Journal of Computational Physics 229 (2010) 2948–2963

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Trefftz difference schemes on irregular stencils

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ARTICLE INFO

Article history:
Received 7 June 2009
Received in revised form 31 October 2009
Accepted 21 December 2009
Available online 4 January 2010

Keywords:
Flexible local approximation
Finite difference schemes
Trefftz functions
Electrostatics
Wave propagation
Wave scattering
Electromagnetic waves
Multiparticle problems
Long-range interactions
Irregular stencils
Meshless methods
Least squares approximation

ABSTRACT

The recently developed Flexible Local Approximation MEthod (FLAME) produces accurate difference schemes by replacing the usual Taylor expansion with Trefftz functions – local solutions of the underlying differential equation. This paper advances and casts in a general form a significant modification of FLAME proposed recently by Pinheiro and Webb: a least-squares fit instead of the exact match of the approximate solution at the stencil nodes. As a consequence of that, FLAME schemes can now be generated on irregular stencils with the number of nodes substantially greater than the number of approximating functions. The accuracy of the method is preserved but its robustness is improved. For demonstration, the paper presents a number of numerical examples in 2D and 3D: electrostatic (magnetostatic) particle interactions, scattering of electromagnetic (acoustic) waves, and wave propagation in a photonic crystal. The examples explore the role of the grid and stencil size, of the number of approximating functions, and of the irregularity of the stencils.

1. Introduction

Traditional finite difference analysis relies primarily on Taylor expansions. These are quite general but are accurate only if the underlying solution has the level of smoothness commensurate with the order of the expansion. In particular, the Taylor approximation breaks down at material interfaces due to jumps in the solution and/or its derivatives. This leads to the well known "staircase effect" in difference schemes (see a discussion of the algebraic nature of this numerical artifact in [1,2]). Other common situations where the Taylor series, and hence the corresponding classical schemes, are inaccurate include boundary layers and sharp peaks or singularities in the vicinity of sources, edges and corners.

The Flexible Local Approximation MEthod (FLAME) [1,2] replaces the Taylor polynomials with much more accurate "Trefftz" approximations by local solutions of the underlying differential equation. As a result, the approximation accuracy and consequently the consistency error of the scheme can be improved dramatically.

Previously, FLAME relied on the point-matching of the nodal values of the local approximation. To fix the key idea, consider a nine-point (3×3) scheme for the Laplace equation in 2D. The solution is approximated locally as a linear combination of eight Trefftz functions, harmonic polynomials being the most natural choice. [1] With nine nodes and only eight free parameters, the nodal values must be linearly dependent. It is the linear relationship between them that constitutes the FLAME

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[1] There are of course other possibilities: e.g. functions $r^m \exp(im\phi)$ $(m = 0, \pm 1, \pm 2, \ldots)$ in a polar coordinate system (r, ϕ) or Green's functions of the form $|\mathbf{r} - \mathbf{r}_{src}|^{-1}$, where the source $\mathbf{r}_{src}$ is located away from the given stencil [3], etc.

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doi:10.1016/j.jcp.2009.12.025

scheme. Details and a large variety of examples can be found in [1,2,4–7]; the applications include electro-and magnetistatics, wave propagation and scattering, the Poisson–Boltzmann equation in macromolecular and colloidal simulation.

One limitation of the point matching procedure is that it links the number of approximating functions and stencil nodes, as evident from the above example of eight basis functions for the nine-point stencil. This connection between functions and nodes has impeded further progress of the method in two different ways.

First, the most natural choices of the stencil and the basis set have not always been feasible. For instance, consider the standard 3×3 stencil in 2D problems involving cylindrical particles. A natural choice of the basis in such cases is cylindrical harmonics [2,5,7] that include the exponential factors $\exp(\mathrm{i}m\phi), m = 0, \pm 1, \pm 2, \ldots$, where ϕ is the polar angle. Since these harmonics come in pairs $\pm m$ for all m except $m = 0$, the "natural" number of functions in this basis is odd.

At the same time, to obtain a FLAME scheme on the nine-point stencil, one must choose eight basis functions, which breaks the natural symmetry: only one index m from the pair $m = \pm 4$ can be taken. This is more of a nuisance than an actual detriment because all harmonics up to order $m = 3$ are still included.

A more serious obstacle is that large stencils (in terms of the number of nodes) require in the established version of FLAME a commensurately large number of basis functions. Unfortunately, expanded basis sets tend to be poorly conditioned. Yet large stencils are highly desirable in some circumstances, in particular for irregular distributions of nodes where small stencils can be strongly distorted and unreliable [8]; including more nodes in the stencil tends to increase robustness.

The disparity between the desirable number of basis functions and stencil nodes became particularly apparent in three-dimensional electromagnetic vector problems. If the number of basis functions is commensurate with the number of the nodal degrees of freedom (number of stencil nodes times three Cartesian components), the basis sets become ill-conditioned. Pinheiro and Webb recently overcame this difficulty by using a relatively small number of approximating functions and applying a least-squares match of the nodal values [9]. It is this idea that is further advanced in the present paper.

The use of least squares matching allows one to relax or even sever the connection between the basis functions and the stencil. This facilitates the construction of FLAME on non-canonical irregular stencils. So far FLAME has mostly been used on regular Cartesian grids – not as a requirement but as a practical matter, to avoid dealing with distorted/skewed stencils. An exception to this practice was adaptive FLAME in [8], where complications due to irregular distributions of nodes in adaptive refinement stencils had to be overcome.

Irregular and adaptive node arrangements are in general highly desirable because the nodes can be concentrated in areas where they are needed the most, in contrast with a regular grid that can only be refined globally. The least squares FLAME described in this paper works on non-canonical stencils more reliably than the previous versions of FLAME.

Irregular stencils are clearly a feature that the new approach, least-squares FLAME, shares with meshless methods (see reviews [10,11]). Another feature that is shared – albeit superficially (see below) – is the least squares matching. I shall, however, refrain from referring to least squares FLAME as a meshless method, for the following reasons.

The primary and defining feature of FLAME is the accurate Trefftz approximation; "meshlessness" is secondary. Approaches that have come to be known as "meshless methods" are associated with quite different approximations. Moving least squares (MLS) techniques, the "reproducing kernel particle method" (RKPM) [11,13,10], and, most recently, maximum-entropy approximations [16,17] are part and parcel of meshless techniques but are quite foreign to FLAME.

Also, the similarity between least squares FLAME and the established meshless methods does not go very far. MLS, RKPM or maximum-entropy functions in meshless methods are subject to costly numerical integration and differentiation. In contrast, no integration or differentiation is needed in FLAME at all.

The use of the least squares fit in both MLS and FLAME is also a superficial similarity. In MLS, the approximation is "moving," in the sense that the coefficients of the relevant polynomial expansion vary from point to point and are found via a least squares match at the nodes. The spatial variation of the coefficients complicates the differentiation and integration that need to be carried out in the numerical procedure. In FLAME, the approximation is usually non-polynomial and "static": the coefficients are fixed for any given stencil. Further notes on meshless methods can be found in Section 6.

Connections of FLAME with other classes of numerical methods such as variational Trefftz methods, GFEM, Discontinuous Galerkin, variational-difference schemes by Moskow *et al.* [18], discontinuous enrichment and others have previously been discussed in great detail [1]; see in particular Sections 1 and 2, Fig. 1, and references in that paper. Here I briefly comment on a few additional contributions, some of them recent.

There is a well established and respectable body of work on special high-order schemes for various types of problems, in particular the Helmholtz equation [19–24]; see Harari's review [19] for further information and references. There is a commonality of goals but not of the methodology between these techniques and FLAME.

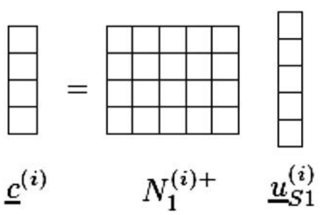

Fig. 1. Matrix dimensions in (14) for $n_1^{(i)} = 5, m = 4$.