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Solution of the Complex-valued Helmholtz Equation using a Dedicated Finite Element Solver

Abstract. This paper describes a numerical FEM model for solving the complex-valued, vector Helmholtz wave equation. The model describes phenomena of electromagnetic wave propagation for high frequencies. The presented model can be used in a larger system seeking an efficient design parameters of electromagnetic energy transfer for high power pulse generation device.

Streszczenie. W niniejszym artykule opisujemy zbudowany model numeryczny MES rozwiązujący zespolone, wektorowe równanie falowe Helmholtza. Pozwala on na modelowanie zjawisk propagacji fal elektromagnetycznych wysokich częstotliwości. Zaprezentowany model może zostać wykorzystany w systemie poszukującym optymalnego projektu urządzenia służącego do przesyłu energii w postaci fali elektromagnetycznej, do generacji silnych impulsów elektromagnetycznych. (Rozwiązywanie zespolonego równania Helmholtza za pomocą dedykowanego oprogramowania MES).

Keywords: finite element method, wave equation, coaxial cable, FEniCS
Słowa kluczowe: metoda elementów skończonych, równanie falowe, kabel koncentryczny, FEniCS.

Introduction

In the paper a finite element simulator of TEM (transverse electromagnetic) waveguide is presented. The need for such a software arises when a fast tool is required to design devices for efficient electromagnetic wave transmission, strong electric field generation and impulse propagation. The design process for radio frequency band devices may require re-evaluations of manufactured prototypes or their corresponding numerical models. For the sake of speed and economy the later approach is dominant nowadays. A numerical simulator (like the one described in this paper) could be used in such a process as an alternative for general commercial packages. Its main advantage lies in a possibility to use it for an automatic evaluation of many potential prototypes by running the simulator in a closed loop for the purpose of an optimization process.

Commercial software for solving electromagnetic wave propagation problems are mostly general purpose software packages, suitable for rapid development of the numerical model. However, once the model is setup the performance can be insufficient for running massive number of simulations evaluating different designs for stochastic optimization algorithms (e.g. evolutionary optimization). On the other hand, an in-house Finite Element Method (FEM) code which can benefit from being highly tailored to the specific problem, is often of a much worse maturity and may contain serious errors which can harm reliability of such a system. In our paper, we use FEniCS project, which benefits from both approaches. FEniCS aggregates many libraries which allow to automatically generate FEM solver for a given PDE problem. The project also allows to automatically parallelize the process of finding solution using MPI or OpenMP.

Mathematical model

The equation that is solved in the simulator is the vector Helmholtz wave equation. It is solved for the complex electric field in 3D (see Eq. 1) [1, 2].

$$(1) \qquad \nabla \times (\mu_r^{-1} \cdot \nabla \times \overline{E}) - k_0^2 \varepsilon_r \cdot \overline{E} = 0$$

In this equation $\overline{E} = E_{re} + jE_{im}$ is a complex-valued 3D vector for an electric field, j is the imaginary unit, μ_r and ε_r are material properties, respectively: relative permeability

and relative permittivity; $k_0 = \omega/c$ is the wavenumber of free-space.

This equation does model wave propagation in a lossless medium with material properties μ_r, ε_r. In this case both the impressed electric current and the impressed magnetic current are assumed to be zero in the whole domain (for a description of a general Helmholtz equation see chapter 2.1 in [1]). The excitation will be provided by the means of a specialized boundary condition.

Finite Element Method requires a discretization of the whole computational domain into a mesh of finite elements. One has to apply a boundary condition on each part of the boundary of the domain. We present three types of such conditions used for truncation of computational domain.

One of the most frequently used boundary conditions for high frequency electromagnetic field simulations is the Perfect Electric Conductor (PEC). Due to skin effect current flows in the metal only in a thin layer beneath the surface of the conductor. In most cases it is valid to approximate it by currents on the boundary of the metal domain. PEC models a perfect (lossless) metallic domain with no electric field inside of it. The electric field on the boundary of PEC satisfies the following equation:

$$(2) \qquad \hat{n} \times \overline{E} = 0$$

This condition restricts the tangential component of $\overline{E}$ to be zero. On PEC boundary only non-zero normal component of $\overline{E}$ is allowed.

A complementary boundary condition is the Perfect Magnetic Conductor (PMC). It can be used to impose a symmetry of electric field. In this case the magnetic field can only have a non-zero normal component:

$$(3) \qquad \hat{n} \times \overline{H} = \hat{n} \times \left(\mu_r^{-1} \cdot \nabla \times \overline{E} \right) = 0$$

PMC is useful if we can find a boundary on which the magnetic field is perpendicular to it. This way, we can truncate our computational domain and assume a symmetric electric field distribution on the other side of such a boundary.

The third boundary condition that is indispensible in most of numerical models is called Waveguide Port Boundary Condition (WPBC). It was introduced by Jin in [1], and is often implemented in commercial software packages, e.g. in COMSOL [2]. WPBC can be used for applying an incident electromagnetic wave.

To derive WPBC a total field formulation should be used. In this formulation all electromagnetic waves are defined as a superposition of (possibly an infinite number) fundamental modes: Traverse Electric (TE), Traverse Magnetic (TM) and Traverse ElectroMagnetic (TEM). So the total field formulation reads [1]:

(4)
$$\overline{E} = \overline{E}^{inc} + \overline{E}^{ref} \quad \Big| \hat{n} \times (\nabla \times)$$
$$\hat{n} \times (\nabla \times \overline{E}) = \hat{n} \times (\nabla \times \overline{E}^{inc}) + a_0 \overline{\gamma}_0^{TEM} e_0^{TEM}$$
$$+ \sum_{m=1}^{\infty} a_m \overline{\gamma}_m^{TE} e_m^{TE} - \sum_{m=1}^{\infty} a_m \overline{\gamma}_m^{TM} e_m^{TM}$$

$\overline{E}^{inc}$ and $\overline{E}^{ref}$ are incident and reflected fields, a_m are amplitudes of the particular modes, $\overline{\gamma}_m^{TE}/\overline{\gamma}_m^{TM}$ are their complex propagation constants and e_m^{TE}/e_m^{TM} are electric fields associated with the modes. However it is often unfeasible to solve the Helmholtz equation for all possible modes of propagation. Often one can truncate such an infinite series by excluding the higher modes (i.e. with $m > 1$) that don't propagate at the given frequency. Situation simplifies itself even further when the incident and the reflected fields are defined as the same mode. Fortunately this is often the case in many engineering problems. For example, if a waveguide port is excited with the TEM mode and it can only absorb TEM mode Eq. 4 simplifies to:

(5) $\hat{n} \times (\nabla \times \overline{E}) = \overline{\gamma}_0^{TEM} [\hat{n} \times (\hat{n} \times \overline{E})] - 2 A_0 \overline{\gamma}_0^{TEM} e_0^{TEM}$

For the coaxial waveguide propagating TEM waves in z-direction the mode's field is defined as: $e_0^{TEM}(x,y) = \left\langle x/(x^2+y^2), y/(x^2+y^2), 0 \right\rangle / (\ln d_0/d_1)$ where r_1 and r_2 are outer and inner radii of the coaxial waveguide and $\overline{\gamma}_0^{TEM} = jk = jk_0\sqrt{\varepsilon_r \mu_r}$. A_0 is the amplitude (in volts) of the excitation on the port. It is worth noting that if $A_0=0$ then the port is passive and can only absorb the given mode.

Numerical formulation

To solve Eq. 1 with Finite Element Method a weak form is derived by multiplying both sides by a test (weighting) function and integrating both sides over the computational domain. It is convenient to apply vector cross product rule:

(6)
$$T \cdot \nabla \times \mu_r^{-1} \cdot (\nabla \times \overline{E}) =$$
$$(\nabla \times T) \cdot \mu_r^{-1} \cdot (\nabla \times \overline{E}) - \nabla \cdot \left[T \times (\mu_r^{-1} \cdot \nabla \times \overline{E}) \right]$$

followed by divergence theorem:

(7) $\iiint\limits_V \nabla \cdot \left[T \times (\mu_r^{-1} \cdot \nabla \times \overline{E}) \right] dV = \iint\limits_S \hat{n} \cdot \left[T \times (\mu_r^{-1} \cdot \nabla \times \overline{E}) \right] dS$

where T and $\overline{E}$ are the test and trial functions, respectively; S is the boundary of the computational domain V. This way one of the volume integrals transforms into a surface integral which allows application the boundary conditions described in this section.

(8)
$$\iiint\limits_V \left[(\nabla \times T) \cdot \mu_r^{-1} \cdot (\nabla \times \overline{E}) - k_0^2 T \cdot \varepsilon_r \cdot \overline{E} \right] dV$$
$$+ \iint\limits_S T \cdot \left[\hat{n} \times (\mu_r^{-1} \cdot \nabla \times \overline{E}) \right] dS = 0$$

It should be noted that in Eq. 8 only $\overline{E}$ is a complex vector function. Weighting function is purely real.

In general such an equation can be discretized on a mesh of finite elements and solved in its complex form:

(9) $\overline{\mathbf{A}}\overline{\mathbf{x}} = \overline{\mathbf{b}}$

where $\overline{\mathbf{A}} = \mathbf{A}_{re} + j\mathbf{A}_{im}$ is a complex bilinear form assembled using Finite Element Method, $\overline{\mathbf{x}} = \mathbf{x}_{re} + j\mathbf{x}_{im}$ is a complex vector with solution of the problem and $\overline{\mathbf{b}} = \mathbf{b}_{re} + j\mathbf{b}_{im}$ is the right-hand side vector. However, not all numerical packages support solving complex-valued systems of equations.

Automatic formulation of the equivalent real-valued system of equations for FEniCS

As mentioned in before, we use FEniCS for an automated solution of the vector Helmholtz wave differential equation using FEM. FEniCS does not support solving of complex differential equations, so the original equation had to be split in both real and imaginary parts [3]. After that one can construct the real-valued system of equations, equivalent to Eq. 9:

(10)
$$\begin{bmatrix} \mathbf{A}_{re} & -\mathbf{A}_{im} \\ \mathbf{A}_{im} & \mathbf{A}_{re} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_{re} \\ \mathbf{x}_{im} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{re} \\ \mathbf{b}_{im} \end{bmatrix}$$

We do this automatically a custom Python module using SymPy library had been developed. SymPy is a Python library for symbolic manipulations of mathematical expressions. It was extended with an implementation of a few operators for complex-valued vectors, i.e. inner vector product, cross vector product, curl, divergence and gradient.
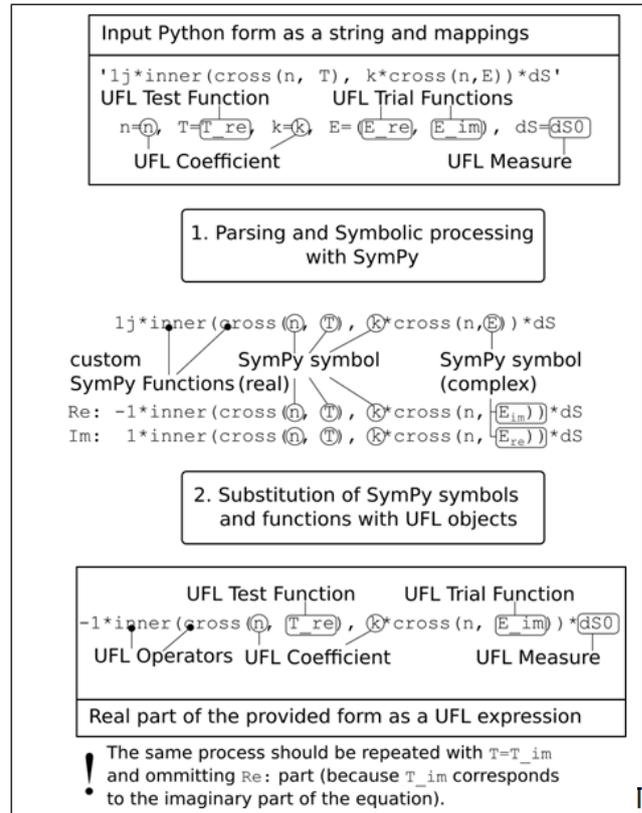
Fig.1. Diagram of a process of complex form splitting

The modules uses SymPy for parsing UFL-like forms into SymPy expressions. The expressions are then simplified and split into real and imaginary expressions. After this phase, our module substitutes SymPy symbols with correct UFL objects. Such objects are then used for assembling

matrices from Eq. 10. Listing 1 shows how the volume integral from Eq. 8 can be assembled using our module `split_complex`.

```
helmholtz_form = """
inner(curl(T), invmur*curl(E))*dV
- k0**2*inner(T, epsr*E)*dV
"""

real_part, _ = split_complex (helmholtz_form,
E=(E_re, E_im),
epsr=epsr, invmur=1./mur, k0=k0,
dV=dV, T=T_re)

_, imag_part = split_complex (helmholtz_form,
E=(E_re, E_im),
epsr=epsr, invmur=1./mur, k0=k0,
dV=dV, T=T_im)

final_ufl_form = real_part + imag_part
```

Listing 1. Separation of the volume integrals from Helmholtz equation using `split_complex` component

In Listing 1 the first invocation of `split_complex` returns a form corresponding to $[A_{re} \ -A_{im}]$ sub-matrix and the second one (`imag_part`) to $[A_{im} \ A_{re}]$.

Numerical model

To verify our simulator a standard coaxial cable problem has been chosen. Coaxial cables are ubiquitous examples of TEM waveguides transferring electromagnetic waves between devices/systems and their strong advantage is that they were thoroughly studied. In this experiment the coaxial cable consists of two conductors (inner and outer) separated by a dielectric material (PTFE). The diameters of the outer and inner conductors are d_0=9.5 mm and d_1=3 mm, respectively. Assuming that PTFE has ε_r=2.0 we can calculate the characteristic impedance of such a coaxial cable using an approximated, analytical formula: $\left(138\Omega/\sqrt{\varepsilon_r}\right)\log_{10}(d_0/d_1)$ which gives us the value 48.85 Ω. This indicates that such a coaxial cable was designed for a 50 Ω systems.

One of the side of the dielectric (S_1) is excited with an electric field by applying on the boundary WPBC. We consider three standard types of termination (see Fig. 2):

a) with a matched impedance at the end (Z_L=50 Ω),
b) with an open end (Z_L=∞ Ω),
c) with a shorted end (Z_L=0 Ω).

Termination in case a) should generate no reflection from the end of the cable (boundary S_0), therefore we could use again WPBC, but this time A_0=0, so the port only absorbs TEM incident electromagnetic wave. Appropriate models for case b) and c) are PMC and PEC, respectively. We expect total reflection from shorted and open ends. The wave should reflect with the same phase from PEC boundary and with the opposite phase from PMC boundary.

Fig. 2. Three types of termination of coaxial cable

Because the inner (S_2) and outer (S_3) conductor are modelled with PEC, there is no need for generating a finite element mesh for any metallic part of the cable (as there is no electric field inside them). Therefore, only the dielectric will be meshed. To decrease the computational effort of the problem we can also take advantage of the symmetry of the cable. In the coaxial cable electric field in TEM mode has only radial component traverse to the direction of propagation. The magnetic field is perpendicular to both the electric field and the direction of propagation. This means that if we consider only one quarter of the coaxial cable, the magnetic field on the sides (S_4 and S_5) of the dielectric will has only the normal component, which is equivalent to applying PMC (see Fig.3).
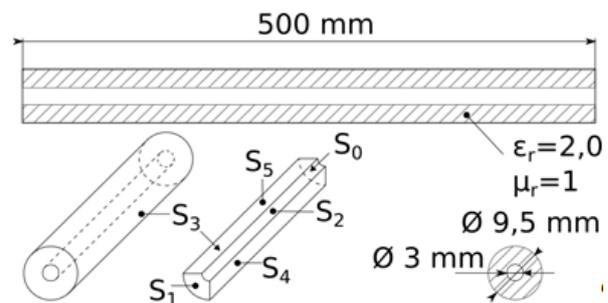
Fig. 3. The illustration of the coaxial cable model

Nédélec (also called vector or edge) finite elements are often used for solving Helmholtz equation. These elements has degrees of freedom (DOF) associated with edges of the finite element mesh. The value in the mesh is the tangential component of the electric field for the edge. They have numerous advantages in this formulation, mainly because of an easy application of boundary conditions. If we want to allow only the normal component of electric field on a boundary we can fix all DOFs as 0 for edges on the boundary. This works because the DOFs contribute only to the component of electric field tangential to the surface. A sample application of PEC in FEniCS is presented in Listing 2.

```
finite_element = "Nedelec 2nd kind H(curl)"
V_re = FunctionSpace(mesh, finite_element, 1)
V_im = FunctionSpace(mesh, finite_element, 1)
V = V_re * V_im
E_re, E_im = TrialFunctions(V)
T_re, T_im = TestFunctions(V)

# ...

pec = Constant((0,0,0), degree=1)
bcs = [
  DirichletBC(V.sub(0), pec, bnds, 2),
  DirichletBC(V.sub(1), pec, bnds, 2),
  DirichletBC(V.sub(0), pec, bnds, 3),
  DirichletBC(V.sub(1), pec, bnds, 3)
]
```

Listing 2. Application of PEC Dirichlet boundary condition. Please note that `V.sub(0)` is the function space describing the real part of electric field, while `V.sub(1)` – the imaginary part

FEniCS provides an interface for different solvers. According to [4] Helmholtz equation is a difficult problem for iterative Krylov space solvers. It appears that solving an equivalent real-valued system of equations makes it even harder for the iterative solvers to converge. In our experiments we weren't able to solve Helmholtz equation with WPBC using any iterative method. Because the size of the problem is moderate, we were able to use a direct method, i.e. MUMPS. It seems to improve time of computation at the cost of extensive memory usage [5].

Results

For a mesh consisting of 39000 tetrahedra with 51507 edges the calculation time on one CPU core was around 30s (Intel(R) Xeon(R) CPU E5-2690 v2 @ 3.00GHz, 32 GB of RAM). The simulations were performed for the frequency 500 MHz, for which the wavelength in PTFE is comparable to the length of the cable (50 cm).
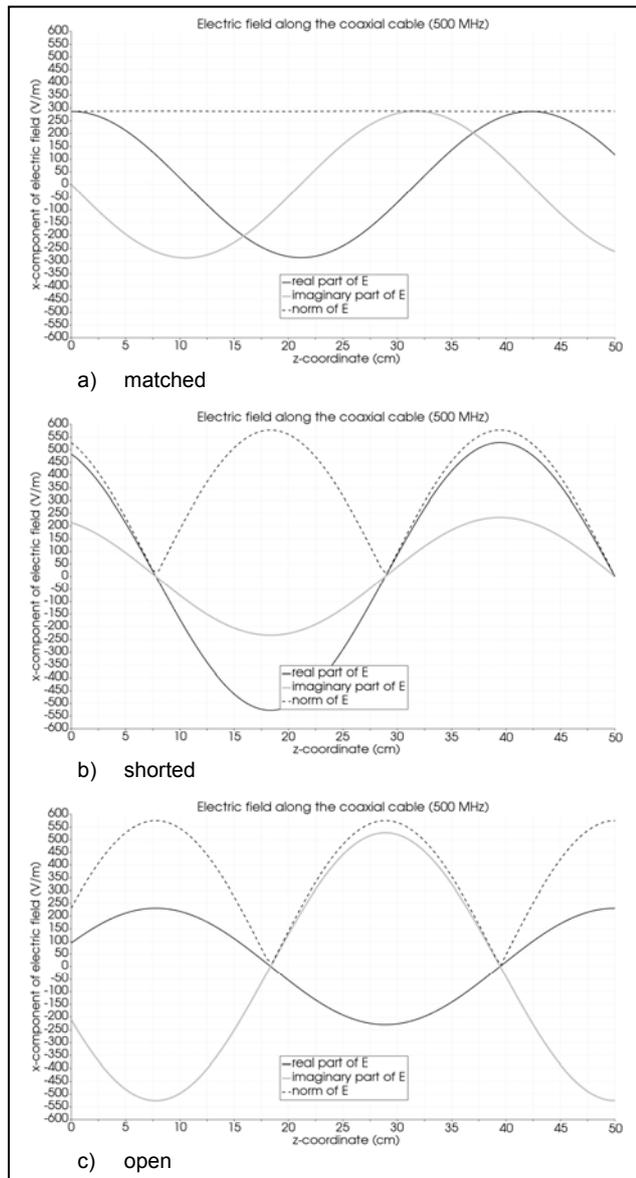
Fig. 4. Radial component of electric field along the coaxial cable (for three types of termination). The evaluation line's endpoints are (3 mm, 0 mm, 0 cm) and (3 mm, 0 mm, 50 cm)

To verify the results for the three types of termination a radial component of the electric field has been plotted along the length of the cable. In Fig. 4 three plots are presented. In the black colour we presented the real part of electric field, while the imaginary part is plotted in grey. The norm of the electric field $|\overline{E}| = \sqrt{E_{re}^2 + E_{im}^2}$ is plotted with a dashed, black line.

We can see that when the cable is terminated with a matching impedance, no standing waves appear (Fig. 4a). When the output of the cable is shorted (Fig. 4b), the electric field at z = 50 cm is 0 V/m and the reflected wave is in phase with the incident one. For the case of the open terminals (Fig. 4c) we can notice a change in phase

between the incident and reflected wave by 180°. Both mismatched cases generate standing wave patterns.

A general view at the electric field overlaid with the finite element mesh can be seen in Fig. 5.
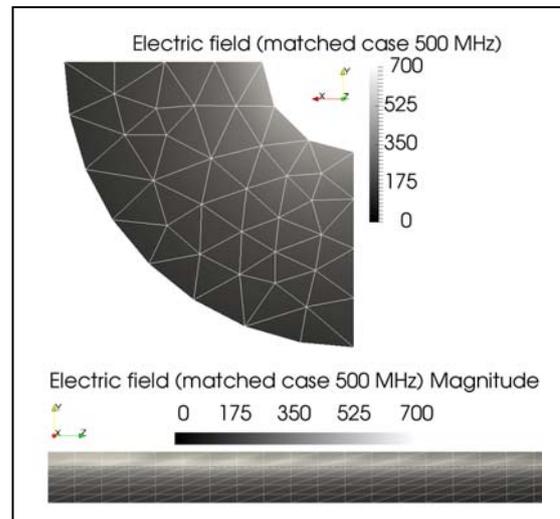
Fig. 5. Radial component of electric field along the coaxial cable (for three types of termination)

Conclusions

To sum up, FEniCS can be used to build a fast and accurate electromagnetic field solver modelling electromagnetic wave propagation. It is possible to solve complex-valued, vector Helmholtz equation in an automatic way at the expense of necessity of constructing an equivalent real-valued system of linear equations.

In general Helmholtz equation needs a special attention to be solved using Krylov space solvers, however a direct method can also be used if only one has enough memory at hand.

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