CHARGE CONSERVATION FOR SPLIT-OPERATOR METHODS IN BEAM DYNAMICS SIMULATIONS *

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Abstract

Split operator schemes have been recently applied for reducing the numerical dispersion in 3D beam dynamic simulations [1]. Another application of split-operator schemes is the unconditionally stable integration of Maxwell's equations in time [2]. However, in comparison to the standard Yee scheme these methods do not fulfill a semi-discrete Gauss law. Theoretically, this circumstances may result in an unbounded growth of the error in semi-discrete Gauss's law in the numerical integration. In this paper it is shown that this is not the case. The existence of modified fully discrete divergence operators for the investigated schemes is shown which guarantee the conservation of a fully discrete charge.

INTRODUCTION

An important aspect of self-consistent particle simulations in the time-domain is the conservation of charge during the simulation. From the Maxwell equations,

$$\text{curl}\ \vec{E} = -\partial_t \vec{B}, \qquad \text{curl}\ \vec{H} = \partial_t \vec{D} + \vec{J} \tag{1}$$

$$\text{div}\ \vec{B} = 0, \qquad \text{div}\ \vec{D} = \varrho \tag{2}$$

it follows that the sources and currents satisfy the continuity equation,

$$\partial_t \varrho + \text{div}\ \vec{J} = 0. \tag{3}$$

This is in general not true for discrete approximations where typically only the first pairs of Maxwell's equations (1) are discretized and solved. The reason for the lack of electric charge conservation in the fully discrete formulations can be categorized as follows:

- First, the semi-discrete approximation of (1) (i.e., discretized space and continuous time) has no appropriate semi-discrete divergence operator, div_h , consistent with (2). One possible reason for this is that, for the semi-discrete *curl* operator, curl_h , the identity, $\text{div}_h\ \text{curl}_h\ = 0$, does not hold.
- Second, the semi-discrete method has an appropriate discrete divergence operator div_h, however, the applied time-marching scheme does not conserve a fully discrete charge in any sense.
- Third, for a fully discrete approximation of (1) an appropriate fully discrete divergence operator div_{ht} exists, however, the fully discrete charge and current distributions do not fulfill the fully discrete continuity equation.

The paper is organized as follows. First, the semi-discrete Finite Integration Technique (FIT) is presented which preserves an appropriate semi-discrete divergence operator. Then, the time-integration of the FIT with split-operator schemes is described. In the following section, appropriate fully discrete divergence operators for the split-operator schemes are constructed. Using these operators, fully discrete continuity equations are derived and conservative fully discrete charge and current interpolation algorithms are constructed. In the last section, two test examples are presented showing the validity of the approach.

FINITE INTEGRATION TECHNIQUE

In this work the investigation is restricted to the FIT [3], however, the same techniques are applicable to other discretization methods. The topological building blocks of the FIT are the discrete operators

$$\begin{aligned} \mathbf{S} &:= \left(\mathbf{P}_x, \mathbf{P}_y, \mathbf{P}_z\right), & \widetilde{\mathbf{S}} &:= -\left(\mathbf{P}_x^T, \mathbf{P}_y^T, \mathbf{P}_z^T\right), \\ [\mathbf{C}]_{ik} &:= \varepsilon_{ijk}\mathbf{P}_j, & \widetilde{\mathbf{C}} &:= \mathbf{C}^T. \end{aligned} \tag{4}$$

Defining the vectors, $\widehat{\mathbf{e}} := (\widehat{\mathbf{e}}_x, \widehat{\mathbf{e}}_y, \widehat{\mathbf{e}}_z)$, of electrical voltages and, $\widehat{\mathbf{h}} := (\widehat{\mathbf{h}}_x, \widehat{\mathbf{h}}_y, \widehat{\mathbf{h}}_z)$, of magnetic voltages the vectors $\widehat{\widehat{\mathbf{d}}}$ of electric fluxes and $\widehat{\widehat{\mathbf{b}}}$ of magnetic fluxes are obtained by the discrete material laws

$$\widehat{\widehat{\mathbf{d}}} := \mathbf{M}_\varepsilon \widehat{\mathbf{e}}, \quad \widehat{\widehat{\mathbf{b}}} := \mathbf{M}_\mu \widehat{\mathbf{h}}. \tag{5}$$

The resulting Maxwell-Grid-Equations (MGE) separate into the dynamic laws

$$\mathbf{C}\widehat{\mathbf{e}} = -\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\widehat{\mathbf{b}}}, \quad \widetilde{\mathbf{C}}\widehat{\mathbf{h}} = \frac{\mathrm{d}}{\mathrm{d}t}\widehat{\widehat{\mathbf{d}}} + \widehat{\widehat{\mathbf{j}}} \tag{6}$$

and the static laws

$$\mathbf{S}\widehat{\widehat{\mathbf{b}}} = 0, \quad \widetilde{\mathbf{S}}\widehat{\widehat{\mathbf{d}}} = \mathbf{q}. \tag{7}$$

The ordinary differential equations (6) are the starting point for the fully discrete methods considered in this work. Equation (6) exactly conserves the semi-discrete charge with respect to the divergence operator,

$$\text{div}_h\ := \widetilde{\mathbf{S}}, \tag{8}$$

which is consistent with the definition of the discrete Gauss law in (7). Hence, only the time integration scheme or charge and current interpolation on the grid may introduce an unbounded growth of the error in Gauss's law.

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SPLIT-OPERATOR SCHEMES

VERLET-LEAPFROG SCHEME

A standard time-marching scheme for (6), with time step Δt, is the Verlet-Leap-Frog (VLF) method

$$\begin{aligned}\widehat{\mathbf{h}}^{(*)} &= \widehat{\mathbf{h}}^{(n)} - \frac{\Delta t}{2}\mathbf{M}_\mu^{-1}\mathbf{C}\widehat{\mathbf{e}}^{(n)},\\ \widehat{\mathbf{e}}^{(n+1)} &= \widehat{\mathbf{e}}^{(n)} + \Delta t\mathbf{M}_\varepsilon^{-1}\widetilde{\mathbf{C}}\widehat{\mathbf{h}}^{(*)},\\ \widehat{\mathbf{h}}^{(n+1)} &= \widehat{\mathbf{h}}^{(*)} - \frac{\Delta t}{2}\mathbf{M}_\mu^{-1}\mathbf{C}\widehat{\mathbf{e}}^{(*)}.\end{aligned} \tag{9}$$

Defining the vectors

$$\mathbf{y} := \left(\widehat{\mathbf{h}}, \widehat{\mathbf{e}}\right)^T, \quad \mathbf{b} := \left(0, -\Delta t\mathbf{M}_\varepsilon^{-1}\widehat{\widehat{\mathbf{j}}}\right)^T \tag{10}$$

it is possible to rewrite the update equations (9), now including the current source by a Godunov splitting, in the more compact form

$$\mathbf{y}^{(n+1)} = \mathbf{G}^{\mathrm{LF}}\left(\Delta t\right)\mathbf{y}^{(n)} + \mathbf{b}^{(n+1/2)} \tag{11}$$

with the propagation matrix $\mathbf{G}^{\mathrm{LF}}\left(\Delta t\right)$.

The VLF scheme preserves the semi-discrete charge defined by the semi-discrete Gauss law (7) if the charge and current are interpolated to the grid such that,

$$\mathbf{q}^{(n+1)} - \mathbf{q}^{(n)} + \Delta t\mathrm{div}_h\,\widehat{\widehat{\mathbf{j}}}^{(n+1/2)} = 0 \tag{12}$$

holds. Consistent charge and current interpolation for (12) are well know in the literature [4] and are in the rest of the paper referred to as standard current and standard shape schemes.

LONGITUDINAL-TRANSVERSAL LEAP-FROG SCHEME

We note that the VLF scheme has a larger maximal stable time step in one- and two-dimensions than in three-dimensions. This motivates a split-operator approach along the spatial directions to achieve stability and a better numerical dispersion along the z-axis. Defining the longitudinal and transversal *curl* operators by

$$\mathbf{C}_L := \begin{pmatrix} 0 & -\mathbf{P}_z & 0\\ \mathbf{P}_z & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \mathbf{C}_T := \mathbf{C} - \mathbf{C}_L \tag{13}$$

the second order accurate longitudinal-transversal VLF (LT-VLF) scheme reads

$$\mathbf{y}^{(n+1)} = \mathbf{G}_T^{\mathrm{LF}}\left(\frac{\Delta t}{2}\right)\mathbf{G}_L^{\mathrm{LF}}\left(\Delta t\right)\mathbf{G}_T^{\mathrm{LF}}\left(\frac{\Delta t}{2}\right)\mathbf{y}^{(n)}. \tag{14}$$

In (14) the propagation matrices $\mathbf{G}_T^{\mathrm{LF}}\left(\Delta t\right)$ and $\mathbf{G}_L^{\mathrm{LF}}\left(\Delta t\right)$ indicate that the VLF method (9) is applied with the partial *curl* operators $\mathbf{C}_L$ and $\mathbf{C}_T$ instead of the full *curl* operator $\mathbf{C}$, respectively. In [1] it is shown that the LT-VLF scheme is stable for an equidistant grid up to a Courant number equal to one and that it has no numerical dispersion along the z-axis at its stability limit. The current term is simply added to (14).

However, the LT-VLF scheme applies only the partial *curl* operators and, therefore, does not conserve the semi-discrete charge in the sense of (7).

ADI SCHEME

The ADI scheme [2] is an unconditionally stable time marching scheme which splits the *curl* operator into the two parts

$$\mathbf{C}_+ := \begin{pmatrix} 0 & 0 & \mathbf{P}_y\\ \mathbf{P}_z & 0 & 0\\ 0 & \mathbf{P}_x & 0\end{pmatrix}, \; \mathbf{C}_- := \mathbf{C} - \mathbf{C}_+. \tag{15}$$

Using these operators the time marching scheme is formulated as

$$\begin{aligned}\frac{\widehat{\mathbf{h}}^{(*)} - \widehat{\mathbf{h}}^{(n)}}{\Delta t/2} &= -\mathbf{M}_\mu^{-1}\left(\mathbf{C}_+\widehat{\mathbf{e}}^{(n)} + \mathbf{C}_-\widehat{\mathbf{e}}^{(*)}\right),\\ \frac{\widehat{\mathbf{e}}^{(*)} - \widehat{\mathbf{e}}^{(n)}}{\Delta t/2} &= \mathbf{M}_\varepsilon^{-1}\left(\widetilde{\mathbf{C}}_+\widehat{\mathbf{h}}^{(n)} + \widetilde{\mathbf{C}}_-\widehat{\mathbf{h}}^{(*)}\right),\\ \frac{\widehat{\mathbf{h}}^{(n+1)} - \widehat{\mathbf{h}}^{(*)}}{\Delta t/2} &= -\mathbf{M}_\mu^{-1}\left(\mathbf{C}_+\widehat{\mathbf{e}}^{(n+1)} + \mathbf{C}_-\widehat{\mathbf{e}}^{(*)}\right),\\ \frac{\widehat{\mathbf{e}}^{(n+1)} - \widehat{\mathbf{e}}^{(*)}}{\Delta t/2} &= \mathbf{M}_\varepsilon^{-1}\left(\widetilde{\mathbf{C}}_+\widehat{\mathbf{h}}^{(n+1)} + \widetilde{\mathbf{C}}_-\widehat{\mathbf{h}}^{(*)}\right).\end{aligned} \tag{16}$$

Scheme (16) separates naturally into two stages, each being implicit in time. In analogy to the VLF method the propagation matrix, $\mathbf{G}^{\mathrm{ADI}}\left(\Delta t\right)$, for the ADI method is defined by (16). Even though the method is implicit, the resulting linear equations can be solved with the sweep method and thus the asymptotic complexity of the method is the same as that of an explicit method. However, also the ADI method (16) does not conserve the charge in the sense of (7).

CONSTRUCTION OF DISCRETE DIVERGENCE OPERATORS

For the construction of an appropriate fully discrete divergence operator the following, general update equation (omitting the explicit dependence on Δt)

$$\mathbf{y}^{(n+1)} = \mathbf{G}\mathbf{y}^{(n)} \tag{17}$$

is considered. Every linear operator $\mathbf{L}$ which defines a scalar grid function φ by $\varphi := \mathbf{L}\mathbf{y}$, which is conserved under the time evolution of (17) has to fulfill the condition

$$\mathbf{L}\mathbf{G} = \mathbf{L}, \quad \left[\mathbf{L}\right]_{ij} := \left[\mathbf{v}_j\right]_i \tag{18}$$

which means that $\mathbf{L}$ is a matrix of left eigenvectors $\mathbf{v}_\mathbf{j}$ with eigenvalue one of the propagation matrix $\mathbf{G}$.

In general, it is not possible to construct $\mathbf{L}$ analytically. However, if boundary conditions are neglected, homogeneous material distributions and grids are assumed, the problem becomes amenable to an analytical treatment. The reason for this is that under these conditions all operators involved in the definition of $\mathbf{G}$ commute. Therefore, it is possible to treat the operators like numbers and hence to find the solutions of (18) with the help of a computer algebra package. In the following, $\sigma := c\Delta t/\Delta$ denotes the Courant number, where Δ is the mesh spacing of a equidistant grid. The appropriate fully discrete divergence operator of the LT-VLF method is given by

$$\mathrm{div}_{ht}^{LT} := \left(\widetilde{\mathbf{S}}_x\mathbf{\Lambda}, \widetilde{\mathbf{S}}_y\mathbf{\Lambda}, \widetilde{\mathbf{S}}_z\right), \; \mathbf{\Lambda} := \mathbf{1} + \frac{\sigma^2}{4}\mathbf{P}_z\mathbf{P}_z^T \tag{19}$$

and that of the ADI method by

$$\mathrm{div}_{ht}^{ADI} := \left(\widetilde{\mathbf{S}}_x\mathbf{\Lambda}_x, \widetilde{\mathbf{S}}_y\mathbf{\Lambda}_y, \widetilde{\mathbf{S}}_z\mathbf{\Lambda}_z\right), \tag{20}$$

$$\mathbf{\Lambda}_x := \mathbf{1} - \frac{\sigma^2}{4}\mathbf{P}_z\mathbf{P}_z^T, \quad \mathbf{\Lambda}_y := \mathbf{1} - \frac{\sigma^2}{4}\mathbf{P}_x\mathbf{P}_x^T,$$
$$\mathbf{\Lambda}_z := \mathbf{1} - \frac{\sigma^2}{4}\mathbf{P}_y\mathbf{P}_y^T.$$

A comparison with (8) shows that (19) and (20) are consistent, second order accurate fully discrete divergence operators in space and time. Using these operators, the fully discrete Gauss laws defined by

$$\mathrm{div}_{ht}^{LT}\widehat{\widehat{\mathbf{d}}} = \mathbf{q}_{ht}, \quad \mathrm{div}_{ht}^{ADI}\widehat{\widehat{\mathbf{d}}} = \mathbf{q}_{ht} \tag{21}$$

are conserved for the LT-VLF and ADI scheme, respectively.

SOLUTION OF THE DISCRETE CONTINUITY EQUATION

Applying div_{ht}^{LT} on the update equations (14) and (16), respectively, results in the fully discrete continuity equations

$$\mathbf{q}^{(n+1)} - \mathbf{q}^{(n)} + \Delta t\,\mathrm{div}_{ht}^{LT/ADI}\widehat{\widehat{\mathbf{j}}}^{(n+1/2)} = 0. \tag{22}$$

In order to derive charge and current interpolations which satisfiy (22) a general technique is proposed which maps every solution of (12) into a solution of (22). This approach has the advantage that well known interpolation methods from the literature for (12) can be applied.

To construct the mapping for the LT-VLF method the operator $\mathbf{\Lambda}$ is applied to (12) and the coefficients are compared with (22) which yield that

$$\mathbf{q}_{ht} = \mathbf{\Lambda}\mathbf{q}, \quad \widehat{\widehat{\mathbf{j}}}_{ht} = \left(\widehat{\widehat{\mathbf{j}}}_x, \widehat{\widehat{\mathbf{j}}}_y, \mathbf{\Lambda}\widehat{\widehat{\mathbf{j}}}_z\right) \tag{23}$$

is a solution of (22).

For the ADI method the VLF continuity equation (12) is rewritten as

$$\mathbf{q}^{(n+1)} - \mathbf{q}^{(n)} + \Delta t\left(\mathbf{S}_x\mathbf{\Lambda}_x\mathbf{\Lambda}_x^{-1}\widehat{\widehat{\mathbf{j}}}_x + \mathbf{S}_y\mathbf{\Lambda}_y\mathbf{\Lambda}_y^{-1}\widehat{\widehat{\mathbf{j}}}_y + \mathbf{S}_z\mathbf{\Lambda}_z\mathbf{\Lambda}_z^{-1}\widehat{\widehat{\mathbf{j}}}_z\right)^{(n+1/2)} = 0. \tag{24}$$

Comparing (24) with the new continuity equation (22) the modified charge and current vectors are obtained as,

$$\mathbf{q}_{ht} = \mathbf{q}, \quad \widehat{\widehat{\mathbf{j}}}_{ht} = \left(\mathbf{\Lambda}_x^{-1}\widehat{\widehat{\mathbf{j}}}_x, \mathbf{\Lambda}_y^{-1}\widehat{\widehat{\mathbf{j}}}_y, \mathbf{\Lambda}_z^{-1}\widehat{\widehat{\mathbf{j}}}_z\right). \tag{25}$$

The operators $\mathbf{\Lambda}_x^{-1}$, $\mathbf{\Lambda}_y^{-1}$ and $\mathbf{\Lambda}_z^{-1}$ can be efficiently calculated by the sweep method.

NUMERICAL VALIDATION

SINGLE PARTICLE

In the first validation example a single macro particle is injected into a cubic cavity of $10\mathrm{cm}$ edge length with perfect electric conducting walls. The macro particle starts at the origin, has an initial velocity of $\beta = 0.3$ and is moving in diagonal direction, i.e., $\vec{v} = 0.3/\sqrt{3}(1,1,1)$. Figure 1 and fig. 3 show the charge densities calculated with the semi-discrete Gauss law (2) for the LT-VLF and ADI method, respectively. As reference, the charge density obtained directly from the particle distribution is shown. When the current is calculated with a standard interpolation scheme large, spatially fluctuating residual charges are left behind the particle on the computational grid. In contrast, the conservative current interpolations (23) and (25) do not show this behavior. For the LT-VLF method this observation is explained in fig. 2 which shows the charge density calculated from the particle position with the shape function defined in (23) and shows that it coincides with the charge density calculated with the fully discrete Gauss law (21). As reference, the charge density obtained from the standard shape function is shown. For the ADI scheme fig. 4 shows that the charge density calculated with the new Gauss law (21) coincides with that obtained directly by the particles with the standard shape function.

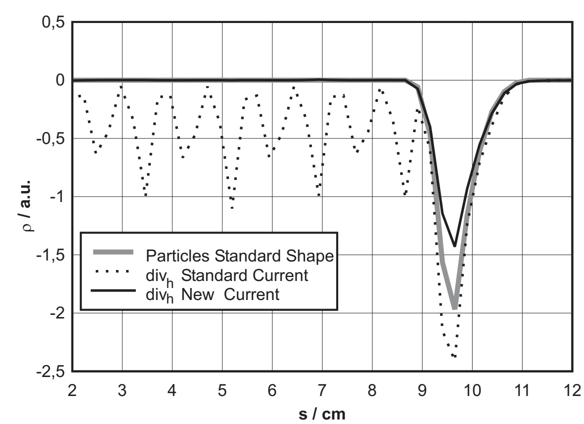

Figure 1: For the LT-VLF scheme the charge distribution obtained by the semi-discrete Gauss law (2) for the standard and newly proposed current scheme is shown. As reference, the charge distribution obtained directly from the particles is shown.

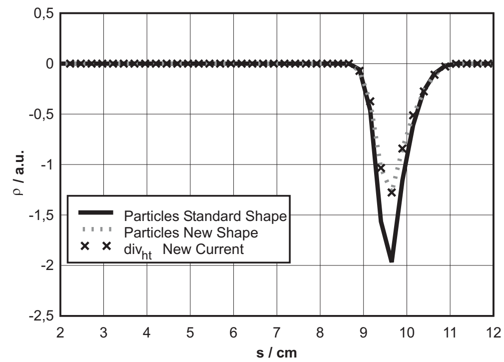

Figure 2: For the LT-VLF scheme the charge distribution obtained from the fully discrete Gauss law (21) is shown. The charge distribution obtained from the fields coincides with that obtained from the particles with the new shape.

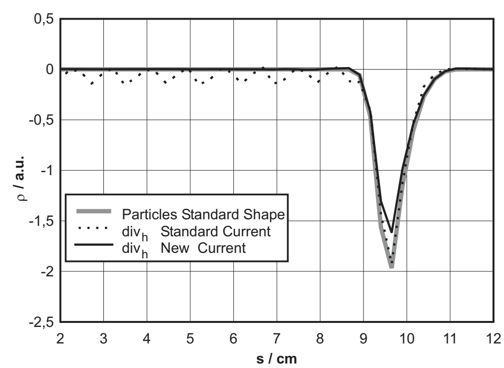

Figure 3: For the ADI scheme the charge distribution obtained by the semi-discrete Gauss law (2) for the standard and newly proposed current scheme is shown . As reference, the charge distribution obtained directly from the particles is shown.

CONVERGING BEAM

In this section a converging electron beam of radius $R = 2\mathrm{cm}$, current $I = 1\mathrm{A}$, with an initial velocity of $v_z = 0.8c$ and a transversal linear varying focusing velocity distribution is considered. The space charge effect in this example is negligible, however, the accumulation of divergence errors in the Gauss law shifts the focal point of the beam. This is demonstrated in fig. 5 where the ADI method is applied with the proposed conservative current calculation (25) and as comparison with a standard current interpolation. The results are compared after approximately twenty beam transitions. An identical simulation results holds true for the LT-VLF method and is therefore not presented.

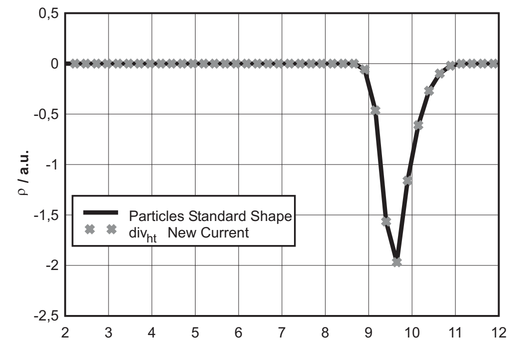

Figure 4: For the ADI scheme the charge distribution obtained from the fully discrete Gauss law (21) is shown and compared to that calculated directly from the particles.

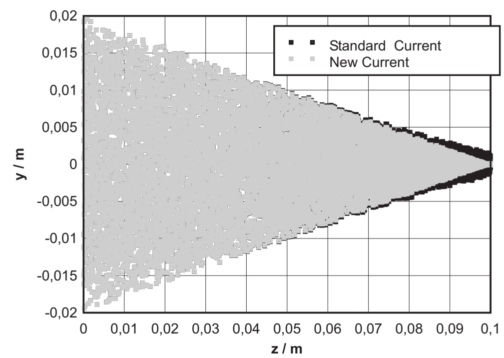

Figure 5: Phase space distribution of the converging electron beam. In gray the simulation for the ADI scheme with the new proposed current scheme and in black the simulation with the standard current scheme is shown. Near the focal point large spurious deviation in phase space are observed.

CONCLUSION

The existence and form of fully discrete Gauss laws appropriate for the LT-VLF and the ADI method have been presented. Additionally, conservative current interpolations for both methods were developed. In two test examples the validity of both approaches have been demonstrated.

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