High performance computing techniques for vortex method calculations

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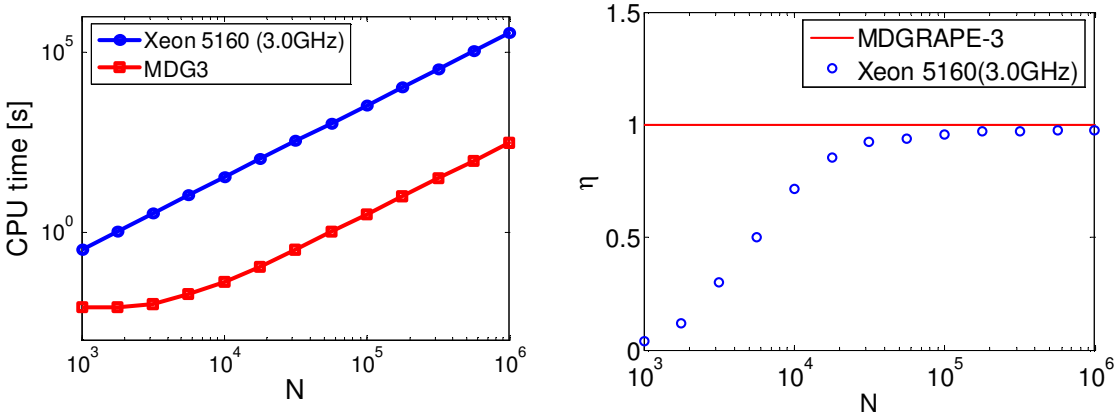
There has always been a strong relationship between progress in vortex methods and advancements in acceleration techniques that utilize this method. When the classical vortex methods became popular nearly 30 years ago, the calculation cost of the N-body solver was $O(N^2)$ for N particles. Due to this 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.

The advent of fast algorithms such as fast multipole method made it possible to achieve a scaling of O(N), and with the help of the rapid development in computational hardware such as a special-purpose computer; MDGRAPE-3, a calculation involving million of vortex elements became possible. The vortex method was recognized as a discretization method rather than an attempt to model vortex dynamics, because the computational power that was necessary to prove these claims became available. Consequently, it was still difficult for vortex methods to be considered as an alternative to conventional methods in computational fluid dynamics.

In the present study, the calculation of vortex method has been accelerated with the simultaneous use of the FMM and MDGRAPE-3 for $N=10^7$. This number is not sufficient for accurate vortex method calculation that can be used in real engineering applications. The present results indicate that for the calculation of significant high Reynolds number, the vortex method requires impractically large N, which is possible by using the proposed acceleration method with the use of high-performance supercomputer.



(a) Performance (b) Efficiency

Fig 1. Performance and efficiency of vortex method calculation

The computation time has been performed and compared with ordinary PC, Xeon 5160 3.0GHz. The CPU-time has been calculated from Biot-Svart law and run for one time step while the number of particles is increased. Figure 1(a) shows the calculation time against the number of vortex elements with and without the use of MDGRAPE-3. It is clearly seen that the computation time is reduced by a factor of 1000 for N ~10^6. This acceleration rate is above the speed of MD simulations and it can be further improved by reducing the number of calls to the MDGRAPE-3 library.

The peak performance of the MDGRAPE-3 board is 330GFlops when the board calculates Coulomb forces for 32000 or more particles. This performance is not the same when vortex method has been calculated using this board.

Result of the efficiency measurements is shown in Figure. Here N is number of particles has been used to calculate the performance of MDGRAPE-3. The solid line represents the peak performance of MDGRAPE-3 board for molecular dynamics calculations and circle represents the maximum efficiency (η) of vortex method calculations. From the results of this measurement, it is proved that the efficiency is improved with increase of number of particles, the board provides high performance if the number of particles is large. It is clearly observed from the figure that the efficiency of the present calculation is 98% compared with the peak performance of MDGRAPE-3 for the largest N of VM calculations.

The global kinetic energy and enstrophy have been investigated to address the numerical accuracy. The results have good agreement when compared with the previous and referenced work. The results with and without the use of the FMM, MDGRAPE-2, MDGRAPE-3 and the combination of FMM and MDGRAPEs do not show any notable difference.

Reference:

T. K. Sheel, R. Yokota, K. Yasuoka, S. Obi, The study of colliding vortex rings using a special-purpose computer and FMM, Transactions of the Japan Society for Computational Engineering and Science, 2008 No. 20080003.