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Using radial basis function-generated finite differences (RBF-FD) to solve heat transfer equilibrium problems in domains with interfaces

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ABSTRACT

When thermal diffusivity does not vary smoothly within a computational domain, standard numerical methods for solving heat equilibrium problems often converge to an inaccurate solution. In the present paper, we discuss a mesh-free, radial basis function-generated finite difference (RBF-FD)-based method for designing stencil weights that can be applied directly to data that crosses an interface. The approach produces a very accurate solution when thermal diffusivity varies smoothly on either side of an interface. It continues to produce high-quality results when a region between two interfaces is much smaller that the distance between adjacent discrete data nodes in the domain (as becomes the case for thin, nearly insulating layers). We give several test cases that demonstrate the method solving heat equilibrium problems to 4th-order accuracy in the presence of smoothly-curved interfaces.

1. Introduction

Since the 1970s and 1980s, significant effort has gone into numerically solving parabolic and elliptic equations that model heat- or otherwise diffusivity-related transport processes in domains with interfaces or challenging boundary conditions. Some of the earliest works in this area include Babuska's finite element approach to elliptic problems [1], Peskin's immersed boundary method used for modeling blood flow in the heart [2], and Mayo's work with integral equations to solve Poisson problems and the biharmonic equations in irregular regions [3].

As with the hyperbolic PDEs that model wave transport, many investigators continue to propose new and improved numerical solutions to diffusive interface problems. A significant amount of this work has involved FEMs or other weak-form methods [4–6].

Other efforts have focused on correcting the error in using traditional finite difference stencils to differentiate non-smooth data across an interface, such as the immersed interface method introduced by LeVeque and Li in [7]. Around the same time, Li and Mayo [8] published work on an alternating direction implicit (ADI) scheme for solving heat equations with interfaces to 2nd-order accuracy. Li and Shen [9] followed up on this method with an ADI approach that allowed smoothly-variable model parameters on either side of an interface. Wiegmann and Bube [10] and Linnick and Fasel [11] presented methods that account for the jump in directional derivatives along Cartesian grid lines when an interface is crossed. Fornberg and Meyer-Spasche [12] and Fornberg [13] described a simple interface correction method for a class of free boundary problems. Some recent interest has been devoted to the study of compact stencils and their correction near interfaces, as in Mittal et al. [14]. Still other approaches use smooth data extensions or "ghost" methods [15,16], the use of embedded domain [17], and coordinate transformation of a curvilinear interface problem into a rectilinear one [18].

A number of very recent studies on the numerical solution of PDEs have focused on the application of a radial basis function-generated finite difference (RBF-FD) approach that allows determination of finite difference-like collocation weights on a mesh-free cloud of data nodes. Fornberg and Flyer [19] published a comprehensive primer on the subject last year, and papers exploring the use of such methods to handle challenging boundary conditions in elliptic problems (e.g. [20,21]) are increasingly seen in computational literature.

The present method is an adaptation of our work with time-dependent wave equations in [22] and [23] that uses RBF-FD with an included support space of piecewise polynomials to solve PDEs to a high degree of accuracy in the presence of interfaces. It offers the following combination of features:

- It can be used on a mesh-free cloud of data nodes whose structure accounts for interfaces, as in [24], or conforms to irregular boundaries, as in [20].
- Stencils that include data nodes on both sides of an interface (or possibly multiple interfaces) include all important mathematical

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information about that interface (curvature, etc.) in the stencil weights. No consideration of the interface is needed after the weights are formed.

- The method requires no formation of fictitious data extensions across interfaces.
- RBF-FD avoids the necessary meshing of FEM techniques.
- Support functions and collocation weights for stencils are determined via relatively small and simple matrix problems.
- The method can achieve any degree of spatial accuracy demanded by the user (though there may be a practical upper limit for stable solutions depending on interface properties in a given problem).

Section 2 of the present paper offers a brief introduction to the isotropic heat equation. Section 2.1 gives a short overview of RBF-FD stencil formation in regions away from interfaces. Section 2.2 explains a simple way to explicitly determine the piecewise polynomial structure of temperature data as that data crosses a curved interface, and how one may use that information within RBF-FD stencils that cross interfaces. When doing so, interfacial thermal diffusion problems may be solved to a high order of accuracy. In Section 3, we present numerical examples which show that the method solves such problems to 4th-order accuracy. Section 3.1 verifies the method presented here vs. an analytical solution in the presence of linear interfaces. Section 3.2 focuses on solution of a simple boundary value problem in a domain with two mildly-curved interfaces. Finally, Section 3.3 presents results from a domain with two circular interfaces that enclose a very thin, strongly insulating region.

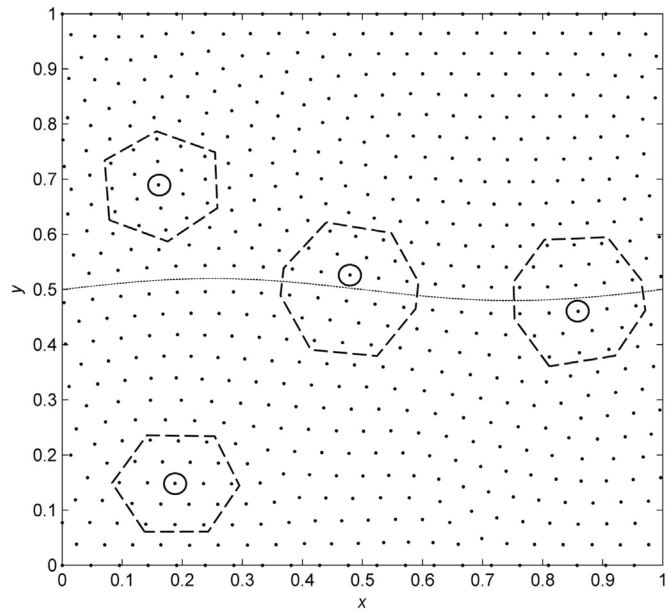

Fig. 1. RBF-FD nodes near a curved interface. The polygonal regions show various stencils, some which cross the interface and some which do not. Stencils are designed to approximate PDE operator values at the circled nodes.

2. RBF-FD methodology

The main goal of the present paper is to solve the isotropic 2-D heat equation in domains where its parameters are discontinuous or non-smooth:

$$u_t = \frac{\partial}{\partial x}\left[\alpha(x, y)\frac{\partial u}{\partial x}\right] + \frac{\partial}{\partial y}\left[\alpha(x, y)\frac{\partial u}{\partial y}\right] = (\alpha u_x)_x + (\alpha u_y)_y \tag{1}$$

In (1), u represents temperature and $\alpha(x, y)$ thermal diffusivity. At an interface, both u and $\mathbf{n}\cdot(\alpha\nabla u)$ must be continuous, where $\mathbf{n}$ is the interface's normal vector. The latter constraint enforces continuity of heat flux across the interface. This paper focuses on solutions to the equilibrium problem where (1) is equal to zero and there is no change in a solution over time. Even so, information from the time-dependent equation will be used to ensure that the equilibrium solutions are correct to a high order of accuracy.

Fig. 1 shows an example 2-D domain containing a single curved interface. The parameter α may change instantly in value between the upper and lower sides of that interface. In this domain, RBF-FD nodes are distributed with a quasi-uniform structure that accounts for the interface shape.

For stencils that do not cross an interface, weights are obtained through standard RBF-FD methodology described briefly in Section 2.1 and in more detail in [19,25]. In stencils that do cross the interface, continuity of temperature and heat flux help to create a special set of RBF-FD weights that ensure high-order accuracy when applied simultaneously to data on both sides of the interface.

2.1. Determination of RBF-FD stencils away from an interface

Traditional finite difference weights for approximating a 2-D operator L (such as $L = \partial/\partial x$ or $L = \partial^2/\partial x^2 + \partial^2/\partial y^2$) cannot be determined in a useful way within an arbitrary stencil of data nodes. Attempting to use the standard polynomial approach from 1-D in a 2-D setting results in unstable and sometimes even singular linear systems that must be solved. However, one can pair a set of 2-D polynomials with RBFs $\phi(\|\underline{x} - \underline{x}_k\|_2)$, with one RBF placed at each stencil point $\underline{x}_k = (x_k, y_k)$. A linear system similar to the one in (2) is then solved to determine stencil weights. Although only constant and linear polynomial terms are seen in (2), higher-order terms may be added to achieve more accurate stencils. Entries in the 1, x, and y columns are evaluations of those polynomial terms at a particular node in the stencil (for example, x_k would represent the evaluation of the function $f(x, y)=x$ at node k).

$$\left[\begin{array}{ccc|ccc} & & & 1 & x_1 & y_1 \\ & A & & \vdots & \vdots & \vdots \\ & & & 1 & x_n & y_n \\ \hline 1 & \cdots & 1 & & & \\ x_1 & \cdots & x_n & & 0 & \\ y_1 & \cdots & y_n & & & \end{array}\right] \left[\begin{array}{c} w_1 \\ \vdots \\ w_n \\ \hline w_{n+1} \\ w_{n+2} \\ w_{n+3} \end{array}\right] = \left[\begin{array}{c} L\phi(\|\underline{x} - \underline{x}_1\|)|_{\underline{x}=\underline{x}_c} \\ \vdots \\ L\phi(\|\underline{x} - \underline{x}_n\|)|_{\underline{x}=\underline{x}_c} \\ \hline L1|_{\underline{x}=\underline{x}_c} \\ Lx|_{\underline{x}=\underline{x}_c} \\ Ly|_{\underline{x}=\underline{x}_c} \end{array}\right] \tag{2}$$

Entries in the (symmetric) matrix A are evaluations of the RBFs placed at each data node (rows) and evaluated at each node (columns): $a_{i,j} = \phi(\|\underline{x}_i - \underline{x}_j\|)$. The RHS terms are evaluated at the evaluation node of the stencil, $\underline{x}_c$. If the stencil node structure is reasonable and if the RBFs are any of the commonly used types, including multiquadrics (MQ): $\phi(r) = \sqrt{1 + (\varepsilon r)^2}$, Gaussians (GA): $\phi(r) = e^{-(\varepsilon r)^2}$, or polyharmonic splines (PHS) $\phi(r) = \begin{cases} r^m & , m \text{ odd} \\ r^m \log r & , m \text{ even} \end{cases}$, the resulting linear system will generally be nonsingular. In the solution vector, $w_1, \ldots, w_n$ are the weights applied to data at nodes $\underline{x}_k$, $k = 1, 2, \ldots, n$. The rest of the w-entries are discarded. For more information about RBF-FD stencil determination, see [19] (its Section 5.1.4 provides a derivation of (2)).

The approach above is used in this paper for stencils that do not cross interfaces. Although the paper focuses on modification of the supplemental support polynomials to enforce interface continuity conditions, we also describe and implement a method for modifying the RBFs to help achieve the same goal. In the case of a stencil that crosses an interface, techniques from Section 2.2 are used to determine exactly how each polynomial term (up to the desired degree of accuracy) changes as the interface is crossed. Evaluation of polynomial terms seen in (2) is then dependent on which side of that interface each node resides.