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Comparison of discrete exterior calculus and discrete-dipole approximation for electromagnetic scattering

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ABSTRACT

In this study, we perform numerical computations of electromagnetic fields including applications such as light scattering. We present two methods for discretizing the computational domain. One is the discrete-dipole approximation (DDA), which is a well-known technique in the context of light scattering. The other approach is the discrete exterior calculus (DEC) providing the properties and the calculus of differential forms in a natural way at the discretization stage. Numerical experiments show that the DEC provides a promising alternative for solving the general Maxwell equations.

1. Introduction

We compare two methods for solving the scattering problems numerically. The first method is the discrete-dipole approximation (DDA), which is a well-known technique in the context of light scattering, see, e.g., [1]. The second approach is based on discrete exterior calculus (DEC), which provides the properties and the calculus of differential forms in a natural way at the discretization stage [2,3]. For electromagnetics the DEC is pioneered by Bossavit and Kettunen [4–6] for antenna applications. Our generalized DEC-formulation for the Maxwell equations [7] works on unstructured grids, and it covers both the classical Yee's FDTD scheme and the Bossavit–Kettunen approach. We concentrate on electromagnetic scattering problems but the methods can be used within other application areas as well. The focus of this paper is comparing the DEC with the DDA to validate the method and to assess the properties in practice.

In particular, we are interested in developing numerical methods tailored for solving large-scale problems efficiently. That is why we pay more attention to the computational efficiency of the methods than to the increase of computing power. The number of computational operations needed for solving the scattering problem with the DDA is of order $\mathcal{O}(N \log N)$, where N is the number of dipoles used for the space discretization. Assuming that the number of time discretization steps is small compared to the number of space discretization elements N, the computational demand for the DEC method is close to $\mathcal{O}(N)$.

The rest of this paper is structured as follows. In Section 2, we present the computational model for the light scattering based on the Maxwell equations. We move on with the discretization methods presented in Sections 3 and 4. Section 5 is devoted to numerical experiments and comparison between the methods. Finally, in Section 6, we present concluding remarks.

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2. Computational model

For both discretization methods, the mathematical model of electromagnetic waves is based on the Maxwell equations:

$$\varepsilon \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{H} = -\sigma \mathbf{E}, \tag{1}$$

$$\mu \frac{\partial \mathbf{H}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \tag{2}$$

where **E** and **H** are the electric and magnetic fields respectively, ε is the electric permittivity, μ is the magnetic permeability, and σ is the electric conductivity. The equations presented above describe the time-dependent wave propagation. For considering the time-harmonic wave propagation, we substitute, into Eqs. (1) and (2), the variables $\mathbf{E} = \mathrm{Re}(\mathcal{E} \exp(\mathrm{i}\omega t))$ and $\mathbf{H} = \mathrm{Re}(\mathcal{H} \exp(\mathrm{i}\omega t))$, where i is the imaginary unit, such that $\mathrm{i}^2 = -1$, and ω is the angular frequency. This relationship between time-dependent and time-harmonic wave formulations has a crucial role in developing efficient computational methods for time-harmonic waves.

3. Discrete exterior calculus and exact controllability approach

The discrete exterior calculus provides the properties and the calculus of differential forms (see, e.g., [8]) in a natural way at the discretization stage. For reader who is familiar with the Finite Difference Time-Domain (FDTD) method, we propose to keep that method in mind; in a special case, the DEC is identical to FDTD [5,6]. The advantage of our DEC-based method is the use of arbitrarily shaped well-centered polyhedron elements and alternative Hodge operators. These modifications can significantly increase the accuracy and efficiency of the simulations. Our DEC-based method is developed for solving three-dimensional time-harmonic problems in domains of size 10–100 wavelengths. Next we give a short introduction to the DEC, which is based on the discretization of differential forms. We also present a staggered time discretization scheme and describe an algorithm for utilizing the exact controllability method.

A discrete analogue of the smooth differential form is called the discrete differential form (see, e.g., [9,2,3] for details). The spatial discretization is based on a decomposition of the domain into a cell complex, a collection of fundamental objects which is called cells (see, e.g., [2]). Basically, a 0-cell is a single point in space, a 1-cell is a differentiable path between two 0-cells, and a p-cell (cell of dimension p) is a connected differentiable p-manifold with a boundary constructed by a finite set of $(p-1)$-cells.

An important property of the differential forms is that a p-form can be integrated on a p-manifold as described in Chapter 7 of Abraham et al. [10]. With this property in mind, the discrete p-form is defined as a set of integration values paired with oriented p-cells of a mesh. For a more detailed description of cells, meshes, and discrete forms we refer the reader to see Hirani's thesis [2].

To discretize the Maxwell equations for the DEC, the vector fields **E**, **B**, **H**, and **D** must be transferred to the corresponding discrete forms E, B, H, and D. The usual procedure is to define E on the primal edges (1-form), B on the primal faces (2-form), H on the dual edges (1-form), and D on the dual faces (2-form). The values of the discrete forms are computed from vector fields by

$$E_i := \int_{L_i} \mathbf{E} \cdot d\mathbf{l},$$

$$B_j := \int_{S_j} \mathbf{B} \cdot d\mathbf{s},$$

$$H_j := \int_{L_j^*} \mathbf{H} \cdot d\mathbf{l},$$

$$D_i := \int_{S_i^*} \mathbf{D} \cdot d\mathbf{s},$$

where L_i and L_j^* are the primal and dual edge elements, and S_i^* and S_j are the corresponding dual and primal face elements respectively. It is notable that, with the well-defined mesh and dual mesh, the corresponding dual elements always exist. The positioning of the discrete form values is illustrated in Fig. 1.

The space-discretization of the Maxwell equations can be carried out exactly by using the discrete differential forms, and the orientation of a cell complex is an important property in the discretization. The Faraday law is written on the primal elements as

$$\partial_t B_j = -\sum_{i=1}^{n} (d_1)_{j,i} E_i,$$

where d_1 is the incidence matrix defining the neighbouring relations and relative orientations of the primal edges and faces. The incidence matrix d_1 corresponds to the curl operator, and it transfers 1-forms to 2-forms. It has non-zero values only, if the current edge L_i is included in the

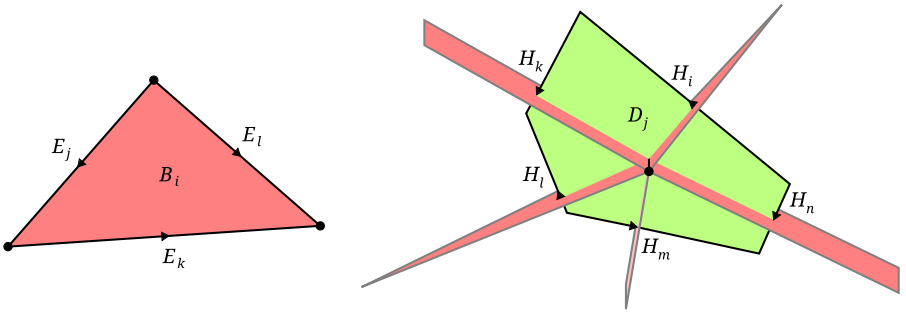

Fig. 1. The **E** and **B** fields are defined on the primal elements (left). Similarly the **H** and **D** fields are defined on the dual elements (right).