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A Parallel Adaptive Treecode Algorithm for Evolution of Elastically Stressed Solids

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Abstract. The evolution of precipitates in stressed solids is modeled by coupling a quasi-steady diffusion equation and a linear elasticity equation with dynamic boundary conditions. The governing equations are solved numerically using a boundary integral method (BIM). A critical step in applying BIM is to develop fast algorithms to reduce the arithmetic operation count of matrix-vector multiplications. In this paper, we develop a fast adaptive treecode algorithm for the diffusion and elasticity problems in two dimensions (2D). We present a novel source dividing strategy to parallelize the treecode. Numerical results show that the speedup factor is nearly perfect up to a moderate number of processors. This approach of parallelization can be readily implemented in other treecodes using either uniform or non-uniform point distribution. We demonstrate the effectiveness of the treecode by computing the long-time evolution of a complicated microstructure in elastic media, which would be extremely difficult with a direct summation method due to CPU time constraint. The treecode speeds up computations dramatically while fulfilling the stringent precision requirement dictated by the spectrally accurate BIM.

AMS subject classifications: 65D30, 65N35, 74B05

Key words: Treecode, parallel, elasticity, boundary integral method.

1 Introduction

Crystal growth problem is of primary interest in different fields of science and technology. One example is the production of binary alloys via solid-solid phase transformations. The second/precipitate phase emerges from the mother/matrix phase by lowering

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the temperature and it then grows by diffusion. The morphological evolution of these precipitates raises keen interest in the materials science community, as these microstructures actually control the macroscopic behavior (e.g. mechanical strength) through their interactions (e.g. elasticity) with the surrounding matrix phase.

Computational approaches to this problem include phase field methods and boundary integral methods (BIM) among many others [5, 6, 18, 19, 24, 30, 32]. We will use a boundary integral method to solve the field equations and to track the motion of the interface between the matrix and the precipitate. The main advantage of the BIM is its high accuracy, dimension reduction, and exact treatment of the boundary conditions. Compared with phase field methods, it is not straightforward for BIM to handle phenomena like precipitate merge or splitting. For the problem studied here, we assume topology change does not occur. A review article on boundary integral methods in fluids and materials can be found in [14]. In a boundary integral method, an iterative method (e.g. GMRES) is often used to solve the dense and asymmetric linear systems for the discretized integral equations. In GMRES, to compute the matrix-vector multiplication, a direct summation method requires $\mathcal{O}(N^2)$ operations, where N is the dimension of the linear system or the number of computational points on the interface. The long time computation is prohibitively expensive for precipitates with complicated morphology, as a large N is necessary to resolve the interface. In practice, a fast summation method is used to reduce the computation cost from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$ or $\mathcal{O}(N\log N)$. Examples include the fast multipole method (FMM) [8, 12] and the treecode method [2, 21].

For our proposed problem, Akaiwa and Meiron studied the diffusional effects without elasticity using FMM [1]. Thornton *et al.* [31] performed a computational study of an anisotropic homogeneous problem. In their work, they used the fast multipole method to evaluate the boundary integrals. Jou, Leo, and Lowengrub [15] investigated an isotropic and inhomogeneous problem without fast summation methods. Note that the inhomogeneity requires solution of dipole strength to be used in the boundary integrals. In this paper, we dramatically improve the original methods in [15] by incorporating a time rescaling scheme [3, 20] and a parallel treecode algorithm. The detailed study of the rescaling scheme for this problem has been published in [3]. Here, we focus on the development of the treecode. In particular, we derive recurrence relations in Subsection 3.2 for various kernels used in our integral equations. We also perform the error analysis associated with the treecode approximation. Moreover, using a novel source dividing strategy, we develop an adaptive parallel treecode algorithm in Subsection 3.4. This approach of parallelization can be readily implemented in other treecodes with either uniform or non-uniform point distribution.

The fundamental idea of a treecode is a divide-and-conquer strategy. The Barnes-Hut treecode divides the space evenly into four children in the two-dimensional space [2], and then approximates a cluster of points by a single point at the cluster center with that point carrying all the weights of points in the cluster. Later, this idea is implemented for various kernels [9, 21]. When the size of a cluster is small compared to the distance between a point and the cluster, the treecode approximates point-cluster interactions us-