Basis Functions for the EMX Software

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***Abstract*— This paper describes the electromagnetic basis functions for the EMX software suite, a package for Electromagnetic and Electrostatic Particle-in-Cell simulation in general geometry. The basis functions are derived in a general differential geometric context, which makes clear how they may be generated from a single scalar function.**

The EMX software suite ([1], where it is referred to as 3DPIC) is routinely used by the Electromagnetics Division of Culham Electromagnetics and Lightning as part of the design process for vacuum electronic devices and components where the interaction of electromagnetic or electrostatic fields and charged particles is of importance [2], [3]. This paper focusses on the basis functions used to represent the electromagnetic field in EMX.

In the language of differential geometry [4], the absence of magnetic 'charge' and Faraday's Law may be expressed as

$$dF = 0 \tag{1}$$

where F is the electromagnetic stress tensor (or 2-form). Since any form A satisfies $d^2A = 0$, it follows that (1) may be solved by setting $F = dA$ where A is an arbitrary vector (or 1-form), usually called the electromagnetic 4-vector potential. However, for many reasons, it is helpful to be able work with a scalar rather than a vector formulation of a problem. Unfortunately, the natural way of introducing a scalar γ such that $A = d\gamma$, is useless, since such γ imply $dA = 0$, ie. no electromagnetic field.

The procedure adopted for the construction of A in EMX is to use the components of $d\gamma$ with respect to some suitable coordinate system $\{x^i, i = 1,2,3,4\}$, to weight the natural basis vectors $dx^i, i = 1,2,3,4$, thus:

$$e^i = \langle d\gamma, \partial/\partial x_i \rangle dx^i \tag{2}$$

where the summation convention is *not* employed. The inner product $\langle , \rangle$ has a particularly simple representation in component form, hence the electromagnetic potential can be written

$$A_\gamma = \sum_{i=1}^{4} A_i dx^i \partial\gamma/\partial x_i \tag{3}$$

In EMX the $\{A_i, i = 1,2,3,4\}$ are chosen to be constants for each γ, and γ and its derivatives have compact support. Thus, expressing $A = \sum_\gamma A_\gamma$ is equivalent to a finite element representation for A in terms of unknown 'nodal' values A_i on a vector basis (2) $e^i = dx^i(\partial\gamma/\partial x_i), i = 1,2,3,4$.

In principle, the functions γ could be chosen from any complete set of basis functions for 4-space. The point of the approach is that it is necessary to consider only *scalar* function bases, and moreover, it applies in any reasonable spatio-temporal coordinate system.

It is of interest to establish a relationship between the basis $\{e^i, i = 1,2,3,4\}$ and the more familiar edge elements. This is most simply achieved in Cartesian coordinates, choosing the unit hyper-cube as support for γ [1]. The γ have to be taken as the (hyper-)pyramidal functions, namely the direct product of 1-D splines called Chapeau functions. Nodal values correspond to the apexes of the (hyper-)pyramids in such a representation of a scalar. However, by differentiating a Chapeau function, two piecewise constant (top-hat) functions of compact support are generated, centred midway between the apexes of the original Chapeaux. Hence, each component of A has a top-hat dependence on the corresponding coordinate. Identifying the centre of all four top-hats with the centre of a (4-)vector finite element, the nodal value for say A_y, is seen to be centred in y, but on the edges in x, z and t. Applying the same correspondence between derivative and centring in a coordinate to dA, gives a spatio-temporally interlaced representation for the electromagnetic field itself, which corresponds to the well-known, staggered, Yee representation.

In conclusion, the basis functions described here have enabled the generalisation of the Yee algorithm to arbitrary geometries. Many aspects remain to be exploited, notably the arbitrariness of the polynomial order and support of the scalar basis function γ, eg. to generate cubic (hyper-)tetrahedral elements. More speculatively, the formalism could be used to hybridise schemes, eg by taking some γ to be complex polynomials and allowing the coefficients A_i to depend on position.

References

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