Scientific Computing – Software Concepts for Solving Partial Differential Equations

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Abstract

Many problems in science and engineering are described by partial differential equations. To solve these equations on non-trivial domains, numerical methods such as the finite element method are required. In this lecture, I will shortly introduce models from mechanical and electrical engineering, and present the numerical methods and algorithms. I will focus on the design of finite element software.

1 Partial Differential Equations in Science and Engineering and the Finite Element Method

In this section, models from electrical and mechanical engineering are introduced. The arising partial differential equations are solved with the finite element package NGSolve. We will discuss the computed results and the solution procedures.

1.1 Electrostatics

The full Maxwell equations describe the interaction of electric and magnetic fields. In a stationary limit, the electric fields can be modeled by a scalar equation, only. Electrostatics models for example a charged capacitor.

The involved quantities are:

Symbol	Unit	
Φ	V	electrostatic potential
E	V/m	electric field intensity
D	As/m^2	dielectric displacement current density
ρ	As/m^3	charge density

Here, V is the abbreviation for Volt, and A is short for Ampere.

The quantities are related by

$$E = \nabla\Phi \qquad D = \varepsilon E \qquad \rho = -\operatorname{div} D. \tag{1}$$

The material parameter ε is the dielectric coefficient.

Putting together the equations above, one ends up with the second order scalar equation

$$-\operatorname{div}(\varepsilon\nabla\Phi) = \rho \tag{2}$$

Still, the potential Φ and the charge density ρ are two unknown fields, and we need more information. Assume the domain consists of conductors and insulators. Then

- inside a conductor the voltage is constant. This implies that E, D, and ρ vanish inside the conductor,
- there are no charges inside of an insulator.

This implies that charges are allowed only at the boundary of conductors. We write ρ_S for the surface charge density.

Now, we pose the full model. Assume that the bounded domain Ω contains M separate conductors $\Omega_1^C \ldots \Omega_M^C$. Let Ω^I be the complement $\Omega \setminus \cup\Omega_i^C$. On $\Gamma := \partial\Omega$ we assume $\Phi = 0$. Then, the problem is described by the boundary value problem

$$\begin{array}{rcll} -\operatorname{div}(\varepsilon\nabla\Phi) & = & 0 & \text{in}\,\Omega^I, \\ \Phi & = & \Phi_i & \text{in}\,\Omega_i^C, \\ \Phi & = & 0 & \text{on}\,\Gamma. \end{array}$$

The scalars Φ_i are assumed to be known. E.g., these are the applied voltages to the plate of a capacitor.

By mean of Gauss´ theorem one obtains

$$D_n = \rho_S,$$

i.e., the Neumann data for the second order equation.

1.1.1 Weak form and discretization

For shorter notation we set $\Gamma_0 := \Gamma$, $\Gamma_i = \partial\Omega_i^c$, and rename $\Omega := \Omega^I$. Then, the bvp is

$$-\operatorname{div}(\varepsilon\nabla\Phi) = 0 \quad \text{in}\ \Omega \tag{3}$$

with Dirichlet boundary conditions

$$\Phi = \Phi_i \quad \text{on}\ \Gamma_i. \tag{4}$$

We have not yet defined a function space for the unknown field Φ. It will come out naturally from the weak formulation. For this, we multiply (3) by an arbitrary smooth function v vanishing on $\cup\Gamma_i$, integrate over the domain Ω, and apply integration by parts:

$$-\int_\Omega \operatorname{div}(\varepsilon\Phi) v \, dx = \int_\Omega \varepsilon \nabla\Phi \cdot \nabla v \, dx = 0.$$

This gives now the definition of the boundary value problem in weak form. Define the function space

$$V := \{v \in L_2(\Omega) : \nabla v \in L_2\}.$$

That space is the Sobolev space $H^1(\Omega)$, which is an Hilbert space with inner product $(u,v)_{L_2} + (\nabla u, \nabla v)_{L_2}$. Now, search $\Phi \in V$ such that

$$\Phi = \Phi_i \qquad \text{on } \Gamma_i$$

and

$$\int_\Omega \varepsilon \nabla\Phi \cdot \nabla v \, dx = 0 \qquad \forall\, v \in V \text{ s.t. } v = 0 \text{ on} \Gamma_i.$$

Due to the choice of the space (H^1 has well defined boundary values, trace theorem), this is a well posed formulation. Indeed, there is a unique solution in V, which follows from the inverse trace theorem, and the Lax-Milgram theorem.

An equivalent formulation (to the weak one) is the constrained minimization problem

$$\min_{\substack{v \in V \\ v=\Phi \text{ on } \Gamma_i}} \int \varepsilon \, |\nabla v|^2 \, dx. \tag{5}$$

Exercise: Show the equivalence

For two reasons which will become clear later, we replace the constrained minimization problem by a penalty approximation with 'large' penalty parameter α:

$$\min_{v \in V} \int_\Omega \varepsilon \, |\nabla v|^2 \, dx + \alpha \int_{\cup\Gamma_i} (v - \Phi_i)^2 \, ds. \tag{6}$$

The corresponding variational form is to find $v \in V$ such that

$$\int_\Omega \varepsilon \nabla\Phi \cdot \nabla v \, dx + \alpha \int_\Gamma \Phi v \, ds = \alpha \int_\Gamma \Phi_i v \, ds \qquad \forall\, v \in V. \tag{7}$$

Now, the identity holds for all $v \in V$ without restriction onto the boundary values.

By performing integration by parts again, one obtains the according b.c. in strong form

$$\varepsilon \frac{\partial \Phi}{\partial n} + \alpha \Phi = \alpha \Phi_i,$$

which is a b.c. of Robin type.

1.1.2 Finite Element Discretization

For the numerical treatment of (7) on replaces the infinite dimensional function space V by a space V_N of finite dimension N. The finite element method is one possibility to construct spaces V_N. The domain Ω is sub-divided into simple domains. Most popular are triangles and quadrilaterals in 2D, and tetrahedra and (deformed) cubes in 3D. On these simple domains, the approximation functions are usually polynomials.

.... basis functions, shape functions, dofs to ensure continuity, hat functions ....

Functions in V_N are expanded in the basis $\{p_1, \ldots, p_N\}$

$$\Phi_N(x) = \sum_{i=1}^N u_i p_i(x).$$

The so called Galerkin approximation to (7) is to find $\Phi_N \in V_N$ such that

$$\int_\Omega \varepsilon \nabla \Phi_N \cdot \nabla v_N \, dx + \alpha \int_\Gamma \Phi_N v_N \, ds = \alpha \int_\Gamma \Phi_i v_N \, ds \qquad \forall \, v_N \in V_N. \tag{8}$$

We plug in the expansion of Φ_N. Testing for all $v \in V_N$ is equivalent to test for all basis functions. This leads to: Find $u = (u_1, \ldots, u_N) \in \mathbb{R}^N$ such that

$$\sum_{i=1}^N \Big\{ \underbrace{\int_\Omega \varepsilon \nabla p_i \cdot \nabla p_j \, dx + \alpha \int_\Gamma p_i p_j \, ds}_{=:A_{ji}} \Big\} u_i = \underbrace{\alpha \int_\Gamma \Phi_i p_j \, ds}_{=:f_j} \qquad \forall \, j \in \{1, \ldots N\}. \tag{9}$$

This is the linear system of equations

$$Au = f.$$

The equation can either be solved by a direct elimination method, or, by an iterative method such as the preconditioned conjugate gradients method. (Sparse) direct methods are appropriate for problems of moderate size (about up to 200 000 unknowns for 2D problems, and 40 000 for 3D problems), but suffer from large memory and CPU requirements for large problems. Iterative methods depend on the type of the applied preconditioner, i.e., an inexact inverse. A simple preconditioners is the diagonal of the matrix, good ones are multigrid and more general Additive Schwarz methods. Preconditioning will be discussed later in Section ..

1.1.3 Simulating a capacitor with NGSolve

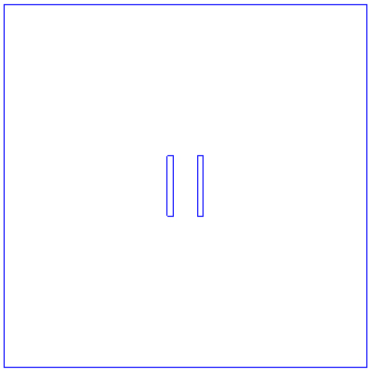
We simulate a plate capacitor as drawn below. The capacity is defined as

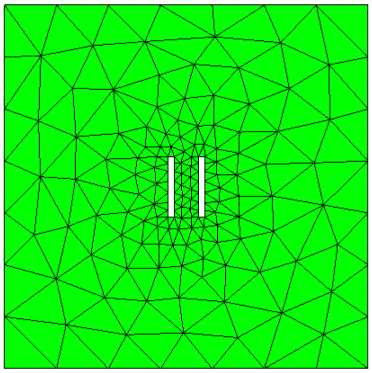
$$C = \frac{Q}{U},$$

where $Q = \int_{\Gamma_+} q_S \, ds$ is the total charge on one plate, and $U = \Phi_+ - \Phi_-$ is the voltage (=difference of potential) between the plates.

Exercise: Show that the capacity is related to (twice of) the stored energy

$$CU^2 = \int_\Omega E \cdot D \, dx.$$





The following Netgen input file describes the geometry above. First, a list of 12 points is specified. The entries are x and y coordinates, and a local relative mesh refinement close to this point. Then, a list of 12 line segments is specified. The first parameters give left and right sub-domain number, 0 means outside. The next number specifies the type of curve, 2 means straight line between the next 2 points. The last number is the relative refinement along this line. Finally, with the `-bc=1` flag, a boundary condition number is specified. We set bc=1 on the outer boundary, and 2 and 3 for the two plates, respectively.

A run of Netgen with this input file generates the triangular mesh drawn above.

```
splinecurves2d
5

12
-3      -3      1
3       -3      1
3       3       1
-3      3       1

0.2     -0.5    10
0.3     -0.5    10
0.3     0.5     10
0.2     0.5     10
-0.3    -0.5    10
-0.2    -0.5    10
-0.2    0.5     10
-0.3    0.5     10
```

```
12
1       0       2       1       2       1  -bc=1
1       0       2       2       3       1  -bc=1
1       0       2       3       4       1  -bc=1
1       0       2       4       1       1  -bc=1

0       1       2       5       6       1  -bc=2
0       1       2       6       7       1  -bc=2
0       1       2       7       8       1  -bc=2
0       1       2       8       5       1  -bc=2

0       1       2       9       10      1  -bc=3
0       1       2       10      11      1  -bc=3
0       1       2       11      12      1  -bc=3
0       1       2       12      9       1  -bc=3
```

The pde we want to solve involves the bilinear form

$$A(\Phi, v) = \int_{\cup\Omega_i} \varepsilon_i \nabla\Phi \cdot \nabla v + \int_{\cup\Gamma_i} \alpha_i \Phi v.$$

The coefficients ε_i and α_i can be specified for each sub-domain, and each piece of the boundary, respectively. There is just one sub-domain, i.e., $\varepsilon = (\varepsilon_1) = (1)$. There are three parts of the boundary, thus $\alpha = (0, 1e5, 1e5)$, where 10^5 is the chosen 'large' penalty parameter.

We apply $+1V$ and $-1V$ onto the electrodes. Thus the right hand side functional is

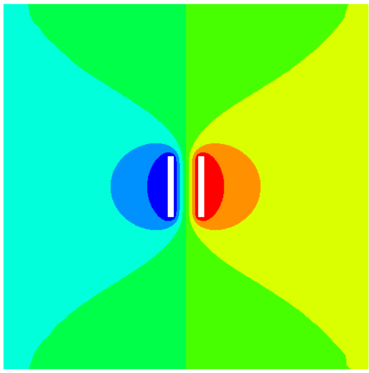
$$f(v) = 10^5 \Big\{ \int_{\Gamma_2} 1\, v\, ds + \int_{\Gamma_3} -1\, v\, ds \Big\} = \int_{\cup\Gamma_i} g_i v\, ds.$$

The coefficient g takes the values $(0, 10^5, -10^5)$ on the pieces Γ_i of the boundary.

The NGSolve input file specifiing that variational problem is given below. First, the filenames of the prepared geometry and mesh files must be specified. Then, one defines coefficient functions, finite element spaces, gridfunctions, bilinear-forms, and linearforms as required by the weak formulation. Several flags are possible to adjust the components. A preconditioner defines an (inexact) inverse. The action starts with the numproc . The numproc bvp takes the matrix provided by the bilinear-form, a right hand side vector provided from the linear-form,and the vector from the gridfunction, and solves the linear system of equations. Each numproc has a unique name such as np1.

```
geometry = demos/capacitor.in2d
mesh = demos/capacitor.vol

define constant geometryorder = 1
# define constant refinep = 1
```

```
define coefficient coef_eps
1,

define coefficient coef_alpha
0, 1e5, 1e5,

define coefficient coef_g
0, 1e5, -1e5,

define fespace v -order=1
define gridfunction u -fespace=v

define bilinearform a -fespace=v -symmetric
laplace coef_eps
robin coef_alpha

define linearform f -fespace=v
neumann coef_g

# define preconditioner c -type=direct -bilinearform=a
# define preconditioner c -type=local -bilinearform=a
define preconditioner c -type=multigrid -bilinearform=a -smoothingsteps=1


numproc bvp np1 -bilinearform=a -linearform=f -gridfunction=u -preconditioner=c -maxsteps=1000

numproc drawflux np2 -bilinearform=a -solution=u -label=flux


# evaluate energy:

define bilinearform aeval -fespace=v -symmetric -nonassemble
laplace coef_eps
numproc evaluate npeval  -bilinearform=aeval -gridfunction=u -gridfunction2=u


# error estimator:

define fespace verr -l2 -order=0
define gridfunction err -fespace=verr

numproc zzerrorestimator np3 -bilinearform=a -linearform=f -solution=u -error=err -minlevel=1
numproc markelements np4 -error=err -minlevel=1 -factor=0.5
```



Computed (double) energy $\int D \cdot E \, dx = \int \varepsilon |\nabla \Phi|^2 \, dx$ is 16.069, which gives a capacity of

$$C = \frac{16.069}{2^2} = 4.017 \frac{As}{V}.$$

1.2 Elasticity

We want to model the mechanical deformation of a body due to applied forces. A body is called elastic, if the deformation returns to the initial state after removing the forces. Otherwise, it is called elasto-plastic. We restrict ourself to the elastic behavior.

1.2.1 One dimensional elasticity

We start with a one-dimensional model. Take a beam (a, b) which is loaded by a force density f in longitudinal (x) direction. We are interested in the displacement $u(x)$ in x-direction.

The involved variables are

- The *deformation* Φ, unit is [m]. The point x of the initial configuration is moved to the point $\Phi(x)$. The *displacement* u is the difference $\Phi(x) - x$.
- The *force density* f, unit [Newton/m] is the applied load inside the body, e.g., the gravity. A *boundary load* g, unit [Newton] can be applied at the end of the beam. Its orientation is in outward direction.
- The *strain* ε, unit [1]: It describes the elongation. Take two points x and y on the beam. After deformation, their distance is $\Phi(y) - \Phi(x)$. The relative elongation of the beam is
$$\frac{(\Phi(y) - \Phi(x)) - (y - x)}{y - x} = \frac{u(y) - u(x)}{y - x}.$$
In the limit $y \to x$, this is u'. We define the strain ε as
$$\varepsilon = u'.$$

- The *stress* σ, unit [Newton]: It describes internal forces. If we cut the piece (x, y) out of the beam, we have to apply forces at x and y to keep that piece in equilibrium. This force is called stress σ. Equilibrium for an internal interval is

  $$\sigma(y) - \sigma(x) + \int_x^y f(s)\,ds = 0,$$

  which leads in differential form to

  $$\sigma' = -f.$$

  Equilibrium on an interval including the boundary (e.g., the point b) is

  $$g(b) - \sigma(x) + \int_x^b f(s)\,ds = 0.$$

  This leads to $\sigma n = g$, where n is the outward unit-vector.

Hook's law postulates a linear relation between the strain and the stress:

$$\sigma = E\varepsilon.$$

Combining the three equations

$$\varepsilon = u' \qquad \sigma = E\varepsilon \qquad \sigma' = -f$$

leads to the second order equation for the displacement u:

$$-(Eu')' = f.$$

Boundary conditions are

- Dirichlet b.c.: Prescribe the displacement at the boundary
- Neumann b.c: Prescibe the boundary load

The weak form is the minimization problem

$$\min_{\substack{v \in H^1 \\ v = g \text{ on } \Gamma_D}} \frac{1}{2} \int_a^b E\,(v')^2 dx - \int_a^b f v\,dx - \int_{\{a,b\}} g v\,ds.$$

The first term can be considered as energy stored due to the deformation of the body, the second and third term is work applied against external forces.

1.2.2 Elasticity in more dimensions

Now, a body $\Omega \subset \mathbb{R}^d$ is deformed due to volume and surface loads. The fields are now

- The *deformation* $\Phi : \Omega \to \mathbb{R}^d$ and the *displacement* $u = \Phi(x) - x$.
- The *volume load density* $f : \Omega \to \mathbb{R}^d$, unit $[N/m^d]$ and the *surface load density* $g : \partial\Omega \to \mathbb{R}^d$, unit $[N/m^{d-1}]$.
- The *strain* is now measured in squared relative distances:

  $$\frac{\|\Phi(x+\Delta x) - \Phi(x)\|^2}{\|\Delta x\|^2} = \frac{\|\Phi'(x)\Delta x\|^2}{\|\Delta x\|^2} + O(|\Delta x|)$$

  The *Cauchy Green strain tensor*

  $$C(x) := \Phi'(x)^T \Phi'(x)$$

  measures the stretching in a direction n via

  $$n^T C n = \lim_{\varepsilon \to 0} \frac{\|\Phi(x+\varepsilon n) - \Phi(x)\|^2}{\|\varepsilon n\|^2}.$$

  A body is undergoing a rigid body motion (i.e., distances are kept constant) if and only if $C = I$, i.e., Φ' is an orthogonal matrix. This means $\det \Phi' \in \{+1, -1\}$. By continuity in time of the deformation process, one excludes -1. Thus a rigid body motions implies that Φ' is a rotation matrix. Φ can be a rotation plus a translation.

Now, we start from the weak formulation, i.e., the principle of minimal energy. For this, let

$$W : \mathbb{R}^{d\times d} \to \mathbb{R}$$

be a function measuring the internal energy density caused by the strain C. The total energy due to a displacement v is

$$V(v) = \int_\Omega W(C(v)) - \int_\Omega fv - \int_{\Gamma_N} gv, \tag{10}$$

and the problem is now

$$\min_{\substack{v \\ v=u_g \text{ on } \Gamma_D}} V(v). \tag{11}$$

A rigid body displacement does not cause internal energy, i.e.,

$$W(C) = 0 \qquad \text{for } C = I.$$

A simple energy funtional is the quadratic one, called Hook's law

$$W(C) = \frac{1}{8} \sum_{i,j,k,l=1}^{d} D_{ijkl}(C-I)_{ij}(C-I)_{kl} = \frac{1}{8} D(C-I) : (C-I).$$

It envolves the fourth order material tensor D. An isotropic material (same properties in all direction) has the special form

$$W(C) = \frac{\mu}{4}|C - I|^2 + \frac{\lambda}{8}(\mathrm{tr}\,(C - I))^2,$$

where μ and λ are called Lamé parameters. Here $A : B = \sum_{i,j} A_{ij}B_{ij}$ is the inner product of tensors, $|A| := (A : A)^{1/2}$ is the norm, and $\mathrm{tr}\, A = \sum_i A_{ii}$ is the trace of the tensor.

We will now evaluate the first order minimum conditions for the minimization probem (11). The directional derivative of the functional $V(u)$ into the direction v is

$$\langle V'(u), v\rangle := \lim_{t\to 0} \frac{1}{t}\left\{V(u + tv) - V(u)\right\}.$$

The first order minimum conditions claim that $V'(u) = 0$, i.e., $\langle V'(u), v\rangle = 0$ for all directions v. We use the chain rule to evaluate the derivatives:

$$\begin{aligned}\langle V'(u), v\rangle &= \int_\Omega \frac{dW(C(u))}{dC} : \langle C'(u), v\rangle - \int_\Omega fv - \int_{\Gamma_N} gv \\ &= \int_\Omega \frac{dW(C(u))}{dC} : \{(I + \nabla u)^T\nabla v + (\nabla v)^T(I + \nabla u)\}\,dx - \int_\Omega fv - \int_{\Gamma_N} gv\end{aligned}$$

Since $\frac{dW}{dC}$ is symmetric, and $A : (B + B^T) = 2A : B$ for symmetric tensors A, the integrand is equal to

$$2\frac{dW}{dC} : (I + \nabla u)^T\nabla v = 2(I + \nabla u)\frac{dW}{dC} : \nabla v = 2\nabla\Phi\frac{dW}{dC} : \nabla v.$$

The variational formulation is now to find u such that $u = u_g$ on Γ_D and

$$\int_\Omega 2(\nabla\Phi)\frac{dW}{dC} : \nabla v\,dx = \int_\Omega fv + \int_{\Gamma_N} gv \qquad \forall\, v \text{ s.t. } v = 0 \text{ on } \Gamma_D. \tag{12}$$

First and second Piola Kirchhoff stress tensor ...

If we plug in Hook's law $W = \frac{1}{8}D(C - I) : (C - I)$, then $\frac{dW}{dC} = \frac{1}{4}\,D(C - I)$, and we observe for the first factor

$$\begin{aligned}\nabla\Phi\frac{dW}{dC} &= \frac{1}{4}(I + \nabla u)D((I + \nabla u)^T(I + \nabla u) - I) \\ &= \frac{1}{4}D(\nabla u + (\nabla u)^T) + O((\nabla u)^2).\end{aligned}$$

In linear elasticity, one neglects the higher oder terms in ∇u. The left hand side becomes

$$\int \frac{1}{2}\{D(\nabla u + (\nabla u)^T)\} : \nabla v\,dx.$$

Again, we use that $D(\nabla u + (\nabla u)^T)$ is symmetric to use also the symmetric form for v:

$$\int \frac{1}{4}\{D(\nabla u + (\nabla u)^T)\} : \{\nabla v + (\nabla v)^T\}\, dx.$$

We introduce a new symbol, called the linearized strain operator, or the symmetric gradient operator

$$\varepsilon(u) = \frac{1}{2}\{\nabla u + (\nabla u)^T\}.$$

With this we arrived at the linear elasticity model: find $u \in [H^1(\Omega)]^d$ such that $u = u_g$ on Γ_D and

$$\int_\Omega D\varepsilon(u) : \varepsilon(v) = \int_\Omega fv\, dx + \int_{\Gamma_N} gv\, ds \qquad \forall\, v \in [H^1(\Omega)]^d \;\text{ s.t. } v = 0 \text{ on } \Gamma_D.$$

The symmetric tensor

$$\sigma := D\varepsilon(u)$$

is called strain tensor. It satisfies

$$\int \sigma\varepsilon(v)\, dx = \int \sigma : \nabla v\, dx = \int -(\text{div }\sigma)\cdot v + \int_{\partial\Omega} \sigma n \cdot v = \int fv + \int_{\Gamma_N} gv.$$

Thus, we have derived the strong from

$$\text{div }\sigma = f$$

and the natural boundary conditions

$$\sigma n = g \qquad \text{on } \Gamma_N$$

1.2.3 Elasticity with NGSolve

```
geometry = ngsolve/pde_tutorial/beam.geo
mesh = ngsolve/pde_tutorial/beam.vol

define constant heapsize = 100000000

define coefficient E
1,

define coefficient nu
0.2,


define coefficient penalty
```

```
1e6, 0, 0, 0, 0, 0

define coefficient coef_force
5e-5,

# finite element space with 3 components
define fespace v -dim=3 -order=5 -eliminate_internal -augmented=1
define gridfunction u -fespace=v

define linearform f -fespace=v
source coef_force -comp=3

define bilinearform a -fespace=v -symmetric  -eliminate_internal -linearform=f
elasticity E nu
robin penalty  -comp=1
robin penalty  -comp=2
robin penalty  -comp=3

# define preconditioner c -type=direct -bilinearform=a
define preconditioner c -type=multigrid -bilinearform=a

numproc bvp np1 -bilinearform=a -linearform=f -gridfunction=u -preconditioner=c -maxstep

# compute stresses:
define fespace vp -dim=6  -order=5
define gridfunction stress -fespace=vp
numproc calcflux np2 -bilinearform=a -solution=u -flux=stress -applyd
```

1.3 Magnetostatics

A second limit problem of Maxwell equations are the equations for a stationary magnetic field. Here, the involved quantities are

Symbol	Unit	
j	A/m^2	a given current density such that div $j = 0$
B	Vs/m^2	magnetic flux density (German: “Induktion”)
H	A/m	magnetic field intensity (German: “Magnetische Feldstärke”)

All these quantities are vector fields. It is assumed that the currents have no sources, i.e.,

$$\operatorname{div} j = 0.$$

Ampere's law is that for every smooth surface S there holds

$$\int_S j \cdot n \, ds = \int_{\partial S} H \cdot \tau ds.$$

By Stokes´ theorem, the right hand side can be rewritten as $\int_S \operatorname{curl} H \cdot n \, ds$. Thus, there holds

$$\operatorname{curl} H = j$$

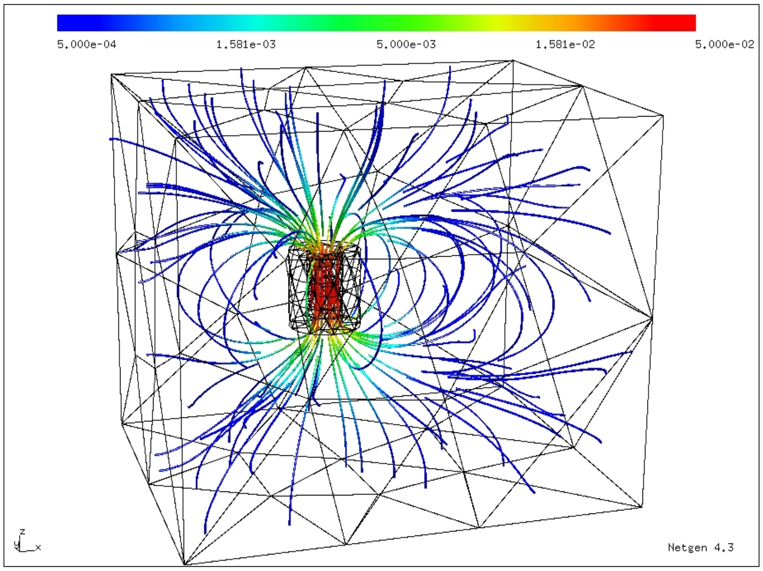
The hypotheses onto the magnetic flux B is that it has no sources, i.e.,

$$\operatorname{div} B = 0$$

The two magnetic quantities B and H are related by the material law

$$B = \mu H,$$

where μ is called permeability. In general, the relation is non-linear, and may depend also on the history. The magnetic flux density B induced by a prescribed current j in a coil is drawn below:



The usual approach to handle these equations is to introduce a vector-potential A such that

$$B = \text{curl } A$$

Since div curl $= 0$, this implies div $B = 0$. On the other hand, $\operatorname{div} B = 0$ holds in $\mathbb{R}^3$, which is simply connected, and thus allows to introduce the potential. Combining the equations leads to the second order problem for A:

$$\operatorname{curl} \mu^{-1} \operatorname{curl} A = j$$

As usual, we go over to the weak form. Multiply with test functions v and using the integration by parts rule $\int_\Omega \operatorname{curl} u \cdot v = \int_\Omega u \cdot \operatorname{curl} v + \int_{\partial\Omega} (n \times u) \cdot v \, ds$:

$$\int_\Omega \mu^{-1} \text{curl } A \cdot \operatorname{curl} v \, ds + \int_{\partial\Omega} (n \times \mu^{-1} \text{curl } A) \cdot v \, ds = \int_\Omega j \cdot v \, dx$$

This variational form shows two canonical boundary conditions:

- Posing the equation for arbitrary v implies that

  $$n \times \mu^{-1} \text{curl } A = n \times H = 0,$$

  i.e., the tangential components of H vanish at the boundary. These are the natural Neumann boundary conditions.

- Prescribe tangential boundary conditions for A, and put the tangential components of v to 0, then

  $$(n \times \mu^{-1} \operatorname{curl} A) \cdot v = \mu^{-1} \text{curl } A \cdot (v \times n) = 0$$

  These are the essential Dirichlet boundary conditions. They imply that $B \cdot n = \operatorname{curl}_n A_\tau = 0$ at the boundary.

The problem is: find A such that

$$\int_\Omega \mu^{-1} \text{curl } A \cdot \operatorname{curl} v \, ds = \int_\Omega j \cdot v \, dx \qquad \forall \, v \tag{13}$$

The solution is not unique. Since $\operatorname{curl} \nabla = 0$, adding an arbitrary gradient field to A gives another solution. One possibility is to ignore the non-uniqueness, and work directly on the factor space. An other approach is to select the unique vector potential being orthogonal to gradients of arbitrary scalar fields, i.e.

$$\int A \cdot \nabla\varphi = 0 \qquad \forall \, \varphi \tag{14}$$

This additional condition is called gauging. The b.c. onto φ have to correspond to the ones of A: If A has 0-tangential b.c., then φ must have 0 b.c. as well.

1.3.1 The classical $\operatorname{curl}\operatorname{curl} + \operatorname{div}\operatorname{div}$ approach

One idea is to perform integration by parts of the gauging-equation to obtain

$$\int_\Omega A\nabla\varphi\,dx = -\int_\Omega \operatorname{div} A\,\varphi\,dx + \int_{\partial\Omega} A\cdot n\varphi\,ds = 0$$

This implies $\operatorname{div} A = 0$, and, for the case of Neumann boundary conditions also $A\cdot n = 0$. The classical approach is to utilize $\operatorname{div} A = 0$ and add a consistent term to the variational equation to obtain

$$\int \mu^{-1}\,\text{curl }A\cdot\text{curl }v\,dx + \int \mu^{-1}\,\text{div }A\cdot\text{div }v\,dx = \int f\cdot v\,dx \qquad \forall\, v,$$

with boundary conditions either $A\cdot\tau = 0$, or $A\cdot n = 0$. For this problem, standard continuous finite elements can be used. This approach was most popular until the 1990s. But, it has serios disadvantages:

- For the case of highly different material parameters μ, the stability of the equation gets really lost. Iteration numbers of iterative solvers go up, there are no robust methods available.

- This approach cannot be used in electro-dynamics, where more terms come in. There, the equation becomes (e.g., for the time harmonic setting in the so called A^* formulation)

  $$\int \mu^{-1}\,\text{curl }A\operatorname{curl} v\,dx - \omega^2\int \varepsilon(x)Av\,dx = \int j\cdot v\,dx,$$

  where ε is the dielectric material parameter. Now, choosing test functions $v = \nabla\varphi$, integration by parts gives the equation

  $$\operatorname{div}(\varepsilon A) = 0,$$

  there is no choice for gauging. In sub-domains with constant coefficients ε, this implies $\operatorname{div} A = 0$ in the sub-domains, but not globally. One could use this hidden equation for stabilization:

  $$\int \mu^{-1}\,\text{curl }A\operatorname{curl} v\,dx + \int \mu^{-1}\operatorname{div}(\varepsilon A)\operatorname{div}(\varepsilon v)\,dx - \omega^2\int \varepsilon Av\,dx = \int j\cdot v\,dx.$$

  But now, one cannot use continuous elements: The $\operatorname{div} - \operatorname{div}$-term is not finite in the case of non-continuous coefficients ε. There are fixes by introducing an additional scalar potential, but things don't get simpler.

1.3.2 The $H(\mathrm{curl})$ formulations

The modern approach is not to stabilize with the div − div term. The theoretical setting is to add the gauging condition as given in (14). In general, when adding equations, one has to add also additional unknowns. We pose the mixed formulation to find the vector field A and the scalar field φ such that

$$\begin{array}{rcl} \int \mu^{-1} \operatorname{curl} A \operatorname{curl} v \, dx \quad + \quad \int v \nabla \varphi & = & \int j \cdot v \, dx \qquad \forall\, v \\ \int A \nabla \psi \, dx \qquad\qquad & = & 0 \qquad\qquad \forall\, \psi \end{array}$$

The proper function space for A is the space

$$H(\mathrm{curl}) = \{ v \in [L_2]^3 : \operatorname{curl} v \in [L_2]^3 \},$$

with the norm

$$\|v\|^2_{H(\mathrm{curl})} = \|v\|^2_{L_2} + \| \operatorname{curl}\ v\|^2_{L_2}.$$

The space for the Lagrange parameter φ is the $(H^1, \|\nabla \cdot\|_{L_2})$. Continuity of the mixed formulation is immediate. The important LBB-condition

$$\sup_{v \in H(\mathrm{curl})} \frac{(v, \nabla \psi)}{\|A\|_{H(\mathrm{curl})}} \geq c\, |\nabla \psi|_{L_2}$$

is also simple to verify: Take $v = \nabla \psi$. This is possible, since

$$\nabla H^1 \subset H(\mathrm{curl}).$$

That property is essential, and will also be inherited onto the discrete level. Kernel-ellipticity is more involved, but also true.

We usually do not want to solve the mixed problem, but a positive definite one. This can be obtained by regularization: Adding a 'small' term

$$\varepsilon \int A v \, dx$$

to the mixed formulation is a regular perturbation, i.e., we change the solution of $O(\varepsilon)$. The perturbed problem is now:

$$\begin{array}{rcl} \int \mu^{-1} \operatorname{curl} A \operatorname{curl} v \, dx + \varepsilon \int A v \, dx \quad + \quad \int v \nabla \varphi & = & \int j \cdot v \, dx \qquad \forall\, v \\ \int A \nabla \psi \, dx \qquad\qquad & = & 0 \qquad\qquad \forall\, \psi \end{array}$$

We choose test functions $v = \nabla \varphi$ for the first line:

$$\underbrace{\int \mu^{-1} \operatorname{curl} A \operatorname{curl} \nabla \varphi \, dx}_{=0} + \varepsilon \underbrace{\int A \nabla \varphi \, dx}_{=0} + \int \nabla \varphi \nabla \varphi = \underbrace{\int j \nabla \varphi \, dx}_{=0},$$

i.e, $\nabla \varphi = 0$, and we can solve the regularized problem in A, only:

$$\int \mu^{-1} \operatorname{curl} A \operatorname{curl} v \, dx + \varepsilon \int A v \, dx = \int j \cdot v \, dx \qquad \forall\, v \in H(\mathrm{curl})$$

With the proper methods, everything (discretization, solvers, error estimators) are robust in the regularization parameter ε.

1.3.3 Finite elements in $\mathbf{H}(\mathrm{curl})$

We first derive the natural continuity properties of $H(\mathrm{curl})$. Let $u \in H(\mathrm{curl})$, and $q = \mathrm{curl}\, u$. Then, for all smooth vector functions φ vanishing at the boundary there holds $\int q \cdot \varphi = \int \mathrm{curl}\, u \cdot \varphi = \int u \cdot \mathrm{curl}\, \varphi$. This relation is used to define the *weak* curl operator: q is called the weak curl of u if there holds

$$\int_\Omega q \cdot \varphi = \int_\Omega u \cdot \mathrm{curl}\, \varphi \qquad \forall \varphi \in [C_0^\infty]^3$$

An L_2 function u is in $H(\mathrm{curl})$ if curl u is in L_2. A sufficient condition is the following:

Theorem 1. *Let $\Omega = \bigcup \Omega_i$ be a domain decomposition. Assume that*

$$u_i = u|_{\Omega_i} \qquad \textit{is smooth}$$

and the tangential components are continuous over sub-domain interfaces, i.e.,

$$u_i \times n_i = -u_j \times n_j \qquad \textit{on } \overline{\Omega_i} \cap \overline{\Omega_j}$$

Then $u \in H(\mathrm{curl}, \Omega)$, and the locally defined curl u *is the global, weak* curl u.

Proof. We check that the local curl satisfies the definition of the weak curl:

$$\begin{aligned}
\int_\Omega (\mathrm{curl}\, u)_i \varphi \, dx &= \sum_{\Omega_i} \int_{\Omega_i} \mathrm{curl}\, u_i \varphi \, dx \\
&= \sum_{\Omega_i} \int_{\Omega_i} u_i \, \mathrm{curl}\, \varphi \, dx + \int_{\partial\Omega_i} (n_i \times u_i) \varphi \, ds \\
&= \int_\Omega u \, \mathrm{curl}\, \varphi \, dx + \underbrace{\sum_{\overline{\Omega_i} \cap \overline{\Omega_j}} \int_{\overline{\Omega_i} \cap \overline{\Omega_j}} [n_i \times u_i + n_j \times u_j] \varphi \, ds}_{=0} .
\end{aligned}$$

□

The opposite is true is well. If $u \in H(\mathrm{curl}, \Omega)$, then u has continuous tangential components.

This characterization motivates the definition of finite element spaces for $H(\mathrm{curl})$ on the mesh $\{T\}$. The type-II Nédélec elements of order k generate the space

$$V_h^k = \{ v : v|_T \in [P^k]^3, \ v \cdot t \text{ continuous over element-interfaces} \}$$

The space is constructed by defining a basis. We start with a P^1-triangular element. In 2D, the $H(\mathrm{curl})$ has 2 vector components. Each component is an affine linear function on the triangle, i.e., has 3 parameters. Totally, the P^1 triangle has 6 parameters. We demand continuity of the tangential component over element boundaries, i.e., the edges.

The tangential component is a linear function on the edge, thus, it is specified by two 2 degrees of freedom. 3 edges times 2 degrees of freedom specifiy the 6 parameters on the element.

We now give a basis. Let E_{ij} be an edge from vertex V_i to vertex V_j. Let φ_i^V and φ_j^V be the corresponding vertex basis functions. Then we define the two basis functions

$$\varphi_{ij}^{E,0} := \varphi_i^V \nabla \varphi_j^V - \nabla \varphi_i^V \varphi_j^V$$

as well as

$$\varphi_{ij}^{E,1} := \nabla(\varphi_i^V \varphi_j^V) = \varphi_i^V \nabla \varphi_j^V + \nabla \varphi_i^V \varphi_j^V$$

associated with the edge E_{ij}.
Exercise: Show that this is a basis for $V_h^1 \subset H(\mathrm{curl})$. Verify that

- $\varphi_{ij}^{E,0}$ and $\varphi_{ij}^{E,1} \subset V_h^1$
- $\varphi_{ij}^{E,0} \cdot \tau = 0$ and $\varphi_{ij}^{E,1} \cdot \tau = 0$ on edges $E \neq E_{ij}$
- $\varphi_{ij}^{E,0} \cdot \tau$ and $\varphi_{ij}^{E,1} \cdot \tau$ are linearly independent on the edge E_{ij}

In magnetostatics, we are only interested in the magnetic flux $B = \operatorname{curl} A$, but not in the vector potential A itself. The basis-functions $\varphi_{ij}^{E,1}$ are gradients, so do not improve the accuracy of the B-field. Thus, we might skip them, and work with the $\varphi_{ij}^{E,0}$, only. This are the Nédélec elements of the first type, also known as edge elements.

1.3.4 Magnetostatics with NGSolve

We first give the definition of a 3D geometry as drawn in the field-lines plot above. We specify the cylindrical coil by cutting out a smaller cylinder from a larger cylinder. The air domain is bounded by a rectangular box. In Netgen, one can specify geometric primitives such as infinite cylinders, half-spaces (called planes), and so on. One can construct more complicated solids by forming the union (or) , intersection (and) or complements (not) of simpler ones. One can specify boundary conditions with the `-bc=xxx` flag. The final sub-domains are called Top-Level-Objects (tlo) and have to been specified. The `-col=[red,green,blue]` flag gives the color for the visualization.

```
algebraic3d
solid coil = cylinder (0, 0, -1; 0, 0, 1; 0.4)
        and not cylinder  (0, 0, -1; 0, 0, 1; 0.2)
        and plane (0, 0, 0.4; 0, 0, 1)
        and plane (0, 0, -0.4; 0, 0, -1);

solid box = orthobrick (-2, -2, -2; 3, 2, 2) -bc=1;
solid air =  box and not coil -bc=3;
```

```
tlo coil -col=[0, 1, 0];
tlo air  -col=[0, 0, 1] -transparent;
```

The input-file for the solver is the tutorial example 'd7_coil.pde': The current source in the sub-domain of the coil is prescribed as function $(y, -x, 0)$ in angular direction. An $H(\text{curl})$ finite element space of arbitrary order is defined by specifiing the `-hcurlho` flag. The flag `-nograds` specifies to skip all gradient basis functions. The keywords for the integrators are

`sourceedge jx jy jz`	$\int j \cdot v \, dx$
`curlcurledge nu`	$\int \nu \,\text{curl}\, u \;\text{curl}\, v \, dx$
`massedge sigma`	$\int \sigma u \cdot v \, dx$

The numproc `drawflux` inserts a field into the visualization dialog-box. It applies the differential operator of the specified bilinear-form to the specified grid-function. The `-applyd` flag specifies whether the field is multiplied with the coefficient function, or not. Recall that the B-field is curl A, and the H-field is $\mu^{-1}\,\text{curl}\; A$.

```
geometry = ngsolve/pde_tutorial/coil.geo
mesh = ngsolve/pde_tutorial/coil.vol

define constant geometryorder = 4
define constant secondorder = 0

define coefficient nu
1, 1,

define coefficient sigma
1e-6, 1e-6,

define coefficient cs1
( y ), 0,
define coefficient cs2
( -x ), 0,
define coefficient cs3
0, 0, 0

define fespace v -hcurlho -order=4 -nograds

define gridfunction u -fespace=v -novisual

define linearform f -fespace=v
sourceedge cs1 cs2 cs3 -definedon=1
```

```
define bilinearform a -fespace=v -symmetric
curlcurledge nu
massedge sigma -order=2


define bilinearform acurl -fespace=v -symmetric -nonassemble
curlcurledge nu


define preconditioner c -type=multigrid -bilinearform=a -cylce=1 -smoother=block -coarse

numproc bvp np1 -bilinearform=a -linearform=f -gridfunction=u -preconditioner=c -maxstep

numproc drawflux np5 -bilinearform=acurl -solution=u  -label=B-field
numproc drawflux np6 -bilinearform=acurl -solution=u  -label=H-field  -applyd
```

2 Mathematical Objects and their implementation

In this chapter, we discuss the building blocks of the finite element method, and how they are implemented in the object-oriented C++ code NGSolve.

2.1 Finite Elements

One has to build a basis for the finite element function space

$$V_h = \{v \in C^0 : v|_T \in P^k \text{ for all elements } T \text{ in the mesh}\},$$

where C^0 are the continuous functions. On triangles (and tetrahedra), the space P^k is the space of polynomials up to the total order k. On quadrilaterals (and 3D hexahedra), the space $P^k = P^{k,k}$ contains all polynomials up to order k in each variable.

The global basis is constructed by defining an local basis on each element such that the local basis functions match at the element boundaries. To define the element basis, the element T is considered as the mapping of one reference element, i.e.,

$$T = F_T(T^R).$$

This reduces the task to define a basis $\{\varphi_1, \ldots, \varphi_{N_T}\}$ on the reference element. The basis functions on the mapped element are

$$\varphi_{T,i}(F_T(x)) := \varphi_i(x) \qquad \forall\, x \in T^R$$

The basis functions on the reference element are called shape functions.

2.1.1 One dimensional finite elements

The lowest order finite element space consists of continuous and piecewise affine-linear functions. A basis for the 1D reference element $T^R = (-1, 1)$ is

$$\varphi_1 = \frac{1+x}{2}, \quad \varphi_2 = \frac{1-x}{2}.$$

These functions are 1 in one vertex, and vanish in the other one. The global basis function associated with the vertex V is $\varphi_{T_l,2}$ on the left element, and $\varphi_{T_r,1}$ for the right element.

To build C^0-continuous elements of higher order, one adds more basis functions which vanish at the boundary $\{-1, +1\}$ to ensure continuity. These functions are called bubble functions. A simple basis is the monomial one

$$\varphi_{i+3} = x^i(1-x^2) \qquad \forall\, i = 0, \ldots p-2.$$

Later, we will have to evaluate matrices like $A_{ij} := \int_{-1}^{+1} \varphi_i \varphi_j \, dx$. When using this basis, the matrix is very ill conditioned (comparable to the Hilbert matrix). Thus, one usually chooses orthogonal polynomials as basis functions.

The k^{th} Legendre polynomial P_k is a polynomial of order k which is $L_2(-1,1)$-orthogonal to all polynomials of order $l < k$, i.e.,

$$\int_{-1}^{1} P_k(x) P_l(x)\, dx = 0 \qquad \forall\, l \neq k.$$

They are normalized such that $P_k(1) = 1$. Legendre polynomials can be evaluated efficiently by the three-term reccurency

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_k(x) &= \frac{2j-1}{j} x P_{k-1}(x) - \frac{j-1}{j} P_{k-2}(x) \qquad k \geq 2. \end{aligned}$$

Legendre polynomials do not vanish at the element boundaries. One possibility to ensure this is to multiply with the quadratic bubble, i.e., to take $(1-x^2)P_k(x)$. A different one (and the most popular one) is to introduce integrated Legendre polynomials

$$L_k(x) := \int_{-1}^{x} P_{k-1}(s)\, ds.$$

For $k \geq 2$, these polynomials vanish in $\{-1, 1\}$. The left end is clear, for the right end there holds

$$L_k(1) = \int_{-1}^{1} P_{k-1}\, ds = \int_{-1}^{1} P_0 P_{k-1}\, dx = 0 \qquad \forall\, k \geq 2.$$

The idea behind the integrated Legendre polynomials is that they are orthogonal with respect to the inner product $(u', v')_{L_2(-1,1)}$.

Legendre polynomials belong to the more general family of Jacobi polynomials $P_k^{(\alpha,\beta)}$ which are orthogonal polynomials with respect to the weighted inner product

$$(u, v) := \int_{-1}^{1} (1-x)^{\alpha} (1+x)^{\beta} uv\, dx.$$

There is a three term reccurency for the Jacobi polynomials as well. The bubble functions

$$\varphi_k = (1-x^2) P_k^{(2,2)}$$

are L_2-orthogonal.

2.1.2 Quadrilateral finite elements

We take the reference square $(-1,1)^2$. The lowest order basis functions are the bilinear ones

$$\varphi_1 = \frac{(1+x)(1+y)}{4} \quad \varphi_2 = \frac{(1-x)(1+y)}{4} \quad \varphi_3 = \frac{(1-x)(1-y)}{4} \quad \varphi_4 = \frac{(1+x)(1-y)}{4}$$

These are functions which are 1 in one vertex, and vanish on all edges not containing this vertex, in particular, in all other vertices. These basis functions are associated with the vertices of the mesh. The restriction to the edges are linear functions. They are continuous since they coincide in the vertices.

Next, we add functions to obtain polynomials of order p on the edges. These additional basis functions must have support only on the elements containing the edge. This is obtained by choosing edge bubble-functions vanishing in the vertices. For example, the edge bubble functions for the edge $(-1,-1)$-$(1,-1)$ on the reference element are defined as

$$\varphi_{E_1,i} := L_{i+2}(x)\frac{y+1}{2} \qquad i = 0, \ldots, p-2$$

These functions vanish on all other edges.

To obtain the full space $P^{k,k}$, one has to add the element bubble functions

$$L_i(x)L_j(y) \qquad i,j = 2, \ldots, p.$$

These functions vanish on the boundary ∂T, and thus are always continuous to the neighbor elements.

There appears one difficulty with the continuity of the edge basis functions: There are even functions and odd functions on the edge. For the odd functions, the orientation of the edge counts. When mapping the reference elements onto the domain, the orientation of the edges do not necessarily match, and thus, the functions would not be continuous. One possibility to resolve the conflict is to transform the basis functions. The odd functions must change sign, if the edge of the reference element is oriented opposite to the global edge. A second possibility is to parameterize the reference element: For each specific element, take the global orientation of the edge onto the reference element. This is a transformation of the arguments x or y. A simple possibility to orient edges is to define the direction from the smaller vertex to the larger one. On the reference element, one has to know the global vertex number to handle the orientation. This second approach is simpler for 3D elements (in particular tetrahedral ones) and thus taken in NGSolve.

2.1.3 Triangular finite elements

The construction of a basis on triangles follows the same lines. It is useful to work with barycentric coordinates λ_1, λ_2, and λ_3. The vertex basis functions are exactly the barycentric coordinates.

The edge-based basis functions on the edge between vertex i and vertex j are defined as

$$\varphi_{E,k} = L_{k+2}\Big(\frac{\lambda_i - \lambda_j}{\lambda_i + \lambda_j}\Big)(\lambda_i + \lambda_j)^{k+2} \qquad k = 0, \ldots, p-2.$$

There holds

1. This is a polynomial of order $k+2$. The first factor is rational of order $k+2$ in the denominator, and this is compensated by the second factor. The implementation of these functions is possible by a division free three-term reccurency.
2. On the edge E_{ij} there holds $\lambda_i+\lambda_j=1$, and thus, the function simplifies to $L_{k+2}(\lambda_i-\lambda_j)$.
3. On the edge E_{jk} there holds $\lambda_i=0$, and the function is $L_{k+2}(-1)\lambda_j^{k+2}=0$. Similar for the edge E_{ik}.

Again, the element bubble functions are defined by a tensor product construction. For this, let

$$\begin{aligned} u_k &= L_{k+2}\Big(\frac{\lambda_1-\lambda_2}{\lambda_1+\lambda_2}\Big)(\lambda_1+\lambda_2)^{k+2} \qquad k=0,\ldots,p-2, \\ v_l &= \lambda_3 P_l(2\lambda_3-1) \qquad l=0,\ldots,p-1 \end{aligned}$$

Then, the element bubble functions are

$$\varphi_{k,l}=u_k v_l \qquad \forall\, k\geq 0, l\geq 0, l+k\leq p-3.$$

The first factor vanishes for the edges $\lambda_1=0$ and $\lambda_2=0$, and the second factor vanishes for the edge $\lambda_3=0$.

2.1.4 Tangential continuous finite elements

To approximate Maxwell equations (in $H(\mathrm{curl})$), we need vector valued finite elements whose tangential components are continuous over element boundaries. We construct such elements for triangles.

The simplest type of basis functions are the high order edge-based basis functions. Take the gradients of the H^1 edge-based basis functions of one order higher:

$$\Phi_{E,i}=\nabla\varphi_{E,i+1} \qquad i=1,\ldots,p$$

Since the global H^1 basis functions are continuous over element boundaries, the tangential component of their derivatives is continuous, as well. Above, we have defined p basis functions up to order p. There is missing one more function. Since for edge bubble functions there holds

$$\int_E \Phi_{E,i}\cdot\tau\,ds=\int_E \nabla\varphi_{E,i+1}\cdot\tau\,ds=\varphi_{E,i+1}(V_{E_1})-\varphi_{E,i+1}(V_{E_2})=0,$$

all these functions are $(\cdot\tau,\cdot\tau)_{L_2(E)}$-orthogonal to the constant. One has to add the lowest order edge-element basis function as defined in Section 1.3:

$$\Phi_{E,0}=\nabla\varphi_{E_1}\varphi_{E_2}-\varphi_{E_1}\nabla\varphi_{E_2}$$

The tangential boundary values of the element-based basis functions must vanish. Recall the construction $\varphi_{T,ij} = u_i v_j$ for the H^1-case. The first factor vanishes on the two edges $\lambda_1 = 0$ and $\lambda_2 = 0$, while the second factor vanishes for $\lambda_3 = 0$. The functions

$$\Phi^1_{T,kl} := (\nabla u_k) v_l$$

have vanishing tangential traces on all edges, since the tangential derivative of a bubble function vanishes. The same holds for

$$\Phi^2_{T,kl} := u_k (\nabla v_l)$$

A third class of functions with vanishing tangential traces are

$$\Phi^2_{T,kl} := \Phi_{E,0} v_l,$$

where $\Phi_{E,0}$ is the lowest order edge-basis function for the edge $\lambda_3 = 0$. One can show that these functions form a basis for $\{v \in [P^p]^2 : v \cdot \tau = 0 \text{ on } \partial T\}$. Instead of taking the first two types a above, one may take the sum and the difference of them. This has the advantage to include gradient basis functions explicitely (since $\nabla(u_k v_l) = (\nabla u_k) v_l + u_k \nabla v_l$).

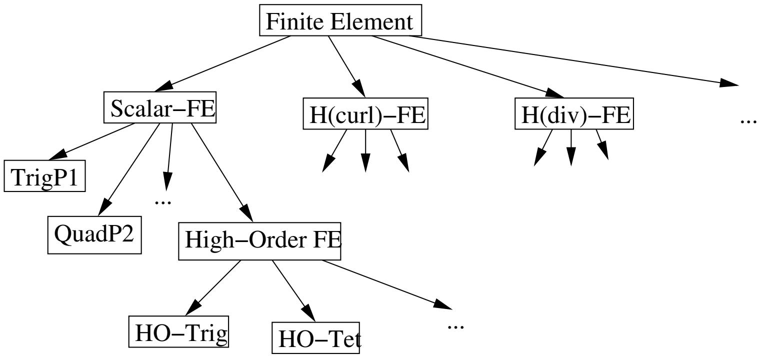
We were sloppy in defining the gradient. We need tangential continuity on the mapped element, so the basis functions must be gradients on the mapped elements. But, on the other hand, we want to define the $H(\text{curl})$ basis functions on the reference element. The remedy is to define the transformation for $H(\text{curl})$-basis functions compatible with gradients by

$$u(F(x)) := (F')^{-T} u^R(x) \qquad \forall\, x \in T^R.$$

If u^R is the gradient ∇w^R on the reference element, then $u = \nabla w$ on the mapped element, where $w(F(x)) = w^R(x)$. This transformation is called covariant transformation.

2.1.5 A class hierarchy for finite elements

In NGSolve, a hierarchy is designed to extract common properties of families of finite elements:



All these types correspond to C++ classes.

The base class must be general enough to include common properties of all type of elements (currently in the mind of the author). These include the type of element, space dimension, number of shape functions, and polynomial order. The C++ realization is:

```
class FiniteElement
{
protected:
  int dimspace;          // space dimension (1, 2, or 3)
  ELEMENT_TYPE eltype;  // element geometry (trig, quad, ...)
  int ndof;              // number of degrees of freedom
  int order;             // polynomial order

public:
  FiniteElement (int adimspace, ELEMENT_TYPE aeltype, int andof, int aorder)
    : dimspace(adimspace), eltype(aeltype), ndof(andof), order(aorder) { ; }
  virtual ~FiniteElement () { ; }

  int SpatialDim () const { return dimspace; }
  int GetNDof () const { return ndof; }
  int Order () const { return order; }
  ELEMENT_TYPE ElementType() const { return eltype; }
};
```

The properties are chosen to be stored as member variables (instead of, e.g., provided by virtual function calls) for faster access. A variable of each specific finite element type is just defined once for the reference element, so additional memory cost is not an issue. The base class has no methods for shape function evaluation since it is not clear whether the shape functions are scalars or vectors.

Finite elements for scalar H^1-problems have in common that they have scalar shape functions, and the gradient is well defined. For historical reasons, H^1 finite elements are called `NodalFiniteElement`. These class inherits the properties of the base `FiniteElement`, and adds methods for shape function evaluation:

```
class NodalFiniteElement : public FiniteElement
{
  ...
  virtual void CalcShape (const IntegrationPoint & ip,
                         Vector<> & shape) const = 0;
  virtual void CalcDShape (const IntegrationPoint & ip,
                          Matrix<> & dshape) const;
};
```

A NodalFiniteElement offers just the interface to compute shape functions, but, it does not know about the specific element, so it cannot compute shape functions. This is provided by the mechanism of virtual functions. The function `CalcShape` computes the vector of all shape functions in a given point `ip` on the reference element. It is a pure virtual function (specified by the syntax `= 0` at the end of the line) which means that every specific finite element must overload the `CalcShape` function. The function `CalcDShape` computes all partial derivatives of shape functions and stores them in the $ndof \times spacedim$-matrix dshape. There is a default implementation by numerical differentiation, but, the specific finite element class may overload this function by computing the derivatives analytically.

A specific finite element is a triangular element with shape functions in P^1. Indeed, also the CalcDShape method is overloaded:

```
class FE_Trig1 : public NodalFiniteElement
{
  FE_Trig1() : NodalFiniteElement (2, ET_TRIG, 3, 1) { ; }
  virtual ~FE_Trig1() { ; }
  virtual void CalcShape (const IntegrationPoint & ip,
                          Vector<> & shape) const
  {
    shape(0) = ip(0);
    shape(1) = ip(1);
    shape(2) = 1-ip(0)-ip(1);
  }
};
```

There were a plenty of elements implemented for fixed order up to 2 or 3.

The newer elements are high order elements of variable order. One can specify a polynomial order for each edge, (and each face for 3D,) and the interior of the element separately. The parametric reference element also contains the global vertex number to compute shape functions with the right orientation. The following class collects the additional properties for all scalar high order elements:

```
class H1HighOrderFiniteElement : public NodalFiniteElement
{
public:
  int vnums[8];   // global vertex number
  int order_inner;
  int order_face[6];
  int order_edge[12];
public:
  H1HighOrderFiniteElement (int spacedim, ELEMENT_TYPE aeltype);
  void SetVertexNumbers (Array<int> & vnums);
  void SetOrderInner (int oi);
  void SetOrderFace (const Array<int> & of);
  void SetOrderEdge (const Array<int> & oe);

  virtual void ComputeNDof () = 0;
};
```

Now, for each element geometry (trig, quad, tet, hex, ..), one high order finite element class is defined. It computes the number of shape functions and the shape functions for a specified order in each edge and the interior:

```
class H1HighOrderTrig : public H1HighOrderFiniteElement
{
  H1HighOrderTrig (int aorder);
  virtual void ComputeNDof();
  virtual void CalcShape (const IntegrationPoint & ip,
                          Vector<> & shape) const;
};
```

In contrast to the `NodalFiniteElement`, the `HCurlFiniteElement3D` computes a matrix of shape functions, and a matrix of the curl of the shape functions:

```
class HCurlFiniteElement3D : public FiniteElement
{
  ...
  virtual void CalcShape (const IntegrationPoint & ip,
                          Matrix<> & shape) const = 0;
  virtual void CalcCurlShape (const IntegrationPoint & ip,
                              Matrix<> & dshape) const;
};
```

2.1.6 The shape tester

The shape tester is a tool to visualize the basis-functions. It was written for debugging the shape functions. There pops up a dialog box to select the index of the basis function.

```
geometry = examples/cube.geo
mesh = examples/cube.vol

define fespace v -h1ho -order=3
define gridfunction u -fespace=v

numproc shapetester np1 -gridfunction=u
```

2.2 Integration of bilinear-forms and linear-forms

After choosing the basis $\{\varphi_1, \ldots, \varphi_N\}$ for the finite element space, the system matrix $A \in \mathbb{R}^{N\times N}$ and right hand side vector $f \in \mathbb{R}^N$ are defined by

$$A_{i,j} := A(\varphi_i, \varphi_j) \qquad \text{and} \qquad f_j := f(\varphi_j).$$

For now, we assume that $A(.,.)$ has the structure

$$A(u, v) = \int_\Omega B(v)^t D B(u)\, dx,$$

where $B(u)$ is some differential operator such as $B(u) = \nabla u$, $B(u) = u$, $B(u) = \operatorname{curl} u$, etc. etc. The matrix D is a coefficient matrix, e.g., $D = \lambda(x) I$. Similar, the linear-form has the structure

$$f(v) = \int_\Omega d^t B(v)\, dx,$$

where d is the coefficient vector. The case of boundary-integrals follows the same lines.

The convenient way to compute the global matrix is to split the integral over Ω into integrals over the elements T, and use that the restriction of the global basis function φ_i onto the element T is a shape function φ_α^T:

$$A_{i,j} = \int_\Omega B(\varphi_j)^t D B(\varphi_i)\, dx = \sum_{T \in \mathcal{T}} \int_T B(\varphi_\beta^T)^t D B(\varphi_\alpha^T)$$

One computes local *element matrices* $A^T \in \mathbb{R}^{N_T \times N_T}$ by

$$A_{\alpha,\beta}^T = \int_T B(\varphi_\beta^T)^t D B(\varphi_\alpha^T)\, dx,$$

and assembles them together to the global matrix

$$A = \sum_T (C^T)^t A^T C^T,$$

where $C_T \in \mathbb{R}^{N_T, N}$ is the *connectivity matrix* relating the restriction of the global basis function φ_i to the local ones via

$$\varphi_i|_T = \sum_{\alpha=1}^{N_T} C_{\alpha,i}^T \varphi_\alpha^T.$$

Usually, the C^T consists mainly of 0s, and has N_T entries 1. E.g., the orientation of edges can be included into the connectivity matrices by -1 entries.

For many special cases, the integrals can be computed explicitely. But for more general cases (e.g., with general coefficients), they must be computed by numerical integration.

For this, let $IR^k = \{(x_i, \omega_i)\}$ be an integration rule or order k for the reference element $\widehat{T}$, i.e.,

$$\int_{\widehat{T}} f(x)\,dx \approx \sum_{(x_i,\omega_i)\in IR^k} \omega_i f(x_i),$$

and the formula is exact for polynomials up to order k. The best integration rules for the 1D reference element are Gauss-rules, which can be generated for an arbitrary order k. On other elements (quads, trigs, tets, hexes, ...) integration rules are formed by tensor product construction.

On a general element T, which is obtained by the transformation F_T, i.e., $T = F_T(\widehat{T})$, the transformed integration rule is

$$\int_T f(x)\,dx \approx \sum_{(x_i,\omega_i)\in IR^k} \omega_i f(F_T(x_i)) \det(F_T'(x_i)).$$

Computing the element matrices by the integration rule gives

$$A^T_{\alpha,\beta} \approx \sum_{(x_i,\omega_i)} \omega_i B(\varphi^T_\beta)(F_T(x_i))^t D B(\varphi^T_\alpha)(F_T(x_i))\ \det(F_T'(x_i)).$$

By combining the vectors $B(\varphi^T_i)(F_T(x_i))$ to a matrix (called B-matrix), the whole matrix A^T can be written as

$$\begin{aligned} A^T &\approx \sum_{(x_i,\omega_i)} \omega_i \begin{pmatrix} B(\varphi^T_1)^t \\ B(\varphi^T_2)^t \\ \vdots \\ B(\varphi^T_{N_T})^t \end{pmatrix} D\Big(B(\varphi^T_1), \ldots, B(\varphi^T_{N_T})\Big) \det(F_T') \\ &= \sum_{(x_i,\omega_i)} \omega_i B^t D B\ \det(F_T') \end{aligned}$$

The advantage of the matrix form is that for the implementation optimized matrix-matrix operations can be used instead of hand-written loops.

2.2.1 Examples of integrator

In the case of the bilinear-form

$$\int \rho(x) uv\,dx,$$

i.e., $B(u) = u$ and $D = \rho(x)$, the B-matrix in $\mathbb{R}^{1\times N_T}$ is

$$B_{j,1} = (\varphi^T_j(x_i))_{i=1,\ldots N_T}.$$

The shape functions φ^T on the mapped element $T = F_T(\widehat{T})$ are defined by means of the shape functions $\hat{\varphi}$ on the reference element

$$\varphi^T(F_T(\hat{x})) := \hat{\varphi}(\hat{x}) \qquad \forall\, \hat{x} \in \widehat{T}.$$

The bilinear-form of a scalar 2^{nd} order problem with general coefficient matrix $a \in \mathbb{R}^{d\times d}$ is

$$\int_\Omega (a\nabla u) \cdot \nabla v \, dx.$$

In this case, the B-matrix is of dimension $d \times N_T$ and has the components

$$B_{k,j} = \frac{\partial \varphi_j^T}{\partial x_k}$$

To express these derivatives by derivatives on the reference element, the chain rule is involved (where $\frac{d}{dx}$ gives a row vector):

$$\frac{d\varphi^T}{dx} = \frac{d}{dx}\hat{\varphi}(F_T^{-1}(x)) = \frac{d\hat{\varphi}}{dx}(F_T^{-1}(x))\frac{dF_T^{-1}(x)}{dx} = \frac{d\hat{\varphi}}{dx}(F_T^{-1}(x))(F')^{-1}(F_T^{-1}(x)).$$

Rewriting for column-vectors $\nabla\varphi$ gives

$$\nabla\varphi^T(F_T(\hat{x})) = (F')^{-T}(\hat{x})(\nabla\hat{\varphi})(\hat{x}).$$

By first setting up the $\widehat{B}$-matrix for the reference element, i.e.,

$$\widehat{B}_{k,j} = \frac{\partial \varphi_j}{\partial x_k},$$

the B-matrix is computed by the matrix-matrix operation

$$B = (F')^{-T}\widehat{B}. \tag{15}$$

The bilinear-form for *linear elasticity* (e.g., for 2D) involves the strain operator $\varepsilon(u) = \frac{1}{2}\{(\nabla u) + (\nabla u)^T\}$. We rewrite this symmetric strain-matrix as a strain-vector in the form

$$B(u) = \begin{pmatrix} \varepsilon_{11}(u) \\ \varepsilon_{22}(u) \\ 2\varepsilon_{12}(u) \end{pmatrix} = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} \\ \frac{\partial u_2}{\partial x_2} \\ \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \end{pmatrix}.$$

A basis for the vector-field (u_x, u_y) is built by taking 2 copies of the scalar basis and arranging it as

$$\left\{ \begin{pmatrix} \varphi_1^T \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_1^T \end{pmatrix}, \begin{pmatrix} \varphi_2^T \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_2^T \end{pmatrix}, \ldots, \begin{pmatrix} \varphi_{N_T}^T \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \varphi_{N_T}^T \end{pmatrix} \right\}.$$

Thus, the B-matrix in $\mathbb{R}^{3\times 2N_T}$ takes the form

$$B = \begin{pmatrix} \frac{\partial\varphi_1^T}{\partial x_1} & 0 & \frac{\partial\varphi_2^T}{\partial x_1} & 0 & \\ 0 & \frac{\partial\varphi_1^T}{\partial x_2} & 0 & \frac{\partial\varphi_2^T}{\partial x_2} & \cdots \\ \frac{\partial\varphi_1^T}{\partial x_2} & \frac{\partial\varphi_1^T}{\partial x_1} & \frac{\partial\varphi_2^T}{\partial x_2} & \frac{\partial\varphi_2^T}{\partial x_1} & \end{pmatrix}$$

2.2.2 A template family of integrators

The element-matrix (and element-vector) integrators are implemented as classes. The base class provides the interface to a function for computing the element matrix. It cannot be implemented for the base-class, so it is a pure virtual function:

```
class BilinearFormIntegrator
{
public:
  virtual
  void AssembleElementMatrix (const FiniteElement & fel,
                              const ElementTransformation & eltrans,
                              Matrix<double> & elmat) = 0;
  ...
};
```

One has to provide a `FiniteElement`, which can evaluate the shape functions on the reference element. The `ElementTransformation` knows about the mapping F_T, and can compute metric quantities such as F_T'. The result is returned in the matrix `elmat`.

The common properties for integrators of the form $\int B(v)^t D B(u) dx$ are combined into the family of classes `T_BDBIntegrator`. Each member of the family has its own differential operator $B(.)$, and coefficient-matrix D. Such families of classes can be realized by class-templates:

```
template <class DIFFOP, class DMATOP>
class T_BDBIntegrator : public BilinearFormIntegrator
{
protected:
  DMATOP dmatop;
public:

  virtual void
  AssembleElementMatrix (const FiniteElement & fel,
                         const ElementTransformation & eltrans,
                         Matrix<double> & elmat) const
  {
     int ndof = fel.GetNDof();
     elmat.SetSize (DIFFOP::DIM * ndof);
     elmat = 0;

     Matrix<double> bmat (DIFFOP::DIM_DMAT, DIFFOP::DIM * ndof);
     Matrix<double> dbmat (DIFFOP::DIM_DMAT, DIFFOP::DIM * ndof);
     Mat<DIFFOP::DIM_DMAT, DIFFOP::DIM_DMAT, double> dmat;
     const IntegrationRule & ir = GetIntegrationRule (fel);

     for (int i = 0 ; i < ir.GetNIP(); i++)
     {
       SpecificIntegrationPoint  ip(ir[i], eltrans);

       DIFFOP::GenerateMatrix (fel, ip, bmat);
       dmatop.GenerateMatrix (fel, ip, dmat);

       double fac = ip.GetJacobiDet() * ip.Weight();

       dbmat = fac * (dmat * bmat);
       elmat += Trans (bmat) * dbmat;
     }
   }
}
```

The dimension of the element matrices depend on the number of shape functions provided by finite element, and of the differential operator. The diff-op provides the dimension of the D-matrix (called DIFFOP::DIM_DMAT), as well as the number of copies of the finite element, e.g., 2 for linear elasticity in 2D, (called DIFFOP::DIM). While the size of the B-matrix depends on the finite element, the size of the D-matrix is fixed at compile-time. For this, once the matrix-class Matrix of dynamic size, and once, the matrix class with fixed size Mat<H,W> is used. The integration rule depends on the geometry of the element, and the polynomial order of the shape functions. The SpecificIntegrationPoint stores the Jacobi matrix, which is computed by the ElementTransformation eltrans.

The DIFFOP class has the function GenerateMatrix to compute the B-matrix. It does not need additional data, so a static function of the class is called. Similar, the DMATOP class computes the D-matrix. But now, data (such as the value of coefficients) are involved, and a function for the variable dmatop is called. The linear algebra expressions compute the element matrix as derived above.

Some more secrets:

- Memory management to avoid many allocate/delete-operations
- combining several integration points for longer inner loops
- B-matrix of fixed height at compile-time

A differential operator has to provide some values such as the dimension of the D-matrix, and has to compute the B-matrix. A gradient differential operator for D dimensions is DiffOpGradient<D>. The B-matrix is computed according to equation (15):

```
/// Gradient operator of dimension D
template <int D> class DiffOpGradient
```

```
{
public:
  enum { DIM = 1 };
  enum { DIM_SPACE = D };
  enum { DIM_ELEMENT = D };
  enum { DIM_DMAT = D };

  static void GenerateMatrix (const FiniteElement & fel,
                              const SpecificIntegrationPoint & ip,
                              Matrix<double> & mat)
  {
    mat = Trans (ip.GetJacobianInverse ()) * Trans (fel.GetDShape(ip));
  }
};
```

To provide a simpler use of the integrators, we have defined classes combining differential operators and coefficient matrices, such as a D-dimensional `LaplaceIntegrator<D>`:

```
template <int D>
class LaplaceIntegrator : public T_BDBIntegrator<DiffOpGradient<D>, DiagDMat<D> >
{
public:
  LaplaceIntegrator (CoefficientFunction * coeff)
    : T_BDBIntegrator<DiffOpGradient<D>, DiagDMat<D> > (DiagDMat<D> (coeff))
  {
    ;
  }
};
```

A tutorial showing how to use the finite elements and integrators is `netgen/ngsolve/tutorial/demo_fem.cpp`

2.3 Linear algebra concepts

Vectors and matrices are central data types for any mathematical simulation software. There are different competing design choices. E.g., if one needs many operations with small matrices, or little operations with large ones. The first type is the one I have in mind for the (dense) element matrix computations, while the second one is the type for the assembled global (sparse) matrices. A related choice is whether matrix-matrix operations are useful, or if just matrix-vector multiplications are efficiently possible.

2.3.1 Matrix and Vector data types

The cheapest useful vector data type stores the size of the vector, and has a pointer to the data. In NGSolve, such a vector is called `FlatVector`. The prefix `Flat` is always used for classes not taking care about memory-management. Such a `FlatVector` is used, when one wants to use ones own allocation, or, if the data already exists in memory, and one wants to put a Vector - data-structure over this array. The `FlatVector` is a template-class, where the template argument specifies the data type for the elements of the vector. Useful types are, e.g., `double` or `std::complex<double>` from the C++ standard library.

In the constructor, the vector-size and the pointer to the memory are set. One can access the size, and one can access the vector's elements with the bracket-operator, for example `u(i) = v(i) + w(i)`:

```
template <typename T = double>
class FlatVector
{
protected:
  int size;
  T * data;
public:
  FlatVector (int as, T * adata) : size(as), data(adata) { ; }

  int Size () const { return size; }

  T & operator() (int i) { return data[i]; }
  const T & operator() (int i) const { return data[i]; }
};
```

The `Vector` class extends the `FlatVector` by memory management. In the constructor, the vector size is given. The `Vector` allocates the required memory, and initializes the base class with it. The `Vector` has a destructor cleaning up the memory:

```
template <typename T = double>
class Vector : public FlatVector<T>
{
```

```
public:
 Vector (int as) : FlatVector<T> (as, new T[as]) { ; }
  ~Vector() { delete [] data; }
};
```

Possible uses of `Vector` and `FlatVector` are:

```
  Vector<double> u(10);
  FlatVector<double> subvec(&u(6), 4);
```

Often, the size of the vector is known at compile-time. For this case, there is the `Vec` template class. It can use static memory, instead of dynamic:

```
template <int SIZE, typename T = double>
class Vec
{
protected:
  T data[SIZE];
public:
  Vec () { ; }

  int Size () const { return SIZE; }

  T & operator() (int i) { return data[i]; }
  const T & operator() (int i) const { return data[i]; }
};
```

Possible uses are for 3D - point coordinates. One can also build `Vector`s, where the elements are `Vec`s:

```
  Vector<Vec<3,double> > u(10);
  u(10)(0) = 5;
```

In a similar way, there exist the matrix types `FlatMatrix`, `Matrix`, and `Mat`. The access operators are of the form `m(i,j)`.

2.3.2 Vector operations

Vectors should provide the vector space operations 'sum of vectors' and 'multiplication with a scalar'. A nice way to code vector-operations is like

```
  Vector<double> u(10), v(10), w(10);
  double alpha;
  u = alpha * v + w;
```

The C++ beginners implementation is to implement the '+' operator, the '*' operator, and the assignment operator '=' as follows:

```
template<typename T>
Vector<T> operator+ (const FlatVector<T> & a, const FlatVector<T> & b)
{
  Vector<T> temp(a.Size());
  for (int i = 0; i < a.Size(); i++) temp(i) = a(i) + b(i);
  return temp;
}

template<typename T>
Vector<T> operator* (double a, const FlatVector<T> & b)
{
  Vector<T> temp(a.Size());
  for (int i = 0; i < b.Size(); i++) temp(i) = a * b(i);
  return temp;
}

class FlatVector<T>
{
  ...
  FlatVector<T> & operator= (const FlatVector<T> & v)
  {
     for (int i = 0; i < size; i++) data[i] = v(i);
     return *this;
  }
};
```

This vector implementation allows the nice notation, but at the costs of low performance: Temporary objects must be allocated inside the operator functions, and, additionally for the return values.

To avoid such temporary objects, one can provide the following assignment methods:

```
class FlatVector<T>
{
  ...

  FlatVector<double> & void Set (double alpha, FlatVector<T> & v)
  {
     for (int i = 0; i < size; i++) data[i] = alpha * v(i);
     return *this;
  }

  FlatVector<double> & Add (double alpha, FlatVector<T> & v)
  {
    for (int i = 0; i < size; i++) data[i] += alpha * v(i);
    return *this;
  }
```

The use of these methods look like:

```
  u . Set (alpha, v) . Add (1, w);
```

... not that nice, but more efficient.

The remedy for this performance-readability conflict are *expression templates*. The above operator notation gets inefficient, since the memory to store the result is not available when just knowing the vector arguments. The idea is to return a symbolic object representing the sum of two vectors. This representation knows how to evaluate the elements of the sum:

```
  template <typename VA, typename VB>
  class SumVector
  {
    const VA & veca;
    const VB & vecb;
  public:
    SumVector (const VA & a, const VB & b) : veca(a), vecb(b) { ; }
    VA::TELEM operator() (int i) { return veca(i)+vecb(i); }
  };

  template <typename VA, typename VB>
  SumVector<VA, VB> operator+ (const VA & a, const VB & b)
  { return SumVector<VA, VB> (a, b); }
```

The computation can only happen at a stage, when the memory for the result is known. This is the case in the assignment operator:

```
  class FlatVector
  {
    ...
    template <typename VA, typename VB>
    void operator= (const SumVector<VA, VB> & sum)
    {
      for (int i = 0; i < size; i++)  data[i] = sum(i);
    }
  }
```

Now, a construct like

```
   u = v + w;
```

is possible. The '+' operator returns the object SumVector<Vector<double>, Vector<double> >. The '*' operator is defined similar:

```
template <typename VB>
class ScaleVector
{
  double scal;
  const VB & vecb;
public:
  ScaleVector (double a, const VB & b) : scal(a), vecb(b) { ; }
  VB::TELEM operator() (int i) { return scal*vecb(i); }
};

template <typename VB>
ScaleVector<VB> operator* (double, const VB & b)
{ return ScaleVector<VB> (a, b); }
```

It is also possible to combine expressions:

```
 u = alpha * v + w;
```

This results in a type SumVector<ScaleVector<Vector<double> >, Vector<double> >.

The above concept has one problem: The operators (e.g., '+') have un-specialized template arguments, which define the operator for every type. This may conflict with other '+' operators (e.g., for connecting strings). One has to introduce a joint base class (called, e.g., VecExpr) for all vector classes (including SumVector etc.), and defines the operators for members of the VecExpr family, only. To find back from the base-class to the specific vector class, the so called *Barton and Nackman*-trick is applied: The base class is a template family, and the derived class instantiates the base-class template argument with itself:

```
template <typename T>
class VecExpr { };

template <typename T>
class FlatVector<T> : public VecExpr<FlatVector<T> >
{ ... };

template <typename VA, typename VB>
class SumVector : public VecExpr<SumVector<VA, VB> >
{ ... };
```

Now, the '+' operator can be defined for members of the VecExpr family, only:

```
  template <typename VA, typename VB>
  SumVector<VA, VB> operator+ (const VecExpr<VA> & a, const VecExpr<VB> & b)
  {
    return SumVector<VA,VB> (static_cast<VA> (a), static_cast<VB> & b);
  }
```

What happens for `u + v`, where the vectors are of type `FlatVector<double>` ? The elements `u` and `v` are derived from `VecExpr<FlatVector<double> >`, thus, the above '+' operator can be applied. The template parameters `VA` and `VB` are initialized with `FlatVector<double>`. Inside the function, the elements `a` and `b`, which are known to be of the base type `VecExpr<FlatVector<double> >`, are up-casted to the derived type `FlatVector<double>`, what is indeed a valid cast. The result will be of the type `SumVector<FlatVector<double>, FlatVector<double> >`.

The assignment operator also takes profit of the `VecExpr` family:

```
template <typename T> class FlatVector : public VecExpr<..>
{
  ...
  template <typename TV>
  FlatVector & operator= (const VecExpr<TV> & v)
  {
    for (int i = 0; i < size; i++) data[i] = static_cast<TV>(v) (i);
    return *this;
  }
}
```

This programming style is called *expression templates*. In NGSolve, these expression templates are implemented in the basic linear algebra for vectors and dense matrices. Vectors are considered to be matrices of width 1. Matrix expressions include matrix-matrix products, sums, differences, negative matrices, and transpose matrices.

Expression templates are a challenge for compilers. Newer compilers (e.g. gcc3.x, Visual.net) are able to generate code comparable to hand-written loops for the matrix-vector operations. It is important to declare all the involved functions as inline to combine everything into one block.

An example file showing the use of the basic linear algebra is *ngsolve/tutorial/demo_bla.cpp*.

2.3.3 Linalg library based on Matrix-Vector multiplication

The above concept applies well to dense matrices, but cannot be used this way for all matrix operations providing just a matrix-vector multiplication. Examples for such matrices are sparse matrices, or linear operators defined by iterative methods like Gauss-Seidel iteration.

Here, I am thinking about matrices of large dimension, where one does not worry about a few virtual function calls.

In this case, we have a base class BaseMatrix providing a matrix-vector multiplication:

```
class BaseMatrix
{
  virtual void MultAdd (double s, BaseVector & x, BaseVector & y) = 0;
     // y += s * Mat * x
};
```

The specific matrices are derived from BaseMatrix and overload the MultAdd method. For virtual functions, template-parameterized arguments are not allowed. Thus, one needs also a BaseVector class. For the large matrices, I decided for a second family of matrices and vectors independent of the Vector from the dense library. Vectors derived from BaseVector were called VVector with V like in virtual. This vector family provides the Set and Add functions:

```
class BaseVector
{
  virtual BaseVector & Set (double s, BaseVector & v) = 0;   // *this = s * v
  virtual BaseVector & Add (double s, BaseVector & v) = 0;   // *this += s * v
};
```

Also for the matrix-vector library, expression templates are defined to allow the 'nice' notation. But now, the evaluation does not access vector/matrix elements, but calls the virtual functions Set, Add, or MultAdd.

3 Key-technologies: Preconditioning and Adaptivity

The performance of the finite element method mainly depends on two components: How to generate good meshes, and how to solve the arising linear matrix equations. In this section, we discuss both of them.

3.1 Preconditioning

Usually, the finite element matrices are huge. Thus, a direct solver (like an LU factorization) would require too much CPU-time as well as memory. Iterative methods have to be applied.

A matrix C is called a preconditioner for A, if

- it approximates A, i.e., $C \approx A$,
- the matrix-vector multiplication with its inverse is possible.

The quality of the preconditioner depends on how well it approximates the matrix, and how efficient is the application of C^{-1}.

Some preconditioners are

- $C = I$: The application is very cheap, but the approximation of A is in general bad.
- The Jacobi preconditioner $C = \operatorname{diag}\{A\}$: The application is also very cheap, the approximation of A might be reasonable. One of the most popular ones.
- Take $C = A$: The approximation is perfect, but the application of C^{-1} is in general too expensive.

A preconditioner is usually applied to solve a linear equation $Ax = b$ by an iterative method. The simplest one is the Richardson iteration:

Take an initial guess x^0, e.g., $x^0 = 0$
Compute iteratively

$$x^{k+1} = x^k + C^{-1}(b - Ax^k)$$

The iteration is stopped as soon as the residual $b - Ax^k$ is small. In the case of a symmetric and positive definite matrix C, a useful norm is

$$\|b - Ax^k\|^2_{C^{-1}} := (b - Ax^k)^T C^{-1} (b - Ax^k).$$

The evaluation requires just one additional inner product. The spectral radius ρ of $I - C^{-1}A$ is the largest absolute value of an eigen-value of $I - C^{-1}A$. If $\rho < 1$, then the Richardson iteration converges with convergence rate ρ.

For symmetric and positive definite matrices A and C, the conjugate gradient iteration can be applied. One step is comparable cheap to the Richardson iteration, but it converges much faster. There exist many extensions for non-symmetric matrices (GMRes, QMR, BiCG, ...).

In NGSolve, preconditioners are defined as follows

```
define preconditioner c1 -type=direct -bilinearform=a
define preconditioner c2 -type=local -bilinearform=a  -test
```

This defines once the preconditioner $C_1 = A$, and the Jacobi preconditioner $C_2 = \text{diag}\{A\}$. The bilinear-form A must be defined in advance. The direct preconditioner is realized by a sparse Cholesky factorization of the (symmetric) matrix A. The `-test` flag specifies that the eigenvalues of $C_2^{-1}A$ will be computed, which is usually of interest when testing the preconditioners.

The preconditioner is applied when solving the linear system by the `numproc bvp`:

```
numproc bvp np1 -bilinearform=a -linearform=f -gridfunction=u -preconditioner=c2
```

This calls the conjugate gradient iteration with preconditioner C_2. If no preconditioner is specified, the trivial one $C = I$ is chosen. One can specify the relative accuracy (with, e.g., `-prec=1e-8`) at which the equation is solved, and the maximal allowed iteration number (with, e.g., `-maxstep=1000`). When adding the flag `-qmr`, the quasi minimal residual (QMR) iteration for non-symmetric matrices is used instead of the conjugate gradient iteration.

3.1.1 Block Jacobi preconditioners

A generalization of the Jacobi preconditioner is to take a block version. This is defined by

$$C^{-1} = \sum_{i=1}^{m} E_i (E_i A E_i^t)^{-1} E_i^t,$$

where E_i is a $n \times n_i$ matrix, where each column vector is a unit vector. One has to invert m matrices $A_i := E_i A E_i^t$ of the 'small' dimension n_i. The original Jacobi preconditioner is included, here is $m = n$ and $E_i = (e_i)$.

It is possible that each unit vector e_j occurs in exactly one matrix E_i, or, it may appear in several ones. These versions are called non-overlapping, and overlapping, respectively. The idea of choosing the blocks is to design robust preconditioners with respect to some (bad) parameters, e.g.,

- Anisotropic meshes: Choose blocks along the short direction(s)
- High order methods: Choose blocks containing all unknowns associated with an edge, face, or cell
- Maxwell equations: Choose blocks containing gradient basis functions

A block-Jacobi preconditioner is defined by adding the `-block` flag:

```
define preconditioner c -type=local -bilinearform=a -block
```

In NGSolve, the blocks are provided by the finite element space (`FESpace`) object. The method `CreateSmoothingBlocks` returns a table of size m. Each entry i of the table contains the set of degrees of freedom associated with the block E_i. The matrix class `BlockJacobiPrecond` implements the matrix-vector operation $C^{-1} \times v$.

3.1.2 Block Gauss-Seidel iteration and preconditioners

A step of the Richardson iteration with a block-Jacobi preconditioner can be written as

```
Compute $d = b - Ax$, set $w = 0$
for $i = 1, \dots m$ do
    Get small vector $d_i = E_i^t d$
    Compute small correction $w_i = A_i^{-1} d_i$
    Collect vector $w = w + E_i w_i$
Update vector $x = x + w$
```

Instead of computing all the updates for the same residual d, an updated residual can be used for each step:

```
for $i = 1, \dots m$ do
    Get small vector $d_i = E_i^t (b - Ax)$
    Compute small correction $w_i = A_i^{-1} d_i$
    Update vector $x = x + E_i w_i$
```

This procedure defines also a preconditioner: Given a right hand side vector, start with $x = 0$, and perform one or more Gauss-Seidel iterations. Then set $C^{-1} b := x$. If one performs the symmetric version, i.e., add the inverse loop for $i = m, \dots, 1$ afterwards, one obtains a symmetric preconditioner (provided that A is symmetric).

The implementation of the (block) Gauss-Seidel iteration depends on the storage of the matrix. Usually, a sparse matrix format stores the non-zero elements (by column indices and values) for each row. This allows a cheap evaluation of the components $d_i = E_i^t (b - Ax)$ of the residual. If only one half of a symmetric matrix is stored, the (block) Gauss Seidel iteration is still possible, bot more tricky. The Gauss-Seidel iteration is implemented in the `GSSmooth` method of the `BlockJacobiPrecond` class.

3.1.3 Twogrid and multigrid preconditioners

The approximation $C \approx A$ of a (block) Jacobi preconditioner gets worse, as the mesh becomes finer. This leads to increasing numbers of necessary iterations. Here, the twogrid (and multigrid) techniques help. The idea is to define additionally a coarse mesh, and assemble the according finite element matrix A_H. Assume that it is much smaller, and a exact factorization is possible. Then, the inverse of the coarse grid matrix can be used as additional component in the preconditioner.

We need a grid transfer operator, called E_H, which transfers finite element functions from the coarse grid to finite element functions on the fine grid. This operator is called *prolongation*. Similar, one has to transfer residuals from the fine grid to residuals on the coarse grid. This operator is called *restriction*, and is usually chosen as the transpose E_h^t. Then, an additive two-grid preconditioner is

$$C^{-1} = E_H A_H^{-1} E_H^t + \sum_{i=1}^{m} E_i A_i^{-1} E_i.$$

The local fine grid steps are the same as in the block-Jacobi version. The quality of the two-grid preconditioner depends now on the ratio of the mesh sizes between the (actual) fine grid, and the (artificial) coarse grid. The additional costs are due to the factorization of the coarse grid matrix. These are competing goals in choosing the best coarse grid. The solution is *multigrid*, which introduces a whole sequence of grids in between. The NGSolve finite element spaces can provide a `Prolongation` object performing the grid transfer operations.

Usually, one starts from a coarse grid, which is refined to obtain the fine grid. In this case of nested grids, the prolongation and restriction operators pop up naturally (e.g., by setting the vertex value on the fine grid as mean value of its two parents on the coarser grid).

Instead of an Jacobi-like additive coarse grid step, it can be also performed Gauss-Seidel like after the local steps. This is indeed the classical two/multigrid method. The collection of local steps is called *smoother*.

In NGSolve, the multigrid preconditioner can be defined as

```
define preconditioner c -type=multigrid -bilinearform=a
      -smoothingsteps=1 -smoother=block
```

One can choose between a Gauss-Seidel (default) and the block-Gauss-Seidel smoother (with `-smoother=block`), and can choose a few parameters. The `-smoothingsteps` choose the number of local steps before and after the coarse grid correction step.

The flag `-cycle` chooses the number of recursive calls to the next coarser level. The default is `-cycle=1`, which is called the multigrid-V-cycle. The 2-cycle is called the multigrid-W-cycle. Choosing `-cycle=0` gives the Gauss-Seidel iteration on the fine grid only. This is the way to choose a Gauss-Seidel preconditioner in NGSolve.

3.1.4 Preconditioning for high order finite elements

The preconditioners for high order finite element matrices are built similar to twogrid preconditioners: Here, one artificially assembles a finite element matrix for the corresponding lowest order finite elements. One runs a block-Jacobi / block-Gauss-Seidel iteration for the high order space (e.g., with blocks related to edges, faces, cells), and then performs a correction step with the low order matrix.

Like a prolongation operator for the twogrid method, one needs a transfer matrix from the low order basis to the high order basis. If the high order basis is built such that the low order basis functions are a subset of the high order basis functions, then the transfer operator is trivial: Just take these coefficients, and set the high order coefficients to 0. In NGSolve, the low order basis functions are always the first basis functions for the high order space.

One can combine both techniques: Define a coarse grid, on which the low order finite element matrix can be factorized. Build the low order finite element matrix on a fine grid as an intermediate level. For this one, only (Gauss-Seidel) smoothing is performed. Finally, do smoothing only for the high order matrix on the fine grid. This sequence of operations is involved when defining the `multigrid` preconditioner. The artificial low order matrices are generated automatically for the high order finite element spaces.

3.2 A posteriori error estimates and Local Mesh Refinement

We will derive methods to estimate the error of the computed finite element approximation. Such *a posteriori* error estimates may use the finite element solution u_h, and input data such as the source term f:

$$\eta(u_h, f)$$

An error estimator is called *reliable*, if it is an upper bound for the error, i.e., there exists a constant C_1 such that

$$\|u - u_h\|_V \leq C_1 \, \eta(u_h, f) \tag{16}$$

An error estimator is *efficient*, if it is a lower bound for the error, i.e., there exists a constant C_2 such that

$$\|u - u_h\|_V \geq C_2 \, \eta(u_h, f). \tag{17}$$

The constants will in general depend on the shape of the triangles, but must not depend on the source term f, or the (unknown) solution u. They should not depend on the shape of the domain Ω.

One use of the a posteriori error estimator is to know the accuracy of the finite element approximation. A second one is to guide the construction of a new mesh to improve the accuracy of a new finite element approximation.

The usual error estimators are defined as sum over element contributions:

$$\eta^2(u_h, f) = \sum_{T \in \mathcal{T}} \eta_T^2(u_h, f)$$

The local contributions should correspond to the local error. For the common error estimators there holds the local efficiency estimates

$$\|u - u_h\|_{V(\omega_T)} \geq C_2 \, \eta_T(u_h, f).$$

The patch ω_T contains T and all its neighbor elements.

We consider variational problems: Find $u \in V$ such that

$$A(u, v) = f(v) \qquad \forall \, v \in V,$$

where $A(.,.)$ is an inf-sup stable bilinear-form:

$$\inf_{u \in V} \sup_{v \in V} \frac{A(u, v)}{\|u\|_V \, \|v\|_V} \succeq 1.$$

In particular, if $A(.,.)$ is coercive ($A(v,v) \succeq \|v\|_V^2$), then $A(.,.)$ is inf-sup stable. The inf-sup stability includes more general problems such as saddle-point problems, or Helmholtz-type problems (if not in resonance). This stability property allows to transfer the error to a residual:

$$\|u-u_h\|_V \preceq \sup_{v\in V} \frac{A(u-u_h,v)}{\|v\|_V} = \sup_{v\in V} \frac{f(v)-A(u_h,v)}{\|v\|_V} = \|f(.)-A(u_h,.)\|_{V^*} \tag{18}$$

We will work on this residual in the following sections.

3.2.1 Partition of unity and the Clément operator

A partition of unity is a family of local functions $\{\psi_i\}$ such that

$$\sum \psi_i = 1 \qquad \text{and} \qquad 0 \leq \psi_i \leq 1.$$

A partition of unity associated with the triangulation $\mathcal{T}$ satisfies

$$\operatorname{supp} \psi_i \subset \omega_{V_i},$$

where ω_{V_i} is the vertex patch $\cup_{V_i \in T} T$. One particular p.u. are the vertex basis functions. They satisfy

$$\|\nabla \psi_i\|_{L_\infty} \preceq h_i^{-1}.$$

The h_i is the maximal diameter of elements connected with the vertex V_i. The constant in this estimate depends on the shape of the triangles.

The p.u. allows to localize a function. Take $v \in H^1(\Omega)$, then $(\psi_i v) \in H_0^1(\omega_{V_i})$, with norm bounds

$$\begin{aligned} \|\nabla(\psi_i v)\|_{L_2} &\leq \|(\nabla\psi)v\|_{L_2} + \|\psi \nabla v\|_{L_2} \\ &\leq h^{-1}\|v\|_{L_2} + \|\nabla v\|_{L_2}. \end{aligned}$$

This is not a stable estimate, since the right hand side blows up for small mesh-sizes h. Except in L_p-spaces, a function cannot be decomposed stable into local functions. But, after subtracting a function resolving the mesh-scale, the localization is stable:

Theorem 2. *Assume there exists an operator $\Pi_h : V \to V_h$. Then following two claims are equivalent:*

- *The operator is bounded and satisfies an approximation property*

$$\|\nabla \Pi_h v\|_{L_2(\Omega)} + \|h^{-1}(v - \Pi_h v)\|_{L_2(\Omega)} \preceq \|\nabla v\|_{L_2(\Omega)}$$

- *The interpolation-rest $v - \Pi_h v$ can be stable localized, i.e.,*

$$v - \Pi_h v = \sum v_i \qquad s.t. \qquad \sum \|\nabla v_i\|_{L_2}^2 \preceq \|\nabla v\|_{L_2}^2$$

with $v_i = \psi_i v$.

Indeed, such operators are available (Clément, Scott-Zhang, ...). The constants depend on the shape of the triangles. The concept is the same for other function spaces.

3.2.2 Error estimators by solving local Dirichlet problems

By (18), there exists a $v \in V$ such that the error is bounded as

$$\|u - u_h\|_V \preceq \frac{f(v) - A(u_h, v)}{\|v\|}$$

Now, use the partition of unity to split the v into finite element part, and local components, i.e., $v = v_h + \sum v_i$ with $\|v_h\|^2 + \sum \|v_i\|^2 \preceq \|v\|^2$. This allows to bound the error

$$\begin{aligned}
\|u - u_h\|_V &\preceq \frac{f(v_h + \sum v_i) - A(u_h, v_h + \sum v_i)}{\{\|v_h\|_V^2 + \sum \|v_j\|_V^2\}^{1/2}} \\
&\leq \frac{|f(v_h) - A(u_h, v_h)|}{\{\|v_h\|_V^2 + \sum \|v_j\|_V^2\}^{1/2}} + \frac{\sum |f(v_i) - A(u_h, v_i)|}{\{\|v_h\|_V^2 + \sum \|v_j\|_V^2\}^{1/2}} \\
&\leq \frac{|f(v_h) - A(u_h, v_h)|}{\|v_h\|_V} + \frac{\sum \|v_i\| \frac{|f(v_i) - A(u_h, v_i)|}{\|v_i\|}}{\{\sum \|v_j\|_V^2\}^{1/2}} \\
&\leq \frac{|f(v_h) - A(u_h, v_h)|}{\|v_h\|_V} + \sum \frac{|f(v_i) - A(u_h, v_i)|^2}{\|v_i\|_V^2} \\
&\leq \frac{|f(v_h) - A(u_h, v_h)|}{\|v_h\|_V} + \Big\{ \sum \frac{|f(v_i) - A(u_h, v_i)|^2}{\|v_i\|_V^2} \Big\}^{1/2}
\end{aligned}$$

Finally, using the Galerkin orthogonality $A(u_h, v_h) = f(v_h)$, we obtain

$$\|u - u_h\|_V^2 = \sum \frac{|f(v_i) - A(u_h, v_i)|^2}{\|v_i\|_V^2} \leq \sum \sup_{\tilde{v}_i \in V_i} \frac{|f(\tilde{v}_i) - A(u_h, \tilde{v}_i)|^2}{\|\tilde{v}_i\|_V^2}$$

The last terms are dual norms in V_i^*, which can be (in principal) computed by solving variational problems:

$$\sup_{\tilde{v}_i \in V_i} \frac{|f(\tilde{v}_i) - A(u_h, \tilde{v}_i)|^2}{\|\tilde{v}_i\|_V^2} = \|w_i\|_V^2,$$

with $w_i \in V_i$ such that

$$(w_i, v_i)_V = f(v_i) - A(u_h, v_i) \qquad \forall\, v_i \in V_i.$$

Of course, the local Dirichlet problem cannot be solved exactly, but it can be approximated by a method of higher order.

3.2.3 Error estimators based on flux averaging

For the standard H^1-problem,

$$-\operatorname{div}(a\nabla u) = f,$$

the residual evaluates to

$$\sup_{v \in H^1} \frac{\int f v \, dx - \int a \nabla u_h \nabla v \, dx}{\|v\|}. \tag{19}$$

Since $a\nabla u_h$ has no divergence in L_2, we cannot integrate by parts. The idea is to compute an approximation for the flux, i.e.,

$$p_h \approx a\nabla u_h$$

such that $p_h \in H(\mathrm{div})$. This can be done by averaging into (normal)-continuous finite elements. Then

$$\begin{aligned}
\|u-u_h\|_V &\preceq \sup_{v\in V} \frac{\int fv\,dx - \int p_h \nabla v\,dx + \int (p_h - a\nabla u_h)\nabla v\,dx}{\|v\|} \\
&= \sup_{v\in V} \frac{\int (f + \operatorname{div} p_h) v\,dx + \int (p_h - a\nabla u_h)\nabla v\,dx}{\|v\|} \\
&\leq \|f + \operatorname{div} p_h\|_{H^{-1}} + \|p_h - a\nabla u_h\|_{L_2}
\end{aligned}$$

The H^{-1}-norm is not a local norm, as it was desired. By subtracting the Clément interpolant in the numerator of (19), one can avoid the dual norm, and achieve a scaled L_2 norm:

$$\|u-u_h\|_{H^1} \preceq \|h\,(f + \operatorname{div} p_h)\|_{L_2} + \|p_h - a\nabla u_h\|_{L_2}$$

Sometimes (e.g., lowest order elements), the first term can be skipped. Then, with averaging to continuous flux-elements, this estimator is the classical and most popular Zienkiewicz-Zhu error-estimator. In the case of jumping coefficients, or high order elements, the averaging into normal-continuous (Raviart-Thomas) elements is of advantage.

3.2.4 Goal driven error estimates

The above error estimators estimate the error in the energy norm V. Some applications require to compute certain values (such as point values, average values, line integrals, fluxes through surfaces, ...). These values are described by linear functionals $b : V \to \mathbb{R}$. We want to design a method such that the error in this goal, i.e.,

$$b(u) - b(u_h)$$

is small. The technique is to solve additionally the dual problem, where the right hand side is the goal functional:

$$\text{Find } w \in V: \qquad A(v,w) = b(v) \qquad \forall\, v \in V.$$

Usually, one cannot solve the dual problem either, and one applies a Galerkin method also for the dual problem:

$$\text{Find } w_h \in V_h: \qquad A(v_h,w_h) = b(v_h) \qquad \forall\, v_h \in V_h.$$

In the case of point values, the solution of the dual problem is the Green function (which is not in H^1). The error in the goal is

$$b(u-u_h) = A(u-u_h, w) = A(u-u_h, w-w_h).$$

A rigorous upper bound for the error in the goal is obtained by using continuity of the bilinear-form, and energy error estimates η^1 and η^2 for the primal and dual problem, respectively:

$$|b(u-u_h)| \preceq \|u-u_h\|_V \|w-w_h\|_V \preceq \eta^1(u_h, f)\, \eta^2(w_h, b).$$

A good heuristic is the following (unfortunately, not correct) estimate

$$b(u-u_h) = A(u-u_h, w-w_h) \preceq \sum_{T\in\mathcal{T}} \|u-u_h\|_{H^1(T)}\, \|w-w_h\|_{H^1(T)} \preceq \sum_{T} \eta^1_T(u_h, f)\, \eta^2_T(w_h, b) \tag{20}$$

The last step would require a local reliability estimate. But, this is not true.

We can interpret (20) that way: The local estimators $\eta^2_T(w_h)$ provide a way for weighting the primal local estimators according to the desired goal.

3.2.5 Mesh refinement algorithms

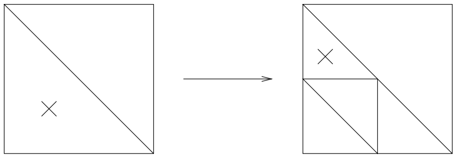
A posteriori error estimates are used to control recursive mesh refinement:

```
Start with initial mesh $\mathcal{T}$
Loop
    compute fe solution $u_h$ on $\mathcal{T}$
    compute error estimator $\eta_T(u_h, f)$
    if $\eta \leq$ tolerance then stop
    refine elements with large $\eta_T$ to obtain a new mesh
```

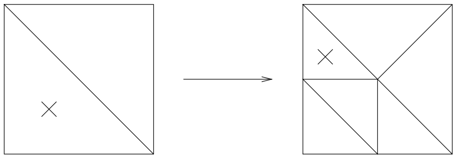
The mesh refinement algorithm has to take care of

- generating a sequence of regular meshes
- generating a sequence of shape regular meshes

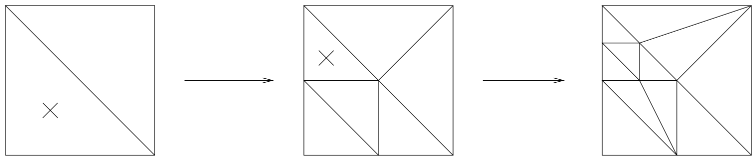
Red-Green Refinement:
A marked element is split into four equivalent elements (called red refinement):



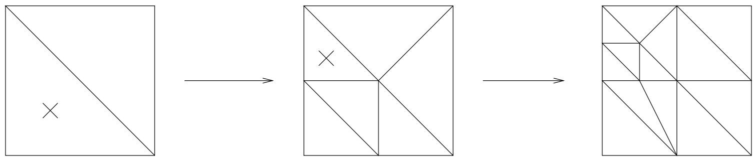
But, the obtained mesh is not regular. To avoid such irregular nodes, also neighboring elements must be split (called green closure):



If one continues to refine that way, the shape of the elements may get worse and worse:



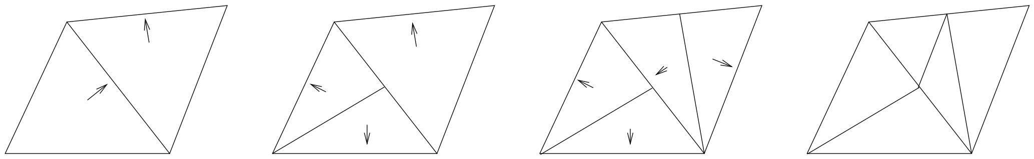
A solution is that elements of the green closure will not be further refined. Instead, remove the green closure, and replace it by red refinement.



Marked edge bisection:

Each triangle has one marked edge. The triangle is only refined by cutting from the middle of the marked edge to the opposite vertex. The marked edges of the new triangles are the edges of the old triangle.

If there occurs an irregular node, then also the neighbor triangle must be refined.



To ensure finite termination, one has to avoid cycles in the initial mesh. This can be obtained by first sorting the edges (e.g., by length), end then, always choose the largest edges as marked edge.

Both of these refinement algorithms are also possible in 3D.

4 Applications

4.1 Structural mechanics

Many engineering applications involve thin structures (walls of a building, body of a car, ...). On thin structures, the standard approach has a problem: One observed that the simulation results get worse as the thickness decreases. The explanation is that the constant in Korn's inequality gets small for thin structures. To understand and overcome this problem, we go over to beam, plate and shell models.

We consider a thin ($t \ll 1$) two-dimensional body

$$\Omega = I \times (-t/2, t/2) \qquad \text{with} \qquad I = (0,1)$$

Recall the bilinear-form in the case of an isotropic material:

$$A(u,v) = \int 2\mu \, \varepsilon(u) : \varepsilon(v) + \lambda \text{ div } u \text{ div } v \, dx$$

The goal is to derive a system of one-dimensional equations to describe the two-dimensional deformation. This we obtain by a semi-discretization. Define

$$\widetilde{V}_M = \left\{ \begin{pmatrix} u_x(x,y) \\ u_y(x,y) \end{pmatrix} \in V : u_x(x,y) = \sum_{i=0}^{M_x} u_x^i(x) y^i, \; u_y(x,y) = \sum_{i=0}^{M_y} u_y^i(x) y^i \right\}.$$

This function space on $\Omega \subset \mathbb{R}^2$ is isomorph to a one-dimensional function space with values in $\mathbb{R}^{M_x+M_y+2}$. We perform semi-discretization by searching for $\tilde{u} \in \widetilde{V}_M$ such that

$$A(\tilde{u}, \tilde{v}) = f(\tilde{v}) \qquad \forall \, \tilde{v} \in \widetilde{V}_M.$$

As $M_x, M_y \to \infty$, $\widetilde{V}_M \to V$, and we obtain convergence $\tilde{u} \to u$.

The lowest order (qualitative) good approximating semi-discrete space is to set $M_x = 1$ and $M_y = 0$. This is

$$\widetilde{V} = \left\{ \begin{pmatrix} U(x) - \beta(x) y \\ w(x) \end{pmatrix} \right\}$$

Evaluating the bilinear-form (of an isotropic material) leads to

$$\begin{aligned} A\left(\begin{pmatrix} U - y\beta \\ w \end{pmatrix}, \begin{pmatrix} \tilde{U} - y\tilde{\beta} \\ \tilde{w} \end{pmatrix} \right) \quad = \quad & (2\mu + \lambda) t \int_0^1 U' \tilde{U}' \, dx + \\ & (2\mu + \lambda) \frac{t^3}{12} \int_0^1 \beta' \tilde{\beta}' + 2\mu \frac{t}{2} \int_0^1 (w' - \beta)(\tilde{w}' - \tilde{\beta}) \, dx \end{aligned}$$

The meaning of the three functions is as follows. The function $U(x)$ is the average (over the cross section) longitudinal displacement, $w(x)$ is the vertical displacement. The function β is the linearized rotation of the normal vector.

We assume that the load $f(x,y)$ does not depend on y. Then, the linear form is

$$f\begin{pmatrix}\tilde{U}-y\tilde{\beta}\\ \tilde{w}\end{pmatrix} = t\int_0^1 f_x\tilde{U}\,dx + t\int_0^1 f_y\tilde{w}\,dx$$

The semi-discretization in this space leads to two decoupled problems. The first one describes the longitudinal displacement: Find $U \in H^1(I)$ such that

$$(2\mu+\lambda)t\int_0^1 U'\tilde{U}'\,dx = t\int_0^1 f_x\tilde{U}'\,dx \qquad \forall\, U' \in H^1(I).$$

The small thickness parameter t cancels out. It is a simple second order problem for the longitudinal displacement.

The second problems involves the 1D functions w and β: Find $(w,\beta) \in V = ?$ such that

$$(2\mu+\lambda)\frac{t^3}{12}\int_0^1 \beta'\tilde{\beta}'\,dx + \mu t\int_0^1 (w'-\beta)(\tilde{w}'-\tilde{\beta})\,dx = t\int_0^1 f_y\tilde{w}\,dx \qquad \forall\,(\tilde{w},\tilde{\beta}) \in V$$

The first term models bending. The derivative of the rotation β is (approximative) the curvature of the deformed beam. The second one is called the shear term: For thin beams, the angle $\beta \approx \tan\beta$ is approximatively w'. This term measures the difference $w'-\beta$. This second problem is called the Timoshenko beam model.

For simplification, we skip the parameters μ and λ, and the constants. We rescale the equation by dividing by t^3: Find (w,β) such that

$$\int \beta'\tilde{\beta}'\,dx + \frac{1}{t^2}\int (w'-\beta)(\tilde{w}'-\tilde{\beta})\,dx = \int t^{-2} f\tilde{w}\,dx. \tag{21}$$

This scaling in t is natural. With $t \to 0$, and a force density $f \sim t^2$, the deformation converges to a limit. We define the scaled force density

$$\tilde{f} = t^{-2} f$$

In principle, this is a well posed problem in $[H^1]^2$:

Lemma 3. *Assume boundary conditions $w(0) = \beta(0) = 0$. The bilinear-form $A((w,\beta),(\tilde{w},\tilde{\beta}))$ of (21) is continuous*

$$A((w,\beta),(\tilde{w},\tilde{\beta})) \preceq t^{-2}(\|w\|_{H^1} + \|\beta\|_{H^1})(\|\tilde{w}\|_{H^1} + \|\tilde{\beta}\|_{H^1})$$

and coercive

$$A((w,\beta),(w,\beta)) \geq \|w\|_{H^1}^2 + \|\beta\|_{H^1}^2$$

Proof: ...

As the thickness t becomes small, the ratio of the continuity and coercivity bounds becomes large ! This ratio occurs in the error estimates, and indicates problems. Really, numerical computations show bad convergence for small thickness t.

The large coefficient in front of the term $\int(w' - \beta)(\tilde{w}' - \tilde{\beta})$ forces the difference $w' - \beta$ to be small. If we use piece-wise linear finite elements for w and β, then w_h' is a piece-wise constant function, and β_h is continuous. If $w_h' - \beta_h \approx 0$, then β_h must be a constant function !

The idea is to weaken the term with the large coefficient. We plug in the projection P^0 into piece-wise constant functions: Find (w_h, β_h) such that

$$\int \beta_h' \tilde{\beta}_h' \, dx + \frac{1}{t^2} \int P^0(w_h' - \beta_h) \, P^0(\tilde{w}_h' - \tilde{\beta}_h) \, dx = \int \tilde{f} \tilde{w}_h \, dx. \tag{22}$$

Now, there are finite element functions w_h and β_h fulfilling $P^0(w_h' - \beta_h) \approx 0$.

In the engineering community there are many such tricks to modify the bilinear-form. Our goal is to understand and analyze the obtained method.

Again, the key is a mixed method. Start from equation (21) and introduce a new variable

$$p = t^{-2}(w' - \beta). \tag{23}$$

Using the new variable in (21), and formulating the definition (23) of p in weak form leads to the bigger system: Find $(w, \beta) \in V$ and $p \in Q$ such that

$$\begin{array}{ccccll} \int \beta' \tilde{\beta}' \, dx & + & \int (\tilde{w}' - \beta) p \, dx & = & \int \tilde{f} \tilde{w} \, dx & \forall \, (w, \beta) \in V \\ \int (w' - \beta) \tilde{p} \, dx & - & t^2 \int p \, \tilde{p} \, dx & = & 0 & \forall \, \tilde{p} \in Q. \end{array} \tag{24}$$

This is a mixed formulation of the abstract structure: Find $u \in V$ and $p \in Q$ such that

$$\begin{array}{ccccll} a(u, v) & + & b(v, p) & = & f(v) & \forall \, v \in V, \\ b(u, q) & - & t^2 c(p, q) & = & 0 & \forall \, q \in Q. \end{array} \tag{25}$$

The big advantage now is that the parameter t does not occur in the denominator, and the limit $t \longrightarrow 0$ can be performed.

This is a family of well posed problems.

Theorem 4 (Brezzi's theorem)**.** *Assume that $a(.,.)$ and $b(.,.)$ are continuous bilinear-forms*

$$a(u, v) \leq \alpha_2 \, \|u\|_V \, \|v\|_V \qquad \forall \, u, v \in V, \tag{26}$$

$$b(u, q) \leq \beta_2 \, \|u\|_V \, \|q\|_Q \qquad \forall \, u \in V, \; \forall \, q \in Q. \tag{27}$$

Assume there holds coercivity of $a(.,.)$ on the kernel,i.e.,

$$a(u, u) \geq \alpha_1 \, \|u\|_V^2 \qquad \forall \, u \in V_0, \tag{28}$$

and there holds the LBB (Ladyshenskaja-Babuška-Brezzi) condition

$$\sup_{u \in V} \frac{b(u,q)}{\|u\|_V} \geq \beta_1 \|q\|_Q \quad \forall\, q \in Q. \tag{29}$$

Then, the mixed problem is uniquely solvable. The solution fulfills the stability estimate

$$\|u\|_V + \|p\|_Q \leq c\{\|f\|_{V^*} + \|g\|_{Q^*}\},$$

with the constant c depending on $\alpha_1, \alpha_2, \beta_1, \beta_2$.

Theorem 5 (extended Brezzi)**.** *Assume that the assumptions of Theorem 4 are true. Furthermore, assume that*

$$a(u,u) \geq 0,$$

and $c(p,q)$ is a symmetric, continuous and non-negative bilinear-form. Then, the big form

$$B((u,p),(v,q)) = a(u,v) + b(u,q) + b(v,p) - t^2\, c(p,q)$$

is continuous and stable uniformly in $t \in [0,1]$.

We check Brezzi's condition for the beam model. The spaces are $V = [H^1]^2$ and $Q = L_2$. Continuity of the bilinear-forms $a(.,.)$, $b(.,.)$, and $c(.,.)$ is clear. The LBB condition is

$$\sup_{w,\beta} \frac{\int (w' - \beta) q\, dx}{\|w\|_{H^1} + \|\beta\|_{H^1}} \succeq \|q\|_{L_2}$$

We construct a candidate for the supremum:

$$w(x) = \int_0^x q(s)\, ds \qquad \text{and} \qquad \beta = 0$$

Then

$$\frac{\int (w' - \beta) q\, dx}{\|w\|_{H^1} + \|\beta\|_{H^1}} \succeq \frac{\int q^2\, dx}{\|w'\|} = \|q\|_{L_2}$$

Finally, we have to check kernel ellipticity. The kernel is

$$V_0 = \{(w,\beta) : \beta = w'\}.$$

On V_0 there holds

$$\begin{aligned} \|w\|_{H^1}^1 + \|\beta\|_{H^1}^2 &\preceq \|w'\|^2 + \|\beta\|_{H^1}^2 = \|\beta\|_{L_2}^2 + \|\beta\|_{H^1}^2 \\ &\preceq \|\beta'\|_{L_2} = a((w,\beta),(w,\beta)) \end{aligned}$$

The lowest order finite element discretization of the mixed system is to choose continuous and piece-wise linear elements for w_h and β_h, and piecewise constants for p_h. The discrete problem reads as: Find $(w_h, \beta_h) \in V_h$ and $p_h \in Q_h$ such that

$$\begin{array}{rcccl} \int \beta_h' \tilde{\beta}_h'\, dx & + & \int (\tilde{w}_h' - \beta_h) p_h\, dx & = & \int \tilde{f} \tilde{w}_h\, dx \qquad \forall\, (w_h, \beta_h) \in V_h \\ \int (w_h' - \beta_h) \tilde{p}_h\, dx & - & t^2 \int p_h\, \tilde{p}_h\, dx & = & 0 \qquad \forall\, \tilde{p}_h \in Q_h. \end{array} \tag{30}$$

This is a inf-sup stable system on the discrete spaces V_h and Q_h. This means, we obtain the **uniform** a priori error estimate

$$\begin{aligned}\|(w-w_h,\beta-\beta_h)\|_{H_1}+\|p-p_h\|_{L_2} &\preceq \inf_{\tilde{w}_h,\tilde{\beta}_h,\tilde{p}_h}\|(w-\tilde{w}_h,\beta-\tilde{\beta}_h)\|_{H_1}+\|p-\tilde{p}_h\|_{L_2}\\ &\preceq h\,\{\|w\|_{H^2}+\|\beta\|_{H^2}+\|p\|_{H^1}\}\end{aligned}$$

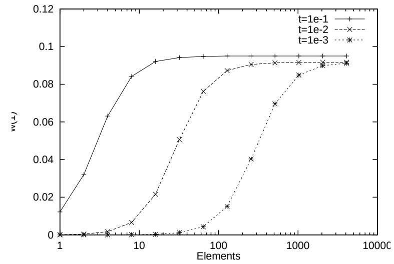
The required regularity is realistic.

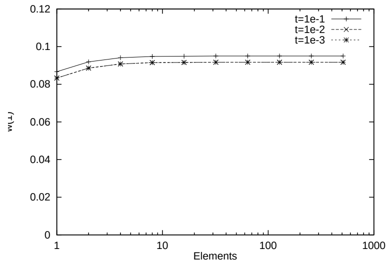
The second equation of the discrete mixed system (30) states that

$$p_h = t^{-2}P^0(w_h' - \beta_h)$$

If we insert this observation into the first row, we obtain exactly the discretization method (22) ! Here, the mixed formulation is a tool for analyzing a non-standard (primal) discretization method. Both formulations are equivalent. They produce exactly the same finite element functions. The mixed formulation is the key for the error estimates.

The two pictures below show simulations of a Timoshenko beam. It is fixed at the left end, the load density is constant one. We compute the vertical deformation $w(1)$ at the right boundary. We vary the thickness t between 10^{-1} and 10^{-3}. The left pictures shows the result of a standard conforming method, the right picture shows the results of the method using the projection. As the thickness decreases, the standard method becomes worse. Unless h is less than t, the results are completely wrong ! The improved method converges uniformly well with respect to t:





4.2 Wave equations

Wave equations can model acoustic, elastic, electro-magnetic, or any other type of waves. Acoustic waves (sound waves) involve as variables the air pressure p, and the velocity v of the air particles. A non-constant pressure accelerates particles, for which we assume the linear relation

$$\dot{v} = -c_1 \nabla p.$$

Sources of the velocity field lead to changing air density, and thus to changing air pressure:

$$\dot{p} = -c_2 \operatorname{div} v.$$

Combining the equations, and setting $c = c_1 c_2$ leads to the second order hyperbolic equation

$$\ddot{p} - c\Delta p = 0.$$

Waves can be excited from boundary values (e.g., vibrating structures), or volume terms. We assume some given volume sources f, and set (after renaming $u = p$)

$$\ddot{u} - c\Delta u = f.$$

Given boundary values, and initial values for u and $\dot{u}$, one can solve the equation in time domain. Most often, one is interested in the behavior of waves at certain frequencies. Thus, one assumes a time-harmonic source, e.g.,

$$f(x,t) = \underline{f}(x)\cos(\omega t)$$

Inserting the Ansatz $u(x,t) = \underline{u}(x)\cos(\omega t)$ into the equation leads to

$$-c\Delta \underline{u} - \omega^2 \underline{u} = \underline{f}.$$

If existent, this gives one solution for the instationary problem with some specific initial values. The weak formulation is to find $u \in H^1$ such that

$$\int_\Omega c\nabla u \nabla v \, dx - \omega^2 \int_\Omega uv \, dx = \int_\Omega fv \qquad \forall\, v.$$

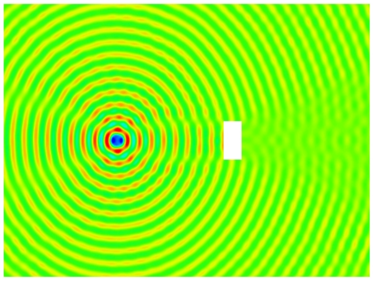
The involved bilinear-form is not elliptic, which does not allow to apply Lax-Milgram to prove existence and uniqueness of a solution. Indeed, it ω is a resonance frequency, i.e., there exists a non-zero u such that

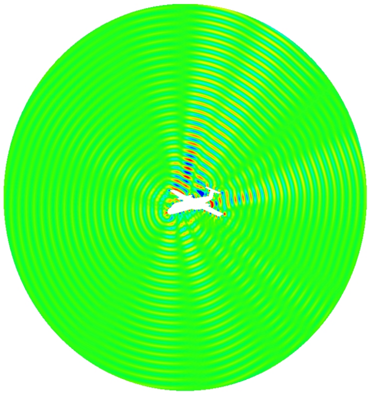
$$\int c\nabla u \nabla v \, dx = \omega^2 \int uv \, dx \qquad \forall\, v,$$

then the right hand side $f = 0$ has a non-trivial solution. ω^2 is an eigen-value, and u is the corresponding eigenfunction. On bounded domains (only !), the eigen-values are discrete (compact embedding of H^1 into L_2). If ω^2 is not an eigen-value, then there is a unique solution (Fredholm-theory).

4.2.1 Wave equations on unbounded domains

Unbounded domains are common for acoustic problems. Sound radiates into the (practically) unbounded atmosphere. If we want to use finite elements, we have to compute on a finite domain, and have to introduce artificial boundary conditions simulating the infinite domain. The picture left shows a sound wave which is scattered on a box (modeled by Neumann b.c.) The outer boundary conditions are so called absorbing boundary conditions, which imitate an infinite domain. The right picture shows a (radar) wave scattered form a 2D-airplane.





We start with the 1D equation $-cu'' + \ddot{u} = 0$ on $\mathbb{R}$. The functions

$$\cos(kx + \omega t + \alpha)$$

such that $ck^2 - \omega^2 = 0$ are solutions. These functions take the same values for all points $x = -\frac{\omega}{k}t$. This means, they travel with the speed of sound $-\frac{\omega}{k}$. If k is positive, then it is a left-going wave, otherwise, it is a right-going wave.

Our model is now:

- there are sources f only in a bounded interval I.
- left from I, the solution should be a left-going wave, and right from I, the solution should be a right-going wave

It will be easier to describe solutions by complex functions. The functions

$$u(x,t) = e^{i(kx+\omega t+\alpha)}$$

are solutions of the homogeneous problem. Taking the real part gives the physical solution. The functions satisfy

$$u'(x,t) = ike^{i(kx+\omega t+\alpha)} = iku(x,t).$$

This can be used as a boundary condition. Let $k = +\frac{\omega}{\sqrt{c}}$. The boundary condition

$$\frac{\partial u}{\partial n} = -iku$$

is satisfied by the right-going wave $u(x,t) = e^{i(-kx+\omega t+\alpha)}$ on the right boundary, and by the left-going wave $u(x,t) = e^{i(kx+\omega t+\alpha)}$ on the left boundary. The same Robin-type boundary conditions can be applied in 2D and 3D. It is exactly satisfied by waves in normal direction to the boundary, but is an approximation to waves in other directions.

The weak form is: Find $u \in H^1(\Omega, \mathcal{C})$ such that

$$\int_\Omega c \nabla u \nabla v \, dx - \omega^2 \int_\Omega uv \, dx - ik \int_{\Gamma_R} uv \, dx = \int_\Omega f v \, dx.$$

This problem has always a unique solution depending continuously on the right hand side.

The bilinear-form is complex and symmetric. The same holds for the arising finite element matrix. Efficient equation solvers are an interesting open problem !