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Compensated optimal grids for elliptic boundary-value problems

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ABSTRACT

A method is proposed which allows to efficiently treat elliptic problems on unbounded domains in two and three spatial dimensions in which one is only interested in obtaining accurate solutions at the domain boundary. The method is an extension of the optimal grid approach for elliptic problems, based on optimal rational approximation of the associated Neumann-to-Dirichlet map in Fourier space. It is shown that, using certain types of boundary discretization, one can go from second-order accurate schemes to essentially spectrally accurate schemes in two-dimensional problems, and to fourth-order accurate schemes in three-dimensional problems without any increase in the computational complexity. The main idea of the method is to modify the impedance function being approximated to compensate for the numerical dispersion introduced by a small finite-difference stencil discretizing the differential operator on the boundary. We illustrate how the method can be efficiently applied to nonlinear problems arising in modeling of cell communication.

1. Introduction

Many nonlinear problems in a broad range of applications in science and engineering lead to models which consist of coupled compartments of different spatial dimensionality (see e.g. [1–7]). For example, in many cell communication systems signaling molecules are emitted, interact with, and induce responses through the surfaces of cells forming a two-dimensional layer of epithelium while diffusing through the three-dimensional extracellular medium surrounding the epithelial layer [8] (for more details on this example, see the following section). Model formulation in such problems is complicated by the need, in general, to consider partial differential equations (PDEs) defined on two-dimensional surfaces (or even one-dimensional curves) in addition to the usual three-dimensional equations in the bulk. This mixture of spatial dimensions, especially on unbounded domains, naturally complicates the computational studies of these models.

Often in such problems, however, the equation in the bulk can be a simple linear PDE, as, e.g., in the case of the cell signaling example mentioned above where the concentration of the signaling molecule in the extracellular medium can be assumed to satisfy the diffusion equation in free space with some effective diffusion constant. In these cases it is possible to reduce the dimensionality of the problem via a boundary integral formulation. At the same time, such a formulation suffers from spatial (as well as temporal in the case of evolution problems) nonlocality which, once again, generally makes numerical studies of such problems difficult (for various approaches to this type of problems, see e.g. [9–14]).

A new approach to computing boundary data for linear second-order problems has been developed over the last decade which utilizes the concept of "optimal grids" [15–19]. This method applies a finite-difference discretization to the second-order elliptic operator, using a judiciously chosen sequence of unequal steps to accurately approximate the Neumann-to-

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Dirichlet (NtD) map associated with that operator in a number of simple geometries. The optimality of the approximation (in the sense which will be discussed in more detail in the following sections) allows to dramatically reduce the number of grid points in the direction normal to the boundary, making the dimensionality of the computational problem essentially equal to that of the boundary. This method has many advantages which make it a natural choice for the numerical studies of non-linear problems [20]. In particular, the method is second order-accurate in the size of spatial discretization of the boundary, and the size of the optimal grid can be chosen to match its accuracy with that of the finite-difference stencil on the boundary for all scales of the problem. When very high accuracy of the solution is not required, this approach results in very compact finite-difference approximation schemes for the original PDEs which are typically adequate for computational purposes.

Apart from increasing the size of the finite-difference grid, the most straightforward way to increase the accuracy of the optimal grid discretization would be to use a higher-order discretization for the transverse part of the differential operator in the bulk. This would increase the size of the stencil and naturally reduce the efficiency of the method. It appears, however, that the optimal grid method has the capacity for increasing the degree of accuracy of the obtained numerical solution on the boundary *without* increasing the size of the discretization stencil. Instead of resorting to higher-order stencils, one can attempt to modify the impedance function (for technical details see the following sections) in a way that it compensates for the numerical dispersion introduced by a small nearest-neighbor stencil. The obtained method, which we term the method of "compensated" optimal grids, is the subject of the present paper. We will illustrate this method with a number of examples in two- and three-dimensional elliptic boundary-value problems relevant to cell communication models. In particular, we will show that for two-dimensional problems on uniform grids along the boundary one could go from second-order to essentially spectral accuracy without increasing the computational complexity of the problem, while in three dimensions one can go from second- to fourth-order accurate method by either utilizing hexagonal lattices on the boundary or using a special 9-point stencil on square lattices.

Our paper is organized as follows. In Section 2, we give a motivating example from modeling cell communication by diffusing ligands. In Section 3, we review the method of optimal grids and introduce the idea of compensated optimal grids. Later on in this section we verify our method for a linear and an exactly solvable nonlinear problem. Then, in Section 4 we discuss ways to extend the two-dimensional version of the compensated optimal grids method to three dimensions. In Section 5, we present an application of our computational approach to a three-dimensional problem arising in cell communication modeling. Finally, in Section 6 we summarize our results.

2. Motivating example

We begin by discussing a typical example of a modeling setting in which the numerical issues discussed in this paper arise naturally [4]. Consider an idealized situation in which a flat epithelial layer is imbedded in a semi-infinite layer of extra-cellular medium (ECM), see Fig. 1. Cells at the bottom of the layer emit various signaling molecules which can then diffuse in the extracellular space and bind to their specific cell-surface receptors [8,22]. Binding of the signaling molecule to its respective receptor, in turn, activates the intracellular signaling cascades which elicit multiple cellular responses. Importantly, such responses may further regulate secretion of the acting signaling molecule, resulting in the establishment of positive and negative feedbacks [23].

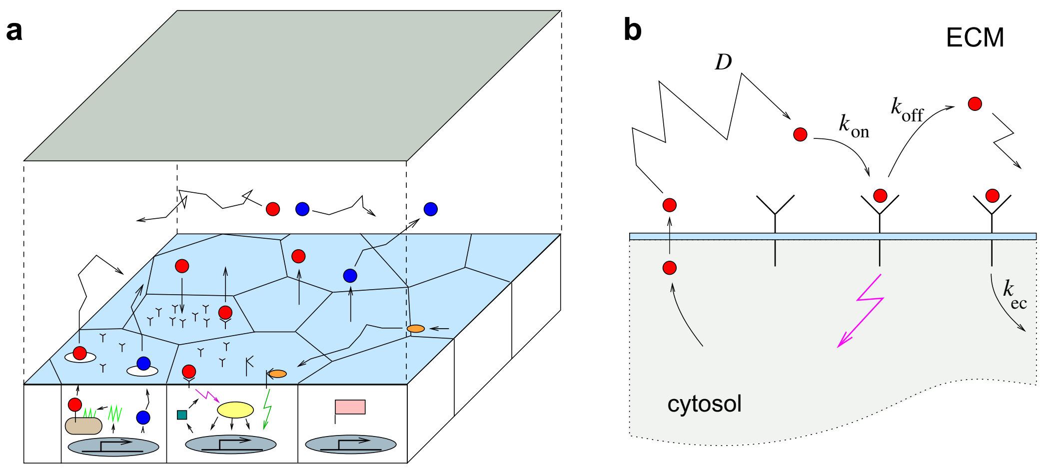

Fig. 1. The schematics of cell-to-cell signaling in an epithelial layer: the geometry of the epithelial layer (a) and the summary of the physical processes at the cell surface (b). In (a), red and blue circles show signaling molecules that are secreted by the epithelial cells, orange ovals represent the molecules of an imposed morphogen gradient. Both the signaling molecules and the morphogen bind to their specific cell-surface receptors, initiating responses by the intracellular machinery, represented by various symbols within cells. Details are taken from the signaling circuitry involved in the *Drosophila* egg development [21]. (For interpretation of the references in colour in this figure legend, the reader is referred to the web version of this article.)