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Creation of Spatial Charge Separation in Plasmas with Rigorously Charge-Conserving Local Electromagnetic Field Solvers

C. Othmer,* U. Motschmann,† and K. H. Glassmeier*

*Institute for Geophysics and Meteorology, Technical University of Braunschweig, Braunschweig, Germany; and †Institute for Theoretical Physics, Technical University of Braunschweig, Braunschweig, Germany
E-mail: c.othmer@tu-bs.de

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Charge-conserving local field solvers are widely used in today's electromagnetic plasma simulations. As in such codes the charge does not appear explicitly, the injection of new particles into the computational volume and their removal upon reaching the boundaries requires some cautiousness. While for quasineutral plasmas a particle injection in accordance with charge conservation can be realized quite easily, the injection of nonneutral plasmas with spatially separated electron and ion sources might lead to the emergence of unwanted divergences in the electric field. With a three-dimensional charge-conserving electromagnetic plasma simulation, we evaluate several injection schemes of nonneutral plasmas and present a method that rigorously respects conservation of charge and thus allows injection of nonneutral plasmas without producing unwanted divergences in the electric field.

Key Words: partial-difference equations; initial-boundary value problem; plasma physics; electromagnetic; electron and ion beams.

1. LOCAL ELECTROMAGNETIC FIELD SOLVERS

While the first proposal of a local field solver for an electromagnetic plasma simulation dates back to as early as 1968 [1], such local methods are widely used in today's electromagnetic plasma simulations (e.g., [2–8]). Electromagnetic simulation codes have to solve the full set of Maxwell's equations. As pointed out by Villasenor and Buneman [9], two of them, namely

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} \quad \text{and} \tag{1}$$

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$$\frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{B} - \vec{j}, \tag{2}$$

where units are chosen such that $\varepsilon_0 = \mu_0 = 1$, already express the possibility of a purely local field update. By "leapfrogging" $\vec{E}$ and $\vec{B}$ in space and time on a suitably staggered grid, these two equations provide new data from old, using present values from the immediate vicinity only (see also [10, 11]).

By contrast, the two divergence equations

$$\nabla \cdot \vec{E} = \rho \quad \text{and} \tag{3}$$

$$\nabla \cdot \vec{B} = 0 \tag{4}$$

require for their solution distant information in the form of spatial boundary conditions. However, one can readily verify that $\nabla \cdot \vec{B}$ remains zero if Eq. (1) is used to update $\vec{B}$, and if $\nabla \cdot \vec{B} = 0$ for $t = 0$. This holds already for simple space-and-time-centered finite-difference representations of $\partial/\partial t$, $\nabla\times$, and $\nabla\cdot$ [9]. Similarly, one can verify that $\nabla \cdot \vec{E}$ remains ρ, if it was so initially, and if the code rigorously satisfies the charge continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{j} \quad \text{for } t = 0 \text{ and all } t. \tag{5}$$

Hence, the "nonlocal" divergence equations (3) and (4) have to be solved only for $t = 0$. While for $\vec{B}$ the initial configuration is known analytically in many cases, the initial electric field $\vec{E}$ for a given charge distribution ρ can be obtained in one of two ways: either by using a common Poisson solver, i.e., employing a nonlocal method at $t = 0$, or, in the case of quasineutral plasmas, by starting with $\vec{E} = \vec{\rho} = 0$ by composing the plasma of electron-ion pairs that initially reside at the same location.

The task one is left with in order to have a purely local field update by virtue of Eqs. (1) and (2) only is to make sure that the code rigorously conserves charge. This requirement affects the current assignment scheme, i.e., how the current contribution of a moving particle is distributed among the grid points, as well as the injection of new and the removal of old particles. Several charge-conserving current assignment techniques have been proposed [1, 9, 12, 13] (see also [11]), the most sophisticated and least noisy of which is the one of Villasenor and Buneman [9]. These authors make use of the particle-in-cell (PIC) method [11, 14] and define the current as normal vectors on the midpoints of the grid cell boundaries. A moving particle sweeps over some of the grid cell boundaries with a certain subvolume of its charge, and the current on each boundary is calculated as the amount of charge that is carried through the boundary during the particle move. This scheme is widely used in today's plasma simulations with local electromagnetic field solvers (e.g., [1–7] and references therein) and has proved to be very efficient.

2. PARTICLE INJECTION AND REMOVAL WITH CHARGE-CONSERVING CODES

A characteristic of charge-conserving local field solvers is that the charge density ρ does not appear explicitly, so particles give rise to electric fields not via their charges but only by virtue of the currents they produce. This has to be taken into account for the injection of new and the removal of old particles.

Suppose a particle of charge $+q$ is "injected" into a vacuum at $\vec{x}_0$ with a velocity $\vec{v}$, moves to $\vec{x}_1 = \vec{x}_0 + \vec{v}\Delta t$ after one time step, and is forced to stay there. As a consequence of charge conservation, the electric field that will develop from such a configuration is not a monopole Coulomb field corresponding to the positive charge at $\vec{x}_1$, but a dipole field caused by $+q$ at $\vec{x}_1$ and a virtual negative charge $-q$ at $\vec{x}_0$ (see also [15]). This emergence of virtual charges of opposite sign, or in other words of divergences of $\vec{E}$, is characteristic of charge-conserving simulation codes.

Similarly, the charge of a particle that leaves the simulation domain does not disappear but gives rise to an electric Coulomb field as though it were stuck right behind the computational boundary. For the simulation of free-space boundaries, this is clearly an unwanted effect, which can, however, be remedied quite easily [15]. Due to the general tendency of a plasma to be charge neutral, the particles that are about to leave the simulation domain can be expected to form a quasineutral plasma (provided there are enough particles of each sign within the simulation). Once stuck behind the boundary, they can compensate for each other when a thin conducting layer is provided adjacent to the simulation boundaries. Such a conducting layer was successfully implemented by Buneman [15] as an efficient way of removing the unwanted stuck charges of outgoing particles.

The emergence of virtual charges upon particle *injection*, however, requires more caution. Obviously, whether these virtual charges are physical or a numerical artifact depends on the physical model one wants to simulate. For example, for an isolated electron emitter, the emergence of virtual charges is consistent with what actually happens physically: For each electron that is emitted, a positive charge remains back on the emitting surface. The continuous emission of electrons will then lead to an accumulation of positive charges on the emitter and hence to the buildup of an emission sheath surrounding the emitter.

There can, however, be situations where such an accumulation of charges of opposite signs and the associated formation of emission sheaths do not correspond to the physical scenario that is to be modeled, e.g., when the emitter is far enough away from the simulation region, or for devices that emit charges of both signs in equal amounts. One example of such a device is the ion thruster. These consist of an electron and an ion source that are spatially separated and eject electrons and ions in practically equal numbers. In contrast to the isolated electron emitter above, an accumulation of charge on the emitters does not take place because they are electrically connected.

For such an emission problem, where no charge is accumulated on the emitter, the emergence of virtual charges associated with the injection of particles in a charge-conserving code is an unwanted phenomenon. How the virtual charges can be eliminated by using an appropriate injection method is illustrated in the following for an emission configuration corresponding to an ion thruster.

3. INJECTION WITH SPATIAL CHARGE SEPARATION

One straightforward way of injecting a particle without generating a virtual charge of opposite sign would be to add the analytically known electrostatic monopole field of the injected particle to each grid point of the simulation volume. This would alter ρ and $\vec{E}$ in a self-consistent manner. However, such a procedure is computationally very expensive, might cause stability problems, as it implicitly involves an indefinite propagation velocity of the electric field, and, above all, is unphysical except in the electrostatic limit.

Similarly to the initialization of $\vec{E}$ and ρ being accomplished by composing the plasma of electron ion pairs that intially reside at the same location (see Section 1), one might think of another cure for unwanted divergences of $\vec{E}$ as follows: to inject an electron-ion pair and give the unwanted charge a large mass and velocity directed back to the surface. After a few time steps, only the desired *particle* would remain in the simulation. Upon reaching the simulation boundary, however, the *charge* of the unwanted particle would get stuck, as discussed above, and give rise to a stationary Coulomb field. Hence, such an injection method would not be capable of eliminating the virtual charge, but would just relocate it from the original injection site to right behind the simulation boundary.

Using a 3D local electromagnetic PIC code with a charge-conserving current assignment method according to Villasenor and Buneman [9], we simulated various injection schemes for a simplified ion thruster configuration. The results of our simulation runs are shown in Figs. 1–3. Randomly distributed over the top box on the left side of the simulation volume, electrons are created at each time step and are injected with a bulk velocity of $v_x = 0.1c$ plus

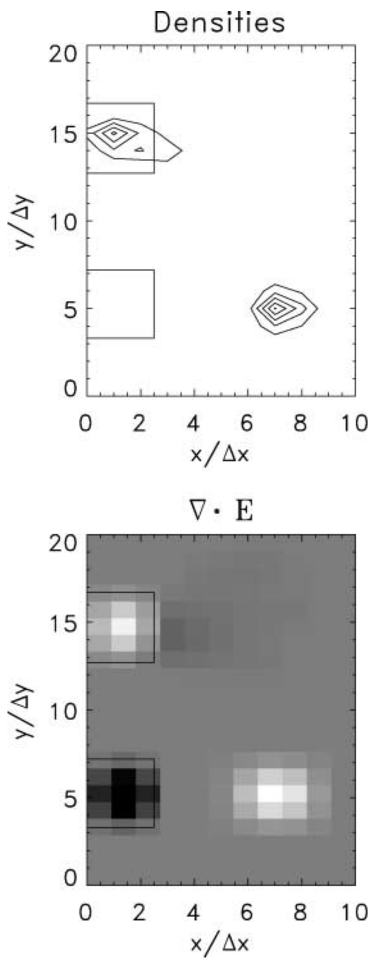

FIG. 1. Cuts through the simulation domain, including the electron and ion injection regions (rectangles adjacent to the left border), for the case of no compensation. (Top panel) Electron and ion densities; (bottom panel) divergence in the electric field. Black and white correspond to negative and positive divergence, respectively. The background grey tone indicates zero divergence.

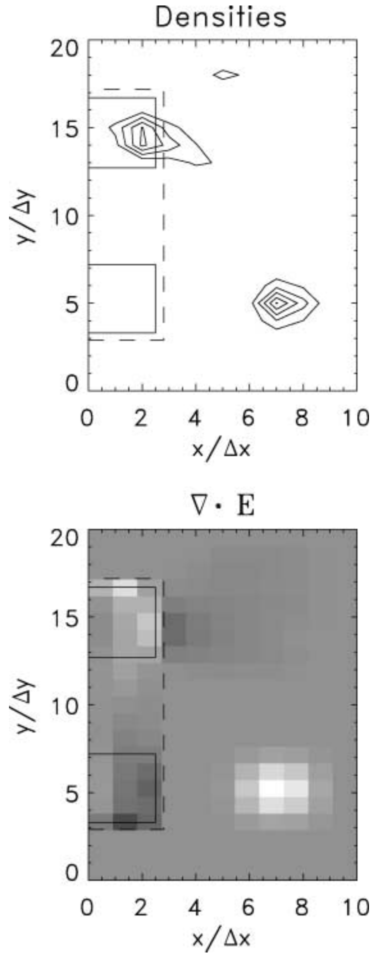

FIG. 2. Same as Fig. 1, but with a conductive region within the dashed rectangle.

an isotropic thermal spread of $0.01c$. With the same number per time step, ions are created in the lower box and leave it with a uniform bulk velocity of $0.1c$ plus a negligibly small thermal spread corresponding to $T_e = T_i$. In order to make the ions practically insensitive to electromagnetic fields, their mass was chosen to be as high as $250{,}000 m_e$. We switched on the injection at $t = 0$, stopped it after a while, and let the system evolve for some time. While the densities (top panels) in Figs. 1–3 were obtained by summing over the particles, the divergences of $\vec{E}$ (bottom panels) were calculated by central differencing the electric field.

Figure 1 shows the results for the case of straightforward injection without any correction to the electric field. As can be seen from the top panel, an injected ion "drop" has left the injection box and has flown up to $x \approx 7$. In accordance with Maxwell's equations, the electric field shows a positive divergence in this region (bottom panel). A divergence of similar amplitude but of opposite sign has emerged within the rectangle where the ions were injected. This is a direct consequence of the charge-conserving character of the code and is exactly what was described in the previous section as the creation of oppositely signed virtual charges.

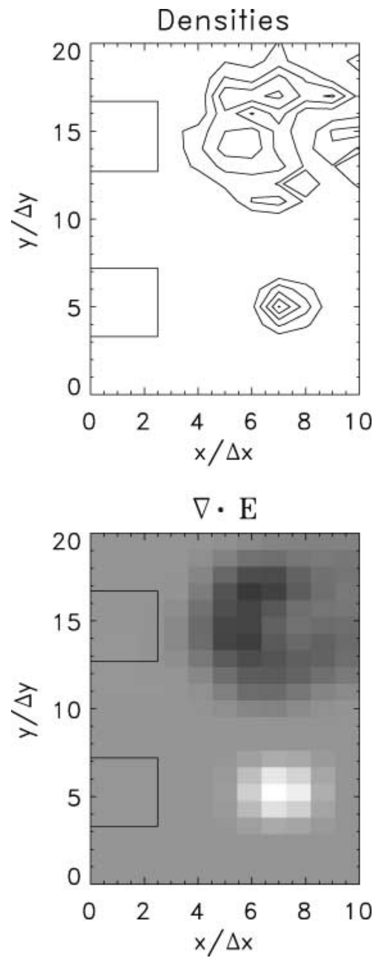

FIG. 3. Same as Fig. 1, but obtained by using the "generator technique." Note the lack of divergence in the electric field in the injection regions and the free expansion of the electrons.

The virtual charges exert an attractive force on the injected particles, as in the case of the isolated emitter described above. While the huge ion mass prevents the ion dynamics from being significantly altered by this force, the effects on the electrons are dramatic. Similarly to the emergence of negative divergences of $\vec{E}$ in the ion source region, the electron injection in the top rectangle gives rise to positive virtual charges there. As a consequence, the relatively light electrons cannot expand freely and are stuck in the injection region, despite having the same bulk velocity as the ions.

As each injected particle creates one virtual charge, a continuous injection of plasma particles would lead to an ever increasing number of charges in the particle source regions. Their electric field would rise correspondingly, such that at a certain point the whole simulation dynamics would be ruled by the virtual charges. Hence, such an injection scheme without any compensation for the emergence of virtual charges is not appropriate for the modeling of an ion-thruster-like emission scenario with electrically connected electron and ion sources.

In the simulated configuration, positive and negative virtual charges emerge at the same rate. Their continuous accumulation could therefore be suppressed if they were allowed to compensate for each other. The easiest way of doing that is to conductively connect both source regions of virtual charges by embedding them in an electrically conductive medium. Such a conductive connection would allow the electric fields of the virtual charges to drive currents that, in turn, contribute to the removal of the unwanted divergences of $\vec{E}$, similar to the mutual compensation between stuck charges of leaving particles in a thin conducting layer adjacent to the simulation boundaries [15]. We therefore embedded the electron and ion injection boxes into a region of finite volumetric electrical conductivity, which is marked by the dashed lines in Fig. 2. Within this region, an *additional* loop runs over the electric field and modifies it according to

$$\vec{E} := (1 - \sigma)\vec{E}. \tag{6}$$

As will be shown now, this manipulation of $\vec{E}$ corresponds exactly to the effect of a conduction current $\vec{j}_c = \sigma\vec{E}$ [15]: As throughout the simulation domain, the $\vec{E}$ field in the conducting region has to be advanced according to

$$\vec{E}_{new} = \vec{E}_{old} + \nabla \times \vec{B} - \vec{j}, \tag{7}$$

where for simplicity we set $\Delta t = 1$. While outside the conducting region $\vec{j}$ is just the current carried by the particles $\vec{j}_p$, inside the conduction current $\vec{j}_c = \sigma\vec{E}$ has to be considered, such that

$$\vec{j} = \vec{j}_p + \vec{j}_c, \tag{8}$$

$$\Rightarrow \vec{E}_{new} = \{\vec{E}_{old} + \nabla \times \vec{B} - \vec{j}_p\} - \vec{j}_c, \tag{9}$$

where the term in braces corresponds to the electric field $\vec{E}'_{new}$, which is determined via the common field update of Eq. (2) when only the particles' contribution to the current is considered. Computing the conduction current now as

$$\vec{j}_c = \sigma\vec{E}'_{new} \tag{10}$$

yields for the updated electric field

$$\vec{E}_{new} = \{\vec{E}_{old} + \nabla \times \vec{B} - \vec{j}_p\} - \sigma\vec{E}'_{new} \tag{11}$$

$$= (1 - \sigma)\vec{E}'_{new}. \tag{12}$$

Hence, a finite volumetric conductivity can be implemented by updating the electric field in the usual manner and then reducing it by a factor of $1 - \sigma$.

We simulated the same scenario as described above for various values of σ. A conductivity around $\sigma = 0.05$ turned out to be a reasonable choice and led to results like the one depicted in Fig. 2. As can be seen from the bottom panel, the conductivity indeed provides a certain degree of compensation for virtual charges compared to that in Fig. 1. However, along the surface of the conductive region, the divergences of $\vec{E}$ are still quite strong and apparently big enough to keep most of the electrons from escaping. These surface divergences could not be significantly reduced by other choices of σ. Hence, while for outgoing particles a conductive layer proved to be efficient in removing unwanted stuck charges via mutual compensation [15], a region of volumetric conductivity does not serve for such a spatially concentrated, massively nonneutral injection of particles as in our example.

A refinement of this conductive injection region would be to embed an electron and ion injection box into *two separate* regions of electrical conductivity and to supply it with a static current flowing on a wire between them. This current could then spread out over each injection box in order to compensate for the emerging virtual charges. Such a configuration would avoid the accumulation of virtual charges that occurred in the case of the straightforward injection (Fig. 1) but would not completely eliminate their effect on the particle motion. The general problem of a conductivity-based charge compensation is that it requires a *finite time* for the compensation to be completed: The virtual charge appears instantaneously once the particle is injected and is gradually removed by virtue of the conductivity only after some time steps. During this time, however, the virtual charge exerts a nonzero force on the particle and thus affects the particle motion in an unwanted manner.

In order to completely remove the effect of the virtual charges on the particles, a rigorous mutual compensation between the virtual charges of both particle source regions has to be enforced. We accomplished this by implementing in the injection process a kind of electrical generator which generates the particles *before* they are injected and therefore *does not produce virtual charges at all*: As in other plasma simulation applications, in our example electrons and ions are injected with the same number per time step and can therefore be grouped into electron-ion pairs. To each of these pairs belongs a set of positions $\vec{x}_e, \vec{x}_i$ and velocities $\vec{v}_e, \vec{v}_i$. The role of the generator now is to place these particles not at their respective injection positions but halfway between $\vec{x}_e$ and $\vec{x}_i$ (see Fig. 4), and to provide them with individually determined transfer velocities $\vec{v}_{tr}$ and $-\vec{v}_{tr}$ that make

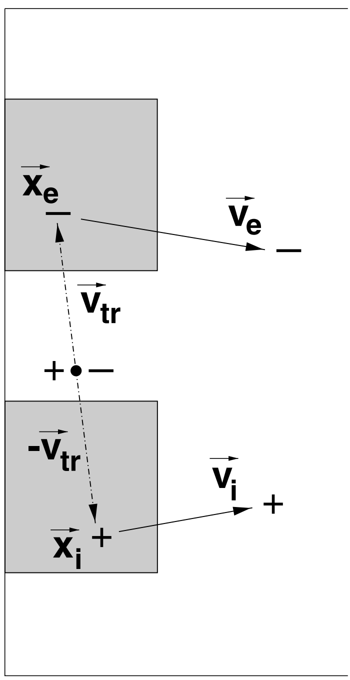

FIG. 4. The "generator." New electrons and ions are placed in pairs halfway between their respective injection positions and are moved to $\vec{x}_e$ and $\vec{x}_i$ without being subjected to electromagnetic fields. The currents they produce during their transfer phase contribute to the field update of Eq. (2).

them reach their respective injection locations $\vec{x}_e$ and $\vec{x}_i$ in a certain number of time steps. During their transfer, the particles are not subjected to electromagnetic fields. However, the currents they produce are collected and enter Eq. (2). Once the particles reach their destinations $\vec{x}_e$ and $\vec{x}_i$, they appear as new particles in the simulation. They can then be subjected to the electromagnetic field or, as in our example, where the details of the particle injection mechanism itself are not of interest, can simply be provided with their desired injection velocities $\vec{v}_e$ and $\vec{v}_i$.

As electrons and ions are created in pairs at the same location, this injection scheme rigorously satisfies conservation of charge and thus guarantees that no unwanted divergences of $\vec{E}$ develop. Figure 3 shows that employing the "generator technique" has indeed dramatic consequences for the injection scenario compared to the previous injection schemes. As expected from a proper ion-thruster-like particle injection, the electric field in the particle source regions is divergence free and the electrons can expand freely.

The generator technique can be thought of as electrically connecting the two injection locations $\vec{x}_e$ and $\vec{x}_i$ with a straight wire on which, for a certain number of time steps, a current in the form of an up-moving negative charge and a down-moving positive charge is flowing. This current enters the field update via Eq. (2) and provides the injection locations with the charges to be injected. Once these charges have reached $\vec{x}_e$ and $\vec{x}_i$, respectively, the "wire" is removed. For each electron-ion pair that is to be injected such a wire is applied. Considering that each wire exists for a certain number of time steps and that—usually—many more than one electron-ion pair is injected at each time step, it becomes clear that a large number of wires are present at the same time. Hence, the generator gives rise to a practically continuous current in space and time. To some extent, the generator mimics the way in which the real plasma device works: It forms a conductive connection between the spatially separated particle sources, where the necessary currents flow to provide each source with the charges to be injected.

We note, however, that the analogy between our generator and currents moving between two emitters is not complete: Such currents are bulk flows of electrons at low velocity, which are driven by an applied voltage. In contrast, the charges in our scheme move at high velocity (see below) and their motion is prescribed externally, i.e., they do not move self-consistently in the ambient electromagnetic field. These deviations of the generator technique from simple currents moving between two emitters require the discussion of two side effects of the proposed injection scheme: enhanced radiation and the static magnetic field caused by the generator current.

4. SIDE EFFECTS OF THE GENERATOR TECHNIQUE

The generator requires additional storage and computing time for the particles that are in the transfer phase. When N_{inj} is the number of electron-ion pairs that are injected at each time step, and T_{tr} is the number of time steps that are needed for the transfer, then this additional work load amounts to $2N_{inj}T_{tr}$ particles. N_{inj} is in general determined by the actual simulation project, such that the only way of reducing storage and computing time is to choose T_{tr} as small as possible. A short duration of the transfer phase T_{tr} can be achieved by a high transfer velocity v_{tr}, whose upper limit is of course the velocity of light c. Allowing v_{tr} to be close to c thus reduces storage requirements and work load. However, this has to be paid for with enhanced emission of radiation: On the transition between the transfer phase and the actual injection of the particles, their velocities change abruptly from $\vec{v}_{tr}$ to $\vec{v}_{e/i}$, possibly involving a 90° direction change, as in our sample simulation. The amount of radiation generated via this massive particle acceleration increases with v_{tr} getting closer to c, which might be troublesome.

Therefore, we carried out a series of simulation runs of our sample configuration with varying transfer velocities between 0.1 and 0.8c and employed Lindman's [16] nonreflecting boundary conditions, which let radiation escape across the computational boundary. As a measure of the impact of the enhanced radiation on the particle motion, we compared the particle positions at the end of each run and computed the maximum deviation between simulation runs with different v_{tr}. This maximum turned out to be around $10^{-8}\Delta x$, which is on the order of numerical noise. Hence, when appropriate radiating boundary conditions such as Lindman's are used, the enhanced radiation of the generator is not a problem.

In our example, the two particle sources are very close, and the region where the generator is operating is therefore quite small. One might wonder what happens when the injection areas are farther separated from each other, as they are, e.g., in a diode-like configuration where electrons and ions are injected on opposite sides of the numerical domain. In such a geometry, the generator would have to transport the charges all around the boundary, and the region of generator operation would therefore cover a much larger fraction of the computational volume than in our example. However, as outlined above, the generator can be regarded as a current-carrying wire that transports charge to the respective injection areas. Its side effects are therefore the generation of a static magnetic field according to the current through the "wire" and the enhanced radiation. While the latter's impact on the particle motion was shown to be negligible, the static magnetic field is physical and consistent with the simulated device, because in order to close the current wedge the real device, e.g., a diode, also needs such a wire to carry precisely the same current as our generator does. In a real experiment this magnetic field can be reduced in the region of interest by arranging the current-carrying wire appropriately. For our generator technique, however, it is necessary to keep the whole "wire" inside the simulation domain. Therefore, reducing the magnetic field in the region of interest is possible in principle, e.g., in our example by extending the simulation domain further to the left and locating the charge-separation process there, but bears the cost of additional computational work for the enlarged grid. Hence, for every simulation project, a trade-off between the desired reduction of the magnetic field impact and the affordable additional computer work has to be made, e.g., based on an estimate of the magnetic field magnitude, which can be obtained simply by Biot–Savart's law.

5. SUMMARY

We have evaluated different injection schemes of nonneutral plasmas for charge-conserving local electromagnetic field solvers. If the particle injection is not rigorously charge conserving, such field solvers create unwanted divergences in the electric field, which were shown to have dramatic consequences on the particle dynamics. With our "generator," which creates the charges in accordance with charge conservation *before* they are injected, we have proposed a method that prevents the emergence of unwanted divergences of $\vec{E}$. It allows injection of nonneutral plasma into charge-conserving local electromagnetic field solvers as it is needed for configurations with spatially separated electron and ion sources. The side effects of the proposed technique, enhanced radiation and a static magnetic field, were shown to be negligible or calculable, respectively.

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