A Localized Implicit Method for Accelerating Conjugate Gradient Method in PDE Simulation

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1 INTRODUCTION

The conjugate gradient (CG) method is a crucial technique in PDE simulations. This study focuses on a CG method that finds an unknown vector $\boldsymbol{x}^{t+1}$ by solving an N-dimensional linear system (1). Let t represent a simulation time step ($t \geq 0$). The linear system is specified by a coefficient matrix $\boldsymbol{A} = (a_{i,j})$ and a right-hand vector $\boldsymbol{b} = (b_i)$.

$$\sum_{j \in T} a_{i,j} x_j^{t+1} = b_i \qquad (\forall i \in T), \tag{1}$$

where $T = \{0, 1, \ldots, N-1\}$ denotes a set of the computational points in the simulation domain.

There have been studies [1, 2] for accelerating CG-based PDE simulation by partitioning the simulation domain. An appropriate partition requires domain knowledge of the simulation model, which limits the applicability of the acceleration methods.

We propose an alternative acceleration method based on the localization in a coefficient matrix. Since the coefficient matrix is an abstraction of the simulation domain, the proposed method is easily applicable without domain knowledge.

2 METHOD

The core idea for acceleration is to approximately divide the linear system into localized subsystems; the k-th subsystem is defined as (2) by a partial coefficient matrix $\boldsymbol{A}_k$, a partial right-hand vector $\boldsymbol{b}_k$, and an approximate partial solution $\boldsymbol{x}_k^{t+1}$. Figure 1 illustrates the concept of the proposed method. The method decomposes $\boldsymbol{A}$ into block sub-matrices on its diagonal.

$$\boldsymbol{A}_k \boldsymbol{x}_k^{t+1} = \boldsymbol{b}_k. \tag{2}$$

In order to solve the subsystems individually, the proposed method ignores the dependency between the subsystems but instead adds approximate boundary conditions (highlighted in red). We use an explicit solution of the entire linear system for the approximation.

The accuracy of the proposed method relies on the distribution of the non-zero elements in a coefficient matrix. The more non-zero elements concentrate in the diagonal, the fewer boundary conditions the proposed method approximates. Consequently, the proposed method is useful for nearest-neighbor interaction models because such models result in a strongly diagonal distribution.

In the localization phase, the proposed method constructs the localized subsystems given the block size B. We determine a subset of computational points T_k to be solved in the k-th subsystem:

$$T_k = \{j \in T \mid \left\lfloor \frac{j}{B} \right\rfloor = k - 1\}. \tag{3}$$

We then approximate x_j^{t+1} for all $j \in (T \setminus T_k)$ in (1) as an explicit solution $\hat{x}_j^{t+1} = \Sigma_{l \neq j} a_{j,l} x_l^t / a_{jj}$. Summing up the approximated terms as a boundary condition $c_i = \sum_{j \notin T_i} a_{i,j} \hat{x}_j^{t+1}$, we obtain the following approximate B-dimensional linear system since $|T_k| = B$.

$$\sum_{j \in T_k} a_{i,j} x_j^{t+1} \approx b_i - c_i \qquad (\forall i \in T_k). \tag{4}$$

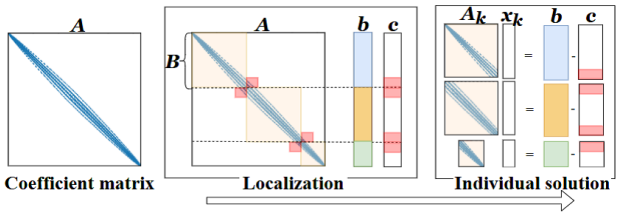

Figure 1: Overview of the proposed method.

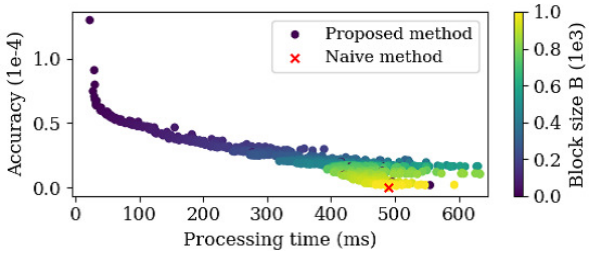

Figure 2: Speed-accuracy tradeoff for varying B.

In the individual solution phase, the proposed method applies a CG method to solve each subsystem derived as (4). The worst computational complexity of the proposed method $O(NZ(\boldsymbol{A}_k))$ is less than that of a naive implicit method $O(NZ(\boldsymbol{A}))$, where $Z(\boldsymbol{A})$ is the number of the non-zero elements in $\boldsymbol{A}$.

3 EVALUATION

We evaluated the processing time and the accuracy per simulation time step with varying B. The accuracy is represented by the mean squared error between the solution with the proposed method and that with the naive implicit method . We employed 2-D FEM that calculates the heat conduction of a cylindrical aluminum plate of 5012 computational points ($N = 5012$).

As shown in Figure 2, a small block reduced the processing time in exchange for an accuracy loss. The rapid decrease in the accuracy against the gentle increase in processing time suggests that an appropriate choice of B provides a fast approximation of the solution with a small accuracy loss.

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