Acceleration of Deterministic Boltzmann Solver with Graphics Processing Units

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Abstract. GPU-accelerated computing of the Boltzmann collision integral is studied using deterministic method with piecewise approximation of the velocity distribution function and analytical integration over collision impact parameters. The acceleration of 40 times is achieved compared to CPU calculations for a 3D problem of collisional relaxation of bi-Maxwellian velocity distribution.

Keywords: Boltzmann equation, direct Boltzmann solver, Graphics Processing Units, CUDA programming model.

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INTRODUCTION

Recent advancements in the development of Graphics Processing Units (GPU) make it possible to achieve teraflop performance on a single desktop computer [1]. To achieve peak performance, special numerical algorithms for GPU architecture should be developed to divide the problem into multiple threads executed in parallel. The acceleration of 30-40 times by GPU computations is reported in [2] for the evaluation of the Boltzmann collision integral with semi-regular methods. Frezzotti et al. [3, 4] have shown that direct solution of the Boltzmann equation (with both the Bhatnagar-Gross-Krook-Welander (BGKW) model and the hard sphere collision integral) can be easily divided into threads to produce more than 2 orders of magnitude speedup on GPU versus CPU.

In the present paper, the GPU-accelerated computing (with NVIDIA cards and the high level CUDA programming language) is studied for computing the Boltzmann collision integral with deterministic (regular) method using a piecewise approximation for the velocity distribution function and analytical integration over impact parameters (see, e.g. [5]). The work utilizes our previous experience on parallelization in velocity space for the deterministic method described in [6] and the development of different parallel algorithms for direct Boltzmann solvers [7, 8].

We describe special GPU algorithms for solving the Boltzmann kinetic equation by the deterministic (regular) method. This method could be particularly attractive for unsteady problems, problems with low gas velocities (such as flows in MEMS) and flows at small Knudsen numbers. A regular grid in velocity space is used with cubic cells in velocity space. The splitting procedure reduces the problem to advection in physical space, and collisional relaxation in velocity space. This paper focuses on the relaxation part of the problem. The GPU-methods for solving the advection part have already been described in [2-4].

THE BOLTZMANN EQUATION AND THE DETERMINISTIC METHOD

The Boltzmann kinetic equation is written in the usual form using standard notations:

$$\frac{\partial f}{\partial t} + \xi_1 \frac{\partial f}{\partial \xi_1} = I(\xi_1, x, t), \quad I(\xi_1, x, t) = \int \left[ f(\xi') f(\xi) - f(\xi) f(\xi') \right] \text{gb} \text{db} d\xi d\xi_1.$$

Here $f$ is the distribution function, $I$ is the collision integral written for a model of hard spheres (or VHS). The deterministic method [5, 6] for calculation of the collision integral is briefly described below. A uniform rectangular 3D computational mesh is introduced in velocity space with cells $\Delta \xi_x \times \Delta \xi_y \times \Delta \xi_z$. The computational domain is...
chosen in such a way that the distribution function is small beyond the domain. The cells are numbered by a 3D index \( i = (i_x, i_y, i_z) \). The location of the center of a cell \( X_i \) is defined in the following manner:

\[
\xi_{i\alpha} = \xi_{i\alpha, \text{MIN}} + (i_{\alpha} + 1/2) \Delta \xi_{\alpha}, \quad \alpha = x, y, z.
\]

As the computational domain is finite the 3D index can be easily converted into a 1D index. A piecewise constant approximation of the distribution function is adopted, i.e. the distribution function is assumed to be constant inside of each cell. This approximation of the distribution function can be written as follows:

\[
f(\xi) = \sum_i f_i e_i(\xi), \quad e_i(\xi) = \begin{cases} 1, & \xi \in X_i, \\ 0, & \xi \notin X_i \end{cases}
\]

The collision integral is computed in the center of each cell \( X_i \):

\[
I_i = \int \left[ f(\xi) f(\xi') - f(\xi) f(\xi) \right] g b d \xi d \varepsilon d\xi_i.
\]

The integration over parameter \( \xi_i \) in (2) is performed numerically using the centered rectangular quadrature formula on the cells of the computational mesh:

\[
I_i = \sum_j \left[ \int f(\xi) f(\xi') - f(\xi) f(\xi) \right] g b d \xi d \varepsilon \Delta \xi_i.
\]

In (3) \( \Delta \xi = \Delta \xi_x \Delta \xi_y \Delta \xi_z \), \( g_{ij} = |\xi_i - \xi_j| \). Substituting (1) into (3) results in:

\[
I_i = \sum_j \left[ \int \left( f_k e_k(\xi') e_i(\xi) - f_i f_j \right) g_{ij} b d \varepsilon \right] \Delta \xi_i.
\]

Equation (4) can be rewritten in the following manner:

\[
I_i = \sum_{k,l} A_{k1} f_k f_i - f_i \sum_j f_j B_{ij}.
\]

The coefficients \( A_{k1} \) and \( B_{ij} \) depend only on the velocity mesh and have the form:

\[
A_{k1} = \Delta \xi \sum_j g_{ij} \left[ e_k(\xi') e_i(\xi) \right]_{j} b d \varepsilon, \quad B_{ij} = \Delta \xi g_{ij} \left[ b d \varepsilon \right].
\]

In [5, 6] it is shown that the coefficients \( A_{k1} \) and \( B_{ij} \) can be computed analytically for the collision model of hard spheres. The practical restriction for the direct application of Eq. (5) in numerical simulations consists of the huge size of the array \( A_{k1} \). To overcome this limitation, the equation (6) should be used. As the velocities \( \xi, \xi_i \) and \( \xi', \xi_i' \) are linked by the momentum conservation law, the indices \( i, j, k \) and \( l \) are not independent: \( i + j = k + l \), and a new index \( n \) can be introduced instead of 2 indices \( k \) and \( l \): \( k = (i + j + n)/2 \), \( l = (i + j - n)/2 \). Thus, instead of summation over indices \( k \) and \( l \) in (5), a summation over indices \( j \) and \( n \) can be used:

\[
I_i = \sum_{j,n} A_{i\cdot j\cdot n} f_{i+j+n} f_{i+j-n} - f_i \sum_j f_j B_{ij}.
\]

The coefficients \( A_{i\cdot j\cdot n} \) are computed as follows:

\[
A_{i\cdot j\cdot n} = \Delta \xi g_{ij} \left[ e_{i+j+n}(\xi') e_{i+j-n}(\xi) \right]_{j} b d \varepsilon.
\]

It can be noted that \( A_{i\cdot j\cdot n} = A_{i\cdot m,j\cdot m,n} \) for the uniform computational mesh, and all the velocities in the equation (9) for \( A_{i\cdot m,j\cdot m,n} \) can be transformed to the velocities in the equation for \( A_{i\cdot j\cdot n} \) by the shift of the coordinate.
system on \(-m \Delta \xi\). So the coefficients \(A'_{i,j,n}\) depends on \(n\) and on the difference \(i-j\): \(A'_{i,j,n} = \hat{A}_{i,j,n}\), and the size of the array \(A'_{i,j,n}\) can be reduced the size of velocity mesh types. The size of array \(B_{ij}\) can also be reduced in similar manner: \(B_{ij} = \hat{B}_{i-j}\). Finally, the collision integral used in our computations has the following form:

\[
I_i = \sum_{j,n} \hat{A}_{i,j,n} f_i f_{i+j,n} - f_i \sum_j f_j \hat{B}_{i-j}.
\]

(10)

The fundamental physical property of the collision integral is the existence of collision invariants. These invariants must be conserved in the numerical computation of the collision integral:

\[
\sum_i I_i \varphi_i (\xi_i) \Delta \xi_i = 0, \quad \varphi_i = 1, \xi_x, \xi_y, \xi_z, \left(\xi_x^2 + \xi_y^2 + \xi_z^2\right).
\]

(11)

In order to maintain the collision invariants (11), the polynomial conservative correction proposed by Aristov and Tcheremissine [9] is used:

\[
f_i^x = f_i \left[a_0 + a_x \xi_x + a_y \xi_y + a_z \xi_z + a_2 \left(\xi_x^2 + \xi_y^2 + \xi_z^2\right)\right].
\]

(12)

The function (12) is substituted instead of \(f_i\) in front of the second summation in (10):

\[
I_i = \sum_{j,n} \hat{A}_{i,j,n} f_i f_{i+j,n} - f_i \sum_j f_j \hat{B}_{i-j}.
\]

(13)

Substituting the collision integral (13) into (11) results in the system of 5 linear equations for 5 unknowns \(a_0, a_x, a_y, a_z\), which can be easily solved.

The advantage of the considered method is the absence of statistical noise, which arises when semi-regular methods (Monte-Carlo procedures or Korobov’s sequences) are used. A serious drawback of the method is its high computational cost (about \(N^{0.3}\) operations, where \(N\) is the number of cells in velocity space). It is expected that the application of GPU can drastically accelerate these computations.

**GPU COMPUTING AND CUDA IMPLEMENTATION**

NVIDIA CUDA technology was taken as a tool to implement deterministic Boltzmann solver on GPU. In order to achieve good performance on a GPU the code must be well parallelized in a fashion similar to the traditional multi-CPU computing. Unfortunately, GPU architecture and CUDA technology impose additional requirements to the numerical algorithms making the process of effective code development quite different from the traditional parallel programming and introducing new “degrees of freedom” for tuning specific applications. These requirements are briefly discussed in the following paragraphs.

A CUDA-enabled device has a set of streaming multiprocessors (e.g. 30 multiprocessors for NVIDIA GeForce GTX 280). Each multiprocessor can support up to 1024 active threads. The smallest executable unit of parallelism on a device is called *warp* and consists of 32 threads. Within one warp multiple execution paths must be avoided, because branching leads to serialization of the code for a diverging path. Besides warp, a thread block must be considered. A thread block is a set of threads executed on one multiprocessor sharing some resources. When developing the CUDA algorithm, a programmer must think not only in terms of threads but also in terms of warps and thread blocks.

Any device has access to several types of memory. One must distinguish a slow DRAM memory (global memory) and a fast on-chip memory (shared memory and registers). Global memory has high access latency (more than 400 clock cycles); otherwise shared memory and registers latency is 2 orders lower. The peak performance of operations with global memory is achieved when the memory is accessed in a coalesced manner (the threads of a warp access sequentially aligned memory blocks). The shared memory size is small – 16 Kb per thread block, while global memory size can be up to 1 Gb. One of the challenges in GPU programming is to replace uncoalesced and redundant accesses to global memory by accesses to shared memory when it is possible.

It has been recently shown (see [2]–[4]) that the use of NVIDIA CUDA technology can provide more than 2 orders speedup for Boltzmann solvers. The threads in these papers correspond to points in physical space. This approach suits well for GPU computing of collision integral because the same code is executed for different threads. The advection of the distribution function in physical space is also well processed by GPUs.
In the present paper we consider the possibility to compute the relaxation problem on GPUs. This problem is a fundamental part of any Boltzmann solver, so efficient GPU relaxation code could be a part of more complex solver. Although the relaxation problem seems less complex than solution of spatially inhomogeneous Boltzmann equation, it is not as well parallelized because the physical coordinate cannot be used as a thread ID parameter for obtaining the same code for a warp.

At first sight, selecting threads equivalent to points in velocity space seems to be natural for GPU computations of the collision integral by the deterministic method. Unfortunately, analysis shows that direct application of this approach does not provide performance benefits. The reasons are the unstructured access to arrays of coefficients which are stored in global memory and multiple execution paths.

The algorithm of collision integral computations has been optimized for the GPU computations in the following manner. In order to reduce accesses to global memory thread blocks were organized in such a way that each thread block processed the part of the collision integral with the 1-st components of the 3D indices \(i, j\) and \(n\) in (10) being constant inside a thread block. This results in that the 1-st components of all 3D indices in (10) being constant inside a thread block. The part of the distribution function with a fixed 1-st component of index is stored in shared memory.

The CUDA code of a kernel for computation of the part of the collision integral, corresponding to collision frequency (the last sum in (10)) is presented in Listing 1. This code is created for the simplest case of a rectangular 3D computational domain where the range of points in each coordinate is constant and independent of other coordinates. The kernel writes the results to a buffer. The buffer is large enough to guarantee that no writing conflict will happen.

Listing 1. CUDA kernel for computations of the collision frequency.
```c
__global__ void compute_inverse_collision_integral (float * f, float * a,
float * inverse_integral_buf)
{
short int i_x, i_y, i_z, j_x, j_y, j_z, n_x, n_y, n_z, m_x, m_y, m_z, index;
short int k_x, k_y, k_z, l_x, l_y, l_z;
__shared__ float f1_shared[N_YZ];
__shared__ float f2_shared[N_YZ];
__shared__ float a_shared[N_YZ];
__shared__ float integral_shared[N_YZ];

j_x = blockIdx.x % N_X; // 1-st components of indices are equivalent computed from block ID
i_x = blockIdx.y;

n_x = (blockIdx.x / N_X) << 1 | ((i_x + j_x) & 1);

k_x = (i_x + j_x + n_x) >> 1; l_x = (i_x + j_x - n_x) >> 1;

for (index = threadIdx.x; index < N_YZ; index+= blockDim.x)
// copy the distribution
f1_shared[index] = f[k_x * N_YZ + index];

for (index = threadIdx.x; index < N_YZ; index+= blockDim.x)
// function to shared memory
f2_shared[index] = f[l_x * N_YZ + index];

for (index = threadIdx.x; index < N_YZ; index+= blockDim.x)
// initialization of shared
integral_shared[index] = 0.0f;

m_x = (i_x > j_x) ? i_x - j_x : j_x - i_x; // abs (i - j)

for (index = threadIdx.x; index < N_YZ; index+= blockDim.x)
// to shared memory buffer
integral_shared[index] += a_shared[m_index] * (f1_shared[k_index] * f2_shared[l_index] + // accumulating the collision integral
f1_shared[l_index] * f2_shared[k_index]); // to shared memory buffer

k_index = get_1D_index_from_y_and_z (k_y, k_z);
l_index = get_1D_index_from_y_and_z (l_y, l_z);
integral_shared[k_index] += a_shared[m_index] * (f1_shared[k_index] * f2_shared[l_index] + // accumulating the collision integral
f1_shared[l_index] * f2_shared[k_index]); // to shared memory buffer

for (index = threadIdx.x; index < N_YZ; index+= blockDim.x)
inverse_integral_buf[(i_x + blockIdx.x * N_X) * N_YZ + index] = integral_shared[index]; // copy the results from shared memory to global memory
}
```

Listing 2. CUDA kernel for computing the inverse collision integral.
The kernel for computing the inverse collision integral is presented in Listing 2. It is the main part of the code, because computations of the inverse collision integral by the deterministic method take more than 99% of time. The structure of the code is similar to that of Listing 1. One should mention that the shared memory buffer is updated twice during the internal loop. This is due to the fact that the components of the index \( n \) could be both positive and negative. The results are stored in a global memory buffer of a size large enough to avoid memory writing conflicts.

After the kernels have completed their work the data from buffers are collected using a simple kernel which sums the parts of the buffer corresponding to the same velocity points. The in the conservative correction procedure (11)-(13) is executed. The moments of the collision integral, which are necessary for the conservative correction are computed by the kernel. The linear system for the 5 unknowns \( a_0, a_x, a_y, a_z, \) and \( a_2 \) is solved in a serial manner. The final value of the collision integral is obtained with the formula (13) by a kernel, which corrects the collision integral.

The results of computations with the developed code with the use of NVIDIA GeForce GTX 295 GPU show the 40 times speedup for the computational mesh 20x20x20 with respect to the CPU version of the program executed on Intel Core 2 3GHz processor. This shows that the speedup of the proposed method is not as great as in the papers [2]-[4] but nevertheless the GPU in this case are several times more efficient than the same price CPU computing.

**SOLUTIONS OF TEST PROBLEMS**

Collisional relaxation of a bi-Maxwellian distribution was studied to explore the GPU acceleration process. The initial distribution is sum of 2 Maxwellians with different mean velocities. The temporal evolution of the velocity distribution function during the relaxation is presented in Fig. 1. The left plot shows the evolution of the distribution function in the cross-section \( \xi_y=0, \xi_z=0 \), the right plot corresponds to the cross-section \( \xi_x=0, \xi_z=0 \).

![Figure 1](image_url)

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**REFERENCES**