A Matrix-Free Conjugate Gradient Method for Cluster Computing ⋆

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Abstract

The conjugate gradient method is applied to a large, sparse, highly structured linear system of equations obtained from a finite difference discretization of the Poisson equation. The matrix-free implementation of the matrix-vector product is shown to be optimal with respect to both memory usage and performance. The parallel implementation of the method can give excellent performance on a cluster of workstations, with the optimal number of processors depending on the quality of the interconnect hardware. This justifies the use of the method as computational kernel for the time-stepping in a system of reaction-diffusion equations.

Key words: Poisson equation, finite difference method, matrix-free iterative method, conjugate gradient method, cluster computing
2000 MSC: 35J05, 65F10, 65F50, 65N06, 65Y05

The concentration of calcium ions (Ca^{2+}) in human heart cells controls the beating of the heart [1–3]. The time-evolution of the concentration of the calcium ions is modeled by a system of coupled non-linear reaction-diffusion equations involving n_s chemical species. The model developed in [1–3] describes this evolution of the concentrations of calcium $c^{(0)}$ and of several indicator and buffer species $c^{(1)}$, …, $c^{(n_s-1)}$ by

$$\frac{\partial c^{(0)}}{\partial t} - \nabla \cdot \left(D^{(0)} \nabla c^{(0)} \right) = \left(\sum_{j=1}^{n_s-1} R^{(j)}(c^{(0)}, c^{(j)}) \right) + R^{(0)}(c^{(0)}) + \sigma(c^{(0)}, x, t),$$
$$\frac{\partial c^{(i)}}{\partial t} - \nabla \cdot \left(D^{(i)} \nabla c^{(i)} \right) = R^{(i)}(c^{(0)}, c^{(i)}), \quad i = 1, \ldots, n_s - 1, \qquad (1)$$

⋆ This work is part of undergraduate research performed by the first author.

with the reaction terms

$$R^{(i)}(c^{(0)}, c^{(i)}) = -k_i^f c^{(0)} c^{(i)} + k_i^b \left(\bar{c}_i - c^{(i)}\right), \quad i = 1, \ldots, n_s - 1, \qquad (2)$$

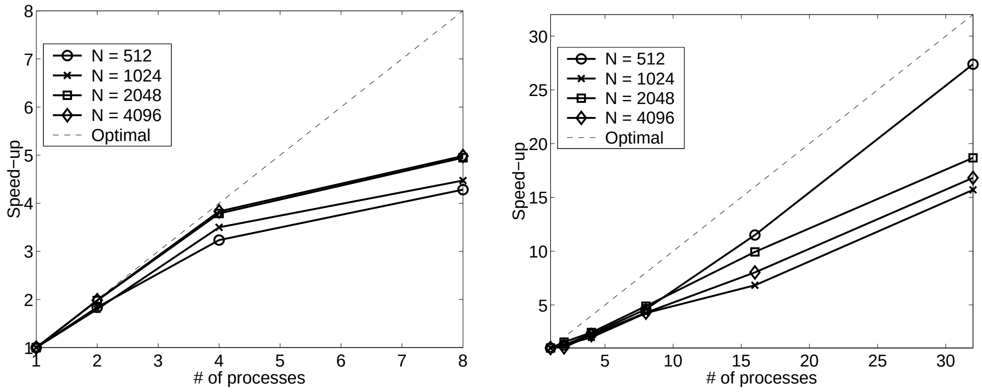
and the short-hand notation $R^{(0)}(c^{(0)}) = -J^{(pump)}(c^{(0)}) + J^{(leak)}$. All functions $R^{(i)}$ are given, and the diffusivity matrices $D^{(i)}$ are constant, diagonal, and positive definite. The term $\sigma(c^{(0)}, x, t)$ models the release of the calcium from the calcium release units throughout the cell by indicator functions in time and Dirac delta functions in space; see [4,5] for more details. The domain $\Omega \subset \mathbb{R}^3$ is the interior of the cell and is reasonably modeled as a parallelepiped.

This paper presents such a fine-grained parallel, matrix-free implementation of the conjugate gradient method and analyzes its parallel performance on a cluster of loosely coupled workstations. Since the iterative method used for all linear solves at every time step will be the computational kernel of the solution of (1), its optimization and careful analysis are relevant to the performance of the overall method.

Instead of the full application problem (1), a classical prototype problem, used in many textbooks is considered to isolate the analysis. We consider a finite difference discretization of a Poisson equation on a unit square with a known solution. The resulting linear system shares all relevant features with the application problem: The system matrix is symmetric positive definite, very sparse, and highly structured with constant coefficients to allow for an efficient matrix-free implementation of the matrix-vector product needed in the conjugate gradient method.

Results for a two-dimensional domain are presented here, but the performance of the method on a three-dimensional domain will be equivalent for comparable numbers of degrees of freedom. The matrix-free implementation allows the solution of an approximation with over 16.7 million degrees of freedom in serial on a machine with 1 GB of memory. Speedup studies for cases up to this size are performed on three different clusters of workstations: One 8-processor cluster and one 64-processor cluster are loosely coupled by 100 Mbps and 1 Gbps ethernet interconnects, respectively; the third cluster is a tightly coupled 64-processor cluster with high-performance Myrinet interconnect. The parallelism of the matrix-free matrix-vector product in the conjugate gradient method gives good performance for only up to 4 processors on the loosely coupled clusters. To obtain excellent performance for up to at least 32 processors, the tighter coupling with a high performance interconnect is needed. These results validate the use of the method as computational kernel for the application problem (1).

In Figure 1 (a), we see as N becomes larger, the factor of speedup approaches a factor of 5 for 8 processes with each plot using nonblocking communication on the 8 processor cluster. We conclude that for this loosely coupled cluster



(a) (b)

Fig. 1. Plot of the observed speedup of the conjugate gradient method for $N = 512$, 1024, 2048, and 4096 using nonblocking communication on the (a) 8 processor cluster with 100 Mbps ethernet interconnect and (b) 64 processor cluster with a Myrinet interconnect. The optimal case of linear speedup is shown for comparison.

with 100 Mbps ethernet interconnect, the use of 4 processors constitutes the most efficient use of resources.

Figure 1 (b) shows that the timings continue to improve significantly all the way up to 32 processors with a high performance Myrinet interconnect.

The parallel performance studies on clusters with three different interconnects show that the conjugate gradient method requires high performance interconnect hardware to scale well beyond 4 processors.

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