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Overview of neutral territory methods for the parallel evaluation of pairwise particle interactions

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Abstract. Particle simulations in fields ranging from biochemistry to astrophysics require evaluation of the interactions between all pairs of particles separated by less than some fixed interaction radius. The extent to which such simulations can be parallelized has historically been limited by the time required for inter-processor communication. Recently, Snir [1] and Shaw [2] independently introduced two distinct methods for parallelization that achieve asymptotic and practical advantages over traditional techniques. We give an overview of these methods and show that they represent special cases of a more general class of methods. We describe other methods in this class that can confer advantages over any previously described method in terms of communication bandwidth and latency. Practically speaking, the best choice among the broad category of methods depends on such parameters as the interaction radius, the size of the simulated system, and the number of processors. We analyze the best choice among a subset of these methods across a broad range of parameters.

1. Introduction.

Simulations in many fields often require the explicit evaluation of interactions between all pairs of particles separated by less than some interaction radius \( R \) (“near interactions”). Examples include molecular dynamics and Monte Carlo simulations in biochemistry and materials science, N-body simulations in astrophysics and plasma physics, and particle-based hydrodynamic simulations in fluid dynamics. The remaining pairwise interactions are either neglected or handled via a less expensive method [3]. The computation of near interactions is often the dominant cost in such simulations. Though the near interaction computations are independent and can generally be evaluated in parallel, the communications required to bring together position and/or other data for pairs of particles on the same processor can severely limit scalability.

In this paper, we consider spatial domain decompositions, in which each processor is assigned a specific region of space (its “home box”), and is responsible for updating the positions and velocities of all particles contained in that box. As some near interactions will occur between particles located in different processors, particle data will need to be communicated between processors to compute all the near interactions. In this paper, we assume that particles are uniformly distributed in space, and that the home boxes are arranged in a uniform Cartesian mesh.

Figure 1 illustrates two strategies for parallelization. In a traditional strategy (a two-dimensional version of which is illustrated in figure 1a), a near interaction is assigned to a processor that contains

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at least one of the particles. Each processor imports the full set of particles with which one of its own particles could interact. Equivalently, the “import region” of each home box is a “full shell” containing all particles within a distance $R$ of the home box boundary. In many simulations, the interaction is “commutative,” in the sense that computing the influence of particle $i$ on particle $j$ requires the same data as computing the influence of particle $j$ on particle $i$, so the import region can be reduced in volume to a “half shell.” The communication required for the method is roughly proportional to the volume of the import region.

In a “neutral territory” method [2], a near interaction may be assigned to a home box that does not contain either particle, and must therefore import both. A two-dimensional analog of one such approach, Shaw’s original NT method [2], is illustrated in figure 1b. In this figure, near interactions occur within the home box in the same row of home boxes as particle $i$, and in the same column as particle $j$.

Both methods shown in the figure can be thought of as having two “zones.” Each zone is a spatial region specified relative to the home box. Each method interacts all particles in one zone with all particles in the other zone (subject to a local filtering process that will be ignored for purposes of this paper). In the traditional method, the first zone comprises the entire import region plus the home box, while the second zone is just the home box itself. In the two-dimensional NT analog illustrated in figure 1b, the first zone comprises the horizontal row of boxes, while the second comprises the vertical column of boxes. In the limit where the number of processors becomes large and the size of each home box thus becomes small, the communication bandwidth per processor is proportional to the sum of the two zone volumes while the expected number of near interactions occurring within each processor is proportional to the product of the two zone volumes.

The expected number of near interactions per home box is fixed, regardless of communication strategy, and this effectively sets a lower bound for the product of the two zone volumes [4]. Ideally, the sum of the two zone volumes should be minimized while holding the product of the zone volumes at the lower bound. Traditional methods have grossly unbalanced zone volumes, but neutral territory methods can be balanced to yield dramatic reductions in inter-process communication requirements.

2. **Summary of previous methods.**

The HS (for “Half-Shell”) method, whose import region is shown in figure 2a, is an example of a traditional spatial domain decomposition strategy for commutative particle interactions. Assuming a cubical home box (which is optimal for this method) with side length $h$, the HS import region consists of 3 rectangular “face” subregions, each with volume $\frac{\pi R h^2}{4}$ each, and 4 spherical octant “corner” subregions of volume $\frac{\pi R^3}{6}$ each, for a total import volume of $3R h^2 + \frac{3\pi R^3}{6} + \frac{2\pi R^3}{4}$. The HS method interacts all particles in the home box with all particles in the union of the home box and the import region (with the exception of certain redundant interactions, which we will ignore for this and the other methods discussed here).

In Shaw’s NT (for “Neutral Territory”) method, whose import region is shown in figure 2b, two particles interact within a box whose $x$ and $y$ mesh coordinates are those of one particle and whose $z$ mesh coordinate is that of the other particle. The home box aspect ratio determines the dimensions of the import region, and is optimized to minimize inter-processor communication. Assuming a home box with dimensions $h_x x h_y y h_z z$, the import region consists of (a) an “outer tower” consisting of two face subregions of volume $h_x z R$ each, and (b) an “outer plate” consisting of two face subregions of volume $h_y x R$ each and two edge subregions of volume $2 \pi R h_z/4$ each, for a total import volume of $2 R h_x^2 + 2 R h_y^2 + \frac{\pi R h_z}{2}$. Optimization of the home box aspect ratio, however, results in an asymptotic import volume of $2 \pi^{1/2} R^{1/2} V_{x,y}$ as the number of processors becomes very large, where $V_x$ is the volume of the home box. The NT method interacts every tower particle with every plate particle.

Snir’s hybrid method [1], referred to here as the “SH method,” employs an import region consisting of (a) one connected subregion, and (b) one non-contiguous subregion consisting of a set of bars oriented along a plane orthogonal to that of the contiguous subregion. Although this method requires more inter-processor communication than the NT method, both asymptotically and in absolute terms, Shaw has shown [2] that with certain NT-like modifications, Snir’s method can
achieve performance approaching (though not equalling, for finite \( p \)) that of the NT method for problems and machines of reasonable size. The import region of this modified version of Snir’s method (referred to as the “SNT method”), is illustrated in figure 2c.

The communication bandwidth requirements of the NT, SH, and SNT methods scale asymptotically as \( O(R^{3/2}p^{-1/2}) \), while those of traditional spatial decomposition methods such as the HS method scale as \( O(R) \). When the number of processors becomes large, the amount of data imported by traditional methods becomes proportional to the volume of a sphere of radius \( R \), while the amount imported by these new methods is proportional to the square root of this volume. In addition, as the number of processors approaches infinity, the amount of data imported by these new methods approaches zero, while that imported by the traditional methods approaches a finite asymptote.

The details of all methods described in this section are discussed more extensively in [2].


While the HS, NT, SH and SNT methods have strikingly different import regions, all of these methods collect local and remote particle data into two zones and interact all particles in one zone with all particles in the other. It is possible to generalize these algorithms to methods based on a larger number of zones, and to modify them in certain other ways, to generate improved methods. These methods are described briefly below and detailed in [4].

In [4], it is shown that the interaction of two zones of complete home boxes is similar to a discrete convolution of the zones. If the result of this convolution covers at least the full shell surrounding the home box (or half of it in the commutative case), all necessary near interactions will be computed at least once. We refer to this is the “convolution criterion.”

A method that satisfies the convolution criterion can be improved by noting that a point in a zone can be eliminated if it is further than \( R \) away from the closest point in the other zones with which the zone interacts. (The use of more than two zones is described below.) We refer to this is the “rounding criterion.” Figure 2d (“Clouds”) and figure 2e (“Foam”) provide additional examples of methods that satisfy both criteria.

All methods considered thus far are based on the use of two zones. There will often be advantages, however, to methods that use three or more zones, each of which interacts with one or all of the others. Consider, for example, a method in which two particles interact within a box whose \( x \) mesh coordinate is that of the particle with the smaller \( x \) coordinate, whose \( y \) mesh coordinate is that of the particle with the smaller \( y \) coordinate, and whose \( z \) mesh coordinate is that of the particle with the smaller \( z \) coordinate. The import region associated with this method is shown in figure 2f. The required computations can be expressed as interactions between eight non-overlapping zones, indicated by different colors in the figure. They are the home box, three face subregions that abut the \(+x, +y\) and \(+z\) home box faces, three edge subregions that abut the \(+x+y, +x+z\) and \(+y+z\) home box edges, and one corner subregion that touches the \(+x+y+z\) home box corner. The home box zone interacts with all of these zones; in addition, each face zone interacts with all other face zones, and with one edge zone.

We refer to this method as the ES (for “Eighth-Shell”) method, since it imports one-eighth of a full shell in the limit as the number of processors approaches infinity. Assuming a cubical home box (which is optimal for this method) with side length \( h \), the total import volume of the this method is \( 3Rh^3 + 3/4 \pi R^2h + 1/6 \pi R^3 \). The ES method is inferior to Shaw’s original NT method when the number of processors is large, but it has an import volume equal to or lower than all known methods in the low parallelism limit. Moreover, it is always superior to the traditional HS method in terms of communication bandwidth.

When there are multiple zones, the set of required zone-zone interactions must be specified. In addition, one may specify the order in which required zone-zone interactions will be computed. This ordering can be used to maximize overlap of communication and computation, thus hiding some of the communication latency associated with the import of particle data from remote zones.

A multiple-zone formulation of Shaw’s original NT method not only hides communication latency but also reveals an additional rounding opportunity. Because particles in the lower half of the outer tower need not interact with the home box particles, the rounding criterion can be used to further reduce the volume of the outer tower.
In [4], bounds are derived for the bandwidth scaling of generalized methods. It is found that the ES method is approximately optimal as the number of processors approaches zero, and that the Foam method is an (exactly) optimal two-zone method as the number of processors approaches infinity. The NT method offers the best performance for a wide range of intermediate values.

Figure 3 plots the normalized import volume against the parallelization parameter \( \alpha_R = R / (h, h) \) for selected methods, using home boxes whose aspect ratios have been independently optimized. The Eighth-Shell method is best for \( \alpha_R < -0.8 \). Shaw’s NT method, improved via the additional rounding opportunity outlined above, is best for \( -0.8 < \alpha_R < 17 \). The Foam method becomes competitive for \( \alpha_R > 17 \). Expressing these results in terms of machine size, and assuming a system with 50,000 particles, an interaction radius \( R = 12 \) Angstoms, and a density of 0.1 particle per cubic Angstrom, the Eighth-Shell method is found to be best for small- to moderate-sized clusters (\( p < -150 \)), the NT method is best for larger clusters and ultra-parallel machines like BlueGene [5] and QCDOC [6] (\( -150 < p < -1,400,000 \)), and the Foam method would be best for a hypothetical machine containing more than \( -1,400,000 \) processors.

It may be noted that in the above example, the Foam method does not become competitive until there are more processors than particles; neutral territory methods, however, can take advantage of a number of processors larger than the number of particles being simulated, since they can calculate pairwise interactions within processors that contain no particles. This phenomenon may be viewed as a form of load-balancing; more generally, the class of neutral territory methods offer significant advantages with regard to the distribution of computational load across all available processors.

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References
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Figure 1. (a) Traditionally, particles \(i\) and \(j\) interact on a processor that contains either \(i\) or \(j\). (b) In a neutral territory method, it may not contain either \(i\) or \(j\). Each interaction box (dark gray) imports all particles in its import region (light gray).

Figure 2. Import regions of select methods. (a) Traditional Half-Shell (HS), (b) Shaw’s original NT, (c) SNT, (d) Clouds, (e) Foam, (f) Eighth-Shell (ES). In (a)-(e), the two zones are red and blue, with their overlap in purple. In (f), each color corresponds to a different zone.

Figure 3. Import volume versus parallelization parameter for select methods.