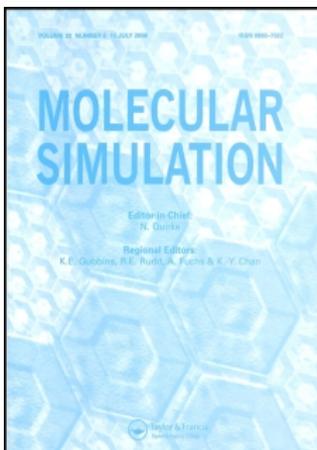


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Harvesting graphics power for MD simulations

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We discuss an implementation of molecular dynamics (MD) simulations on a graphic processing unit (GPU) in the NVIDIA CUDA language. We tested our code on a modern GPU, the NVIDIA GeForce 8800 GTX. Results for two MD algorithms suitable for short-ranged and long-ranged interactions, and a congruential shift random number generator are presented. The performance of the GPU's is compared to their main processor counterpart. We achieve speedups of up to 40, 80 and 150 fold, respectively. With the latest generation of GPU's one can run standard MD simulations at 10⁷ flops/\$.

Keywords: molecular dynamics simulation; GPGPU; random number generator

1. Introduction

Over the last 30 years computer simulations have become an important tool in materials science, often bridging the gap between theory and experiment. Simulations can be used both to predict the outcome of experiments and to test the assumptions of theories. The basic idea of most classical simulations is to calculate the forces acting on all particles, and then integrate Newton's equations of motion using these forces. This approach is not limited to single atoms or molecules: the same approach can be used to model the motion of stars within galaxies.

With the rapid increase of available computational power, more systems become tractable for simulations. Nowadays it is possible to simulate the time evolution of simple molecules over microseconds with atomistic detail on a conventional personal computer. However, for many systems, the computational power of a single processor (CPU) is not sufficient. In this case, simulations are run in parallel on many processors, which allows us to simulate hundreds of thousands of molecules over time-spans of milliseconds. The increase of computational power comes at a price: the different processors have to exchange information on the simulated system continuously. This communication costs time, reducing the effective performance of a parallel system to typically less than 80% [1,2] of the total performance of all its individual CPUs. And although there are standardised software tools for the implementation of this communication, such as PVM [3], MPI [4] or OpenMP [5], writing a code for parallel execution is not trivial. Moreover, the necessary very low

latency, high throughput communication hardware often costs as much as the processing units themselves.

An alternative approach speeds up the simulations by using special purpose hardware. For example, in simulations of stars or charged molecules, more than 90% of the computation time is typically spent on the calculation of the gravitational or electrostatic interaction. Most prominently, the GRAPE board [6] is a special purpose hardware designed to calculate such interactions; recently, a variant called MDGRAPE [7] has been put forward to calculate the interactions of more general pair potentials. Due to their specificity, these boards can achieve several orders of magnitude higher throughput compared to conventional CPUs, but are only of interest for a limited community of researchers. This makes these boards relatively expensive and their development cycle long.

Since 2003, a new route to gain additional computational power has opened: the graphics processors (graphic processing units, GPUs) of recent PC hardware have become general purpose processors, which can be programmed using C-like programming environments such as the GL shader language [8], C for graphics (Cg) [9] or the NVIDIA compute unified device architecture (CUDA) [10]. Their computational power exceeds that of the CPU by orders of magnitude: while a conventional CPU has a peak performance of around 20 Gigafllops, a NVIDIA GeForce 8800 Ultra reaches theoretically 500 Gigafllops. This means, that 4 graphics cards can replace a complete 64 processor PC cluster, saving space and reducing the necessary power supply from 15 kW to around 2 kW. Moreover, graphics processors follow a Moore-law with a computational power doubling every 9

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months, in contrast to 18 months for conventional CPUs. For the end of 2007, the first Teraflops-cards are expected.

There have been early attempts to harvest this computational power for various applications, including fast Fourier transforms [11], matrix operations [12], lattice Boltzmann simulations [13] or Monte Carlo (MC) simulations of the 2D Ising model [14]. Recently, Portegies Zwart *et al.* [15,16] presented a N -body simulation with gravitational interactions, where the force calculation was performed on the GPU. For the latter application, the graphics cards are in direct competition with the GRAPE boards, and achieve similar performances at much lower costs and higher reliability. Yang *et al.* already presented a proof-of-concept molecular dynamics (MD) simulation for the thermal conductivity of solid argon [17]; their implementation is however limited to the simulation of defect-free solids.

In this article, we aim to assess the portability of classical molecular simulation systems onto GPUs using NVIDIA's CUDA [10]. Unlike the previous attempts of putting only the computationally most expensive parts of the simulation onto the graphics cards, we demonstrate that in fact the entire simulation can be ported to the graphics cards. The resulting program reproduces all data obtained from a standard single-processor simulation. We report benchmarks of three codes: two simulating the classical "work-horse" of coarse-grained molecular simulation, the Lennard-Jones system, and a classical rand48 random number generator [18]. We tested these codes on a system consisting of an Intel Xeon CPU running at 3.2 GHz and a NVIDIA GeForce 8800 GTX (16 multiprocessors (MPs), running at 675 MHz each). For

both the simulation and the calculation of random numbers, we achieve an about 25- to 150-times speedup using the GPU compared to the CPU.

1.1 GPU architecture

To facilitate the discussion on the technical implementations, it is necessary to briefly summarise the key aspects of the GPU's hardware architecture and its nomenclature (see also Figure 1). We use the NVIDIA CUDA system for programming the GPU, which allows to write functions for the GPU, so-called *kernels*, in a C-like language. For detailed information we refer to NVIDIA CUDA programming guide [10].

The NVIDIA GeForce 8800 GTX consists of 16 MPs. Each MP has a single-instruction-multiple-data (SIMD) architecture and is capable of performing the same operation on different data 32 times per two clock cycles. Many copies of a kernel, so-called *threads*, are executed in parallel on all available MPs on the GPU. To fit the SIMD architecture, groups of 32 threads form a *warp* which is executed on the same MP. If a kernel contains a branch and threads of the same warp take different routes, then both routes are executed sequentially and the total run time is the sum of both branches. This *warp divergence* can have a serious impact on performance.

Threads can store data in 8192 32-bit registers per MP, and a high-speed *shared memory* of 16 kB per MP is available to share data among threads running on the same MP. For this, threads are grouped into *blocks* of up to 512 threads which are forced to run on the same MP. A

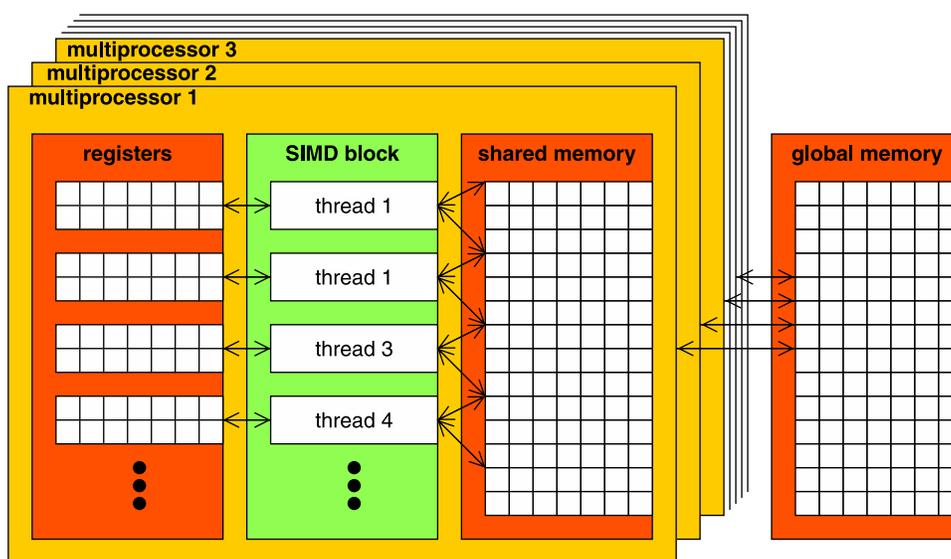


Figure 1. Schema of the multiprocessor and memory organisation of current NVIDIA GPUs. While registers are bound to a thread, all threads of the same SIMD block have access to a common shared memory, and all threads on all MPs have access to the global memory.

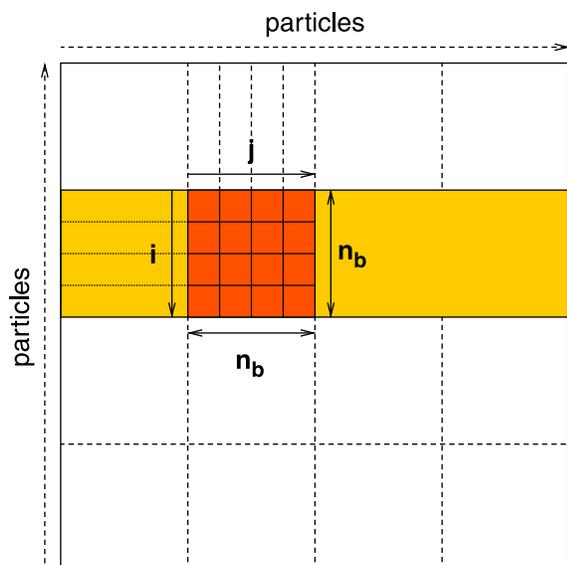


Figure 2. Schema of the splitting of the force calculation into blocks. Each of the n_b threads is dedicated to calculating all interactions of particle i . All particles j are loaded in blocks of again n_b particles, which are then shared among all threads.

slower *global memory* of 768 MB is also available that is shared among all MPs. To hide register read–write latencies of one to two clock cycles, it is recommended that block sizes of 192 or more threads be used, and more than one block per MP should be scheduled in order to hide the much larger global memory read latencies of 200 to 400 clock cycles. Note however, that GPU global memory is still ten times faster than the main memory of recent PCs.

As a final remark we point out that nowadays graphics hardware only supports single precision floating point arithmetic. This might not suffice for systems where energy conservation is crucial. But for systems in thermal equilibrium, i.e. with a stochastic thermostat, this forms no limitation.

2. N-squared MD

We start with the most simple MD algorithm in which each particle interacts with all other particles. Therefore, the total force calculation scales quadratic with the particle number N . The force \vec{f}_i on a particle i is given by

$$\vec{f}_i = - \sum_{\substack{j=1 \\ j \neq i}}^N f(|\vec{r}_j - \vec{r}_i|) \frac{\vec{r}_j - \vec{r}_i}{|\vec{r}_j - \vec{r}_i|}, \quad (1)$$

where $f(r)$ is the well-known Lennard–Jones pair force, truncated at a distance $r_c = 2.5\sigma$ and shifted such that the force at the cutoff distance was zero. The full Lennard–

Jones pair force is given by

$$f_{\text{LJ}}(r) = 24\epsilon \left[2 \left(\frac{\sigma}{r} \right)^{13} - \left(\frac{\sigma}{r} \right)^7 \right], \quad (2)$$

our truncated and shifted force by

$$f(r) = \begin{cases} f_{\text{LJ}}(r) - f_{\text{LJ}}(r_c) & r < r_c \\ 0 & r \geq r_c \end{cases}. \quad (3)$$

The Velocity Verlet algorithm was applied to integrate Newton’s equations of motion [19].

2.1 Implementation details

A MD simulation is naturally suited for a SIMD architecture, because it performs the same set of operations on each particle. The most simple way to parallelise this algorithm is to have one independent thread per particle. However, naively implementing Equation (1) turns out to be far from efficient. The reason for this is that every thread loads all particle positions from global memory, which is not cached. Each read access comes with some latency, causing the processor to idle until the data arrives. A huge improvement can be achieved by taking advantage of the fact that all threads need the same data. By grouping threads into blocks, data can be shared among them, effectively reducing memory bandwidth and idle times.

Our implementation works as follows: each thread loads one different particle from global memory and stores it into shared memory. Then all threads of a block are synchronised to ensure loading has finished. Now the data of all threads are accessible through high-speed shared memory, and each thread can calculate the interactions of its dedicated particle with all other particles in shared memory (see Figure 2). For a block of n_B threads, this reduces memory bandwidth by a factor $1/n_B$. In addition, each thread can now compute more interactions per memory read, allowing the thread scheduler to more efficiently hide global memory latencies. The optimal block size depends on the resources used by the kernel: number of registers and shared memory size. A block size of $n_B = 64$ turned out to be the optimal choice for our program. For details about the interplay between register usage, shared memory usage, block size and number of blocks per MP, we refer to NVIDIA’s CUDA programming guide [10].

2.2 Results

To compare the performance of the GPU and CPU implementations on our test system, we measured the time required to integrate a single MD time step as a function of

system size N . The speedup factor x is defined as

$$x = \frac{T_{\text{CPU}}}{T_{\text{GPU}}}, \quad (4)$$

where T_{CPU} is the time used by the CPU implementation and T_{GPU} the time used by the GPU implementation. In addition to the GPU implementation with CUDA, we also present results from a GPU implementation in Cg [9], a language designed for graphic processing. It is supported by the majority of current graphics hardware, but does not provide the flexibility required for more complex MD algorithms.

The left graph in Figure 3 shows the average time used to integrate a single MD time step. The quadratic scaling of run time with system size is clearly visible for the CPU version. For the GPU code at small system sizes, the overhead of invoking the graphic program is comparable to the actual computation time. Therefore, the quadratic scaling regime is reached when this overhead becomes negligible, which corresponds to a system size of approximately 4000 particles.

The speedup factor for the GPU implementation is depicted in the right graph in figure 3. Although the GPU version is faster for all our system sizes, it requires a system size larger than 4000 particles to reach its full speedup of around 80.

3. Cell-lists MD

If the pair interaction is short-ranged, the simulation box is typically decomposed into smaller domains, so-called cells, with a side length equal to or greater than the maximum interaction range. For a given particle, all interaction partners are then located in the same and directly neighbouring cells. Therefore, the algorithm scales linearly with the number of particles, but suffers some

penalty due to the overhead associated with maintaining the cell structure. For small systems, this might be disadvantageous compared to the N -squared algorithm, but for large systems it generally results in a huge performance gain. The system size at which both algorithms perform equally well is called *break-even point*.

Another way of optimisation are the so-called Verlet lists. For each particle, a list holds all neighbour particles within a sphere of $r_V = r_c + \Delta r$, the Verlet radius. The Verlet lists *skin* with width Δr prevents particles to move into interaction range unnoticed and generally acts as an invalidation criterion. Every time a particles list is updated, the particles current position is stored as Verlet list centre. If this particle moved further than $\Delta r/2$ away from its Verlet list centre, the list has expired and needs to be rebuild. Obviously, the larger Δr , the less frequent the lists have to be updated, but the more unnecessary interactions with $r > r_c$ have to be computed. Updating Verlet lists is rather expensive and scales like $O(N^2)$. Therefore, cell lists are often used to reduce its costs to $O(N)$. Compared to cell lists, Verlet lists further reduce the number of possible interaction partners and result in a theoretical seven fold speedup.

Yang *et al.* [17] used the Verlet lists approach to compute the thermal conductivities in solid argon on a GPU. However, their Verlet lists were computed only once (on the CPU) and never updated, which restricts its use to defect-free solids. To fit the SIMD architecture, they added virtual particles to obtain the same list size for all particles. Moreover, to avoid inner-loop branching which deteriorates the performance, the interaction cutoff distance was set to the Verlet list radius r_V . In doing so, they removed the essential skin from their Verlet lists allowing interactions due to fluctuations to be ignored. This shows that Verlet lists are not particularly suited for a SIMD architecture. The MD code of [17] is therefore useful as a proof of concept, but cannot be used for production runs.

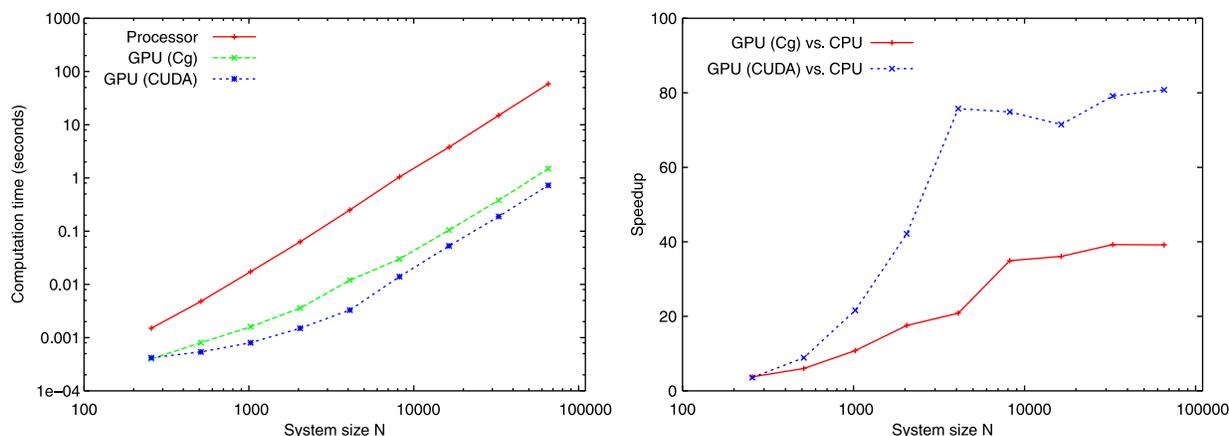


Figure 3. Left: Time (in seconds) required to integrate a single MD time step as a function of system size N . Right: Speedup factor for both GPU implementations, Cg and CUDA. The speedup saturates once both the processor and GPU versions have reached the quadratic scaling regime.

In our program we applied only cell lists. They seem more suitable for the hardware architecture and could be implemented to run entirely on the GPU. Care was taken not to neglect any interactions and to include cell list updates.

3.1 Implementation details

There are plenty of schemes to implement the cell lists technique [19]. One approach uses one linked list per cell to store the identities of the particles located in it. The advantage is that this scheme works well for all densities without parameter modifications, because there are no size limitations on a linked list. The disadvantage is that memory access is random, not sequential, and therefore a linked list cannot be loaded in parallel.

Another way is to assign a fixed sized array of placeholders (AOP) to every cell and physically copy particles position into this array. The advantage of this scheme is that interacting particles are physically close together in memory allowing for fast parallel loading. The disadvantage is that it generally requires more memory, because each AOP has to provide space enough to store particles at the highest possible density.

Our implementation uses the latter scheme. Per cell, one thread is devoted to one placeholder. Empty places are filled with virtual particles. Each thread i of a cell c_0 loads the data of placeholder i of cell c_n from global memory and stores it into shared memory. It synchronises with the other threads of the same cell c_0 to ensure loading has finished. Now it computes the interactions of particle i with all particles in shared memory. Note that this is done for virtual particles, too. These steps are performed for the centre cell, $c_n = c_0$, and all neighbour cells, $n = 1, \dots, 26$.

But the force computation is not the only task. As particles move, the cell lists have to be updated. While this is straightforward on a single CPU, the parallel version comes with some difficulties. If a cell realises that one of its particles is about to move to a neighbour cell, it cannot move the particle there without the risk of memory-write conflicts and data inconsistency.

To safely update a cell in a parallel environment, we first remove all particles from the list which left the cell. Then all particles from neighbouring cells are checked to see if they moved in and need to be added to this list. Double-buffering ensures that all old lists stay intact until all cells have updated their list. Both for removing the particles from a cell that have left the cell and adding the particles that have moved in, we have to first test where a particle belongs, and then update the corresponding particle list by either deleting or adding particles.

Testing particles can be done in parallel. Each thread of a cell computes the cell id for one particle and stores it

in shared memory. Now one thread sequentially loops over these particles and adds those with a correct cell id to the list. To prevent memory-write conflicts, this task has to be performed by a single thread per cell, leaving all other threads idle.

Updating a cell list requires all particles from this cell and its neighbour cells to be loaded from memory. In order not to load the same data twice, we perform this task during force calculation, not directly after the integration of positions. As a drawback the cell lists are not precisely up-to-date, but one time-step behind. In order not to neglect any interactions, the cells have to have a side length larger than the maximum interaction range plus a so-called skin of thickness λ , where λ is the maximum particle displacement per time step. For MD simulations it is common practise to use an even larger skin and therefore update the cell lists only every couple of time steps.

3.2 Results

As for the N -squared MD algorithm in Section 2, we compared the GPU implementation with its CPU counterpart. Because the algorithmic complexity exceeded the capabilities of Cg, only CUDA could be used.

The system size lower limit is given by the requirement to have at least 3 cells per dimension at a density of $\rho = 1.0$. The upper limit for the density was given by the array size associated with every cell, which was $n = 32$ in the data presented here. For a minimum cell size of $r_c = 2.5\sigma$ and a density of $\rho = 1.0$, on average $\rho r_c^3 \approx 16$ places per cell are occupied. This implies that most of the time half of the threads are calculating interactions of virtual particles which do not contribute. This deteriorates at lower densities.

The run time is density dependent: the more particles per cell, the more interactions have to be computed, and the computation time rises. This is true for the CPU version. However, our GPU version behaves differently. In contrast to the CPU version, the GPU version's run time is dominated by the total number of cells, not by the number of interactions per cell. This is because interactions are always calculated for all placeholders; at low densities, most of them are however empty. At constant number of particles, the number of cells decreases with the density, and therefore the run time decreases. This effect saturates once all placeholders of a cell are used.

The left graph of figure 4 shows the speedup factor for our GPU implementation. At the lowest density of $\rho = 0.1$, the GPU version is twice as fast as the CPU version. At higher densities, the GPU outperforms the CPU by up to a factor 40. The errors for these speedup factor are smaller than the symbol sizes and the kinks and bumps reproducible. They relate to the cell size, which fluctuates in order to get an integer number of cells per

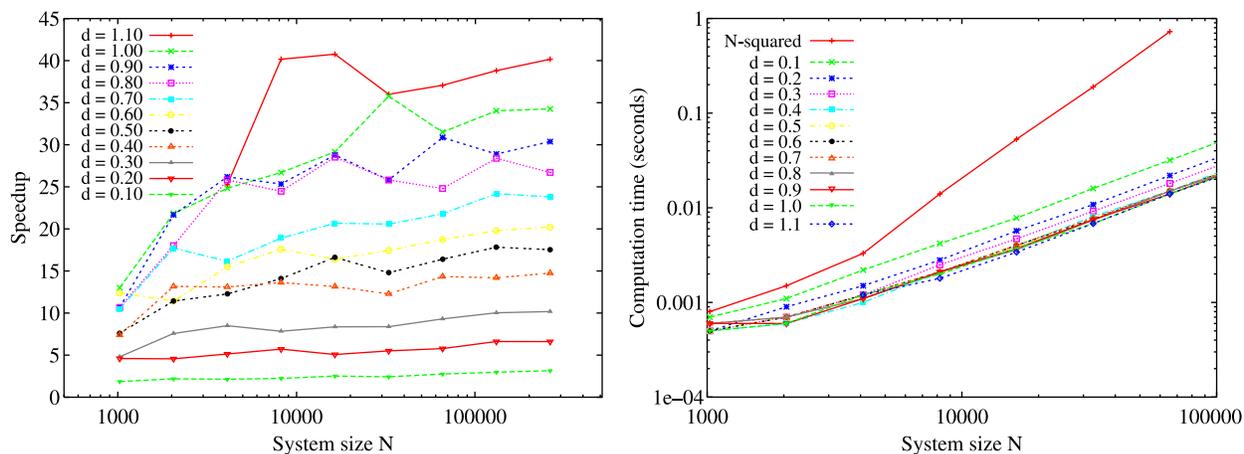


Figure 4. Left: Speedup of the GPU version at various densities. The kinks and bumps are reproducible. For details, see main text. Right: absolute times (in seconds) for a single MD step. The density-independent N -squared MD data is presented as a reference. The intersection points with this reference data would indicate the break-even points for the cell-lists algorithm. But for all system sizes shown here, the cell-lists MD is faster than its N -squared counterpart.

dimension. Assume a box length of $L_x = 11\sigma$ and a minimum cell size of $r_c = 2.5\sigma$, then the number of cells for this dimension is $n_x = \text{int}[L_x/r_c] = \text{int}[4.4] = 4$ and the actual cell size is $r'_c = L_x/n_x = 2.75\sigma$. This increase of 10% results in 33% more particles per cell, leading to 77% more interactions, decreasing the CPU performance. But for the GPU version a few more threads compute real particle interactions instead of virtual ones, resulting in no penalty.

The absolute computation times required per MD time step are depicted in the right graph of Figure 4. For comparison, the (density independent) N -squared MD data is shown as well. The cell-list data feature a different slope than the N -squared data, indicating linear and quadratic scaling, respectively. Intersection points with the N -squared curve would indicate the break even points, where both algorithms perform equally well. However, for all system sizes and densities depicted in Figure 4, the cell-lists version performed better than its N -squared counterpart.

4. Random number generation

For many applications in computer simulations, e.g. MC simulations or MD simulations with a stochastic thermostat, a large quantity of (pseudo-)random numbers is required. Typically, simple linear congruential generators such as the Irand48 are used [18]. Given a number x_n , the following number in its series is generated as follows:

$$x_{n+1} \equiv ax_n + c \pmod{2^{48}}, \quad (5)$$

where a and c are some integer constants. The pseudo-random number x_{n+1} is then converted to the pseudo-

random number Y_{n+1} of the required data type. For Y_{n+1} , one uses the d most-significant bits of x_{n+1} , where d is the bit size of the required data type (e.g. $d = 31$ for nonnegative 32-bit integers).

4.1 Implementation details

To parallelise generation rule (5), we note that

$$x_{n+m} \equiv Ax_n + C \pmod{2^{48}}, \quad (6)$$

where

$$A \equiv a^m \pmod{2^{48}} \quad \text{and} \quad C \equiv \sum_{i=0}^{m-1} a^i c \pmod{2^{48}}. \quad (7)$$

The random number generator is then implemented as follows. We choose a number S of random numbers to generate in parallel. To start the random number generator, we choose a seed x_0 , and generate the first x_i , $i = 1, \dots, S$ according to the serial rule (5). The next set of S pseudo-random numbers is then generated from this set according to rule (6). Since the calculation of x_{i+S} only requires knowledge about x_i , all x_{i+S} , $i = 1, \dots, S$ can be calculated in parallel. If some multiple RS of S random numbers is required, each set $x_i, x_{i+S}, \dots, x_{i+(R-1)S}$ can be calculated independently by an isolated processor.

For the implementation on current GPUs, this is very convenient: using S independent threads, each thread first loads its current state x_i . Then, it generates the following pseudo-random numbers x_{i+S} , calculates the output value Y_{i+S} and stores it. This step is repeated for all x_{i+nS} , until in total R random numbers have been generated and stored. Finally, the thread saves the current state $x_{i+(R-1)S}$. For

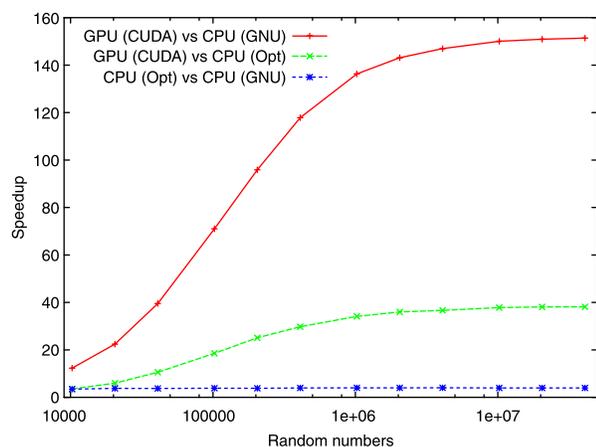


Figure 5. Speedup of a self-written CPU and a GPU version of the rand48 random number generator versus the standard glibc implementation.

our test, we used $S = 6144$ independent threads, grouped into 32 blocks of 192 threads each.

Note that all arithmetics is done modulo 2^{48} . However, GPUs (as well as standard CPUs) do not offer 48-bit data types. In principle, a 48-bit number can be represented by three 16-bit numbers, but for performance reasons it is better to represent the 48-bit number as one 64-bit integer or two 32-bit integers. We have chosen to represent the x_n by two 32-bit integers, which contain the 24 most-significant and 24 lowest-significant bits.

4.2 Results

We compare our implementation of the lrand48 random number generator on the GPU both to the standard GNU-libc lrand48() function as well as a self-written CPU version using 64-bit arithmetics. For each implementation, we measured the time necessary to generate the first N random numbers of the lrand48 series for $10,240 \leq N \leq 40,960,000$. The resulting speedup factors of our implementations relative to the GNU-libc implementations are shown in Figure 5.

The optimised CPU version is consistently faster than the system implementation by a factor of almost four. This simply demonstrates the high 64-bit performance of current PC processors. However, the GPU achieves a much higher performance. For generating more than a million random numbers, the GPU is faster than the standard-libc lrand48 by a factor of 150. Compared to our optimised CPU-version, the speedup is still almost 40.

Although the speedup factor for this pure integer arithmetics problem is therefore not as high as for typical floating-point problems, the GPU is still competitive for the generation of random numbers. Moreover, our

implementation stores the output random numbers in the relatively slow main memory of the graphics card. Depending on the problem at hand, it is however often possible to generate random numbers on the fly, which will increase the speedup factor.

5. Summary and outlook

The computational power of recent graphics cards is fifty times as large as the power of a conventional processor. It has been shown previously that this speed can be harvested for many problems, e.g. matrix multiplication or the calculation of electrostatic interactions. In this article, we have demonstrated that it is possible to run a conventional MD simulation entirely on a graphics card. The simulations run 25–80 times faster than on a single conventional processor, at comparable prices. Similar results are reported by Anderson *et al.* [20] using a different technical approach. This shows that it is also possible to harvest this computational power for MD simulations.

Although our code features only the simple Lennard-Jones potential, it is trivial to replace this potential by other pair-potentials, including the coulombic interaction. By this, our code can in fact be used for many systems of interest. Moreover, the GPUs are indeed general purpose processors by now, and therefore it should be possible to implement many other techniques equally efficiently, such as Ewald summation methods or SHAKE for constrained dynamics. Currently the GPUs are limited to single precision floating point operations. For long non-thermalized simulations, in which energy conservation is crucial, this precision might not be sufficient. However, double-precision GPUs are expected for the end of this year.

While MD simulation techniques can be easily ported onto the GPU architecture, this does not hold for the equally wide-spread family of MC methods. Tomov *et al.* [14] have implemented a MC scheme for the 2D Ising model showing that lattice-based probabilistic simulations can be ported to the GPUs SIMD architecture. However, off-lattice many particle MC simulations are difficult to parallelise, both on conventional parallel architectures and on SIMD hardware. Reasons for this are the random acceptance moves causing unpredictable branching, and the permanent access to global information to obey detailed balance.

The difference in computational power between conventional processors and GPUs is expected to increase further. At the end of this year, NVIDIA GPUs are expected to reach Teraflops performance on a single card, and will feature double precision floating point operations, at a rate of 250 Gigaflops. Even with current off-the-shelf PC mainboards it is possible to build systems equipped

with four graphics cards. A single PC can therefore obtain Teraflops performance, and a small cluster of such PCs provides a computational power of 10 Teraflops for a price of less than \$100,000.

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