

ACCELERATION OF VORTEX METHODS CALCULATION USING MDGRAPE-2 AND MDGRAPE-3: A COMPARATIVE STUDY

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Abstract: *The calculation of vortex method has been accelerated by using special-purpose computers, MDGRAPE-2 and MDGRAPE-3, respectively. The similar algorithm has been implemented and the improvement in speed of MDGRAPE-2 was 100 times while MDGRAPE-3 was 1000 times faster when compared with the ordinary PC Xeon 5160(3.0GHz) for $N=10^6$. In addition, the speed of MDGRAPE-3 was 25 times faster compared with MDGRAPE-2. The round off errors have been investigated in both cases.*

Keywords: *Vortex Method, Special-Purpose Computer, MDGRAPE-2, MDGRAPE-3, Scaling Error*

1 Introduction

There has always been a strong relationship between progress in vortex methods and advancements in acceleration techniques that utilize this method. When the classical vortex methods became popular nearly 30 years ago, the calculation cost of the N-body solver was $O(N^2)$ for N particles. Due to this enormous calculation cost, the intention at that time was not to fully resolve the high Reynolds number fluid flow, but to somewhat mimic the dominant vortex dynamics using discrete vortex elements. One of the main difficulties of vortex methods to be accepted in the mainstream of computational fluid dynamics is the numerical complexity of calculating the velocity using the Biot-Savart law, which is in fact analogous to an "N-body problem" and hence requires $O(N^2)$ operations for N vortex elements.

The large numbers of elements are required for accurate vortex methods calculation at high Reynolds number flows that is very high computation cost. Therefore, significant acceleration techniques are necessary to reduce the computation cost of N-body interaction calculation for millions of particles having the cost of $O(N^2)$ with growing N [1-3].

There are two techniques to reduce the force calculation cost of an N-body simulation which hardware and software techniques. In the hardware techniques, there are two techniques, one is a parallel computer and the other is a special-purpose computer. To accelerate the vortex methods calculation, parallel calculation has been widely used in previous studies [6, 9-10]. Even though accelerate the calculation significantly; there are some difficulties to use parallel computations for longer calculations. It has limitations with parallelization according to hardware specifications. The memory bandwidth is a big problem to calculate for large number of vortex elements, which required special consideration. Power consumption and heat dissipation interrupt the longer time calculations. These problems are becoming serious for advanced scientific computation. Shortcomings of parallel computers, the special-purpose approach can solve parallelization limit thoroughly. It has relaxed power consumption according to hardware specification. The cost-performance is minimum ~100 times better than that of parallel computation using ordinary cluster computers [14].

In the present research, the special-purpose computers MDGRAPE-2 and MDGRAPE-3 have been used rigorously to accelerate the vortex method calculation [11-12], separately. In this paper, a comparative study between MDGRAPE-2 and MDGRAPE-3 has been investigated for high Reynolds number flows.

2 Vortex Method

The vortex method describes the flow field by the superposition of particles with a smooth distribution of vorticity [3]. From this vorticity, the velocity of vortex elements is calculated by the Biot-Savart equation. The vortex elements are then convected according to this velocity, and at the same time, the vorticity is updated

according to the stretching and diffusion term of the vorticity equation. We will only show the final discretized form of each equation here.

The discretized form of the Biot-Savart equation with the high order algebraic cutoff function by [15] can be written as

$$\mathbf{u}_i = -\frac{1}{4\pi} \sum_{j=1}^N \frac{|\mathbf{r}_{ij}|^2 + (5/2)\sigma_j^2}{\left(|\mathbf{r}_{ij}|^2 + \sigma_j^2\right)^{5/2}} \boldsymbol{\gamma}_j \times \boldsymbol{\gamma}_j \quad (1)$$

he subscript i stand for the target elements, while j stands for the source elements, thus $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ is the distance vector. $\boldsymbol{\gamma}$ is the vortex strength and σ is the core radius of the vortex element. Using the same high order algebraic function as above, the stretching term becomes [15]

$$\frac{d\boldsymbol{\gamma}_i}{dt} = \frac{1}{4\pi} \sum_{j=1}^N \left\{ -\frac{|\mathbf{r}_{ij}|^2 + (5/2)\sigma_j^2}{\left(|\mathbf{r}_{ij}|^2 + \sigma_j^2\right)^{5/2}} \boldsymbol{\gamma}_i \times \boldsymbol{\gamma}_j + 3 \frac{|\mathbf{r}_{ij}|^2 + (7/2)\sigma_j^2}{\left(|\mathbf{r}_{ij}|^2 + \sigma_j^2\right)^{7/2}} (\boldsymbol{\gamma}_i \cdot (\mathbf{r}_{ij} \times \boldsymbol{\gamma}_j)) \mathbf{r}_{ij} \right\} \quad (2)$$

For the calculation of the diffusion term, we use the core spreading method [5], which uses the relation

$$\frac{d\sigma_i}{dt} = \frac{\nu}{\sigma_i} \quad (3)$$

The radial basis function interpolation [2] is used every ten time steps to ensure the convergence of the core spreading method [17]. The convection is solved by updating the position of vortex elements according to their velocity

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i \quad (4)$$

In summary, the vortex method sequentially solves Eqs. (1), (2), (3), and (4). The MDGRAPE-2 and MDGRAPE-3 are used to calculate Eqs. (1) and (2).

3 The MDGRAPE-2

The MDGRAPE-2 is a calculation accelerator board that dramatically increases the speed of molecular dynamics calculations by calculating the general force exerted between all pairs of particles in an N-body particle simulations [13]. A single board increases the computing speed of an ordinary PC to 64GFlops comparable to a supercomputer. The calculation of interactions between particles as represented by potential

and force are carried out in MDGRAPE-2. In case of calculating the potential,

$$\Phi_i = \sum_{j=1}^N b_{ij} g(w) = \sum_{j=1}^N b_{ij} g\left(a_{ij} \left(|\mathbf{r}_{ij}|^2 + \varepsilon_{ij}^2\right)\right) \quad (5)$$

and the force calculations are treated similarly, where $g(w)$ is an arbitrary function equivalent to an intermolecular force, and a_{ij} , b_{ij} , and ε_{ij} are arbitrary coefficients which are settled down for every model.

$$\mathbf{f}_i = \sum_{j=1}^N b_{ij} g(w) \mathbf{r}_{ij} = \sum_{j=1}^N b_{ij} g\left(a_{ij} \left(|\mathbf{r}_{ij}|^2 + \varepsilon_{ij}^2\right)\right) \mathbf{r}_{ij} \quad (6)$$

To apply these libraries to the calculation of a vortex method, Biot-Savart law in Eq. (1) is expressed as follows.

$$\mathbf{u}_i = \sum_{j=1}^N B_j g\left(A_j \left(|\mathbf{r}_{ij}|^2 + \varepsilon_{ij}^2\right)\right) \mathbf{r}_{ij} \quad (7)$$

where A_j , B_j are arbitrary constants. The details mathematical formulations are introduced in [3, 7, 11-12, 16].

The function $g()$ for an arbitrary value $a|\mathbf{r}_{ij}|^2$ is calculated by interpolation, from values that are tabulated prior to the execution of the main program. If the inter-particle distance is such that $a|\mathbf{r}_{ij}|^2$ falls out of this tabulated domain, the MDGRAPE-2 assumes $g()$ is zero. The number of tabulated points is constant. Thus, defining the table in a large domain would result in larger spacing between the tabulated points, and therefore a larger interpolation error. On the contrary, defining the table in a small domain would yield a higher probability that the inter particle spacing would fall outside the tabulated domain, which can also cause errors. The optimum range has been investigated for the vortex ring calculation by [11] for MDGRAPE-2.

4 The MDGRAPE-3

The MDGRAPE-3 is a special-purpose computer exclusively designed for molecular dynamics simulations. A typical MDGRAPE-3 system consists of a general-purpose computer and a special-purpose hardware connected via a PCI board. The MDGRAPE chips can only handle two types of calculations. The Coulomb potential

$$p_i = \sum_{j=1}^N b_j g\left(a|\mathbf{r}_{ij}|^2\right) \quad (8)$$

and Coulomb force

$$f_i = \sum_{j=1}^N b_j g\left(a|\mathbf{r}_{ij}|^2\right) \mathbf{r}_{ij} \quad (9)$$

where $g(\cdot)$ is an arbitrary function, which must be defined prior to the calculation. a and b_j are constants, which can be used for scaling. The direct form of the Biot-Savart equation (1) and the stretching term (2) can be calculated by using a combination of (8) and (9).

The three critical issues regarding the implementation of the MDGRAPE on vortex methods are the efficient calculation of the Biot-Savart and stretching equation, the optimization of the table domain, and the minimization of the round-off error caused by the partially single precision calculation in the MDGRAPE. These problems were investigated by [11] for the preceding but similar machine; MDGRAPE-2. The only difference between the MDGRAPE-2 and MDGRAPE-3 is that the latter can simultaneously calculate along with the host machine, but can only handle a small number of source particles at once [8]. However, these differences do not have any effect on the above-mentioned critical issues, and the findings of [11] can be directly used for the MDGRAPE-3.

5 Comparative Study

The difficulties to use MDGRAPE-3 are the same as of MDGRAPE-2 and which has been solved in details for MDGRAPE-2. The only difference between them is that MDGRAPE-3 can simultaneously calculate along with the host machine, but can only handle a small number of source particles at once [8]. However, these differences do not have any effect on the same critical issues once solved and the findings of MDGRAPE-2 can be directly used for MDGRAPE-3.

5.1 Scaling Error

Here we will first confirm that MDGRAPE-3 outputs the same results as the previous calculations using MDGRAPE-2. Figure 1 shows typical velocity distribution on a logarithmic scale, calculated from Eq. (1), with and without the use of MDGRAPE for six different input ranges, where a single source particle is positioned at the origin and 1000 target particles are distributed from 10^{-4} to 10^4 . Xeon 5160(3.0GHz), MDG2, and MDG3 stand for calculations without MDGRAPE, with MDGRAPE-2, and with MDGRAPE-3, respectively. The velocity becomes zero when $|\mathbf{r}_{ij}|/\sigma_j$ falls outside of the range of the table. Otherwise, the results of the Biot-Savart calculation on MDGRAPE-2 and MDGRAPE-3

match those of the results on the host computer in each case.

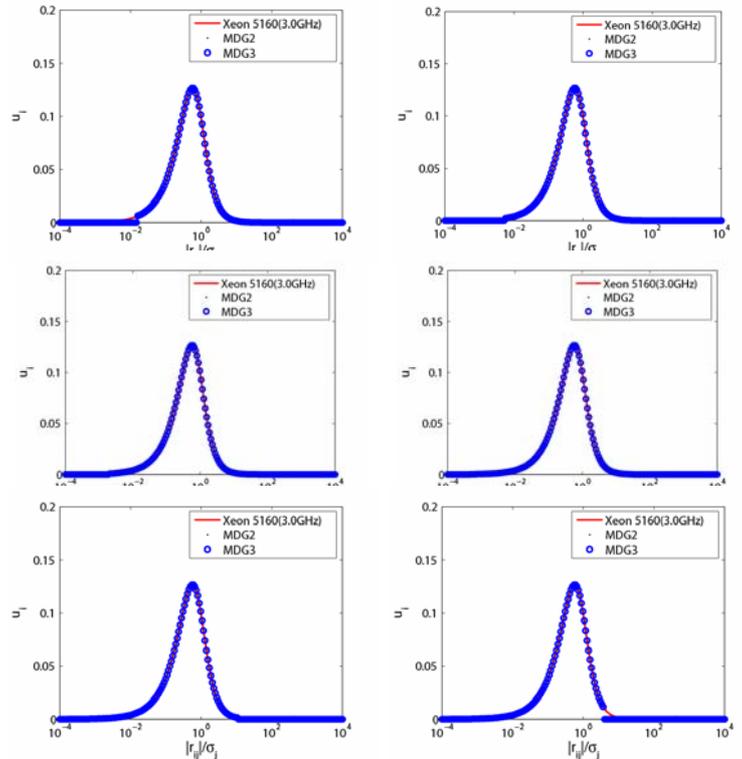
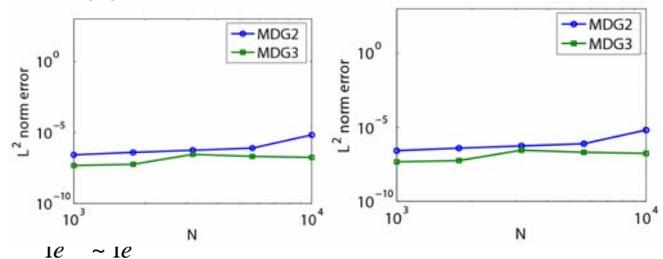


Fig. 1 Different ranges of a function table

Figure 2 shows the comparative error for different input ranges between MDGRAPE-2 and MDGRAPE-3. It can be easily observed that the errors are different for different ranges. The errors in figures 2(a) and 2(b) are below 10^{-5} . The rest of errors are larger and are not satisfactory in the vortex method calculations. The optimum range is determined $1e^{-2} \sim 1e^6$ for entire calculations.

5.2 CPU-time and L^2 norm error

The calculation cost and accuracy are important issues for any numerical simulation. In this calculation these two factors have been investigated carefully. The calculation has been accelerated retained the accuracy at an acceptable label. The CPU-time has been compared with different acceleration techniques at one time step by changing the number of



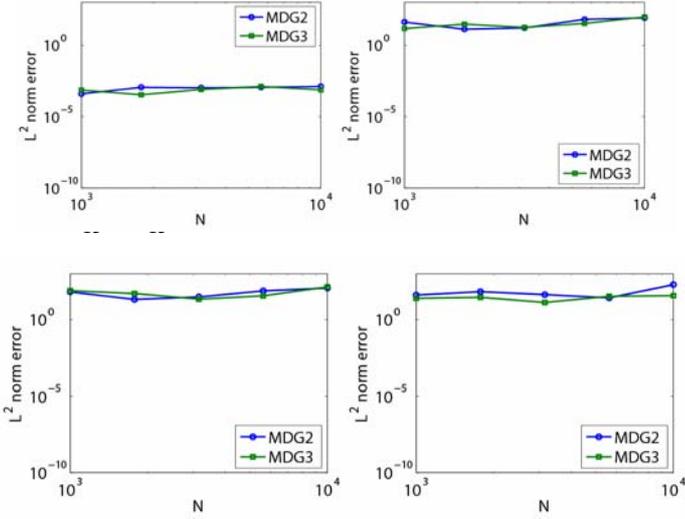


Fig. 2 Comparative scaling error between MDGRAPE-2 and MDGRAPE-3

The L^2 norm error is defined as the difference in the induced velocity of the same particles between the host and MDGRAPE for the same time step as follows.

$$L^2(\text{norm error}) = \frac{\sum (u_{\text{host}} - u_{\text{md}})^2 + (v_{\text{host}} - v_{\text{md}})^2 + (w_{\text{host}} - w_{\text{md}})^2}{\sum (u_{\text{host}}^2 + v_{\text{host}}^2 + w_{\text{host}}^2)}$$

where the suffices *md* and *host* represent with and without the use of MDGRAPE, respectively.

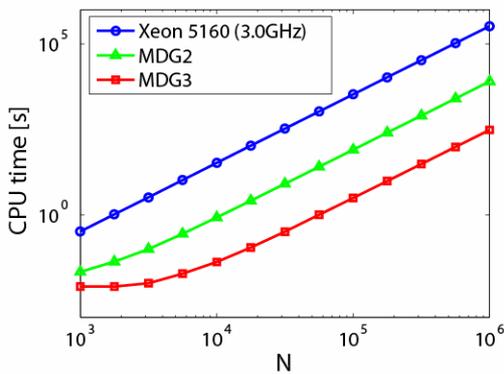


Fig. 3 Acceleration using MDGRAPE-2 and MDGRAPE-3

Figure 3 shows the cpu-time for one time step against the number of vortex elements with and without the use of MDGRAPE. The legends 'Xeon 5160(3.0GHz)', 'MDG2', and 'MDG3' correspond to the calculations without the use of MDGRAPE and with the use of MDGRAPE-2 and MDGRAPE-3. It is clearly seen that the calculation time has been reduced with the use of both schemes for $N \sim 10^6$ when compared with

the host calculation time. From the figure it is shown that MDGRAPE-3 calculation has been further accelerated than MDGRAPE-2 when compared with host calculation. The MDGRAPE-3 is 1000 times faster when compared with the host calculation and 25 times faster compared with the MDGRAPE-2. This means that MDGRAPE-3 implies much faster calculation than MDGRAPE-2 which leads to use the new special-purpose computer.

Numerical accuracy is an important issue for any numerical simulation and engineering applications as well. Therefore, here we will check the accuracy of MDGRAPE-3 calculations compared with that of MDGRAPE-2.

It is already observed in Fig. 3 that MDGRAPE-3 is faster compared with MDGRAPE-2. I must check the accuracy of present calculation before going to implement the actual calculation on it.

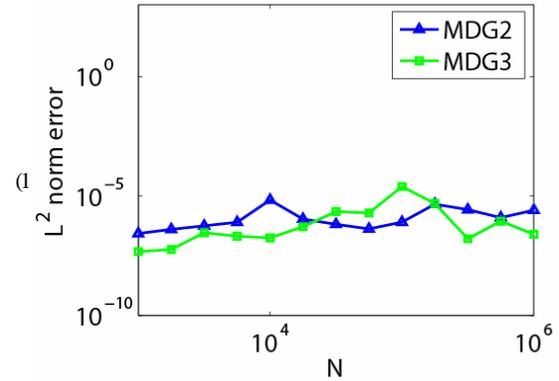


Fig. 4 Accuracy of MDGRAPE-2 and MDGRAPE-3

Figure 4 represent the L^2 norm error as of Eq. (10) for Biot-Savart calculation compared between the old and new board. It is shown that both errors are in the same order of magnitude and below 10^{-5} . On the one hand MDGRAPE-3 gives less error for small number of elements but it keeps the same order of magnitude compared to large numbers. On the other hand MDGRAPE-2 gives large error for large number of elements but it keeps the same order of magnitude with small number of elements. This negligible discrepancy may cause by slightly different hardware specifications and the floating-point operations between them.

6 Conclusions and Future Work

The vortex method calculation has been accelerated using MDGRAPE-2 and MDGRAPE-3, respectively. It is observed that MDGRAPE-3 has been reduced computation

cost is 1000 times while MDGRAPE-2 was 100 times when compared with Xeon 5160(3.0GHz) PC. The CPU-time and accuracy of both boards have been investigated for vortex method calculations and compared with the host PC. The speed of MDGRAPE-3 is 25 times faster when compared with MDGRAPE-2. The accuracy has been retained in acceptable level.

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Websites

MDGRAPE-2 can be found in

atlas.riken.go.jp/mdm/mdgrape2.html

MDGRAPE-3 can be available in mdgrape.gsc.riken.jp

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