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A spectral mimetic least-squares method*

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ABSTRACT

We present a spectral mimetic least-squares method for a model diffusion-reaction problem, which preserves key conservation properties of the continuum problem. Casting the model problem into a first-order system for two scalar and two vector variables shifts material properties from the differential equations to a pair of constitutive relations. We use this system to motivate a new least-squares functional involving all four fields and show that its minimizer satisfies the differential equations exactly. Discretization of the four-field least-squares functional by spectral spaces compatible with the differential operators leads to a least-squares method in which the differential equations are also satisfied exactly. Moreover, the latter are reduced to purely topological relationships for the degrees of freedom that can be satisfied without reference to basis functions. Numerical experiments confirm the spectral accuracy of the method and its local conservation.

1. Introduction

We consider the model diffusion-reaction problem

$$-\nabla \cdot \mathbb{A}\nabla\phi + \gamma\phi = f \quad \text{in } \Omega,$$

$$\phi = g \quad \text{on } \Gamma_D,$$

$$\mathbf{n} \cdot \mathbb{A}\nabla\phi = h \quad \text{on } \Gamma_N,$$
(1)

where $\Omega \subset \mathbb{R}^n$, n = 2, 3, has a Lipschitz-continuous boundary $\partial \Omega = \Gamma_D \cup \Gamma_N$ and **n** is the outward unit normal to $\partial \Omega$. We assume that \mathbb{A} is a symmetric positive definite tensor and γ is a real-valued, strictly positive function, i.e., there exist constants $f_{\min}, f_{\max}, \gamma_{\min}, \gamma_{\max} > 0$ such that

$$f_{\min}\boldsymbol{\xi}^{\mathrm{T}}\boldsymbol{\xi} \leq \boldsymbol{\xi}^{\mathrm{T}}\mathbb{A}(\mathbf{x})\boldsymbol{\xi} \leq f_{\max}\boldsymbol{\xi}^{\mathrm{T}}\boldsymbol{\xi} \quad \text{and} \quad \gamma_{\min} \leq \gamma(\mathbf{x}) \leq \gamma_{\max},$$
(2)

for all $\mathbf{x} \in \Omega$ and $\mathbf{\xi} \in T_{\mathbf{x}}\Omega$. The tensor \mathbb{A} and the function γ describe material properties. For instance, in heat transfer applications \mathbb{A} is the thermal conductivity of the material and γ can be related to the specific heat capacity.

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Almost all published² least-squares methods for (1) start with the reformulation of the governing equations into an equivalent first-order system

$$\nabla \cdot \mathbf{u} + \gamma \phi = f \quad \text{in } \Omega,$$

$$\mathbf{u} + \mathbb{A} \nabla \phi = 0 \quad \text{in } \Omega,$$

$$\phi = g \quad \text{on } \Gamma_D,$$

$$\mathbf{n} \cdot \mathbf{u} = -h \quad \text{on } \Gamma_N$$
(3)

followed by setting up a least-squares functional

$$\mathcal{J}(\boldsymbol{u},\boldsymbol{\phi};f) \coloneqq \frac{1}{2} \left(\|\nabla \cdot \boldsymbol{u} + \gamma \boldsymbol{\phi} - f\|_X^2 + \|\boldsymbol{u} + \mathbb{A}\nabla \boldsymbol{\phi}\|_Y^2 \right), \tag{4}$$

and a least-squares principle, which is the following unconstrained minimization problem:

$$(\boldsymbol{u}, \boldsymbol{\phi}) = \underset{\boldsymbol{v} \in U, \, \varphi \in V}{\arg\min} \, \mathcal{J}(\boldsymbol{v}, \varphi; f).$$
(5)

We will refer to ϕ and \mathbf{u} as the *potential* and *flux* variables. In (4)–(5) *X*, *Y* and *U*, *V* are some appropriate *data* and *solution* spaces. The key juncture in the definition of a well-posed least-squares method is to choose these spaces such that \mathcal{J} is norm-equivalent, i.e., the residual "energy" $|||(\mathbf{u}, \phi)||| := \mathcal{J}(\mathbf{u}, \phi; 0)$ defines an equivalent norm on the solution spaces:

$$C_{1}\left(\|\boldsymbol{v}\|_{U}^{2}+\|\varphi\|_{V}^{2}\right) \leq \||(\boldsymbol{v},\varphi)\||^{2} \leq C_{2}\left(\|\boldsymbol{v}\|_{U}^{2}+\|\varphi\|_{V}^{2}\right), \quad \forall \boldsymbol{v} \in U, \ \varphi \in V.$$
(6)

This guarantees the strong coercivity of the Euler–Lagrange equation for (5), which is the least-squares variational problem. As a result, restriction of the least-squares principle (5) to finite dimensional subspaces $U^h \subset U$ and $V^h \subset V$ yields a well-posed discrete least-squares problem with symmetric and positive definite linear system. This obviates the need for an inf–sup compatibility condition between the variables and makes the method amenable to well-established iterative solvers. The latter is one of the key advantages of least-squares methods. Furthermore, norm-equivalence (6) implies that minimization of \mathcal{J} amounts to minimization of the error in \boldsymbol{u} and ϕ in their respective norms. Therefore, the least-squares functional provides a natural a posteriori error estimator [2], which is another important advantage of least-squares methods.

One common choice for which (6) holds is $X = Y = L^2(\Omega)$, $U = H(\text{div}, \Omega)$ and $V = H^1(\Omega)$. Because strong coercivity is inherited on subspaces, one can approximate both solution spaces by standard C^0 elements. Since the inception of least-squares methods this has often been quoted as one of their principal advantages. However, when formulated in this way, the least-squares method is not conservative [3–5] and in some cases solutions can be very inaccurate; see [6,7] for examples.

The use of div-conforming elements for the flux, such as Raviart–Thomas elements [8], has been suggested in [9] as a way to improve the accuracy and conservation of least-squares methods for (1). Analysis in [9] shows that div-conforming elements enable optimal L^2 convergence of the flux, which does not hold true for nodal elements. Furthermore, the flux approximation becomes locally conservative.

In this paper we extend these ideas to develop a *spectral* mimetic least-squares method for (1) that is locally conservative. Reformulation of the model problem into a *four-field* first-order system involving two scalar and two vector variables allows us to shift material parameters from the differential operators into a pair of constitutive relations. The four-field system prompts the inclusion of two new equation residuals to the standard least-squares formulation (4). We show that the resulting least-squares principle satisfies exactly the differential equations, while the constitutive relations are satisfied approximately. The key idea then is to approximate the four fields by finite elements from a discrete exact sequence. This allows us to satisfy exactly the differential equations in the discrete setting and yields a locally conservative least-squares method.

In contrast to other high-order methods, which utilize modal or purely nodal degrees of freedom, our approach uses compatible spectral elements with geometrically localized degrees of freedom; see, e.g., [10] for a related construction of high-order Whitney elements on simplices. Because these degrees of freedom live on geometric mesh entities, they are co-chains of the same order as the dimension of the entity. This reduces the action of differential operators such as div, grad and curl to the action of the co-boundary operator on the corresponding co-chain, i.e., the discretized differential operators are purely topological and independent of the size or shape of the mesh. As a result, our approach transforms the differential equations into purely topological relationships for the degrees of freedom that can be satisfied without reference to basis functions. In so doing we obtain a least-squares method in which the discrete differential equations are satisfied exactly, and the approximation takes place in the constitutive relations involving A and γ .

The rest of the paper is organized as follows. Section 2 transforms (1) into a first-order four field system and explains the formulation of the mimetic least-squares method. Section 3 derives topological discretizations of the differential equations, which are independent of the basis functions. Section 4 presents the corresponding compatible spectral elements used in this work. We discuss approximation of constitutive laws, which depends on the basis functions, in Section 5. In Section 6 the behavior under mappings will be presented. We conclude with numerical examples in Section 7 and conclusions in Section 8.

² The negative norm least-squares method for second order elliptic equations [1] is one notable exception.

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