

EPFL

PROJECT CSE I

Notes

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1 FINITE ELEMENT METHOD

1.1 THE GENERAL APPROACH

Summarizes Chapter 1 in Quarteroni: Introduction to Finite Elements Method

Usually, the problems may be expressed in a simple equation

$$\begin{cases} Lu = f & \text{in } \Omega \\ u = u_D & \text{on } \partial\Omega \end{cases} \quad (1.1)$$

where L denotes a linear differential operator (e.g. $-\Delta$ in the Poisson equation), u the solution to be found, and f is a source term independent of u . Some boundary condition u_D is imposed on the solution u .

However, equation (1.1) usually does not allow all physically significant solutions (particularly non-differentiable ones). Therefore, we convert the problem to a weak form. This is achieved by multiplying (1.1) with a test function $v \in V$, and integrating over the whole domain Ω :

$$\int_{\Omega} (Lu)v = \int_{\Omega} fv, \quad \forall v \in V \quad (1.2)$$

Usually, integration by parts allows us to “transfer” the derivatives from the Lu term to the test function v , such that the order (with respect to the derivatives taken) is more “balanced” between the two terms. As a trade-off, a boundary term appears and needs to be eliminated to facilitate the finite element solution. This term can often be eliminated by restricting ourselves to test functions from a subspace $V' \subset V$. The weak problem then reads

$$\int_{\Omega} (L_u u)(L_v v) = \int_{\Omega} fv, \quad \forall v \in V' \quad (1.3)$$

with a linear differential operator L_u acts on the solution u , and a linear differential operator L_v , appearing due to the integration by parts, acts on the test function v . For simplicity, we refer to the left-hand side as the bilinear form

$$a(u, v) = \int_{\Omega} (L_u u)(L_v v) \quad (1.4)$$

and the right-hand side as the linear form

$$F(v) = \int_{\Omega} fv \quad (1.5)$$

To solve (1.3), we prefer to look for approximate solutions u_h in a finite dimensional space V_h with $\dim(V_h) = N_h$ (what role does V'_h , the space wherein v lies to satisfy the boundary conditions, play? as far as I can tell V'_h is the subspace of V_h , in which all functions vanish at the boundary where u is known). Choosing a basis $\{\varphi_i\}_{i \leq N_h}$ then allows us to represent the approximate solution as

$$u_h = \sum_{j \leq N_h} u_j \varphi_j \quad (1.6)$$

for some coefficients u_i that need to be determined. We thus see, that (1.3) turns into a linear system, since we only need to test the equality for the basis elements φ_i of V_h :

$$\sum_{j=1}^{N_h} u_j a(\varphi_j, \varphi_i) = F(\varphi_i), \quad i \in \{1, \dots, N_h\} \quad (1.7)$$

If we write $A_{ij} = a(\varphi_j, \varphi_i)$ and $\mathbf{F} = (F(\varphi_1), \dots, F(\varphi_{N_h}))^T$, we have reduced the problem to finding $\mathbf{u} = (u_1, \dots, u_{N_h})^T$, such that

$$\mathbb{A}\mathbf{u} = \mathbf{F} \quad (1.8)$$

and have identified an approximate solution to (1.1) as $u \approx u_h = \sum_{j \leq N_h} u_j \varphi_j$.

Choosing the space V_h is fundamental to have an accurate method that gives a good approximation u_h of u . Furthermore, the choice of basis $\{\varphi_i\}_{i \leq N_h}$ influences how \mathbb{A} ends up looking. Of particular interest are bases for which $a(\varphi_j, \varphi_i)$ vanishes for almost all i and j , thus yielding a sparse matrix \mathbb{A} . The choice of basis also controls the conditioning of \mathbb{A} (need to find an example to illustrate this).

1.2 THE POISSON EQUATION

Taken from FEniCS manual (too lazy for bibtex...)

We aim to solve an equation of the form

$$-\Delta u(\mathbf{x}) = f(\mathbf{x}) \quad (1.9)$$

on a domain $\mathbf{x} \in \Omega$, with a solution $u(\mathbf{x})$ that satisfies a certain boundary condition $u(\mathbf{x}) = u_d(\mathbf{x})$ for all $\mathbf{x} \in \partial\Omega$ that lie on the border of Ω .

To do this, we first convert this equation to its weak form by multiplying both sides with an arbitrary test function $v(\mathbf{x})$, which vanishes on the border (i.e. $v(\mathbf{x}) = 0, \forall \mathbf{x} \in \partial\Omega$), and by then integrating over all of Ω :

$$-\int_{\Omega} \Delta u(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} = \int_{\Omega} f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} \quad (1.10)$$

We may now rearrange the gradient product rule $\nabla(ab) = (\nabla a)b + a(\nabla b)$ and Gauss' theorem (as long as $v(\mathbf{x})$ is differentiable in a neighborhood of Ω) combined with the fact that $v(\mathbf{x})$ vanishes on $\partial\Omega$ to convert the right-hand side to

$$\begin{aligned} -\int_{\Omega} \Delta u(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} &= -\int_{\Omega} \nabla(\nabla u(\mathbf{x}) v(\mathbf{x})) d\mathbf{x} + \int_{\Omega} \nabla u(\mathbf{x}) \nabla v(\mathbf{x}) d\mathbf{x} \\ &= -\int_{\partial\Omega} \nabla u(\mathbf{x}) v(\mathbf{x}) d\boldsymbol{\omega} + \int_{\Omega} \nabla u(\mathbf{x}) \nabla v(\mathbf{x}) d\mathbf{x} \\ &= \int_{\Omega} \nabla u(\mathbf{x}) \nabla v(\mathbf{x}) d\mathbf{x} \end{aligned} \quad (1.11)$$

Consequently, the weak formulation of the problem is to find $u(\mathbf{x})$, such that for arbitrary $v(\mathbf{x})$, we have

$$\int_{\Omega} \nabla u(\mathbf{x}) \nabla v(\mathbf{x}) d\mathbf{x} = \int_{\Omega} f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} \quad (1.12)$$

To simplify and generalize the notation, we may use the linear form $L : V \rightarrow \mathbb{R}$ as

$$L(v) = \int_{\Omega} f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} \quad (1.13)$$

and also the bilinear form $a : V \times V \rightarrow \mathbb{R}$

$$a(u, v) = \int_{\Omega} \nabla u(\mathbf{x}) \nabla v(\mathbf{x}) d\mathbf{x} \quad (1.14)$$

1.3 EXAMPLE: ONE DIMENSIONAL POISSON EQUATION

Initial idea taken from Wikipedia article about FEM.

To illustrate the choice of basis functions, we will now consider the simple one dimensional case $\Omega = [a, b]$, such that the weak formulation of the problem turns into

$$\int_a^b u'(x) v'(x) dx = \int_a^b f(x) v(x) dx \quad (1.15)$$

We now subdivide the domain $[a, b]$ into M subintervals, each of length $h = (b - a)/M$, with nodes at $x_k = a + hk, k \in \{0, 1, \dots, M\}$. We proceed to choose as the basis functions the class of the piecewise linear Lagrange interpolating polynomials on $[x_k, x_{k+1}], k \in \{0, 1, \dots, M\}$, defined as

$$v_k(x) = \frac{x - x_{k-1}}{x_k - x_{k-1}} \mathbf{1}_{\{x \in [x_{k-1}, x_k]\}} + \frac{x_{k+1} - x}{x_{k+1} - x_k} \mathbf{1}_{\{x \in [x_k, x_{k+1}]\}} \quad (1.16)$$

If we now interpolate $f(x)$ and $u(x)$ as piecewise linear Lagrange polynomials, we get the representation

$$\begin{aligned} f(x) &\approx \sum_{i=1}^M f(x_{i-1}) \frac{x - x_i}{x_{i-1} - x_i} + f(x_i) \frac{x - x_{i-1}}{x_i - x_{i-1}} \\ &= \sum_{i=1}^{M-1} f(x_i) v_i(x) \end{aligned} \quad (1.17)$$

and analogously

$$u(x) = \sum_{i=1}^{M-1} u(x_i) v_i(x) \quad (1.18)$$

We now restricted ourselves to the discrete variational formulation of the problem

$$\sum_{i=1}^{M-1} u(x_i) \int_a^b v_i'(x) v_j'(x) dx = \sum_{i=1}^{M-1} f(x_i) \int_a^b v_i(x) v_j(x) dx \quad (1.19)$$

which needs to be satisfied for all $j \in \{0, 1, \dots, M\}$.

This equation can be rewritten in terms of two matrices \mathbf{K} and \mathbf{L} which we define as

$$K_{ij} = \int_a^b v_i(x) v_j(x) dx \quad (1.20)$$

$$L_{ij} = \int_a^b v_i'(x) v_j'(x) dx \quad (1.21)$$

such that we get

$$\sum_{i=1}^{M-1} u(x_i) L_{ij} = \sum_{i=1}^{M-1} f(x_i) K_{ij} \quad (1.22)$$

Notice, that we only need the entries K_{ij} and L_{ij} with $i \in \{1, 2, \dots, M-1\}$, since we already know the boundary conditions of $u(x)$ at $x = x_0$ and $x = x_M$.

We realize, that the L_2 inner product of $v_i(x)$ with $v_j(x)$ (and consequently also the one of $v_i'(x)$ with $v_j'(x)$) is zero for all $|i - j| > 1$, hence, we distinguish two different cases.

1. $i = j$: Here, the inner product turns out to be

$$\begin{aligned} \int_a^b v_i(x) v_i(x) dx &= \int_a^b \left(\frac{x - x_{i-1}}{x_i - x_{i-1}} \right)^2 \mathbf{1}_{\{x \in [x_{i-1}, x_i]\}} + \left(\frac{x_{i+1} - x}{x_{i+1} - x_i} \right)^2 \mathbf{1}_{\{x \in [x_i, x_{i+1}]\}} dx \\ &= 2 \int_{x_{i-1}}^{x_i} \left(\frac{x - x_{i-1}}{x_i - x_{i-1}} \right)^2 dx \\ &= \frac{2}{h^2} \int_{x_{i-1} - x_{i-1}}^{x_i - x_{i-1}} u^2 du \\ &= \frac{2}{h^2} \frac{1}{3} h^3 \\ &= \frac{2h}{3} \end{aligned} \quad (1.23)$$

and for the derivatives it is

$$\begin{aligned}
\int_a^b v_i'(x) v_i'(x) dx &= \int_a^b \left(\frac{1}{x_i - x_{i-1}} \right)^2 \mathbf{1}_{\{x \in [x_{i-1}, x_i]\}} + \left(\frac{-1}{x_{i+1} - x_i} \right)^2 \mathbf{1}_{\{x \in [x_i, x_{i+1}]\}} dx \\
&= 2 \int_{x_{i-1}}^{x_i} \left(\frac{1}{x_i - x_{i-1}} \right)^2 dx \\
&= \frac{2}{h^2} \int_0^h 1 du \\
&= \frac{2}{h}
\end{aligned} \tag{1.24}$$

2. $|i - j| = 1$: Here, we can limit ourselves to the case where $j = i + 1$, since the other case is fully symmetric. We calculate

$$\begin{aligned}
\int_a^b v_i(x) v_{i+1}(x) dx &= \int_a^b \frac{x_{i+1} - x}{x_{i+1} - x_i} \frac{x - x_i}{x_{i+1} - x_i} \mathbf{1}_{\{x \in [x_i, x_{i+1}]\}} dx \\
&= \int_{x_i}^{x_{i+1}} \frac{x_{i+1} - x}{x_{i+1} - x_i} \frac{x - x_i}{x_{i+1} - x_i} dx \\
&= \frac{1}{h^2} \int_{x_i - x_i}^{x_{i+1} - x_i} (x_{i+1} - x_i - u) u du \\
&= \frac{1}{h^2} \int_0^h (h - u) u du \\
&= \frac{1}{h^2} \left(\frac{h^3}{2} - \frac{h^3}{3} \right) \\
&= \frac{h}{6}
\end{aligned} \tag{1.25}$$

and for the derivative it is

$$\begin{aligned}
\int_a^b v_i'(x) v_{i+1}'(x) dx &= \int_a^b \frac{-1}{x_{i+1} - x_i} \frac{1}{x_{i+1} - x_i} \mathbf{1}_{\{x \in [x_i, x_{i+1}]\}} dx \\
&= -\frac{1}{h^2} \int_{x_i}^{x_{i+1}} 1 dx \\
&= -\frac{1}{h}
\end{aligned} \tag{1.26}$$

Now, using the previously defined matrices \mathbf{K}_{ij} and \mathbf{L}_{ij} , we get the matrix equation

$$\mathbf{L} \mathbf{u} = \mathbf{K} \mathbf{f} \tag{1.27}$$

with

$$\mathbf{u} = (u_0, u(x_1), \dots, u_M)^T \quad (1.28)$$

$$\mathbf{f} = (f(x_0), f(x_1), \dots, f(x_M))^T \quad (1.29)$$

$$\mathbf{L} = \begin{pmatrix} 1 & & & & \\ \frac{2}{h} & -\frac{1}{h} & & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & -\frac{1}{h} & \frac{2}{h} & \ddots & \\ & & -\frac{1}{h} & \ddots & -\frac{1}{h} \\ & & & \ddots & \frac{2}{h} \\ & & & & 1 \end{pmatrix} \quad (1.30)$$

$$\mathbf{K} = \begin{pmatrix} \frac{u_0}{f(x_0)} & & & & \\ \frac{2h}{3} & \frac{h}{6} & & & \\ \frac{h}{6} & \frac{2h}{3} & \frac{h}{6} & & \\ & \frac{h}{6} & \frac{2h}{3} & \ddots & \\ & & \frac{h}{6} & \ddots & \frac{h}{6} \\ & & & \ddots & \frac{2h}{3} \\ & & & & \frac{u_M}{f(x_M)} \end{pmatrix} \quad (1.31)$$

$$(1.32)$$

Here, we have adjusted the first rows in \mathbf{L} and \mathbf{K} , such that the boundary conditions are necessarily satisfied. To obtain the finite element solution, we simply solve this linear system.

2 MAXWELL'S EQUATIONS

Let $\mathbf{E} = (E_1, E_2, E_3)^T$ denote the electric field, $\mathbf{B} = (B_1, B_2, B_3)^T$ the magnetic field strength, and $\mathbf{j} = (j_1, j_2, j_3)^T$ the electric current density. We suppose Maxwell's equations hold:

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

$$\nabla \cdot \mathbf{B} = 0 \quad (2.2)$$

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B} \quad (2.3)$$

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

2.1 VECTOR POTENTIAL FORMULATION

We can therefore use (2.2) to write $\mathbf{B} = \nabla \times \mathbf{A}$ for some vector potential \mathbf{A} . Furthermore, we can identify from (2.3) that $\mathbf{E} = -\nabla \phi - \partial_t \mathbf{A}$ can be written for some scalar potential ϕ .

The physical quantities \mathbf{E} and \mathbf{B} remain unchanged if we transform $\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla\psi$ and $\phi \rightarrow \phi' = \phi - \partial_t\psi$ (gauge transformations), as can be explicitly verified by plugging these transformed potentials into the definitions of \mathbf{E} and \mathbf{B} . Choosing as the gauge field as

$$\psi = \int_0^t \phi dt' \quad (2.5)$$

we see that $\phi' = \phi - \partial_t \int_0^t \phi dt' = \phi - \phi = 0$. Hence, if we now express the electric field \mathbf{E} in terms of these transformed potentials, we realize that $\mathbf{E} = -\nabla\phi' - \partial_t\mathbf{A}' = -\partial_t\mathbf{A}'$ because we have transformed ϕ exactly in such a way, which makes ϕ' vanish (not symbolically, but due to its actual value being zero). As for the magnetic field \mathbf{B} , we have $\mathbf{B} = \nabla \times \mathbf{A}'$.

Plugging these identities into (2.4), and for simplicity replacing the symbol \mathbf{A}' with \mathbf{A} again, we get

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{A}) = -\epsilon \partial_t^2 \mathbf{A} + \mathbf{j} \quad (2.6)$$

We may want to introduce a harmonic time dependence of \mathbf{A} and \mathbf{j} with frequencies ω , such that $\mathbf{A}(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}) \exp(i\omega t)$ and $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}(\mathbf{x}) \exp(i\omega t)$. Plugging this into (2.6) yields us

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{A}) - \epsilon \omega^2 \mathbf{A} = \mathbf{j} \quad (2.7)$$

We reduce this equation to its weak formulation, by multiplying it with a vector-valued function $\mathbf{v} \in H_{\text{curl}}(\Omega)$, where we denoted

$$H_{\text{curl}}(\Omega) = \{\mathbf{u} : \Omega \rightarrow \mathbb{C}, \text{ such that } \mathbf{u} \in L^2(\mathbb{C})^3, \nabla \times \mathbf{u} \in L^2(\mathbb{C})^3\} \quad (2.8)$$

and by integrating over all of Ω :

$$\int_{\Omega} (\nabla \times (\mu^{-1} \nabla \times \mathbf{A})) \cdot \mathbf{v} - \epsilon \omega^2 \int_{\Omega} \mathbf{A} \cdot \mathbf{v} = \int_{\Omega} \mathbf{j} \cdot \mathbf{v} \quad (2.9)$$

To further simplify this expression, we will derive an identity for the scalar product of a vector-valued function \mathbf{v} with the curl of a vector-valued function \mathbf{u} . For this, we use the completely antisymmetric tensor ε_{ijk} (frequently referred to as the Levi-Civita tensor), to rewrite the k -th component of the curl as

$$(\nabla \times \mathbf{u})_k = \sum_i \sum_j \varepsilon_{ijk} \partial_i u_j \quad (2.10)$$

where ∂_i denotes the partial derivative with respect to the i -th coordinate direction. Rewriting the scalar product as a sum and identifying $\mathbf{u} = \mu^{-1} \nabla \times \mathbf{A}$, we apply the product rule to get

$$\begin{aligned}
(\nabla \times \mathbf{u}) \cdot \mathbf{v} &= \sum_k (\nabla \times \mathbf{u})_k v_k \\
&= \sum_k \left(\sum_i \sum_j \varepsilon_{ijk} \partial_i u_j \right) v_k \\
&= \sum_k \sum_i \sum_j \partial_i (\varepsilon_{ijk} u_j v_k) - \sum_k \sum_i \sum_j u_j (\varepsilon_{ijk} \partial_i v_k) \\
&= \sum_k \sum_i \sum_j \partial_i (\varepsilon_{jki} u_j v_k) - \sum_k \sum_i \sum_j u_j ((-\varepsilon_{ikj}) \partial_i v_k) \\
&= \sum_i \partial_i (\mathbf{u} \times \mathbf{v})_i + \sum_j u_j (\nabla \times \mathbf{v})_j \\
&= \nabla \cdot (\mathbf{u} \times \mathbf{v}) + \mathbf{u} \cdot (\nabla \times \mathbf{v})
\end{aligned} \tag{2.11}$$

Consequently, we may rewrite the double curl term as

$$\begin{aligned}
\int_{\Omega} (\nabla \times (\mu^{-1} \nabla \times \mathbf{A})) \cdot \mathbf{v} &= \int_{\Omega} \nabla \cdot ((\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{v}) + \int_{\Omega} (\mu^{-1} \nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v}) \\
&= \int_{\partial\Omega} ((\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{v}) \cdot \mathbf{n} + \int_{\Omega} (\mu^{-1} \nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v})
\end{aligned} \tag{2.12}$$

Again denoting $\mathbf{u} = \mu^{-1} \nabla \times \mathbf{A}$, we can rearrange

$$\begin{aligned}
(\mathbf{u} \times \mathbf{v}) \cdot \mathbf{n} &= \sum_k \left(\sum_i \sum_j \varepsilon_{ijk} u_i v_j \right) n_k \\
&= \sum_j \left(\sum_i \sum_k (-\varepsilon_{ikj}) u_i n_k \right) v_j \\
&= -(\mathbf{u} \times \mathbf{n}) \cdot \mathbf{v}
\end{aligned} \tag{2.13}$$

and therefore have

$$\int_{\partial\Omega} ((\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{v}) \cdot \mathbf{n} = - \int_{\partial\Omega} ((\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{n}) \cdot \mathbf{v} \tag{2.14}$$

We can finally identify the weak form of the problem as

$$\int_{\Omega} (\mu^{-1} \nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v}) - \epsilon \omega^2 \int_{\Omega} \mathbf{A} \cdot \mathbf{v} = \int_{\Omega} \mathbf{j} \cdot \mathbf{v} + \underbrace{\int_{\partial\Omega} ((\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{n}) \cdot \mathbf{v}}_{\text{boundary integral term}} \tag{2.15}$$

where \mathbf{n} denotes the normal vector to $\partial\Omega$. Notice how we placed the boundary integral term on the right hand side, since along the border $\partial\Omega$ we usually either know $\nabla \times \mathbf{A} = \mathbf{B} = \mathbf{B}_D$ (or even only $\mathbf{B} \times \mathbf{n}$) as the Neumann boundary condition or $-i\omega \mathbf{A} = \mathbf{E}_D$ as the Dirichlet boundary condition.

2.2 ELECTRIC FIELD FORMULATION

Multiplying both sides of (2.3) with μ^{-1} and taking the curl allows us to substitute (2.4) in, such that we get

$$\begin{aligned}\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) &= -\partial_t (\nabla \times (\mu^{-1} \mathbf{B})) \\ &= -\partial_t (\partial_t (\epsilon \mathbf{E}) + \mathbf{j}) \\ &= -\partial_t^2 (\epsilon \mathbf{E}) + \partial_t \mathbf{j}\end{aligned}\tag{2.16}$$

Introducing a harmonic time dependence of \mathbf{E} and \mathbf{j} with frequencies ω , such that $\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}) \exp(i\omega t)$ and $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}(\mathbf{x}) \exp(i\omega t)$, we obtain

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} = i\omega \mathbf{j}\tag{2.17}$$

The i on the right-hand side is giving me (and most likely FEniCS too) a major headache, hence why I will try my luck with finding a formulation involving \mathbf{B} in the next section.

2.3 MAGNETIC FIELD FORMULATION

Multiply both sides of (2.4) with ϵ^{-1} and take the curl to obtain, with the help of (2.3), the expression

$$\begin{aligned}\nabla \times (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) &= \nabla \times (\partial_t \mathbf{E} + \epsilon^{-1} \mathbf{j}) \\ &= \partial_t (\nabla \times \mathbf{E}) + \nabla \times (\epsilon^{-1} \mathbf{j}) \\ &= -\partial_t^2 \mathbf{B} + \nabla \times (\epsilon^{-1} \mathbf{j})\end{aligned}\tag{2.18}$$

Introducing a harmonic time dependence of \mathbf{B} and \mathbf{j} with frequencies ω , such that $\mathbf{B}(\mathbf{x}, t) = \mathbf{B}(\mathbf{x}) \exp(i\omega t)$ and $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}(\mathbf{x}) \exp(i\omega t)$, we obtain

$$\nabla \times (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) - \omega^2 \mathbf{B} = \nabla \times (\epsilon^{-1} \mathbf{j})\tag{2.19}$$

Converting this equation to its weak form by multiplying both sides with a vector valued function $\mathbf{v} \in H_{\text{curl}}(\Omega)$ and integrating over all of Ω yields

$$\int_{\Omega} (\nabla \times (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B}))) \cdot \mathbf{v} - \omega^2 \int_{\Omega} \mathbf{B} \cdot \mathbf{v} = \int_{\Omega} (\nabla \times (\epsilon^{-1} \mathbf{j})) \cdot \mathbf{v}\tag{2.20}$$

Using the above derived identity

$$(\nabla \times \mathbf{u}) \cdot \mathbf{v} = \nabla \cdot (\mathbf{u} \times \mathbf{v}) + \mathbf{u} \cdot (\nabla \times \mathbf{v})\tag{2.21}$$

we may write using Gauss' theorem

$$\begin{aligned}
\int_{\Omega} (\nabla \times (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B}))) \cdot \mathbf{v} &= \int_{\Omega} \nabla \cdot ((\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) \times \mathbf{v}) \\
&+ \int_{\Omega} (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) \cdot (\nabla \times \mathbf{v}) \\
&= \int_{\partial\Omega} ((\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) \times \mathbf{v}) \cdot \mathbf{n} \\
&+ \int_{\Omega} (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) \cdot (\nabla \times \mathbf{v})
\end{aligned} \tag{2.22}$$

and

$$\begin{aligned}
\int_{\Omega} (\nabla \times (\epsilon^{-1} \mathbf{j})) \cdot \mathbf{v} &= \int_{\Omega} \nabla \cdot ((\epsilon^{-1} \mathbf{j}) \times \mathbf{v}) + \int_{\Omega} (\epsilon^{-1} \mathbf{j}) \cdot (\nabla \times \mathbf{v}) \\
&= \int_{\partial\Omega} ((\epsilon^{-1} \mathbf{j}) \times \mathbf{v}) \cdot \mathbf{n} + \int_{\Omega} (\epsilon^{-1} \mathbf{j}) \cdot (\nabla \times \mathbf{v})
\end{aligned} \tag{2.23}$$

Since $(\mathbf{u} \times \mathbf{v}) \cdot \mathbf{n} = \mathbf{u} \cdot (\mathbf{v} \times \mathbf{n})$ (as was shown above), the boundary integrals vanish if we have

$$\mathbf{v} \times \mathbf{n} = 0, \text{ on } \partial\Omega \tag{2.24}$$

In that case, we end up with the following (simplified) weak form

$$\int_{\Omega} (\epsilon^{-1} \nabla \times (\mu^{-1} \mathbf{B})) \cdot (\nabla \times \mathbf{v}) - \omega^2 \int_{\Omega} \mathbf{B} \cdot \mathbf{v} = \int_{\Omega} (\epsilon^{-1} \mathbf{j}) \cdot (\nabla \times \mathbf{v}) \tag{2.25}$$

3 WAVEGUIDES

In Section 2 we have derived the weak form of the time-harmonic Maxwell equation for the vector potential \mathbf{A} . Let us now apply it to a small collection of illustrative examples.

3.1 TWO-DIMENSIONAL PERFECTLY CONDUCTING WAVEGUIDE

Consider a two-dimensional rectangular box of length l and width w enclosing a vacuum (depicted in Figure 3.1).

Defining $\mathbf{g} = (\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{n} = \mu^{-1} \mathbf{B} \times \mathbf{n}$ on the boundary $\partial\Omega$ and setting $\mathbf{j} = 0$, we can convert (2.15) into

$$\int_{\Omega} (\mu^{-1} \nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v}) - \epsilon \omega^2 \int_{\Omega} \mathbf{A} \cdot \mathbf{v} = \int_{\partial\Omega} \mathbf{g} \cdot \mathbf{v} \tag{3.1}$$

If we only consider $\mathbf{A} = (0, 0, A_z)^T$ and $\mathbf{v} = (0, 0, v_z)^T$, the two curls can be rewritten as the dot product of two gradients, since

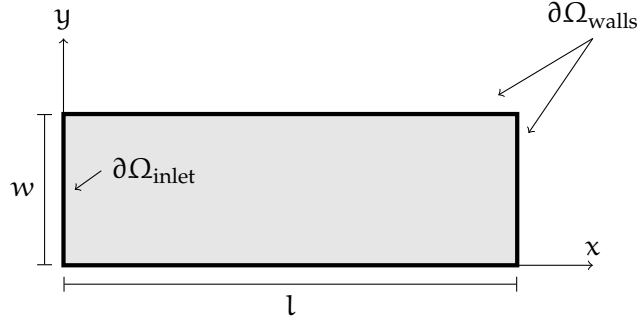


FIGURE 3.1 – Waveguide

$$\nabla \times \mathbf{A} = (\partial_y A_z, -\partial_x A_z, 0) \quad (3.2)$$

and similarly for $\nabla \times \mathbf{v}$, such that

$$(\nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v}) = (\nabla A_z) \cdot (\nabla v_z) \quad (3.3)$$

We thus end up with the following simplified weak form of the problem

$$\int_{\Omega} (\mu^{-1} \nabla A_z) \cdot (\nabla v_z) - \epsilon \omega^2 \int_{\Omega} A_z v_z = \int_{\partial\Omega} g_z v_z \quad (3.4)$$

3.1.1 CONSTANT FIELD (OLD AND FLAWED VERSION)

Suppose we observe an electromagnetic wave at frequency ω and with the magnetic field of strength B_0 aligned with the y -direction incident on the waveguide at $x = 0$. Symbolically, we thus have $\mathbf{B}(t) = (0, B_0, 0)^T \exp(i\omega t)$ at $x = 0$ for $y \in [0, w]$.

From this, we can calculate the function g_z on the “inlet” boundary to be (knowing that we have already taken account of the harmonic time-dependence of \mathbf{B} in deriving (3.4))

$$\mathbf{g}_{\text{inlet}} = \mu^{-1} \mathbf{B} \times \mathbf{n} = \mu^{-1} B_0 (\mathbf{e}_y \times \mathbf{e}_x) = -\mu^{-1} B_0 \mathbf{e}_z \quad (3.5)$$

Referring to Section 3.2, we know that for perfectly conducting walls the magnetic field \mathbf{B} in our case (with walls on top and bottom) must satisfy

$$\mathbf{n} \cdot \mathbf{B} = 0 \implies B_y = 0 \quad (3.6)$$

This, in turn, means that **different orientation of \mathbf{n} for bottom wall!**

$$\mathbf{g}_{\text{walls}} = \mu^{-1} \mathbf{B} \times \mathbf{n} = \mu^{-1} B_x (\mathbf{e}_x \times \mathbf{e}_y) = \mu^{-1} B_x \mathbf{e}_z \quad (3.7)$$

Therefore, in general, we have (assuming all other walls to be perfect conductors)

$$g_z = \begin{cases} -\mu^{-1} B_0, & \text{at the inlet} \\ 0 & \text{at the walls} \end{cases} \quad (3.8)$$

Ok, this is not entirely right, because this implicitly assumes that $B_x = 0$ at the walls (which would be correct for purely transversal waves in the waveguide, but not in general). Will somehow have to find a way to correct this later.

Alternatively, the problem can be equivalently solved using Dirichlet instead of Neumann boundary conditions (mental note: the function \mathbf{g} encodes a Neumann boundary condition, since it contains $\nabla \times \mathbf{A}$, hence partial derivatives of \mathbf{A}). Here, we no longer have a right-hand side term in (3.4), because for Dirichlet boundary conditions we **require the test functions \mathbf{v} to vanish wherever we already know the exact value of \mathbf{A} (i.e. on the boundary $\partial\Omega$)**.

Because we only consider time-harmonic electric fields $\mathbf{A} = \mathbf{A}(\mathbf{x}) \exp(i\omega t)$, and the relation $\mathbf{E} = -\partial_t \mathbf{A} = -i\omega \mathbf{A}$ holds, we should be able to impose boundary conditions on \mathbf{A} based on an unput field \mathbf{E} . Again making use of the two-dimensionality of the problem, we allow an input field $\mathbf{E}(t) = (0, 0, E_0)^T \sin(\omega t)$ (because I currently do not feel too comfortable dealing with complex numbers in FEniCS), and have to therefore impose a boundary condition $A_z = -E_0/\omega$ at $x = 0$ for $y \in [0, w]$.

3.1.2 CONSTANT FIELD (NEW VERSION)

We consider two types of boundaries. An inlet $\partial\Omega_{\text{inlet}}$ at $x = 0$ (left boundary) and perfectly conducting walls $\partial\Omega_{\text{walls}}$ at all other boundaries.

Suppose we observe an electromagnetic wave at frequency ω and with the magnetic field of strength B_0 aligned with the y -direction incident on the waveguide at $x = 0$. Symbolically, we thus have $\mathbf{B}(t) = (0, B_0, 0)^T \exp(i\omega t)$ at $\partial\Omega_{\text{inlet}}$.

From this, we can calculate the function g_z on the inlet boundary $\partial\Omega_{\text{inlet}}$ to be (knowing that we have already taken account of the harmonic time-dependence of \mathbf{B} in deriving (3.4))

$$g_z = (\mu^{-1} \mathbf{B} \times \mathbf{n})_z = \mu^{-1} B_0 (\mathbf{e}_y \times (-\mathbf{e}_x))_z = \mu^{-1} B_0, \text{ on } \partial\Omega_{\text{inlet}} \quad (3.9)$$

For the other boundaries $\partial\Omega_{\text{walls}}$, we preferably use the boundary conditions on \mathbf{A} derived in Section 3.2. Particularly the one following from looking at \mathbf{E} , i.e.

$$\mathbf{n} \times \mathbf{A} = 0 \quad (3.10)$$

is useful, since it tells us that $\mathbf{A} = (0, 0, A_z)^T = 0 \implies A_z = 0$ on $\partial\Omega_{\text{walls}}$ (because \mathbf{n} points either in the x - or y -direction, so the curl of \mathbf{n} with \mathbf{A} will always explicitly contain A_z in one of its components that are required to vanish).

TABLE 3.1 – Boundary conditions for a waveguide with a field $\mathbf{B}(t) = (0, B_y, 0)^T \exp(i\omega t)$ incident on an inlet $\partial\Omega_{\text{inlet}}$ and perfectly conducting walls $\partial\Omega_{\text{walls}}$ otherwise.

Type	$\partial\Omega_{\text{inlet}}$	$\partial\Omega_{\text{walls}}$
Dirichlet	$A_z = -\frac{1}{i\omega} E_z$	$A_z = 0$
Neumann	$g_z = \mu^{-1} B_y$	$g_z = \pm \mu^{-1} B_x$ ($-\mu^{-1} B_y$ for outlet)

Only the combination of Neumann boundary conditions for $\partial\Omega_{\text{inlet}}$ and Dirichlet boundary conditions for $\partial\Omega_{\text{walls}}$ seem to be practical for now, since we do not have to deal with complex numbers, and do not have to know the B_x component at the walls (since setting it to zero is only really viable for \mathbf{B} -fields that exclusively oscillate in the y -direction).

(Remark: The Neumann boundary condition for $\partial\Omega$ may be compactly summarized as $g_z = \mu^{-1}(-B_y, B_x, 0)^T \cdot \mathbf{n} = (\mathbf{e}_z \times \mu^{-1}\mathbf{B}) \cdot \mathbf{n}$.)

3.2 BOUNDARY CONDITIONS

Monk2003, Page 8

At an interface $\partial\Omega$, separating the waveguide Ω from its environment, the electric field \mathbf{E} and the magnetic field \mathbf{B} satisfy the following boundary conditions:

$$\mathbf{n} \times (\mathbf{E} - \mathbf{E}_{\text{ext}}) = 0, \text{ on } \partial\Omega \quad (3.11)$$

$$\mathbf{n} \cdot (\mathbf{B} - \mathbf{B}_{\text{ext}}) = 0, \text{ on } \partial\Omega \quad (3.12)$$

<https://farside.ph.utexas.edu/teaching/jk1/Electromagnetism/node112.html> Inside perfect conductors, the electric fields vanish. Therefore, also the curl of the electric field vanishes, and for time-harmonic problems it follows that also the magnetic field is zero.

Consequently, supposing the waveguide's walls are perfectly conducting, we end up with the simplified boundary conditions

$$\mathbf{n} \times \mathbf{E} = 0, \text{ on } \partial\Omega \quad (3.13)$$

$$\mathbf{n} \cdot \mathbf{B} = 0, \text{ on } \partial\Omega \quad (3.14)$$

Expressing the fields \mathbf{E} and \mathbf{B} in terms of the vector potential \mathbf{A} (using the time-harmonic relations $\mathbf{E} = -i\omega\mathbf{A}$ and $\mathbf{B} = \nabla \times \mathbf{A}$), we have

$$\mathbf{n} \times \mathbf{A} = 0, \text{ on } \partial\Omega \quad (3.15)$$

$$\mathbf{n} \cdot (\nabla \times \mathbf{A}) = 0, \text{ on } \partial\Omega \quad (3.16)$$

3.3 EIGENVALUE PROBLEM

We want to find the resonant modes of a waveguide. For the unforced case, we have only sinusoidal oscillations in the x - and y -direction. Therefore, the axial frequencies must be integer multiples of π/w or π/l respectively, yielding the superimposed frequency modes

$$\omega_{nm} = \sqrt{\left(\frac{n}{w}\right)^2 + \left(\frac{m}{l}\right)^2} \quad (3.17)$$

Also, we could numerically obtain these eigenfrequencies using the generalized eigenvalue problem

$$\int_{\Omega} (\mu^{-1} \nabla \times \boldsymbol{\varphi}) \cdot (\nabla \times \mathbf{v}) = \lambda \int_{\Omega} \boldsymbol{\varphi} \cdot \mathbf{v} \quad (3.18)$$

for all $\mathbf{v} \in V$, which then yields $\lambda = \sqrt{\omega}$. With the finite element discretization of the above integrals, we obtain a generalized eigenvalue problem of the form

$$\mathbb{K}\mathbf{u} = \lambda \mathbb{M}\mathbf{u} \quad (3.19)$$

There is a small pitfall when using scipy's sparse hermitian eigenvalue solver: When trying to find the smallest magnitude eigenvalue (which is zero, because similarly to what was seen in Section 1.3, the stiffness matrix \mathbb{L} has row sums identically equal to 0, such that a constant solution would always yield zero eigenvalues. This is also obvious from the explicit problem, since constant functions let the left-hand side vanish, and for non-zero \mathbf{u} , the eigenvalue must essentially be zero.) the method does not seem to converge (**why is that so?**). However, when switching to the shift-invert mode, this problem no longer persists.

For the forced problem, the inlet acts as an oscillation amplitude. The x-direction modes must therefore lie between two integer multiples of π/l , for a resonant mode. The general rule is

$$\omega_{nm} = \sqrt{\left(\frac{n}{w}\right)^2 + \left(\frac{m + 1/2}{l}\right)^2} \quad (3.20)$$

3.4 EIGENVALUES OF THE FORCED SYSTEM

In the presence of a boundary term $\mathbf{L} = \int_{\partial\Omega} \mathbf{g}\mathbf{v}$, the eigenvalue problem becomes

$$\mathbb{K}\mathbf{u} - \omega^2 \mathbb{M}\mathbf{u} = \mathbf{L} \quad (3.21)$$

Suppose we know a complete set of eigenpairs $\{\mathbf{u}_j, \lambda_j\}_{j \in \mathbb{N}}$ that solve the system with $\mathbf{L} = 0$. We may then expand any \mathbf{u} in this eigenbasis to $\mathbf{u} = \sum_j \alpha_j \mathbf{u}_j$. Consequently, we may rewrite (3.21) as

$$\begin{aligned} \mathbf{L} &= \sum_j \alpha_j (\mathbb{K}\mathbf{u}_j - \omega^2 \mathbb{M}\mathbf{u}_j) \\ &= \sum_j \alpha_j (\lambda_j \mathbb{M}\mathbf{u}_j - \omega^2 \mathbb{M}\mathbf{u}_j) \\ &= \sum_j \alpha_j (\lambda_j - \omega^2) \mathbb{M}\mathbf{u}_j \end{aligned} \quad (3.22)$$

Taking the scalar product with \mathbf{u}_i , we conclude that

$$\begin{aligned} \langle \mathbf{u}_i, \mathbf{L} \rangle &= \sum_j \alpha_j (\lambda_j - \omega^2) \langle \mathbf{u}_i, \mathbb{M}\mathbf{u}_j \rangle \\ &= \alpha_i (\lambda_i - \omega^2) \end{aligned} \quad (3.23)$$

where we used the fact that there exist \mathbf{u}_i , that are \mathbb{M} -orthonormal. Consequently, we may write

$$\mathbf{u} = \sum_j \alpha_j \mathbf{u}_j \text{ with } \alpha_j = \frac{\langle \mathbf{u}_j, \mathbf{L} \rangle}{\lambda_j - \omega^2} \quad (3.24)$$

What we recognize is that for frequencies ω^2 close to one of the eigenvalues λ_j , the solution \mathbf{u} will “explode” in magnitude, provided \mathbf{u}_j is not orthogonal to \mathbf{L} . If, however, $\langle \mathbf{u}_j, \mathbf{L} \rangle = 0$, we may observe that there is no peak to be found at $\omega^2 = \lambda_j$ in the L2-norm frequency sweep $\|\mathbf{u}(\omega)\|_2$.

3.5 THREE-DIMENSIONAL PERFECTLY CONDUCTING WAVEGUIDE

We again start from

$$\int_{\Omega} (\mu^{-1} \nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{v}) - \omega^2 \int_{\Omega} \epsilon \mathbf{A} \cdot \mathbf{v} = \int_{\partial\Omega} \mathbf{g} \cdot \mathbf{v} \quad (3.25)$$

where we defined $\mathbf{g} = (\mu^{-1} \nabla \times \mathbf{A}) \times \mathbf{n} = \mu^{-1} \mathbf{B} \times \mathbf{n}$ on the boundary $\partial\Omega$.

Yet again, for perfectly (electrically) conducting walls we have (see boundary conditions from Section 3.2)

$$\mathbf{n} \times \mathbf{A} = 0, \text{ on } \partial\Omega \quad (3.26)$$

We can split \mathbf{A} into its normal and tangential component $\mathbf{A} = A_n \mathbf{n} + A_t \mathbf{t}$ with $\mathbf{n} \perp \mathbf{t}$. (3.26) then reads $A_t = 0$, meaning all tangential components of the vector potential \mathbf{A} with respect to the boundary $\partial\Omega$ must vanish. (Problem: Only two degrees of freedom are restricted in this way, when implementing the Dirichlet boundary condition. Need to find an expression or condition on A_n as well...)

As for the inlet, if $\mathbf{n}|_{\text{inlet}} = \mathbf{e}_z$, then we have

$$\mathbf{g} = \mu^{-1} \mathbf{B} \times \mathbf{e}_z = \mu^{-1} (B_y, 0, -B_x)^T \quad (3.27)$$

3.5.1 NÉDÉLEC ELEMENTS OF THE FIRST KIND

Nédélec: <https://link.springer.com/content/pdf/10.1007/BF01396415.pdf>

Monk: <https://www.sciencedirect.com/science/article/pii/037704279390093Q>

“In order to ensure that $\mathbf{n} \times \mathbf{A} = 0$ on $\partial\Omega$, we need only set those degrees of freedom associated with edges and faces on $\partial\Omega$ to zero.”

4 RATIONAL INTERPOLATION

Bonizzoni, Pradovera, Ruggeri: Rational-based model order reduction of Helmholtz frequency response problems with adaptive finite element snapshots

Our aim is to find an alternative way of determining the frequency response of a frequency dependent system on an alternative way, which does not require us to solve a potentially large generalized eigenvalue problem. This can be achieved by

“sampling” N approximate finite element solutions of the system at a set of support points/frequencies $\omega_1, \omega_2, \dots, \omega_N$. Performing a generalized QR-decomposition (Householder triangularization) on the snapshot matrix $\mathbf{A} = [A(\omega_1), A(\omega_2), \dots, A(\omega_N)] = \mathbf{QR}$. In a singular value decomposition the smallest right singular vector of \mathbf{R} is used to define a barycentric rational interpolant of the solution $A(\omega)$.

Our goal is to find the last column of the matrix \mathbf{V} in the singular value decomposition of the Gramian matrix

$$G_{ij} = \langle A(\omega_i), A(\omega_j) \rangle = \int_{\Omega} A(\omega_i) \cdot A(\omega_j) \approx A(\omega_i)^T \mathbf{M} A(\omega_j) \quad (4.1)$$

denoted as $\mathbf{G} = \mathbf{A}^T \mathbf{M} \mathbf{A} = \mathbf{V} \mathbf{\Sigma} \mathbf{V}^T$ with the matrix \mathbf{M} approximating the inner product in $L^2(\Omega)$. By computing a Householder triangularization of the snapshot matrix $\mathbf{A} = \mathbf{QR}$ with \mathbf{R} being an upper triangular matrix and the columns of \mathbf{Q} satisfying $\langle Q_i, Q_j \rangle = \delta_{ij}$. Then, we can realize that

$$\mathbf{G} = \mathbf{A}^T \mathbf{M} \mathbf{A} = \mathbf{R}^T \mathbf{Q}^T \mathbf{M} \mathbf{Q} \mathbf{R} = \mathbf{R}^T \mathbf{R} \quad (4.2)$$

coincides with the Cholesky decomposition of the Gramian matrix \mathbf{G} . Consequently, computing the singular value decomposition of $\mathbf{R} = \mathbf{U} \mathbf{S} \mathbf{V}^T$ will give us

$$\mathbf{G} = \mathbf{R}^T \mathbf{R} = \mathbf{V} \mathbf{S}^T \mathbf{U}^T \mathbf{U} \mathbf{S} \mathbf{V}^T = \mathbf{V} \mathbf{S}^2 \mathbf{V}^T = \mathbf{V} \mathbf{\Sigma} \mathbf{V}^T \quad (4.3)$$

In summary, we perform the following algorithm:

Algorithm 1 Minimal rational interpolation

Require: Support points $\{\omega_i\}_{i=1}^N$

Require: Finite element formulation of the problem $a(A, v; \omega) = L(v)$

Solve $a(A, v; \omega_i) = L(v)$ to obtain $A(\omega_i)$ for $i \in \{1, 2, \dots, N\}$

Assemble snapshot matrix $\mathbf{A} = [A(\omega_1), A(\omega_2), \dots, A(\omega_N)]$

Compute Householder triangularization $\mathbf{A} = \mathbf{QR}$

Compute singular value decomposition of $\mathbf{R} = \mathbf{U} \mathbf{S} \mathbf{V}^T$

Define $\mathbf{q} = (q_1, q_2, \dots, q_N)^T = \mathbf{V}(:, N)$

return $\tilde{A}(\omega) = \sum_i \frac{q_i A(\omega_i)}{\omega - \omega_i} / \sum_i \frac{q_i}{\omega - \omega_i}$

4.1 HOUSEHOLDER TRIANGULARIZATION

Trefethen: Householder triangularization of a quasimatrix

The goal is to obtain the QR factorization of a matrix $\mathbf{A} = \mathbf{QR}$, where the matrix \mathbf{Q} is orthonormal. The Householder triangularization offers a numerically stable and robust way to perform this factorization even for matrices that are rank-deficient or ill-conditioned.

4.2 SINGULAR VALUE DECOMPOSITION

Why the last (smallest singular value) column?

4.3 BARYCENTRIC ROOT FINDING

Klein G: Applications of Linear Barycentric Rational Interpolation

Given a rational function r in barycentric coordinates representation

$$r(z) = \frac{\sum_{i=1}^N \frac{p_i}{z-z_i}}{\sum_{i=1}^N \frac{q_i}{z-z_i}} \quad (4.4)$$

we are interested in finding z for which $r(z)$ exhibits a singularity. To do so, we need only analyze the roots of the denominator. This problem may be elegantly converted to a generalized eigenvalue problem by translating

$$\begin{aligned} 0 &= \sum_{i=1}^N q_i v_i \\ 1 &= v_i(z - z_i), i \in \{1, 2, \dots, N\} \end{aligned} \quad (4.5)$$

into the generalized eigenvalue problem

$$\begin{pmatrix} 0 & q_1 & q_2 & \dots & q_N \\ 1 & \omega_1 & & & \\ 1 & & \omega_2 & & \\ \vdots & & & \ddots & \\ 1 & & & & \omega_N \end{pmatrix} \mathbf{v} = z \begin{pmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} \mathbf{v} \quad (4.6)$$

whose solutions z satisfy $r(z) = 0$.

4.4 GREEDY APPROACH

Pradovera, Nobile: Frequency-domain non-intrusive greedy Model Order Reduction based on minimal rational approximation

In order to algorithmically find out where (and how many) support points/frequencies are needed to achieve a certain interpolation precision, one can employ the following greedy strategy: As the next support point to be added to an existing set of support points, choose the minimizer ω^* of the absolute value of the denominator rational polynomial $Q(\omega)$ in the barycentric representation of the surrogate $\tilde{A}(\omega) = \tilde{P}(\omega)/\tilde{Q}(\omega)$:

$$\omega^* = \operatorname{argmin}_{\omega} |\tilde{Q}(\omega)| \quad (4.7)$$

The stopping criterion is based on the relative deviation in the L2-norm of the surrogate $\tilde{A}(\omega)$ from the finite element solution $A(\omega)$ exhibited at ω^* :

$$\frac{\|A(\omega^*) - \tilde{A}(\omega^*)\|}{\|A(\omega^*)\|} \quad (4.8)$$

Algorithm 2 Greedy minimal rational interpolation

Require: Tolerance τ

Require: Test points $\Omega_{\text{test}} = \{\omega_i\}_{i=1}^N$

Require: Initial support points $\omega_a, \omega_b \notin \Omega_{\text{test}}$

Build initial surrogate $\tilde{A}_2(\omega) = \tilde{P}_2(\omega)/\tilde{Q}_2(\omega)$ using ω_a, ω_b

$s = 2$

while $\Omega_{\text{test}} \neq \emptyset$ **do**

Find $\omega^* = \operatorname{argmin}_{\omega \in \Omega_{\text{test}}} |\tilde{Q}_s(\omega)|$

Remove ω^* from Ω_{test}

Compute $A(\omega^*)$

if $\|A(\omega^*) - \tilde{A}_s(\omega^*)\| \leq \tau \|A(\omega^*)\|$ **then**

$s = s + 1$

Build surrogate $\tilde{A}_s(\omega)$ using additional support point ω^*

return $\tilde{A}_s(\omega)$

end if

Build surrogate $\tilde{A}_{s+1}(\omega)$ using additional support point ω^*

if $\tilde{A}_{s+1}(\omega)$ could not be built in a stable way **then**

return $\tilde{A}_s(\omega)$

end if

$s = s + 1$

end while

return $\tilde{A}_s(\omega)$

5 WEAK DERIVATIVE

Taken from Quarteroni: Introduction to Finite Elements Method

Let $\Omega \subset \mathbb{R}^d$ open. The support of $f : \Omega \rightarrow \mathbb{R}$ is defined as

$$\operatorname{supp}(f) = \overline{\{x \in \Omega \mid f(x) \neq 0\}} \quad (5.1)$$

f has compact support, if there exists a compact subset $K \subset \Omega$, such that $\operatorname{supp}(f) \subset K$, and define

$$\mathcal{D}(\Omega) = \{f \in C^\infty(\Omega) \mid f \text{ has compact support}\} \quad (5.2)$$

(If I remember correctly, extending this notion to $f \in C^1(\Omega)$ should yield an almost identical treatment, unless we also include higher order (weak) partial derivatives). Let $T : \mathcal{D} \rightarrow \mathbb{R}$, $\varphi \mapsto \langle T, \varphi \rangle = T(\varphi)$ be a linear map. We say that T is continuous, if

$$\lim_{n \rightarrow \infty} \langle T, \varphi_n \rangle = \langle T, \varphi \rangle \quad (5.3)$$

with $\{\varphi_k\}_{k \in \mathbb{N}} \subset \mathcal{D}(\Omega)$ converging to φ . Such (linear and continuous) maps are called distribution on $\mathcal{D}(\Omega)$, and they form the space of distributions $\mathcal{D}'(\Omega)$.

The (weak) partial coordinate-derivatives of T (namely $\partial_i T$, $i \in \{1, \dots, d\}$) are characterized by distributions that satisfy

$$\langle \partial_i T, \varphi \rangle = -\langle T, \partial_i \varphi \rangle \quad (5.4)$$

for all $\varphi \in \mathcal{D}(\Omega)$.

Interesting for us is mainly the following case: Given a function $f \in L^2(\Omega)$, we define a distribution $T_f \in \mathcal{D}'(\Omega)$ to be

$$\langle T_f, \varphi \rangle = \int_{\Omega} f(x) \varphi(x) dx \quad (5.5)$$

for all $\varphi \in \mathcal{D}(\Omega)$.

This allows us to define a weak derivative to functions that are (in the classical sense) not differentiable (i.e. not in $C^1(\Omega)$). Consider for example the absolute value function $|\cdot| \in L^2(K)$ where $K \subset \mathbb{R}$ is compact. Since

$$\begin{aligned} \int_K (\partial_x |x|) \varphi(x) dx &= - \int_K |x| \varphi'(x) dx \\ &= - \int_{K \cap \mathbb{R}_+} x \varphi'(x) dx - \int_{K \cap \mathbb{R}_-} (-x) \varphi'(x) dx \\ &= \int_{K \cap \mathbb{R}_+} \varphi(x) dx + \int_{K \cap \mathbb{R}_-} (-1) \varphi(x) dx \\ &= \int_K \text{sign}(x) \varphi(x) dx \end{aligned} \quad (5.6)$$

we may conclude that the weak derivative of the absolute value function is therefore the signum function. Notice, how the derivative of the absolute value function is only not well-defined at $x = 0$, i.e. on a set of zero measure. This nuisance is circumvented when talking about the weak derivative, since the measure zero sets have zero integral.

6 RANDOM

6.1 MODIFIED POTENTIAL

Consider, for instance, solving the following equation:

$$\nabla \times (\nabla \times \mathbf{A}) - \mathbf{A} = \mathbf{j} \quad (6.1)$$

Even if we only care about the quantity $\mathbf{B} = \nabla \times \mathbf{A}$, and therefore would not even “realize” if \mathbf{A} was modified to $\mathbf{A}' = \mathbf{A} + \mathbf{c}$ for a constant vector \mathbf{c} , this modification significantly changes the solution to the equation, because

$$\nabla \times (\nabla \times \mathbf{A}') - \mathbf{A}' = \mathbf{j} \quad (6.2)$$

turns, when plugging in the above-mentioned expression for \mathbf{A}' , into

$$\nabla \times (\nabla \times \mathbf{A}) - \mathbf{A} = \mathbf{j} + \mathbf{c} \quad (6.3)$$

yielding a possibly entirely different solution \mathbf{A} than initially wanted.

Therefore, we cannot adjust \mathbf{A} in such a way that it vanishes on the boundary of a radial symmetric domain, because we would implicitly change the physical outcome of the solution.

6.2 KERNEL OF CURL OPERATOR

Supposedly, the kernel of the curl operator $\nabla \times$ is precisely ∇F in simply connected regions, meaning $\nabla \times f = 0$ iff $f = \nabla F$ for some twice differentiable F . Vague parallel to complex analysis: On simply connected domains any holomorphic function f may be written as $f = F'$ for a holomorphic antiderivative F .

6.3 COMPLEX SYSTEMS

We want to be able to solve $\mathbb{A}\mathbf{x} = \mathbf{b}$ for a complex-valued system. Since

$$wz = (\Re(w) + i\Im(w))(\Re(z) + i\Im(z)) = \Re(w)\Re(z) - \Im(w)\Im(z) + i(\Re(w)\Im(z) + \Im(w)\Re(z)) \quad (6.4)$$

and both \Re and \Im are linear, we can split the system into its real and imaginary components:

$$\Re(\mathbb{A}\mathbf{x}) = \Re(\mathbb{A})\Re(\mathbf{x}) - \Im(\mathbb{A})\Im(\mathbf{x}) = \Re(\mathbf{b}) \quad (6.5)$$

$$\Im(\mathbb{A}\mathbf{x}) = \Re(\mathbb{A})\Im(\mathbf{x}) + \Im(\mathbb{A})\Re(\mathbf{x}) = \Im(\mathbf{b}) \quad (6.6)$$

This is easily rewritten as a purely real system twice the size of the old one

$$\begin{pmatrix} \Re(\mathbb{A}) & -\Im(\mathbb{A}) \\ \Im(\mathbb{A}) & \Re(\mathbb{A}) \end{pmatrix} \begin{pmatrix} \Re(\mathbf{x}) \\ \Im(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \Re(\mathbf{b}) \\ \Im(\mathbf{b}) \end{pmatrix} \quad (6.7)$$

This now also allows us to enforce complex boundary conditions on \mathbf{x} , which we can do by appropriately conditioning on the real or imaginary part of it.

6.4 MIRRORING

If a waveguide composition is symmetric along one axis, then we could mirror it and apply Neumann boundary conditions to the one side which would have been in the center.

7 IDEAS

What might be really interesting is to instead look at the problem in space-time using the Maxwell tensor

$$\mathbb{F} = \begin{bmatrix} 0 & -E_1/c & -E_2/c & -E_3/c \\ E_1/c & 0 & B_3 & -B_2 \\ E_2/c & -B_3 & 0 & B_1 \\ E_3/c & B_2 & -B_1 & 0 \end{bmatrix} \quad (7.1)$$

In the covariant formulation of the Maxwell theory, the inhomogeneous Maxwell equations reduce to a single equation

$$\partial_a F^{ab} = -J^b \quad (7.2)$$

with the four current density $\mathbf{J} = (\mu c \rho, \mu \mathbf{j})$. The weak formulation of the problem could then be stated as (using Einstein's sum convention, i.e. summing over repeated indices)

$$\int_{\Omega \times \mathbb{R}} F^{ab} \partial_a v_b = \int_{\Omega \times \mathbb{R}} J^b v_b \quad (7.3)$$

where boundary conditions are yet to be determined. If we somehow would manage to find a suitable function space for the four-dimensional \mathbf{v} , it might be possible to find both \mathbf{E} and \mathbf{B} from a finite element method.