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An a posteriori-driven adaptive Mixed High-Order method with application to electrostatics ☆

Daniele A. Di Pietro [a], Ruben Specogna [b,*]

[a] University of Montpellier, Institut Montpelliérain Alexander Grothendieck, 34095 Montpellier, France
[b] University of Udine, Polytechnic Department of Engineering and Architecture, 33100 Udine, Italy

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ABSTRACT

In this work we propose an adaptive version of the recently introduced Mixed High-Order method and showcase its performance on a comprehensive set of academic and industrial problems in computational electromagnetism. The latter include, in particular, the numerical modeling of comb-drive and MEMS devices. Mesh adaptation is driven by newly derived, residual-based error estimators. The resulting method has several advantageous features: It supports fairly general meshes, it enables arbitrary approximation orders, and has a moderate computational cost thanks to hybridization and static condensation. The a posteriori-driven mesh refinement is shown to significantly enhance the performance on problems featuring singular solutions, allowing to fully exploit the high-order of approximation.

1. Introduction

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, denote a bounded connected polyhedral domain of boundary $\partial\Omega$, f a square-integrable volumetric source term, and $\boldsymbol{K}$ a bounded tensor-valued diffusion coefficient piecewise constant on a polyhedral partition P_Ω of Ω, and with eigenvalues in the interval $[\underline{K}, \overline{K}]$, $0 < \underline{K} \leq \overline{K} < +\infty$. We consider the problem that consists in seeking a vector-valued field $\boldsymbol{\sigma} : \Omega \to \mathbb{R}^d$ and a scalar-valued field $u : \Omega \to \mathbb{R}$ such that

$$\boldsymbol{K}^{-1}\boldsymbol{\sigma} - \nabla u = 0 \qquad \text{in } \Omega, \tag{1a}$$

$$-\nabla\cdot\boldsymbol{\sigma} = f \qquad \text{in } \Omega, \tag{1b}$$

$$u = 0 \qquad \text{on } \partial\Omega. \tag{1c}$$

Our goal is to develop an a posteriori-driven, adaptive version of the Mixed High-Order method of [1] for the numerical approximation of problem (1); cf. also [2] for more general diffusion coefficients and boundary conditions. The performance of the proposed method is thoroughly demonstrated on a comprehensive set of academic and industrial test cases.

Problems of the form (1) arise in a variety of fields, ranging from porous media flows to heat transfer and electrostatics. The latter application provides the original motivation for this work. In this context, the variable u represents the electric

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* Corresponding author.
E-mail addresses: daniele.di-pietro@umontpellier.fr (D.A. Di Pietro), ruben.specogna@uniud.it (R. Specogna).

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scalar potential, whereas $\boldsymbol{e} = -\nabla u$ is the electric field. Since $\boldsymbol{e}$ is conservative by assumption, the harmonic field component is assumed to be zero. The inverse of the diffusion coefficient, $\boldsymbol{K}^{-1}$, represents the electrical permittivity, usually denoted by $\boldsymbol{\varepsilon}$. The vector variable $\boldsymbol{\sigma}$ represents the electric displacement vector field, often denoted by $\boldsymbol{d}$, whereas f is a known volumetric source charge density. Thus, (1b) represents Gauss's law, whereas (1a) results from the composition of the constitutive law $\boldsymbol{d} = \boldsymbol{\varepsilon}\boldsymbol{e}$ and the definition of the scalar potential u.

In electrostatics, the solution of the scalar pure diffusion problem (1) plays a fundamental role, e.g., in the extraction of parasitic circuit parameters in integrated circuits [3,4], in the solution of forward problems in Electrical Capacitance Tomography [5], and in the optimization of epoxy spacers in high-voltage direct current transmission lines [6]. Moreover, multi-physics problems involving electrostatics coupled with elastostatics or with the Schrödinger problem are fundamental to simulate the behaviour of micro electro mechanical systems (MEMS) [7] and nano-electronic devices [8]. Solving the Poisson–Boltzmann electrostatic problem is used to produce an implicit solvation to speed up molecular dynamics simulations, see [9,10]. Finally, the electrostatic problem is similar to the steady-state current conduction problem which has applications, e.g., to the solution of forward problems in Electrical Impedance Tomography [11] and to the computation of stationary 3D halo currents in fusion devices [12]. In all of the above examples, the exact solution typically contains singularities due to both the geometry and the problem data. Disposing of efficient mesh adaptation strategies is thus paramount to benefit from the use of high-order methods.

Several classical methods have been used to numerically solve problem (1) or variations thereof in the context of computational electromagnetism. A (by far) non-exhaustive list includes, in particular, [13–16,4,17,18] and the high-order method of [19]. Such methods are limited to standard element shapes and, in most cases, do not support nonconforming mesh refinement. Other methods exist, on the other hand, that support more general meshes, among which we cite, in particular, the Discrete Geometric Approach (DGA) of [20] (which, however, is restricted to the lowest-order). Recently, novel paradigms have appeared that enable arbitrary approximation orders on general polyhedral meshes. Our focus here is on the Mixed High-Order (MHO) method of [1] which, in its lowest-order version, can be linked to the DGA method (cf. Remark 5). The MHO scheme considered here has several advantageous features which set it apart from the aforementioned methods: (i) Unlike standard finite element methods, it supports fairly general meshes possibly containing polyhedral elements and nonmatching interfaces; (ii) unlike the DGA method, it allows arbitrary approximation orders; (iii) these features come at only a moderate computational cost thanks to the existence of an equivalent primal formulation (cf. [21]) together with the possibility to reduce the global number of degrees of freedom by static condensation.

The main results of this work are new a posteriori error estimate for the MHO method and the use of the corresponding estimators in the context of an adaptive resolution algorithm for problems in electrostatics. For the derivation of our error estimators, we use a residual-based approach that relies on an abstract estimate inspired by [22]; cf. also [23]. We also cite [24] for the idea of relying on the equivalent primal formulation to derive a posteriori bounds for mixed methods. A key point to use the abstract error estimate in our context is a new reformulation of the stabilization term in the MHO method, which establishes a new connection with the hybridized version studied in [21]. The upper bound thus derived has no undetermined constants and, possibly up to minor modifications, also extends to sibling schemes such as the Hybrid High-Order method of [25] (cf. also [26]) and the DGA method of [20]. Adaptive resolution methods for related high-order polyhedral discretization methods, each with its own distinguishing features, are developed in [27–29].

The performance of the proposed error estimators to drive mesh adaptivity is thoroughly demonstrated on several three-dimensional academic and industrial test cases. Two strategies are explored for the mesh adaptation: a standard refinement procedure based on matching simplicial meshes, and an adaptive coarsening procedure inspired by [30]. The former strategy has a clear interest in engineering applications due to the fact that many efficient, automatic mesh generators exist for meshes composed of standard elements. Such mesh generators are also well-integrated in computer-assisted modeling chains. The adaptive coarsening strategy, on the other hand, is a new procedure enabled by the availability of polyhedral methods which shows promise as a simple means to reduce the number of degrees of freedom without the need to regenerate a new mesh. The idea consists in starting from an initial mesh composed of standard elements fine enough to capture the geometric features of the domain and the scales of the exact solution, and performing the actual computations on a sequence of polyhedral meshes obtained by adaptive coarsening of the former.

Our numerical tests show that the adaptive algorithm delivers a significant advantage with respect to computations on uniformly refined mesh sequences, both in terms of error vs. number of degrees of freedom and in terms of error vs. computational wall time. In academic test cases with analytical singular solutions, we show in particular that the optimal orders of convergence are recovered on sequences of adaptively refined meshes. In the industrial test cases, for which an exact solution is not available, we show, on the other hand, that the adaptive algorithm yields a much better approximation of the capacitance with respect to computations on uniformly refined meshes.

The paper is organized as follows. In Section 2 we introduce the notion of general mesh along with the principal notations. In Section 3 we recall the Mixed High-Order method, its equivalent primal reformulation, and we state our a posteriori bound in Theorem 2. An extensive numerical validation of an adaptive resolution algorithm based on the estimators of Section 3 is presented in Section 4. Section 5 contains the proof of Theorem 2 preceded by the required preparatory material. Readers mainly interested in the numerical recipe and results can skip this section at first reading.