Journal of Computational Physics 274 (2014) 393–412

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A fast marching approach to multidimensional extrapolation

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ARTICLE INFO

Article history:
Received 14 February 2014
Received in revised form 4 June 2014
Accepted 12 June 2014
Available online 19 June 2014

Keywords:
Fast marching method
Extrapolation
Hamilton–Jacobi equation
Eikonal equation
Level set method

ABSTRACT

A computationally efficient approach to extrapolating a data field with second order accuracy is presented. This is achieved through the sequential solution of non-homogeneous linear static Hamilton–Jacobi equations, which can be performed rapidly using the fast marching methodology. In particular, the method relies on a fast marching calculation of the distance from the manifold Γ that separates the subdomain Ω_{in} over which the quantity is known from the subdomain Ω_{out} over which the quantity is to be extrapolated. A parallel algorithm is included and discussed in the appendices. Results are compared to the multidimensional partial differential equation (PDE) extrapolation approach of Aslam (Aslam (2004) [31]). It is shown that the rate of convergence of the extrapolation within a narrow band near Γ is controlled by both the number of successive extrapolations performed and the order of accuracy of the spatial discretization. For m successive extrapolating steps and a spatial discretization scheme of order N, the rate of convergence in a narrow band is shown to be $\min(N+1, m+1)$. Results show that for a wide range of error levels, the fast marching extrapolation strategy leads to dramatic improvements in computational cost when compared to the PDE approach.

1. Introduction

Many applications of computational science and engineering involve extrapolating data located in a subregion of a computational space to the rest of the simulation domain. This is especially pertinent to the propagation of discontinuous fronts, which is a significant component of phenomena such as multiphase flows [1–10], supersonic flows [11], reacting flows [12–14], multiphase electrohydrodynamics [15,16], crack propagation [17,18], and image processing [19–21]. Calculations involving discontinuous fronts often suffer from numerical artifacts such as nonphysical oscillations and low orders of convergence [22,23], unless relevant quantities are extrapolated or extended across the front in order to avoid differentiating across discontinuities. A typical way of achieving this is by performing a constant extrapolation through the solution of a Hamilton–Jacobi type equation, as is the case in the original ghost fluid method [22,24,25] and a variety of other level set applications [1,26,2]. Another approach that circumvents Courant–Friedrichs–Lewy (CFL) limitations of a partial differential equation (PDE) extrapolation is the fast marching method (FMM), developed by Sethian [27] and Adalsteinsson and Sethian [28] for the solution of static Hamilton–Jacobi equations in the context of level set methods [29]. Constant FMM extrapolation has been recently employed to improve the accuracy of the conservative level set method [9]. The fast marching approach is proven to be much faster than a PDE approach, but Aslam [30] has argued that it would suffer from lower accuracy and a reduced rate of convergence under mesh refinement in some instances.

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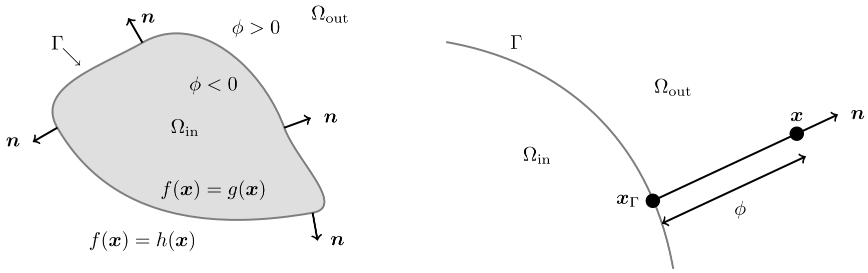
http://dx.doi.org/10.1016/j.jcp.2014.06.023
0021-9991/



(a) Various parameters for the extrapolation. (b) Close-up version of image to the left.

Fig. 1. Schematics illustrating the extrapolation scenario.

Multidimensional extrapolation in the context of the PDE method has been described by Aslam [31] and subsequently used in application to the Stefan problem [32,33]. Despite its straightforward adaptivity to multidimensional extrapolation, the FMM has not yet been analyzed in detail for higher order extrapolations, which may be attributed to the aforementioned concerns regarding rate of convergence and accuracy. The goal of this study is to present a quantitative comparison between the PDE-based and FMM-based extrapolation methods, analyzing both the speed and accuracy of each method.

This paper is organized as follows: in the next section, the mathematical framework for multidimensional extrapolation is given, including a derivation of the expected order of accuracy, followed by discussions of both PDE and FMM solution approaches in Sections 2.3 and 2.4, respectively. Provided in Section 3 is a discussion of the PDE and FMM implementations used in this work. The PDE methodology is similar to the implementation of Aslam [31]. Parallel implementation of the FMM procedure for level set re-initialization and subsequent data extrapolation is provided in Appendix A and Appendix B, respectively. Section 4 presents multidimensional extrapolation results for the canonical test case used by Aslam [31]. Finally, this test case is also adapted to an additional shape in Section 5, revealing some subtleties of the method that are worth consideration. From these tests it is shown that the FMM provides a computationally efficient means of performing second order accurate extrapolation.

2. Mathematical formulation

2.1. Problem description

Consider a domain Ω that contains a continuous surface Γ, such that it divides Ω into an inner subdomain Ω_{in} and an outer subdomain Ω_{out}, as illustrated in Fig. 1(a). Then consider the function $g(\boldsymbol{x})$ to be extrapolated, defined for all $\boldsymbol{x} \in \Omega$. To simplify the discussion, the function $g(\boldsymbol{x})$ is considered here to be a scalar without loss of generality. There exists a signed distance level set $\phi(\boldsymbol{x}) = \pm\|\boldsymbol{x} - \boldsymbol{x}_\Gamma\|$, where $\boldsymbol{x}_\Gamma$ is the location on Γ that provides the minimum Euclidean distance from location $\boldsymbol{x}$, as shown in Fig. 1(b). The sign of ϕ is negative in the domain Ω_{in} and positive in the domain Ω_{out}. The level set ϕ is an auxiliary function to our discussion and, given ϕ, a smooth field of normal vectors is obtained from

$$\boldsymbol{n} = \frac{\nabla\phi}{\|\nabla\phi\|}, \tag{1}$$

oriented outward from Ω_{in}.

For any point $\boldsymbol{x} \in \Omega_{\text{out}}$, the function $h(\boldsymbol{x})$ is defined as the mth order Taylor Series expansion of g from $\boldsymbol{x}_\Gamma$, i.e.,

$$h(\boldsymbol{x}) = \sum_{k=0}^{m} \frac{\phi^k}{k!} \frac{\partial^k g}{\partial\phi^k}\bigg|_{\boldsymbol{x}_\Gamma}. \tag{2}$$

Note that the $\boldsymbol{x}$ dependence of ϕ has been dropped for simplicity. We will build our extrapolation of g in the form of the function $f(\boldsymbol{x})$, written as

$$f(\boldsymbol{x}) = \begin{cases} g(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in \Omega_{\text{in}}, \\ h(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in \Omega_{\text{out}}. \end{cases} \tag{3}$$

It is clear that $f(\boldsymbol{x})$ should be $\mathcal{C}^m$ continuous across Γ.

2.2. Expected accuracy

When obtaining f for a set of numerical data, it is clear from Eqs. (2) and (3) that the resulting accuracy of the extrapolated f field in Ω_{out} will depend on both m and the accuracy of the discrete representation of $\partial^k g/\partial\phi^k|_{\boldsymbol{x}_\Gamma}$. Assuming that $\boldsymbol{n}$ is horizontal and $\boldsymbol{x}_\Gamma = 0$ such that the distance from Γ is described by the variable x, we introduce a discrete upwind operator $\mathcal{U}$ that approximates the first derivative of a function with order of accuracy N such that

$$g'_i = \mathcal{U}(g_i) + \mathcal{O}(\Delta x^N), \tag{4}$$