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A class of difference schemes with flexible local approximation

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Abstract

Solutions of many physical problems have salient local features that are qualitatively known a priori (for example, singularities at point sources, edge and corners; boundary layers; derivative jumps at material interfaces; strong dipole field components near polarized spherical particles; cusps of electronic wavefunctions at the nuclei; electrostatic double layers around colloidal particles, etc.) The known methods capable of providing flexible local approximation of such features include the generalized finite element – partition of unity method, special variational-difference schemes in broken Sobolev spaces, and a few other specialized techniques. In the proposed new class of Flexible Local Approximation MEthods (FLAME), a desirable set of local approximating functions (such as cylindrical or spherical harmonics, plane waves, harmonic polynomials, etc.) defines a finite difference scheme on a chosen grid stencil. One motivation is to minimize the notorious 'staircase' effect at curved and slanted interface boundaries. However, the new approach has much broader applications. As illustrative examples, the paper presents arbitrarily high order 3-point schemes for the 1D Schrödinger equation and a 1D singular equation, schemes for electrostatic interactions of colloidal particles, electromagnetic wave propagation and scattering, plasmon resonances. Moreover, many classical finite difference schemes, including the Collatz "Mehrstellen" schemes, are direct particular cases of FLAME.

Keywords: Generalized finite difference method; Flexible approximation; Multiparticle problems; The Schrödinger equation; The Poisson–Boltzmann equation; Wave propagation; Scattering; Photonic crystals; Plasmon particles

1. Introduction: computational methods with flexible approximation

In many physical problems some salient features of the solution are qualitatively known a priori. Such features include singularities at point sources, edge and corners; boundary layers; derivative jumps at material interfaces; strong dipole field components near polarized spherical particles; cusps of electronic wavefunctions

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at the nuclei; electrostatic double layers around colloidal particles – and countless other examples. Such "special" behavior of physical fields is arguably a rule rather than an exception. Clearly, taking this behavior into account in numerical simulation will tend to produce more accurate and physically meaningful results.

The special features of the field are typically local, and in numerical modeling it is therefore desirable to employ various *local* approximations of the field. The focus of this paper is precisely on "flexible local approximation" and on methods capable of providing it – that is, employing a variety of approximating functions not at all limited to polynomials. It is from this angle that the existing approaches are reviewed (Section 2) and new ideas are considered. Section 4 introduces a new class of Flexible Local Approximation MEthods (FLAME), where the difference scheme is defined by the chosen set of local basis functions and the grid stencil.

One motivation for developing this class of methods is to minimize the notorious 'staircase' effect at curved and slanted interface boundaries on regular Cartesian grids. In the spirit of "flexible local approximation", the behavior of the solution at the interfaces is represented *algebraically*, by suitable basis functions on simple grids, rather than *geometrically* on conforming meshes. More specifically, fields around spherical particles can be approximated by several spherical harmonics; fields scattered from cylinders – by Bessel functions, and so on. Such analytical approximations are incorporated directly into the difference scheme.

This approach can be contrasted with very well known, and very powerful, finite element (FE) methodology, where the geometric features of the problem are represented on complex conforming meshes. The flexibility of approximation in FEM is achieved through adaptive mesh refinement: changing the mesh size (h-refinement) or the order of approximation (p-refinement). Still, approximation remains piecewise-polynomial; in fact, the polynomial space is an integral part of the standard definition of a finite element [22,17].

FEM is indispensable in many problems where the geometries are complex and material parameters vary. In addition to mechanical, thermal and electromagnetic modeling of traditional devices and machines, FEM has recently penetrated new areas of macromolecular simulation. Molecular interface surfaces can be viewed as intersections of hundreds or thousands of spheres and consequently are geometrically extremely complex. These interfaces separate the interior of the molecule, that can be approximated by an equivalent relative dielectric constant on the order of 1–4, from the solvent that in "implicit" models is considered as a continuum with equivalent dielectric and Debye parameters ([9,46,58,30,41,94,98] and references therein).

However, the computational overhead of mesh generation and matrix assembly in FEM is significant, and for geometrically simple problems FEM may not be competitive with finite difference (FD) schemes and other methods operating on simple Cartesian grids. One extreme example of geometric simplicity comes from molecular dynamics simulations, where charges or dipoles are typically considered in a cubic box with periodic boundary conditions. The Ewald algorithm (taking advantage of fast Fourier transforms) is then usually the method of choice.

Problems with multiple moving particles, such as for example in magnetically driven assembly [121,122], also call for development and application of new techniques. Generation of geometrically conforming FE meshes is obviously quite complicated or impractical when the particles move and their number is large (say, on the order of a hundred or more). Parallel adaptive generalized FEM has been developed [47–49], but the procedure is quite complicated both algorithmically and computationally. Standard FD schemes would require unreasonably fine meshes to resolve the shapes of all particles. An alternative approach is to use two types of grid: spherical meshes around the particles and a global Cartesian grid [44,36]. The electrostatic potential then has to be interpolated back and forth between the grids, which reduces the numerical accuracy.

The celebrated fast multipole method (FMM) has clear advantages for systems with a large number of known charges or dipoles in free space (or a homogeneous medium). For inhomogeneous media (e.g. a dielectric substrate, or finite size particles with dielectric or magnetic parameters different for those of free space) FMM can still be used as a fast matrix–vector multiplication algorithm imbedded in an iterative