# Implementation of a Parallel Tree Method on a GPU

Naohito Nakasato<sup>a</sup>

<sup>a</sup> Department of Computer Science and Engineering University of Aizu Aizu-Wakamatsu, Fukushima 965-8580, Japan Email: nakasato@u-aizu.ac.jp

#### **─** Abstract

The kd-tree is a fundamental tool in computer science. Among other applications, the application of kd-tree search (by the tree method) to the fast evaluation of particle interactions and neighbor search is highly important, since the computational complexity of these problems is reduced from  $O(N^2)$  for a brute force method to  $O(N \log N)$  for the tree method, where N is the number of particles. In this paper, we present a parallel implementation of the tree method running on a graphics processing unit (GPU). We present a detailed description of how we have implemented the tree method on a Cypress GPU. An optimization that we found important is localized particle ordering to effectively utilize cache memory. We present a number of test results and performance measurements. Our results show that the execution of the tree traversal in a force calculation on a GPU is practical and efficient.

Keywords:

#### 1. Introduction

A technique for gravitational many-body simulations is a fundamental tool in astrophysical simulations because the gravitational force drives structure formation in the universe. The length scales that arise in structure formation range from less than 1 cm for the aggregation of dust to more than  $10^{24}$  cm for the formation of cosmological structures. At all scales, gravity is a key physical process for the understanding of structure formation. The reason behind this is the long-range nature of gravity.

Suppose we simulate structure formation with N particles. The flow of the many-body simulation is as follows. First, we calculate the mutual gravitational forces between the N particles, then integrate the orbits for the N particles, and repeat this process as necessary. Although it is simple in principle, the force calculation is a challenging task from the point of view of computer science. A simple, exact method for the force calculation requires  $O(N^2)$  computational complexity, which is prohibitively compute-intensive for large N. An exact force calculation is necessary in some types of simulations, such as few-body problems, the numerical integration of planets orbiting around a star (e.g., the Solar System), and the evolution of dense star clusters. For simulations that do not require exact forces, however, several approximation techniques have been proposed (Hockney & Eastwood, 1981; Barnes & Hut, 1986; Greengard & Rokhlin, 1987). The particle-mesh/particleparticle-mesh method (Hockney & Eastwood, 1981) and the tree method (Barnes & Hut, 1986) reduce the computational complexity of the force calculation to  $O(N \log N)$ . fast multipole method (FMM) reduces it further to O(N)(Greengard & Rokhlin, 1987). Of these methods, the tree method has been used extensively in astrophysical simulations,

since its adaptive nature is essential for dealing with clumpy structure in the universe (e.g., Bouchet & Hernquist, 1988).

Despite the  $O(N \log N)$  complexity, computational optimization of the tree method by techniques such as vectorization and parallelization is necessary to accommodate demands for simulations with larger and larger N. Hernquist (1990), Makino (1990), and Barnes (1990) have reported various techniques to vectorize the force calculation with the tree method. Warren et al. (1992), Dubinski (1996), and Yahagi et al. (1999) have reported a parallel tree method for massively parallel processors (MPPs). In a recent publication (Springel et al., 2005), a simulation of large-scale structure formation in the universe with more than ten billion particles, using a parallel tree code running on an MPP, has been reported. Another computational technique to speed up the tree method utilizes the GRAPE special-purpose computer (Sugimoto et al., 1990; Makino & Taiji, 1998). Using a combination of vectorization techniques for the tree method, the tree method can be executed efficiently on a GRAPE system (Makino, 1991).

Cosmological simulations are a "grand challenge" problem. The Gordon Bell prizes have been awarded many times for cosmological simulations (Warren & Salmon, 1992; Fukushige & Makino, 1996; Warren et al., 1997, 1998; Kawai et al., 1999; Hamada et al., 2009). In those simulations, both parallel tree codes (Warren & Salmon, 1992; Warren et al., 1997, 1998) and a tree code running on a GRAPE system (Fukushige & Makino, 1996; Kawai et al., 1999) and a graphics processing unit (GPU) (Hamada et al., 2009) were used to perform cosmological simulations.

In the present paper, we describe our implementation of the tree method on a GPU. The rise of the GPU forces us to rethink our way of doing parallel computing, since the perfor-

Preprint submitted to Elsevier October 25, 2018

mance of recent GPUs has reached the impressive level of > 1 Tflops. Acceleration techniques for many-body simulations with a GPU have already been reported (e.g., Nyland et al., 2007; Portegies Zwart et al., 2007; Hamada & Iitaka, 2007; Belleman et al., 2008); however, these techniques have implemented an exact, brute force method with  $O(N^2)$  complexity. It is apparent, however, that for applications that do not require exact forces, it is possible to do much more efficient computation by the tree method. We have directly implemented the tree method on a GPU so that we can enjoy the speed of an  $O(N \log N)$  algorithm. For small N < 30,000, the brute force method on a GPU is faster than the tree method owing to extra work concerning the tree data structure. However, our results show that the tree method significantly outperforms the brute force method on a GPU for  $N \gg 10,000$ , which is the standard size in current astrophysical simulations is. Our code is simple and easy to extend to other numerical algorithms that require a neighbor list or a short-range force, such as algorithms for the smoothed particle hydrodynamics (SPH) method (Gingold & Monaghan, 1977; Lucy, 1977).

#### 2. GPU architecture

In this section, we briefly summarize the architecture of the Cypress GPU that we used in the present work (most of the information is taken from AMD Inc. (2010)).

#### 2.1. Cypress architecture

The Cypress GPU, from AMD, is the company's latest GPU and has many enhancements for general-purpose computing. It has 1600 arithmetic units in total. Each arithmetic unit is capable of executing single-precision floating-point fused multiplyadd (FMA) operation. Five arithmetic units make up a fiveway very-long-instruction-word (VLIW) unit called a stream core (SC). Therefore, one Cypress processor has 320 SCs. One SC can execute a several combinations of operations such as (1) five 32-bit integer operations, (2) five single-precision FMA operations, (3) four single-precision FMA operations with one transcendental operation, (4) two double-precision add operations, or (5) one double-precision FMA operations. Each SC has a register file of 1024 words, where one word is 128 bits long (four single-precision words or two double-precision words). A group of 16 SCs make up a unit called a compute unit. At the top level of the GPU, there are 20 compute units, a controller unit called an ultra-threaded dispatch processor, and other units such as units for graphics processing, memory controllers, and DMA engines.

All SCs in the compute unit work in a single-instruction-multiple-thread (SIMT) mode, i.e., 16 SCs execute the same instructions for four clock cycles to accommodate the latency of the arithmetic units. That is, we have 64 threads proceeding as a wavefront on the Cypress GPU. At the time of writing, the fastest Cypress processor runs at 850 MHz and offers a peak performance of  $1600 \times 2 \times 850 \times 10^6 = 2.72$  Tflop/s in single-precision operations. With double-precision operations, we have  $320 \times 2 \times 850 \times 10^6 = 544$  Gflop/s.

The external memory attached to the Cypress consists of 1 GB of GDDR5 memory with a 256 bit bus. It has a data clock rate of 4.8 GHz and offers a bandwidth of 153.6 GB/s. This external memory is accessed through four banks, as shown in Figure 1. In each bank, there is a second-level read cache (L2 cache). The total size of the second-level cache is 512 KB, i.e., 4 × 128 KB. Twenty compute units and memory controllers are interconnected through a crossbar. Each compute unit has a first-level read cache (L1 cache) and a local data share (LDS), as depicted in Figure 1. The sizes of the L1 cache and LDS are 8 KB and 32 KB, respectively. The L1 cache can fetch data at 54.4 GB/s when the cache is hit; namely, the aggregate bandwidth of the L1 cache on the Cypress GPU is  $54.4 \text{ GB/s} \times 20$ = 1.088 TB/s. This high memory bandwidth is a notable feature of this GPU. As we shall describe in the following section, taking advantage of the hardware-managed cache is critical to obtaining high performance on the Cypress GPU.

## 2.2. Programming the Cypress GPU

In the present work, we programmed the Cypress GPU using an assembly-like language called IL (Intermediate Language). IL is like a virtual instruction set for GPUs from AMD. With IL, we have full control of every VLIW instruction. The programming model supported by IL is a single-instruction-and-multiple-data (SIMD) model at the level of the SC. In this programming model, a sequence of instructions generated from an IL program is executed on all SCs simultaneously with different input data.

A block of code written in IL is called a compute kernel. The device driver for a GPU compiles IL instructions into the corresponding machine code when we load a kernel written in IL. In a compute kernel, we explicitly declare what type of variable the input data is. In the main body of the IL code, we write arithmetic operations on the input data. Logically, each SC is implicitly assigned data that is different from that for every other SC. In the case of a simple compute kernel, the SC operates on the assigned data. Operations such as this, as arise in pure stream computing, seem to work with the highest efficiency. In a complex compute kernel, which we explore in the present work, each SC not only operates on the assigned data but also explicitly loads random data that might be assigned to another SC. To accomplish a random access to external memory, we explicitly calculate the address of the data in the compute kernel.

The ATI Stream software development kit (SDK) for the Cypress GPU also supports OpenCL, which is a standard API with an extended C language (hereafter referred to as C for OpenCL) for writing a compute kernel. In this work, we also present a compute kernel written in C for OpenCL (see Appendix A for the code). We believe that it is instructive to present our algorithm in C for OpenCL and that this makes the algorithm easy to understand. Both programming methods (using IL and using C for OpenCL) have pros and cons. With IL, we have the advantage of full control of the VLIW instructions, but a compute kernel written in IL is somewhat cumbersome. On the other hand, it is is easier to start writing a compute kernel in C for OpenCL, but optimization for any particular GPU

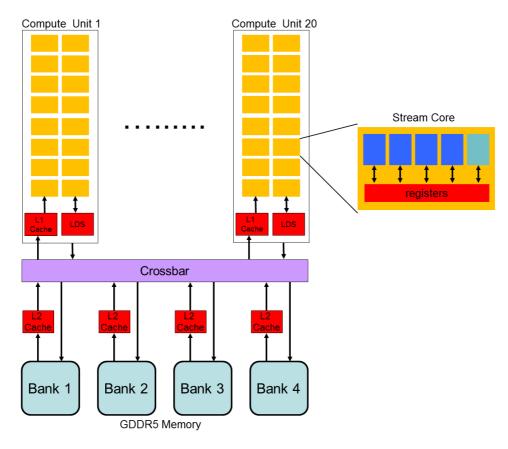


Figure 1: Block diagram of the Cypress GPU, with emphasis on the memory system.

architecture is not straightforward. An advantage of programming with OpenCL is that we can use OpenCL to program a general-purpose many-core CPU. In the following section, we compare implementations of the tree method on a GPU based on compute kernels written in IL and in C for OpenCL. We also compare the performance of a compute kernel written in C for OpenCL on a GPU and on a CPU.

### 3. Bare performance of brute force method on a GPU

So far, we have developed around a dozen kernels in IL that we use for astrophysical many-body simulations. In this section, we report the performance of our implementation of a brute force method for computing gravitational forces. This code served as a basis for us to implement a more sophisticated algorithm later.

To be precise, we have implemented a set of conventional equations expressed as

$$p_{i} = \sum_{j=1, j\neq i}^{N} p(\mathbf{x}_{i}, \mathbf{x}_{j}, m_{j}) = \sum_{j=1, j\neq i}^{N} \frac{m_{j}}{(|\mathbf{x}_{i} - \mathbf{x}_{j}|^{2} + \epsilon^{2})^{1/2}},$$

$$\mathbf{a}_{i} = \sum_{j=1, j\neq i}^{N} f(\mathbf{x}_{i}, \mathbf{x}_{j}, m_{j}) = \sum_{j=1, j\neq i}^{N} \frac{m_{j}(\mathbf{x}_{i} - \mathbf{x}_{j})}{(|\mathbf{x}_{i} - \mathbf{x}_{j}|^{2} + \epsilon^{2})^{3/2}},$$
(1)

where  $a_i$  and  $p_i$  are the force vector and potential for a particle i, and  $x_i$ ,  $m_i$ ,  $\epsilon$  are the position of the particle, its mass, and a parameter that prevents division by zero, respectively. We can solve these equations by two nested loops on a general-purpose CPU. In the inner loop, we simultaneously evaluate the functions p and f, and require 22 arithmetic operations, which include one square root and one division, to compute the interaction between particles i and j. Since previous authors, starting from Warren et al. (1997), have used a conventional operation count for the evaluation of  $f_i$  and  $p_i$ , we have adopted a conventional count of 38 throughout this paper.

Elsen et al. (2006) reported an implementation of a brute force method for gravitational and other forces on an old GPU from AMD/ATi. One of the main insights obtained was that a loop-unrolling technique greatly enhanced the performance of the code. We have followed Elsen et al.'s approach and tried several different methods of loop unrolling. Fujiwara & Nakasato (2009) have reported our optimization efforts for old GPUs. Here, we present a summary of our results. In Figure 2, we plot the computing speed of our optimized IL kernel for computing Eq.(1) as a function of N. We tested three GPU boards, namely RV770 GPUs running at 625 and 750 MHz and a Cypress GPU running at 850 MHz. The three systems had peak computing speeds in single precision of 1.04, 1.2, and 2.72 Tflop/s, respectively. So far, we have obtained a maximum performance of  $\sim 2.6$  Tflop/s on the Cypress GPU

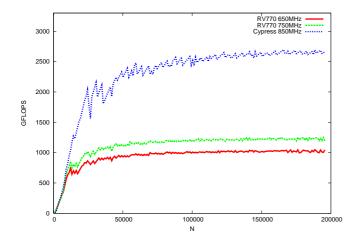


Figure 2: Performance of the brute force method on various GPUs

for N > 150,000. For N = 195,584, our optimized brute force method took roughly 0.5 s on the Cypress GPU. As far as we know, the performance that we obtained is the fastest ever with one GPU chip.

Even with the massive computing power available on such GPUs, however, we cannot escape from a computational complexity of  $O(N^2)$ . Therefore, if we need to do an astrophysical many-body simulation for large N, we need a smart algorithm to do the job, since the recent standard for N in astrophysical simulations is at least 100,000 for complex simulations with baryon physics and 1,000,000 for simple many-body simulations.

## 4. Tree method on a GPU

### 4.1. Tree method

The tree method (Barnes & Hut, 1986) is a special case of the general kd-tree algorithm. This method has been optimized to efficiently calculate the mutual forces between particles, and reduces the computational complexity of the force calculation from  $O(N^2)$  for the brute force method to  $O(N \log N)$ . A trick used is that instead of computing the exact force by a brute force method, it approximates the force from distant particles using a multipole expansion. It is apparent that there is a trade-off between the approximation error and the way in which we replace a group of distant particles by a multipole expansion. A tree structure that contains all particles is used to judge this trade-off efficiently.

The force calculation in the tree method is executed in two steps: (1) a tree construction and (2) the force calculation. In the tree construction, we divide a cube that encloses all of the particles into eight equal sub-cells. The first cell is the root of a tree that we construct; it is called the root cell. Then, each sub-cell is recursively subdivided in the same say until each cell contains zero or one particle. As the result of this procedure, we obtain an oct-tree.

In the force calculation, we traverse the tree to judge whether we should replace a distant cell that contains a group of particles

Figure 3: Pseudocode for the force calculation by traversing the tree

that are geometrically close together with the multipole expansion of those particles. If we do not replace the cell, we then traverse sub-cells of the distant cell. If we do replace the cell, we calculate a particle—cell interaction. When we encounter a particle, we immediately calculate a particle—particle interaction. Given a particle with index i which we want to compute the force acting on, this procedure is expressed as pseudocode in Figure 3. Note that subcell[] is a pointers to its own sub-cells. In this pseudocode, f is a function that computes the particle—particle interaction, and f\_multipole is a function that computes the particle—cell interaction. In the work described in this paper, since we considered only the monopole moment of a cell, both functions were expressed exactly as in Eq. (1). In principle, we can use any high-order moment in the particle—cell interaction.

We follow this procedure starting from the root cell, with the following condition that tests whether a cell is far enough away. Let the distance between the particle and the cell be d. The cell is well separated from the particle if  $l/d < \theta$ , where l is the size of the cell and  $\theta$  is a parameter that controls the trade-off. Since the smaller l/d is, the more distant the cell is from the particle, this condition (called the opening condition) tests geometrically whether the cell is far from the particle. This recursive force-calculation procedure is almost the same as in the original algorithm of Barnes & Hut (1986).

An important feature of the tree method is that with tree traversal, the force calculations for different particles are completely independent of each other. Therefore, after we have completed the tree construction, the force calculation is a massively parallel problem. There are two possible ways to implement the tree method on a GPU to take advantage of this feature.

### 4.2. Tree method with GRAPE

One way is a method proposed by Makino (1991). This method was proposed as a tree method for the special-purpose computer GRAPE. A GRAPE system consists of a host computer and a GRAPE board or boards. The host computer controls the GRAPE board. For a program running on the host, the GRAPE board acts like a subroutine that calculates the gravitational forces for given particles.

So, we need the following two steps to use a GRAPE system for a force calculation using the tree method: (1) construction of

an interaction list on the host computer, and (2) the actual force calculation on the GRAPE board. The interaction list is a list of particles and distant cells that are supposed to interact with a given particle. After the construction of interaction lists for all particles is completed, we compute the force on each particle by sending the interaction lists to the GRAPE board. These two steps are necessary because the GRAPE board does not have the ability to traverse the tree. Many authors have used this method extensively. Three winners and a finalist of the Gordon Bell prize have used a variant of this method with a different version of the GRAPE system and a GPU (Fukushige & Makino, 1996; Kawai et al., 1999; Hamada et al., 2009; Kawai & Fukushige, 2006). A drawback of this approach is that the performance is limited by the speed of the host computer that is responsible for the tree traversal. This possible bottleneck, which is similar to Amdahl's law, might be critical without a highly tuned implementation of treewalk() running on the host. Furthermore, in all of the results presented by Fukushige & Makino (1996), Kawai et al. (1999), Kawai & Fukushige (2006), and Hamada et al. (2009), extra force evaluations by a factor of two were required to obtain the best performance. Note that because of the extra force evaluations, the maximum error in the force that these authors have reported was better than the error obtained with the conventional tree method for a given  $\theta$ .

#### 4.3. General tree walk

Another way to implement the tree method, which we have followed in the present work, is to implement the whole procedure shown in Figure 3 on a GPU. The advantage of this approach is that only the tree construction, which requires relatively little time, is executed on the host, so that we utilize the massive computing power of the GPU as much as possible. More importantly, we can use our method in applications that require short-range interaction forces (Warren & Salmon, 1995). This is because it is possible to implement a neighbor search algorithm as a general tree-walk procedure of the kind shown in Figure 4. Two procedures, proc\_particle and proc\_cell, are used to process the particle-particle and particle-cell interactions, respectively. In addition, a function distance\_test is used to control the treatment of a distant cell. The calculation of the gravitational force is an application of the general tree-walk procedure that has been very success-

#### 4.4. Our GPU implementation

In our implementation of the tree method on a Cypress GPU, we first construct an tree on the host computer that controls the GPU. At this stage, there is no difference between our original tree code and the newly developed code for the GPU.

We need to take special care in implementing the tree-walk procedure on the GPU. Currently, GPU architecture does not support recursive procedures except when it is possible to fully expand a recursion. Such a full expansion is possible only if the level of the recursion is fixed, but in the tree method, it is impossible to know how deep the recursion will be without performing the tree traversal. So, we adopted a method proposed

```
procedure general_treewalk(i, cell)
  if cell has only one particle
    proc_particle(i, cell)
  else
    if distance_test(i, cell) is true
      proc_cell(i, cell)
    else
      for i = 0, 7
        if cell->subcell[i] exists
            general_treewalk(i, cell->subcell[i])
```

Figure 4: Pseudocode for a general tree-walk procedure.

```
procedure treewalk_iterative(i)
  cell = the root cell
  while cell is not null
   if cell has only one particle
     force += f(i, cell)
     cell = cell->next
  else
   if cell is far enough from i
     force += f_multipole(i, cell)
     cell = cell->next
  else
     cell = cell->more
```

Figure 6: Pseudocode for an iterative tree-walk procedure.

by Makino (1990) that transforms a recursion in treewalk() into an iteration. A key feature is that for a given cell, we do not need whole pointers (subcell[]) to traverse the tree. We need only two pointers, to the cells that we will visit next when the opening condition is true and when it is false, respectively. These two pointers (hereafter called next[] and more[]) are easily obtained by a breadth-first traversal of the tree. Figure 5 shows next[] and more[] schematically. Note that a cell that has sub-cells has both a next[] and a more[] pointer, while a leaf cell (a particle in the present case) with no sub-cells has only a next[] pointer. An iterative form of treewalk() with these two pointers is shown in Figure 6.

We implemented the iterative procedure treewalk() rather directly in IL. The input data for this compute kernel is four arrays. The first contains the positions and masses of the particles and cells. We pack a position and a mass into a vector variable with four elements. Therefore, this array is an array of four-element vectors. The mass of a cell equals the total mass of the particles in the cell, and the position of the cell is at the center of mass of the particles. The second and third arrays contain the "next" and "more" pointers, respectively. Both of these are simple arrays. The fourth array contains the sizes of the cells. The size of the cell is necessary for testing the opening condition. See the description in Appendix Appendix A for the definitions of these arrays.

In the present work, we adopted the following modified

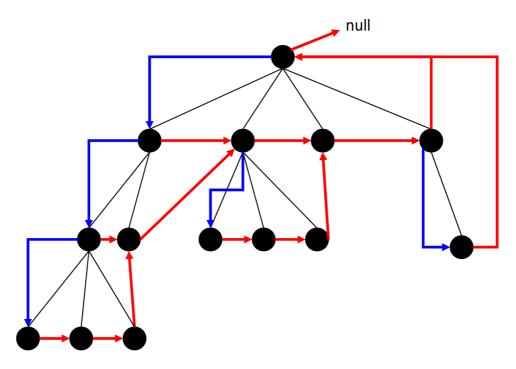


Figure 5: A tree with "more" and "next" pointers, shown by blue and red arrows, respectively.

opening condition, expressed as

$$\frac{l}{\theta} + s < d,\tag{2}$$

where s is the distance between the center of the cell and the center of mass of the cell. The modified condition of Eq. (2) takes the particle distribution in the cell into account through s since if particles gather at a corner of a cell, the effective size of the cell becomes larger. In Figure 7, we present a schematic view of a distant cell and a particle which we are trying to calculate the force acting on. In practice, we precomputed the square of the effective size  $S_{\text{effective}}$  as

$$S_{\text{effective}} = \left(\frac{l}{\theta} + s\right)^2,$$
 (3)

and sent  $S_{\text{effective}}$  instead of l for each cell. With  $S_{\text{effective}}$ , we do not need to compute the square root of d, and we simply compare  $S_{\text{effective}}$  and  $d^2$  during the tree traversal.

In Figure 8, we present an abstract version of our compute kernel written in IL. In IL programming, each SC executes the compute kernel with the assigned data in parallel. In this code, own represents the specific cell assigned to each SC; =, load, and  $\rightarrow$  are not real IL instructions or operations but conventional symbols used here for the purpose of explanation. We have omitted the calculation of the load addresses for the arrays since it is too lengthy to show in detail. In addition, the particle—particle and particle—cell interaction codes have been omitted because they simply compute the functions f and p in Eq. (1). In Appendix A, we present a working compute kernel written in C for OpenCL. We present a performance comparison between the IL and OpenCL implementations in the next section.

Table 1: Our test system

CPU	Intel Xeon E5520 × 2			
Memory	DDR3 800 1GB × 6			
GPU	Radeon 5870 memory 1GB			
OS	Ubuntu 9.10 (64 bit)			
Driver	Catalyst 10.8 (fglrx 8.76.7 [Aug 3 2010])			
SDK	ATI Stream SDK 2.2			

With the compute kernel shown, the flow of our tree method on the Cypress GPU is as follows.

- 1. Construct a tree (host).
- 2. Compute the total mass, the center of mass, and the effective size of each cell (**host**).
- 3. Compute the "next" and "more" pointers (host).
- 4. Send the input data to the GPU (host).
- 5. Iterative tree walk associated with the force calculation for each particle (**GPU**).
- 6. Receive the force for each particle from the GPU (host).

We have indicated whether the corresponding part is executed on the host or the GPU in bold text at the end of each step.

# 5. Tests and optimization

Here, we describe the results of some basic tests to show that our code worked correctly, and to obtain some performance characteristics. We used the configuration shown in Table 1 for

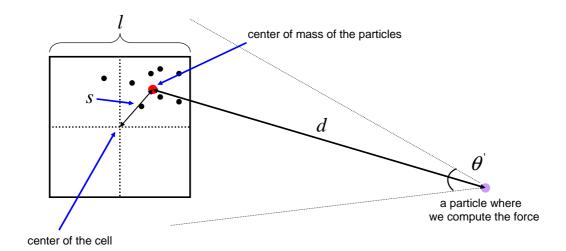


Figure 7: Schematic view of a distant cell and a particle (shown by a solid purple point). The black solid points are particles that belong to the cell. The large red point is the center of mass of the particles in the cell.

all results presented in this paper. In the basic tests, we used a set of particles randomly distributed in a sphere.

First, Table 2 shows how the computing time depends on N. Each value of computing time was obtained by averaging the results of 20 runs. In this test, we set  $\theta=0.6$ .  $T_{\rm total}$  and  $T_{\rm construction}$  are the total time required for the force calculation and the time spent on the construction of the tree, respectively. Roughly, the tree construction took 20–28% of  $T_{\rm total}$ . For all values of N used, we checked that there was effectively no error in the force computed by the GPU. <sup>1</sup> All operations on the GPU were done with single-precision, and we observed that the error was comparable to the machine epsilon,  $\sim 10^{-6}$ . We believe that the error originates from a difference in the implementations of the inverse of the square root on the host and on the GPU. We consider that this is not at all significant for our purpose of astrophysical many-body simulations.

Regarding computing speed, randomly distributed particles are the most severe test because two successive particles in the input data have a very high chance of being at different posi-

Table 2: Dependence of computing speed on N: no sorting

N	$T_{\text{total}}$ (s)	$T_{\text{construction}}$ (s)
50K	$3.95 \times 10^{-2}$	$1.1 \times 10^{-3}$
100K	$9.65 \times 10^{-2}$	$2.5\times10^{-2}$
200K	$2.34 \times 10^{-1}$	$6.1 \times 10^{-2}$
400K	$5.83 \times 10^{-1}$	$1.5\times10^{-1}$
800K	$1.36 \times 10^{0}$	$3.8 \times 10^{-1}$

<sup>&</sup>lt;sup>1</sup>Here, the "error" is not the error due to the approximations in the force calculations.

Table 3: Dependence of computing speed on N: particles sorted in Morton order

N	$T_{\text{total}}$ (s)	$T_{\rm construction}$ (s)
50K	$3.00 \times 10^{-2}$	$9.1 \times 10^{-3}$
100K	$6.08 \times 10^{-2}$	$1.8\times10^{-2}$
200K	$1.27\times10^{-1}$	$3.9\times10^{-2}$
400K	$2.65 \times 10^{-1}$	$8.0 \times 10^{-2}$
800K	$5.66 \times 10^{-1}$	$1.6 \times 10^{-1}$

```
...declaration of I/O arrays and constants...
...initialize variables for accumulation...
xi = load own->x
yi = load own->y
zi = load own->z
cell = root
whileloop
  break if cell is null
  xj = load cell->x
  yj = load cell->y
  zj = load cell->z
  mj = load cell->m
  s_eff = load cell->s_eff
  dx = xj - xi
  dy = yj - yi
  dz = zj - zi
  r2 = dx*dx + dy*dy + dz*dz
  if cell is a particle
    ...compute particle-particle interaction...
    cell = load next
  else
    if r2 > s_eff
      ...compute particle-cell interaction...
      cell = load cell->next
      cell = load cell->more
  endif
```

Figure 8: Abstract IL code for our compute kernel that executes the iterative tree walk

endloop

tions. By the nature of the tree method, if two particles are close to each other, those particles are expected to be in the same cell and to interact with a similar list of particles and distant cells. This means that if two successive particles in the input data are geometrically close, the tree walk for the second particle almost certainly takes less time owing to a higher cache-hit rate. To accomplish such a situation, we can sort the particles to ensure that successive particles are as close as possible together. Fortunately, such sorting is easily available with the tree method by traversing the tree in depth-first order. In the course of the traversal, we add each particle encountered at a leaf node to a list. After the tree traversal, we can use the list obtained to shuffle the particles so that the order of particles is nearly the desired order. This ordering of particles is called the Morton ordering. With this preprocessing, the speed of our method was altered as shown in Table 3. Note that the time in Table 3 does not contain the time required for the preprocessing. This is adequate, since in astrophysical many-body simulations, the tree structure is repeatedly constructed at each time step so that we can automatically obtain this sorting for free. We observed that  $T_{\text{total}}$  obtained with the Morton ordering was faster by a factor of 1.5-2.2, depending on N, than without the preprocessing. Moreover,  $T_{\text{construction}}$  also decreased in all cases owing to better cache usage on the host. With the Morton ordering, the tree construction took roughly 14–27% of  $T_{\text{total}}$ .

The programming API for the Cypress GPU has a facility to report the cache-hit rate for the GPU. In Table 4, we show how the cache-hit rate depends on N and the ordering of the particles. The results indicate that the performance of our method is significantly affected by the ordering of the particles. In the tests described in the following, we always used preprocessing. Note that we could have obtained even better results if we had sorted the particles in the Peano–Hilbert order, which has been reported to be the optimal order for locality of data access, and is used by some tree codes (e.g., Warren & Salmon, 1993).

In Figure 9, we present  $T_{\rm total}$  as a function of N for three cases: the tree method with Morton ordering, the tree method without sorting, and the brute force method. Except for N < 30,000, the tree method with Morton ordering ( $\theta = 0.6$ ) outperforms the brute force method on the GPU.

In Figure 10, we compare the performance for the following three cases: (a) a kernel written in IL running on a Cypress GPU, (b) a kernel written in C for OpenCL running on a Cy-

Table 4: Dependence of cache-hit rate on N for different orderings of the particles

N	No sorting (%) Morton ordering (	
50K	75	93
100K	63	91
200K	55	87
400K	48	85
800K	43	80

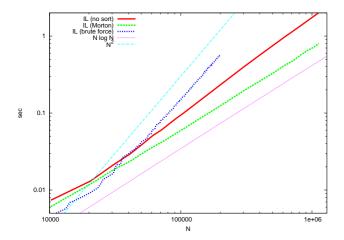


Figure 9: Comparison between the tree method on a GPU and the brute force method on a GPU.  $T_{\rm total}$  as a function of N is plotted for three cases. The  $N^2$  and  $N \log N$  scaling lines are also plotted for reference.

press GPU, and (c) a kernel written in C for OpenCL running on a multicore CPU. Since our test system had eight physical (16 logical) cores, the OpenCL kernel ran on the CPU with 16 threads. The last two cases show almost identical performance even though the theoretical performance in single precision for the Cypress GPU is  $\sim\!20$  times faster. In fact, the tree method is not compute-intensive but is limited by memory bandwidth, and hence the effective performance of the compute kernel written in IL is roughly  $\sim 1\%$  of the theoretical performance in single-precision. On the other hand, the performance gap between the two kernels written in IL and C for OpenCL is a factor of  $\sim\!2.5$ . We believe that one of the main reasons is that our compute kernel written in C for OpenCL is executed without using L1 cache. We will investigate further optimizations of the OpenCL kernel in future work.

Next, we examine how  $T_{\rm total}$  depends on  $\theta$ , which controls the error bound for the tree method. A larger  $\theta$  means that more of the distant particles are replaced by a multipole expansion. In other words, for a smaller  $\theta$ , we need to perform a larger number of force calculations, and hence the computation will take a longer time. At the same time, the error due to the multipole expansion decreases. Practically, a force calculation by the tree method with  $\theta < 0.1$  is reduced to almost the same level as a brute-force computation. In such a regime, effectively, we do not have any preference for the tree method. In Table 5, we

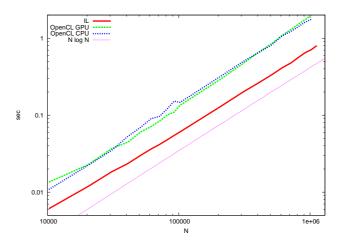


Figure 10: Comparison between the tree method using a kernel written in IL, the tree method using a kernel written in OpenCL on a GPU, and the tree method using a kernel written in OpenCL on a CPU. The  $N \log N$  scaling line is also plotted for reference.

Table 5: Dependence of  $T_{\text{total}}$  and the cache-hit rate on  $\theta$  for N = 800K

$\theta$	$T_{\text{total}}$ (s)	Cache-hit rate (%)
0.2	$1.65 \times 10^{1}$	23
0.3	$5.24 \times 10^{0}$	36
0.4	$2.24 \times 10^{0}$	48
0.5	$1.14 \times 10^{0}$	59
0.6	$6.82 \times 10^{-1}$	68
0.7	$4.92 \times 10^{-1}$	75
0.8	$3.98 \times 10^{-1}$	80
0.9	$3.43 \times 10^{-1}$	80
1.0	$3.10 \times 10^{-1}$	82

show the dependence of  $T_{\rm total}$  and the cache-hit rate on  $\theta$ . In this test, we used  $N=800 {\rm K}$  particles. In all of the tests that we have presented so far, a clear trend is that the computing time seems to be determined solely by the cache-hit rate. Before we had done these tests, we expected that branch operations would be a bottleneck for the compute kernel. In reality, all that matters is the cache-hit rate.

Finally, we measured the average error in the accelerations using the following equation:

$$a_{\text{error}} = \frac{1}{N} \sum_{i=0}^{N-1} \frac{|\boldsymbol{a}_{i}^{\text{tree}} - \boldsymbol{a}_{i}^{\text{direct}}|}{|\boldsymbol{a}_{i}^{\text{direct}}|}, \tag{4}$$

where  $a_i^{\text{tree}}$  and  $a_i^{\text{direct}}$  are the acceleration forces obtained by the tree method on the GPU and by the brute force method on the host computer, respectively. We use a similar definition for the error in the potential,  $p_{\text{error}}$ . For this test, we used a realistic particle distribution that represented a disk galaxy. We used GalactICS (Kuijken & Dubinski, 1995) to generate the particle distribution. The particle distribution had three components,

namely a bulge, a disk, and a halo, with a mass ratio of approximately 1:2:12. Tables 6 and 7 present  $a_{\text{error}}$  and  $p_{\text{error}}$ , respectively, for several different values of N and  $\theta$ . Both  $a_{\text{error}}$  and  $p_{\text{error}}$  depend on  $\theta$  as expected. Except for N=500K, we have a smaller  $a_{\text{error}}$  for larger N. We found no systematic error in  $a_i$  computed by the tree code on the GPU. However, it would be desirable to use double-precision variables for accumulation of  $a_i$  to reduce  $a_{\text{error}}$  for large  $N>10^5$ . There is only a negligible difference between the results computed by the compute kernels written in IL and in C for OpenCL.

## 6. Comparison with other work

#### 6.1. Octree textures on a GPU

Lefebvre et al. (2005) have implemented an tree data structure for a texture-mapping and tree traversal algorithm on a GPU. Owing to the limitations of GPUs and on the SDK for the GPUs at that time, their method seemed to be restricted to applications in computer graphics. A critical point is that the possible depth of the tree was limited, so that we cannot directly employ this implementation for our purposes.

#### 6.2. Another tree implementation on a GPU

Gaburov et al. (2010) have reported another implementation of the tree method on a GPU. Our implementation and their approach share the same strategy, but there are differences in detail, aside from the GPU architecture adopted. Both of us have implemented a tree walk on a GPU. The implementation of Gaburov et al. (2010) constructs interaction lists by means of a tree walk on a GPU and then computes the force on the GPU using these interaction lists. This implementation requires three invocations of kernels. In contrast, we do a tree walk and compute the force on-the-fly with one kernel invocation.

Both approaches have pros and cons. With the Gaburov et al. (2010) approach, a fairly high compute efficiency (~ 100 Gflops) has been obtained, whereas our code shows low efficiency (~ 30 Gflops). On the other hand, Gaburov et al. (2010)'s code requires more floating-point operations than does our optimal tree code. We believe that our implementation is simpler than that of Gaburov et al. (2010), which requires multi-pass computations. And we also believe that our implementation is easier to extend to a general tree walk. In fact, we have extended our compute kernel written in IL to the SPH method (Gingold & Monaghan, 1977; Lucy, 1977) and obtained fairly good performance.

# 6.3. Fast multipole method on a GPU

Gumerov & Duraiswami (2008) have reported an implementation of a fast multipole method (FMM) on a GPU. The FMM is a sophisticated algorithm to evaluate long-range interaction forces with a computational complexity of O(N). In the FMM, in addition to the replacement of distant particles with multipole expansions, local expansions are utilized to evaluate the force acting on a group of particles. Gumerov & Duraiswami (2008) reported that for N=1,048,576, the algorithm took 0.68 s with p=4 (Table 8 of Gumerov & Duraiswami (2008)),

where p is a parameter that controls the error bound. Figure 10 of Gumerov & Duraiswami (2008) indicates that the average relative error obtained with p = 4 was  $\sim 2 \times 10^{-4}$  for the potential. The error is comparable to the relative error obtained with the tree method with  $\theta \sim 0.5$ –0.6. Note that Gumerov and Duraiswami used a random particle distribution in a cube. For comparison, we did a test with a similar particle distribution. Our kernel written in IL took 0.65 s for N = 1,048,576 with $\theta = 0.6$ . The cache-hit rate of the test was 81%. The performance of our tree code and that obtained by Gumerov and Duraiswami with the FMM is comparable. Note that the Cypress GPU used in the present work was different from and newer than the GPU that Gumerov and Duraiswami used. Generally, the FMM is well suited to applications that require long-range interaction forces for uniformly distributed particles or sources, whereas the tree method is more robust to the highly clustered particles that typically arise in astrophysical many-body simulations. We believe that our method is more suitable than that of Gumerov & Duraiswami (2008) for our purpose of astrophysical applications.

# 7. Conclusions

In this paper, we have described our implementation of the tree method on a Cypress GPU. By transforming a recursive tree traversal into an iterative procedure, we have shown that the execution of a tree traversal together with a force calculation on a GPU can be practical and efficient. In addition, our implementation shows performance comparable to that of a recently reported FMM code on a GPU.

We can expect to get further performance gains by fully utilizing the four-vector SIMD operations of the SCs of the GPU. Moreover, since 10–20% of  $T_{\text{total}}$  is spent on the tree construction, parallelization of this part on a multicore CPU will be an effective way to boost the total performance. Provided that we can easily extend our code to implement a force calculation for short-range interactions by a method such as the SPH method, we believe that a future extended version of our code will enable us to do a realistic astrophysical simulation that involves baryon physics with N > 1,000,000 very rapidly. It is fairly easy to incorporate higher-order multipole expansion terms into our method, and it would be a natural extension to the present work. Another good application of the tree method on a GPU would be to simulations that adopt a symmetrized Plummer potential (Saitoh & Makino, 2010). We believe that our method is the best for implementing that proposal, and hence that we shall certainly obtain better accuracy and good performance in simulating galaxy evolution and formation with different mass resolutions.

# Acknowledgments

The author would like to thank M. Sato and K. Fujiwara for their efforts to utilize RV770 GPUs for astrophysical manybody particle simulations. Part of this work is based on their undergraduate theses of 2008 at the University of Aizu. The

Table 6: Dependence of the average acceleration error  $a_{\text{error}}$  on N and  $\theta$ . N is a multiple of 1024.

$\theta$	N = 10K	N = 50K	N = 100K	N = 200K	N = 500K
0.2	2.93e-04	1.69e-04	1.48e-04	2.24e-04	5.73e-03
0.3	6.37e-04	4.42e-04	3.98e-04	4.52e-04	5.90e-03
0.4	1.23e-03	8.86e-04	8.16e-04	8.27e-04	6.20e-03
0.5	2.04e-03	1.50e-03	1.41e-03	1.36e-03	6.64e-03
0.6	3.15e-03	2.31e-03	2.20e-03	2.06e-03	7.20e-03
0.7	4.39e-03	3.35e-03	3.18e-03	2.94e-03	7.91e-03
0.8	5.94e-03	4.51e-03	4.33e-03	3.98e-03	8.77e-03
0.9	7.85e-03	5.95e-03	5.69e-03	5.22e-03	9.86e-03
1.0	9.95e-03	7.69e-03	7.34e-03	6.81e-03	1.13e-02

Table 7: Dependence of the average potential error  $p_{\text{error}}$  on N and  $\theta$ .

$\theta$	N = 10K	N = 50K	N = 100K	N = 200 K	N = 500K
0.2	4.46e-05	4.39e-05	5.37e-05	5.52e-05	4.64e-05
0.3	9.87e-05	1.07e-04	1.41e-04	1.42e-04	1.02e-04
0.4	1.84e-04	1.90e-04	2.70e-04	2.66e-04	1.80e-04
0.5	2.98e-04	2.96e-04	4.30e-04	4.23e-04	2.88e-04
0.6	4.42e-04	4.34e-04	6.23e-04	6.10e-04	4.28e-04
0.7	6.05e-04	5.82e-04	8.26e-04	8.12e-04	5.79e-04
0.8	7.71e-04	7.29e-04	1.04e-03	1.02e-03	7.29e-04
0.9	9.57e-04	8.99e-04	1.27e-03	1.24e-03	8.99e-04
1.0	1.15e-03	1.09e-03	1.51e-03	1.47e-03	1.10e-03

author is grateful to Dr. H. Yahagi for his comments on a draft version of this paper. This work was supported in part by a Grant-in-Aid from the Ministry of Education (No. 21244020).

# Appendix A. Working OpenCL code

In this appendix, we present our compute kernel written in C for OpenCL. We have tested this kernel with ATI Stream SDK 2.2. The function tree\_gm is an entry point to the kernel. n is the number of particles. pos[i] is a float4 variable for the positions and masses, i.e.,  $x_i$  and  $m_i$ . acc\_g[i] is a float4 variable for the accelerations and the potential, i.e.,  $a_i$  and  $p_i$ . next[] and more[] are arrays that contains the two pointers described in Section 4.4. For all arrays, we assume that the data for the particles is at indices i from 0 to n-1. The data for the cells resides at i >= n. Finally, size[] contains softening parameters of the particles for i < n and the size of the cells for i >= n. We believe that it will be straightforward to prepare these arrays from any tree implementation.

#### References

- AMD Inc. (2010). ATI Stream Computing OpenCL Programming Guide, rev1.05.
- Barnes, J. (1990). A Modified Tree Code: Don't Laugh: It Runs. Journal of Computational Physics, 87, 161–170.
- Barnes, J., & Hut, P. (1986). A Hierarchical  $O(N \log N)$  Force-Calculation Algorithm. *Nature*, 324, 446–449.
- Belleman, R. G., Bédorf, J., & Portegies Zwart, S. F. (2008). High Performance Direct Gravitational N-body Simulations on Graphics Processing Units II: An Implementation in CUDA. New Astronomy, 13, 103–112.
- Bouchet, F. R., & Hernquist, L. (1988). Cosmological Simulations using the Hierarchical Tree Method. *Astrophysical Journal Supplement*, 68, 521–538.
- Dubinski, J. (1996). A Parallel Tree Code. New Astronomy, 1, 133–147.
- Elsen, E., Houston, M., Vishal, V., Darve, E., Hanrahan, P., & Pande, V. (2006). *N*-body simulation on GPUs. In *SC '06: Proceedings of the 2006 ACM/IEEE Conference on Supercomputing* (p. 188). New York: ACM.
- Fujiwara, K., & Nakasato, N. (2009). Fast Simulations of Gravitational Manybody Problem on RV770 GPU. ArXiv e-prints, .
- Fukushige, T., & Makino, J. (1996). In *Proceedings of Supercomputing '96*. Los Alamitos: IEEE Computer Society Press.
- Gaburov, E., Bédorf, J., & Portegies Zwart, S. F. (2010). Gravitational Treecode on Graphics Processing Units: Implementation in CUDA. *Procedia Computer Science*, 1, 1113–1121. ICCS 2010.
- Gingold, R. A., & Monaghan, J. J. (1977). Smoothed Particle Hydrodynamics: Theory and Application to Non-spherical Stars. *Monthly Notices of the Royal Astronomical Society*, 181, 375–389.
- Greengard, L., & Rokhlin, V. (1987). A Fast Algorithm for Particle Simulations. *Journal of Computational Physics*, 73, 325–348.
- Gumerov, N. A., & Duraiswami, R. (2008). Fast multipole methods on graphics processors. *Journal of Computational Physics*, 227, 8290–8313.
- Hamada, T., & Iitaka, T. (2007). The Chamomile scheme: An Optimized Algorithm for N-body Simulations on Programmable Graphics Processing Units. ArXiv Astrophysics e-prints, .
- Hamada, T., Narumi, T., Yokota, R., Yasuoka, K., Nitadori, K., & Taiji, M. (2009). 42 TFlops Hierarchical N-body Simulations on GPUs with Applications in Both Astrophysics and Turbulence. In SC '09: Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis (pp. 1–12). New York: ACM.
- Hernquist, L. (1990). Vectorization of tree traversals. *Journal of Computational Physics*, 87, 137–147.
- Hockney, R., & Eastwood, J. (1981). Computer Simulation Using Particles. New York: McGraw-Hill.
- Kawai, A., & Fukushige, T. (2006). \$158/GFLOPS astrophysical N-body simulation with reconfigurable add-in card and hierarchical tree algorithm. In

- SC '06: Proceedings of the 2006 ACM/IEEE Conference on Supercomputing (p. 48). New York: ACM.
- Kawai, A., Fukushige, T., & Makino, J. (1999). \$7.0/Mflops astrophysical N-body simulation with treecode on GRAPE-5. In Supercomputing '99: Proceedings of the 1999 ACM/IEEE Conference on Supercomputing (CDROM) (p. 67). New York: ACM.
- Kuijken, K., & Dubinski, J. (1995). Nearly self-consistent disc/bulge/halo models for galaxies. Monthly Notices of the Royal Astronomical Society, 277, 1341–1353
- Lefebvre, S., Hornus, S., & Neyret, F. (2005). Octree Textures on the GPU. GPU Gems, 2, 595–614.
- Lucy, L. B. (1977). A Numerical Approach to the Testing of the Fission Hypothesis. Astronomical Journal, 82, 1013–1024.
- Makino, J. (1990). Vectorization of a treecode. *Journal of Computational Physics*, 87, 148–160.
- Makino, J. (1991). Treecode with a special-purpose processor. Publications of the Astronomical Society of Japan, 43, 621–638.
- Makino, J., & Taiji, M. (1998). Scientific Simulations with Special-Purpose Computers: The GRAPE Systems. New York: John Wiley and Sons.
- Nyland, L., Harris, M., & Prins, J. (2007). Fast N-body Simulation with CUDA. In GPU Gems3 (pp. 677–696). New York: Addison-Wesley.
- Portegies Zwart, S. F., Belleman, R. G., & Geldof, P. M. (2007). High-performance Direct Gravitational N-body Simulations on Graphics Processing Units. New Astronomy, 12, 641–650.
- Saitoh, T. R., & Makino, J. (2010). The Natural Symmetrization for Plummer Potential. ArXiv e-prints, .
- Springel, V., White, S. D. M., Jenkins, A., Frenk, C. S., Yoshida, N., Gao, L., Navarro, J., Thacker, R., Croton, D., Helly, J., Peacock, J. A., Cole, S., Thomas, P., Couchman, H., Evrard, A., Colberg, J., & Pearce, F. (2005). Simulations of the Formation, Evolution and Clustering of Galaxies and Quasars. *Nature*, 435, 629–636.
- Sugimoto, D., Chikada, Y., Makino, J., Ito, T., Ebisuzaki, T., & Umemura, M. (1990). A Special-purpose Computer for Gravitational Many-body Problems. *Nature*, 345, 33–35.
- Warren, M., Germann, T., Lomdahl, P., Beazley, D., & Salmon, J. (1998).
  Avalon: An Alpha/Linux cluster achieves 10 Gflops for \$15k. In Super-computing '98: Proceedings of the 1998 ACM/IEEE Conference on Super-computing (CDROM) (pp. 1–11). Washington, DC: IEEE Computer Society.
- Warren, M., & Salmon, J. (1992). Astrophysical N-body simulations using hierarchical tree data structures. In Supercomputing '92: Proceedings of the 1992 ACM/IEEE Conference on Supercomputing (pp. 570–576). Los Alamitos, CA, USA: IEEE Computer Society Press.
- Warren, M., & Salmon, J. (1993). A parallel hashed oct-tree *N*-body algorithm. In *Supercomputing '93: Proceedings of the 1993 ACM/IEEE Conference on Supercomputing* (pp. 12–21). New York: ACM.
- Warren, M., Salmon, J., Becker, D., Goda, M., Sterling, T., & Wickelmans, G. (1997). In *Proceedings of Supercomputing '97*. Los Alamitos: IEEE Computer Society Press.
- Warren, M. S., Quinn, P. J., Salmon, J. K., & Zurek, W. H. (1992). Dark Halos Formed via Dissipationless Collapse. I: Shapes and Alignment of Angular Momentum. Astrophysical Journal, 399, 405–425.
- Warren, M. S., & Salmon, J. K. (1995). A Portable Parallel Particle Program. Computer Physics Communications, 87, 266–290.
- Yahagi, H., Mori, M., & Yoshii, Y. (1999). The forest method as a new parallel tree method with the sectional Voronoi tessellation. *Astrophysical Journal Supplement*, 124, 1–9.

```
float4 g(float4 dx, float r2, float mj)
{
  float r1i = native_rsqrt(r2);
  float r2i = r1i*r1i;
  float r1im = mj*r1i;
  float r3im = r1im*r2i;
  float4 f;
  f.x = dx.x*r3im;
  f.y = dx.y*r3im;
  f.z = dx.z*r3im;
  f.w = r1im;
  return f;
__kernel void
tree_gm(__global float4 *pos,
        __global float *size,
        __global int *next,
        __global int *more,
        __global float4 *acc_g,
        int root, int n)
{
  unsigned int gid = get_global_id(0);
  float4 p = pos[gid];
  float4 acc = (float4)(0.0f, 0.0f, 0.0f, 0.0f);
  int cur = root;
  while(cur !=-1) {
   float4 q = pos[cur];
   float mj = q.w;
   float s = size[cur];
    float4 dx = q - p;
    float r2 = dx.x*dx.x + dx.y*dx.y + dx.z*dx.z;
    if (cur < n) {
      if (r2 != 0.0f) {
       r2 += s;
        acc += g(dx, r2, mj);
      cur = next[cur];
    } else {
      if (s < r2) {
       acc += g(dx, r2, mj);
        cur = next[cur];
      } else {
        cur = more[cur];
   }
  }
 acc_g[gid] = acc;
```

Figure A.11: Working OpenCL code that that executes the iterative treewalk. The compute kernel that we have written in IL is mostly similar to this code.