Conformal Electromagnetic Particle in Cell: A Review

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***Abstract*— Conformal (or body-fitted) electromagnetic particle-in-cell (EM-PIC) numerical solution schemes are reviewed. Included is a chronological history of relevant particle physics algorithms often employed in these conformal simulations. Brief mathematical descriptions of particle-tracking algorithms and current weighting schemes are provided, along with a brief summary of major time-dependent electromagnetic solution methods. Several research areas are also highlighted for recommended future development of new conformal EM-PIC methods.**

***Index Terms*— Computational electromagnetics, conformal mesh, particle in cell (PIC), plasma simulation, reviews.**

I. Introduction

The ELECTROMAGNETIC particle-in-cell (EM-PIC) numerical simulation technique is commonly used to model systems of interacting electromagnetic fields and charged particles. The advantages that EM-PIC exhibits over other numerical simulation techniques include its ability to accurately predict the behavior of many complex physical systems, its validity over a wide range of operating regimes (extending to relativistic phenomena), and the simplicity of its underlying solution algorithm. Since its inception over half a century ago [1], [2], many contributions have resulted in improved physics fidelity and computational performance [3]–[6]. EM-PIC has also been used to simulate and analyze numerous physical systems including high-power microwave sources, accelerator beams, high-frequency semiconductor devices, and deposition reactors. The scalability of the EM-PIC method is limited only by the choice of hardware. While the first EM-PIC simulations were limited to a few hundred particles along a single dimension, the present simulations may contain billions of particles simulated in three dimensions while running on massively parallel computer architectures.

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In EM-PIC, the electromagnetic fields are traditionally assigned to fixed locations on a virtual mesh structure, while the particles are tracked in continuous physical space [4]–[6]. Regular quadrilateral (or hexahedron) meshes are often chosen as the EM-PIC unit cell in two (or three) dimensions, suggesting a finite-difference time-domain (FDTD) electromagnetic field solution algorithm. The FDTD method is simple in theory, easily implemented, and extensively studied. However, the well-known drawbacks of the FDTD method include its failure to accurately capture field behavior in the presence of irregular (curved or misaligned) boundaries and numerical dispersion. The representation of these irregular boundaries is often addressed using the well-known *staircasing* approximation. The limitations of the staircasing approximation when using the FDTD method to simulate electromagnetic fields are well documented in [7]–[13]. Further limitations are also present in FDTD-based EM-PIC simulations, where staircasing can lead to inaccurate particle behavior at these boundaries. A common work around is to increase the mesh resolution in the immediate vicinity of these irregular boundaries, thereby reducing the effective distance separating the numerical representation of the physical system boundaries [14]. However, this approach can significantly increase the total number of system unknowns and the overall time to solution. It can also severely limit the maximum simulation time step [9], [15]–[22], without completely solving the problem of accurate particle emission. Finally, the staircase approximation can lead to singularities in the field solution at convex corners as the cell size approaches zero.

The accurate simulation of irregular boundaries is also possible through the application of conformal FDTD-based EM-PIC algorithms. Such schemes avoid unnecessary mesh refinement and lead to more accurate particle behavior in the vicinity of such boundaries. Numerous conformal EM-PIC schemes have been published, with several of these mathematical and geometric methods adapted, or borrowed, from other computational science communities. With many available algorithms to choose from, it can be a daunting and time-consuming task to choose the algorithm suited best for a particular problem. Since this group of relevant references has yet to be compiled into a single source, it is the primary objective of this work to gather these sources and provide comparisons of their main features. Of course, this is not the first review of conformal electromagnetic solution schemes. Instead, it builds upon many previous reviews [6], [23]–[31] while updating and including newly developed methods. It is the hope of the authors that this grouping of references will aid the reader in selecting appropriate EM-PIC algorithms and perhaps even aid in the development of future conformal EM-PIC solution methods. Specifically, this review will address the following:

1) provide records of and citations to published conformal EM-PIC schemes and related algorithms;
2) provide brief mathematical descriptions of and summarize relevant conformal EM-PIC algorithms;
3) highlight areas for recommended future conformal EM-PIC development.

Conformal EM-PIC remains only one simulation technique with a multitude of other PIC solution frameworks. As such, the present scope must be limited, so the following topics will *not* be addressed in this review (except when relevant for historical context):

1) early PIC history and related works (see [6], [27], [32]–[35]);
2) nonconformal EM-PIC schemes (including adaptive mesh refinement);
3) non-EM-PIC methods (unless necessary to provide historical context);
4) nonparticle or hybrid-particle schemes (i.e., fluid-based plasma simulation methods);
5) computer-science-based and hardware developments (e.g., graphics processor unit and parallel implementations).

Before proceeding, the meaning of conformal must be addressed. In what follows, *conformity* (also referred to as *body fitting*) will refer to solution domains and corresponding meshes that closely match material interfaces and physical boundaries. Note that the traditional staircased mesh (see Fig. 1) is considered nonconforming in this work when considering a curved or misaligned boundary (or misaligned with respect to the simulation coordinate axes). The term *closely* here includes both *approximate* and *exact* conformity. For example, a virtual domain and/or mesh with outer boundaries or material interfaces exactly matching the physical location and shape of their corresponding physical boundaries and interfaces demonstrates *exact* conformity. On the other hand, if simulation boundaries and interfaces only partially or closely match the position and shape of their physical counterparts, then the mesh is only *approximately* conformal. Visual depictions of both conformal and nonconformal meshes are provided in Fig. 1.

It should be noted that a hexahedron-based mesh aligned along all three Cartesian coordinates is in fact typically exactly conforming when representing a brick structure. However, the discussion from hereon will address irregular boundaries and interfaces as those representing curved or slanted features when referring to systems and methods demonstrating conformity.

This paper is organized as follows. Due to its parallel development history and strong influence on conformal EM-PIC methods, a brief review of conformal electromagnetic simulations is first outlined in Section II. Many particle physics and related algorithms often used in conformal EM-PIC simulations are presented in Section III. Finally, Section IV highlights areas of recommended research in conformal EM-PIC methods, while a brief summary of this paper is provided in Section V.

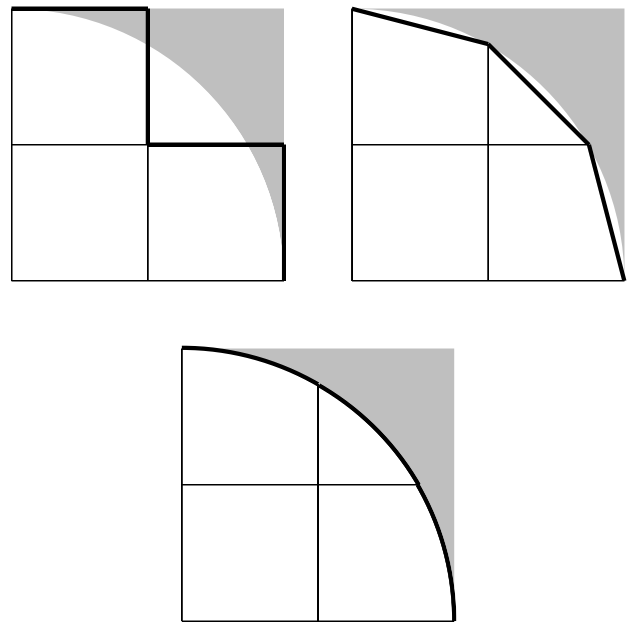

Fig. 1. Examples of (top left) nonconformal (e.g., *staircased*), (top right) approximately conformal, and (bottom) exactly conformal meshes representing a curved physical boundary.

II. Conformal Electromagnetic Solution Methods

The conformity of any simulation is intimately related to its virtual solution domain, which in the case of EM-PIC is determined by the mesh structure. Since electromagnetic field samples are located on this mesh, the electromagnetic solution itself is an integral part of a conformal EM-PIC model. Furthermore, since EM-PIC schemes are almost always time-dependent solutions (in order to capture nonlinear temporal effects), the following algorithms are limited to temporal electromagnetic schemes. The mesh-based electromagnetic field solution algorithms cited here were first developed by the computational electromagnetics community prior to their inclusion in EM-PIC schemes. Thus, due to both their important role in conformal EM-PIC schemes and their previous chronological development, an overview of conformal electromagnetic field solution methods is warranted, but only a brief review is provided here. Further reading may be obtained elsewhere in the many review papers on the subject [23], [24], [26], [29]–[31], [36].

A. Finite-Difference Time Domain

Arguably the first, simplest, and most widely used time-domain electromagnetic field solution algorithm is the FDTD method, first developed and published in 1966 [37]. Although fast and based upon simple theory, the Yee FDTD algorithm is not conformal for irregular boundaries and is thus available (without staircasing) only for a small subset of mesh structures. In light of these drawbacks, many have proposed augmented FDTD methods in attempts to achieve conformity while maintaining its attractive qualities. Such conformal FDTD methods are discussed in the following.

The first conformal electromagnetic FDTD schemes were published in [38]–[42], albeit for straight-edged domains. These early methods were later extended to curved boundaries [43]–[45] and curvilinear meshes [46], [47]. Other conformal FDTD implementations of note have included the use of both overlapping conformal and nonconformal grids [48], the inclusion of conformal dielectric weights in the FDTD algorithm [49], [50], simple area weighting for diagonal cells [51], [52], the introduction of a field correction step [53], improved stability [54], and localized boundary implementations [55].

One of the most popular conformal FDTD algorithms is the *Dey–Mittra* scheme (after its developers) [56]–[62]. Generalizing [51] and [58], the Dey–Mittra algorithm employs the integral form of Faraday's law by calculating modified face areas and realizing that the tangential electric field in any conformal surface must go to zero. While simple in theory, the Dey–Mittra scheme is applicable only when perfect electric conductors (PECs) are present, and can also reduce the maximum allowable time step in order to maintain stability. Zagorodnov *et al.* [63], [64] and Xiao and Liu [65], [66] later developed area-extending interpolation schemes that successfully addressed this issue. Other related methods involve grouping electric flux calculations and local time-stepping schemes [67], and flux-limiting methods adapted from the computational fluid dynamics (CFD) community [68].

On the other hand, irregular interfaces separating two dielectrics have been effectively treated by employing whole cell weighting [49], [50], [69], [70], applying material differences at individual cell edges [71], and borrowing similar algorithms from photonic bandgap methods [72]–[74]. Schemes citing second-order accuracy have also been developed for various material interface combinations [75], [76], while recent implementations have cited even higher order accuracy [67], [77]–[80]. Of course, these works represent only a small subset of available methods for effectively simulating systems containing dielectric interfaces.

Finally, many FDTD-based schemes have been designed for curvilinear meshes (which preserve the exact conformity of even curved boundaries), including early works by Holland [81]. More recent works have included efficient temporal schemes [82], higher order algorithms [83], and Lagrangian-based approaches [84].

B. Finite-Volume Time Domain

The first to apply finite-volume time-domain (FVTD) methods in simulating electromagnetic fields on conformal meshes were Madsen and Ziolkowski [85], Shankar *et al.* [86], and Mohammadian *et al.* [87]. Holland *et al.* [88] improved upon these early methods by introducing second-order accuracy for nonuniform and nonorthogonal grids. Gedney and Lansing [89] and Madsen [90] later independently developed a method guaranteeing the preservation of local charge divergence, while Hermeline [91] introduced energy-conserving algorithms. The stability of the FVTD algorithm was later analyzed in [92]–[96].

C. Finite-Element Time Domain

Following several early methods originally developed for simulating temporal electromagnetic scattering [97]–[105], Lynch and Paulsen [106] were the first to publish an explicit finite-element time-domain (FETD) formulation. Still others independently developed and published similar explicit FETD algorithms the same year [107], [108]. Recent applications of the explicit FETD method have included inhomogeneous media [109], hybrid boundary integral schemes [110], the use of various cell shapes [111]–[116] and mesh structures [117], finite difference-based schemes [118], unconditionally stable explicit time-stepping [119], [120], mass lumping [121], sparse matrix approximations [122], and higher order accuracy [123].

Implicit FETD schemes were first published in [124] and [125], with unconditionally stable schemes later introduced in [126] and [127]. Recent implicit FETD developments have included the use of mixed basis functions [128]–[130], Whitney element schemes for vector bases [131]–[134], variational integrators [135], [136], and the application of other implicit time-stepping schemes [115], [137], [138].

D. Discontinuous Galerkin Time Domain

The discontinuous Galerkin (DG) time domain (DGTD) method remains attractive for its ability to achieve higher-order accuracy independent of the original mesh resolution [139], [140]. Recent DGTD applications have included cavity mode analysis [141], and local mesh refinement [142] and time stepping [143].

E. Hybrid Methods

Some of the first hybrid electromagnetic solutions combined both FDTD and FVTD algorithms on conformal hybrid meshes [144]–[146]. Yee *et al.* [48] and Yee and Chen [147] later proposed a hybrid FVTD/FDTD scheme employing overlapping meshes assuming edge- and node-based field assignments. Later extensions included 3-D nonhexahedral-based meshes [147], separate curvilinear and rectangular meshes [148], and impedance boundary conditions [149]. Yang *et al.* [150] adapted this overlapping mesh scheme for curvilinear PEC boundaries with inhomogeneous cell filling, while Donderici and Teixeira [151] extended it to arbitrary mesh orientations. Although accurate [48], [147], early FVTD/FDTD schemes proved unstable at later time steps (often referred to as *late-time instability*) [17], [152]. Riley and Turner [17], [152], [153] were the first to develop a hybrid FVTD/FDTD method that avoided the late-time instabilities associated with earlier methods [146], [154] by introducing artificial numerical damping.

Wu and Itoh [155], [156] developed the first FETD/FDTD hybrid methods in the mid-1990s independently of Darve and Loehner [157]. Feliziani and Maradei [158] later employed Whitney elements in the independent development of a more accurate hybrid FETD/FDTD scheme, while Koh *et al.* [159] developed an interpolation scheme for passing between nonconforming meshes. Others have extended these works to dispersive materials [160], simplified formulations [161]–[164], and DG-like flux passing schemes [165]–[168].

As with the FVTD/FDTD hybrid schemes, computational issues quickly arose in these hybrid FETD/FDTD schemes, taking the form of nonphysical reflections and late-time instabilities [161], [169]–[171]. Hwang and Wu [169] were the first to address these problems in FETD/FDTD methods by applying a numerical low-pass filter, while Rylander and Bondeson [170] and Rylander [172] later interpreted the wrapper layer by applying trapezoidal integration, thus avoiding the late-time instability previously observed. Riley [173], Riley *et al.* [174], Montgomery *et al.* [175], Edelvik [176], Abenius *et al.* [177], El Hachemi *et al.* [178], [179], and Rylander *et al.* [180] have more recently adapted this hybrid FETD/FDTD algorithm for numerous electromagnetic scattering applications, while Monorchio *et al.* [181] interfaced it with still more boundary methods.

Driscoll and Fornberg [182] and Fomberg [183] were the first to lay the foundations of DGTD/FDTD, while Garcia *et al.* [184], [185] were the first to explicitly publish a hybrid DGTD/FDTD scheme.

Although too numerous to name them all here, other hybrid schemes have included FVTD/FETD schemes [186], Taylor–Galerkin methods borrowed from CFD [187], FETD/DGTD hybrid schemes [188], and finite-integration technique (FIT)/FVTD schemes [189].

III. Electromagnetic Particle-in-Cell Schemes

The electromagnetic field update represents only one of the four major components of the EM-PIC solution algorithm (the others being force interpolation, particle push/tracking, and current weighting) [4]–[6], [190]. The particle push in any EM-PIC scheme is unaffected by the choice of mesh structure due to its representation in a continuum domain. Thus, only the interpolation between fields and particles (force interpolation), particle tracking across mesh cells, and current weighting are affected. It should be noted the absorption and emission of particles from material and domain boundaries are also affected by the choice of either an approximate or exact conformal mesh, although its inclusion in the EM-PIC algorithm depends on the system being simulated. A summary of the various numerical methods employed by conformal EM-PIC schemes during these algorithm steps will be discussed in the following.

A. Conformal FDTD-PIC

Prior to conformal EM-PIC developments, Quintenz [191] introduced the first electrostatic PIC (ES-PIC) scheme capable of simulating slanted emission surfaces. Although limited in conformity to diagonally bisected quadrilaterals in two dimensions, his work represented the first conformal PIC code.

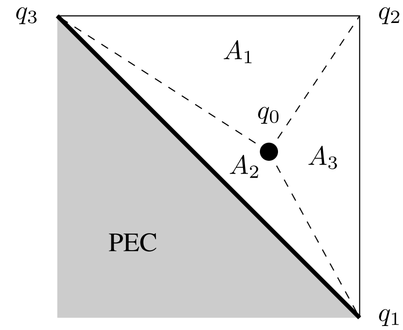

Fig. 2. Triangle area weighting scheme used for the electrostatic simulation of slanted boundaries. Figure adapted from [192].

The same diagonally bisected conformal cell scheme was later adapted in [192] for a fully time-dependent EM-PIC scheme. Mezzanotte *et al.* [51] later independently developed a similar algorithm to simulate purely electromagnetic fields. Accurate charge assignment within the conformal bisected Cartesian cells was ensured by modifying the standard bilinear interpolation schemes of earlier EM-PIC works. For example, a point charge located within a given triangular cell may be distributed to its three surrounding cell nodes via inverse area weighting according to

$$q_i = \frac{q_0 A_i}{\sum_{j=1}^{3} A_j} \tag{1}$$

where q_i is the fraction of the original charge mapped to the ith node and A_i is its associated fractional area. A visual representation of this charge assignment algorithm is shown in Fig. 2.

Pointon [192] also addressed accurate particle emission at slanted boundaries and around corners by solving Gauss' law at local boundary cells. The same slanted boundary particle emission method was later generalized to Cartesian meshes in three dimensions [193].

Grote *et al.* [194] published the first application of true cut cells when describing their ES-PIC code, WARP. Cut cells were first implemented in an EM-PIC computational framework, VORPAL, two years later [195], [196], and became one of its important capabilities and features [197]–[201]. Nieter *et al.* [195], Smithe *et al.* [197], and Nieter *et al.* [198] originally developed a conformal emission scheme based upon extending the particle path from its nearest exterior node. Although simple in theory, this method introduced more noise than comparable algorithms [197] and did not guarantee charge conservation [195], [198]. It also incorrectly assigned emitted charge to the two closest interior nodes *prior*, leading to spurious charges [195], [197]. Improved emission algorithms (visually depicted in Fig. 3) were later developed to avoid these shortcomings [199].

The particle seen in Fig. 3 is initially assigned to either the nearest node or opposing edge (face) in two (three) dimensions, and is then emitted normal to the conformal boundary. This two-step process avoids the problem of premature space charge introduction prior to physical emission [199]. Both of the above node and edge (or face) emission algorithms are essentially identical in accuracy and charge positioning,

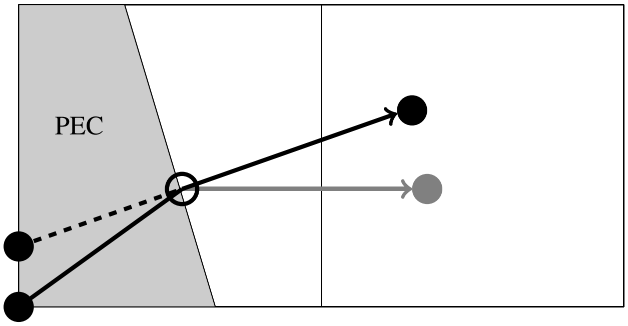

Fig. 3. Charge-conserving cut-cell particle emission via corner (solid line) and edge (dashed line) schemes. Emission via the noncharge-conserving orthogonal edge scheme (gray line) is also shown.

only differing in their coding complexity [199]. In each case, emission uniformity was addressed via a stochastic surface area weighting scheme [197].

One potential issue introduced by these two emission algorithms includes the particle move itself. For example, if the physical lengths of these two moves are significantly different, then nonphysical fields can result at the emission surface [199]. This currently remains an unsolved problem in Dey–Mittra EM-PIC schemes and is recommended for future research.

Particle behavior (both absorption and emission) in the vicinity of domain boundaries and material surfaces is paramount to the operation of many real-world plasma systems. This also holds true for their corresponding EM-PIC simulations. As the most accurate and flexible choice, several EM-PIC simulations have been developed for curvilinear (or nonorthogonal) meshes in efforts to capture this important behavior.

Although Halter [202] was the first to develop an ES-PIC code on nonorthogonal meshes, Jones [203] was the first to develop an EM-PIC code on nonorthogonal meshes. Seldner and Westermann [204] later published the first particle push algorithm tailored specifically for curvilinear meshes by interpolating between nonorthogonal (physical) and orthogonal (logical) meshes. Westermann [205]–[208] pursued this work, developing algorithms for transformed coordinate frames, while Friedman *et al.* [209] also employed similar methods. Grote *et al.* [194], [210] later developed a suite of tools for use in their WARP code, which included cut cells and the ability to process *warped* meshes.

Recent work in FDTD-based PIC schemes on nonorthogonal meshes has included 3-D ES-PIC formulations developed in [211]–[214] with 3-D versions currently under development. Citing the benefits of a structured mesh with exact geometric representation, curvilinear EM-PIC simulations remain promising and are also recommended for future research and development.

B. FVTD-PIC

The improved geometric flexibility and accuracy often associated with FV-based PIC methods developed for unstructured meshes lead to added complexity when simulating particle behavior. Most notably, the incremental cell indexing associated with structured meshes is no longer available in unstructured meshes. As a result, more complex algorithms with additional computational costs are required to accurately capture the corresponding particle physics and track particles through the mesh. Several of these algorithms are described below.

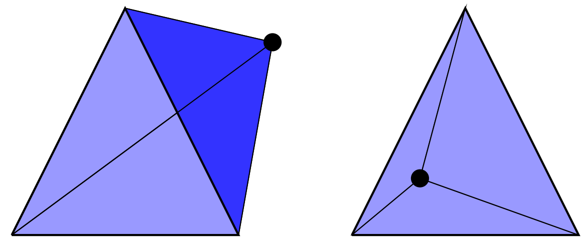

Fig. 4. Visual representation of triangle area summation. Noncontained (left) and contained particles (right) with correspondingly shaded areas.

The first FV-based PIC scheme developed specifically for an unstructured mesh was published in [215]. Based upon the earlier methods of Winslow [216] and limited to a 2.5- dimensional ES-PIC formulation, this work by Matsumoto and Kawata represented the first PIC scheme capable of simulating system behavior within a tetrahedron-based unstructured mesh. After updating particle velocities and positions, the containing mesh cell for every particle must be identified. Matsumoto and Kawata performed this search within a two-dimensional unstructured mesh by summing particle-edge triangle areas and testing with the original cell area, as visually depicted in Fig. 4.

For example, the total area of the image on the right in Fig. 4 is equal to that of the test cell, while the total area associated with the left particle position is larger than the test cell. Thus, the particle in the image on the right in Fig. 4 belongs to the current mesh cell, while the particle in the left image does not.

If the cells are not efficiently searched, the testing phase can prove prohibitively expensive for a large unstructured mesh. Matsumoto and Kawata [215] limited this search to those cells falling within a maximum particle traversal radius as determined by the simulation time step. Although significantly more efficient than the exhaustive brute force method described previously, this maximum radius search method neglects all cells traversed on the way from the original to the final cell, if they exist. In this case, these traversed cells are required for assigning current weights prior to updating the electromagnetic fields at the start of the next solution cycle.

These particle–mesh interpolations were calculated by first choosing a maximum radius of the searchable area, or typically the maximum length of any cell edge. Assuming node-based fields, the total force acting upon any given particle was then calculated by summing over all enclosed effective forces via [215]

$$\vec{F}_P = \sum_{i=1}^{N} \frac{\vec{F}_i}{l_i} \Big/ \sum_{i=1}^{N} \frac{1}{l_i} \tag{2}$$

where N is the total number of enclosed nodes (or fields in this case), $\vec{F}_i$ is the force on the particle at P due to the fields associated with node i, $\vec{F}_p$ is the total force on the particle, and l_i are the distances separating the ith mesh node and the particle position P. A visual representation

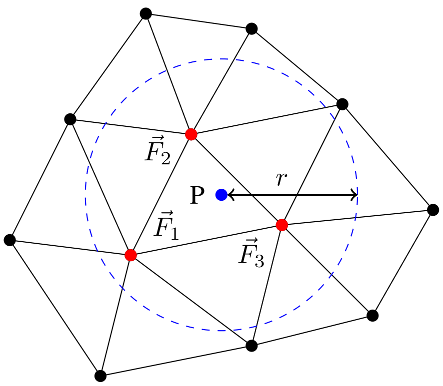

Fig. 5. Visual representation of the Matsumoto and Kawata particle–mesh interaction space.

of this calculation is provided in Fig. 5, with the enclosed (red dots) nodes highlighted. Charges and current densities were assigned to mesh nodes in a similar manner. Matsumoto and Kawata [215] reported the conservation of numerous physical quantities, citing the use of reciprocal interpolation schemes.

Hermeline [217] and Adolf *et al.* [218] published the first electromagnetic FVTD-PIC code around the same time. FVTD electromagnetic field solution methods were paired with a PIC update scheme on unstructured grids in two dimensions for the cylindrical coordinate frame. Unlike [215], the FVTD-PIC scheme used in [217] and [218] employed a Delaunay–Voronoï dual-mesh structure [219], [220]. Here, particle tracking was performed using fully vectorized search scheme [221], while charge assignment employed weighted distributions [218]. Hermeline [222] later extended their method to three dimensions and solved the Maxwell-Vlasov system.

Karmesin *et al.* [223] later developed particle-tracking and current assignment schemes on nonorthogonal meshes for use in FVTD-PIC codes by updating the particle velocity in the physical frame, with the particle position updated in the logical frame. This was similar to the method developed in [204]–[206], which was adapted in [224]. Charge and current density assignments were then available through the application of the well-known Villasenor and Buneman scheme [225] on the logical mesh [223]. While accurate and extremely flexible, these transformations between logical and physical spaces contribute added complexity to the overall EM-PIC algorithm. Earlier weighting methods developed in [226] remained applicable, while more recent schemes have demonstrated decreased computational effort [227].

Gatsonis and Spirkin [228], [231] and Spirkin and Gatsonis [229], [230] later published an improved particle search algorithm for unstructured meshes using the known particle velocity to dictate the search direction. Based upon [221], it required solving [228]

$$\mathbf{r}_0(t) + \mathbf{v}(t)\tau = \alpha\mathbf{r}_{12} + \beta\mathbf{r}_{13} \tag{3}$$

as a matrix equation for the unknown scalar values

$$\begin{bmatrix} \alpha \\ \beta \\ \tau \end{bmatrix} = [\,\mathbf{r}_{12} \quad \mathbf{r}_{13} \quad -\mathbf{v}\,]^{-1}[\,\mathbf{r}_0\,] \tag{4}$$

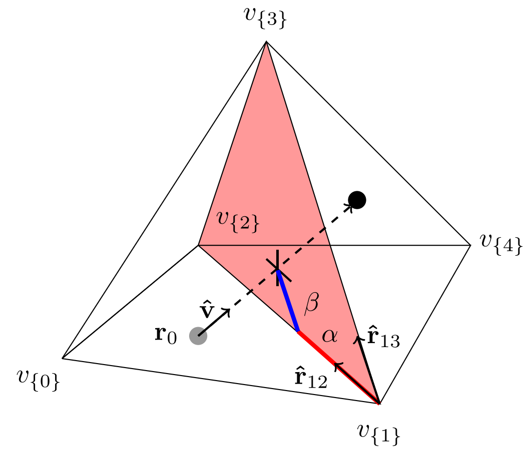

Fig. 6. Gatsonis and Spirkin particle search algorithm displaying a particle-intersecting face, f_{123} (shaded region).

where the scalar unknowns τ, α, and β represent the time of flight from $\mathbf{r}_0$ to the intersection point with face f_{123}, and the intersection points in the skewed coordinate frame, respectively. If $0 < \tau < 1$ and $0 < \alpha + \beta < 1$, then the particle-intersected face f_{123} and the adjacent cell must be checked for further face intersections. Conversely, if τ is negative or greater than one for all tested faces, the particle is assumed to belong to the current cell. In all other cases, a particle–face intersection does not exist, and the next face is checked. This particle search algorithm is visually depicted in Fig. 6.

The Gatsonis and Spirkin particle search algorithm identifies all traversed cells (in order) and locates their point of intersection, with the latter being useful in the case of boundary intersection. However, this method does require solving a matrix equation for each particle and every corresponding face tested, which can be computationally expensive when tracking billions of particles.

Further FVTD-PIC applications have included charge-conserving schemes employing higher order time stepping [232], drift–diffusion models for simulating glow discharges [233], atmospheric plasma simulations [234], development for parallel architectures [223], [235], charge correction [18], [236], [237] and conservation schemes [238], time splitting of the particle push update [239], and stochastic collision modeling [228]–[230], [240], [241].

C. FETD-PIC

The first FE-based particle codes were purely electrostatic in nature, simulated only electron gun systems, and solved the Vlasov–Poisson equations [242]–[247]. Physical–logical space interpolations for nonorthogonal meshes [242], [243] and with bilinear interpolation within elements [244]–[246] were developed. Other early works in FE-based PIC included Galerkin testing methods [248]–[250] and particle pushing algorithms [251].

Although earlier works have been cited [252], [253], the first full and *detailed* descriptions of FETD-PIC schemes were independently published in [218] and [254]–[256]. Degond *et al.* [256] introduced mass lumping in order to

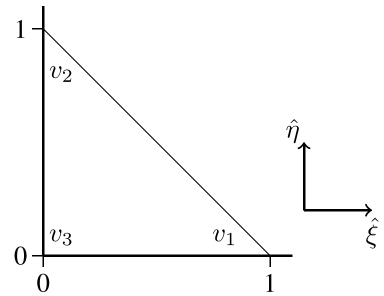

Fig. 7. Scalar basis function assignment in the transformed coordinate frame [257].

decrease the computation time of the field solve, while mesh-to-particle electromagnetic field interpolations were computed using area weighting techniques. The first tracking algorithms for unstructured meshes were published by Löhner and Ambrosiano [257] who borrowed heavily from the CFD community. Here, each triangular cell within the 3-D unstructured mesh was mapped to a regular right triangle with edge length unity. The three nodal basis functions within these transformed coordinates then become

$$N_1(\xi, \eta) = \xi, \quad N_2(\xi, \eta) = \eta, \quad N_3(\xi, \eta) = 1 - \xi - \eta \qquad (5)$$

where ξ and η represent the transformed coordinate frame unit vectors corresponding to $\hat{x}$ and $\hat{y}$ in the physical frame. A visual representation of this is provided in Fig. 7.

This transformation between coordinate frames drastically simplified the particle search algorithm. For instance, once the corresponding ξ and η positions were computed for a given particle position in the physical frame, the particle belonged to the current cell if [257]

$$\min\{N_1, N_2, N_3\} \geq 0, \quad \max\{N_1, N_2, N_3\} \leq 1 \qquad (6)$$

which avoids the matrix inversions from (4) entirely, although the calculation of all N_i values at the current particle position is still required. The resulting vectorized particle search algorithm is as follows [257].

1) Perform the scalar basis function test from (6), starting with the previous known cell.
2) If the particle belongs to the current cell, move on to the next particle. If not, continue.
3) Gather the cell index opposite the present node with the lowest basis function value.
4) Recompute basis functions in (6).
5) Repeat Steps 2–4 until all particles are located, moving those particles to the end of the *active* list.

A visual representation of a particle traversing an unstructured grid is provided in Fig. 8.

Degond *et al.* [256] later implemented a node-based vectorized search, allowing for the simultaneous updating of both cell location and charge assignments. Further enhancements were later introduced in [221] and [258]–[261].

Although computationally more efficient than the unstructured mesh particle search of Gatsonis and Spirkin, the Löhner and Ambrosiano particle search does not necessarily identify only traversed mesh cells. Instead, their particle search

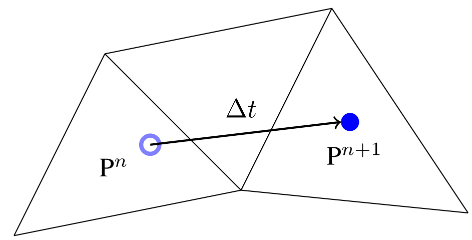

Fig. 8. Particle tracking across an unstructured mesh of triangles.

method may identify external cells through which the particle never entered. This is due to the identification of the most likely traversed adjacent cell based solely on the minimum nodal basis function value. As a result, those cells identified as traversed by a particle may extend outside the path of the particle and may contain erroneous cells. This may not only lead to assigning current and charge to incorrect mesh edges, but may also result in errors in particle–surface interactions (including absorption).

In an attempt to capture exact geometric conformity, FETD-PIC schemes have been developed for nonorthogonal meshes as well. Arter and Eastwood [262], Eastwood [263], and Eastwood *et al.* [264]–[267] were the first to develop such an FETD-PIC method. Similar to other methods developed for nonorthogonal meshes, coordinate transformations between physical and logical spaces were employed in [264], [267], and [268], removing the need for complex particle search algorithms or mesh–particle interpolations. Charge and current conservation in unstructured and nonorthogonal meshes was also developed and reported in [263] and [267].

FETD-PIC schemes have more recently been applied in the simulation of traveling-wave tubes [269], ion thrusters [270], beam dynamics [271]–[279], high current sources [280]–[282], and gas cells [283], [284]. Electrostatic FETD-PIC schemes [285]–[289], higher order basis functions [290], adaptive meshing [291], [292], charge and current conservation [136], [293]–[296], parallelization [297], and others works [298], [299] have also been reported.

D. DGTD-PIC

Much like its corresponding and purely electromagnetic formulations, DGTD-PIC has received increased interest in recent years. Jacobs and Hesthaven [300], [302] and Jacobs *et al.* [301] were the first to publish a DGTD-PIC scheme, while also proposing and implementing a unique particle search algorithm. For any particle leaving its parent cell during the particle push, the node in closest proximity to its traveled path is identified and stored. All adjacent mesh cells connected to this identified node were then searched in logical space for particle containment. Due to the large size of the higher order elements employed, particles were typically found within this first grouping of adjacent cells [300].

Of particular interest to Jacobs and Hesthaven was the accurate assignment of charge back to the unstructured mesh. In their original DGTD-PIC work, they proposed and analyzed a series of charge assignment functions based upon continuous and differentiable functions [300]. These functions were chosen to avoid grid heating and instability, along with

Gibbs-like phenomena [4], [300]. Comparing against an analytic solution, weighting functions with more confined representations were found to exhibit less noise, although at the cost of increased run time [300]. Several charge conservation methods were also developed and detailed in [300].

DGTD-PIC methods have recently been used to simulate many real-world systems, including linear accelerator cavities [19], electron guns [21], and gyrotrons [303]. The DGTD-PIC method has also been used to solve Vlasov–Poisson [304]–[309] and Vlasov–Ampere systems [310], [311] and to accurately capture physical phenomena [312].

E. Hybrid Methods

Unlike their purely electromagnetic counterparts, few hybrid PIC schemes have been developed. In fact, Seidel *et al.* [313] developed one of the only hybrid PIC schemes, employing a hybrid FVTD/FDTD electromagnetic solution. As usual, tetrahedral elements lining curved and slanted domain boundaries were interfaced with hexahedron elements forming a wrapper layer. FVTD was applied within all tetrahedra and the wrapper layer, while FDTD was applied within all remaining elements. Particle tracking was performed using the previously detailed methods, while charge and current density were assigned via volume weighting. Although too numerous to mention here, Seidel *et al.* [313] discussed many other issues encountered in this hybrid PIC method.

To date, the authors know of no other published hybrid PIC schemes. Although references to other hybrid PIC methods do exist, their authors either avoid detailed development citing complexity concerns [314] or the code remains untested or incomplete [315]–[317]. Hybrid PIC schemes could prove very successful and advantageous in future applications, and are recommended as an area of future research.

F. Other EM-PIC Methods

Numerous other EM-PIC schemes have also been published. For example, Weiland *et al.* [318] adapted the FIT method to simulate accelerator beam physics, while Friedman *et al.* [209] and Grote *et al.* [194], [210] later employed spatial transformations to predict particle behavior in bent beams. More recent developments have included the application of phase-space methods in solving the Vlasov equation [319], Green's function-based approaches [320], and improved data extraction FIT methods [321].

IV. Future Directions

There is much potential for continued research into conformal EM-PIC schemes. As previously highlighted, recommended areas of future research and development into conformal EM-PIC methods include finite difference-based EM-PIC schemes for nonorthogonal meshes, hybrid EM-PIC frameworks, and improved particle emission for cut-cells. All of these methods promise significant improvements over current conformal EM-PIC simulation capabilities. But if such simulations were developed, what algorithms would they likely draw upon? What advances might they provide in terms of computational cost and improved accuracy or flexibility?

For a 3-D EM-PIC code on a curvilinear mesh, the electromagnetic field solve would likely expand upon [46], [47], [211]–[214], and [264]–[268]. This could then be paired with particle push, tracking, and scattering algorithms developed specifically for curvilinear meshes [214], [264], [265], [267]. The resulting conformal EM-PIC code would likely be much less computationally expensive compared with the FE-based nonorthogonal mesh field solve developed in [264], [265], and [267]. However, the stability and accuracy of such a solution when including particles and related current sources may still present issues and may need to be addressed.

Hybrid EM-PIC schemes also promise much improved geometric conformity while simultaneously minimizing any cost increases. Such schemes would employ both unstructured and structured mesh regions, similar to previous hybrid mesh electromagnetic works [170], [171], [174], [180]. The electromagnetic field solve would likely draw upon the methods developed in [170], [171], [174], and [180], while particle tracking and current assignment could be updated, employing any one of the above-mentioned algorithms. It appears that such a hybrid EM-PIC scheme is presently achievable by merely gathering and combining various currently independent algorithms.

Finally, any improved particle emission method developed for cut cell-based conformal FDTD (CFDTD) EM-PIC schemes would need to address the path length issue described by Loverich [199]. Moreover, since several CFDTD-based EM-PIC codes are presently used [200], [322], improving upon this two-step emission algorithm in CFDTD-based EM-PIC is highly recommended.

V. Conclusion

Conformal EM-PIC solution methods and algorithms have been presented, discussed, and detailed. Brief mathematical descriptions for many important and popular methods were provided and also visually depicted. Conformal finite difference, volume, and element along with discontinuous Galerkin electromagnetic solution methods were also briefly discussed. Various algorithms developed for particle tracking and current weighting for unstructured and nonorthogonal meshes were detailed. The advantages and disadvantages associated with many of these methods were also highlighted. Differences between similar algorithms were highlighted where relevant.

Many conformal EM-PIC schemes currently exist, with very good mathematical and theoretical descriptions readily available. In many cases, the reader needs only to select a handful of numerical algorithms that conform to a given set of criteria (including computational cost, desired accuracy, generic applicability, etc.) to successfully simulate complex systems.

Finally, several areas of future research in conformal EM-PIC methods were recommended. These included EM-PIC frameworks on both nonorthogonal and hybrid meshes and an accurate particle emission algorithm for cut cells, which avoids erroneous field generation.

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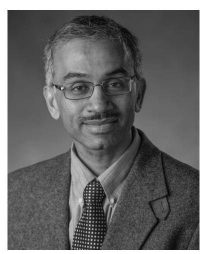

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