TSC method using semi-implicit method for spring mass simulation

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1. INTRODUCTION

There are two possible ways to parallelize time evolution simulations: in the time direction and in the spatial direction. TSC method [1] parallelizes the simulation in the time direction. It approximately calculates Jacobi matrix of the whole time step equations and updates all variables over all-time steps iteratively. However, the approximated Jacobi matrix often becomes unstable especially when the number of time steps becomes large.Semi-implicit method [2] was proposed to increase the time step width in molecular dynamics simulations. It reveals the method to stabilize the Jacobi matrix by neglecting the negative eigenvalue parts of the elemental Hessians.

We incorporate the stabilized Jacobi matrix calculation of Semi-implicit method to TSC method, and evaluate the performance.

2. TSC METHOD

The TSC method approximately solves the Jacobi matrix equation derived from the Newton method for all time steps. In the method, the coarsening in the time direction is used to reduce the computational cost.

All time steps of the time evolution problem can be written in the form of a nonlinear system of simultaneous equations (1). where u_i denotes the variable for the i-th time step, g_i denotes the constant term for each time step. This simultaneous equation can be solved by iterative solution of linearized equation (2) as in Newton method. $\Delta \boldsymbol{u_i}$ and $\Delta \boldsymbol{r_i}$ denote the corrected solution and residual at each time step, respectively.

$$\begin{cases} \boldsymbol{u_0} = \boldsymbol{g_0} \\ \boldsymbol{A}(\boldsymbol{u_1}, \boldsymbol{u_0}) = \boldsymbol{g_1} \\ \boldsymbol{A}(\boldsymbol{u_2}, \boldsymbol{u_1}) = \boldsymbol{g_2} \\ \vdots \\ \boldsymbol{A}(\boldsymbol{u_i}, \boldsymbol{u_{i-1}}) = \boldsymbol{g_i} \end{cases} (1) \quad \begin{pmatrix} J_0 & & & \\ K_1 & J_1 & & \\ & \ddots & & \\ & & K_i & J_i \end{pmatrix} \begin{pmatrix} \Delta \boldsymbol{u_0} \\ \Delta \boldsymbol{u_1} \\ \Delta \boldsymbol{u_2} \\ \vdots \\ \Delta \boldsymbol{u_i} \end{pmatrix} = \begin{pmatrix} \Delta \boldsymbol{r_0} \\ \Delta \boldsymbol{r_1} \\ \Delta \boldsymbol{r_2} \\ \vdots \\ \Delta \boldsymbol{r_i} \end{pmatrix} (2)$$

3. SEMI-IMPLICIT METHOD

The semi-implicit method is a stable method for solving simulations by correcting the eigenvalues of the Jacobi matrix so that they do not become negative. When the eigenvalue of the Jacobian matrix becomes less than a certain value, correction is performed based on the coefficient of friction. It is possible to set how much negative values are allowed by the parameter ω. In this study, only the method for generating the Jacobi matrix of the semi-implicit method is used to stabilize the Jacobi matrix calculation of TSC method.

4. RESULTS

The time evolution simulation is a spring mass point simulation, in which three mass points are connected in a triangle in two dimensions to simulate the motion in a viscous liquid.

Figure 1 shows the results of running the conventional and proposed methods for 16384 time-step simulation. The horizontal axis is the number of parallelism, and the vertical axis is the speed up ratio between the sequential and the parallel runs. The speed up ratio is calculated by theoretical execution time based on the number of iteration for convergence.

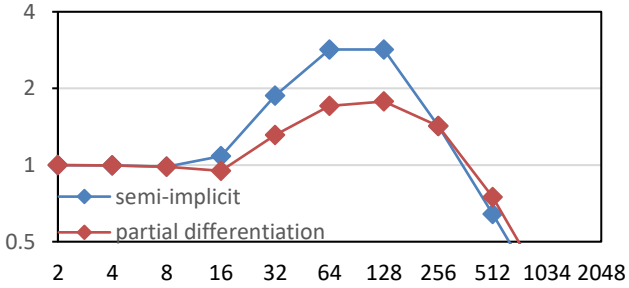

Figure 1. Speed up ratio of the TSC methods with different degrees of parallelism

5. CONCLUSION

The introduction of the semi-implicit method to the TSC method in spring mass point simulations increases stability and accelerates convergence. However, there are other time step simulations where the number of iterations does not improve or deteriorates. Therefore, it is necessary to analyze under what conditions convergence improves.

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