

A locally conservative high-order least-squares formulation in curvilinear coordinates

Marc Gerritsma and Pavel Bochev

Abstract We present a locally conservative spectral least-squares formulation for the scalar diffusion-reaction equation in curvilinear coordinates. Careful selection of a least squares functional and compatible finite dimensional subspaces for the solution space yields the conservation properties. Numerical examples confirm the theoretical properties of the method.

1 Introduction

Least-squares finite element methods for partial differential equations reformulate PDEs into unconstrained minimization problems. The sum of weighted equation residuals measured in suitable Sobolev norms defines the least-squares functional. Norm-equivalent least-squares functionals give rise to symmetric and strongly coercive variational problems. These properties are inherited on conforming finite dimensional subspaces of the solution space. Therefore, conforming finite element discretizations circumvent inf-sup conditions and are always symmetric, positive definite, which make these discrete systems amenable to well-established iterative solvers.

Exceptional stability of least-squares formulations has led to the widespread use of standard C^0 elements in their discretization. Unfortunately, resulting finite element methods are only approximately conservative, which generally leads to vi-

Marc Gerritsma

TU Delft, Kluyverweg 1, 2629 HS Delft, The Netherlands e-mail: M.I.Gerritsma@tudelft.nl

Pavel Bochev

Sandia National Laboratories, Computational Mathematics, Mail Stop 1320, Albuquerque, NM 87185, USA e-mail: pbboche@sandia.gov. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

olation of fundamental physical properties, such as loss of mass or artificial vorticity generation in potential flows. In many cases this drawback can outweigh potential advantages of least squares methods; see [10, 19]. As a result, improving conservation properties of least-squares methods has attracted significant attention [5, 6, 8, 10, 12, 13, 14].

2 Conservative least-squares functional

We explain our approach using the following diffusion-reaction problem [2]

$$\begin{aligned} -\nabla \cdot \mathbb{A} \nabla \phi + \gamma \phi &= f \text{ in } \Omega, \\ \phi &= g \text{ on } \Gamma_D, \\ n \cdot \mathbb{A} \nabla \phi &= h \text{ on } \Gamma_N, \end{aligned} \quad (1)$$

where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, 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

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

for all $x \in \Omega$ and $\xi \in T_x \Omega$. 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.

This scalar problem can be recast as an equivalent four-field problem, given by

$$\begin{aligned} \nabla \cdot \mathbf{u} + \psi &= 0 \text{ in } \Omega, & \mathbf{v} &= \mathbb{A}^{-1} \mathbf{u} \text{ in } \Omega, & \text{and} & \phi &= g \text{ on } \Gamma_D, \\ \mathbf{v} + \nabla \phi &= 0 \text{ in } \Omega, & \psi &= \gamma \phi - f \text{ in } \Omega, & & -n \cdot \mathbf{u} &= h \text{ on } \Gamma_N. \end{aligned} \quad (3)$$

We will refer to the equations $\nabla \cdot \mathbf{u} + \psi = 0$ and $\mathbf{v} + \nabla \phi = 0$ as the *conservation laws*. The first one expresses the fact that the net amount of outflow, \mathbf{u} , over the surface of any body $\omega \subset \Omega$ balances the volumetric production terms ψ . The second equation states that circulation of \mathbf{v} over any closed loop is zero. We call such equations *topological* because they are independent of material parameters and only involve geometric concepts like surface, body and closed loop. With proper selection of discrete variables these equations can be satisfied exactly.

On the other hand, the equations $\mathbf{v} = \mathbb{A}^{-1} \mathbf{u}$ and $\psi = \gamma \phi - f$ depend explicitly on the material parameters \mathbb{A} and γ and the right hand side term f . We refer to these equations as the *constitutive relations*. Their association with geometry is less obvious; for instance $\mathbf{v} = \mathbb{A}^{-1} \mathbf{u}$ equates circulation of \mathbf{v} along a curve to the flux of \mathbf{u} across a surface. This geometrical incompatibility between the variables is an important source of errors in many numerical methods.

The two sets of equations play very different mathematical and physical roles. The constitutive relations prescribe functional relationships between the variables,

which represent simplified summaries of more complex physical phenomena, i.e., these equations are *based on modeling assumptions*. The material-dependent data is generally obtained through experiment and is not known exactly. On the other hand, the conservation laws express fundamental balance relationships between global quantities that hold universally, i.e., these equations *do not involve modeling assumptions*.

In this paper we consider a least-squares functional originally proposed in [2]:

$$\begin{aligned} \mathcal{J}((\phi, \mathbf{v}), (\psi, \mathbf{u}); f) = & \frac{1}{2} \left(\|\mathbb{A}^{-1/2}(\mathbf{u} + \mathbb{A}\nabla\phi)\|_0^2 + \right. \\ & \left. \|\gamma^{-1/2}(\gamma\phi + \nabla \cdot \mathbf{u} - f)\|_0^2 \|\mathbf{v} + \nabla\phi\|_0^2 + \|\nabla \cdot \mathbf{u} + \psi - f\|_0^2 \right), \end{aligned} \quad (4)$$

and its associated least-squares principle

$$\min_{(\phi, \mathbf{v}) \in U, (\psi, \mathbf{u}) \in V} \mathcal{J}((\phi, \mathbf{v}), (\psi, \mathbf{u}); f) \quad (5)$$

where $U = H^1(\Omega) \times (L^2(\Omega))^n$ and $V = L^2(\Omega) \times H(\text{div}, \Omega)$.

Proposition 1. *The least-squares functional (4) is norm-equivalent with respect to the solution space $U = H^1(\Omega) \times (L^2(\Omega))^n$ and $V = L^2(\Omega) \times H(\text{div}, \Omega)$.*

Proof. See [2].

Proposition 2. *The solution of (5) satisfies the conservation laws in the L^2 sense.*

Proof. The proof follows by taking variations of (4) with respect to \mathbf{v} and ψ .

3 A mimetic least-squares method

Because strong coercivity is inherited on subspaces, conforming finite element spaces of $H^1(\Omega)$ and $H(\text{div}, \Omega)$ such as standard C^0 elements will give a well-posed least-squares finite element method. Since the inception of least-squares methods this has often been quoted as one of its principal advantages. However, if we want Proposition 2 to hold at the discrete level, we need to ensure that the discrete conservation laws, $\nabla \cdot \mathbf{u} + \psi = 0$ and $\mathbf{v} + \nabla\phi = 0$, can be represented on these subspaces, i.e. if $(\phi^h, \mathbf{v}^h) \in G^h \times C^h$ with $G^h \subset H^1(\Omega)$ and $C^h \subset (L^2(\Omega))^n$, we need to have that $\nabla\phi^h \in C^h$ for all $\phi^h \in G^h$. Similarly, for $(\psi^h, \mathbf{u}^h) \in S^h \times D^h$ with $S^h \subset L^2(\Omega)$ and $D^h \subset H(\text{div}, \Omega)$ we require that $\nabla \cdot \mathbf{u}^h \in S^h$ for all $\mathbf{u}^h \in D^h$. Thus, the finite dimensional spaces forming $U^h = G^h \times C^h$ and $V^h = S^h \times D^h$ need to belong to a discrete DeRham complex, [5, 17]. With the spectral element basis functions from [11] this is indeed the case. With these spectral basis functions, the conservation laws can be exactly satisfied and reduce to simple relations between the expansion coefficients. In addition, the discrete conservation laws do not depend on the size or shape of the grid and will be independent of the order of the spectral element

approximation. The discrete conservation laws only depend on the topology of the grid, see for instance [2, 16] for a more extensive explanation.

Let $\Omega_0 = [-1, 1]^2$ be the reference spectral element with coordinates (ξ, η) and $\Phi : \Omega_0 \rightarrow \Omega$, $(x, y) = \Phi(\xi, \eta)$. We expand the pullback of the potential, $\Phi^* \phi^h$, in terms of a tensor product of Lagrange polynomials, h_i , associated with the GLL points of polynomial degree N in both ξ - and η -direction, see also [9] and [2] for the transformations

$$\Phi^* \phi^h(\xi, \eta) = \sum_{i=0}^N \sum_{j=0}^N \phi_{i,j} h_i(\xi) h_j(\eta), \quad (6)$$

and $\Phi^* \mathbf{v}$ as

$$\Phi^* \mathbf{v}^h(\xi, \eta) = \sum_{i=1}^N \sum_{j=0}^N u_{i,j} e_i(\xi) h_j(\eta) + \sum_{i=0}^N \sum_{j=1}^N v_{i,j} h_i(\xi) e_j(\eta), \quad (7)$$

where the edge $e_i(\xi)$ are given by, [11]

$$e_i(\xi) = - \sum_{k=0}^{i-1} dh_k(\xi). \quad (8)$$

In terms of these expansions the conservation law $\mathbf{v} + \nabla \phi = 0$ assumes the form

$$\begin{aligned} \Phi^* \mathbf{v}^h + \nabla \Phi^* \phi^h &= \sum_{i=1}^N \sum_{j=0}^N (u_{i,j} + \phi_{i,j} - \phi_{i-1,j}) e_i(\xi) h_j(\eta) + \\ &\quad \sum_{i=0}^N \sum_{j=1}^N (v_{i,j} + \phi_{i,j} - \phi_{i,j-1}) h_i(\xi) e_j(\eta) = 0. \end{aligned} \quad (9)$$

Since basis functions are linear independent, (9) holds if and only if

$$u_{i,j} + \phi_{i,j} - \phi_{i-1,j} = 0 \quad \text{and} \quad v_{i,j} + \phi_{i,j} - \phi_{i,j-1} = 0. \quad (10)$$

The pullback of the fluxes, $\Phi^* \mathbf{u}^h$, is expanded in terms of tensor products of edge functions and Lagrange polynomials as, see [2, 11, 15] for details

$$\Phi^* \mathbf{u}^h(\xi, \eta) = \sum_{i=0}^N \sum_{j=1}^N p_{i,j} h_i(\xi) e_j(\eta) - \sum_{i=1}^N \sum_{j=0}^N q_{i,j} e_i(\xi) h_j(\eta). \quad (11)$$

Finally, the pullback of ψ^h , $\Phi^* \psi^h$ is expanded as

$$\Phi^* \psi^h(\xi, \eta) = \sum_{i=1}^N \sum_{j=1}^N \psi_{i,j} e_i(\xi) e_j(\eta). \quad (12)$$

With these particular expansions the conservation law $\nabla \cdot \mathbf{u} + \psi = 0$ can be expressed as a relation between the expansion coefficients

$$p_{i,j} - p_{i-1,j} + q_{i,j} - q_{i,j-1} + \psi_{i,j} = 0. \quad (13)$$

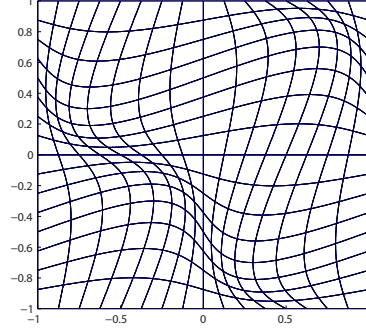


Fig. 1 Curvilinear coordinate system generated by the mapping (14) for $K=16$.

4 Numerical example

In [2] we demonstrated the conservation properties of (4) on affine elements. In this section we extend these results to non-affine, curvilinear grids.

In order to show that even in curvilinear coordinates the conservation laws are satisfied up to machine precision we solve the scalar diffusion-reaction problem on the spectral element grid shown in Figure 3. The spectral element mesh consists of $K \times K$ elements

$$\begin{aligned} x(\xi, \eta) &= \xi + c \sin(\pi\xi) \sin(\pi\eta), \\ y(\xi, \eta) &= \eta + c \sin(\pi\xi) \sin(\pi\eta), \end{aligned} \quad (\xi, \eta) \in [-1, 1]^2. \quad (14)$$

This curvilinear mesh was also used in [7, 9, 17].

For this test problem we use $\mathbb{A} = \mathbb{I}$ and $\gamma = 1$ and as exact reference solution $\phi_{ex}(x, y) = \sin(\pi x) \sin(\pi y)$. Although the material parameters are trivial in the (x, y) -coordinates, this is no longer the case when the equations are transformed to (ξ, η) -coordinates, see [2]. In Figure 2 h -convergence of the unknowns ϕ , \mathbf{v} , \mathbf{u} and ψ in the L^2 -norm is depicted for $K = 1, \dots, 16$ and $N = 1, \dots, 6$. The convergence rates are optimal in all unknowns. In Figure 3 the residuals of $\nabla \cdot \mathbf{u} + \psi$ and $\nabla \times \mathbf{v}$ are plotted in the L^∞ -norm as a function of $h = 2/K$ and N . The conservation relations are satisfied up to machine precision, independent of the mesh size, the particular mesh shape (i.e. curved grid) and polynomial degree. The slight increase in error with h -refinement and p -enrichment is a result of the increase in condition number,

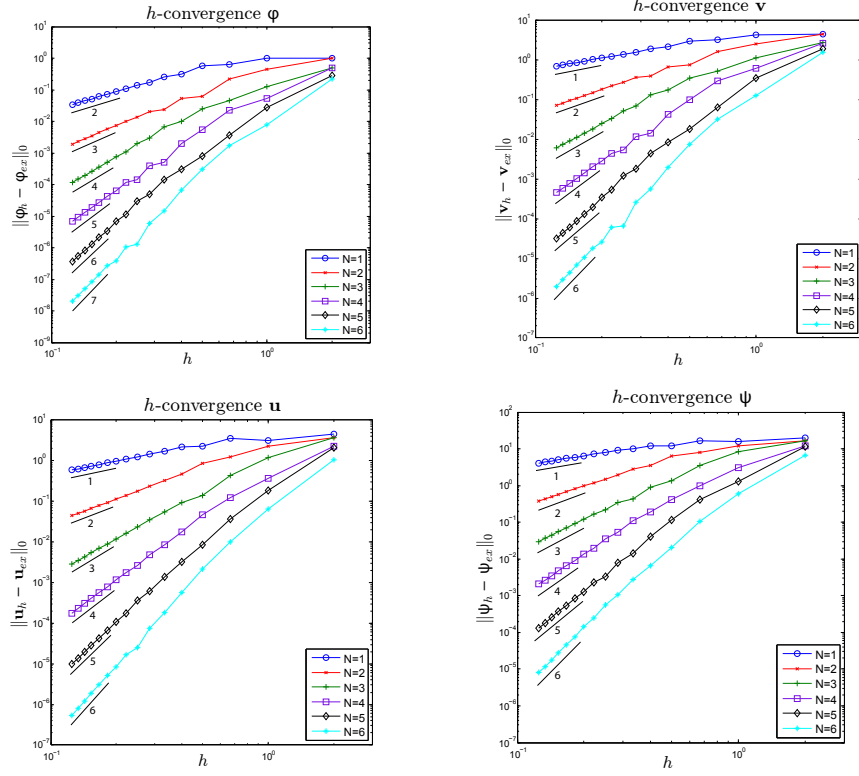


Fig. 2 Convergence plots of ϕ , \mathbf{v} , \mathbf{u} and ψ with h -refinement for various polynomial approximations.

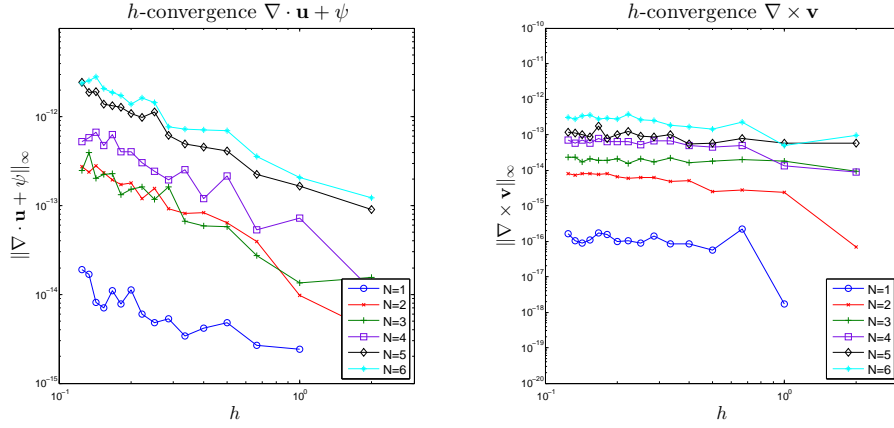


Fig. 3 Convergence plots of $\nabla \cdot \mathbf{u} + \psi$, and $\nabla \times \mathbf{v}$ with h -refinement for various polynomial approximations.

since in this study the full system resulting from (4) was solved. In practice this is not necessary, because if we know a priori that we can satisfy the conservation laws exactly, we might as well use the reduced functional

$$\mathcal{J}^R((\phi, \mathbf{u}); f) = \frac{1}{2} \left(\|\mathbb{A}^{-1/2}(\mathbf{u} + \mathbb{A}\nabla\phi)\|_0^2 + \|\gamma^{-1/2}(\gamma\phi + \nabla \cdot \mathbf{u} - f)\|_0^2 \right), \quad (15)$$

and determine \mathbf{v} from ϕ and ψ from \mathbf{u} in a post-processing step using (10) and (13). In summary,

when the reduced least-squares functional (15) is used to calculate ϕ^h and \mathbf{u}^h and \mathbf{v}^h and ψ^h are derived in a post-processing step using (10) and (13) and the associated expansions (9) and (12) for \mathbf{v}^h and ψ^h , then for all meshes and all polynomial degrees

$$\|\nabla \times \mathbf{v}^h\|_{L^\infty} = 0 \quad \|\nabla \cdot \mathbf{u}^h + \psi^h\|_{L^\infty} = 0,$$

that is, the least-squares formulation is exactly locally conservative.

5 Conclusions

Despite all its advantages, lack of conservation is one of the major drawbacks of least-squares finite element methods implemented using standard C^0 elements. In this paper we have shown that by combining an appropriate choice of a least-squares functional with compatible finite element spaces, one can define a least-squares method that is conservative up to a machine accuracy.

In practice, one can use the reduced functional (15) in which case the conservation laws are identically satisfied regardless of the coarseness and shape of the grid as well the approximation order. The price we pay is that we can no longer use our favorite C^0 -elements.

Acknowledgements This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR).

References

1. J.H. Adler, P.S. Vassilevski, *Error analysis for constrained first-order system least-squares finite element methods*, SIAM J. Sci. Comput., 38(3), pp. A 1071 - A 1088, 2014.
2. P.B. Bochev, M.I. Gerritsma, *A spectral mimetic least-squares method*, to appear CAMWA, 2014.

3. P.B. Bochev, M.D. Gunzburger, *A locally conservative least-squares method for Darcy flows*, Commun. Numer. Meth. Engng., 24, pp. 97-110, 2008.
4. P.B. Bochev, M.D. Gunzburger, *Least-squares finite element methods*, Springer 2009.
5. P.B. Bochev, M.D. Gunzburger, *A locally conservative mimetic least-squares finite element method for the Stokes equations* In *Proceedings of LSSC 2009*, Vol 5910, Lirkov I, Margenov S, Wasniewski J (eds.), Springer Lecture Notes in Computer Science, pp. 637-644, 2009.
6. P.B. Bochev, J. Lai, L. Olson, *A non-conforming least-squares finite element method for incompressible fluid flow problems*, Int. J. Numer. Meth. Fluids, 72, pp. 375-402, 2013.
7. P.B. Bochev, D. Ridzal, *Rehabilitation of the lowest-order Raviart-Thomas element on quadrilateral grids*, SIAM J. Numer. Anal., 47(1), pp. 487-507, 2008.
8. P. Bolton, R.W. Thatcher, *On mass conservation in least-squares methods*, J. Comput. Phys., 203(1), pp. 287-304, 2005.
9. M. Bouman, A. Palha, J.J. Kreeft, M.I. Gerritsma, *A conservative spectral element method on curvilinear domains*, In *Spectral and Higher Order Methods for Partial Differential Equations*, J. Hesthaven and R. Rønquist (eds.), Vol 76, Springer Lecture Notes in Computational Science and Engineering, pp. 111-119, 2011.
10. C.L. Chang, J.J. Nelson, *Least-squares finite element method for the Stokes problem with zero residual of mass conservation*, SIAM J. Numer. Anal., 34(2), pp. 480-489, 1997.
11. M.I. Gerritsma, *Edge functions for spectral element methods*, In *Spectral and Higher Order Methods for Partial Differential Equations*, J. Hesthaven and R. Rønquist (eds.), Vol 76, Springer Lecture Notes in Computational Science and Engineering, pp. 199-208, 2011.
12. J.J. Heys, E. Lee, T.A. Manteuffel, S.F. McCormick, *An alternative least-squares formulation for the Navier-Stokes equations with improved mass conservation*, J. Comput. Phys., 226(1), pp. 994-1006, 2007.
13. J.J. Heys, E. Lee, T.A. Manteuffel, S.F. McCormick, J.W. Ruge, *Enhanced mass conservation in least-squares methods for Navier-Stokes equations*, SIAM J. Sci. Comput., 31(3), pp. 2303-2321, 2009.
14. T. Kattelans, W. Heinrichs, *Conservation of mass and momentum of the least-squares spectral element collocation scheme for the Stokes problem*, J. Comput. Phys., 228(13), pp. 4649-4664, 2009.
15. J.J. Kreeft, M.I. Gerritsma, *Mixed mimetic spectral element method for Stokes flow: A point-wise divergence-free solution*, J. Comput. Phys., 240, pp. 284-309, 2013.
16. J.J. Kreeft, A. Palha, M.I. Gerritsma, *Mimetic framework on curvilinear quadrilaterals of arbitrary order*, arXiv:1111.4304, 2011.
17. A. Palha, M.I. Gerritsma, *Spectral element approximations of the Hodge- \star operator in curved elements*, In *Spectral and Higher Order Methods for Partial Differential Equations*, J. Hesthaven and R. Rønquist (eds.), Vol 76, Springer Lecture Notes in Computational Science and Engineering, pp. 283-291, 2011.
18. A. Palha, P. Rebelo, R. Hiemstra, J.J. Kreeft, M.I. Gerritsma, *Physics-compatible discretization techniques on single and dual grids, with application to the Poisson equation for volume forms*, J. Comput. Phys., 257, pp. 1394-1422, 2014.
19. M.M.J. Proot, M.I. Gerritsma, *Mass- and momentum conservation of the least-squares spectral element method for the Stokes problem*, J. Sci. Comput., 27, pp. 389-401, 2006.