An exact charge-conserving gather-scatter algorithm for particle-in-cell simulations on unstructured grids

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Abstract

We present a novel charge-conserving gather-scatter algorithm for particle-in-cell simulations on unstructured grids. Charge conservation is obtained from first principles, i.e., without the need for any post-processing or correction steps. The key ingredients that enable this property are (1) the use of (discrete) differential forms to represent the electromagnetic fields, currents, and charged particles and to provide consistent localization rules for the degrees of freedom thereof on the different types of geometrical elements (nodes, edges, facets) comprising the unstructured grid, and (2) use of Whitney forms as basic interpolants of such discrete differential forms to continuum space. The present algorithm discretizes the first-order Maxwell’s system directly to avoid any spurious modes with secular growth (otherwise present on approaches based on a single field formulation) and on the use of a Galerkin-Whitney representation for the discrete Hodge star operators (i.e., the metric datum of the grid) that is applicable to irregular, unstructured grids. Examples are provided to verify exact preservation of discrete Gauss’ law for all times.

Keywords: gather-scatter, particle-in-cell (PIC), Whitney forms, finite elements, unstructured grids, differential forms.

1. Introduction

Particle-in-cell (PIC) algorithms have been extensively used for several decades in the simulation of problems involving space charges [1234], including plasma-related applications such as electron accelerators [5], laser ignited devices [6], and high-power microwave generation [7], to name a few. A key challenge to PIC algorithms is how to achieve exact charge conservation properties on unstructured, irregular grids. Otherwise, undesired charge accumulation may occur at grid points leading to violation of Gauss’ law and spurious solutions. The traditional approach to enforce charge conservation is to apply correction terms to the electric fields in order to satisfy Gauss’ law at every time step [8910]. An alternative approach is to enforce the (discrete) continuity equation directly at every grid cell [111213141516]. However, this latter approach is predicated on the use of rectangular grids. In order to more accurately represent general curved geometries, the use of unstructured grids is highly desirable [1718].

In this paper, we present a novel gather-scatter algorithm with exact charge conserving properties for use in PIC simulations on unstructured grids. Charge conservation is achieved from first principles, i.e., without resorting to any correction steps. The main ingredients that enable exact conservation properties are (1) the representation of the electromagnetic fields, currents, and charged particles as discrete differential forms (of different degrees) via an exterior calculus formalism that provides precise and consistent localization rules for the degrees of freedom thereof in the different geometric elements (nodes, edges, faces, etc.) that comprise

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the unstructured grid and (2) the use of Whitney forms as basic interpolants of such discrete differential forms to continuum space \[19, 20, 21\].

We note that an algorithm based upon similar tenets was proposed in \[22, 23\]; however, that algorithm relies on the vector-wave equation and on the use of the time-integrated electric field as a dynamical variable. Compared to Maxwell’s equations, the vector-wave equation admits an enlarged solution space that includes gradient-like solutions exhibiting secular growth in time, i.e., of the form \(t \nabla \phi\). These solutions, even if not initially excited by (properly set) initial conditions, can nevertheless emerge at late times due to the accumulation of round-off errors and pollute the numerical solution unless specialized strategies such tree-cotree decomposition (gauging) \[21\], grad-div regularization \[25\], or ad hoc corrections \[26\] are utilized. In addition, the approach in \[22, 23\] requires a numerical differentiation in time to compute the electric field \(E\). This causes the (temporal) order of accuracy for \(E\) to be one order less than the order of accuracy of the time integration scheme itself. Further, a Newmark-Beta scheme is adopted in \[22, 23\] for the numerical time integration. This scheme has the advantage of producing an unconditionally stable update, but has the disadvantage of yielding a linear system with deteriorating condition numbers for large Courant factors that may occur, for example, in highly refined grids or multiscale problems \[27\]. On the other hand, the present algorithm is based directly on the coupled first-order Maxwell’s curl equations and a mixed Whitney form representation for the electromagnetic fields devoid of spurious solutions. We also employ a leap-frog type update in time that only requires the solution of a symmetric positive-definite system with no condition number deterioration across different mesh-refinement scales \[27\].

Another charge-conserving and multi-symplectic PIC scheme utilizing discrete differential forms was very recently presented in \[18\]. This algorithm is based on variational vector-potential formulation with manifest gauge symmetry; however, the authors employ discrete Hodge star operators (i.e., which encode the spatial metric) represented as diagonal matrices. This representation is only accurate on grids in which a (geometrically) orthogonal dual grid exists, such as Delaunay triangulations with a Voronoi dual. This diagonal approximation is not well suited for more general types of irregular grids. In contrast, the present algorithm is applicable to unstructured simplicial grids in general, i.e., with arbitrary element geometries. This is made possible by making use of a Galerkin-Whitney representation \[21, 28\] for the Hodge star operators, as given by \(9\) and \(10\) below. Also very recently, Campos-Pinto et al. \[29\] put forth a comprehensive charge-conserving PIC scheme based on a finite element Maxwell solver using curl-conforming elements of arbitrary order, arbitrary shape factors, and piecewise polynomial trajectories of particles. Upon identification of curl- and div-conforming finite elements with the proper spaces of differential forms, it can be seen that the field solver part utilized in \[29\] is formally equivalent, to lowest order, to the field solver proposed here. The key difference between the approaches lies on the gather-scatter algorithm: While the algorithm in \[29\] hinges upon the more traditional use of shape factors (describing the charge distribution) and on the use of the \(J = \rho v\) relation for the current deposition by charged particles, the gather-scatter algorithm introduced here exploits the same family of functions used to represent the fields to consistently represent the particle currents and charges (by Whitney 1-forms and 0-forms, resp.) on the grid as well. As shown below, this novel charge and current assignment scheme is simple and geometrically intuitive, and yield exact charge conservation irrespective of the shape of the irregular cells comprising the unstructured grid.

\[1\]Recall that a simplicial grid is such that all its elements are \textit{simplices}, i.e., elements whose boundaries are the union of a minimal number of lower-dimensional elements. Therefore, in a 3-D simplicial grid for example, any face is a triangle and any volume cell is a tetrahedron.
2. Formulation

2.1. Field update

On unstructured grids, the electric field intensity $\mathbf{E}(\mathbf{r}, t)$ and the magnetic flux density $\mathbf{B}(\mathbf{r}, t)$ can be expanded using Whitney basis functions as \[19, 20, 21\]

$$
\mathbf{E}(\mathbf{r}, t) = \sum_{i=1}^{N_e} e_i(t) \mathbf{W}_1^i(\mathbf{r}),
$$

(1)

$$
\mathbf{B}(\mathbf{r}, t) = \sum_{i=1}^{N_f} b_i(t) \mathbf{W}_2^i(\mathbf{r}),
$$

(2)

where $N_e$ and $N_f$ are the number of edges and faces in the grid, so that there is a 1:1 correspondence (localization) of the degrees of freedom $e_i(t)$ and $b_i(t)$ to edges and faces, resp., in the grid. In the above, $\mathbf{W}_1^i(\mathbf{r})$ and $\mathbf{W}_2^i(\mathbf{r})$ are (Whitney) edge and face basis functions \[19, 20, 21\], respectively. The units of $\mathbf{W}_1^i(\mathbf{r})$ and $\mathbf{W}_2^i(\mathbf{r})$ are $[m^{-1}]$ and $[m^{-2}]$, respectively. The edge and face Whitney functions above are vector proxies of Whitney 1-forms and Whitney 2-forms, respectively. For details about Whitney functions, see Appendix A. Note that the units of the time-dependent coefficients $e_i(t)$ and $b_i(t)$ are Volts [V] and Webers [Wb].

The above expansions are informed by the fact that electric field is a 1-form and magnetic flux density is a 2-form in the language of differential forms \[30, 31, 32, 33\]. Furthermore, if an electric current density is present in the grid, current density is defined such that

$$
\mathbf{J}(\mathbf{r}, t) = \sum_{i=1}^{N_e} i_i(t) \mathbf{W}_1^i(\mathbf{r}).
$$

(3)

so that the degrees of freedom $i_i(t)$ are associated to the edges of the grid, like those of $\mathbf{E}(\mathbf{r}, t)$ \[7\]. With the aid of Galerkin testing, Maxwell’s equations can be spatially discretized as \[21\]

$$
\mathbf{C} \cdot \mathbf{e} = -\frac{d}{dt} \mathbf{b},
$$

(4)

$$
\mathbf{C}^T \cdot [\star_{\mu^{-1}}] \cdot \mathbf{b} = \frac{d}{dt} [\star_\epsilon] \cdot \mathbf{e} + \mathbf{i}.
$$

(5)

$\mathbf{C}$ is an incidence matrix with elements in the set $\{-1, 0, 1\}$, providing the (discrete) representation of curl operator distilled from the metric \[34, 35\]. The superscript $T$ indicates the transpose. The arrays of degrees of freedom are defined as

$$
\mathbf{e} = [e_1(t), e_2(t), \cdots, e_{N_e}(t)]^T,
$$

(6)

$$
\mathbf{b} = [b_1(t), b_2(t), \cdots, b_{N_f}(t)]^T,
$$

(7)

$$
\mathbf{i} = [i_1(t), i_2(t), \cdots, i_{N_e}(t)]^T.
$$

(8)

In addition, $[\star_{\mu^{-1}}]$ and $[\star_\epsilon]$ in (5) are discrete Hodge star operators given by the following integrals \[21, 28\],

$$
[\star_\epsilon]_{ij} = \int_{\Omega} \epsilon \mathbf{W}_1^i(\mathbf{r}) \cdot \mathbf{W}_1^j(\mathbf{r}) dV,
$$

(9)

$$
[\star_{\mu^{-1}}]_{ij} = \int_{\Omega} \frac{1}{\mu} \mathbf{W}_2^i(\mathbf{r}) \cdot \mathbf{W}_2^j(\mathbf{r}) dV,
$$

(10)

\[2\]We employ a star subscript on $\mathbf{J}$, because, strictly speaking, the electric current density $\mathbf{J}$ is a (twisted) 2-form that should be discretized in the dual grid. The above $\mathbf{J}_*$ is the Hodge dual representation of $\mathbf{J}$, on the primal grid \[32\].
which, for a given grid, are pre-computed using quadratures. This property is necessary to ensure stability of the time updating scheme. It should be pointed out that the Hodge matrix associated with \( \mathbf{i} \) in (5) is the identity matrix.

Using the leap-frog scheme, the semi-discrete equations (4) and (5) can be fully discretized as

\[
\mathbf{b}^{n+\frac{1}{2}} = \mathbf{b}^{n-\frac{1}{2}} - \Delta t \mathbf{C} \cdot \mathbf{e}^n, \tag{11}
\]

\[
[\mathbf{e}] \cdot \mathbf{e}^{n+1} = [\mathbf{e}] \cdot \mathbf{e}^n + \Delta t \left( \mathbf{C}^T \cdot [\mathbf{e}] \cdot \mathbf{b}^{n+\frac{1}{2}} - \mathbf{b}^{n+\frac{3}{2}} \right). \tag{12}
\]

Since (9) and (10) are positive-definite, it can be easily shown that the above update scheme is conditionally stable, obeying a Courant-like stability criterion \([21],[35]\). From the discrete values \( \mathbf{e}^{n+1} \) and \( \mathbf{b}^{n+\frac{1}{2}} \) obtained from (11) and (12), the temporal coefficients \( e_i(t) \) in (1) and \( b_i(t) \) in (2) can be interpolated as \([36]\).

\[
e_i(t) = \sum_n e_n \Pi^\mathbf{i}(t), \tag{13}
\]

\[
b_i(t) = \sum_n b_n^{\frac{1}{2}} \Lambda^{\mathbf{i}+\frac{1}{2}}(t), \tag{14}
\]

where \( \Pi^\mathbf{i}(t) \) is a piecewise constant (pulse) function centered on integer times and \( \Lambda^{\mathbf{i}+\frac{1}{2}}(t) \) is a piecewise linear (rooftop) function centered on half-integer times. The choice of (13) and (14) is inspired by (4), where time derivative of \( \mathbf{b} \) should be the same form of \( \mathbf{e} \). Also, \( i_{\mathbf{i}}(t) \) in (3) can be likewise expanded in the piecewise linear function centered on half-integer time indices (see (5)).

2.2. Gather step

In the gather step, field values are interpolated at the positions of particles. Since Whitney basis functions are used to represent the field values, (1) and (2) can be directly used for the interpolation. Using (13) and (14), \( \mathbf{E} \) and \( \mathbf{B} \) in their respective discrete times are expressed as

\[
\mathbf{E}(\mathbf{r}_p, n\Delta t) = \mathbf{E}^n(\mathbf{r}_p) = \sum_{i=1}^{N_e} e_i^n \mathbf{W}_i^1(\mathbf{r}_p), \tag{15}
\]

\[
\mathbf{B}(\mathbf{r}_p, (n+1/2)\Delta t) = \mathbf{B}^{n+\frac{1}{2}}(\mathbf{r}_p) = \sum_{i=1}^{N_f} b_i^{n+\frac{1}{2}} \mathbf{W}_i^2(\mathbf{r}_p), \tag{16}
\]

where \( \mathbf{r}_p \) is the position of the \( p \)-th particle.
2.3. Particle update

The next step is to update particle attributes such as position \( \mathbf{r}_p(t) \) and velocity \( \mathbf{v}_p(t) \). The equation of motion and Lorentz-Newton equation are utilized. For simplicity, we consider here a non-relativistic case:

\[
\frac{d\mathbf{r}_p}{dt} = \mathbf{v}_p, \\
\frac{d\mathbf{v}_p}{dt} = \frac{q}{m} (\mathbf{E} + \mathbf{v}_p \times \mathbf{B}).
\]

In (18), \( q \) and \( m \) are the charge and mass of the particle, respectively. Using the leap-frog time update, (17) and (18) are discretized as

\[
\mathbf{r}_p^{n+1} - \mathbf{r}_p^n = \Delta t \mathbf{v}_p^{n+\frac{1}{2}},
\]

(19)

\[
\mathbf{v}_p^{n+\frac{1}{2}} - \mathbf{v}_p^{n-\frac{1}{2}} = \frac{q\Delta t}{m} (\mathbf{E}^n + \mathbf{v}_p^n \times \mathbf{B}^n).
\]

(20)

Note that (19) is the explicit update whereas (20) is implicit. Furthermore, the interpolated values of \( \mathbf{v}_p^n \) and \( \mathbf{B}^n \) in the right hand side of (20) should be calculated a priori. We assume that \( \mathbf{v}_p^n \) is expanded in the piecewise linear function because \( \mathbf{v}_p^n \) and \( \mathbf{B}^n \) are centered on the same time. Therefore, when \( t = n\Delta t \),

\[
\mathbf{v}_p^n = \frac{1}{2} \left( \mathbf{v}_p^{n+\frac{1}{2}} + \mathbf{v}_p^{n-\frac{1}{2}} \right),
\]

(21)

\[
\mathbf{B}^n = \frac{1}{2} \left( \mathbf{B}^{n+\frac{1}{2}} + \mathbf{B}^{n-\frac{1}{2}} \right).
\]

(22)

In contrast to \( \mathbf{v}_p \), \( \mathbf{B} \) is the function of space as well, so it is assumed that \( \mathbf{B}^{n+\frac{1}{2}}(\mathbf{r}_p) = \mathbf{B}^{n+\frac{1}{2}}(\mathbf{r}_p^n) \). Therefore, (20) is modified to

\[
\mathbf{v}_p^{n+\frac{1}{2}} - \mathbf{v}_p^{n-\frac{1}{2}} = \frac{q\Delta t}{m} \left[ \mathbf{E}^n + \frac{1}{4} \mathbf{v}_p^{n+\frac{1}{2}} \times \left( \mathbf{B}^{n+\frac{1}{2}} + \mathbf{B}^{n-\frac{1}{2}} \right) + \frac{1}{4} \mathbf{v}_p^{n-\frac{1}{2}} \times \left( \mathbf{B}^{n+\frac{1}{2}} + \mathbf{B}^{n-\frac{1}{2}} \right) \right].
\]

(23)

After some algebra, (23) can be succinctly expressed as

\[
\mathbf{v}_p^{n+\frac{1}{2}} = \mathbf{N}^\top \cdot \mathbf{v}_p^{n-\frac{1}{2}} + \frac{q\Delta t}{m} \mathbf{N}^\top \cdot \mathbf{E}^n,
\]

(24)

where

\[
\mathbf{N} = \begin{bmatrix}
1 & -\frac{q\Delta t}{2m} B_z^n & \frac{q\Delta t}{2m} B_y^n \\
\frac{q\Delta t}{2m} B_z^n & 1 & -\frac{q\Delta t}{2m} B_x^n \\
\frac{q\Delta t}{2m} B_y^n & \frac{q\Delta t}{2m} B_x^n & 1
\end{bmatrix},
\]

(25)

\[
B_s^n = \frac{1}{2} \left( B_s^{n+\frac{1}{2}} + B_s^{n-\frac{1}{2}} \right), \quad s = x, y, \text{ or } z.
\]

(26)

Note that \( \mathbf{N} \) is unitless. In summary, (19) together with (24) constitute the well-known (non-relativistic) equation of motion for a charged particle in an electromagnetic field. Note that the particle velocity should be updated before the update of the particle position.

2.4. Scatter step

This step is to assign charge density and current density back to the grid using the updated particle attributes. Of course, the fundamental question here is how to assign the particle charge to grid vertices (nodes) consistent to the assignment of the respective currents to grid edges. To achieve this, we use the same
family of interpolatory functions for both, viz. Whitney functions. The advantage of using such functions is two-fold: (i) they preserve the total amount of the vertex-distributed charge for each particle and (ii) they exactly preserve the charge continuity equation (more on this below) and guarantee that no spurious charges arise in Gauss’ law during the particle motion on the grid.

To examine this, let us first consider the charge assignment. The charge $Q$ of the $p$-th particle is represented as a 0-form and distributed to the grid vertices so that

$$q_i = Q W^0_i(r_p) = Q \lambda_i(r_p),$$

(27)

where the subscript $i$ is the index of vertices and $W^0_i$ is the Whitney 0-form associated with vertex $i$. The value of the function $W^0_i(r_p)$ is simply equal to the barycentric coordinate of the point $r_p$ referred to the node $i$, i.e., $W^0_i(r_p) = \lambda_i(r_p)$ (see Appendix A). When (27) is summed over all possible $i$ values,

$$\sum_i q_i = \sum_i Q \lambda_i(r_p) = Q \sum_i \lambda_i(r_p) = Q,$$

(28)

since $\sum_i \lambda_i(r_p) = 1$ holds (a partition of unity). The charge assignment (27) is illustrated in Fig. 2a with the local numbering of vertices and edges. Vertices and edges are represented by $\nu$ and $e$, respectively. Note that the charge values are only associated to the vertices of the triangle on which the particle is located.

Fig. 2b describes the current assignment. The $p$-th particle of charge $Q$ moves from $r_{p,s}$ to $r_{p,f}$ during $\Delta t$ along straight path $L$. For example, the current assigned to $e_1$ (edge 1) is

$$i_1 = \frac{Q}{\Delta t} \int_{r_{p,s}}^{r_{p,f}} W^1_1(r_p) \cdot dL = \frac{Q}{\Delta t} \left( \lambda^s_1 \lambda^f_2 - \lambda^f_1 \lambda^s_2 \right),$$

(29)

where $\lambda^s_i$ and $\lambda^f_i$ are shorthands of $\lambda_i(r_{p,s})$ and $\lambda_i(r_{p,f})$, respectively (see Appendix B for further details on the evaluation of this line integral). The current values $i_2$ and $i_3$ can be obtained similarly. During the scatter step $\Delta t$, particles might travel beyond a single triangle element and cross element edges. In this case, the path can be simply divided into smaller segments whereby each segment resides entirely within a single triangle. The scatter step above can then be applied to each segment.

2.5. Charge conservation

To verify charge conservation, let us consider the semi-discrete continuity equation

$$\frac{d}{dt} q + \dot{S} : i = 0,$$

(30)
where the array \( q \) represents the amount of charge at all vertices, i.e., \( q = [q_1(t), q_2(t), \cdots, q_{Nv}(t)]^T \), \( N_v \)
being the number of vertices in the grid, and \( \tilde{S} \) being the incidence matrix associated with the (discrete)
divergence operator in the dual grid [28, 32, 34, 37]. Note that, similarly to \( C \), all elements of \( \tilde{S} \) are in the
set \{-1,0,1\}. Applying a leap-frog time update to (30), we obtain
\[
\frac{q^{n+1} - q^n}{\Delta t} + \tilde{S} \cdot i^{n+\frac{1}{2}} = 0. \tag{31}
\]
Then, let us consider \( \nu_1 \) (vertex 1) without loss of generality. The time rate of charge variation at \( \nu_1 \)
is
\[
\frac{q_1^{n+1} - q_1^n}{\Delta t} = Q_1 \frac{\lambda_1'}{\Delta t} - Q_2 \frac{\lambda_2'}{\Delta t} = Q \frac{\lambda_1' - \lambda_2'}{\Delta t}. \tag{32}
\]
On the other hand, the current flowing out of \( \nu_1 \) can be computed as
\[
(\tilde{S} i^{n+\frac{1}{2}})_1 = i_1 + i_2
\]
\[
= \frac{Q}{\Delta t} \left[ \int_{r_{p,s}}^{r_{p,j}} W_1^1(r_p) \cdot dL + \int_{r_{p,s}}^{r_{p,j}} W_2^1(r_p) \cdot dL \right]
\]
\[
= \frac{Q}{\Delta t} \left[ \left( \lambda_1^1 \lambda_2^1 - \lambda_1^j \lambda_2^j \right) + \left( \lambda_1^1 \lambda_3^1 - \lambda_1^j \lambda_3^j \right) \right] = \frac{Q}{\Delta t} \left[ \lambda_1' - \lambda_2' \right], \tag{33}
\]
where the property \( \lambda_1 + \lambda_2 + \lambda_3 = 1 \) has been used, and the Whitney edge basis functions are indexed in
an ascending order fashion (instead of a cyclic order) such that
\[
W_1^1(r_p) = \lambda_1(r_p) \nabla \lambda_2(r_p) - \lambda_2(r_p) \nabla \lambda_1(r_p), \tag{34}
\]
\[
W_2^1(r_p) = \lambda_1(r_p) \nabla \lambda_3(r_p) - \lambda_3(r_p) \nabla \lambda_1(r_p), \tag{35}
\]
\[
W_3^1(r_p) = \lambda_2(r_p) \nabla \lambda_3(r_p) - \lambda_3(r_p) \nabla \lambda_2(r_p). \tag{36}
\]
As the sum of (32) and (33) equals zero, the continuity equation is verified exactly.

The above derivation can be interpreted geometrically by understanding the geometrical representation
of Whitney 0-forms and 1-forms. Let us consider \( \nu_1 \) again. As explained in Appendix A and illustrated
in Fig. 3a, barycentric coordinates can be visualized as a ratio of two areas. The variation on the charge
assigned to \( \nu_1 \) during \( \Delta t \) is illustrated in terms of such areas in Fig. 3a and is expressed as
\[
\frac{Q}{\Delta t} (\lambda_1' - \lambda_2') = \frac{Q}{\Delta t} \frac{A_{q1,n+1} - A_{q1,n}}{A}, \tag{37}
\]
where \( A_{q1,n+1} \) and \( A_{q1,n} \) are the triangle areas as indicated in Fig. 3a and \( A \) is the area of the whole
triangle (grid element) defined by \( \nu_1, \nu_2 \) and \( \nu_3 \). On the other hand, the current flowing out of \( \nu_1 \) is the sum
of the currents along the edges touching \( \nu_1 \), that is \( e_1 \) and \( e_2 \). Referring to the geometrical interpretation of
the integral of Whitney 1-forms provided in Appendix A, the sum of these two currents is evaluated as
\[
i_1 + i_2 = \frac{Q}{\Delta t} \left[ - \int_{r_{p,s}}^{r_{p,j}} W_1^1(r_p) \cdot dL - \int_{r_{p,s}}^{r_{p,j}} W_2^1(r_p) \cdot dL \right] = - \frac{Q}{\Delta t} \left[ \frac{A_{e1}}{A} + \frac{A_{e2}}{A} \right], \tag{38}
\]
where \( A_{e1} \) and \( A_{e2} \) are indicated in Fig. 3b and the minus sign is due to the relative orientations of the path
\( L \) and Whitney 1-forms. Since
\[
A_{q1,n+1} - A_{q1,n} = A_{e1} + A_{e2}, \tag{39}
\]
the sum of (37) and (38) is identically zero.
2.6. Gauss’ law preservation

We next demonstrate that Gauss’ law is automatically satisfied for all time steps if proper initial conditions are used. By left-multiplying both sides of (12) by the discrete divergence matrix $\tilde{S}$, we obtain

$$\tilde{S} \cdot [\epsilon] \cdot \left( \frac{e^{n+1} - e^n}{\Delta t} \right) = \tilde{S} \cdot C^T \cdot [\mu_{n-1}] \cdot b^{n+\frac{1}{2}} - \tilde{S} \cdot i^{n+\frac{1}{2}}. \tag{40}$$

The first term of the right-hand side of (40) vanishes due to the exact sequence property for the dual grid, i.e., $\tilde{S} \cdot C^T = 0$. Using the discrete continuity equation (31), we can rearrange (40) as

$$\tilde{S} \cdot [\epsilon] \cdot \left( \frac{e^{n+1} - e^n}{\Delta t} \right) = q^{n+1} - q^n, \tag{41}$$

which is the discrete version of

$$\frac{\partial}{\partial t} \nabla \cdot D = \frac{\partial}{\partial t} \rho. \tag{42}$$

Therefore, Gauss’ law is preserved for all time steps if the initial condition $\tilde{S} \cdot [\epsilon] \cdot e^0 = q^0$ is met.

For completeness, we show next that Gauss’ law for magnetism is also satisfied if appropriate initial conditions are used. By taking discrete divergence matrix $S$ in both sides of (11), we have

$$S \cdot \left( \frac{b^{n+\frac{1}{2}} - b^{n-\frac{1}{2}}}{\Delta t} \right) = -S \cdot C \cdot e^n = 0, \tag{43}$$

where the second equality is from the exact sequence property in the primal grid, i.e., $S \cdot C = 0$. The relation (43) is the discrete version of

$$\frac{\partial}{\partial t} \nabla \cdot B = 0. \tag{44}$$

Therefore, Gauss’ law for magnetism is also preserved for all times if $b^0$ is such that $S \cdot b^0 = 0$.

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\footnote{The identity $\tilde{S} \cdot C^T = 0$ can be recognized as the discrete analogue of $\nabla \cdot \nabla \times = 0$.}

\footnote{Note that $S$ is distinct from $\tilde{S}$ since $S$ refers to the primal grid (i.e., the computational mesh itself) whereas $\tilde{S}$ refers to the dual grid (See [32][34]).}
2.7. Time-update sequence

Using the above equations, the overall time-update procedure is carried out in the following sequence. Initial conditions for \( E_0 \), \( B^{-\frac{1}{2}} \), \( v_p^{-\frac{1}{2}} \), and \( r_p^0 \) are first assumed. During each cycle, \( b^{n+\frac{1}{2}} \) is first calculated. Then, \( E^n \) and \( B^{n+\frac{1}{2}} \) are interpolated at particle positions. Next, after the particle acceleration \( v^{n+\frac{1}{2}}_p \) is performed, the particle push \( r^{n+1}_p \) is performed for all particles. Next, currents \( i^{n+\frac{1}{2}} \) are assigned (scattered) to grid edges. Finally, \( e^{n+1} \) is updated. Note that \( v_p \) and \( r_p \) are 3×1 column vectors. The procedure is illustrated in Fig. 4 and each step is enumerated below.

1) \( B \) update : \[ b^{n+\frac{1}{2}} = b^{n-\frac{1}{2}} - \Delta t \cdot C \cdot e^n \]

2) \( E \) gather : \[ E^n = \sum_{i=1}^{N_e} e^{n\frac{1}{2}}_i W^1_i(r^n_p) \]

3) \( B \) gather : \[ B^{n+\frac{1}{2}} = \sum_{i=1}^{N_f} b^{n+\frac{1}{2}}_i W^2_i(r^n_p) \]

4) Particle acceleration : \[ v^{n+\frac{1}{2}}_p = N^{-1} \cdot N^T \cdot v^{n-\frac{1}{2}}_p + \frac{q\Delta t}{m} \cdot N^{-1} \cdot E^n \]

5) Particle push : \[ r^{n+1}_p = r^n_p + \Delta t \cdot v^{n+\frac{1}{2}}_p \]

6) \( I \) scatter : \[ i^{n+\frac{1}{2}}_i = \frac{Q}{\Delta t} \int_{r^{p,f}_{p,s}} W^1_i(r_p) \cdot dL \]

7) \( E \) update : \[ \star \cdot e^{n+1} = \star \cdot e^n + \Delta t \left( C^T \cdot [s_{\mu-1}] \cdot b^{n+\frac{1}{2}} - i^{n+\frac{1}{2}} \right) \]

The algorithm utilizes an "intelligent" mesh for tracking particles at each time step without resorting to iterative search or lookup tables. The intelligent mesh is constructed (initialized) once the input mesh is loaded and it includes (adds) the necessary connectivity information among mesh elements to efficiently determine the element location of each particle in the next time step. The computing time of this process is minimal because it always starts the particle search from adjacent elements. It should also be stressed that the proposed gather-scatter algorithm is independent of the time integration scheme and it can be combined with other schemes as well. One advantage of the leap-frog time-stepping scheme chosen here is that it is both symplectic and energy-conserving (non-dissipative), as already observed in [18].
3. Validation

Let us consider a simple cyclotron motion for which a uniform static magnetic field is excited along the z-direction. The static magnetic flux density is $B_z = 2.275 \times 10^{-3}$ Wb/m$^2$, which produces the gyroradius of 0.25 m using

$$B_z = \frac{mv}{rq},$$

where $m = 9.1 \times 10^{-31}$ kg, $v = 10^8$ m/s, and $q = -1.6 \times 10^{-19}$ C.

Fig. 5 shows the snapshots of the movement of a single particle at selected time steps. As the scheme is conditionally stable, time step should be less than the Courant limit $\Delta t_c = 0.14887$ ns, which is the function of the mesh element sizes and is computed from the maximum eigenvalue of the stiffness matrix [27].

Fig. 5 shows the snapshots of the movement of a single particle at selected time steps. As the scheme is conditionally stable, time step should be less than the Courant limit $\Delta t_c = 0.14887$ ns, which is the function of the mesh element sizes and is computed from the maximum eigenvalue of the stiffness matrix [27]. This $\Delta t_c$ is less than $\Delta t/|v_p| \approx 0.1/10^8 = 10^{-9}$ s, where $\Delta t$ is the typical edge length of the triangular grid elements. It can be observed that the particle exactly shows the circular motion of 0.25 m radius. In this simulation, a pair of particles with the opposite charges are initially placed in the same location, so that net charge density and electric fields are initially zero. In contrast to the negatively charged particle, the particle with positive charge is assumed to be stationary due to its much larger mass, which is not shown in Fig. 5.

Table 1 shows similar results as Fig. 6, but extended up to $10^6$ time steps to further verify charge and energy conservation.

Next, Fig. 7 shows the movement of three negatively-charged particles at different time steps. Similarly as before, these particles describe circular motions because the influence of the static magnetic field is more dominant than interactions among the particles. Particles with positive charges, which are not shown in Fig. 7, are again stationary at all time steps due to their much larger masses. We select three random vertices
Figure 6: Charge and energy conservation: (a) Distributed amounts of charge to local vertices and their sum at all time steps and (b) Absolute value of the particle velocity at all time steps.

Table 1: Charge and energy conservation at large time steps.

| n   | $q_1$ | $q_2$ | $q_3$ | $Q$          | $|v_p|_{10^8}$ |
|-----|-------|-------|-------|--------------|---------------|
| $10^4$ | -6.410056 × $10^{-20}$ | -9.245821 × $10^{-20}$ | -3.441224 × $10^{-21}$ | -1.600000 × $10^{-19}$ | 9.999999 × $10^7$ |
| $10^5$ | -7.635486 × $10^{-20}$ | -7.154041 × $10^{-20}$ | -1.210471 × $10^{-20}$ | -1.600000 × $10^{-19}$ | 9.999999 × $10^7$ |
| $10^6$ | -6.187120 × $10^{-20}$ | -7.726390 × $10^{-21}$ | -1.472014 × $10^{-19}$ | -1.600000 × $10^{-19}$ | 9.999999 × $10^7$ |
| $10^7$ | -5.772639 × $10^{-21}$ | -2.809120 × $10^{-20}$ | -7.423930 × $10^{-20}$ | -1.600000 × $10^{-19}$ | 1.000000 × $10^8$ |
| $10^8$ | -5.766949 × $10^{-20}$ | -7.721123 × $10^{-20}$ | -2.091755 × $10^{-20}$ | -1.600000 × $10^{-19}$ | 1.000000 × $10^8$ |

$\nu_5, \nu_{21}, \nu_{42}$ as illustrated in Fig. 7(a) for the verification of Gauss’ law. The discrete version of Gauss’ law at $t = n\Delta t$, i.e., $\mathbf{S} \cdot [x] \cdot \mathbf{e}^n = \mathbf{q}^n$ is computed in double-precision floating-point arithmetic. Table 2 shows the left- and right-hand side values of this equation and the residuals at several time steps up to $10^8$. The agreement is excellent, and includes at least thirteenth significant digits in all cases and relatively negligible residuals at very large time steps. Note that Gauss’ law for magnetism $\mathbf{S} \cdot \mathbf{b}^n = 0$ is trivially preserved because only the $B_z$ component is present in this case, and is invariant with respect to $z$.

4. Concluding Remarks

A new charge-conserving gather-scatter algorithm for the PIC simulations of Maxwell’s equations with space charges has been presented. The algorithm is suited for arbitrary-unstructured grids and relies upon the representation of the various dynamical quantities as discrete differential forms of different degrees, and on their self-consistent interpolation by Whitney forms. The preservation of Gauss’ law is demonstrated for all times, both analytically and by means of numerical tests.

Acknowledgments

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Figure 7: Movement of three particles in the uniform static magnetic field at different time instants ($\Delta t = 0.1$ ns): (a) $t = 0$, (b) $t = 50\Delta t$, (c) $t = 100\Delta t$, and (d) $t = 200\Delta t$.

Appendix A. Whitney forms: Basic properties

For convenience, we provide here the explicit expressions of Whitney forms [39] in 3-D. In the past, Whitney forms have proved useful in finite element modeling of electromagnetic fields [40, 41, 42], to suppress spurious modes. Although Whitney forms can be more succinctly and elegantly expressed using the exterior calculus of differential forms [21, 32, 33, 39], we adopt here the more familiar notation of vector calculus.

In 3-D, there are four types of Whitney $p$-forms, according to their degree $p$. A Whitney 0-form is a continuous scalar function simply expressed as

$$W^0_i(r) = \lambda_i(r),$$  \hspace{1cm} (A.1)

where the subscript $i$ represents vertex $i$ and $\lambda_i$ is the barycentric coordinate [43] associated with vertex $i$. The geometrical construction for barycentric coordinates is illustrated in Fig. A.8. For a 1-D simplex (i.e. edge), the barycentric coordinates associated to the vertices $\nu_1$ and $\nu_2$ of any point $r$ in the simplex are equal to ratios $\lambda_1 = L_1/(L_1 + L_2)$ and $\lambda_2 = L_2/(L_1 + L_2)$, respectively, with $L_1$ and $L_2$ as indicated in Fig. A.8. For a 2-D simplex (triangle), the barycentric coordinates associated to the three vertices $\nu_1$, $\nu_2$ and $\nu_3$ of any point $r$ in the simplex are equal to $\lambda_1 = A_1/A$, $\lambda_2 = A_2/A$, and $\lambda_3 = A_3/A$, respectively, with the areas $A_1$, $A_2$, and $A_3$ as indicated and $A = A_1 + A_2 + A_3$. In a 3-D simplex, which is a tetrahedron, the barycentric coordinates can be similarly written as volume ratios. It is clear that $0 \leq \lambda_i \leq 1$ for all $i$ and that the sum of the barycentric coordinates of any given point $r$ associated to the neighbor vertices equals one. Hereinafter, the dependence on $r$ is dropped for notational simplicity, i.e., $\lambda_i(r) = \lambda_i$.

The vector (function) proxy of a Whitney 1-form associated with an arbitrary edge $ij$ bounded by

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5For the sake of clarity, we adopt in this Appendix a vertex-based indexing for all types of elements. This is in contrast to...
vertices \(i\) and \(j\) is expressed as \[^{32}\]

\[
W_{ij}^r(r) = \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i. \tag{A.2}
\]

For a brief geometrical illustration of the Whitney 1-form, let us consider Fig. A.9. The area \(A_{e1}\), which is associated with \(e_1\), is

\[
A_{e1} = A \left[ \lambda_1^1 \lambda_2^1 - \lambda_2^1 \lambda_1^1 \right], \tag{A.3}
\]

where \(\lambda_1^r\) and \(\lambda_2^r\) are shorthands of \(\lambda_i(r_i)\) and \(\lambda_j(r_j)\), respectively. As Fig. A.9b shows, \(A_{e1}\) can be regarded as the sum of small triangles such that

\[
A_{e1} = A \sum_n \left[ \lambda_1^n \lambda_2^{n+1} - \lambda_2^n \lambda_1^{n+1} \right]
\]

\[
= A \sum_n [\lambda_1^n (\lambda_2^n + \Delta \lambda_2^n) - \lambda_2^n (\lambda_1^n + \Delta \lambda_1^n)]
\]

\[
= A \sum_n [\lambda_1^n \Delta \lambda_2^n - \lambda_2^n \Delta \lambda_1^n]. \tag{A.4}
\]

After taking the limit of infinitesimally small triangles and transforming this summation to an integral, we obtain

\[
A_{e1} = A \int_{r_s}^{r_f} [\lambda_1 \nabla \lambda_2 - \lambda_2 \nabla \lambda_1] \cdot d\mathbf{L} = A \int_{r_s}^{r_f} W_{12}^r (r) \cdot d\mathbf{L}. \tag{A.5}
\]

the single-indexing adopted for all element types elsewhere in the paper.

Table 2: Verification of the discrete Gauss’ law at different time steps and (global) vertices.

| Vertex | \(n\) | \(\mathbf{S} \cdot [\kappa] \cdot \mathbf{e}^n\) | \(\mathbf{q}^n\) | \(\mathbf{S} \cdot [\kappa] \cdot \mathbf{e}^n - \mathbf{q}^n\) |
|--------|------|---------------------------------------|----------------|---------------------------------------|
| \(\nu_5\) | 10\(^1\) | -6.206610172341678 \times 10^{-36} | 0 | -6.206610172341678 \times 10^{-36} |
| | 10\(^2\) | -3.655787431057314 \times 10^{-34} | 0 | -3.655787431057314 \times 10^{-34} |
| | 10\(^3\) | -3.996030839096777 \times 10^{-20} | -3.996030839096777 \times 10^{-20} | 6.620384183831123 \times 10^{-35} |
| | 10\(^4\) | -3.581126715387582 \times 10^{-20} | -3.581126715387582 \times 10^{-20} | -2.074587661969626 \times 10^{-32} |
| | 10\(^5\) | 1.442950348685220 \times 10^{-31} | 0 | 1.442950348685220 \times 10^{-31} |
| | 10\(^6\) | -2.830713776667131 \times 10^{-30} | 0 | -2.830713776667131 \times 10^{-30} |
| \(\nu_{21}\) | 10\(^1\) | 3.385423730368188 \times 10^{-36} | 0 | 3.385423730368188 \times 10^{-36} |
| | 10\(^2\) | -2.045237819570873 \times 10^{-20} | -2.045237819570873 \times 10^{-20} | -6.981496048403730 \times 10^{-34} |
| | 10\(^3\) | -3.751623558930333 \times 10^{-20} | -3.751623558930333 \times 10^{-20} | -5.970382827600431 \times 10^{-33} |
| | 10\(^4\) | -6.8014480186811823 \times 10^{-20} | -6.8014480186811823 \times 10^{-20} | -1.690035261998000 \times 10^{-32} |
| | 10\(^5\) | -1.26463438238650 \times 10^{-31} | 0 | -1.26463438238650 \times 10^{-31} |
| | 10\(^6\) | -1.345470547792998 \times 10^{-30} | 0 | -1.345470547792998 \times 10^{-30} |
| \(\nu_{42}\) | 10\(^1\) | -4.98803347936703 \times 10^{-20} | -4.98803347936703 \times 10^{-20} | 1.70926285643672 \times 10^{-33} |
| | 10\(^2\) | -3.1591942392524 \times 10^{-20} | -3.1591942392524 \times 10^{-20} | 2.26896215731212 \times 10^{-33} |
| | 10\(^3\) | -3.9155004100283 \times 10^{-20} | -3.9155004100283 \times 10^{-20} | 8.73890722657083 \times 10^{-33} |
| | 10\(^4\) | 8.443811020826656 \times 10^{-32} | 0 | 8.443811020826656 \times 10^{-32} |
| | 10\(^5\) | 7.91991669552179 \times 10^{-31} | 0 | 7.91991669552179 \times 10^{-31} |
| | 10\(^6\) | -5.373841942680172 \times 10^{-21} | -5.373841942680172 \times 10^{-21} | 7.859451526095034 \times 10^{-30} |
Figure A.8: Geometrical illustration for Whitney 0-forms (barycentric coordinates) of a point \( \mathbf{r} \) in simplices of various degrees: (a) 1-D simplex and (b) 2-D simplex.

The areas associated with \( e_2 \) and \( e_3 \) can be derived in a similar fashion. The last integral above can be viewed as the generalization of the concept of barycentric coordinates from 0-dimensional objects (points) to 1-dimensional objects (segments). That is, this relation illustrates that, in the same manner as the Whitney 0-forms (barycentric coordinates) are used to represent a point as a weighted sum of nearby vertices \( i = 1, 2, 3 \) (with respective weights \( A_i/A \)), Whitney 1-forms represent any segment \([\mathbf{r}_s, \mathbf{r}_f]\) in terms of the nearby edges \( e_1, e_2, \) and \( e_3 \) (now with weights \( A_{e_1}/A, A_{e_2}/A, \) and \( A_{e_3}/A, \) respectively). In both cases, the weights are computed by the “contraction” \([32]\) of the corresponding Whitney form with the geometrical object. For a 0-form, this contraction simply means an evaluation of \( W_0^i \) at the point \( \mathbf{r} \), i.e., \( W_0^i(\mathbf{r}) \) as in (A.1), whereas for a 1-form, this contraction means an evaluation of the line integral of \( W_1^{ij} \) along the segment \([\mathbf{r}_s, \mathbf{r}_f]\) as in (A.5). For a more general description of these Whitney form properties, see [44]. A comprehensive discussion of the integral of Whitney 1-forms along a straight segment is presented in Appendix B below.

Likewise, the vector proxy of a Whitney 2-form associated with a triangular cell \( ijk \) is a vector function expressed as [32]

\[
W^2_{ijk}(\mathbf{r}) = 2 \left[ \lambda_i \nabla \lambda_j \times \nabla \lambda_k + \lambda_j \nabla \lambda_i \times \nabla \lambda_k + \lambda_k \nabla \lambda_i \times \nabla \lambda_j \right].
\] (A.6)

Finally, in 3-D, the proxy of a Whitney 3-form associated with a tetrahedral cell \( ijk\ell \) in 3-D is a scalar function written as [32]

\[
W^3_{ijk\ell}(\mathbf{r}) = 6 \left[ \lambda_i \nabla \lambda_j \cdot (\nabla \lambda_k \times \nabla \lambda_\ell) + \lambda_j \nabla \lambda_i \cdot (\nabla \lambda_k \times \nabla \lambda_\ell) + \lambda_k \nabla \lambda_i \cdot (\nabla \lambda_j \times \nabla \lambda_\ell) \right]
+ \lambda_\ell \nabla \lambda_i \cdot (\nabla \lambda_j \times \nabla \lambda_k) + \lambda_i \nabla \lambda_\ell \cdot (\nabla \lambda_j \times \nabla \lambda_k) + \lambda_j \nabla \lambda_\ell \cdot (\nabla \lambda_i \times \nabla \lambda_k) \right],
\] (A.7)

Despite the complicated-looking expression [A.7], \( W^3_{ijk\ell} \) can be shown in 3-D to be simply equal to

\[
W^3_{ijk\ell}(\mathbf{r}) = \begin{cases} 
\frac{1}{V}, & \text{if } \mathbf{r} \text{ is in the tetrahedron } ijk\ell, \\
0, & \text{otherwise}, 
\end{cases}
\] (A.8)

where \( V \) is the volume of the tetrahedron \( ijk\ell \) [32]. Whitney forms are interpolatory in the precise sense that they are equal to one when “evaluated on” the respective elements (vertices, edges, triangles, and tetrahedra) and to zero on all remaining elements of the grid, where “evaluated on” in the case of \( W^1_{ij}, W^2_{ijk}, \) and \( W^3_{ijk\ell} \) means “integrated over” edges, triangles, or tetrahedrons respectively\(^6\). Furthermore,
Figure A.9: Geometrical illustration of the weight assigned to Whitney 1-forms representing a segment \( L \) in a 2-D simplex: (a) In red color is the area \( A_{e_1} \) associated with the Whitney 1-form on \( e_1 \) (edge 1) that represents \( L \). The associated weight is given by \( A_{e_1}/A \), where \( A \) is the total area of the triangle composed of \( \nu_1, \nu_2, \) and \( \nu_3 \). A similar construction can be made for the other two edges \( e_2 \) and \( e_3 \). (b) Area represented by a sum of small triangles. See the main text for more details.

Whitney forms inherit the same type of continuity of the fields they represent. Specifically, \( W_0^i(r) \) is a continuous scalar function (representing scalar potentials for example), \( W_1^{ij}(r) \) is a tangentially continuous vector function (representing “intensity” vector fields for example), \( W_2^{ijk}(r) \) is a normally continuous vector functions (representing “flux density” vector fields or volumetric current densities for example) and \( W_3^{ijkl}(r) \) is a discontinuous scalar field (representing volumetric charge densities for example).

In 2-D, as in the numerical examples considered here, \( W_0^i(r) \) and \( W_1^{ij} \) write exactly as above, but \( W_2^{ijk} \) reduces to a scalar discontinuous function

\[
W_2^{ijk}(r) = \begin{cases} 
\frac{1}{A}, & \text{if } r \text{ is in the triangle } ijk, \\
0, & \text{otherwise,} 
\end{cases} \tag{A.9}
\]

where \( A \) is the area of the triangle \( ijk \). Furthermore, \( W_3^{ijkl} \) is identically zero in 2-D. For these and more properties of Whitney forms, the reader is referred to [19, 20, 45, 46, 44] and references therein.

Appendix B. Line integral of Whitney 1-forms

The scatter step of the proposed algorithm and the analytical verification of charge conservation provided above both rely upon the evaluation of line integrals of Whitney 1-forms. In this Appendix, we consider this in more detail. An arbitrary segment \( L \) from \( r_{p,s} \) to \( r_{p,f} \) on a triangle is illustrated in Fig. B.10. The segment can be decomposed into two vectors \( a \) and \( b \). \( \lambda_1(\cdot) \) and \( \lambda_2(\cdot) \) are barycentric coordinates associated with \( \nu_1 \) and \( \nu_2 \). \( h_1 \) and \( h_2 \) are the heights of the triangle for the base of \( e_3 \) and \( e_2 \), respectively. The edge vectors \( e_1 \), \( e_2 \), and \( e_3 \) are oriented in an ascending fashion of the associated vertex numbers. Note that the edge numbers do not coincide with the vertex numbers.

A simple way to evaluate the line integral

\[
\int_{r_{p,s}}^{r_{p,f}} W_1^i(r_p) \cdot dL, \tag{B.1}
\]

Alternatively, one could consider it as a discontinuous vector function with such amplitude and oriented along the \( z \)-direction, i.e., transverse to a 2-D domain in the \( xy \)-plane, so that expressions such as \( [10] \) remain invariant with the volume element \( dV \) representing an area (2-D volume).
is to use a parametric representation such that
\[ W_1^1(r_p) = W_1^1(s) \quad \text{and} \quad dL = dL(s). \] (B.2)

\( W_1^1(s) \) and \( dL(s) \) are simply assumed to be a linear function of the parameter \( s \) and the range of \( s \) is set to \( 0 \leq s \leq 1 \). As an example, the line integral of the Whitney edge basis function associated with \( e_1 \), \( W_1^1(r_p) = \lambda_1 \nabla \lambda_2 - \lambda_2 \nabla \lambda_1 \), is derived here.

As preliminaries, several variables are calculated. Vectors \( a \) and \( b \) can be expressed as
\[ a = - \left( \lambda_f^2 - \lambda_s^2 \right) e_3 = -\Delta_2 e_3, \] (B.3)
\[ b = - \left( \lambda_f^1 - \lambda_s^1 \right) e_2 = -\Delta_1 e_2. \] (B.4)

First, the path and its space derivative are parameterized through \( s \) such that
\[ L = L(s) = (a + b)s = -(\Delta_2 e_3 + \Delta_1 e_2)s, \] (B.5)
and \( dL = -(\Delta_2 e_3 + \Delta_1 e_2)ds \). Next, barycentric coordinates and their gradients are parameterized through \( s \) as well, i.e.,
\[ \lambda_1(s) = \left[ \lambda_f^1 - \lambda_s^1 \right] s + \lambda_s^1 = \Delta_1 s + \lambda_s^1 \] (B.6)
\[ \lambda_2(s) = \left[ \lambda_f^2 - \lambda_s^2 \right] s + \lambda_s^2 = \Delta_2 s + \lambda_s^2 \] (B.7)

The gradients of the barycentric coordinates are constant, so they are not the function of \( s \), that is
\[ \nabla \lambda_1 = \frac{1}{2A} \hat{z} \times e_3, \quad \nabla \lambda_2 = \frac{1}{2A} \hat{e}_2 \times \hat{z}, \] (B.8)
where \( A \) is the area of the triangle. Some dot products used for the line integral are summarized below.
\[ \nabla \lambda_1 \cdot e_2 = -1, \quad \nabla \lambda_1 \cdot e_3 = 0 \] (B.9a)
\[ \nabla \lambda_2 \cdot e_2 = 0, \quad \nabla \lambda_2 \cdot e_3 = -1 \] (B.9b)

Therefore, (B.1) for \( e_1 \) is computed as
\[ \int_{r_{p,s}}^{r_{p,f}} W_1^1(r_p) \cdot dL = \int_{r_{p,s}}^{r_{p,f}} (\lambda_1 \nabla \lambda_2 - \lambda_2 \nabla \lambda_1) \cdot dL \]
Similarly, the other two line integrals can be computed as

\[
\int_0^1 \left[ (\Delta_1 s + \lambda_1^s) \nabla \lambda_2 - (\Delta_2 s + \lambda_2^s) \nabla \lambda_1 \right] \cdot \left( -\Delta_2 e_3 - \Delta_1 e_2 \right) ds
\]

\[
= -\Delta_2 \left( \nabla \lambda_2 \cdot e_3 \right) \int_0^1 (\Delta_1 s + \lambda_1^s) ds + \Delta_1 \left( \nabla \lambda_1 \cdot e_2 \right) \int_0^1 (\Delta_2 s + \lambda_2^s) ds
\]

\[
= \Delta_2 \left[ \frac{\Delta_1}{2} + \lambda_1^s \right] - \Delta_1 \left[ \frac{\Delta_2}{2} + \lambda_2^s \right] = \Delta_2 \lambda_1^s - \Delta_1 \lambda_2^s
\]

\[
= \left( \lambda_1^f - \lambda_2^f \right) \lambda_1^s - \left( \lambda_1^f - \lambda_1^s \right) \lambda_2^f = \lambda_1^s \lambda_2^f - \lambda_1^f \lambda_2^s. \quad (B.10)
\]

Similarly, the other two line integrals can be computed as

\[
\int_{r_{p,s}}^{r_{f,t}} W_2^s(r_p) \cdot dL = \lambda_1^s \lambda_3^f - \lambda_1^f \lambda_3^s \quad (B.11)
\]

\[
\int_{r_{p,s}}^{r_{f,t}} W_3^s(r_p) \cdot dL = \lambda_2^s \lambda_3^f - \lambda_2^f \lambda_3^s \quad (B.12)
\]

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