BALANCING THE LOAD: A VORONOI BASED SCHEME FOR PARALLEL COMPUTATIONS

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ABSTRACT

The use of numerical simulations in science is ever increasing and with it the computational size. In many cases single processors are no longer adequate and simulations are run on multiple core machines or supercomputers. One of the key issues when running a simulation on multiple CPUs is maintaining a proper load balance throughout the run and minimizing communications between CPUs.

We propose a novel method of utilizing a Voronoi diagram to achieve a nearly perfect load balance without the need of any global redistributions of data. As a show case, we implement our method in RICH, a 2D moving mesh hydrodynamical code, but it can be extended trivially to other codes in 2D or 3D. Our tests show that this method is indeed efficient and can be used in a large variety of existing hydrodynamical codes as well as other applications.

1. INTRODUCTION

Large computational tasks require machines with distributed memory, since in such systems, the number of CPUs and the size of the total available memory is not set by the capacity of a single machine. An important downside to the distributed memory approach is that communications between processors may take a significant fraction of the computation time since information is carried over a network.

Ensuring proper load balance during parallel calculations of partial differential equations (e.g. hydrodynamics) using the distributed memory approach, is essential for achieving superior performance. In this paper we present a general scheme that is applicable to any problem that can be solved with domain decomposition. Since our implementation is for hydrodynamics, the rest of the paper uses nomenclature of hydrodynamics without loss of generality. For uniform fixed mesh codes (e.g. Athena\textsuperscript{2} (Stone et al. 2008)) load balancing is no great challenge. Partitioning the domain into equal sized static partitions is straightforward, results in balanced loading and minimal communications. For static but nonuniform mesh, a tree based partitioning can be used (e.g. Dubinski (1996)) to divide the domain among the different CPUs. Smooth particle hydrodynamics (SPH), Adaptive Mesh Refinement (AMR) and moving mesh codes differ from the above since the number of cells/points in a given part of the domain is not constant in time. Pluto (Mignone et al. 2012), an AMR code, achieves load balancing by implementing the Kernighan-Lin algorithm for solving knapsack problems (see Schloegel et al. (2000) for more details). Recently it has become very popular to use space filling curves (e.g. Morton curve (Warren and Salmon 1995), or a Peano-Hilbert curve (Shirokov and Bertschinger 2005) to map the cells/points among the different CPUs and to define their boundaries (Shirokov and Bertschinger 2005; Springel 2005; Teyssier 2002). However, as the points move during the time evolution, the load balance between processors deteriorates and redistribution among CPUs is necessary.

2. A VORONOI BASED PARALLELIZATION SCHEME

The novel method introduced here uses a Voronoi diagram to decompose the domain. This is not to be confused with hydrodynamic Voronoi schemes, like AREPO or TESS (Springel 2010; Duffell and MacFadyen 2011), or own code RICH, which use Voronoi diagram to determine the computational cells boundaries. The basic building blocks of the method are CPU mesh points. The corresponding Voronoi diagram based on these mesh points defines for each CPU a region within the computational domain. Each CPU retains in its memory only the hydro points that lie inside its Voronoi cell. At the beginning of the calculation, the domain is decomposed via the Voronoi diagram, and each CPU is assigned its relevant hydro points.

At the beginning of each subsequent time step, we check which hydro points moved between different CPU Voronoi cells, and send their information to the new CPU in which they lie now. This can be done extremely easily and efficiently since the Voronoi diagram already contains the information of who are the neighbors of each CPU. Since typically hydro points can not move in a single time step distances that are larger than their size, the number of communications required is limited to about $O(N^{2/3})$ for 2D, or $O(N^{4/3})$ for 3D, where $N$ is the number of hydro points per CPU. Therefore, for large enough $N$ the communication time is guaranteed to be a small fraction of the computational time even if communications are relatively slow.

Another novelty of this method is that the CPU mesh points can be moved in such a manner as to try and maintain a constant workload per CPU. To determine how the CPU mesh points are to be moved, each CPU is given a merit based on its current workload.

Specifically, we following a scheme which we call “Pressure Balancing Scheme”. For each time step (or every few time steps if the problem is “smooth” with regards to its hydro points distribution) we implement the following procedure:
1. Every CPU constructs the Voronoi diagram of all of the CPU mesh points.

2. The information of Hydro points that moved outside the CPU’s Voronoi cell to which they belonged in the previous time step are sent to their new CPU and new Hydro points are received from the neighboring CPUs.

3. At the end of the computational time step, each CPU determines its merit, which in our scheme we call “pressure”, by counting how many Hydro points are in its domain and this data is broadcasted to the neighboring CPUs.

4. Every CPU determines its new location by

\[
\delta x_i = M_{\text{best}} \cdot \left( \sum_{j=0}^{\text{Neighbors}} (x_i^n - x_j^n) / (M_j + 1) \right) - 1 / (M_i + 1)
\]

where \(M_{\text{best}}\) is the total number of Hydro points divided by the number of processors, \(M_i\) is the number of Hydro points in the \(i\)-th CPU, \(R_i\) is the CPU’s effective radius calculated as \(\pi R_i^2 = A_i\) for 2D and \(4 \pi R_i^3 / 3 = V_i\) for 3D where \(A_i\) is the area of the \(i\)-th CPU Voronoi cell in 2D and \(V_i\) is its volume in 3D, \(n\) is the temporal index and we set \(\alpha = 0.04\).

5. Optionally, a Lloyd iteration can be performed (e.g. eq 63 in \cite{Springel2010}) in order to ensure that the CPU cells remain rather round.

This scheme allows the domains of CPUs to “drift” with the flow of the points, maintaining a good load balance and diminishing the amount of data exchange between CPUs.

If the initial load balance is poor, or an abrupt shift in the load balance occurs, the number of time steps to regain good load balance can be roughly estimated as the number of time steps it takes a CPU mesh point to travel the distance of the domain size. If \(A\) is the area of the domain, then the distance that a badly load balanced CPU mesh point has to travel, \(\Delta r\), is of order

\[
\Delta r \approx \sqrt{A}
\]

The distance that a CPU mesh point travels in a single time step, \(\delta r\), is roughly

\[
\delta r \approx \alpha R \approx \alpha \sqrt{A / N_{\text{CPU}}}
\]

where \(N_{\text{CPU}}\) is the number of CPUs. The number of time steps required to find a good load balance should typically be

\[
\frac{\Delta r}{\delta r} \approx \sqrt{N_{\text{cpu}} / \alpha}
\]

For the 3D case it is

\[
\frac{\Delta r}{\delta r} \approx \frac{N_{\text{cpu}}^{1/3}}{\alpha}.
\]

3. PERFORMANCE

In the following section we run several benchmarks to test our method. All tests are using the RICH moving mesh hydrodynamics code (2014 In preparation), which solves the Euler equations on a moving Voronoi mesh. RICH is made parallel by using MPI and the Voronoi based parallelization scheme described in this paper. All of the tests are run on the Astric cluster in Hebrew University, which hosts 56 Intel E5-2670 Xeon processors for a combined total of 896 threads connected via InfiniBand FDR non-blocking connection. For all of the following tests the load balance is defined to be the ratio between the CPU with the highest number of cells to the average zones per CPU, i.e. \(\max M_i / M_{\text{best}}\).

3.1. Load Balancing

We use a simple blast wave problem in order to check the performance of our new load balancing scheme. The initial problem is set up with a random mesh of uniform density, with a total of \(10^4\) hydro points distributed equally among 128 CPUs. In order to measure the effectiveness of our parallelization scheme, we plot the load balancing max \(M_i / M_{\text{best}}\) as a function of time in figure 1. The test starts with almost perfect load balance, and as the hydro points begin to redistribute themselves, the work is no longer perfectly distributed. However, the average load balance is close to unity (mean value of 1.11), and thus the parallelization is efficient considering that there are no global redistributions of data.

3.2. Weak Scaling

In a perfect parallelization scheme, increasing the number of CPUs while keeping the workload per CPU constant should result with a constant computational time per time step; this is known as weak scaling. However, the need to communicate information between processors and load imbalance prevent this from happening in practice.

In order to check the weak scaling of our scheme, the same blast wave problem as in the previous section is run. First we keep a constant workload of \(10^5\) hydro points per thread, while increasing the number of threads, and a second time keeping \(10^4\) hydro points per thread. Fig-
ure [2] shows that for a small number of threads the time per time step increases slightly as the number of threads is increased. We identify two main factors responsible for this increase. The first is the ability of a CPUs to increase its speed while the number of threads on it that are being used is low (this is known as Turbo Boost). Secondly, our implementation of creating the boundary conditions is more efficient for the single thread case than the multi thread one, this will be addressed in future versions of RICH. The big, almost factor of two, decrease in efficiency that is exhibited between 16 and 32 threads is the change from a single thread per core to two threads per core. From 32 threads up to 512 threads, the computing time for a hydro time step is roughly constant (only 10% change).

The same problem as before is ran, once with a total workload 10^7 hydro points and once with 10^5 cells while each thread hosts 10^3 hydro points. Figure 4 shows the load balancing, as defined above, as a function of time. It is evident that good efficiency is maintained at all times.

3.3. Strong Scaling

Ideally, for a fixed number of hydro points, the computational time should scale inversely proportional to the number of processors used. It should be equal to the computational time on a single processor divided by the number of processors used. In practice this is not achieved due to imperfect load balancing and time spent on communication between processors. Strong scaling, defined as keeping the total workload constant while the number of CPUs increases, is another way to measure the efficiency of the parallelization scheme.

The same problem as before is ran, once with a total workload of 10^6 hydro points and once with 10^7 hydro points. The same qualitative behavior as in the weak scaling can be seen in figure 3. Up to 16 threads the scaling is one over the number of threads, then there is a performance decrease, by almost a factor of two, once we switch to two threads per core. For the smaller workload, using more than 256 threads actually increases the time it takes for a single hydro iteration. This is because the workload per thread is so low that the overhead in constructing the boundaries (with their communication) dominates the computation. At least for this implementation, running with less than 4000 hydro points per thread is counterproductive.

3.4. Uniform Distribution

3.5. Achieving Load Balance

This scheme can also quickly achieve excellent load balance even when the initial distribution of work is very unbalanced. To show this, we set up a static mesh problem, where the hydro points are distributed in the domain \([-1, 1]^2\], with random position picked from an exponential distribution that is described such that the probability of having a hydro point between \(r\) and \(r + dr\), where \(r\) is the radius, is given by \(\lambda \exp(-\lambda r) dr\) with \(\lambda = 10\). The initial positions of CPU mesh points is randomly chose from a uniform distribution in the unit square. This initial setup gives an inefficient configuration, and our goal is to show how the processors position move according to our algorithm and advance towards more efficient load
balance. The hydro mesh points are kept fixed and, in fact, no hydro is calculated.

The system is then iterated using the load balancing steps described in the previous section, and the load balance is recorded for each iteration. This test is preformed with 96 CPUs and a total of $9.6 \times 10^8$ hydro mesh points. With our initial setup the load balance is 66 and the configuration of the CPUs is shown in fig. 5. The load balance as a function of the iteration number is plotted in fig. 6 while the final configuration of the CPUs is shown in fig. 5. Our scheme improves the load balance which eventually saturates on the average value of 1.4. It takes about $\sim 300$th iterations to achieve this load balance, which is comparable to our estimate of $\sqrt{N_{\text{cpu}}}/\alpha = 100$. The mean value of the load balance after 300 iterations is 1.4, a dramatic improvement in efficiency over the initial load balance of 60.

4. FURTHER EXTENSIONS

Our merit system can easily be extended to deal with more complex scenarios where the computational time per hydro point is not constant. Hydro points whose computational time is longer than other points can simply be taken into account as more than one hydro point

when the effective pressure is calculated. An effective implementation of this option is to calculate the time it took each CPU to advance a single time step and give a merit based on that time. This way, the algorithm will tend to even out the computational time among the CPUs even if additional calculations other than hydrodynamics are taking place.

In some cases a large dynamical range of time steps, which are different for differenthydro points, is present. Some codes (e.g. [Katz et al. 1996]) have an option to advance in time only a subset of hydro points with their relevant time step, thus while one hydro point is advanced one large time step, another hydro point with a smaller time step can be advanced many smaller time steps. Defining a pressure just as the time it takes each CPU cell, will results in good load balance, but could create a very large memory imbalance between CPUs, since some CPUs will have many hydro points with a large time step and some will have a small number of hydro points with small time steps. One way to overcome this issue is to use a MultiGrid approach. A Voronoi diagram of the processors should be created for every time step level, and then our method for load balancing should be applied to each time step level individually while taking into account only hydro points with the corresponding time step. Note that there is no reason for the CPU to have its domains overlap between the different time step levels.

5. DISCUSSION

We present here a novel method to parallelize a computational code on a distributed memory machine. It is relevant for handling the load balance of partial differential equations that can be solved with domain decompositions. This method, which uses a moving Voronoi diagram to determine the CPU domains, ensures that there is no need for global data redistribution throughout the whole computation but only exchange of points adjacent to the edges of the CPU’s domain. The ability of the CPUs to “flow” with the hydro points greatly reduces the need to transfer data between CPUs. Tests run with the RICH moving mesh code, show very good scaling up to 512 threads.

The main caveat for this parallelization scheme is that it is efficient only as long as the number of CPUs is smaller than the number of hydro points per CPU. Since typically the number of hydro points per CPU is much larger than the number of CPUs, this caveat does not impose a strong constraint.

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