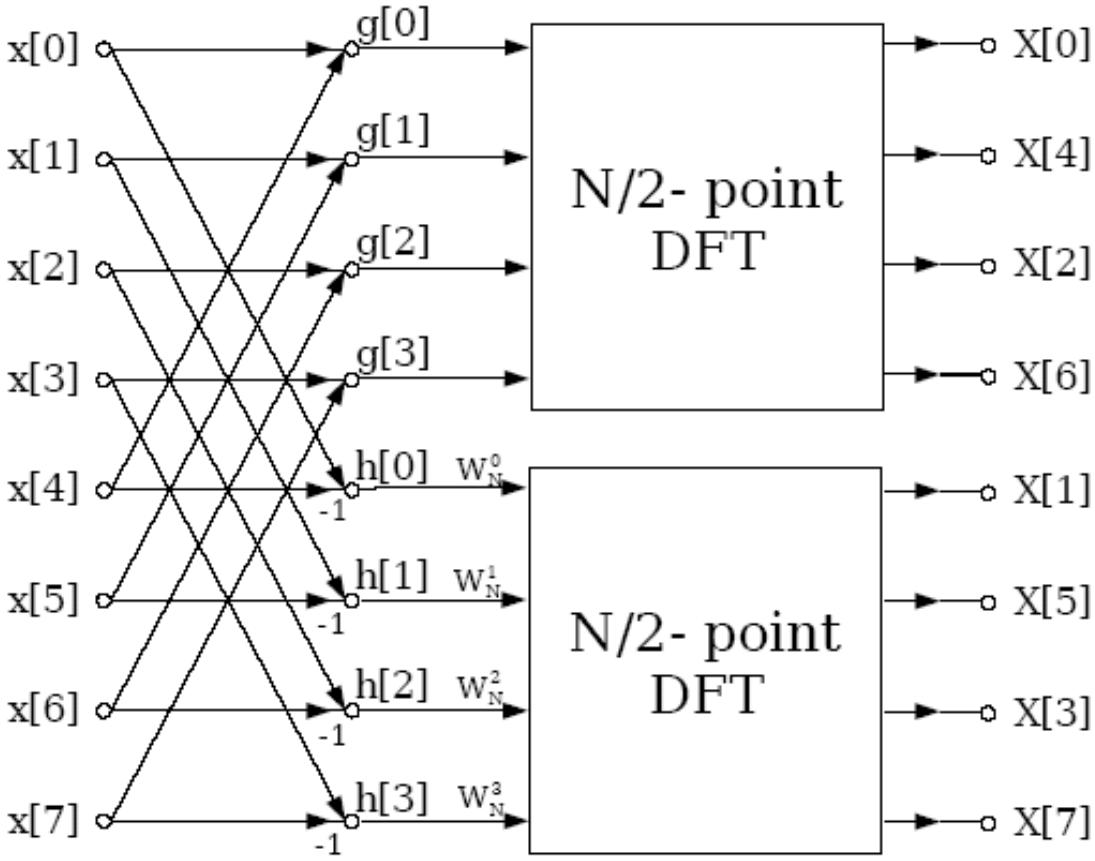
$$X(k)=\sum_{j=0}^{N-1} x(j)e^{\frac{2\pi i}{N}jk}$$

then the result can be written in terms of two transforms of half the length, one for the even elements of the result, and one for the odd:

$$X(2\mathrm{r})=\sum_{j=0}^{N/2-1} x(j)e^{\frac{2\pi i}{(N/2)}(2\mathrm{r})j}+\sum_{j=0}^{N/2-1} x(j+N/2)e^{\frac{2\pi i}{(N/2)}(2\mathrm{r})j}$$

$$X(2\mathrm{r}+1)=\sum_{j=0}^{N/2-1} x(j)e^{\frac{2\pi i}{(N/2)}(2\mathrm{r}+1)j}-\sum_{j=0}^{N/2-1}\left[x(j+N/2)e^{\frac{2\pi i}{N}j}\right]e^{\frac{2\pi i}{(N/2)}(2\mathrm{r}+1)j}$$

Graphically this can be represented as

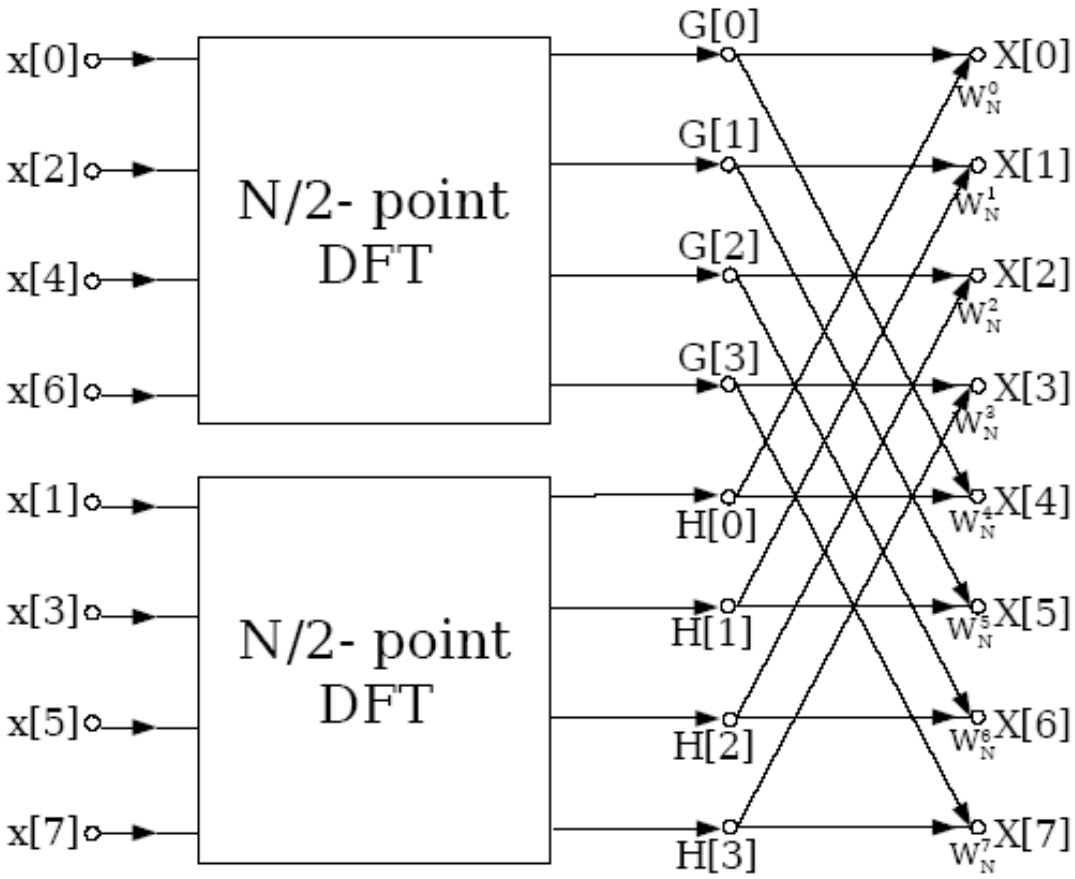


Thus using 2 MPI processes a distributed memory FFT of length 8 can be performed by distributing the data such that process 0 has elements 0-3 and process 2 elements 4-7. The two processes then send their data to each other which is combined as described above, and then finally a library routine is called to perform the final FFT which is completely local to the process. This divide and conquer method can obviously be generalised to any power of two number of processes calculating an FFT which is of length a power of 2; in general for P processes there will be $Log_2(P)$ stages where data is exchanged and combined by pairs of processes, and then each of the processes will perform a length N/P serial FFT by use of a standard library routine.

It can also be seen that the data distribution in the above is the 1 dimensional analogue of the domain decomposition used by DL_POLY. The generalisation of the above to 3 dimensions is clear. The processors are split into a $P_x*P_y*P_z$ grid ("the processor grid"), the parallel 1D transforms in the x direction are all performed at once, and this is repeated for y and z. This results in a FFT algorithm that precisely matches that required by DL_POLY and therefore avoids any initial or final data redistribution. It is this method that I earlier implemented. The resulting code, the Daresbury Fourier Transform (DaFT), was then used by DL_POLY_3.

The only apparent problem is the vectors produced by the DIF method are not in natural order; it is in so called "bit reversed" order, and to return it to natural order would require extensive communications so apparently defeating the point of the exercise. In fact for DL_POLY_3 and DL_POLY_4 this is not an issue because the operations required in Fourier space are, as noted above,

local. As a result the operations in Fourier space can be performed very easily in bit reversed order as all that is required to be known is the value of **m** for the grid point under consideration, and in particular it is *not* necessary to know the value on the grid for any other vector **m'**, thus obviating the need for any communication. Further if the inverse Fourier transform required for the calculation of the forces is performed by the Cooley and Tukey algorithm, a decimation in time (DIT) algorithm, and the input values are provided in bit reversed order, the final result is returned in the natural ordering in real space. The graphical representation of the DIT method is



It can be seen that in parallel a very similar method to that employed for the forward transform can be employed, except the data exchange and serial FFT steps are reversed. Further because the inverse transform takes its input in bit reversed order no communication is required between the two FFT stages.

The resulting code performs very well, and it was shown in [xiv] that while as a stand alone routine it is often slower than the standard slab based 3D FFT methods, in DL_POLY_3 DaFT was almost always superior within DL_POLY due to the extra communications that slab based methods require to bring the data into the appropriate distribution.

However the code as described above is limited to process counts that are powers of 2. As at large processor counts the separation between neighbouring powers of 2 increases this restriction can result in the scientist having to markedly "scale up" his computational system simply so that he or she can run on the next lowest power of 2 cores, so resulting in an appreciable increase in cost of the calculation. This is a waste of their computational budget. Further

with HECToR phase2a for the first time the nodes themselves were not powers of 2, forcing the scientist to under-populate at least 1 of the nodes in most runs. As HECToR accounting is "by the node" this was another waste of computational resources. Both these above points led to the current work, to remove the above restrictions.

On the other hand it should be noted that the dimensions of the FFT grid, as opposed to the processor grid, are *not* restricted to powers of 2. Rather the dimensions are restricted to the values $P_\mu N_{FFT}$, where P_μ is the number of processors down a given dimension (x,y or z) of the processor grid, and N_{FFT} is a length which the serial FFT library routine can perform. In other words the restriction is that the length must be a multiple of the number of processors, and the allowed multiples are determined by the capabilities of the serial FFT library function. In practice the GPFA routines of Temperton[xv] are used. These can perform FFTs for sequences whose lengths have prime factors 2, 3, or 5. Thus DaFT in its original formulation was capable of 3 dimensional parallel FFTs where the dimensions of the FFT had length $P_\mu*2^a*3^b*5^c$, for zero or positive integer a, b and c and P_μ a power of 2. However DL_POLY_3 imposed the restriction that the dimensions of the FFT grid must be a power of 2, a point I shall return to when describing the current work.

Thus the overall 3D DaFT algorithm is actually very simple, in many ways much simpler than the standard "transpose" based methods. Given a processor grid of size $P_x*P_y*P_z$ and an FFT grid of size $N_x*N_y*N_z$

1. Perform the 1D FFTs in the x direction. Each of these are split over P_x cores, and each core has $(N_y/P_y)*(N_z/P_z)$ of these to perform, and obviously only one message need be sent for all the 1D FFTs at each stage, thus ensuring long messages
2. As 1 but for the y direction
3. As 1 but for the z direction

Thus to be effective it is necessary only to achieve good scaling of the 1D FFTs to approximately $P^{1/3}$ cores, where P is the total number of cores used by the job, since each 1D FFT is only distributed across ~ $P^{1/3}$ cores.

4 DaFT (Mixed Radix)

The major limitation on DaFT is that it limited to powers of 2 number of processes, a limit that is not commensurate with either some modern computational systems or the needs of some users of DL_POLY. Thus for DL_POLY_4 work has been funded by the dCSE mechanism to provide a generalisation of the above. The original proposal was to allow process grids which had factors of the form $2^a*3^{0-2}*5^{0-1}$, this form being chosen to

1. Fit the architecture of the then current phase2a HECToR system which had 24 core nodes
2. Allow some future proofing to possible future architectures
3. Allow sufficient flexibility to the scientist so that waste of computational resources due to using "oversized" systems was markedly reduced.

In fact what was implemented was a full mixed radix domain decomposed

parallel FFT. This allows for ***any*** number of processes to be used for the FFT, though due to the nature of the both the algorithm and implementation it is most efficient if the prime factors of the number of processes used be small integers.

The mixed radix algorithm depends upon the following identity: If the length of a Fourier Transform is N and it can be factored as $N=N_1*N_2$ then

$$X(k)=\sum_{j=0}^{N-1} x(j)e^{\frac{2\pi i}{N}jk}$$

can be written in terms of the two factors as

$$X(N_2k_1+k_2)=\sum_{j_1=0}^{N_1-1}\left[e^{\frac{2\pi i}{N}j_1k_2}\right]\left(\sum_{j_2=0}^{N_2-1} x(N_1j_2+j_1)e^{\frac{2\pi i}{N_2}j_2k_2}\right)e^{\frac{2\pi i}{N}j_1k_1}$$

It can be see that again the Fourier transform has been decomposed into 2; the term in parentheses is an FT of length N_2, while the outer sum is an FT of length N_1 with some extra phase ("twiddle") factors. Thus each of the two FTs could be calculated by the parallel DIF algorithm described above, generalising it where necessary to deal with the case where 2 is not the factor of interest.

However in practice to deal with a general number of processes efficiently would be somewhat complicated by this method as the communication patterns depend fundamentally on the value of the prime factor of interest. Instead the pragmatic decision was made to split the factors into two sets, *short* and *long*. Short factors are small primes, and thus the factorisation of the number of processors will typically contain these factors raised to high powers. As such these are performed by either a DIF or DIT FFT algorithm, depending on the direction of the transform. Long factors are larger primes, and thus they will be (typically) raised to low powers in the factorisation. In this case the FFT algorithm often gives little gain compared to a simple, straightforward quadrature based discrete Fourier transform (DFT - in fact if the power is unity the DFT and FFT are identical), and as such the longer factors are all amalgamated and a single DFT is performed. Currently the only short factor supported is 2, but the code has been designed to allow easy addition of other primes numbers to this set.

To clarify the above consider the case where the 1D FFT in a given direction is being performed by 36 cores. As $36=2^2*3^2$ the short factors are 2, and will use the distributed FFT algorithm outlined above, while the long factor is $3^2=9$, and this FT associated with this factor will be performed by a simple DFT.

In the above equation the long factors correspond to the summation over j_2, while the short factors are the j_1 sum. Thus the method for the mixed radix forward transform is

1. Perform the DFT for the long factors
2. Scale with the appropriate twiddle factors
3. Perform the FFT for the short factors

To perform the DFT the data has to be circulated amongst the processors that

hold the DFT of length N_2. If the factorisation of the number of processors along the dimension is P_μ=S*L, where S is the product of the short factors and L the same for the long, then there will be S of these transforms, and each of these transforms require the data to be communicated between the L processes that hold the data for it. A number of different ways of performing this data circulation were investigated, but the in practice a simple systolic loop with double buffering was found most effective. This is possibly because it allows some overlap of computation and communication as can be seen from the code excerpt below:

```
which = 0
work = a
a = 0.0_wp
rank = desc%rank; rem_rank = rank
Do pulse = 0, desc%size - 1
   t = Exp( Cmplx( 0.0_wp, &
       ( sign * 2.0_wp * pi * rank * rem_rank ) / desc%length, Kind = wp ) )
   If ( which == 0 ) Then
      If ( pulse /= desc%size - 1 ) Then
         Call MPI_IRECV(  work2, 2 * Size( work2 ), wp_mpi, down, down, &
              desc%comm, comms_request1, comms_error )
         Call MPI_ISEND( work , 2 * Size( work  ), wp_mpi,   up, rank, &
              desc%comm, comms_request2, comms_error )
      End If
      a = a + t * work
      If ( pulse /= desc%size - 1 ) Then
         Call MPI_WAIT( comms_request1, comms_status, comms_error )
         Call MPI_WAIT( comms_request2, comms_status, comms_error )
      End If
   Else
      If ( pulse /= desc%size - 1 ) Then
         Call MPI_IRECV(  work , 2 * Size( work  ), wp_mpi, down, down, &
              desc%comm, comms_request1, comms_error )
         Call MPI_ISEND( work2, 2 * Size( work2 ), wp_mpi,   up, rank, &
              desc%comm, comms_request2, comms_error )
      End If
      a = a + t * work2
      If ( pulse /= desc%size - 1 ) Then
         Call MPI_WAIT( comms_request1, comms_status, comms_error )
         Call MPI_WAIT( comms_request2, comms_status, comms_error )
      End If
   End If
   which = Mod( which + 1, 2 )
   rem_rank = Mod( rem_rank + 1, desc%size )
End Do
```

The algorithm described above will work for any number of processors provided the length of the 1D FFTs in each direction is a multiple of size of the processor grid in the corresponding dimension. For DL_POLY_4 in practice this is not an issue. The user input that determines the grid size is a minimum accuracy for the SPME method. As increasing the FFT grid size increases the

accuracy of the SPME method, it is therefore sufficient to simply increase the grid size until both the accuracy criterion and the above restriction are satisfied. In practice the overhead is small; the cube root of the number of processors on HECToR is roughly 35, thus indicating that in a bad case the FFT grid is 34 bigger than necessary in each direction. Compare this to a factor of 2 for the previous version! As a job on so many cores would have a grid of the order of 1000s in each of the 3 directions the overhead is obviously small.

5 Other Changes

After the FFT was generalised to deal with arbitrary numbers of processes it was necessary to do the same for DL_POLY. Earlier version of the application assumed

1. The number of cores was a power of 2
2. The dimensions of the FFT grid were powers of 2

The former is the major restriction, once it is removed the later follows naturally; indeed the general procedure is described in the previous section, namely to pick a size that satisfies the minimum accuracy criterion and then increase it until the dimension was consistent with the requirements of the new DaFT routines.

The removal of restriction 1 required a number of changes to code. By far the largest of these was to implement an algorithm to determine the domain decomposition for an arbitrary number of processes. For a given number of cores the chosen decomposition should

1. Enable DL_POLY to run as efficiently as possible
2. Reproduce the results of earlier versions of the code where appropriate

To develop such an algorithm note that

1. Just as for halo exchange codes the time spent in message passing is proportional to the surface area of the parallelipipeds into which the unit cell is decomposed
2. For a given process count the volume each process holds is constant, irrespective of the decomposition
3. Therefore as to maximise efficiency one has to minimise the ratio of surface area of the parallelipipeds to their volume, the problem reduces to finding that decomposition which minimises the surface area of the parallelipipeds

Thus the problem reduces to an optimisation. There are, however, two slight complications when different decompositions can result in the same surface area. This can occur due to symmetry of the system, e.g. on 16 processors with a cubic unit cell 4*2*2, 2*4*2 and 2*2*4 decompositions all obviously give the same surface area for the parallelipipeds. However it can occur for more general cases where no such apparent symmetry exists. To choose a decomposition in such “degenerate” cases the new code

1. Chooses the factorisation which minimises the maximum number of cores along any dimension in the process grid as this should maximise

the efficiency of DaFT

2. If 1 does not remove all degeneracies choose the case such that $P_x \geq P_y \geq P_z$. This ensures that results from earlier versions of DL_POLY are reproduced

Thus the full algorithm for choosing the decomposition for P cores is

- Calculate the prime factorisation of P
- Loop over all Px = Possible factors of P
  - Pyz=P/Px
  - Calculate the prime factorisation of Pyz
  - Loop over all Py = Possible factors of Pyz
    - Pz=Pyz/Py
    - Calculate the S=the surface area of the parallelipipeds
    - If S < the previous best store S, Px, Py, Pz
    - If S = the previous best
      - If Min(Px,Py,Pz)<Min(Best Px,Py,Pz) store S, Px, Py, Pz
      - If Min(Px,Py,Pz)=Min(Best Px,Py,Pz)
        - If Px< Best Px store S, Px, Py, Pz
        - If Px=Best Px and Py < Best Py store S, Px, Py, Pz
  - Finish Py loop
- Finish Px loop

6 Testing and Verification

The new code was verified against all the standard DL_POLY test cases found at [xvi] and also a number of supercells of Sodium Chloride. In all cases when run on powers of two cores the results from the earlier versions of the code were reproduced. For cases that were not on powers of 2 the calculated thermodynamic properties of the system were the same as those calculated for runs on powers of 2.

7 Benchmarking

The new code was benchmarked by studying NaCl with a system comprising 216,000 ions and run for 2000 time steps. This is a sufficient number of steps to minimise the effect of the start up and close down time. Configuration dumping was also turned off. The time taken for studying such a system is dominated by the electrostatics, and so it is ideal for studying the effect of this work. In particular the major concern was that the performance of the code may be significantly degraded when the processor grid was not a power of 2.

Figure 1 shows the performance, measured as MD time steps per second:

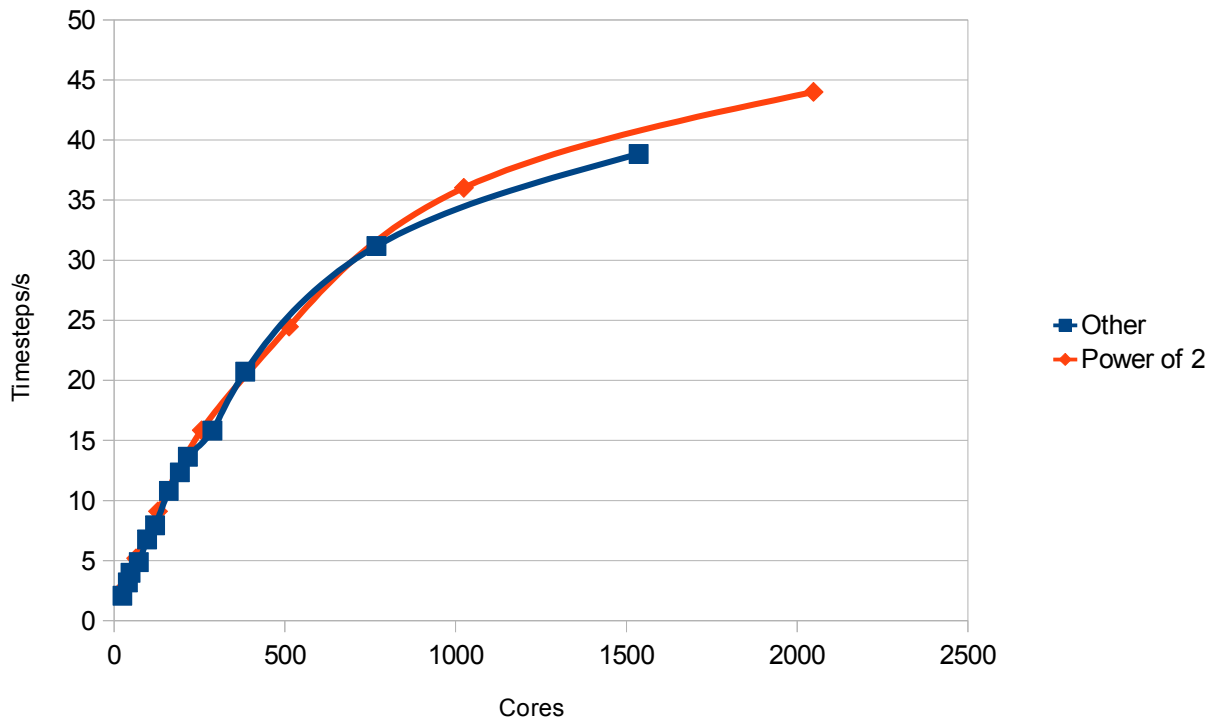


Figure 1: Performance of the new code

The two curves are for those runs that are on powers of two (in red) and those that are *not* (in blue). It can be seen that there is little difference in the two curves. Thus the concerns about the efficiency on non-powers of 2 were unwarranted.

Table 1 shows the raw numbers used to generate the above curves, along with the prime factorisations of the number of cores

Cores	Prime factorisation	Timesteps/s (non power of 2)	Timesteps/s (power of 2)
24	2^3*3	2.08	
32	2^5		2.8
40	2^3*5	3.19	
48	2^4*3	3.98	
64	2^6		5.19
72	2^3*3^2	4.87	
96	2^5*3	6.76	
120	2^3*3*5	7.93	
128	2^7		9.1
160	2^5*5	10.8	
192	2^6*3	12.34	
216	2^3*3^3	13.65	
256	2^8		15.85
288	2^5*3^2	15.82	
384	2^7*3	20.72	
512	2^9		24.48
768	2^8*3	31.18	
1024	2^{10}		36.02
1536	2^9*3	38.84	
2048	2^{11}		44.01

Table 1: Performance of the new code

It can be seen that factorisations involving low powers of 3 and 5 are very effectively dealt with by the new routines, and certainly the initial aim of core counts that factored as $2^a*3^{0-2}*5^{0-1}$ has been more than met.

The new code has been released to users, and is part of the standard release of DL_POLY_4.

8 Conclusion

A new multi-radix parallel FFT has been implemented within DL_POLY_4. Like the old FFT this fits exactly the same domain decomposition that DL_POLY_4 uses, but is not restricted to using powers of 2 number of cores. This new flexibility has been shown to come at little performance penalty, and thus the new code both better fits modern multicore architectures, such as HECToR phase 2, and also allows the scientist to study the system of interest without having to artificially inflate it to fit the restrictions of the code.

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