Diagnosing Spurious Cherenkov Radiation from Numerical Dispersion on Unstructured Grids

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***Abstract*—We investigate the numerical dispersion (phase velocity slow-down) of plane waves propagating on unstructured grids to examine the onset of numerical (spurious) Cherenkov radiation when high-energy charged particles are utilized for particle-in-cell (PIC) simulations. By comparing the numerical dispersion on structured and unstructured grids, we show that, by default, unstructured grids produce less numerical Cherenkov radiation than structured grid of same average cell size.**

I. Introduction

Particle-in-cell (PIC) algorithms have been widely used to model Maxwell-Vlasov equations [1]–[5] describing collisionless plasmas, and utilized for applications related to vacuum electronic devices (VED), astrophysics, and so forth [6]–[9]. Yee's finite-difference time-domain (FDTD) algorithm [10], [11] is typically chosen as the field-solver in PIC algorithms on structured grids, due to simplicity and ease of implementation. Any grid-based field solver such as FDTD produces numerical dispersion, i.e., the resulting 'free-space' electromagnetic (EM) plane wave solutions exhibit phase velocities which are frequency- and direction-dependent [10], [12], [13]. The resulting phase velocities are slower than in the continuum limit and decrease gradually with frequency (in the limit of high frequencies, they approach zero and cannot propagate beyond the grid cut-off frequency, f_{gc}) [14]. When particles are present on the grid, numerical (spurious) Cherenkov radiation can be produced whenever the particle velocities exceed the numerical phase velocity. Spectral low-pass filters or modified finite-difference stencils can be used to mitigate numerical Cherenkov radiation; however, the former may subtly alter the physics of Cherenkov radiation and the latter has a difficulty in dealing with grid boundaries and interfaces [14]. Recently, an exactly charge-conserving PIC algorithm on unstructured grids has been proposed [4], [5], which is devoid of staircasing error and is well-suited for applications involving complex geometries. Numerical dispersion effects on unstructured grids have been investigated in the past [15], [16] in the low-frequency limit (i.e., far from the cut-off frequency of the grid). Here, in order to diagnose the performance of PIC solvers on unstructured grids and compare it to the structured-grid case, we extend the numerical dispersion analysis to tackle the issue of numerical Cherenkov radiation on unstructured grids. In particular, we analyze numerical dispersion on unstructured grid elements with respect to wider bands (up to f_{gc}) and for all propagation directions $\phi_p \in [0^o, 360^o]$. For simplicity, we consider the two-dimensional case.

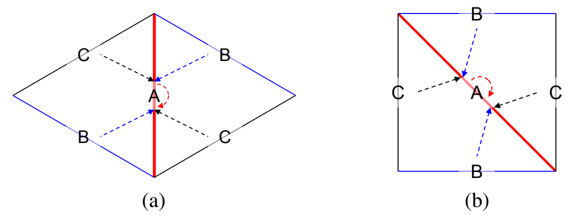
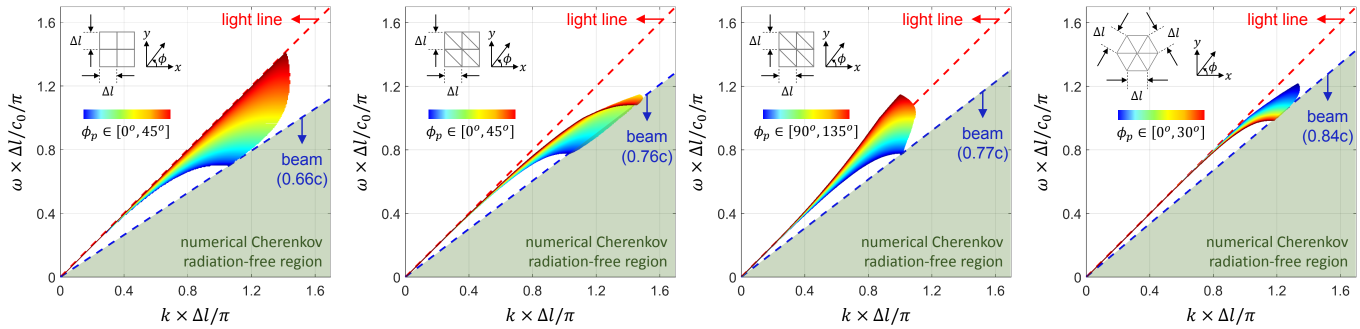


Fig. 1: Contributions of neighbor B- and C-type edges to the A-type edge for the system matrix. (a) is equilateral- and (b) is one-directional-shaped unstructured meshes.

II. Numerical dispersion relation

In the language of differential forms [12], [13], [17], the second-order source-free vector wave equation for electric field intensity is written as $d \star_{\mu^{-1}} d\mathcal{E} + \omega^2 \star_\epsilon \mathcal{E} = 0$ where d is an exterior derivative, $\mathcal{E}$ is a 1−form, $\star_\epsilon$ and $\star_{\mu^{-1}}$ are Hodge star operators associated to the permittivity and inverse permeability, respectively, and ω is the angular frequency. Expanding $\mathcal{E}$ by Whitney 1−form (edge based element) and applying Galerkin method, we can obtain a discrete eigenvalue equation as $\left(\left[\tilde{\mathcal{D}}_{\text{curl}}\right] \cdot \left[\star_{\mu^{-1}}\right] \cdot \left[\mathcal{D}_{\text{curl}}\right] - \omega^2 \left[\star_\epsilon\right]\right) \cdot [\mathbb{E}] = 0$ where $[\mathcal{D}_{\text{curl}}]$ is an incidence matrix analogous to the curl operator $\vec{\nabla}\times$ and having elements in the set of $\{-1, 0, 1\}$, $\left[\star_{\mu^{-1}}\right]$ and $[\star_\epsilon]$ are (symmetric positive-definite) discrete Hodge matrices, $[\mathbb{E}]$ denotes the column vector of degrees of freedom (Dof) for $\mathcal{E}$. Quantities with tilde symbols are associated to the dual mesh [12], [18]. In order to obtain the numerical dispersion relation, we follow a procedures similar to the one considered in [15]. On unstructured meshes, we assume three kinds of edges with respect to direction, which are denoted as A, B, and C as shown in Fig. 1. For a plane wave propagating along $\hat{k}$, the electric field is given by $\vec{E}(\vec{r}) = \vec{E}_0 e^{-j\tilde{k}\hat{k}\cdot\vec{r}}$, where $\vec{E}_0$ is a constant vector. Projecting the plane wave solution into $\mathbb{E}_j$ defined at the j-th edge, it yields $\mathbb{E}_{m(j)} = \hat{t}_{m(j)} \cdot \vec{E}_{0,m(j)} e^{-j\tilde{k}\hat{k}\cdot\vec{r}_{m(j)}}$ where $m(j)$ is a function for the j-th edge depending on the set $\{A, B, C\}$. Substituting the Dofs for the plane wave solution we obtain a discrete eigenvalue equation. Setting the associated determinant to zero provides the *local* numerical dispersion



(a) (b) (c)

Fig. 2: Dispersion relations for numerical plane waves propagating on the mesh. (a) is solved by the FDTD scheme with the structured grids, (b) and (c) are solved by FEM with unstructured grids of one-directional and equilateral cases, respectively.

relation for a plane wave propagating on the unstructured mesh. Note that this relation is only a local approximation because the size and shape of the elements an unstructured mesh does not in general remain constant.

III. Numerical examples

We compare the numerical dispersion properties on unstructured (locally) and structured grids to diagnose the possibility of numerical Cherenkov radiation. Fig. 2a illustrates the dispersion relation for the (structured-grid) FDTD algorithm. The dispersion relation is displayed for ϕ ranging from 0^o to 45^o (half period) since it follows a symmetric pattern for the other angles. In the low-frequency limit very small dispersion is observed, but at higher frequencies (larger wavenumber k) deviations from the light line become more pronounced. The region free from numerical Cherenkov radiation corresponds to a maximum beam velocity of $0.66c$. The local dispersion relations for ‘one-directional’ and equilateral unstructured grids are shown in Fig. 2b (two graphs) and Fig. 2c, respectively. Note that phase errors can be positive or negative on unstructured grids [15]. In the one-directional case, we plot the the results in the intervals $\phi \in [0^o, 45^o]$ and $\phi \in [90^o, 135^o]$, according to the azimuthal symmetry pattern of the local grid. It is seen that the region free from numerical Cherenkov radiation corresponds to a maximum beam velocity of $0.76c$ in this case. For the equilateral case, the dispersion relation is locally periodic under $\phi = 60^o$ rotations, and the half-period $\phi \in [0^o, 30^o]$ is displayed in Fig. 2c. The region locally free from numerical Cherenkov radiation in this case corresponds to a maximum beam velocity of $0.84c$. These results show that equilateral triangle cells provide least absolute values of (positive) phase errors across all angles and hence they are less prone to numerical Cherenkov radiation.

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