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A Second Order Cell Method for Poisson's Equation

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The Cell Method, similar to the Finite Integration Technique, is a well-established numerical method for the solution of field problems, however an often raised criticism is that it is limited to constant fields within elements. In this paper we show that for the case of Poisson's equation the Cell Method can be extended to the second order convergence. Numerical results showing the order of convergence of the method are presented.

Index Terms—Cell Method, Edge elements, Finite Integration Technique, Higher order elements.

I. INTRODUCTION

FOR several physical problems the Cell Method (CM) [1], as well as the Finite Integration Technique (FIT) [2], allows a direct construction of a system of linear algebraic equations starting from integral field equations. The basic building block of the CM are: *topological operators*, represented by rectangular incidence matrices, defined on pairs of dual grids, which express flux, circulation or difference laws which are exactly satisfied and *material operators* (often called discrete “Hodge operators”), represented by square matrices, which express, in an approximate way, physical relationships between different physical quantities.

Both CM and FIT have received considerable interest in the electromagnetics community and are at the heart of successful research and commercial codes. However, such methods have been criticized because they have been limited up to now to first order convergence of the potentials. Notwithstanding the great effort for the definition of material operators for hexahedra [3], tetrahedra [4], [5], [6], [7], [8], and generic polyhedra [9], very few attempts have been targeted at increasing the order of convergence [10], [11] while remaining within the above mentioned framework. In fact some results for 2d problems have been obtained but the resulting methods are quite far from the CM or FIT basic philosophy [12].

In this paper we show how the above-defined characteristic building blocks of the CM (dual topological operators and material operators) can be extended to second order and substantiate this novel method with numerical evidence.

II. TOPOLOGICAL OPERATORS

The CM requires the definition of two cell complexes, usually referred to as primal and dual, linked by duality relations. If N is the dimensionality of the manifold, duality implies a one-to-one correspondence between a generic primal p -geometrical entity (node, edge, face or volume) and the correspondent dual $N - p$ one (volume, face, edge, node, respectively). Each physical variable is univocally associated to an oriented spatial element. When global variables are used

(e.g. integration of pointwise quantities on the spatial element they are related to), this geometric set up allows the use of discrete operators which are representative of the continuous gradient, curl and divergence. It is easy to prove that these discrete operators are the incidence matrices $\mathbf{G}$ (edge-to-node), $\mathbf{C}$ (face-to-edge), $\mathbf{D}$ (volume-to-face). Geometric duality is required to maintain the duality relation between primal and dual topological operators [1]. As far as Poisson's problems are concerned, duality requires that:

$$\tilde{\mathbf{D}} = -\mathbf{G}^T \quad (1)$$

where the $\sim$ indicates that the incidence matrix is constructed on the dual mesh.

III. DISCRETE HODGE OPERATOR

Material operators, represented by square matrices $\mathbf{M}$, link together quantities associated to dual pairs of cell complexes. In the case of Poisson's equation such operator links surface integrals (fluxes) to line integrals. Without loss of generality, in the remainder of this paper we will refer to an electrostatic problem. The stiffness matrix representing the discretized version of the continuous problem can be assembled by the product of topological and constitutive matrices:

$$\mathbf{K} = \tilde{\mathbf{D}}\mathbf{M}\mathbf{G} = -\mathbf{G}^T\mathbf{M}\mathbf{G} \quad (2)$$

Algebraic techniques like CM and FIT are less flexible than Finite Elements because they require that variables associated to edges have the physical meaning of line integrals of the tangential component of the field [13].

A. Interpolating function

In [14] Kameari proposed second order edge elements which are suitable for building a discrete Hodge operator. Given a tetrahedral discretization, six additional nodes are added at the middle of each edge and four at face centers (see Fig. 1(a)). The resulting element has 14 nodes, 24 edges and 12 faces. This second order cell fulfills the necessity of expanding the Nedelec functional space with additional degrees of freedom. Fig. 1(b) shows a possible choice of corresponding dual geometric entities which satisfy the duality relations, namely

Fig. 1. Degrees of freedom (a) and dual faces and volumes (b).

dual faces in one-to-one correspondence with primal edges bounding dual volumes in one-to-one correspondence with primal nodes. It should be noted that the position and shape of the dual surfaces is by no means unique and the presented configuration is just one of the infinite possibilities. Our choice is based on an analogy with first order case and because, since each dual face consists of two triangles, simple quadrature formulas can be implemented.

The degrees of freedom of Kameari's element are allocated onto 24 edges defined on a tetrahedron and can be expressed in terms of barycentric coordinates, which facilitates their numerical integration. Calling λ_i the barycentric coordinate associated to the i th vertex of a tetrahedron, two sets of edge-based interpolating functions can be defined: $\vec{w}_{ij}$ is associated to the first order half-edge connecting nodes i and j , and $\vec{w}_i$ is associated to the short edge connecting the mid-edge and mid-face nodes (see Fig. 1(a)):

$$\begin{aligned}\vec{w}_{ij} &= \frac{1}{10} ((63\lambda_i + 30\lambda_j - 33) \lambda_i \nabla \lambda_j \\ &\quad - (18\lambda_i - 15\lambda_j + 5) \lambda_j \nabla \lambda_i) \\ \vec{w}_i &= \frac{3}{5} (31\lambda_j \lambda_k \nabla \lambda_i + 7\lambda_i \lambda_j \nabla \lambda_k + 7\lambda_i \lambda_k \nabla \lambda_j)\end{aligned}\quad (3)$$

This physical meaning of the degrees of freedom is ensured since the orthogonality condition (the line integrals of the basis functions on each edge are independent from each other) is explicitly imposed in the construction of the interpolating functions. The edge shape functions 3 derive from the following corresponding second order nodal functions related to vertices i , mid-edge nodes ij and mid-face nodes ijk :

$$\begin{aligned}N_i &= 2\lambda_i^2 - \lambda_i + 3\lambda_i (\lambda_j \lambda_k + \lambda_k \lambda_l + \lambda_l \lambda_j) \\ N_{ij} &= 4\lambda_i \lambda_j - 12\lambda_i \lambda_j (\lambda_k + \lambda_l) \\ N_{ijk} &= 27\lambda_i \lambda_j \lambda_k\end{aligned}\quad (4)$$

B. Whitney Hodge operator

The discrete Whitney Hodge operator, sometimes also described as the canonical discrete Hodge operator [15], [16] consists in the sequential application in each tetrahedron of:

- an interpolation operator (the second order Kameari edge element in this case)

$$\vec{E} = \sum_{k=1}^{24} \vec{w}_k e_k, \quad (5)$$

which allows to express a quantity associated to line integrals (the electric field $\vec{E}$) as a linear combination of edge basis functions;

- a continuous Hodge operator (the constitutive equation)

$$\vec{D} = \varepsilon \vec{E}$$

linking a quantity associated to surface integrals (the electric induction field $\vec{D}$) to a quantity associated to line integrals;

- a discretization operator (the de Rham map, consisting of surface integration in this case)

$$d' = \int_{\vec{S}} \vec{D} \cdot \vec{n} dS$$

where the ' symbol indicates that this is a partial contribution coming from a single element (which will then be assembled with those of neighboring elements sharing the same edge).

The discrete Whitney Hodge operator can thus be constructed element-by-element by assembling local contributions of the form

$$m'_{jk} = \int_{\vec{S}_j} \varepsilon \vec{w}_k \cdot \vec{n}_j dS \quad (6)$$

where the subscript j refers to the local dual face of Fig. 1(b) and subscript k refers to the local primal edge of Fig. 1(a).

The final assembled material operator matrix $\mathbf{M}$ is not symmetric. This may not be a major issue for some lowest order Cell Methods, as shown e.g. in [15], [16], because the non-symmetric part of $\mathbf{M}$ may vanish in the multiplication with the topological operator matrices, but this is not the case when the Whitney hodge is inserted in (2)

C. Galerkin Hodge operator

A different way to build a discrete Hodge operator is to ensure that the energy calculated as the volume integral of the energy density in each element W is equal to the discrete energy calculated by resorting to global quantities:

$$W = \frac{1}{2} \sum_{k=1}^{24} e_k d'_k \quad (7)$$

where e_k is electric voltage and d'_k the dielectric flux. For a generic tetrahedron, the energy density is

$$w = \frac{1}{2} \vec{D} \cdot \vec{E} = \frac{1}{2} \varepsilon \vec{E} \cdot \vec{E} \quad (8)$$

By using the interpolator (5), the total energy becomes:

$$\begin{aligned}W &= \frac{1}{2} \int_{\Omega} \varepsilon \left(\sum_{k=1}^{24} \vec{w}_k e_k \right) \cdot \left(\sum_{j=1}^{24} \vec{w}_j e_j \right) d\Omega \\ &= \frac{1}{2} \sum_{k=1}^{24} e_k \int_{\Omega} \varepsilon \vec{w}_k \cdot \left(\sum_{j=1}^{24} \vec{w}_j e_j \right) d\Omega\end{aligned}\quad (9)$$

By imposing the equality of (9) and (7) the following definition of dielectric flux must hold:

$$d'_k = \int_{\Omega} \varepsilon \vec{w}_k \cdot \left(\sum_{j=1}^{24} \vec{w}_j e_j \right) d\Omega \quad (10)$$

Finally, the constitutive matrix is made by terms of the form

$$m'_{jk} = \int_{\Omega} \varepsilon \vec{w}_j \cdot \vec{w}_k d\Omega \quad (11)$$

With this approach the Hodge operator is clearly symmetric and therefore also the final stiffness matrix (2) is symmetric. Furthermore, it can be easily shown that the final stiffness matrix (2) coincides with the one which can be obtained from a Finite Element method based on the second order nodal shape functions (3).

IV. NUMERICAL RESULTS

Results shown in this section refer to the solution of Laplace equation on the unit cube with imposed exact solution on the whole boundary. The first test case is a consistency benchmark, i.e. the ability to reconstruct the quadratic potential:

$$V = x^2 + y^2 - 2z^2 + xy + xz + zy + x + y + z + 6$$

and results are shown in Fig. 2. It can be noted that while the standard first order CM converges as h^2 the proposed second order Whitney and Galerkin approaches have constant error and the solution is almost exact since it is contained in the basis function space. The difference between these latter two cases is examined in the next subsection.

The second benchmark refers to a case for which the solution is not contained in the basis function space:

$$V = \cos(x) \sin(y) e^{\sqrt{2}z}$$

and results are shown in Fig. 3. The first order CM and second order Galerkin converge as h^2 and h^3 , respectively, as expected. Contrary to expectations the second order Whitney CM converges as h^2 and an explanation of the cause of such behavior is presented in the next subsection.

From a computational point of view a comparison with respect to CPU time is more interesting than the one with respect to the average element size h . Fig. 4 clearly shows the benefits of the second order approach since a much higher accuracy can be obtained for a given computational time. Results have been obtained with a direct sparse solver.

A. Critical analysis

While the behavior of the second order Galerkin CM is in line with theoretical predictions due to its coincidence with FEM, the second order Whitney CM does not have the expected dependence on h^3 for benchmark 2 and has a very small constant error for benchmark 1 which is nonetheless definitely not in the order of the machine epsilon. Differently from the first order CM, the two approaches do not give raise to the same stiffness matrix. In fact, in the first order CM, the identity of the final matrices is due to the fact that some particular properties hold only for first order edge elements, e.g. the volume integral of the k th basis function equals the k th dual face area vector [17]:

$$\int_{\Omega} \vec{w}_k d\Omega = \vec{S}_k \quad (12)$$

together with additional constraints imposed by the discrete grad operator.

Fig. 2. Comparison of standard CM, Galerkin and Whitney second order CM on benchmark 1.

Fig. 3. Comparison of standard CM, Galerkin and Whitney second order CM on benchmark 2.

Fig. 4. Timing comparison between first order and second order Cell Methods

Fig. 5. Eigenvalue spectra (eigenvalue magnitude vs eigenvalue index in a sorted list by increasing magnitude) for the Galerkin and Whitney approaches on a sample mesh.

TABLE I
CONDITIONING OF GALERKIN AND WHITNEY MATRICES

Nodes	Cond. Galerkin	Cond. Whitney	Ratio
1593	4.01	12.58	3.14
5005	19.90	174.03	8.75
16093	49.20	3243.70	65.93
28865	90.37	8310.60	91.97
58493	143.30	16971.60	118.43

Although our analysis of this behavior is not entirely satisfactory, a possible cause may be related to the widely different conditioning of the stiffness matrix in the Galerkin and Whitney cases. Fig. 5 shows the eigenvalue spectrum of the two approaches for one of the meshes. It can be seen that while the spectra look similar the conditioning of the matrix obtained from the Whitney approach is much worse than the one of the Galerkin approach. Furthermore, Table I shows that things get worse as the mesh is refined with the conditioning of the matrix obtained from the Whitney approach becoming orders of magnitude worse than the one of the Galerkin approach.

It should also be noted that the Galerkin approach, in spite of its convergence properties, may be considered somewhat incoherent with the philosophy of the CM since (10) specifies the computation of a flux in terms of a volume integral and thus does not specify explicitly the dual face associated to such flux. This on the other hand suggests that a different choice of the faces used for the definition of the fluxes in the Whitney approach may lead to an improved convergence performance.

V. CONCLUSION

This paper presents a first attempt at developing second order discrete Hodge operators suitable for the construction of second order Cell Method or FIT schemes based on tetrahedral meshes. The merits and deficiencies of two possible alternatives, based on Whitney and Galerkin construction schemes, are discussed. Work is in progress to combine the

methodological advantages of the Whitney-type operator with the computational efficiency of the Galerkin-type one.

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