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Parallel re-initialization of level set functions on distributed unstructured tetrahedral grids

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ABSTRACT

Level set functions are employed to track interfaces in various application areas including simulation of two-phase flows and image segmentation. Often, a re-initializing algorithm is incorporated to transform a numerically instable level set function to a signed distance function. In this note, we present a parallel algorithm for re-initializing level set functions on unstructured, three-dimensional tetrahedral grids. The main idea behind this new domain decomposition approach is to combine a parallel brute-force re-initializing algorithm with an efficient way to compute distances between the interface and grid points. Time complexity and error analysis of the algorithm are investigated. Detailed numerical experiments demonstrate the accuracy and scalability on up to 128 processes.

1. Introduction

Moving boundaries occur in various scientific and engineering problems. Burning flames, gas–liquid mixtures, and oil droplets in a surrounding liquid are illustrating examples of multi-phase flows. The boundaries between phases can be described either implicitly or explicitly. In this paper, we are concerned with an implicit representation of boundaries by the level set approach [1]. Here, the boundary is represented by the zero level of a scalar-valued level set function φ whose movement is described by a partial differential equation (PDE). In the context of multi-phase flow problems, the flow is commonly governed by a set of time dependent PDEs involving the level set function to distinguish the different phases from each other.

When solving the PDEs for the flow and the level set function, numerical stability requires to preserve the level set function to be smooth in the vicinity of the interface. To this end, the aim of extension velocities [2,3] is to construct a flow field for moving φ such that the level set function is kept smooth. An alternative is given by re-initializing the level set function whenever the smoothness is lost. The discussion of pros and cons of these two alternatives is beyond the scope of this paper. Here, the focus is on re-initializing the level set function. The objective of the re-initialization procedure is to re-parametrize the level set function φ in the computational domain $\Omega \subset \mathbb{R}^d$, where $d = 2, 3$. More precisely, given a level set function with zero-level on an interface $\Gamma \subset \Omega$, determine φ such that the zero level is preserved, i.e.,

$$\varphi(\mathbf{x}) = 0, \quad \mathbf{x} \in \Gamma,$$

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and, furthermore, the Eikonal equation

$$\|\nabla\varphi\|_2 = h(\mathbf{x}), \quad \mathbf{x} \in \Omega, \tag{1}$$

is satisfied. Here, h denotes a given speed function in Ω. In the context of two-phase flow problems on adaptively refined grids, it is useful to consider the special case of (1) where the property

$$\|\nabla\varphi\|_2 = 1, \quad \mathbf{x} \in \Omega, \tag{2}$$

allows to measure the distances of any $\mathbf{x} \in \Omega$ to the interface. Here, φ is called a signed distance function with numerical advantages addressed in [4]. This property is also of interest when evaluating the surface tension force [5].

For real-world two-phase problems arising from different scientific and engineering disciplines, parallel computing is mandatory to cope with the high demand of time and storage requirement when solving these problems numerically. From a serial point of view, the time for the re-initialization is typically only a small fraction of the time to solve the flow problem. Thus, one might wonder that parallelization of the re-initialization procedure is not important. However, Amdahl's law [6] states that, even using infinitely many processes, the speedup of the overall time to solution is limited by the inverse of the fraction spent in the part of the solution that is not parallelized. For the parallel solution of the two-phase flow problem, this suggests to also take care of the parallelization of the re-initialization procedure. Moreover, today's dominating parallel programming model is based on a distributed-memory approach in which all parts of a simulation need to be parallelized. Therefore, in practice, it is indispensable to employ a parallel re-initialization algorithm.

The new contribution of our work is a parallel algorithm for re-initializing level set functions on unstructured, distributed grids. The main feature of this parallel algorithm is that a single grid of this type is used for both, the flow variables as well as the level set function. To this end, we combine two known algorithmic elements in a novel way. The first element consists of a brute-force re-initialization strategy. As the second element, a suitable multidimensional data structure is employed to reduce the time complexity. Neighborhood relations are computed with this tree data structure rather than with the data structure representing the unstructured grid. The main advantage of our approach is a high degree of parallelism. In summary, the main features of the new algorithm are:

1. applicability to unstructured three-dimensional grids,
2. serial expected runtime of $\mathcal{O}(N\log(N))$, where N is the number of degrees of freedom to represent φ,
3. high degree of parallelism.

The paper is organized as follows. In Section 2, we give a brief overview on related algorithms for solving the Eikonal equation. Our motivation of re-initializing level set functions stems from two-phase flow problems that are described in the context of the level set approach in Section 3. Then, we describe the brute-force algorithm to re-initialize level set functions in Section 4. The use of a suitable tree data structure to handle neighborhood relations in the re-initialization algorithm is sketched in Section 5. The new parallel re-initialization algorithm is described in Section 6 and analyzed in Section 7. Finally, in Section 8, we present various results with respect to complexity, accuracy, and performance.

2. Algorithms for solving the Eikonal equation

There are mainly the following classes of numerical techniques for solving the Eikonal equation (1). The first class consists of PDE-based methods. These methods offer the advantage of exploiting the full range of well-studied numerical techniques for structured as well as unstructured grids. In particular, PDE-based methods are known to be amenable to parallel computing [7] and provide a viable alternative for finite volume and finite difference methods. However, previous research using serial techniques based on finite elements indicated that such approaches tend to be numerically inadequate for two-phase flows [8]. Therefore, this class is not considered further in this paper; see [9] for a recent survey on PDE-based methods for the solution of (1).

The archetype of another class is the fast marching method (FMM), originally developed by Sethian [10] for Cartesian grids. It was later generalized to arbitrary triangulated surfaces [11], unstructured meshes [12], and any d-dimensional implicit hyper-surfaces [13]. The algorithmic complexity of the FMM is $\mathcal{O}(N\log(N))$ where N is the number of grid points. The reader is referred to [1] for a detailed overview. The FMM is based on a front propagation scheme and uses a heap data structure which makes it difficult to parallelize using a domain decomposition strategy. The first discussion on a parallel implementation of the FMM is given in [14] where four different strategies are compared for Cartesian grids. A recent technique [15] determines the flow field on an unstructured grid whereas the level set function is described on a Cartesian grid. Both grids are adaptively refined and distributed among processes. In [16], the FMM is separately applied on each sub-domain. This process is iteratively refined exchanging data across sub-domain boundaries. In contrast to a domain decomposition approach, the parallel FMM presented in [17] is based on distributing the interface and is discussed for Cartesian grids. To the best of our knowledge, there is no publication of any parallel FMM on unstructured grids.

In [18], the authors introduce the fast iterative method (FIM) which is designed for parallel computation on Cartesian grids. This recent method relies on a modification of a label correction scheme coupled with an iterative procedure for the grid point update. In contrast to the FIM, the fast sweeping method (FSM) [19] solves the Eikonal equation on a d-dimensional grid by performing 2^d directional sweeps in a Gauss–Seidel fashion. This sweeping idea of visiting nodes in a