Partitioning 3D space for parallel many-particle simulations

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Abstract

In a common approach for parallel processing applied to simulations of many-particle systems with short-ranged interactions and uniform density, the simulation cell is partitioned into domains of equal shape and size, each of which is assigned to one processor. We compare the commonly used simple-cubic (SC) domain shape to domain shapes chosen as the Voronoi cells of BCC and FCC lattices. The latter two are found to result in superior partitionings with respect to communication overhead. Other domain shapes, relevant for a small number of processors, are also discussed. The higher efficiency with BCC and FCC partitionings is demonstrated in simulations of the sillium model for amorphous silicon.

Key words: parallel computing, particle simulations, space partitioning
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1 Introduction

Realistic simulations of molecular dynamics and other dynamic many-particle systems demand increasingly larger models. Calculations on these large models can be distributed over several processors of a parallel computer to improve performance. An excellent review of the state-of-the-art of parallel atomistic simulations has recently been published by Heffelfinger [1]. According to this work, and to the best of our knowledge, spatial decomposition of the simulation cell is done almost exclusively by partitioning into cubic domains of equal size, each of which is assigned to a processor. Exceptions to this rule

are earlier work by Esselink and Hilbers [2] and Chynoweth et al. [3], who use a 2D decomposition motivated by the square mesh topology of their parallel machine. In case of density fluctuations, load imbalance between the processors might occur; here, we limit ourselves to homogeneous systems with a uniform density, such as bulk materials or liquids. Other methods are necessary for heterogeneous systems such as proteins in vacuum or stellar systems. In homogeneous many-particle systems, the major source of inefficiency inherent to the domain decomposition approach lies in the fact that particles interact over some distance, so that in particular particles near the surface of these domains interact with particles in neighbouring domains. These particles near the surface thus cause communication with neighbouring processors, redundant calculations, or both. For brevity, we call this entire extra work the communication overhead. In the case that the interaction range is much smaller than the lateral size of the domains, the communication overhead will roughly scale with the surface area of the domain. Hence, the optimal domain shape for many-particle systems with a uniform density and a short-range potential is a space-filling shape with minimal surface-to-volume ratio.

This paper is organized as follows. First, we explore domain shapes that are derived from simple-cubic (SC), body-centered-cubic (BCC) and face-centered-cubic (FCC) lattices. We determine their properties with respect to their use in parallel processing and discuss several implementation details. We then apply these domain shapes in a representative many-particle simulation: the *sillium* model of amorphous silicon, as proposed by Wooten, Winer and Weaire. Finally, we present our conclusions.

2 Domain shapes

In this section, several domain shapes are discussed, regarding their properties relevant for parallel processing. All lengths and distances are measured in fractions of the system to be simulated, which thus by definition has unit length edges. The domains assigned to each processor are equal in shape and size, and consequently have a volume of $1/p$ where p is the number of processors. The following discussion assumes a cubic simulation cell, but extension to other regular-shaped simulation cells is straightforward. The interaction range (distance over which particles exert forces) equals r_c, where $r_c \ll 1$. Relevant for our purpose is the volume of the *halo*: the region outside the domain but within a distance r_c. Particles in this halo interact with those inside the domain, causing communication overhead.

2.1 SC partitioning

The most straightforward three-dimensional division of a cube into identical domains is a division into $p = k^3$ smaller cubes, with k a positive integer. The resulting cubic domains have an edge length of $1/k$. The volume V_{cubic} of the halo with radius r_c around each domain equals

$$V_{cubic} = \frac{6r_c}{k^2} + \frac{3\pi r_c^2}{k} + \frac{4}{3}\pi r_c^3. \tag{1}$$

The first term is dominant and equal to r_c times the surface area of the domain. The second and third terms correspond to the extra volume of the halo located near the edges and corners of the domain, respectively. In simulations with short-range interactions as discussed here, usually $r_c k < 1$, so that these terms are small compared to the first.

In the limit of very short-range interaction our problem reduces to the well known Kelvin problem, which is to find a partitioning of space with minimal surface area. Kelvin [4] conjectured that the optimal solution is the Voronoi cell of the BCC lattice, slightly curved to satisfy Plateau's rules [5], but Weaire and Phelan [6] produced an even better partitioning, based on two different cells, and related to the β-tungsten structure. We limit ourselves to proposing partitionings that can be shown to be better than SC and that can be implemented in a relatively simple way.

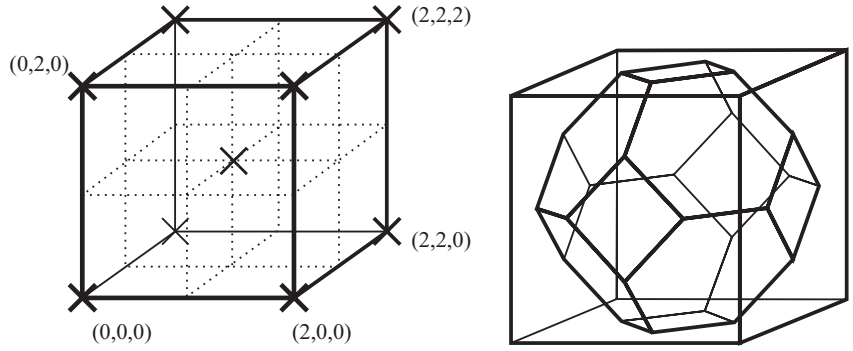
In the case of SC, the surface area is equal to

$$S_{cubic} = \frac{6}{k^2} = \frac{6}{p^{\frac{2}{3}}}. \tag{2}$$

2.2 BCC partitioning

Given that we strive for a small surface-to-volume ratio, it is natural to investigate sphere packings. In one of the better sphere packings, the spheres are located on the sites of a body-centred-cubic (BCC) lattice, with spheres at the corners and the centres of cubic cells. The BCC unit cell is displayed in Figure 1(a). Each unit cell adds two sphere centres to the lattice, as only one corner point is part of the unit cell; the other seven corner points are considered part of neighbouring cells. By repeating this unit cell the BCC lattice is generated. The lattice is then rescaled, such that the length of the edges of a unit cell becomes $\frac{1}{k}$.

The domain of a processor is formed by the Voronoi cell of a lattice point,



(a) (b)

Fig. 1. (a) The basic BCC lattice cell. Sphere centres are marked by '×'. (b) The BCC Voronoi cell, a truncated octahedron.

i.e., the space closest to that point. The model cube can now be divided into $p = 2k^3$ Voronoi cells, as generated by the BCC lattice. It turns out that each Voronoi cell is a truncated octahedron, as shown in Figure 1(b). This is also the shape that Kelvin proposed as a solution to the Kelvin problem.

Each truncated octahedron generated by the BCC lattice fits into a cube with edge length $\frac{1}{k}$. Each of the six square faces has a surface area of $\frac{1}{8k^2}$ and each of the eight hexagonal faces has a surface area of $\frac{3\sqrt{3}}{16k^2}$. This results in a total surface area of

$$S_{BCC} = \frac{6\sqrt{3}+3}{4k^2}, \tag{3}$$

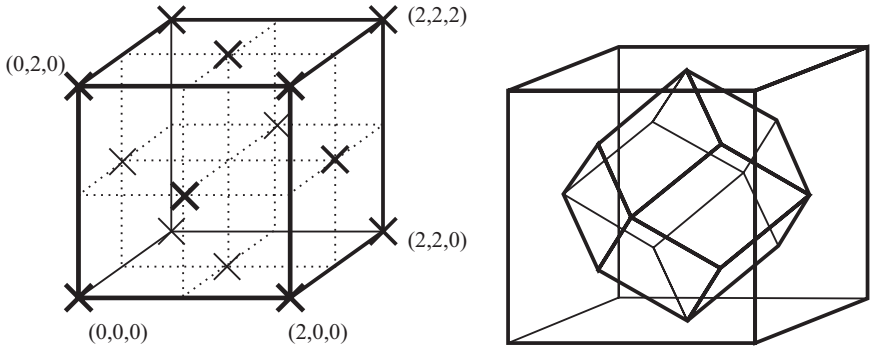
which, after substitution of $k = (p/2)^{\frac{1}{3}}$, gives

$$S_{BCC} = \frac{6\sqrt{3}+3}{2^{\frac{4}{3}}p^{\frac{2}{3}}} \approx \frac{5.3147}{p^{\frac{2}{3}}}. \tag{4}$$

This is over eleven percent better than for SC.

2.3 FCC partitioning

In one of the optimal dense sphere packings, the spheres are placed at sites of a face-centered-cubic (FCC) lattice, with spheres at the corners of cubic cells and at the centres of the faces. The FCC unit cell is shown in Figure 2(a). The corresponding Voronoi cell is a rhombic dodecahedron, as shown in Figure 2(b). Each cubic unit cell adds four points to the lattice, so with this partitioning $p = 4k^3$ processors can be used. After the lattice is rescaled such that each unit cell has an edge of length $\frac{1}{k}$, the Voronoi cell can be considered



(a) (b)

Fig. 2. (a) The FCC basic lattice cell. Sphere centres are marked by '×'. (b) The FCC Voronoi cell, a rhombic dodecahedron, translated to the centre of the cube for reference.

as being made up of a cube with edge length $\frac{1}{2k}$ and six pyramids with height $\frac{1}{4k}$, each covering one face of the small cube. The surface area of the rhombic dodecahedron equals 24 times the surface area of one of the triangular faces of the pyramid, which is $\frac{1}{8\sqrt{2}k^2}$. The surface area of the domain in the FCC partitioning therefore equals

$$S_{FCC} = \frac{3}{\sqrt{2}k^2}, \tag{5}$$

which, after substitution of $k = \sqrt[3]{p/4}$, yields

$$S_{FCC} = \frac{3 \cdot 2^{\frac{5}{6}}}{p^{\frac{2}{3}}} \approx \frac{5.3454}{p^{\frac{2}{3}}}, \tag{6}$$

which is slightly more than for BCC, but still almost eleven percent better than for SC.

Most parallel computers are equipped with $p = 2^q$ processors. With the three partitionings presented above, we can now use $p = k^3$, $p = 2k^3$ and $p = 4k^2$ processors, which includes all powers of two. This means that most parallel computers can be used to their full potential.

2.4 Domain shapes with few processors

Two other simple partitionings exist that have not been mentioned yet. The first is the partitioning into slices with dimensions $1 \times 1 \times \frac{1}{k}$. Each slice has

two sides with unit surface area where communication overhead is generated,

$$S_{slices} = 2. \tag{7}$$

The domain surface area does not decrease with an increasing number of processors, in contrast to the three-dimensional partitionings discussed above. For this reason, this domain shape is only useful when p is small. For $p = 2$, partitioning into slices is better than BCC partitioning (with area 2 vs. 3.35) and for $p = 4$ it is better than FCC partitioning (with area 2 vs. 2.12), but it is worse in all other cases where one of the SC, BCC, or FCC partitionings is applicable.

Another partitioning is that into columns with dimensions $1 \times \frac{1}{k} \times \frac{1}{k}$. Each column has a surface area of

$$S_{columns} = \frac{4}{p^{\frac{1}{2}}}. \tag{8}$$

For $p = 4$ this is as efficient as using slices. Three-dimensional partitioning is better at higher p.

3 Practical implementation issues

In implementations, one needs an efficient procedure to determine the processor to which a particle with coordinates (x, y, z) is assigned. Note that we can break ties arbitrarily in case particles are located exactly on the boundary of two domains (or within a distance corresponding to machine precision), since this event is very unlikely to occur. With SC partitioning for $p = k^3$ processors, the processor number s can then be found by:

$$s = \lfloor kx \rfloor + k\lfloor ky \rfloor + k^2 \lfloor kz \rfloor, \tag{9}$$

where $\lfloor x \rfloor$ is the largest integer smaller than or equal to x.

To assign processor numbers to domains with the BCC shape, it is helpful to note that a BCC lattice consists of two simple-cubic lattices, shifted with respect to each other over a vector $(\frac{1}{2k}, \frac{1}{2k}, \frac{1}{2k})$. One simply determines the nearest site in each of the two sublattices, compares the two, and takes the nearest. Here, one can take Manhattan distances, defined by $\|(x, y, z)\|_1 = |x|+|y|+|z|$, because these are cheaper to compute than Euclidean distances. Since the sum of the Manhattan distances of an arbitrary point to the two nearest sites equals $\frac{3}{2k}$, the nearest one is located at a Manhattan distance of less than $\frac{3}{4k}$. The

procedure to calculate the processor number for the BCC partitioning is outlined in the pseudo-code below, where '$[x]$' denotes the integer nearest to x and 'mod' denotes the modulo operator (needed to wrap around the periodic boundaries):

$D = |kx - [kx]| + |ky - [ky]| + |kz - [kz]|$
if $D < \frac{3}{4}$ **then**
  $s = ([kx] \bmod k) + k([ky] \bmod k) + k^2([kz] \bmod k)$
else
  $s = k^3 + \lfloor kx \rfloor + k\lfloor ky \rfloor + k^2\lfloor kz \rfloor$
end if

For the FCC lattice, it is helpful to note that it can be obtained from a cubic superlattice by removing all grid points for which the total of the coordinates is odd. First, we determine the nearest grid point of this cubic superlattice. If the sum of the coordinates of that grid point is even, that point was the nearest FCC lattice site. If the sum is odd, the closest lattice point can be found by rounding one of the coordinates in the 'wrong' direction, i.e., in the opposite direction of the nearest integer coordinate; the coordinate that should be rounded 'wrongly' is the one with the largest rounding error (and hence the smallest error in the opposite direction). Using the notation $]x[$ for rounding 'wrongly' (in contrast to $[x]$ for usual rounding), defined by the relation $[x]+]x[= \lfloor x \rfloor + \lceil x \rceil$, this procedures thus becomes:

$(P_x, P_y, P_z) = ([2kx], [2ky], [2kz])$
if $P_x + P_y + P_z$ is odd **then**
  if $|2kx - P_x| > |2ky - P_y|$ **and** $|2kx - P_x| > |2kz - P_z|$ **then**
    $P_x =]2kx[$
  else if $|2ky - P_y| > |2kz - P_z|$ **then**
    $P_y =]2ky[$
  else
    $P_z =]2kz[$
  end if
end if
$(P_x, P_y, P_z) = (P_x \bmod 2k, P_y \bmod 2k, P_z \bmod 2k)$
$s = P_x + 2kP_y + 4k^2\lfloor P_z/2 \rfloor$

4 Related partitionings

FCC is only one of the optimal sphere packings; another one is hexagonal-close-packed (HCP). The Voronoi cells of HCP have the same volume and surface area as those of FCC. The HCP packing, however, is not derived from

p	partitioning	p	partitioning
1	—	24	6FCC
2	slices	27	SC
3	slices	32	FCC
4	slices	64	SC
8	SC	128	BCC
16	BCC	256	FCC

Table 1
Best partitioning for typical numbers of processors.

a cubic grid, so in an implementation it is more difficult to assign processor numbers to particles.

The FCC partitioning can be used as the basis for yet another partitioning, which we call 6FCC. The FCC cell can be further subdivided into six (non-regular) octahedra, so $p = 6 \cdot 4k^3 = 24k^3$ processors can be used. This can be rewritten as $p = 3k'^3$, with $k' = 2k$. Each octahedron consists of two pyramids with height $\frac{1}{2k'}$ and base edges of length $\frac{1}{k'}$. The surface area of this shape equals $\frac{4}{\sqrt{2}k'^2}$, which, after the substitution $k' = (p/3)^{\frac{1}{3}}$, yields

$$S_{6FCC} = \frac{3^{\frac{2}{3}}4}{2^{\frac{1}{2}}p^{\frac{2}{3}}} \approx \frac{5.8833}{p^{\frac{2}{3}}}. \tag{10}$$

This is still slightly better than SC, but only really useful when a parallel computer with $p = 3k^3$ processors is used. The case with $p = 3$ is an exception, since using three slices is more efficient. Note that this partitioning is equivalent to the FCC partitioning with only the centres of the faces retained in the lattice.

A summary of recommended partitionings for typical numbers of processors is given in Table 1. This table illustrates the added flexibility that is the result of having several different partitioning methods in our toolbox.

5 Application: amorphous silicon

We have applied SC, BCC, and FCC partitioning to the construction of models of amorphous silicon, following the *sillium* model proposed by Wooten, Winer and Weaire [7,8], with recent algorithmic improvements [9]. This has produced the best models of amorphous silicon that are available to date.

Within the sillium approach, an atomic configuration consists of the coordinates of all N atoms, together with a list of the $2N$ bonds between them. The energy of a configuration is obtained from the Keating potential [10]:

$$E = \frac{3}{16}\frac{\alpha}{d^2}\sum_{\langle ij\rangle}\left(\mathbf{r}_{ij}\cdot\mathbf{r}_{ij} - d^2\right)^2 + \frac{3}{8}\frac{\beta}{d^2}\sum_{\langle jik\rangle}\left(\mathbf{r}_{ij}\cdot\mathbf{r}_{ik} + \frac{1}{3}d^2\right)^2. \tag{11}$$

Here, α and β are the bond-stretching and bond-bending force constants, respectively; $d = 2.35$ Å is the equilibrium Si-Si bond length in the diamond structure. Usual values are $\alpha = 2.965$ eV/Å^2 and $\beta = 0.285\ \alpha$.

The construction of a well-relaxed configuration starts from a configuration in which atoms with random coordinates are four-fold connected. This network is then relaxed through a sequence of many proposed bond transpositions, accepted with the Metropolis acceptance probability [11] given by

$$P = \min\left[1, \exp\left(\frac{E_b - E_f}{k_b T}\right)\right], \tag{12}$$

where k_b is the Boltzmann constant, T the temperature, and E_b and E_f are the total *quenched* energies of the system before and after the proposed bond transposition.

With the approach given above, and described in more detail in Refs. [7,8], Wooten, Winer and Weaire obtained 216-atom structures of *a*-Si with a bond angle deviation as low as 10.9 degrees. A decade later, using the same approach but more computing power, Djordjević, Thorpe and Wooten [12] produced larger (4096-atom) networks of even better quality, with a bond angle deviation of 11.02 degrees for configurations without four-membered rings and 10.51 degrees when these rings were allowed [12]. With some additional algorithmic improvements, Barkema and Mousseau generated 1000-atom configurations with a bond angle deviation of 9.2 degrees [9], and one 4096-atom configuration with a bond angle deviation of 9.89 degrees. Exploiting parallel processing, we have generated a 10,000-atom sample with a bond-angle deviation as low as 9.88 degrees and a 20,000-atom sample, used primarily for our benchmarking. For a discussion of all structural and electronic properties of the 10,000-atom sample, we refer to a forthcoming publication [13]; here we focus on computational aspects.

In our parallel program, the model box containing 10,000 atoms was divided using SC, BCC, and FCC partitionings, depending on the number of processors used. Due to the three-body term in the Keating potential, two extra layers of atoms are needed near the surface of the domains. Communication of these extra atoms is determined by the connectivity information in the

model. It turned out that the amount of communication needed can be well approximated by using a cutoff distance of 1.3 times the average bond length of 2.35Å. For the 10,000-atom and 20,000-atom sample, with box sizes 57.5Å and 72.6Å, we find $r_c \approx 0.053$ and 0.042, respectively.

The program was tested for different values of p on a Cray T3E parallel computer, using the BSPlib communications library [14], and applied to the 20,000-atom sample. As a simple performance metric, we take the efficiency E_p, defined as

$$E_p = \frac{T_1}{pT_p}, \tag{13}$$

where T_p is the execution time of one iteration of the global relaxation procedure on p processors and T_1 is the time for one processor without communication overhead.

The results of the efficiency measurements are shown in Figure 3. It is clear that in general the efficiency deceases as p increases. However, the sudden increase in efficiency when going from $p = 27$ to $p = 32$ shows most clearly that FCC partitioning is better than SC. A similar effect can also be observed, though less pronounced, at $p = 16$ for BCC partitioning.

As an illustration, the 20,000-atom sample was partitioned by the different methods and the atoms in the inner region and the halos were counted. Both the maximum and the average over the p processors were determined. (The maximum number of interior atoms determines the computation time, whereas the maximum number of halo atoms determines the communication time.) The results are listed in Table 2. Also displayed is the ratio of the average number of halo atoms to the average number of interior atoms, a metric that corresponds to the surface-to-volume ratio. (The ratio of the averages is the best measure of the effects studied, since it is less noisy than the ratio of the maxima.) The ratios found explain the jumps in efficiency shown in Figure 3.

6 Conclusion

We have proposed two space partitionings, based on Voronoi cells of the BCC and FCC lattices, that can be used in parallel particle simulations with uniform density and short-ranged interactions. The advantage of these new partitionings is two-fold: (i) they reduce the communication volume by about eleven percent compared to the commonly used SC partitioning; (ii) they extend the range of possible processor numbers, so that now we can use, among others,

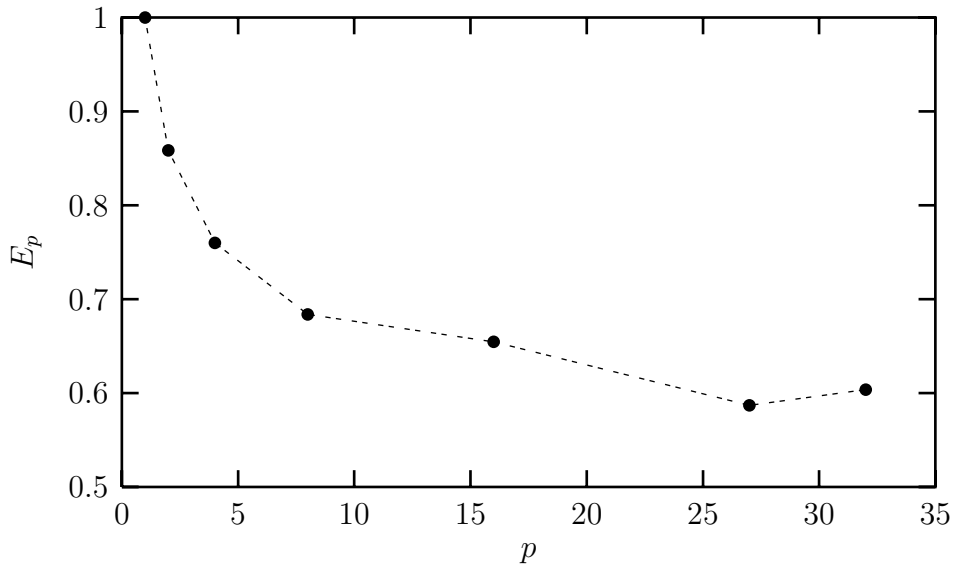


Fig. 3. Measured efficiency as a function of the number of processors p.

p	partitioning	interior		halo		ratio
		max	avg	max	avg	halo/interior
1	—	20000	20000	0	0	0.000
2	BCC	10009	10000	2382	2377	0.238
4	FCC	5019	5000	2156	2139	0.428
8	SC	2551	2500	1546	1517	0.607
16	BCC	1277	1250	904	874	0.699
27	SC	765	741	723	706	0.953
32	FCC	653	625	614	581	0.930

Table 2
The maximum and average number of atoms in the interior of the processor domains and in the halos. Also listed is the ratio between the average numbers of halo atoms and interior atoms.

all powers of two as a number of processors. These two partitionings are of practical use, because they are almost as easy to implement as SC.

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