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Continuously differentiable PIC shape functions for triangular meshes

D.C. Barnes *

Sandia National Laboratory, P.O. Box 5800, Mail stop 0878, Albuquerque, NM 87185, United States

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ABSTRACT

A new class of continuously-differentiable shape functions is developed and applied to two-dimensional electrostatic PIC simulation on an unstructured simplex (triangle) mesh. It is shown that troublesome aliasing instabilities are avoided for cold plasma simulation in which the Debye length is as small as 0.01 cell sizes. These new shape functions satisfy all requirements for PIC particle shape. They are non-negative, have compact support, and partition unity. They are given explicitly by cubic expressions in the usual triangle logical (areal) coordinates. The shape functions are not finite elements because their structure depends on the topology of the mesh, in particular, the number of triangles neighboring each mesh vertex. Nevertheless, they may be useful as approximations to solution of other problems in which continuity of derivatives is required or desired.

1. Introduction

Plasma simulation using the Particle-in-cell (PIC) method is one of the most valuable tools for describing kinetic phenomena [1,2]. Some applications of PIC to two-dimensional (2D) geometries employ triangular elements [3–5]. The use of triangles allows almost complete flexibility in obtaining a mesh for domains with complex shapes and/or which contain internal structures of complex shape, and are unmatched in this flexibility by any alternative meshing of such domains.

In these previous approaches, the particle shape function, which provides interpolation between the particles and mesh in both directions is usually a linear "tent" function which is continuous but has discontinuous derivative(s). Thus, for example, if the electromagnetic field is assumed to be electrostatic only, the electrical potential will be continuous, but its derivative which gives the electric field used to advance particle velocities is not. In this way, particles receive piece-wise constant accelerations as they move within a triangular element and experience jumps in this acceleration as they cross element boundaries. These jumps lead to increased particle noise and are suspected to exacerbate the aliasing instabilities which limit application of PIC to cold, drifting plasmas (*e.g.* beam problems).

In fact, it has become evident in practice that a much superior algorithm results from the use of continuously-differentiable particle shape functions, and it is often the case that the optimum continuity is realized by the use of C_1 elements, such as tensor-product, quadratic B-splines for regular rectangular meshes. That is to say, there appears empirically to be a great advantage to the use of quadratic splines for PIC shape functions, and the advantages of higher-order splines (with more continuous derivatives) is only of marginal advantage in usual applications. Recent work has shed more light on this observation by quantitative analysis of several methods [6].

* Permanent address: Coronado Consulting, Lamy, NM 87540, United States.
E-mail address: dbarnes@sandia.gov.

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The reason for choosing linear, C_0 elements for triangular mesh PIC is, of course, not because the advantages of C_1 elements do not apply, but simply because such elements are not readily available. Only a few practical C_1 interpolation schemes are known for triangular meshes [7,8], and these do not actually improve the usual PIC algorithms because of the following limitation. These C_1 schemes introduce additional quantities per triangle to describe the elements. For example, the relatively economical scheme of Ref. [7] requires 6 quantities per vertex to determine the shape functions. If such a scheme is applied to a given number of particles per element, there will then be fewer PIC markers per degree-of-freedom, increasing the noise by the square root of this multiplicity. In this way, the additional advantages accrued by the increased smoothness are largely or completely canceled by this increase in noise. In contrast, consider the application of the usual quadratic B-spline on a rectangular mesh. In this case, there is but a single degree-of-freedom per vertex, and the shape function extends over a larger portion of the mesh. In this case, there are actually more PIC markers per degree-of-freedom, so the advantages of smoothness are supplemented by the reduction of noise associated with this gain.

There has been significant related work on this subject, both within PIC applications and in related finite-element applications to continuum problems. Unstructured PIC has been extended to three dimensional domains with complicated boundary conditions using usual C_0 elements [9,10], while other authors have employed direct numerical convolution of smooth particle shapes to move toward C_1 elements [11,12]. These applications might benefit from the reduced noise and improved dispersion properties of C_1 elements given by analytic (polynomial) expressions, with obvious potential computational advantages. All of these PIC algorithms employ a "momentum conserving" algorithm in which forces are interpolated from mesh to particles using the same shape functions as used to deposit charge from particles to mesh, and hence are restricted in cell size to a small multiple of Debye length [6].

There has also been a large body of work on higher-order polynomial elements within the general FEM framework [see for example the nice summary in [13]]. In the present work, we have borrowed heavily from some of the methods used in this work, including our pseudo-polar coordinates used later. Such approaches, when applied to unstructured meshes, are formally C_0 but offer higher-order convergence because of providing a better approximation to a smooth solution. Introduction of additional degrees of freedom limits the advantages of smoother fields, as already noted. This is avoided in the present approach which broadens the support of a single particle.

In this paper, a new class of C_1 interpolation is developed and applied as shape functions to triangular PIC. The shape functions described here are perhaps the direct analog of the rectangular mesh quadratic B-spline. The development follows a simple observation, which is that the quadratic B-spline is obtained as a moving average of the linear B-spline, in which the window for averaging is a simple square wave (often referred to as "boxcar" averaging). It is shown how to generalize this to the triangular case, and how to resolve difficulties which arise because of the intrinsically unstructured nature of the mesh, which then presents a multiplicity of cases of different connectivity which must be resolved. This first paper is focused on the mechanics of obtaining the desired functions. Nevertheless, their application to a full nonlinear PIC simulation is illustrated by a single application and a cursory comparison with usual C_0 elements. Such testing cannot provide a full verification and/or validation of the method, nor quantify many of its (low) collisional properties, but space does not permit a deeper study and presentation, which subjects is left for future investigation.

While our discussion is focused on the application of the resulting interpolation functions to PIC and the development accordingly described in the language of PIC, many other applications of these functions are possible. For example, the finite-element solution of higher-order partial differential equations is most conveniently done using elements with higher continuity. The C_1 elements derived here are useful for solution of fourth-order elliptic problems, for example. Some additional applications are mentioned in the discussion section here.

The remainder of this paper is organized as follows. The following section describes the mathematics of the approach, while section 3 works out the details for all required cases. Section 4 gives examples of the resulting shape functions, and section 5 shows their prototype application to triangular PIC. The final section contains a discussion and conclusions and points toward generalization of this approach to three dimensions.

2. The moving window approach

2.1. 1D formulation

Consider first the case of a 1D non-uniform (trivially) rectangular grid. There is a "logical coordinate" ξ which assumes integer values at each mesh point and varies continuously between, so that a continuous mapping from logical (L-space) to Cartesian (C-space) coordinate $x(\xi)$ exists. We derive a (the usual) set of C_1 (functions of a single variable with continuous derivative) useful for interpolation on this mesh. For this, we will first consider the usual linear interpolation which provides a C_0 interpolation and then modify this accordingly. Consider the usual "tent functions" which span the space of linear interpolation functions. The i-th such function is simply

$$X_i^0(\xi) = \begin{cases} \xi - i + 1, & i - 1 < \xi < i \\ i + 1 - \xi, & i < \xi < i + 1 \\ 0, & \text{elsewhere} \end{cases} \tag{1}$$

We then have a C_0 interpolate in C-space of a nodal field $\{\phi_i\}$ given parametrically by