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Minimal Rational Interpolation for Time-Harmonic Maxwell's Equations

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ABSTRACT

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2.1 VECTOR POTENTIAL FORMULATION OF THE TIME-HARMONIC MAXWELL'S EQUATIONS

Let $\mathbf{E}$ denote an electric field, $\mathbf{B}$ a magnetic field strength, ρ an electric charge density, and $\mathbf{j}$ an electric current density. Maxwell's equations are stated in [?] as

$$\nabla \cdot (\epsilon \mathbf{E}) = \rho \tag{2.1}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{2.2}$$

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B} \tag{2.3}$$

$$\nabla \times (\mu^{-1}\mathbf{B}) = \partial_t(\epsilon \mathbf{E}) + \mathbf{j} \tag{2.4}$$

with ε being the permittivity and μ the permeability.

Equation (2.2) allows for an expression of the magnetic field $\mathbf{B} = \nabla \times \mathbf{u}$ in terms of a vector valued function $\mathbf{u}$, the vector potential (in literature commonly denoted with $\mathbf{A}$). Similarly, (2.3) suggests rewriting the electric field $\mathbf{E} = -\nabla \phi - \partial_t \mathbf{u}$ using a scalar function ϕ, referred to as the scalar potential.

The physical quantities $\mathbf{E}$ and $\mathbf{B}$ remain unchanged if we transform $\mathbf{u} \to \mathbf{u}' = \mathbf{u} + \nabla \psi$ or $\phi \to \phi' = \phi - \partial_t \psi$ for arbitrary functions ψ. A convenient choice of ψ is suggested in [?] to be

$$\psi = \int_0^t \phi \, dt' \tag{2.5}$$

which transforms $\phi \to \phi' = 0$ and $\mathbf{u} \to \mathbf{u}' = \mathbf{u} + \nabla \int_0^t \phi \, dt'$. Thus, the expressions for the electrical and magnetic field become

$$\mathbf{E} = -\partial_t \mathbf{u} \tag{2.6}$$

$$\mathbf{B} = \nabla \times \mathbf{u} \tag{2.7}$$

where I renamed the variable $\mathbf{u}'$ to $\mathbf{u}$ for simplicity.

Plugging the identities (2.6) and (2.7) into (2.4) yields

$$\nabla \times (\mu^{-1}\nabla \times \mathbf{u}) = \epsilon \partial_t^2 \mathbf{u} + \mathbf{j} \tag{2.8}$$

For the rest of this report, I restrict myself to vector potentials $\mathbf{u}$ that exhibit a harmonic dependence on time t, i.e. may be factorized into a term solely depending on the position $\mathbf{x}$ and a complex exponential

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}) \exp(i\omega t) \tag{2.9}$$

Substituting this expression into (2.8) results in the

Time-harmonic potential equation
$$\nabla \times (\mu^{-1}\nabla \times \mathbf{u}) - \epsilon\omega^2 \mathbf{u} = \mathbf{j} \qquad (2.10)$$

2.2 WEAK FORMULATION FOR THE TIME-HARMONIC POTENTIAL EQUATION

Equation (2.10) may be multiplied by a vector-valued function $\mathbf{v} \in H_{\text{curl}}(\Omega)$, where

$$H_{\text{curl}}(\Omega) = \{\mathbf{u} : \Omega \to \mathbb{C}, \text{ such that } \mathbf{u} \in L^2(\mathbb{C})^3, \nabla \times \mathbf{u} \in L^2(\mathbb{C})^3\} \tag{2.11}$$

and then integrated over all of Ω to obtain

$$\int_\Omega (\nabla \times (\mu^{-1}\nabla \times \mathbf{u})) \cdot \mathbf{v} - \omega^2 \int_\Omega \epsilon\mathbf{u} \cdot \mathbf{v} = \int_\Omega \mathbf{j} \cdot \mathbf{v} \tag{2.12}$$

This may further be simplified (2.12) to (see Section for details)

Weak formulation of the time-harmonic potential equation

$$\int_\Omega (\mu^{-1}\nabla \times \mathbf{u}) \cdot (\nabla \times \mathbf{v}) - \omega^2 \int_\Omega \epsilon\mathbf{u} \cdot \mathbf{v} = \int_\Omega \mathbf{j} \cdot \mathbf{v} + \int_{\partial\Omega} \underbrace{((\mu^{-1}\nabla \times \mathbf{u}) \times \mathbf{n})}_{=\mathbf{g}} \cdot \mathbf{v} \tag{2.13}$$

---

where $\mathbf{n}$ denotes the surface normal to the boundary $\partial\Omega$.

Boundary conditions on the electric field $\mathbf{E}$ may be enforced in a Dirichlet-type fashion through the relation (2.6) and the assumption (2.9)

$$\mathbf{u}|_{\partial\Omega} = -\frac{1}{i\omega} \mathbf{E}|_{\partial\Omega} \tag{2.14}$$

Those on the magnetic field $\mathbf{B}$ through a Neumann-type condition following from (2.7) and again (2.9)

$$\mathbf{g}|_{\partial\Omega} = (\mu^{-1} \mathbf{B}|_{\partial\Omega}) \times \mathbf{n} \tag{2.15}$$

2.3 TWO-DIMENSIONAL RESONANT CAVITY

A resonant cavity is a region Ω enclosed by a boundary $\partial\Omega$. The boundary is subdivided into one (or more) inlets Γ_N and a perfect electrically conducting wall $\Gamma_D = \partial\Omega \setminus \Gamma_N$.
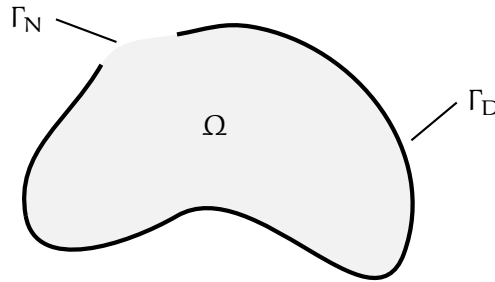

FIGURE 2.1 – 2d resonant cavity.

Suppose the current density $\mathbf{j} \equiv 0$ and orient the coordinate system in such a way that $\mathbf{u} = u_z \mathbf{e}_z$ and $\mathbf{v} = v_z \mathbf{e}_z$. Consequently,

$$(\mu^{-1}\nabla \times \mathbf{u}) \cdot (\nabla \times \mathbf{v}) = (\mu^{-1}\nabla u_z) \cdot (\nabla v_z) \tag{2.16}$$

Use $g_z = (\mathbf{g})_z$ along the boundary Γ_N, to convert (2.13) into the weak formulation for a two-dimensional resonant cavity

$$\int_\Omega (\mu^{-1}\nabla u_z) \cdot (\nabla v_z) - \omega^2 \int_\Omega \epsilon u_z v_z = \int_{\partial\Omega} g_z v_z \tag{2.17}$$

Let $\mathbf{E}$ and $\mathbf{B}$ refer to the electric and magnetic fields inside the cavity. For now, I distinguish two types of boundaries.

For the perfectly conducting boundary, treated in [?], it holds that

$$\mathbf{n} \times \mathbf{E} = 0, \quad \text{on } \Gamma_D \tag{2.18}$$

For the boundaries in a two-dimensional resonant cavity (see Figure 2.1), this only holds true if $E_z = 0$, which translates to the Dirichlet boundary condition $\mathbf{u}|_{\Gamma_D} = 0$ in light of (2.14).

For the inlet, it is easiest to enforce the boundary condition through the magnetic field $\mathbf{B}$ (considering $\mathbf{n} = -\mathbf{e}_x$ as depicted in Figure 2.1):

$$g_z = ((\mu^{-1}\mathbf{B}) \times (-\mathbf{e}_x))_z = \mu^{-1}B_x \tag{2.19}$$

2.4 WAVEGUIDE

2.5 IMPERFECT CONDUCTOR

At an imperfect boundary **?**, (2.6), with (2.9)

$$\mathbf{g} = (\mu^{-1}\nabla \times \mathbf{u}) \times \mathbf{n} = i\omega\lambda(\mathbf{n} \times \mathbf{u}) \times \mathbf{n} \tag{2.20}$$

which, supposing that $\mathbf{u} = u_z \mathbf{e}_z$ and only treating a two-dimensional domain, simplifies (using the fact that $\mathbf{n} \perp \mathbf{u}$ and $\|\mathbf{n}\| = 1$, so $(\mathbf{n} \times \mathbf{u}) \times \mathbf{n} = \mathbf{u}$

$$g_z = i\omega\lambda u_z \tag{2.21}$$

Therefore, reuse (2.17) as it is, but split boundary integral term for Neumann and impedance boundary.

3 FINITE ELEMENT APPROXIMATION WITH FEniCS

$a_\omega(u, v) = L(v)$.

In the style of **?**. Problem (2.13) with Ω being a cubic cavity with an inlet on one side and all other sides with $\mu = \epsilon = 0$, $\mathbf{j} = 0$ for simplicity.

Required packages

```
0  import numpy as np
1  import fenics as fen
2  import matplotlib.pyplot as plt
```

Mesh

```
5  nx, ny, nz = 10, 10, 10
6  mesh = fen.UnitCubeMesh(nx, ny, nz)
```

Function space (Nédélec elements of the first kind **?**)

```
9  V = fen.FunctionSpace(mesh, 'N1curl', 1)
```

Inlet (at $x = 0$)

```
12  class Inlet(fen.SubDomain):
13      def inside(self, x, on_boundary):
14          return on_boundary and fen.near(x[0], 0)
```

PEC boundary

```
17  class PECWalls(fen.SubDomain):
18      def inside(self, x, on_boundary):
19          return on_boundary and not Inlet().inside(x, on_boundary)
```

Boundary ids

```
22  boundary_id = fen.MeshFunction('size_t', mesh, mesh.topology().dim()-1)
23  boundary_id.set_all(0)
24  Inlet().mark(boundary_id, 1)
25  PECWalls().mark(boundary_id, 2)
```

Dirichlet boundary (0 for PEC, because Nédélec)

```
28  u_D = fen.Expression(('0.0', '0.0', '0.0'), degree=2)
29  bc = fen.DirichletBC(V, u_D, boundary_id, 2)
```

Neumann boundary (1 for ...)

```
32  g_N = fen.Expression(('0.0', '0.0', '1.0'), degree=2)
33  ds = fen.Measure('ds', subdomain_data=boundary_id)
```

Trial and test functions

```
36  u = fen.TrialFunction(V)
37  v = fen.TestFunction(V)
```

Neumann boundary integral term

```
40  N = fen.assemble(fen.dot(g_N, v) * ds(2))
```

Stiffness matrix

```
43  K = fen.assemble(fen.dot(fen.curl(u), fen.curl(v)) * fen.dx)
44  bc.apply(K)
```

Mass matrix

```
47  M = fen.assemble(fen.dot(u, v) * fen.dx)
48  bc.zero(M)
```

L2 norms

```
51  def L2_norm(u):
52      u_vec = u.vector().get_local()
53      return pow(((M * u_vec) * u_vec).sum(), 0.5)
```

Solution at frequencies

```
56  omegas = np.linspace(6.2, 6.8, 200)
57  norms = []
58  u = fen.Function(V)
59  for omega in omegas:
60      fen.solve(K - omega**2 * M, u.vector(), N)
61      norms.append(L2_norm(u))
```

Plotting the L2-norms

```
64  plt.plot(omegas, norms)
65  plt.yscale('log')
```

4 MINIMAL RATIONAL INTERPOLATION FOR THE TIME-HARMONIC MAXWELL'S EQUATIONS

Let $u : \mathbb{R} \to \mathbb{C}$. Given $u_j = u(\omega_j)$ for $j \in \{1, \dots, S\}$. Want to find a surrogate

$$\tilde{u}(\omega) \approx u(\omega) \tag{4.1}$$

4.1 MOTIVATION

Equations of the type (2.10), in the most simple case (dropping all constants)

$$\nabla \times (\nabla \times \mathbf{u}) - \omega^2 \mathbf{u} = \mathbf{j} \tag{4.2}$$

Writing the double-curl operator in terms of a matrix $\underline{\mathbf{A}}$

$$\mathbf{u} = (\underline{\mathbf{A}} - \omega^2)^{-1} \mathbf{j} \tag{4.3}$$

Eigenvalue decomposition $\underline{\mathbf{A}} = \underline{\mathbf{V}} \, \underline{\mathbf{\Lambda}} \, \underline{\mathbf{V}}^H$ leads us to a form proposed in **?**

$$\mathbf{u} = \underline{\mathbf{V}}(\underline{\mathbf{\Lambda}} - \omega^2 \underline{\mathbf{1}})^{-1} \underline{\mathbf{V}}^H \mathbf{j} = \sum_i \frac{\mathbf{v}_i \mathbf{v}_i^H \mathbf{j}}{\lambda_i - \omega^2} = \sum_i \frac{\mathbf{r}_i}{\lambda_i - \omega^2} \tag{4.4}$$

which follows from the fact that $\underline{\mathbf{\Lambda}}$ is diagonal, hence also $(\underline{\mathbf{\Lambda}} - \omega^2 \underline{\mathbf{1}})^{-1}$. Here, we denoted the diagonal elements of $\underline{\mathbf{\Lambda}}$ with λ_i (the eigenvalues of $\underline{\mathbf{A}}$) and the columns of $\underline{\mathbf{V}}$ with $\mathbf{v}_i$ (the eigenvectors of $\underline{\mathbf{A}}$).

Hence, it would make sense to search for an approximation of the solution $\mathbf{u}$ that is able to "model" the singularities at $\omega^2 = \lambda_i$, e.g. rational polynomials

$$\tilde{u}(\omega) = \frac{P(\omega)}{Q(\omega)} \tag{4.5}$$

[?]

Algorithm 1 Minimal rational interpolation

Require: $\omega_1, \dots, \omega_S$
Require: $U = [u(\omega_1)| \dots |u(\omega_S)]$ ▷ Snapshot matrix
    Compute G with $g_{ij} = \langle u(\omega_i), u(\omega_j) \rangle_M$, $i, j \in \{1, \dots, S\}$ ▷ Gramian matrix
    Compute the singular value decomposition $G = V\Sigma V^H$
    Define $q = V[:, S]$
    Define $\tilde{u}(\omega) = P(\omega)/Q(\omega)$ with $P(\omega) = \sum_{j=1}^{S} \frac{q_j u(\omega_j)}{\omega - \omega_j}$ and $Q(\omega) = \sum_{j=1}^{S} \frac{q_j}{\omega - \omega_j}$

[?]
[?]
Defining

$$\nu_i = (\omega - \omega_i)^{-1} \tag{4.6}$$

and requiring

$$0 = Q(\omega) = \sum_{i=1}^{S} q_i \nu_i(\omega) \tag{4.7}$$

Algorithm 2 Greedy minimal rational interpolation

Require: $\tau > 0$ ▷ Relative L_2-error tolerance
Require: $\Omega_{test} = \{\omega_i\}_{i=1}^M$ ▷ Set of candidate support points
Require: $a_\omega(u,v) = L(v)$ ▷ Finite element formulation of the problem
  Choose $\omega_1, \ldots, \omega_t \in \Omega_{test}$ ▷ Usually the smallest and largest element
  Remove $\omega_1, \ldots, \omega_t$ from Ω_{test}
  Solve $a_{\omega_i}(u_i, v) = L(v)$ for $i \in \{1, \ldots, t\}$
  Build surrogate $\tilde{u}_t = P_t(\omega)/Q_t(\omega)$ using the solutions $u_1, \ldots, u_t$
  while $\Omega_{test} \neq \emptyset$ **do**
    $\omega_{t+1} \leftarrow \text{argmin}_{\omega \in \Omega_{test}} |Q_t(\omega)|$
    Solve $a_{\omega_{t+1}}(u_{t+1}, v) = L(v)$
    Build surrogate $\tilde{u}_{t+1} = P_{t+1}(\omega)/Q_{t+1}(\omega)$ using the solutions $u_1, \ldots, u_{t+1}$
    if $\|u_{t+1}(\omega_{t+1}) - \tilde{u}_{t+1}(\omega_{t+1})\|_M / \|u_{t+1}(\omega_{t+1})\|_M < \tau$ **then return**
    end if
    $t \leftarrow t + 1$
  end while

---

can be equivalently expressed as a generalized eigenvalue problem

$$\underline{\mathbf{A}}\mathbf{u} = \omega \underline{\mathbf{B}}\mathbf{u} \tag{4.8}$$

with

$$\underline{\mathbf{A}} = \begin{pmatrix} 0 & q_1 & q_2 & \cdots & q_S \\ 1 & \omega_1 & & & \\ 1 & & \omega_2 & & \\ \vdots & & & \ddots & \\ 1 & & & & \omega_S \end{pmatrix} \text{ and } \underline{\mathbf{B}} = \begin{pmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ \vdots & & & \ddots & \\ & & & & 1 \end{pmatrix} \tag{4.9}$$

[?]

Algorithm 3 Additive Householder triangularization
___

Require: $U[1\dots s, 1\dots N]$ ▷ Next snapshot matrix
Require: $R[1\dots S, 1\dots S]$ ▷ Previous triangular matrix
Require: $E[1\dots S, 1\dots N]$ ▷ Previous orthonormal matrix
Require: $V[1\dots S, 1\dots N]$ ▷ Previous Householder matrix
    Extend size of R to $(S+s) \times (S+s)$
    Extend E with S orthonormal columns to $(S+s) \times N$
    Extend size of V to $(S+s) \times N$
    for $j = S+1 : S+s$ **do**
        $u = U[j]$
        for $k = 1 : j-1$ **do**
            $u \leftarrow u - 2\langle V[k,:], u\rangle_M V[k,:]$
            $R[k,j] \leftarrow \langle E[k,:], u\rangle_M$
            $u \leftarrow u - R[k,j]E[k,:]$
        end for
        $R[j,j] \leftarrow \|u\|_M$
        $\alpha \leftarrow \langle E[j,:], u\rangle_M$
        if $|\alpha| \neq 0$ **then**
            $E[j,:] \leftarrow E[j,:](-\alpha/|\alpha|)$
        end if
        $V[j,:] \leftarrow R[j,j]E[j,:] - u$
        $V[j,:] \leftarrow V[j,:] - \langle E[S+1:j], V[j,:]\rangle_M E[S+1:j,:]$
        $\sigma \leftarrow \|V[j,:]\|_M$
        if $\sigma \neq 0$ **then**
            $V[j,:] \leftarrow V[j,:]/\sigma$
        else
            $V[j,:] \leftarrow E[j,:]$
        end if
    end for
___

5 EXAMPLES

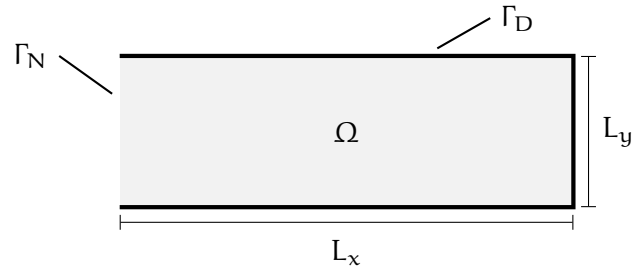## 5.1 TWO-DIMENSIONAL RECTANGULAR CAVITY

FIGURE 5.1 – TODO.

Analytical roots

$$ax = b \tag{5.1}$$

5.2 DUAL MODE CIRCULAR WAVEGUIDE FILTER

FIGURE 5.2 – Dual-mode circular waveguide filter.

5.3 IMPERFECTLY CONDUCTING BOUNDARIES

6 Conclusion and outlook

7 APPENDIX

7.1 DETAILED DERIVATION FOR THE WEAK FORMULATION OF THE TIME-HARMONIC POTENTIAL EQUATION

The goal is to rewrite the curl-integral on the left-hand side of (2.12):

$$\int_\Omega (\nabla \times (\mu^{-1} \nabla \times \mathbf{u})) \cdot \mathbf{v} \tag{7.1}$$

In order to simplify the curls and apply the Gauss theorem, I first show the following vector calculus identity:

Curl product rule

$$(\nabla \times \mathbf{a}) \cdot \mathbf{b} = \nabla \cdot (\mathbf{a} \times \mathbf{b}) + \mathbf{a} \cdot (\nabla \times \mathbf{b}) \tag{7.2}$$

---

where $\mathbf{a}$, $\mathbf{b}$ are vector-value functions. The completely antisymmetric tensor ε_{ijk}, frequently referred to as the Levi-Civita tensor, may be employed to rewrite the components of the curl of a vector-function $\mathbf{a}$ as the sum

$$(\nabla \times \mathbf{a})_k = \sum_i \sum_j \varepsilon_{ijk} \partial_i u_j \tag{7.3}$$

where ∂_i denotes the partial derivative with respect to the i-th coordinate direction. This yields

$$\begin{aligned}
(\nabla \times \mathbf{a}) \cdot \mathbf{b} &= \sum_k (\nabla \times \mathbf{a})_k b_k \\
&= \sum_k (\sum_i \sum_j \varepsilon_{ijk} \partial_i a_j) b_k \\
&= \sum_k \sum_i \sum_j \partial_i (\varepsilon_{ijk} a_j b_k) - \sum_k \sum_i \sum_j a_j (\varepsilon_{ijk} \partial_i b_k) \\
&= \sum_k \sum_i \sum_j \partial_i (\varepsilon_{jki} a_j b_k) - \sum_k \sum_i \sum_j a_j ((-\varepsilon_{ikj}) \partial_i b_k) \\
&= \sum_i \partial_i (\mathbf{a} \times \mathbf{b})_i + \sum_j u_j (\nabla \times \mathbf{b})_j \\
&= \nabla \cdot (\mathbf{a} \times \mathbf{b}) + \mathbf{a} \cdot (\nabla \times \mathbf{b}) \tag{7.4}
\end{aligned}$$

by expressing the scalar product as a component-sum, using the product rule and applying the symmetry and anti-symmetry properties of the Levi-Civita tensor. Now the identity (7.2) to (7.1) together with Gauss' theorem gives

$$\begin{aligned}
\int_\Omega (\nabla \times (\mu^{-1} \nabla \times \mathbf{u})) \cdot \mathbf{v} &= \int_\Omega \nabla \cdot ((\mu^{-1} \nabla \times \mathbf{u}) \times \mathbf{v}) + \int_\Omega (\mu^{-1} \nabla \times \mathbf{u}) \cdot (\nabla \times \mathbf{v}) \\
&= \int_{\partial\Omega} ((\mu^{-1} \nabla \times \mathbf{u}) \times \mathbf{v}) \cdot \mathbf{n} + \int_\Omega (\mu^{-1} \nabla \times \mathbf{u}) \cdot (\nabla \times \mathbf{v})
\end{aligned}$$
$$\tag{7.5}$$

For later convenience, the boundary integral can further be simplified using the

Commutative behavior of the scalar triple product

$$(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = -(\mathbf{a} \times \mathbf{c}) \cdot \mathbf{b} \tag{7.6}$$

This identity follows immediately from a small manipulation with the Levi-Civita tensor:

$$
\begin{aligned}
(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} &= \sum_k \left(\sum_i \sum_j \varepsilon_{ijk} a_i b_j \right) c_k \\
&= \sum_j \left(\sum_i \sum_k (-\varepsilon_{ikj}) a_i c_k \right) b_j \\
&= -(\mathbf{a} \times \mathbf{c}) \cdot \mathbf{b} \tag{7.7}
\end{aligned}
$$

The boundary integral becomes

$$\int_{\partial\Omega} ((\mu^{-1}\nabla \times \mathbf{u}) \times \mathbf{v}) \cdot \mathbf{n} = -\int_{\partial\Omega} ((\mu^{-1}\nabla \times \mathbf{u}) \times \mathbf{n}) \cdot \mathbf{v} \tag{7.8}$$

This concludes the short derivation, because now (7.1) may be rewritten as

$$-\int_{\partial\Omega} ((\mu^{-1}\nabla \times \mathbf{u}) \times \mathbf{v}) \cdot \mathbf{n} + \int_{\Omega} (\mu^{-1}\nabla \times \mathbf{u}) \cdot (\nabla \times \mathbf{v}) \tag{7.9}$$