Structural Aspects of Regularized Full Maxwell Electrodynamic Potential Formulations Using FIT

Sascha Baumanns 1, Markus Clemens 2, Sebastian Schöps 3

1 Universität zu Köln, Mathematical Institute Gyrhofstr. 8b, 50931 Köln, Germany
abaumann@math.uni-koeln.de
2 Bergische Universität Wuppertal, Chair of Electromagnetic Theory 42119 Wuppertal, Germany
clemens@uni-wuppertal.de
3 Technische Universität Darmstadt, Graduate School CE, Dolivostr. 15, 64293 Darmstadt, Germany
schoeps@gsc.tu-darmstadt.de

Abstract—In this paper regularized electrodynamic potential formulations for full Maxwell are presented within the framework of the Finite Integration Technique. The reformulation of the semi-discrete Maxwell Equations into two second order wave equations for the magnetic vector potential and a scalar electric potential is feasible with a Lorenz-type gauge condition. On the other hand, a Coulomb-type condition yields a numerically ill-posed formulation. This is shown using the differential-algebraic equation index concept.

I. INTRODUCTION

Electrodynamic potential formulations, based on \( \vec{A} \)-\( \phi \), are very popular in low and high frequency applications. Many formulations are known and they are well understood and various discretization methods allow efficient simulations in frequency and time domain. Nonetheless the ambiguity of the curl operator still causes inconvenience, for example when applying multigrid solvers, [8]. To this end several regularization have been proposed. In particular grad-div formulations that based on the Coulomb gauge, e.g. for low frequency [2, 6, 5] and high frequency applications [7].

In this paper the Lorenz and Coulomb gauges are discussed for full Maxwell in terms of the Finite Integration Technique (FIT). The numerical implications of both variants are discussed. The paper is structured as follows: the remaining two subsections of the introduction cover the continuous and discrete formulations including the special case of D’Alembert equations. In Section II the discrete curl-curl equation is introduced and different choices for gaugings are discussed. In Section III numerical issues for time-integration are analyzed in terms of the differential index concept for differential-algebraic equations, e.g. [3] and finally the paper closes with a numerical example in Section IV and conclusions.

A. Continuous Formulation

Maxwell’s equations are given in their differential form by

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}, \quad \nabla \cdot \vec{D} = \rho, \quad \nabla \cdot \vec{B} = 0,
\]

where \( \vec{E}, \vec{H} \) are the electric and magnetic field strength, \( \vec{D}, \vec{B} \) the electric and magnetic flux density, \( \rho, \vec{J} = \vec{J}_e + \vec{J}_s \) the electric charge and total electric current density. The equations are related to each other by the material laws

\[
\vec{D} = \varepsilon \vec{E}, \quad \vec{J}_s = \kappa \vec{E}, \quad \vec{B} = \mu \vec{H},
\]

with the permittivity \( \varepsilon \), conductivity \( \kappa \) and permeability \( \mu = \nu^{-1} \) (inverse reluctivity). They can be reformulated in conductive, uniform, isotropic and linear media to a pair of decoupled damped wave equations

\[
\begin{align*}
\Delta - \mu \kappa \frac{\partial}{\partial t} - \mu \varepsilon \frac{\partial^2}{\partial t^2} \vec{A} &= -\mu \vec{J}_s \\
\Delta - \mu \kappa \frac{\partial}{\partial t} - \mu \varepsilon \frac{\partial^2}{\partial t^2} \phi &= -\frac{\rho}{\varepsilon}
\end{align*}
\]

where \( \Delta \) denotes the (scalar and vector) Laplace operators, \( \vec{A} \) denotes the magnetic vector potential and \( \phi \) the electric scalar potential and \( \vec{J}_s \) is an external source current density, [9]. In the undamped case (\( \kappa = 0 \)) this system reduces to the well-known D’Alembert equations.

The formulation (1)-(2) exploits the ambiguity of the electrodynamic potentials to obtain two decoupled equations. It implies a particular regularization of the electrodynamic potentials by the (generalized) Lorenz gauge

\[
\nabla \cdot \vec{A} + \mu \kappa \phi + \mu \varepsilon \frac{\partial \phi}{\partial t} = 0.
\]

They are still coupled via the continuity equation

\[
\nabla \cdot \vec{J}_s + \frac{\kappa}{\varepsilon} \rho + \frac{\partial \rho}{\partial t} = 0.
\]

When solving the system (1)-(2) and (4) we have to ensure that the (generalized) Lorenz gauge (3) is fulfilled implicitly in order to solve Maxwell’s equations.

In the following we derive a space-discrete formulation in terms of FIT but a Whitney finite element will yield analogous results. Later the properties for time-integration of the semi-discrete system will be addressed.

B. Discrete Formulation

Based on a staggered discretization similar to the FDTD-scheme of Yee FIT was introduced [12, 11]. They are widely used within commercially available tools for the time domain
simulation of electromagnetic wave phenomena. This approach is based on the integral form of Maxwell’s Equations and it yields the so-called Maxwell-grid equations (MGE), [11]
\[
Ce = -\frac{d}{dt}b, \quad Ch = \frac{d}{dt}d + j, \quad Sd = q, \quad Sb = 0, \tag{5}
\]
with discrete curl operators \( C \) and \( \overline{C} \), divergence operators \( S \) and \( \overline{S} \) on the primal and dual grid, respectively. The discrete field quantities are integrated on edges, facets and volumes s.t. \( e, h \) describe the electric and magnetic fields, \( d, b \) the electric and magnetic fluxes and \( q, b \) the electric charges. The matrices
\[
d = M_e e, \quad j_k = M_e e, \quad h = M_e b, \tag{6}
\]
contain the permittivities, conductivities and reluctivities (inverse permeabilities). For simplicity only linear materials are considered, i.e., constant matrices. The total current \( j = j_k + j_s \) can include an external source current \( j_s \). For numerical simulations, the MGEs are often restated in a curl-curl formulation.

Starting from Ampère’s Law and inserting (5) and (6) into each other, one derives the discrete curl-curl equation
\[
\overline{CM}_e Ce + M_\nu \frac{d}{dt} e + M_\nu \frac{d^2}{dt^2} e = -\frac{d}{dt} j_s. \tag{7}
\]
The discrete curl-curl operator \( \overline{CM}_e C \) is well understood, [11] and wave propagation problems based on (7) are commonly solved in time domain e.g. by the implicit Newmark-Beta time integration scheme [10]. In the absence of space charges and conductive materials, i.e., \( \overline{SM}_e e = 0 \) and \( M_\nu = 0 \) equation (7) can be augmented by a discrete grad-div-matrix part. This gives the discrete wave equation
\[
L_\nu e + M_e \frac{d^2}{dt^2} e = -\frac{d}{dt} j_s, \tag{8}
\]
where \( L_\nu := \overline{CM}_e C - M_\nu \overline{GM}_e \overline{SM}_e \) is the discrete vector Laplacian, i.e., the curl-curl matrix extended by a regularization featuring the gradient \( \nabla \Phi := \nabla^T \) and a norm-matrix \( M_\nu \approx \frac{1}{\nu} \) that assures correct units, [7]. If space charges are considered a potential formulation can be used.

II. ELECTRODYNAMIC POTENTIALS

Semi-discrete electromagnetic wave propagation problems can be formulated in terms of the the magnetic vector \( a \) and electric scalar potential \( \Phi \). In FIT they are defined as line-integrals located on primary edges and or values at primary grid nodes, respectively. They allow us to represent the electric field and magnetic fluxes in the form
\[
e = -\frac{d}{dt}a - G\Phi \quad \text{and} \quad b = Ca \tag{9}
\]
The approach fulfills the discrete Faraday’s law and the non-existence of magnetic charges in MGE, because vector calculus properties are preserved on the discrete level, [1].

A. Discrete Continuity Equation

Let us derive a MGE based formulation of the continuity equation (10). This involves two discrete scalar Laplacians
\[
L_\nu := -\overline{SM}_e G \quad \text{and} \quad L_\kappa := -\overline{SM}_e G, \tag{10}
\]
for the permittivity and conductivity, respectively. They are clearly positive definite matrices because of the definition of the gradient matrix \( G = -\nabla^T \). The derivations starts from Ampère’s and Gauß’ Law:
\[
\overline{CM}_e Ca + M_\nu \left[ \frac{da}{dt} + G\Phi \right] + M_\nu \left[ \frac{d^2 a}{dt^2} + G \frac{d\Phi}{dt} \right] = j_s \tag{11}
\]
\[
-\overline{SM}_e \frac{da}{dt} + L_\nu \Phi = q \tag{12}
\]
They are coupled by the potentials and right-hand-sides via the continuity equation
\[
\overline{SM}_e a + M_\nu^{-1}L_\nu^{-1}q + \frac{da}{dt} = \left[ \overline{SM}_\kappa - L_\nu L_\nu^{-1} \overline{SM}_\nu \right] \frac{da}{dt}, \tag{13}
\]
that is obtained by a left-multiplication of Ampère’s Law by \( \overline{S} \) and inserting Gauß’ Law etc. The steps are the same as in the continuous case, e.g., applying the divergence operator. Nonetheless, the discrete continuity equation (10) is more general than its continuous counterpart (4). It covers anisotropic and non-homogeneous material distributions.

In the following section the ambiguity of the potentials is fixed by a gauge condition.

B. Regularizations

The generalized discrete Lorenz gauge (3) for a conductive domain in FIT notation is given by
\[
M_\nu G M_\nu \overline{SM}_\nu a + M_\kappa G \Phi + M_\nu \frac{d\Phi}{dt} = 0 \tag{14}
\]
with a norm-matrix \( M_\nu \) as introduced for (7). This regularization is similar to the Lagrange-multiplier formulation for eddy current problem, [4]. Transferring this idea to the present case, we obtain the choice \( M_\nu := \eta L_\nu^{-1} \) with an artificial material parameter \( \eta \sim \nu/\epsilon \) to ensure correct units. Based on this matrix and left-multiplying with \( -\overline{S} \) a much simpler version of the discrete Lorenz’ gauge can be obtained.

When neglecting the scalar potential in (11), one arrives at a Coulomb-type gauge w.r.t. the permittivities
\[
\overline{SM}_\nu a = 0. \tag{15}
\]
C. The Damped Wave Equation

To obtain a discrete version of the damped wave equation (1)-(2), we start by left-multiplying the Lorenz gauge (11) by \( M_\nu^{-1}L_\nu^{-1} \overline{S} \). This yields
\[
\overline{SM}_\nu a + M_\nu^{-1}L_\nu^{-1}L_\nu \Phi + M_\nu^{-1} \frac{d\Phi}{dt} = 0. \tag{16}
\]
Now, using (11) and (13) the system (8)-(9) becomes two discrete damped wave equations
\[
L_\nu a + M_\nu \frac{da}{dt} + M_\nu \frac{d^2 a}{dt^2} = j_s \tag{17}
\]
\[
L_\nu \Phi + M_\nu^{-1}L_\nu^{-1}L_\nu \Phi + M_\nu^{-1} \frac{d\Phi}{dt} = q \tag{18}
\]
with given right-hand-sides \( j_s \) and \( q \) that fulfill the continuity equation (10). The resulting problem (14)-(15) is a system of second-order ordinary differential equations (ODE).
On the other hand, if we solve the full Maxwell problem, i.e., \( q \) is not prescribed, we need an additional equation.

### III. Structural Properties of Full Maxwell

When solving the full Maxwell equations in a discrete electrodynamical potential formulation, both gauge conditions, i.e., Lorenz (11) and Coulomb (12) yield uniquely solvable semi-discrete systems, but they have different structural properties. This will be discussed in this section using the index concept for (linear) differential-algebraic equations of the form

\[
A \frac{d}{dt}x(t) + Bx(t) = q(t)
\]

where \( A, B \in \mathbb{R}^{n \times n} \) are matrices, \( x : [t_0, T] \rightarrow \mathbb{R}^n \) is the time-dependent unknown and \( q : [t_0, T] \rightarrow \mathbb{R}^n \) is an input.

**Definition 1.** The system (16) is called a (linear) differential-algebraic equations (DAE) if \( A \) is singular.

Roughly speaking, the index can be seen as a measure of the equations’ sensitivity to perturbations of the input and the numerical difficulties when integrating. It quantifies the difference to an ODE.

**Definition 2 (Differential Index, [3]).** The DAE (16) has differential index-\( \vartheta \) if \( \vartheta \) is the minimal number of analytical differentiations with respect to the time \( t \) that are necessary to obtain an ODE for \( \frac{dx}{dt} \) as a continuous function in \( x \) and \( t \).

**Definition 3.** A vector \( x_0 \in \mathbb{R}^n \) is a consistent initial value of the DAE (16) if there exists a solution that fulfills \( x_0 = x(t_0) \).

#### A. Full Maxwell with Lorenz Gauge

The first formulation is derived from Lorenz’ Gauge (11). Left-multiplication of the equation by \(-S\) yields

\[
L_\nu M_\nu \tilde{S}M_\nu a + L_\nu \Phi + L_\nu \frac{d\Phi}{dt} = 0.
\]

Together with equations (8)-(9) and introducing the derivative of the magnetic vector potential as an additional unknown \( \pi := da/dt \) we can formulate the problem as a DAE (16) given by

\[
L_\nu M_\nu \tilde{S}M_\nu a = -L_\nu \Phi + L_\nu \frac{d\Phi}{dt} = 0, \quad \text{(17)}
\]

\[
\tilde{C}M_\nu Ca + M_\nu [\pi + G\Phi] + M_\nu \left[ \frac{d\pi}{dt} + G\frac{d\Phi}{dt} \right] = j_s, \quad \text{(18)}
\]

\[
\tilde{S}M_\nu \pi = L_\nu \Phi + q = 0, \quad \text{(19)}
\]

\[
\frac{da}{dt} - \pi = 0, \quad \text{(20)}
\]

with \( x = (q, \Phi, a, \pi) \). Next we determine the differential index of the system (17)-(20). Equation (17) is an ODE for \( \Phi \):

\[
\frac{d\Phi}{dt} = -M_\nu \tilde{S}M_\nu a - L_\nu^{-1}L_\nu \Phi, \quad \text{(21)}
\]

Then, we deduce from (18) and (21) an ODE for \( \pi \):

\[
\frac{d\pi}{dt} = -M_\nu^{-1} \left[ L_\nu a + M_\nu [\pi + G\Phi] + M_\nu GL_\nu^{-1}L_\nu \Phi - j_s \right]
\]

Finally, only one differentiation with respect to time of (19) is needed to obtain an ordinary differential equation for \( q \):

\[
\frac{dq}{dt} = \tilde{S}M_\nu \pi - L_\nu \Phi - \tilde{S}j_s.
\]

Hence we conclude the following result

**Theorem 1.** The system (17)-(20) has differential index-1 and the initial vector \( x_0 = (q_0, \Phi_0, a_0, \pi_0) \) is a consistent initial value if \( q_0 = L_\nu \Phi_0 - \tilde{S}M_\nu \pi_0 \) is fulfilled.

#### B. Full Maxwell with Coulomb Gauge

Instead of augmenting MGE by a Lorenz-type gauge, one can choose the Coulomb gauge (12). Starting by left-multiplying Coulomb’s gauge by \( M_\nu \tilde{G} M_\nu \) we obtain

\[
M_\nu \tilde{G} M_\nu \tilde{S}M_\nu a = 0, \quad \text{(22)}
\]

Using (12) and (22) the system (8)-(9) becomes a semi-discrete damped wave equation accompanied by a Laplace equation. The system reads

\[
L_\nu a + M_\nu \left[ \frac{da}{dt} + G\Phi \right] + M_\nu \left[ \frac{d^2a}{dt^2} + G\frac{d\Phi}{dt} \right] = j_s
\]

\[
L_\nu \Phi = q
\]

with right-hand-sides that fulfill the continuity equation (10) and thus for given \( j_s \) the resulting semi-discrete problem is a system of differential-algebraic equations. The Coulomb gauged system reads

\[
\tilde{S}M_\nu \pi = 0, \quad \text{(23)}
\]

\[
\tilde{C}M_\nu Ca + M_\nu [\pi + G\Phi] + M_\nu \left[ \frac{d\pi}{dt} + G\frac{d\Phi}{dt} \right] = j_s, \quad \text{(24)}
\]

\[
\tilde{S}M_\nu \pi = L_\nu \Phi + q = 0, \quad \text{(25)}
\]

\[
\frac{da}{dt} - \pi = 0, \quad \text{(26)}
\]

This indicates already that the differential index is at least \( \vartheta \geq 2 \). Left-multiplying (24) by \( S \) and applying (27) yields:

\[
\frac{d\pi}{dt} = -L_\nu^{-1} \left[ L_\nu \Phi - \tilde{S}M_\nu \pi + \tilde{S}j_s \right]
\]

Furthermore from (24) we obtain:

\[
\frac{d\pi}{dt} = -M_\nu^{-1} \left[ (M_\nu G - M_\nu GL_\nu^{-1}L_\nu) \Phi + \tilde{C}M_\nu Ca + (M_\nu + M_\nu GL_\nu^{-1} \tilde{S}M_\nu) \pi - (I + M_\nu GL_\nu^{-1} \tilde{S}) j_s \right]
\]

Finally, one differentiation w.r.t. time of (25) results in

\[
\frac{dq}{dt} = \tilde{S}M_\nu \pi - L_\nu \Phi - \tilde{S}j_s
\]

and thus the overall problem has a differential index-2.
Theorem 2. The system (23)-(26) has differential index-2, and the initial vector $x_0 = (q_0, \Phi_0, a_0, \pi_0)$ is a consistent initial value if $SM_a a_0 = 0$, $SM_{\pi} \pi_0 = 0$ and $q_0 = L_\cdot \Phi_0 - SM_{\pi} \pi_0$ are fulfilled.

On the one hand Lorenz and Coulomb yield systems that describe the same phenomena and have the same analytical solutions. On the other hand the structural properties are different, while the Lorenz Gauge yields an index-1 problem the Coulomb Gauge gives index-2. Hence the latter formulation will be much more affected by perturbations.

IV. NUMERICAL EXAMPLES

Let us consider a metal bar surrounded by air and discretized by the Finite Integration Technique, see Figure 1. The contacts are excited by a sinusoidal source. This can either be implemented as an external source current

$$j_s = \sin(2\pi t)$$

or as a Dirichlet boundary condition for the electric scalar potential $\phi$. The simulations were carried out by the implicit Euler scheme with fixed steps $h = 8 \cdot 10^{-5}s, 4 \cdot 10^{-5}s, 2 \cdot 10^{-5}s, 1 \cdot 10^{-5}s$ on the time interval $[0s, 0.5s]$. The numerical solution of the Lorenz (index-1) and Coulomb gauged (index-2) formulations are given in Figures 2a and 2c. Both formulations give solutions as expected.

To analyze the sensitivity, we perturb the source current by a very small high-frequent noise

$$\tilde{j}_s = j_s + 10^{-k} \sin(2 \cdot 10^k + 5\pi t).$$

We have chosen $k = 4$ for the simulations in this paper. As expected, the numerical solution of the perturbed Lorenz-based formulation (index-1) is not affected, Figure 2b. On the other hand the solution of the index-2 formulation suffers strongly from the perturbation, see Figure 2d.

Please note, the effect occurs even for tiniest perturbations, i.e. very large $k >> 1$, due to the chain rule and the effect increases with a reduction in step size, i.e., it cannot be compensated by a finer temporal mesh.

V. CONCLUSIONS

In this paper several electrodynamic potential formulations for full Maxwell were presented in terms of the matrix formalism of FIT. They required the introduction of a new generalized discrete Lorenz gauge. The Lorenz and Coulomb gauged systems have been compared in terms of a DAE index concept. Structural analysis and numerical examples show that the Coulomb gauged system is much more sensitive to small perturbation than its Lorenz counterpart.

Acknowledgements: This work was supported by the BMBF SOFA Verbundprojekt with grand numbers 03MS648A, 03MS648D and 03MS648E.

REFERENCES

[2] A. Bossavit. “Stiff problems in eddy-current theory and the regular-