The Chamomile Scheme: An Optimized Algorithm for \( N \)-body simulations on Programmable Graphics Processing Units

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Abstract

We present an algorithm named “Chamomile Scheme”. The scheme is fully optimized for calculating gravitational interactions on the latest programmable Graphics Processing Unit (GPU), NVIDIA GeForce8800GTX, which has (a) small but fast shared memories (16 K Bytes \( \times \) 16) with no broadcasting mechanism and (b) floating point arithmetic hardware of 500 Gflop/s but only for single precision. Based on this scheme, we have developed a library for gravitational \( N \)-body simulations, “CUNBODY-1”, whose measured performance reaches to 173 Gflop/s for 2048 particles and 256 Gflop/s for 131072 particles.

Key words: Stellar Dynamics, Methods: numerical, Methods: \( N \)-body simulations

1 Introduction

1.1 The \( N \)-body simulation

Astronomical \( N \)-body simulations have been widely used to investigate the formation and evolution of various astronomical systems, such as planetary systems, globular clusters, galaxies, clusters of galaxies, and large scale structures of the universe. In such simulations, we treat planetesimals, stars, or
galaxies as particles interacting with each other. We numerically evaluate interactions between the particles and advance the particles according to the Newton’s equation of motion.

In many cases, the size of an astrophysical N-body simulation is limited by the available computational resources. Simulation of pure gravitational N-body system is a typical example. Since the gravity is a long-range interaction, the calculation cost for interactions between all particles is $O(N^2)$ per time-step for the simplest scheme, where $N$ is the number of particles in the system. We can reduce this $O(N^2)$ calculation cost to $O(N \log N)$, by using some approximated algorithms, such as the Barnes-Hut tree algorithm[1], but the scaling coefficient is pretty large. Thus, the calculation of the interaction between particles is usually the most expensive part of the entire calculation, and thus limits the number of particles we can handle. Smoothed Particle Hydrodynamics (SPH)[2][3], in which particles are used to represent the fluid, is another example. In SPH calculations, hydro-dynamical equation is expressed by short-range interaction between particles. The calculation cost of this SPH interaction is rather high, because the average number of particles which interact with one particle is fairly large, typically around 50, and the calculation of single pairwise interaction is quite a bit more complex compared to gravitational interaction.

In astrophysical N-body simulations, the most important interaction is gravitational force. Using computer resources, we calculate the gravitational force of an $i$-th particle from many $j$-th particles in the following equation:

$$a_i = \sum_j \frac{m_j r_{ij}}{(r_{ij}^2 + \varepsilon^2)^{3/2}} \tag{1}$$

where $a_i$ is the gravitational acceleration of $i$-th particle (here after, we call as $i$-particle), $r_j$ and $m_j$ are the position and mass of $j$-th particle (here after $j$-particle) respectively, and $r_{ij} = r_j - r_i$.

Astrophysics is not the only field where the N-body simulation is used. Molecular dynamics (MD)[4] simulation and boundary element method (BEM) are examples of numerical methods where each element of the system in principle interacts with all other elements in the system. In both cases, approaches similar to the Barnes-Hut tree algorithm or FMM[5] help to reduce the calculation cost, but the interaction calculation still dominates the total calculation cost.

One extreme approach to accelerate the N-body simulation is to build a special-purpose computer for the interaction calculation. Two characteristics of the interaction calculation make it well suited for such approach. Firstly, the calculation of pairwise interaction is relatively simple. In the case of gravitational interaction, the total number of floating-point operations (counting
all operations, including square root and divide operations) is only around 20. So it is not inconceivable to design a fully pipelined, hard-wired processor dedicated to the calculation of gravitational interaction. For other application like SPH or molecular dynamics, the interaction calculation is more complicated, but still hardware approach is feasible. Secondly, the interaction is in its simplest form all-to-all. In other words, each particle interacts with all other particles in the system. Thus, there is lots of parallelism available. In particular, it is possible to design a hardware so that it calculate the force from one particle to many other particles in parallel. In this way we can reduce the required memory bandwidth. Of course, if the interaction is of short-range nature, one can implement some clever way to reduce calculation cost from \(O(N^2)\) to \(O(N)\), and the reduction in the memory bandwidth is not as effective as in the case of true \(O(N^2)\) calculation.

The approach to develop specialized hardware for gravitational interaction, materialized in the GRAPE ("GRAvity piPE") project \([6][7]\), has been fairly successful, achieving the speed comparable or faster than the fastest general-purpose computers. A major limitation of GRAPE is that it can’t handle anything other than the interaction through \(1/r\) potential. It is certainly possible to build a hardware that can handle arbitrary central force, so that molecular dynamics calculation can also be handled\([8][9][10][11][12]\).

However, to design a hardware that can calculate both the gravitational interaction and, for example, an SPH interaction is quite difficult. Actually, to develop the pipeline processor just for SPH interaction turned out to be a rather difficult task \([13][14][15][16][17]\). This is provably because the SPH interaction is much more complex than gravity.

Instead of design a hardware, we can use a programmable hardware to accelerate many kinds of interaction. The Graphics Processing Unit (GPU) is one of such programmable hardware.

### 1.2 The Graphics Processing Unit

The history of Graphics Processing Unit (GPU) is important to understand its possibility.

In early times, GPU was a special-purpose device for processing graphics. The GPU implemented numbers of graphics pipelines in a way that makes running them much faster than drawing directly to the screen with the conventional CPU. For decades, the GPU basically had been very similar to GRAPE, which had many hard-wired pipelines strictly dedicating to graphics processing such as drawing rectangles, triangles, circles, and arcs on the screen.
Recently, the GPU had been very efficient in calculating and displaying computer graphics with their highly parallel structure. Corresponding with the advent of graphics libraries (such as the 8th-generation DirectX, or OpenGL), GPU vendors began to add some programmable hardware instead of the hard-wired pipeline.

In this generation of GPU, such programmable hardware was called the programmable shader. After the GPU implemented the programmable shader, the generality of GPU had improved a little. Using the programmable shader, graphics programmer was able to control GPUs not only in polygon level but also in pixel level through their program code.

As the shading calculation has much compute-intensive and highly parallel characteristic, GPU vendors had to implement large numbers of arithmetic hardwares onto their GPUs. As a result, the performance improvement of GPU had surpassed that of CPU.

1.3 The GPU-based Computing

As the GPU had general-purpose functionality and the performance of GPU were improving rapidly, some people thought they wanted to use the GPU not only for graphics processing but for numerical computing such as physics, chemistry or astrophysics simulations. Such demands pierced and moved GPU vendors to open methods for people in numerical computing, and GPU vendors began to supply methods for accessing general-purpose functions on GPU for numerical computing. People began to call such method as the General-Purpose Computation on GPUs (GPGPU) [18] or GPU-based computing.

In \(N\)-body simulations, the GPU-based computing also could offer the level of flexibility that was impossible to achieve with the conventional GRAPE approaches. GPU is a mass-produced hardware, consisting of a large number of floating-point hardwares in a SIMD (Single Instruction stream, Multiple Data stream) fashion. By programming these floating-point hardwares, we can implement an arbitrary pipeline processor on GPU. Thus, a single hardware can be used to implement various interactions, such as that for gravity, SPH, and others.

Recently the approach to accelerate \(N\)-body simulations with GPUs has become an active area of research. For molecular dynamics simulation, Nyland et al. reported 4096 body simulation with \(290 \times 10^6\) (pair/second) \(\times 38\) (flop/pair) \(\simeq 11\) (Gflop/s) [19]. Mark Harris reported \(N\)-body simulation of 8192 body system with \(480 \times 10^6\) (pair/second) \(\times 38\) (flop/pair) \(\simeq 18\) (Gflop/s) [20], and \(672 \times 10^6\) (pair/second) \(\times 38\) (flop/pair) \(\simeq 26\) (Gflop/s) [18].
There were some more requirements needed for applying the conventional GPUs to $N$-body simulations. The most important requirement was about the performance of the conventional GPUs. Compared with that of the conventional GRAPE, the GPUs used by Harris and Nyland had the peak performance of only around 100 Gflop/s. On the other hand, in the same age, the GRAPE-6Af[21] in a PCI add-in fashion already had the peak performance of 131.3 Gflop/s. According to these performance differences, people in astrophysics did not try to use GPUs as their computing resources.

1.4 The Compute Unified Device Architecture (CUDA)

There also existed another requirement for the conventional GPU. It was the programming method for GPU, which remained quite tricky.

One of widely used methods for programming GPU is the Cg language. The Cg language was developed by the NVIDIA corporation. Using Cg, we can use both of NVIDIA’s and ATI’s GPUs as computing devices. However we should access the GPUs only through the graphics libraries, such as OpenGL or DirectX, in the Cg language. Such programming methods are often quite tricky for people in astrophysics.

Naturally, the GPU vendors had known such circumstances. In November 2006, the NVIDIA corporation opened a quite smart programming method for their GPUs, the Compute Unified Device Architecture (CUDA). Using the CUDA, we can write the GPU’s program as if we use the standard C language and we don’t need to suffer with any graphics libraries.

1.5 The GeForce8800GTX system

Returning our explanation to about the peak performance of GPU, the situation has been changed dramatically in these several months.

At the middle of November 2006, the NVIDIA corporation has released a modern GPU, NVIDIA GeForce8800GTX. Its peak performance reaches even 500 Gflop/s.

Figure. 1 shows the basic structure of GeForce8800GTX system. It is connected to a host computer, which works as an attached processor. The GeForce8800GTX system is composed of one GPU chip and device memory of 768 M Bytes.

1 [http://www.nvidia.com/](http://www.nvidia.com/)
2 [http://www.nvidia.com/](http://www.nvidia.com/)
GDDR3-DRAM (Graphics Double Data Rate 3 Dynamic Random Access Memory). The GPU chip consists of 128 processors (Stream Processors in Figure 1).

The stream processor is a general-purpose processor, which has three floating-point units (floating-point multiply, floating-point multiply and addition). Each stream processor works at 1.35 GHz. Then the peak performance of the GeForce8800GTX equals 518.4 Gflop/s (128 [processors] × 3 [float/processor] × 1.35 [GHz]).

The detailed features of the GPU chip in the GeForce8800GTX system are as follows. All of the processors are divided into 16 blocks (SIMD Blocks in Figure 1). Each block has 8 processors in a SIMD fashion and a quite fast but small shared memory (16 K Bytes each). The 8 processors in a SIMD block can work with a single instruction, and they can synchronize and communicate with each other through the shared memory. On the other hand, the processors in different SIMD blocks can not synchronize with each other. Each processor can execute many tasks with time-multiplexing as many as the processor can allocate its registers to different tasks.

1.6 Glanced difference between the GPU and the GRAPE

Then, what is the fundamental difference between the modern GPU and the conventional GRAPE in N-body simulations?
Figure 2. The basic structure of GRAPE system

Figure 2 shows the basic structure of GRAPE system. The GRAPE implements many pipelines with hard-wired arithmetic units on a chip to calculate the interactions between particles in the equation (1). All pipelines on GRAPE chips are connected directly with large amount of memory (8 M Bytes of SS-RAMS per chip for GRAPE-6) and have a broadcasting mechanism. The path between all pipelines and memory hang in the same line and the data elements of \( j \)-particle can be broadcasted to all pipelines for every clock cycles. Then, the pipelines can calculate the gravitational interactions clock by clock and the time spent for the data moving can be hidden behind the pipeline computations.

Another feature of the GRAPE is that the pipeline implements accumulation units for high precision. The pipeline of GRAPE implements accumulation unit with 64-bit accuracy. In the case of accumulating force exerted from large number of particles, it is quite important because the subtraction between two values with similar size causes a very big error (cancellation of significant digits) and the error accumulates when repeated many times (Here after, we call such error in accumulation as the cumulative error).

For \( N \)-body simulations, the big memory with broadcasting mechanism and the high precision arithmetic hardware for accumulation are the most important features of the traditional GRAPE. On the other hand, small but fast shared memories (16 K Bytes \( \times \) 16) with no broadcasting mechanism and floating point arithmetic hardware of 500 Gflop/s but only for single precision are the most important features of the modern GPU.

Then, what everyone wants to know is the possibility of the modern GPU in \( N \)-body simulations. Is the modern GPU suitable for \( N \)-body simulations?
Our conclusion described in this paper is "almost yes", but a lot of discussions should be done by many people in astrophysics. And it is glad that our scheme named “Chamomile Scheme” becomes the first one step for future discussions.

The plan of this paper is as follows. In section 2, we describe the Chamomile Scheme. In section 3, we demonstrate the performance of the modern GPU by our library, CUNBODY-1. And the section 4 is for discussions.

2 The Chamomile Scheme

2.1 Overview of the Chamomile Scheme

In this section, we describe our Chamomile Scheme (CS), which is fully optimized for calculating gravitational interactions on the modern GPU, NVIDIA GeForce8800GTX. The advantage of the CS is that we can use the features of the GPU:

(1) small but fast shared memories with no broadcasting mechanism,
(2) single precision floating point arithmetic hardware but ultra high-speed, effectively.

Firstly, we show the overview of our CS in Figure 3. The blue locus expresses the behavior of a GPU chip, and the red lines represents the data transfers between the GPU chip and the device memory. The device memory are divided into three regions: a region for all \( j \)-particles (here after, \( j \)-particle memory), a region for all \( i \)-particles (here after, \( i \)-particle memory), and a region for all force (here after, force memory).
At first, the GPU chip takes segmental $j$-particles (hereafter, J-BAG) into its shared memory. After taking the J-BAG, the GPU runs through between $i$-particle memory and force memory, and come back to $j$-particle memory again. This GPU chip’s behavior expressed by the blue locus is repeated again and again until all J-BAGs are taken from $j$-particle memory.

While the GPU chip are running, the J-BAG interacts with all $i$-particles and the force calculated by this interaction are stored into force memory again and again (hereafter, FORCE-LOOP).

Our idea of CS comes from such behavior of GPU chip. When we were taking chamomile tea, suddenly we got an image of such GPU’s behavior illustrated in Figure. 4. So we have named our algorithm as the “Chamomile Scheme”.

### 2.2 Details of the Chamomile Scheme

Figure 5 shows the detailed implementation of the CS on the GeForce8800GTX system. The device memory implements $i$-particle memory, $j$-particle memory and force memory. The shared memory on each SIMD block implements the J-BAG for segmental $j$-particles. The stream processor executes just as if many pipelines are implemented and work simultaneously. The stream processor implements registers for $i$-particles (hereafter, $i$-particle registers) and force (hereafter, force registers). The force registers are divided into two regions, backup force registers and current force registers.

Based on the CS, calculation proceeds in the following steps:

(a) The Host computer sends all of $i$- and $j$-particles to $i$-particle memory and $j$-particle memory, respectively.
(b) The GPU divides $j$-particles into J-BAGs with the size of shared memory.
(c) The GPU divides $i$-particles into blocks (hereafter, I-POTs) with the size of all pipelines.
(d) All pipelines gather the J-BAG from $j$-particle memory to their shared memory. (J-PACKING)
   (e) All pipelines gather $i$-particles from $i$-particle memory to $i$-particle registers.
   (f) All pipelines gather force calculated previously to the backup force registers.
   (g) All pipelines clear the current force registers by zero.
   (h) All pipelines calculate interactions between the I-POT and the J-BAG while summing up the current force registers.
   (i) All pipelines add their current and backup force registers, and scatter the force to force memory.
   (j) GPU repeats (e) $\sim$ (j) for all I-POTs.
(k) The GPU repeats (d) $\sim$ (k) for all J-BAGs.
(l) The GPU sends back all of force to the host computer.

Here, we call the process of (d) as J-PACKING, and (f) $\sim$ (i) as FORCE-LOOP.

Using J-PACKING, we can reduce the transfer time for $j$-particles, because the shared memory is much faster than the device memory. For the GeForce8800GTX system, the latency of the shared memory is about 2 clock cycles. On the other hand, the latency of the device memory is about 200 $\sim$ 300 clock cycles.

The J-PACKING in process (d) needs additional time compared with the case without the shared memory. For every J-PACKING, we need to shift the $j$-particles from the device memory to the shared memory.
Fig. 6. The sequential accessing for the J-PACKING.

Fig. 7. An example of 3-way virtual multiple pipelines (VMPs) for a Stream Processor in the CS algorithm. In fact, we use 16-way VMPs for our implementation.

However the time spent for the J-PACKING doesn’t become a bottleneck. This is because the J-PACKING occurs only once while the GPU are running through between $i$-particle memory and force memory.

Though the J-PACKING is not a bottleneck, there is a slight technique for advancing the bandwidth of J-PACKING. Figure 6 shows the technique. The device memory consists of GDDR3-DRAMs, by which we can use a burst accessing. While building the J-BAG, each pipeline sends each request and the device memory outputs $j$-particles. If the requests are sequential, the outputs also become sequential and the bandwidth of J-PACKING improves.

2.2.1 The Virtual Multiple Pipelining

To improve the bandwidth of the J-BAG more, we can use the NVIDIA’s multi-threading function on the stream processor. The J-BAG doesn’t have no broadcasting mechanism while sending $j$-particles to pipelines. Using the multi-threading, we can hide the time for gathering $j$-particles behind the arithmetic operations on pipelines. Here after, we call such the usage of the multi-threading as virtual multiple pipelining and the multi-threaded pipelines as the virtual multiple pipelines (VMPs).
The original idea of VMP comes from Makino et al. (1997) [22]. The only difference between Makino et al. and the CS is just the substance actually working. For Makino et al., the substance is the hard-wired pipeline and for the CS, it is the stream processor.

Figure 7 illustrates the VMPs on a stream processor. In this figure, the time goes by left to right in each clock cycle. At the first clock cycle, the first pipeline (pipeline 0 in Figure 7) requests a j-particle to the J-BAG. At the same time, the second pipeline (pipeline 1) executes an arithmetic operation, and the last pipeline (pipeline 2) receives j-particle from the J-BAG simultaneously. At the next clock cycle, each operation shift to the next pipeline. The last stage is also the same manner. So, applying the virtual multiple pipelining, the time for gathering j-particles can be hidden by arithmetic operations on the stream processor.

Up to now, we can understand that the CS uses one of the feature of GPU: (1) small but fast shared memories with no broadcasting mechanism, effectively.

2.2.2 The FORCE-LOOP

Secondly, we explain how the CS uses another feature of the GPU: (2) single precision floating point arithmetic hardware but ultra high-speed, effectively.

We named the process between (f) ~ (i) as the FORCE-LOOP in previous sub-
void force(double xj[][],
           double mj[],
           double xi[][],
           double eps2,
           double a[][],
           int ni,
           int nj);

Fig. 9. The structure of subroutine of our library section. Figure 8 shows the steps of the FORCE-LOOP. In the first stage, each pipeline gathers force (old force in this figure) previously calculated from the force memory to the backup force registers. Simultaneously, the pipeline clears the current force register by zero. At the next stage, the pipeline calculates interactions between J-BAG and I-POT. While the calculation, the pipeline is summing up the current force register. After the calculation is finished, the pipeline adds the current force register and the backup force register, and gets back the force added to the force memory.

In this manner, the calculation of interaction for equation (1) can be reformed to the following equation:

\[
\mathbf{a}_i = (\ldots (\sum_{j=0}^{n_{jb}-1} \frac{m_j r_{ij}}{(r_{ij}^2 + \varepsilon^2)^{3/2}}) + \sum_{j=n_{jb}}^{2n_{j}-1} \frac{m_j r_{ij}}{(r_{ij}^2 + \varepsilon^2)^{3/2}}) \ldots ) + \sum_{j=n_j-n_{jb}}^{n_j-1} \frac{m_j r_{ij}}{(r_{ij}^2 + \varepsilon^2)^{3/2}}), \quad (2)
\]

where \( n_j \) is the number of all \( j \)-particles stored in \( j \)-particle memory. \( n_{jb} \) is the number of \( j \)-particles in a J-BAG. By this reformation, the cumulative error strongly depends on the total number of J-BAG, \( (\frac{n_j}{n_{jb}}) \). For GeForce8800GTX, the size of the shared memory is 16 K Byte and \( \frac{n_j}{n_{jb}} \) becomes around 4 (for 2048 particles) \( \sim 256 \) (for 131072 particles) at most. For this reason, we can reduce the cumulative error by the FORCE-LOOP.

3 CUNBODY-1 and the Performance

Based on the Chamomile Scheme, we have developed a library for gravitational \( N \)-body simulations, CUNBODY-1 (CUDA N-BODY version 1). And in this section, we describe the performance results of the CUNBODY-1.
int ni, nj;
double rj[131072][3];
double mj[131072];
double ri[131072][3];
double a[131072][3];
double eps2 = 0.01;

int main()
{
    ...(A)... /* get initial condition for rj, mj, ri, a, and n */
    ...(B)... /* prepare result previously calculated by host */
    ...(C)... /* start stopwatch */
    force(rj, mj, ri, eps2, a, ni, nj);
    ...(D)... /* stop stopwatch and get the lap time */
    ...(E)... /* check results and calculate maximum cumulative error */
}

Fig. 10. A C program for measuring the performance and cumulative error of the CUNBODY-1.

3.1 The Library Structure

Figure.9 shows the subroutine structure of the CUNBODY-1. \( n_i \) and \( n_j \) are the total number of \( i \)-particles and \( j \)-particles, respectively. \( x_j \) represents position of \( j \)-particles (three dimensions), \( m_j \) represents mass of \( j \)-particles, \( x_i \) represents position of \( i \)-particles (three dimensions), \( \text{eps} \) is a softening parameter, and \( a \) represents force calculated by a GPU. The CUNBODY-1 library can be used from standard C/C++/Fortran languages, because we use the CUDA library to implement the CUNBODY-1. We can see the CUNBODY-1 library interface is simple and available not only for the direct integration algorithms but also for other clever algorithms such as the Barnes-Hut tree algorithm[1], etc.

Figure.10 shows our test program written by the standard C language to measure the performance and cumulative error with the CUNBODY-1. In this code, \( r_i \) and \( r_j \) represent positions of \( i \)-particles and \( j \)-particles, respectively. \( m_j \) represents mass of \( j \)-particles, \( a \) represents force calculated by a GPU thorough the CUNBODY-1 library, and \( \text{eps2} \) is for a softening parameter. At the first step (A), the test program initializes all values described above. At next step (B), the program prepares results previously calculated by the host computer with double precision. In (C), the time measurement begins and completes at (D). Then the program checks the errors for all forces calculated by the CUNBODY-1 library (force). Note that, in the actual experiment, we execute the \text{force} function many times and average the times for reducing the measurement deviation.
Table 1
The system details for our experiment

| Component          | Comment                        |
|--------------------|--------------------------------|
| **Hardware**       |                                |
| GPU Board          | ASUS EN8800GTX/HTDP/768MByte    |
| System Board       | ASUS P5WDG2 WS Professional     |
| System Memory      | Transcend TS128MLQ64V8J DDR2-800 1 G Bytes |
| CPU                | Intel Core2Duo E6600 2.40 GHz   |
| **Software**       |                                |
| GPU driver         | NVIDIA Linux Display Driver Version 97.51 [http://www.nvidia.com/cuda/] |
| CUDA SDK           | CUDA SDK Version 0.8 for Linux x86 32-bit [http://www.nvidia.com/cuda/] |
| OS                 | Debian GNU/Linux, kernel 2.6.18 |
| Compiler           | gcc version 4.0.4               |

3.2 System Details for Experiments

Our library is implemented using the CUDA C language. So we need the CUDA library and also a GPU board and a GPU driver. In Table.1, we illustrate the details of our system for the performance experiments.

3.3 Initial conditions

We use the NEMO toolbox[23] to construct the initial condition of a Plummer sphere with equal mass particles with mkplummer command. And we evaluate the cumulative errors between force computed by the host computer with double precision and force computed by the GPU.

3.4 Cumulative Error

In Table.2, we present the results of cumulative force error with the initial conditions of a Plummer sphere with $N$ particles ($N = 2048 \sim 131072$). The cumulative force errors listed mean the maximum force error for all of $N$ particles, which is calculated by the following equation:

$$E_{\text{max}} = \max_{i=0 \sim N-1} \left| \frac{a_{\text{gpu},i} - a_{\text{host},i}}{a_{\text{host},i}} \right|.$$  

(3)
Table 2
Results of the maximum cumulative errors for a Plummer sphere with \( N \) equal mass particles initially in virial equilibrium

| \( N \)   | DIRECT style | Chamomile Scheme |
|---------|--------------|------------------|
| 2048    | \( 2.2 \times 10^{-6} \) | \( 5.4 \times 10^{-7} \) |
| 4096    | \( 3.0 \times 10^{-6} \) | \( 3.3 \times 10^{-7} \) |
| 8192    | \( 5.4 \times 10^{-6} \) | \( 5.0 \times 10^{-7} \) |
| 16384   | \( 7.0 \times 10^{-6} \) | \( 4.3 \times 10^{-7} \) |
| 32768   | \( 1.2 \times 10^{-5} \) | \( 6.8 \times 10^{-7} \) |
| 65536   | \( 1.4 \times 10^{-5} \) | \( 1.0 \times 10^{-6} \) |
| 131072  | \( 2.2 \times 10^{-5} \) | \( 1.5 \times 10^{-6} \) |

where \( a_{\text{gpu},i} \) is force, which asserts on \( i \)-particle, calculated by the GPU. \( a_{\text{host},i} \) is force on \( i \)-particle calculated by the host computer. \( E_{\text{max}} \) is the maximum error of the force.

The first column in Table 2 represents the number of particles, the second column is for the maximum error obtained by direct accumulation of all \( N \) \( j \)-particles in single precision (hereafter, the DIRECT style accumulation). The last column is for the maximum error by the Chamomile Scheme. Using the DIRECT style accumulation, the maximum cumulative error becomes around \( 10^{-6} \). On the other hand, our Chamomile Scheme is better than the DIRECT style, in which the maximum cumulative error is suppressed around \( 10^{-7} \).

3.5 Performance

At the end of this section, we give our results of the measured performances in Table 3. The first column represents the number of particles, the second column is the time spent for the CUNBODY-1 library (force). The last column is the performance in Gflop/s (Giga flop/s).

We count flop/s by the following equation:

\[
S = n_{\text{flop}}N^2/t \quad [\text{flop/s}],
\]  

(4)
Table 3
Results of the performance measurements for a Plummer sphere with $N$ equal mass particles initially in virial equilibrium, using single GPU board and the CUNBODY-1 library

| $N$  | Computing time (sec) | Performance (Giga flop/s) |
|------|----------------------|---------------------------|
| 2048 | $9.21 \times 10^{-4}$ | 173                       |
| 4096 | $2.99 \times 10^{-3}$ | 213                       |
| 8192 | $1.08 \times 10^{-2}$ | 235                       |
| 16384| $4.14 \times 10^{-2}$ | 246                       |
| 32768| 0.162                | 251                       |
| 65536| 0.642                | 254                       |
| 131072| 2.548               | 256                       |

where $N$ is the number of the particles. $t$ is time spent for the CUNBODY-1 library. $n_{flo}$ is the total number of the floating-point operations for force calculation. In this paper, we use 38 as $n_{flo}$. This convection was introduced by Warren et al (1997)[24], and we follow it here since many researches use the same number [25] [21] [26] [27] [28].

4 Discussion

4.1 Comparison of the GPU and the GRAPE in practical applications

It seems to be almost clear that the performance of the GPU is much better than that of the GRAPE in the measured performances. For the case of force calculation only, the theoretical peak performance of GRAPE-6Af with four GRAPE-6 processor is only 87.5 Gflop/s[21]. Oppositely, the GeForce8800GTX has the peak performance of 518.4 Gflop/s, and our CUNBODY-1 with one GeForce8800GTX has the measured performance of 173 $\sim$ 256 Gflop/s.

Of course, there remain many discussions in our insistence. The main discussion is about performance for other cases, such as the direct integration with
float4 force(float2 ij : WPOS,
    uniform sampler2D pos) : COLOR0
{
    // Pos texture is 2D, not 1D, so we need to
    // convert body index into 2D coords for pos tex
    float4 iCoords = getBodyCoords(ij);
    float4 iPosMass = texture2D(pos, iCoords.xy);
    float4 jPosMass = texture2D(pos, iCoords.zw);
    float3 dir = iPos.xyz - jPos.xyz;
    float r2 = dot(dir, dir);
    dir = normalize(dir);
    return dir * g * iPosMass.w * jPosMass.w / r2;
}

Fig. 11. Mark Harris’s code

a Hermite Scheme. In this case, we should calculate not only force but also its
time derivatives simultaneously. For this remained discussion, we have already
pot the measured performance for force and its time derivatives calculation in
simultaneous. Our current result has achieved 179 Gflop/s for 131072 particles
with single GeForce8800GTX[29].

4.2 Comparison with similar research projects

For \(N\)-body simulations, Nyland et al.[19] and Harris et al.[20][18] reported \(N\)-
body simulations with GPUs. Fig.11 shows a part of Harris’s implementation
[20][18] written in the Cg language. This implementation is same as Nyland et
al[19]. These implementations of force calculation are based on the parallelism
of particle pair, \((i, j)\). They build an \(N \times N\) force matrix (texture), \(f_{ij}\). The
float4 vector iPposMass contains three dimensional position vector and mass
of \(i\)-particle. The total force acting on \(i\)-particle is calculated by summing up
with \(j\)-particles by using binary tree summation. This scheme is performed
very efficiently in parallel on a GPU, because it has \(N^2\)-parallelism in the
most heavy force calculation and \(N\)-parallelism in relatively light calculation
of summation. A minor drawback of this algorithm is that the size of \(f_{ij}\) ta-
ble grows up in proportion to \(O(N^2)\), and is limited to the maximum texture
size (2048 particle for their implementations). For more particles, their im-
plementations also need similar scheme to our Chamomile Scheme, where the
particles should be divided into blocks and the total force should be calculated
block by block.

4.3 Performance modelling and more fine optimization

There is a possibility that the performance will improve more for the Chamomile
Scheme. When we almost completed this work, a new version of CUDA library
was released from the NVIDIA corporation. The new version of CUDA library
offers us a method to access the texture memory spaces on the device mem-
ory. The texture memory spaces are implemented as read only region of the
device memory and cached in on-chip memory spaces so as to improve the effective bandwidth and latency. With the texture memory spaces, the sampling costs one memory read from the device memory only on a cache miss. Current CUNBODY-1 library doesn’t use any texture memory spaces. So, if we implement the I-POT on the texture memory spaces, the performance might improve more. The improvement work needs to measure the number of clock cycles for each internal operations. We can easily measure the clock cycles for this purpose, because the CUDA library offers us a method to measure the internal clock cycles. And we can construct the performance model for the modified Chamomile Scheme[30].

4.4 Applying our scheme to the Hierarchical Tree Algorithm

Hierarchical tree algorithm[1] is one of useful algorithms which reduce the calculation cost from $O(N^2)$ to $O(N \log N)$. Recently, the hierarchical tree algorithm is widely used for investigating extremely large-scale cosmological simulations with billions of particles. In such simulations with extreme numbers, we can effectively use special-purpose hardwares for $O(N^2)$ interaction by use of the modified tree algorithm developed by Barnes (1990)[31], firstly used on GRAPE-1A by Makino (1990)[32], and recently used on GRAPE-6Af by Fukushige (2005)[21].

In the modified tree algorithm, not only the computing speed but also the communication speed between the host computer and the special-purpose hardware becomes very important, especially with the small number of particles (around several thousands of particles). In the modified tree algorithm, the GPU seems to be quite suitable because we can use quite high-speed link, the PCI-Express link. Using CUNBODY-1, the average transfer speed has got over 1.3 GByte/s with 2048 particles [33] through the beta version of NVIDIA’s driver, currently limiting up to 2.0 GByte/s in maximum.

4.5 Applying our scheme to other forms of interaction

To tell the truth, our CUNBODY-1 library is implemented as a general fashion to deal with arbitrary forms of interaction. We have already implemented libraries for other types of interaction not only for gravitational force but also for smoothed particle hydrodynamics(SPH) interactions, the time derivative of acceleration, gravitational potential, van der Waals molecular interactions, boundary element method (BEM) interactions, computer generated hologram(CGH) interactions and Kolmogorov-Smirnov test interactions, working with quite enough performance. We call such the generalized library as
CUNBODY (CUDA N-body)-1 kernel. Using CUNBODY-1 kernel, we can implement a function which deals with arbitrary function form of interaction just for users specifying the dimension of particles (i-particle, j-particle and the result of interactions) etc, and its pipeline description (the CUNBODY pipeline description). In appendix A, we present how we specify the dimension and how we specify the pipeline description by CUNBODY-1 kernel[30]. We are planning to release the CUNBODY-1 kernel under the license of GPL (GNU general Public License) soon.

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#define IDIM (4)
#define JDIM (4)
#define FDIM (3)

#include <cunbody_api.h>

static double p_xj[NMAX][JDIM];
static double p_xi[NMAX][IDIM];

void force(double xj[][3],
            double mj[],
            double xi[][3],
            double eps2,
            double a[][3],
            int ni,
            int nj)
{
    for(int i=0;i<ni;i++){
        for(int d=0;d<3;d++) p_xi[i][d] = xi[i][d];
        p_xi[i][3] = eps2;
    }
    for(int j=0;j<nj;j++){
        for(int d=0;d<3;d++) p_xj[j][d] = xj[j][d];
        p_xj[j][3] = mj[j];
    }

cunbody_api(p_xj, p_xi, a, ni, nj);
}

Fig. A.1. A CUNBODY-1 driver code for force function.

A  CUNBODY-1 user specified drivers and pipeline descriptions
#define IDIM (6)
#define JDIM (7)
#define FDIM (7)

#include <cunbody_api.h>

static double p_xj[NMAX][JDIM];
static double p_xi[NMAX][IDIM];
static double p_fi[NMAX][FDIM];

void force(double x[], int n)
{
    for(int i=0; i<n; i++)
    {
        for(int d=0; d<3; d++)
        {
            p_xi[i][d] = x[i][d];
            p_xi[i][d+3] = v[i][d];
            p_xj[i][d] = x[i][d];
            p_xj[i][d+3] = v[i][d];
        }
        p_xj[i][6] = m[i];
    }
    cunbody_api(p_xj, p_xi, p_fi, n, n);

    for(int i=0; i<n; i++)
    {
        for(int d=0; d<3; d++)
        {
            a[i][d] = p_fi[i][d];
            jk[i][d] = p_fi[i][d+3];
        }
        p[i] = p_fi[i][6];
    }
}

Fig. A.2. A CUNBODY-1 code for force, jerk and potential function.

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float eps2 = 1.0/(256.0*256.0);
float xj_0, xj_1, xj_2, xi_0, xi_1, xi_2, dx_0, dx_1, dx_2, dx2_0, dx2_1, dx2_2;
float vj_0, vj_1, vj_2, vi_0, vi_1, vi_2, dv_0, dv_1, dv_2, xv_0, xv_1, xv_2;
float r2, r1i, r2i, r3i, r5i, mj, mf, mr5i, mf3a, fx_0, fx_1, fx_2, pot;
float jk_0, jk_1, jk_2, jk1_0, jk1_1, jk1_2, jk2_0, jk2_1, jk2_2;

xi_0 = INPUT_I[0];
xi_1 = INPUT_I[1];
xi_2 = INPUT_I[2];
vi_0 = INPUT_I[3];
vi_1 = INPUT_I[4];
vi_2 = INPUT_I[5];

xj_0 = INPUT_J[0];
xj_1 = INPUT_J[1];
xj_2 = INPUT_J[2];
vj_0 = INPUT_J[3];
vj_1 = INPUT_J[4];
vj_2 = INPUT_J[5];
mj = INPUT_J[6];

dx_0 = xj_0 - xi_0;
dx_1 = xj_1 - xi_1;
dx_2 = xj_2 - xi_2;
dx2_0 = dx_0 * dx_0;
dx2_1 = dx_1 * dx_1;
dx2_2 = dx_2 * dx_2;
r2 = dx2_0 + dx2_1 + dx2_2 + eps2;
r1i = 1/sqrt(r2);
r2i = r1i * r1i;
r3i = r1i * r2i;
r5i = r2i * r3i;
mr5i = mj * r5i;
mf = mr5i * r2;
pot = mf * r2;
fx_0 = mf * dx_0;
fx_1 = mf * dx_1;
fx_2 = mf * dx_2;
dv_0 = vj_0 - vi_0;
dv_1 = vj_1 - vi_1;
dv_2 = vj_2 - vi_2;
jk1_0 = mf * dv_0;
jk1_1 = mf * dv_1;
jk1_2 = mf * dv_2;
xv_0 = dx_0 + dv_0;
xv_1 = dx_1 + dv_1;
xv_2 = dx_2 + dv_2;
mf3a = 3.0 * mr5i * (xv_0 + xv_1 + xv_2);
jk2_0 = mf3a * dx_0;
jk2_1 = mf3a * dx_1;
jk2_2 = mf3a * dx_2;

OUTPUT[0] += fx_0; // acc_x
OUTPUT[1] += fx_1; // acc_y
OUTPUT[2] += fx_2; // acc_z
OUTPUT[3] += jk_0; // jerk_x
OUTPUT[4] += jk_1; // jerk_y
OUTPUT[5] += jk_2; // jerk_z
OUTPUT[6] -= pot; // pot

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