COMPARATIVE STUDY OF PARALLELIZATION METHODS USING OPEN-MP AND MPI WITH AN UNSTRUCTURED RANS SOLVER FOR PRACTICAL APPLICATIONS

Kunihide Ohashi^{1*}, Yohei Sato² and Takanori Hino³

 ¹ National Maritime Research Institute, 6-38-1 Shinkawa Mitaka Tokyo Japan ,k-ohashi@nmri.go.jp
² Paul Scherrer Institute, Villigen PSI 5232, Switzerland, yohei.sato@psi.ch
³ Yokohama National University, 79-5 Tokiwadai Hodogaya Yokohama Kanagawa Japan, hino@ynu.ac.jp

Key words: OpenMP, MPI, Hybrid, RANS, Parallel computing

Abstract. The speed up ratio of three parallel computing method, pure OpenMP, flat MPI and hybrid method is compared on practical applications. Flow computations around 2D flat plate and a practical ship hull form are selected as test cases. Pure MPI method shows a good performance on the number of the data communication cells which is under 10% of all cells. Hybrid method with lowest number of MPI succeeds to reduce the data communication when the data communication load is heavy, and shows better performance than other methods.

1 INTRODUCTION

Recently, RANS simulations are being applied to practical design problems including ship hull form design, and the reduction of computational time is required to obtain many results for design trials. Processors are also remarkably progressing in year by year and most of CPUs have many cores in one architecture with large cache. There are two major ways of parallel computing, OpenMP and MPI. OpenMP uses stored data in shared memories without domain decomposition and communication across nodes, although it is limited to a single node. A computational domain is divided during pre-process and data is stored in distributed memories in case of MPI. Generally, MPI has an advantages in a large scale computing and it has already proved. Additionally, a hybrid method of OpenMP and MPI is effective when the communication across nodes consumes larger time as in case of using supercomputers[1]. However, parallel computations are usually limited to a few nodes in a practical use.

A comparative study of parallelization methods using OpenMP, MPI and hybrid method in practical applications is carried out in the present study. The flow computations around a flat plate and a practical hull form are selected as test cases. The computational grids of both cases are divided until 32 domains for MPI method. All computations are carried out on practical cluster nodes, and the speed up ratio of three parallel computing methods is compared.

2 COMPUTATIONAL METHOD

An in-house unstructured CFD solver[2, 3] is used. This solver employs unstructured grids and has capability of handling complex geometry. The governing equations are 3D RANS equations for incompressible flows. Artificial compressibility approach is used for the velocity-pressure coupling. A cell-centered layout is adopted in which flow variables are defined at the centroid of each cell. Spatial discretization is based on a finite-volume method and inviscid fluxes are evaluated by the second-order upwind scheme based on the flux-difference splitting of Roe. The evaluation of viscous fluxes is also second-order accurate. The linear equation system is solved by the symmetric Gauss-Seidel (SGS) method, and the multi-color Gauss-Seidel method(MCGS)[4] is employed in case of OpenMP to avoid the data race condition. In case of MCGS method, the solution of linear equation can be obtained from the following equations

$$x_i^{m+1} = \frac{1}{a_i} \left(b_i - \sum_{j=j}^{j+nf} a_{ij} x_j^m \right) \quad (i: cells \ painted \ with \ 1st \ color) \tag{1}$$

$$x_i^{m+1} = \frac{1}{a_i} \left(b_i - \sum_{j=j}^{j+nf} a_{ij} x_j^{m \text{ or } m+1} \right) \quad (i: cells \text{ painted with } 2nd \text{ color})$$
(2)

x is an unknown variable, a and b are known coefficient or variable. The subscript i is cell index, j is cell index adjacent to the cell i which has n_f faces, m is iteration counter of the Gauss-Seidel method. The cells are painted as the way, (i) a target cell is specified, (ii) check the colors of the neighbor cells of the target cell. If there exists a color, paint the target cell in the new color, (iii) iterate until all the cells painted. The data race condition is avoided by the coloring method which paint the neighbor cells with the other colors of the specified cell. Then, unknown variable x is obtained by the equation (1)(2) with the iteration count m on each color level.

Agglomeration multigrid method and the local time stepping method is adopted for the fast convergence. The MCGS method is also applied to the grid in each multi grid level. Domain decomposition is achieved by using METIS[5] for MPI and hybrid method. The computational grid is divided into the grids which have almost the equal cell number to each other to maintain the load balance. The boundary faces are minimized to reduce the data communication. Data communications on MPI are required several times to set the boundary conditions in one time step and in each Gauss-Seidel iteration to synchronize the solutions of neighboring domains. All the computations are carried out on the SMP cluster with Intel Xeon E5-2680(2.7GHz, 8 cores), 64GB memory and 1GbE for communication.

3 RESULTS



Figure 1: Speed up ratio of case1

At first, a flow computation around 2D flat plate is carried out (case1). The computational grid consists of 97,000 structured cells. Three level multigrid is adopted. The grid is painted with two colors by the coloring algorithm on the fine grid, then six colors on the medium and coarse grids in OpenMP and hybrid method. Almost 2% cells are the domain-decomposition boundary cells (communication cells) in case of 32 decompositions. Fig.1 shows the results of the speed up ratio. The speed up ratio of MPI is excellent and shows the ideal performance. The result of OpenMP is less efficient than MPI. The iteration process of MCGS with fewer cells in each color may spend more time. The results of hybrid method is also less efficient than MPI results. The speed up ratio is improved with the increase of the number of MPI processes and the decrease of the thread number of OpenMP.

Next, the flow around a practical hull form[6] is computed (case2). The computational grid has about 900,000 of structured cells. Three level multigrid is adopted again. The grid is painted with two colors on the fine grid, then 8 colors on the medium and 10 colors on the coarse grids in OpenMP and hybrid method. Fig.2 shows the computational grid of 32 parallel MPI. Almost 25% cells are communication cells in case of 32 domain decomposition. Fig.3 shows surface meshes and pressure distribution on the ship hull surface. Surface pressure shows typical distributions, fore region is high, then lower pressure regions appear in the ship hull shoulder region.



Figure 2: Computational grids of 32 parallel MPI

Fig.4 shows the results of speed up ratio. The results of OpenMP show better performance than the results of case1. The number of cells in each color of MCGS increases and the time for iteration process is relatively decreasing. Although the speed up ratio of MPI shows a good performance up to 8 processes, the ratio gradually deviates from the ideal. The data communication requires longer time due to the larger number of communication cells. The hybrid method shows a good performance with 2 MPI processes and 16 threads. Fig.5 shows the fine grid which is divided and painted with the coloring algorithm on hybrid method of 2 parallel MPI with 16 threads. Blue color region is the cells for the data communication of MPI. OpenMP with shared memories succeeds to reduce the data communication on the hybrid method in this case.

4 CONCLUSIONS

The following conclusions are addressed.

- OpenMP with the MCGS method shows better performance with fixed amount of cells in each color and the hybrid method shows a good performance in case data communication load is heavy.
- At most 10% of all cells for data communication cells is preferable for the flat MPI method in the present study.

REFERENCES

[1] Nakajima, K., Three-level hybrid vs. flat MPI on the Earth Simulator: Parallel iterative solvers for finite-element method, *Applied Numerical Mathematics* (2005)



Figure 3: Surface meshes and pressure distribution on ship hull surface with 32 parallel MPI



Figure 4: Speed up ratio of case2

54(2):237–255.

- [2] Hino, T., A 3D Unstructured Grid Method for Incompressible Viscous Flows, J. of the Soc. Naval Archit. Japan (1997) 182.
- [3] Hino, T., An Interface Capturing Method for Free Surface Flow Computations on Unstructured Grids, J. of the Soc. Naval Archit. Japan (1999) 186.
- [4] Sato, Y., Hino, T., Ohashi, K. Parallelization of an unstructured Navier-Stokes solver using a multi-color ordering method for OpenMP, *Computers & Fluids* (2013) 88:496–509.



Figure 5: Computational grid painted with the coloring algorithm on hybrid method of 2 parallel MPI with 16 threads

- [5] Karypis, G. and Kumar, V., A Fast and Highly Quality Multilevel Scheme for Partitioning Irregular Graphs, SIAM Journal on Scientific Computing (1999) 20 No. 1:359–392.
- [6] Larsson, L., Stern, F., Visonneau, M., A Work shop on Numerical Ship Hydrodynamics Gothenburg 2010