Abstract

Commercial graphics processors (GPUs) have high compute capacity at very low cost, which makes them attractive for general purpose scientific computing. In this paper we show how graphics processors can be used for N-body simulations to obtain improvements in performance over current generation CPUs. We have developed a highly optimized algorithm for performing the $O(N^2)$ force calculations that constitute the major part of stellar and molecular dynamics simulations. In some of the calculations, we achieve sustained performance of nearly 100 GFlops on an ATI X1900XTX. The performance on GPUs is comparable to specialized processors such as GRAPE-6A and MDGRAPE-3, but at a fraction of the cost. Furthermore, the wide availability of GPUs has significant implications for cluster computing and distributed computing efforts like Folding@Home.

Keywords: Celestial Mechanics, N-Body Simulations, Stellar Dynamics, Molecular Dynamics, Molecular Simulation, Data Parallel Computing, Stream Computing, Programmable Graphics Hardware, GPU Computing, Brook

1 Introduction

The classical N-body problem consists of obtaining the time evolution of a system of N mass particles interacting according to a given force law. The problem arises in several contexts, ranging from molecular scale calculations in structural biology to stellar scale research in astrophysics.

Molecular dynamics (MD) has been successfully used to understand how certain proteins fold and function, which have been outstanding questions in biology for over three decades [Snow et al. 2005, Gomez et al. 2004]. Exciting new developments in MD methods offer hope that such calculations will play a significant role in future drug research [Fujitani et al. 2005]. In stellar dynamics where experimental observations are hard, if not impossible, theoretical calculations may often be the only way to understand the formation and evolution of galaxies.

Analytic solutions to the equations of motion for more than 2 particles or complicated force functions are intractable which forces one to resort to computer simulations. A typical simulation consists of a force evaluation step, where the force law and the current configuration of the system are used to compute the forces on each particle, and an update step, where the dynamical equations (usually Newton’s laws) are numerically stepped forward in time using the computed forces. The updated configuration is then reused to calculate forces for the next time step and the cycle is repeated as many times as desired.

The simplest force models are pairwise additive, that is the force of interaction between two particles is independent of all the other particles, and the individual forces on a particle add linearly. The force calculation for such models is of complexity $O(N^2)$. Since typical studies involve a large number of particles ($10^3$ to $10^6$) and the desired number of integration steps is usually very large ($10^6$ to $10^{15}$), the computational requirements often limit both the problem size as well as the simulation time and consequently, the useful information that may be obtained from such simulations. Numerous methods have been developed to deal with these issues. For molecular simulations, it is common to reduce the number of particles by treating the solvent molecules as a continuum. In stellar simulations, one uses individual time stepping or tree algorithms to minimize the number of force calculations. Despite such algorithmic approximations and optimizations, the computational capabilities of current hardware remain a limiting factor.

Typically N-body simulations utilize neighborlists, tree methods or other algorithms to reduce the order of the force calculations. Previous work [Elsen et al. 2005] demonstrated a GPU implementation of a neighbor list based method to compute non-bonded forces. However, since the GPU so far outperformed the CPU, the neighborlist creation quickly became a limiting factor. Building the neighborlist on the GPU is extremely difficult due to the lack of specific abilities (namely indirected
output) and research on computing the neighborlist on the GPU is still in progress. Other simplistic simulations that do not need neighborlist updates have been implemented by others [Juekuan Yang 2006]. However, for small N, we find we can do an $O(N^2)$ calculation significantly faster on the GPU than an $O(N)$ method using the CPU (or even with a combination of the GPU and CPU). This has direct applicability to biological simulations that use continuum models for the solvent. We note also that in many of the reduced order methods such as tree based schemes, at some stage an $O(N^2)$ calculation is performed on a subsystem of the particles, so our method can be used to improve the performance of such methods as well. When using GRAPE accelerator cards for tree based algorithms, the host processor takes care of building the tree and the accelerator cards are used to speed up the force calculation step; GPUs could be used in a similar way in place of the GRAPE accelerator boards.

Using the methods described below, we are able to accelerate the force calculation on GPUs over 25 times compared to highly optimized SSE code running on an Intel Pentium 4. This performance is in the range of the specially designed GRAPE-6A [Fukushige et al. 2005] and MGRAPE-3 [Tajji et al. 2003] processors, but uses a commodity processor at a much better performance/cost ratio.

2 Algorithm

General purpose CPUs are designed for a wide variety of applications and take limited advantage of the inherent parallelism in many calculations. Improving performance in the past has relied on increasing clock speeds and the size of high speed cache memories. Programming a CPU for high performance scientific applications involves careful data layout to utilize the cache optimally and careful scheduling of instructions.

In contrast, graphics processors are designed for intrinsically parallel operations, such as shading pixels, where the computations on one pixel are completely independent of another. GPUs are an example of streaming processors, which use explicit data parallelism to provide high compute performance and hide memory latency. Data is expressed as streams and data parallel operations are expressed as kernels. Kernels can be thought of as functions that transform each element of an input stream into a corresponding element of an output stream. When expressed this way, the kernel function can be applied to multiple elements of the input stream in parallel. Instead of blocking data to fit caches, the data is streamed into the compute units. Since streaming fetches are predetermined, data can be fetched in parallel with computation. We describe below how the N-body force calculation can be mapped to streaming architectures.

In its simplest form the N-body force calculation can be described by the following pseudo-code:

```plaintext
for i = 1 to N
   force[i] = 0
   for j = 1 to N
      rj = coordinates[j]
      force[i] = force[i] + force_function( ri, rj )
   end
end
```

The kernel `kforce` is applied to each element of the stream `coordinates` to produce an element of the `forces` stream. Note that the kernel can perform an indexed fetch from the `coordinates` stream inside the j-loop. An out-of-order indexed fetch can be slow, since in general, there is no way to prefetch the data. However in this case the indexed accesses are sequential. Moreover, the j-loop is executed simultaneously for many i-elements; even with minimal caching, rj can be reused for many N i-elements without fetching from memory thus the performance of this algorithm would be expected to be high. The implementation of this algorithm on GPUs and GPU-specific performance optimizations are described in the following section.

There is however one caveat in using a streaming model. Newton’s Third law states that the force on particle i due to particle j is the negative of the force on particle j due to particle i. CPU implementations use this fact to halve the number of force calculations. However, in the streaming model, the kernel has no ability to write an out-of-sequence element (scatter), so `forces[j]` can not be updated while summing over the j-loop to calculate `forces[i]`. This effectively doubles the number of computations that must be done on the GPU compared to a CPU.

Several commonly used force functions were implemented to measure and compare performance. For stellar dynamics, depending on the integration scheme being used, one may need to compute just the forces, or the forces as well as the time derivative of the forces (jerk). We have designated the corresponding kernels `GA` (Gravitational Acceleration) and `GAJ` (Gravitational Acceleration and Jerk). In molecular dynamics,
it is not practical to use \( O(N^2) \) approaches when the solvent is treated explicitly, so we restrict ourselves to continuum solvent models. In such models, the quantum interaction of non-bonded atoms is given by a Lennard-Jones function and the electrostatic interaction is given by Coulomb’s Law suitably modified to account for the solvent. The \( \text{LJC}(\text{constant}) \) kernel calculates the Coulomb force with a constant dielectric, while the \( \text{LJC}(\text{linear}) \) and \( \text{LJC}(\text{sigmoidal}) \) kernels use distance dependent dielectrics. The equations used for each kernel as well as the arithmetic complexity of the calculation are shown in Table 1.

3 Implementation and Optimization on GPUs

3.1 Brook

BrookGPU [Buck et al. 2004] is a C-like high-level language that can be used to program GPUs as streaming processors. Streams are stored as textures and kernels are implemented as fragment programs. The BrookGPU run-time library can utilize a number of graphics interfaces; for this work we used the Microsoft DirectX 9.0c API and the Pixel Shader 3.0 specification Microsoft 2006. DirectX Microsoft 2003 provides a vendor-independent abstraction of hardware features. In the Pixel Shader 3.0 specification, the shader has access to 32 general purpose, 4-component, single precision floating point (float4) registers, 16 float4 input textures, 4 float4 render targets (output streams) and 32 float4 constant registers. A shader consists of a number of assembly-like instructions. Current GPUs have a maximum static program length of 512 (ATI) or 1024 (NVIDIA) instructions. There is a loop limit of 255 iterations of a loop body, but loops can be nested to increase the total numbers of iterations. NVIDIA is limited to 65,535 dynamic instructions and ATI can support an unlimited number. The BrookGPU compiler translates kernels into a high level shader language like CG or HLSL, which is then compiled into pixel shader assembly by an appropriate shader compiler like Microsoft’s fxc or NVIDIA’s cgc. The graphics driver finally maps the Pixel Shader assembly code into hardware instructions as appropriate to the architecture.

3.2 Precision

Recent graphics boards have 32-bit floating point arithmetic. Consequently we have done all the calculations in single precision. Whether or not this is sufficiently accurate for the answers being sought from the simulation is often a subject of much debate and the authors do not intend to settle it here. We are of the opinion that in many cases, though certainly not all, single precision is enough to obtain useful results. Furthermore, if double precision is necessary, it is usually not required throughout the calculation, but rather only in a select few instances. For reference, GRAPE-6 [Makino et al. 2003] performs the accumulation of accelerations, subtraction of position vectors and update of positions in 64-bit fixed point arithmetic with everything else in either 36, 32 or 29 bit floating point precision. It is quite common to do the entire force calculation in single precision for molecular simulations while using double precision for some operations in the update step. If and where necessary, the appropriate precision could be emulated on graphics boards [Göddeke et al. 2005]. The impact on performance would depend on where and how often it would be necessary to do calculations in double precision.

3.3 General Optimization

The algorithm was implemented for several force models. For simplicity, in the following discussion, we only talk about the GA kernel, which corresponds to the gravitational attraction between two mass particles, given by

\[
\mathbf{a}_i = -G \sum_{j \neq i} \frac{m_j}{r_{ij}^2 + \epsilon^2} r_{ij}
\]

where \( \mathbf{a}_i \) is the acceleration on particle \( i \), \( G \) is a constant (often normalized to one), \( m_j \) is the mass of particle \( j \), and \( r_{ij} \) is the vector displacement between particles \( i \) and \( j \). The performance of the kernel for various input sizes are shown in Figure 1.

The algorithm outlined in Section 2 was implemented in BrookGPU and targeted for the ATI X1900XTX. Even this naive implementation performs very well, achieving over 40 GFlops, but its performance can be improved. This kernel executes 48 Giga-instructions/sec and has a memory bandwidth of 33 GB/sec. Using information from GPUBench [Buck et al. 2004], we expect the X1900XTX to be able to execute approximately 30-50 Giga-instruction/sec (it depends heavily on the pipelining of commands) and have a cache memory bandwidth of 41GB/sec. The nature of the algorithm is such that almost all the memory reads will be from the cache since all the pixels being rendered at a given time will be accessing the same j-particle. Thus this kernel is limited by the rate at which the GPU can issue instructions (compute bound).

To achieve higher performance, we used the standard technique of loop unrolling. This naive implementation is designated as a 1×1 kernel because it is not unrolled in either \( i \) or \( j \). The convention followed hereafter when designating the amount of unrolling will be that \( A \times B \) means \( A \) unrolled \( A \) times and \( j \) unrolled \( B \) times. The second GA kernel (1×4) which was written unrolled the
| Kernel                | Formula                                                                 | Flops per Intrxn. | Unroll | Input (bytes) | Inner Loop Insns. | BW (GB/s) | Useful GFLOPS | Giga Intrxn per sec | System Size |
|-----------------------|--------------------------------------------------------------------------|--------------------|--------|---------------|-------------------|-----------|---------------|---------------------|-------------|
| Gravity (accel)       | \( \frac{m_j}{(r_{ij}^2 + \xi^2)^{3/2}} r_{ij} \)                      | 19                 | 4x4    | 64            | 125               | 19.9      | 94.3          | 4.97                | 65,536      |
| Gravity (accel & jerk)| \( m_j \left[ \frac{v_{ij}}{(r_{ij}^2 + \xi^2)^{3/2}} - 3 \frac{(r_{ij} v_{ij})}{r_{ij}^3 (r_{ij}^2 + \xi^2)^{5/2}} \right] \) | 42                 | 1x4    | 128           | 104               | 40.6      | 53.5          | 1.27                | 65,536      |
| LJC (constant)        | \( \frac{q_i q_j}{r_{ij}} r_{ij} + \xi_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 - \left( \frac{\sigma_{ij}}{\xi} \right)^{12} \right] \) | 30                 | 2x4    | 104           | 109               | 33.6      | 77.6          | 2.59                | 4096        |
| LJC (linear)          | \( \frac{q_i q_j}{r_{ij}} r_{ij} + \xi_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 - \left( \frac{\sigma_{ij}}{\xi} \right)^{12} \right] \) | 30                 | 2x4    | 104           | 107               | 34.5      | 79.5          | 2.65                | 4096        |
| LJC (sigmoidal)       | \( \xi_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 - \left( \frac{\sigma_{ij}}{\xi} \right)^{12} \right] \) | 43                 | 2x4    | 104           | 138               | 27.3      | 90.3          | 2.10                | 4096        |

Table 1: Values for the maximum performance of each kernel on the X1900XTX. The instructions are counted as the number of pixel shader assembly arithmetic instructions in the inner loop. Intrxn = Interaction; Insns = Instructions; BW = Bandwidth.

Figure 1: GA Kernel with varying amounts of unrolling j-loop four times, enabling the use of the 4-way SIMD instructions on the GPU. This reduces instructions that must be issued by around a factor of 3. (We cannot reduce instructions by a factor of 4 because some Pixel Shader instructions are scalar). The performance for this kernel is shown in Figure 1. It achieves a modest speedup compared to the previous one, and we have now switched from being compute bound to bandwidth bound (35 Giga-Instructions/sec and ≈40GB/sec).

Further reducing bandwidth usage is somewhat more difficult. It involves using the multiple render targets (MRT) capability of recent GPUs which is abstracted as multiple output streams by BrookGPU. By reading in 4 i-particles into each kernel invocation and outputting the force on each into a separate output stream, we reduce by a factor of four the size of each output stream compared with original. This reduces input bandwidth requirements to one quarter of original bandwidth because each j-particle is only read by one-quarter as many fragments. To make this more clear, we show the pseudo-code for this kernel below. This kernel is designated as a 4x4 kernel.

```
stream coordinates;
stream index = range( 1 to N skip 4 );
stream forces1, forces2, forces4, forces4;
kernel kforce4x4( i )
force1 = 0
force2 = 0
force3 = 0
force4 = 0
ri1 = coordinates[i]
ri2 = coordinates[i+1]
ri3 = coordinates[i+2]
ri4 = coordinates[i+3]
for j = 1 to N skip 4
  rj1 = coordinates[j]
  rj2 = coordinates[j+1]
  rj3 = coordinates[j+2]
  rj4 = coordinates[j+3]
  force1 += force_function4( ri1, rj1, rj2, rj3, rj4 )
  force2 += force_function4( ri2, rj1, rj2, rj3, rj4 )
  force3 += force_function4( ri3, rj1, rj2, rj3, rj4 )
  force4 += force_function4( ri4, rj1, rj2, rj3, rj4 )
end
return force1, force2, force3, force4
end kernel
forces1, forces2, forces3, forces4 = kforce4x4( indices )
```

In the above code, the input is the sequence of integers 1, 5, 9, ..., N and the output is 4 force streams. force_function4 uses the 4-way SIMD math available on the GPU to compute 4 forces at a time. The four output streams can be trivially merged into a single one if needed. Results for this kernel can be seen in Figure 1.
Once more the kernel has become instruction-rate limited and its bandwidth is half that of the maximum bandwidth of the ATI board, but the overall performance has increased significantly.

### 3.4 Optimization for small systems

In all cases, performance is severely limited when the number of particles is less than about 4000. This is due to a combination of fixed overhead in executing kernels and the lack of sufficiently many parallel threads of execution. It is sometimes necessary to process small systems or subsystems of particles ($N \approx 100 - 1000$).

For example, in molecular dynamics where forces tend to be short-range in nature, it is more common to use $O(N)$ methods by neglecting or approximating the interactions beyond a certain cutoff distance. However, when using continuum solvent models, the number of particles is small enough ($N \approx 1000$) that the $O(N^2)$ method is comparable in complexity while giving greater accuracy than $O(N)$ methods.

It is common in stellar dynamics to parallelize the individual time step scheme by using the block time step method [McMillan 1986]. In this method forces are calculated on only a subset of the particles at any one time. In some simulations a small core can form such that the smallest subset might have less than 1000 particles in it. To take maximal advantage of GPUs it is therefore important to get good performance for small output stream sizes.

To do this, we can increase the number of parallel threads by decreasing the j-loop length. For example, the input stream can be replicated twice, with the j-loop looping over the first $N/2$ particles for the first half of the replicated stream and looping over the second $N/2$ particles for the second half of the stream. Consider the following pseudocode that replicates the stream size by a factor of 2:

```plaintext
stream coordinates;
stream indices = range( 1 to 2N );
stream partial_forces;

kernel kforce( i )
    force = 0
    if i <= N:
        ri = coordinates[i]
        for j = 1 to N/2
            rj = coordinates[j]
            force = force + force_function( ri, rj )
        end
    else
        ri = coordinates[i-N+1]
        for j = N/2+1 to N
            rj = coordinates[j]
            force = force + force_function( ri, rj )
        end
    endif
    return force
end kernel

partial_forces = kforce( indices )
```

In this example, the stream `indices` is twice as long as the `coordinates` stream and contains integers in sequence from 1 to 2N. After applying the kernel `kforce` on `indices` to get `partial_forces`, the force on particle $i$ can be obtained with by adding `partial_forces[i]` and `partial_forces[i+N]`, which can be expressed as a trivial kernel. The performance of the LJC(sigmoidal) kernel for different number of replications of the i-particles is shown in Figure 2 for several system sizes.

### 4 Results

All kernels were run on an ATI X1900XTX PCIe graphics card on Dell Dimension 8400 with ATI Catalyst version 7.2 drivers and the latest DirectX SDK (December 2006). A number of different force models were implemented with varying compute-to-bandwidth ratios (see Table 1). A sample code listing is provided in the appendix [A.1] to show the details of how flops are counted.

To compare against the CPU, a specially optimized version of the GA and GAJ kernels were written since no software suitable for a direct comparison to the GPU existed. The work of [Nitadori et al. 2005] uses SSE for the GAJ kernel but does some parts of the calculation in double precision which makes it unsuitable for a direct comparison. The performance they achieved is comparable to the performance achieved here. Using SSE intrinsics and Intel’s C++ Compiler v9.0, we were able to obtain sustained performance of 3.8 GFlops on a 3.0 GHz Pentium 4.

GROMACS [Lindahl et al. 2001] is currently the fastest performing molecular dynamics software with hand-written SSE assembly loops. As mentioned in Section 2 the CPU can do out-of-order writes without a significant penalty. GROMACS uses this fact to halve the number of calculations needed in each force calculation step. In the comparison against the GPU in Table 2 the interactions per second as reported by GROMACS have
been doubled to reflect this. In MD it is common to use neighborlists to reduce the order of the force computation to $O(N)$. The performance of GROMACS doing an $O(N^2)$ calculation as well as an $O(N)$ calculation for a 80 residue protein (lambda repressor, 1280 atoms) is shown in Table2. Despite using a fairly modest cutoff length of 1.2 nm for the $O(N)$ calculation, the $O(N^2)$ GPU calculation represents an order-of-magnitude performance improvement over existing methods on CPUs.

5 Discussion

5.1 Comparison to other Architectures

In Figure 3 is a comparison of interactions/sec between the ATI X1900XTX, GRAPE-6A and a Pentium 4 3.0GHz. The numbers for the GPU and CPU are observed values, those for GRAPE-6A are for its theoretical peak. Compared to GRAPE-6A, the GPU can calculate over twice as many interactions when only the acceleration is computed, and a little over half as many when both the acceleration and jerk are computed. The GPU bests the CPU by 35x, 39x and 15x for the GA, LJC(constant) and GAJ kernels respectively.

Another important metric is performance per unit of power dissipated. These results can be seen in Figure 5. Here the custom design and much smaller on-board memory allows GRAPE-6A to better the GPU by a factor of 4 for the GAJ kernel, although they are still about equal for the GA kernel. The power dissipation of the Intel Pentium 4 3.0 GHz is 82W [Intel 2006], the X1900XTX is measured to be 85W, we estimate GRAPE-6A's dissipation to be 48W since each of the 4 processing chips on the board dissipates approximately 12W [Makino et al. 2003b] and MDGRAPE-3's (MD3-PCIX) dissipation is 40W [Peta Computing Institute 2006].

The advantages of the GPU become readily apparent when the metric of performance per dollar is examined (Figure 4). The current price of an Intel Pentium 4 630 3.0GHz is $100, an ATIX1900XTX is $350, and an MDGRAPE-3 board costs $16000 [Peta Computing Institute 2006]. The GPU outperforms GRAPE-6A by a factor of 22 for the GA kernel and 6 for the GAJ kernel.

5.2 Hardware Constraints

The $4 \times 4$ unrolling that is possible with the GA kernel does not work for the other, more complicated kernels. For example, the GAJ kernel requires two outputs per particle (jerk in addition to acceleration). This reduces the maximum unrolling possibility to $2 \times 4$ because the GPU is limited to a maximum of 4 outputs per kernel. However, even this amount of unrolling doesn’t work...
Table 2: Comparison of GROMACS (GMX) running on a 3.2 GHz Pentium 4 vs. the GPU showing the simulation time per day for an 80 residue protein (lambda repressor) *GROMACS does not have an SSE inner loop for LJC(linear)

| Kernel              | GMX Million Interactions/sec | GMX \( O(N^2) \) ns/day | GMX \( O(N) \) ns/day | GPU Million Interactions/sec | GPU ns/day |
|---------------------|------------------------------|--------------------------|------------------------|-----------------------------|------------|
| LJC(constant)        | 66                           | 5.6                      | 18.2                   | 1327                        | 140        |
| LJC(linear)*         | 33                           | 2.06                     | 9.08                   | 1327                        | 140        |
| LJC(sigmoidal)       | 40                           | 2.5                      | 11                     | 1203                        | 127        |

because the compiler cannot fit the kernel within the 32 available registers. The number of registers is also what prevents the LJC kernels from being unrolled by \( 4 \times 4 \) instead of \( 2 \times 4 \).

This apparent limitation due to the number of registers appears to result from compiler inefficiencies; the authors are currently hand coding a \( 2 \times 4 \) GAJ kernel directly in pixel shader assembly which should cause the kernel to become compute bound and greatly increase its performance. The performance gain of unrolling the LJC kernels to \( 4 \times 4 \) by rewriting them in assembly would most likely be small since these kernels are already compute bound.

While the maximum texture size of \( 4096 \times 4096 \) and 512 MB would make it possible to store up to 16 million particles on the board at a time, this really isn’t necessary. In fact, GRAPE-6A only has storage for 131,000 particles on the board at any one time. This is small enough to occasionally seem restrictive - a good balance is around 1 million particles which could easily be accommodated by 64MB. If board manufacturers wanted to produce cheaper boards specifically for use in these kinds of computations they could significantly reduce the cost without affecting the functionality by reducing the amount of onboard RAM.

The current limits on the number of instructions also impacts the efficiency of large GPGPU programs. On ATI hardware, the maximum shader length of 512 instructions limits the amount of loop unrolling and the complexity of the force functions we can handle.

5.3 On-board Memory vs. Cache Usage

As mentioned in Section 5.3 we expect the kernels to make very efficient use of the cache on the boards. There is a maximum of 512 threads in flight on the ATI X1900XTX at any one time [ATT 2006], and in the ideal situation, each of these threads will try and access the same j-particle at approximately the same time. The first thread to request a j-particle will miss the cache and cause the particle to be fetched from on-board memory, however once it is in the cache, all the threads should be able to read it without it having to be fetched from on-board memory again.

For example, in the case of the GA kernel with 65,536 particles, there would be 16,384 fragments to be processed, and if fragments were processed in perfectly separate groups of 512, then 32 groups would need to be processed. Each group would need to bring in 65,536 particles from main memory to the cache resulting in an extremely low memory bandwidth requirement of 38.2 MB/sec.

Of course, the reality is that particles are not processed in perfectly separate groups of 512 particles that all request the same particle at the same time, but by using ATI Tool [ATT 2000] to adjust the memory clock of the board we can determine how much bandwidth each kernel actually needs to main memory. The results of this testing can be seen in Figure 6.

The performance degradation occurs at approximately 11.3, 5.2, and 2.1 GB/sec for the LJC, GAJ and GA kernels respectively. The LJC kernels must also read in an exclusion list for each particle which does not cache as well as the other reads, and is the reason why their bandwidth to main memory is higher than that of the gravity kernels. The number for the GA kernel suggests that approximately 10 particles are accessing the same j-particle at once.

At memory speeds above 500MHz all the kernels run very near their peak speed, thus board manufacturers could not only use less RAM, they could also use cheaper RAM if they were to produce a number of boards that would only be used for these calculations. This would reduce the cost and power requirements over the standard high end versions used for gaming.
5.4 Distributed Computation

Most biological phenomena of interest occur on timescales currently beyond the reach of MD simulations. For example, the simplest proteins fold on a timescale of 5 to 20 microseconds, while more complex proteins may take milliseconds to seconds. MD simulations on current generation CPUs are usually limited to simulating about 10 nanoseconds per day - it would take several years to obtain a 10 microsecond simulation. However, with the speed increases afforded by the algorithms and hardware discussed here, we are now be able to simulate protein dynamics with individual trajectories on the 10 microsecond timescale in under three months. This will allow the direct simulation of the folding of fast-folding proteins. Moreover, by incorporating this methodology into a distributed computing framework, we are now situated to build Markovian State Models to simulate even longer timescales, likely approaching seconds [Jaychandran et al. 2006]. Thus with the combined effort of GPUs and distributed computing, one would be able to reach timescales of essentially all single-domain, two-state folding proteins. Compared to the donations of CPUs from over 150,000 Windows computers currently producing 145 TFlops, we have 550 GPUs donated to the project producing over 34 TFlops. Thus each GPU is providing roughly 60 times the performance of the average donated x86 CPU.

6 Conclusion

We have successfully taken advantage of the processing power available on GPUs to accelerate pairwise force calculations for several commonly used force models in stellar and molecular dynamics simulations. In some cases the GPU is more than 25 times as fast as a highly optimized SSE-based CPU implementation and exceeds the performance of custom processors specifically designed for these tasks such as GRAPE-6A. Furthermore, our performance is compute bound, so we are well poised to take advantage of further increases in the number of ALUs on GPUs, even if memory subsystem speeds do not increase significantly. Because GPUs are mass produced, they are relatively inexpensive and their performance to cost ratio is an order of magnitude better than the alternatives. The wide availability of GPUs will allow distributed computing initiatives like Folding@Home to utilize the combined processing power of tens of thousands of GPUs to address problems in structural biology that were hitherto computationally infeasible. We believe that the future will see some truly exciting applications of GPUs to scientific computing.

A Appendix

A.1 Flops Accounting

To detail how we count flops we present a snippet of the actual Brook code for the GA kernel. The calculation of the acceleration on the first i-particle has been commented with our flop counts for each instruction. In total, the calculation of the acceleration on the first i-particle performs 76 flops. Since four interactions are computed, this amounts to 19 flops per interaction.

```c
float3 d1, d2, d3, d4, outaccel1;
float4 jmass, r, rinv, rinv cubed, scalar;
d1 = jpos1 - ipos1; //3
d2 = jpos2 - ipos1; //3
d3 = jpos3 - ipos1; //3
d4 = jpos4 - ipos1; //3
r.x = dot( d1, d1 ) + eps; //6
r.y = dot( d2, d2 ) + eps; //6
r.z = dot( d3, d3 ) + eps; //6
r.w = dot( d4, d4 ) + eps; //6
rinv = rsqrt( r ); //4
rinv cubed = rinv * rinv * rinv; //8
scalar = jmass * rinv cubed; //4
outaccel1 += scalar.y * d2 + scalar.z * d3 + scalar.w * d4; //18
if ( Ilist.x != Jlist1.x ){ //don't add force due to ourself
outaccel1 += scalar.x * d1; //6
}
```

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