Multigrid

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1 Introduction

Multi grid is a method for the fast summation of long range forces, i.e. Coulomb force, in a system consisting of a large number of particles. For N-particle system, multi grid has a time complexity of O(N), where the direct solution, the Ewald Sum and Particle Mesh Ewald are of order $O(N^2)$, $O(N^{\frac{3}{2}})$ respectively $O(N \log N)$. Multi grid decomposes the Coulomb interaction between the particles into a local and a smooth part.

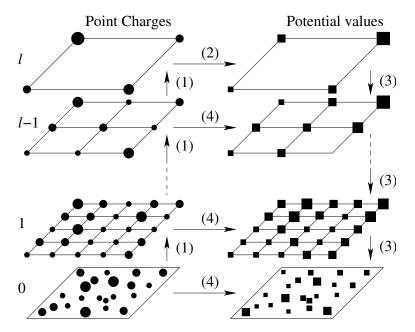


Figure 1: The multilevel scheme of the multi-grid algorithm. (1) Aggregate to coarser grids; (2) Compute potential induced by the coarsest grid; (3) Interpolate potential values from coarser grids; (4) Local corrections.

2 Input parameters

This sections gives the definition of the multi grid input parameters for PROTOMOL .

2.1 General syntax

PROTOMOL expects the following input for multi grid:

```
-algorithm MultiGrid -interpolation <Hermite |BSpline> -kernel <C1|C2|C3|C4>
-direct -smooth -correction
               <real,positive>
  -5
  -toplevelgrid <uint,positive> <uint,positive> <uint,positive> # PBC
                <coordinates,non-zero>
                                                                 # Vacuum
  -h
  -origin
                <coordinates=0 0 0>
                                                                 # Vacuum
  -levels
                <int, positive>
  -order
                <uint=4, positive>
                <uint=2,positive>
  -ratio
```

, where =*value* defines the default value, i.e. optional input.

Note that Coulomb can be replaced by a new, user defined potential, which is of the form cr^a , where c is a constant and r is the distance between particle pairs. The new potential also requires re-definition of C1, C2, C3 and C4. For the Lennard-Jones potential a new template is required due to the sum in the potential definition.

2.2 Interpolation

-interpolation defines the interpolation scheme between the grids the particle level. For the moment PROTOMOL does only accept Hermitian interpolation (Hermite). Other interpolations like b-splines (BSpline) did not improve the accuracy.

2.3 Kernel

-kernel defines how the kernel G(r) (i.e. the Coulomb potential, $r = |\vec{r_i} - \vec{r_j}|$) is softened. To smooth the kernel we only modify in a local range r < s, where s is the softening distance. The smoothed kernel is defined as follow:

$$G_{smooth}(r) \begin{cases} G_s(r) &: r < s \\ G(r) &: \text{ otherwise} \end{cases}$$
(1)

, where $G_s(r)$ is the *smoothing function*. C1, C2, C3 and C4 are smoothing functions $G_s(r)$, which satisfy the the C^1 , C^3 , C^3 respectively C^4 property. The smoothing functions fit only together with the Coulomb potential $(C \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|})$.

2.4 Direct, smooth part and correction

-direct -smooth and -correction indicate the part to be evaluated. -correction accounts the point self energy and the intra molecular term. By default (none of them set) all parts are computed.

2.5 S - softening distance

-s defines the softening distance of the smoothed kernel $G_{smooth}(r)$. It defines also the local correction at each grid level. The softening distance is scaled according the ratio and the actual level.

An increased softening distance will increase the accuracy, but also the computational work. A softening distance of order of the simulation box results in a $O(N^2)$ time complexity.

2.6 Toplevelgrid and gridsize

-toplevelgrid defines the number of grid points in each dimension (n_x, n_y, n_z) for the coarsest grid for vacuum systems, the one on the top. PROTOMOL will itself figure out the number of grid points required, for each finer grid. -h defines the size (length, not grid points) of the finest grid under PBC.

In case of periodic boundary conditions the relation of grid points between to grids is defined by the ratio (-ratio) and mesh size of the finest grid (-g):

$$n_f = n_c \cdot \text{ratio}$$
 (2)

Obviously, the length, depth and high of the grids are the same $(d_f = d_c)$, defined by the cell basis vectors. The number of grid points of the toplevel is equivalent to the number of subdivision for the coarsest grid (Fig. 2).

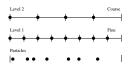


Figure 2: 2-level, periodic boundaries, ratio, $n_1 = n_2 = 8$, $d_1 = d_2$, .

For the case of vacuum (i.e. no boundaries) the relation between two grids and its dimensions depends on the ratio, the interpolation and order of interpolation:

$$n_f = (n_c - \text{ order } + 1) \text{ ratio } + 1 \tag{3}$$

, assuming Hermitian interpolation, where for other interpolation schemes the inner +1 may fall away. For the correctness of interpolation the coarser grid must overlap the finer grid (Fig. 3). The length, depth and high of the finer grid is computed as follow:

$$d_f = \frac{d_c n_f - 1}{\text{ratio (order - 2)}} \tag{4}$$

, assuming Hermitian interpolation, where for other interpolation schemes the -2 may change to -1.

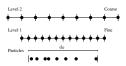


Figure 3: 2-level, no boundaries, 4-order, ratio 2, $n_1 = 13$, $n_2 = 9$, $d_1 = \frac{6}{5}d_0$, $d_2 = \frac{8}{5}d_0$.

From experiments we see that the number of grid points in each dimension for the coarsest grid should be at least the double of the interpolation order, this yields especially for vacuum. Further the number of grid points for the finest grid should reflect a mesh size of the order of the average distance between particles.

2.7 Origin - optional, vacuum

-origin defines the origin of the finest grid. It's optional and only available for vacuum.

2.8 Levels

-levels defines the number of levels (grids).

From experiments we know that finest grid should reflect a mesh size of order of the average distance between particles. Note that the number of levels and the ratio (-ratio) define roughly the relation of grid points between the fines and the coarsest grid. The relation is of ratio^{levels}.

2.9 Order - optional

-order defines the interpolation order. The interpolation order must be even, where 4 and 6 stand for a *cubic* and *quintic* interpolation respectively.

From experiments we see that the interpolation order and the smoothing function $G_S(r)$ must correspond.

2.10 Ratio

-ratio defines the ratio of grid points between a fine and coarse grid. Mostly 2 is used as ratio. For higher order interpolations a ratio more than 2 may be an option.

3 Optimization

An efficient and equivalent definition of the force filed is compute the direct part along with the Lennard-Jones. A separate definition for van der Waals nonbonded interactions (LennardJones) and electrostatics and be rewritten as following:

```
# LennardJones and direct part of multi grid
# Only LennardJones by cutoff
force time LennardJones
                                force time LennardJones CoulombMultiGridDirect
   -switchingFunction C2
                                    -kernel C3
                                    -switchingFunction C2
   -algorithm NonbondedCutoff
   -switchon 0.1
                                    -switchingFunction Cutoff
                                    -algorithm NonbondedCutoff
   -cutoff 10.0
# Only Coulomb bt multi grid
                                    -switchon 0.1
                                    -cutoff 10.0
force time Coulomb
                                    -s 10
   -algorithm MultiGrid
   -interpolation Hermite
                                # Only smooth and correction part of multi grid
                               force time Coulomb
   -kernel C3
   -levels 2
                                    -algorithm MultiGrid
                                    -interpolation Hermite
   -s 10
                                    -kernel C3
   -order 6
   -ratio 2
                                    -smooth
   -h 3 3 3
                                    -correction
   -origin 0 0 0
                                    -levels 2
                                    -s 10
                                    -order 6
                                    -ratio 2
                                    -h 3 3 3
                                    -origin 0 0 0
```

One can expect speed up of 25% or more with this equivalant (mathematically) definition. Note that, one have to expect some energy differences at some point, since the summation oder of forces and energies has changed. Furthermore, one may consider to use a look-up-table for the direct part of multi grid (i.e., CoulombMultiGridDirectTable). In most cases one will not gain much performance, only with great loss of accuracy, i.e., small look-up-table size (-size). In case of PME or plain Ewald, this approach can improve performance with reasonable accuracy, since the direct part of PME or plain Ewald is much more expensive than the direct part of of multi grid.

4 Compilation

For experimental purpose the multi grid has several conditional compilation flags. DEBUG_MULTIGRID Debug DEBUG_MULTIGRID_TIMING Printing the different timings