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A localized meshless method for diffusion on folded surfaces ☆

Ka Chun Cheung [a,*], Leevan Ling [a], Steven J. Ruuth [b]

[a] Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong
[b] Department of Mathematics, Simon Fraser University, Burnaby, BC V5A 1S6, Canada

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ABSTRACT

Partial differential equations (PDEs) on surfaces arise in a variety of application areas including biological systems, medical imaging, fluid dynamics, mathematical physics, image processing and computer graphics. In this paper, we propose a radial basis function (RBF) discretization of the closest point method. The corresponding localized meshless method may be used to approximate diffusion on smooth or folded surfaces. Our method has the benefit of having an a priori error bound in terms of percentage of the norm of the solution. A stable solver is used to avoid the ill-conditioning that arises when the radial basis functions (RBFs) become flat.

1. Introduction

A variety of numerical methods have been proposed to approximate the solution of partial differential equations on surfaces. These include discretizations on parameterized surfaces, finite difference and finite element methods on triangulated surfaces, and embedding methods.

Each class of methods is characterized by certain advantages and disadvantages. Parametrization methods can be very efficient, but these methods require a parametrization of the surface. Typically, the construction of a parameterization leads to distortions in the surface as well as singularities [1–4]. We may avoid this complication by discretizing on triangulated surfaces. Unfortunately, finite difference discretizations on triangulated surfaces are more difficult to construct on curved surfaces than on the plane and it can be difficult to compute geometric quantities such as the curvature and the normal to the surface [5–7]. On the other hand, finite element methods on triangulated surfaces can be effective when applied to problems of elliptic or parabolic type [8,9]. In the embedding class of methods, the surface and the corresponding surface PDE are represented in the underlying d-dimensional embedding space (e.g., a problem posed on a two-dimensional curved surface might be represented and solved in a three-dimensional neighborhood of the surface) thereby enabling the use of standard Cartesian grid methods in $\mathbb{R}^d$. The most popular finite difference [5,6] and RBF discretizations [10,11] of this type project the surface Laplacian to the tangent space of the surface. Often, a level set representation of the surface is used, in which case there is no direct generalization to open surfaces or surfaces without orientation. Moreover, embedding methods typically introduce artificial boundary conditions at the boundary of the computational domain, leading to an addition error and first-order accuracy for diffusion problems. These complications can be overcome by using the closest point method

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* Corresponding author.
E-mail addresses: kachun.charles@gmail.com (K.C. Cheung), sruuth@sfu.ca (S.J. Ruuth).

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[12], which is a high-order accurate method that embeds the surface within the Euclidean embedding space by means of a closest point mapping. The standard explicit closest point method is comprised of an evolution step and an interpolation step: the method must interpolate function values on the surface at each time step in order to replace derivatives intrinsic to the surface with standard Cartesian operators.

In [13], Piret proposed to discretize the closest point method using radial basis functions. As a consequence of using radial basis functions, the method is not restricted to Cartesian grids. This allows for two fundamental advantages over the standard closest point method. First, it is straightforward to use irregular or refined grids according to the needs of the problem. Second, the freedom of selecting nodal points naturally allows one to eliminate the interpolation step of the closest point method by making an appropriate node selection. By avoiding the interpolation step, the computational error and cost associated with interpolation is eliminated. The method proposed in this paper also combines the closest point method and the radial basis function projection method to solve PDEs on surfaces. As in Piret's approach, our approach does not involve an interpolation step, thereby eliminating a source of error and opening the possibility of significant savings in computational cost. Apart from this, we will show that our proposed method is error optimal, i.e., the spatial approximation has a minimal error bound among all meshless methods. Moreover, the error bound is of a-priori type: it depends only on the distribution of nodes and the type of kernel or basis function. On the other hand, the discretization of the spatial variables in our approach leads to a differentiation matrix W such that $\mathbf{u}_t = W\mathbf{u}$. While the differentiation matrix W is error optimal, it is also very ill-conditioned when the radial basis functions become flat or when the nodal points are very dense. Consequently, as we refine our discretization, the differentiation matrix becomes ill-conditioned [14–16]. This trade-off is inherent in meshless methods. See [17,18] for a strategy to handle the ill-conditioning by changing the basis function to an orthogonal basis, thereby stabilizing the computation for flat radial basis functions. Throughout this paper, the differentiation matrix W arising in numerical experiments is solved by this RBF-QR strategy.

In addition to the development of an error-optimal RBF discretization, this paper introduces a generalization of the closest point method appropriate for diffusion on folded surfaces. The standard closest point method is built on the assumption that the closest point function is sufficiently smooth within the computational band. As a consequence, the standard method cannot be used to compute the solutions of PDEs on curves with corners or surfaces with folds. In [19], a transformation was introduced to give a smooth, transformed problem which is amenable to computation via the standard closest point method. Unfortunately, the transformed problem has increased dimensionality, and consequently is computationally expensive. In this paper, we develop an extension of the closest point method for solving diffusion on curves with corners and on folded surfaces. The method computes within the original embedding space and uses node placement along the folds. This makes a radial basis function discretization particularly appropriate. Numerical experiments demonstrate that the proposed method retains high-order accuracy for smooth curves and surfaces, while giving first order convergence for computations on geometries with folds.

2. Surface embedding

The closest point method, originally proposed by Ruuth and Merriman [12], is an embedding method for solving PDEs on surfaces. The method embeds the surface operator to the Euclidean space $\mathbb{R}^n$ using a closest point mapping. Such an embedding is called a closest point extension. By alternating the closest point extension with a traditional PDE solver on $\mathbb{R}^n$, we can obtain an explicit method for solving a surface PDE in the embedding space.

Let $\mathcal{S} \subset \mathbb{R}^n$ be a smooth surface and ∇ be the standard Euclidean gradient in $\mathbb{R}^n$. Then, the surface gradient, denoted by $\nabla_{\mathcal{S}}$, is defined as:

$$\nabla_{\mathcal{S}} := \nabla - \hat{n}(\hat{n} \cdot \nabla), \tag{1}$$

where $\hat{n}$ is the unit normal to the surface $\mathcal{S}$. Consider a C^1 vector field $\phi : \mathbb{R}^n \to \mathbb{R}^n$ that is constant along the normal direction to $\mathcal{S}$. The directional derivative satisfies

$$0 = \frac{d}{d\hat{n}}(u \circ \phi) = \hat{n} \cdot \nabla(u \circ \phi),$$

which we combine with (1) to obtain

$$\nabla_{\mathcal{S}}(u \circ \phi) = \nabla(u \circ \phi) - \hat{n} \cdot \nabla(u \circ \phi)\hat{n} = \nabla(u \circ \phi), \text{ on } \mathcal{S}. \tag{2}$$

Thus, for any C^1 function that is constant along the normal direction to $\mathcal{S}$, we observe that, on the surface, standard Euclidean gradients (defined on the embedding space) coincide with the desired surface gradients. A particularly convenient vector field $\phi : \mathbb{R}^n \to \mathcal{S}$ is the *closest point mapping*

$$\phi_{\mathcal{S}}(x) = \arg\min_{s \in \mathcal{S}} |x - s|, \text{ for all } x \in \overline{\mathcal{S}}, \tag{3}$$

where $\overline{\mathcal{S}} \subseteq \mathbb{R}^n$ is a neighborhood of $\mathcal{S}$ over which the closest point mapping $\phi_{\mathcal{S}}$ is C^1. Generally, the maximum possible $\overline{\mathcal{S}}$ is determined by the curvature of $\mathcal{S}$. For any C^1 surface, we can properly embed $\mathcal{S} \subset \overline{\mathcal{S}}$. For example, if $\mathcal{S} \in \mathbb{R}^2$ is circle, then the maximum possible $\overline{\mathcal{S}}$ will be the whole plane $\mathbb{R}^2$ except the center of $\mathcal{S}$.