More general formulation of finite-element method

- spaces for solutions of weak formulation of PDEs

  - as in the model problem, weak solutions can be with anadvantage looked for in much larger spaces than solutions of the PDEs

  - for many physical problems it is even more natural (systems with shocks waves, for example)

- a reminder of some basic notions on the linear space V:

  - linear form $L : V \to \mathbb{R}$: for all $v, w \in V$ and $\alpha, \beta \in \mathbb{R}$:
$$L(\alpha v + \beta w) = \alpha L(v) + \beta L(w)$$

  - bilinear form $a : V \times V \to \mathbb{R}$ is linear in both arguments

  - symmetric bilinear form : $a(v,w) = a(w,v)$ for all $v, w \in V$

  - inner (scalar) product is a symmetric bilinear form for which : $a(v,v) > 0$ for all $v \in V$

  - norm $\|\cdot\|_a$ corresponding to an inner product $a(\cdot,\cdot)$ is $\|v\|_a = \sqrt{a(v,v)}$ for all $v \in V$

  - Cauchy inequality for an arbitrary inner product
$$|a(v,w)| \leq \|v\|_a \|w\|_a$$

- Hilbert space is a linear space V with an inner product $(\cdot,\cdot)$ and a corresp. norm $\|\cdot\|$ which is complete

  i.e. every Cauchy sequence converges in the norm $\|\cdot\|$:

$$\left[\begin{array}{l} \text{if for } \forall \varepsilon > 0 \ \exists N \text{ such that } \|v_i - v_j\| < \varepsilon \text{ for all } i,j > N \\ \quad \text{then there is } v \in V : \|v - v_i\| \to 0 \text{ for } i \to \infty \end{array}\right]$$

- basic Hilbert spaces for elliptic problems

  1) on the interval $\langle a,b\rangle = I$

     a) a space of square-integrable functions
$$L_2(I) = \left\{ v,\ v \text{ is defined on } I \text{ and } \int_a^b v^2\,dx < \infty \right\}$$

with $(v,w) = \int_a^b v\,w\,dx$ and $\|v\|_{L_2(I)} = \sqrt{(v,v)}$

and thank to the Cauchy inequality (v,w) is well defined

b) for an elliptic problem, a more natural space is

$$H^1(I) = \{ v : v \text{ and } v' \text{ belong to } L_2(I) \}$$

with the inner product

$$(v,w)_{H^1(I)} = \int_a^b (vw + v'w')\,dx$$

and the norm $\|v\|_{H^1(I)} = \left(\int_a^b (v^2 + v'^2)\,dx \right)^{1/2}$

or its subspace

$$H_0^1(I) = \{ v \in H^1(I) : v(a) = v(b) = 0 \}$$

with the same inner product and norm

Example: our model problem $-\frac{d^2u}{dx^2} = f(x)$ on $\langle a,b\rangle$
and $v(a) = v(b) = 0$

can be reformulated as:

Find $u \in H_0^1(I)$ such that $(u',v') = (f,v)$ for all $v \in H_0^1(I)$
$\uparrow$ inner product on $L_2(I)$

- notice that $H_0^1(I)$ is larger than our original space and it is actually the largest space where the weak formulation makes sense

2) on the domain Ω in $\mathbb{R}^d$ which is bounded — now element in $\mathbb{R}^d$

$$L_2(\Omega) = \{ v : v \text{ is defined on } \Omega \text{ and } \int_\Omega v^2\,dx < \infty \}$$
$$\cup$$
$$H^1(\Omega) = \{ v \in L_2(\Omega) : \frac{\partial v}{\partial x_i} \in L_2(\Omega) \text{ for } i = 1, \dots, d \}$$

with inner products and norms

$$(v,w) = \int_\Omega v\,w\,dx \Rightarrow \|v\|_{L_2(\Omega)} = \left(\int_\Omega v^2\,dx \right)^{1/2}$$

$$(v,w)_{H^1(\Omega)} = \int_\Omega (vw + \nabla v \cdot \nabla w)\,dx \Rightarrow \|v\|_{H^1(\Omega)} = \sqrt{(v,v)_{H^1(\Omega)}}$$

and $H_0^1(\Omega) = \{ v \in H^1(\Omega) : v = 0 \text{ on the boundary } \Gamma \text{ of } \Omega \} \subset H^1(\Omega)$

again with the same inner product and norm as in $H^1(\Omega)$

Example: let us consider a Poisson equation in $\mathbb{R}^d$:

$$(D) \qquad \begin{aligned} -\Delta u &= f \quad \text{on } \Omega \\ u &= 0 \quad \text{on } \Gamma \end{aligned} \qquad \text{with } \Delta = \frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_n^2}$$

the weak formulation is (using Green's identity)

is

$$\int_\Omega \nabla v \cdot \nabla w \, dx = \underbrace{\int_\Gamma v \frac{\partial w}{\partial n} ds}_{\text{"0 for test functions}} - \int_\Omega v \Delta w \, dx$$

(W) Find $u \in H_0^1(\Omega)$ such that

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, dx = \int_\Omega f v \, dx = (f,v) \text{ for all } v \in H_0^1(\Omega)$$

and the variational formulation is

(V) Find $u \in H_0^1(\Omega)$ such that $F(u) \le F(v)$ for all $v \in H_0^1(\Omega)$

where $F(v) = \frac{1}{2} a(v,v) - (f,v)$

- note: in general it is simpler to prove the existence of a solution for (W) than for (D)

  and for nonlinear PDEs we can prove the existence only for the weak formulation

- note: the spaces $H^1(\Omega)$ and $H_0^1(\Omega)$ are special cases of the Sobolev spaces $W^{k,p}(\Omega)$ for $p=2$ (starting from $L_2(\Omega)$)

  in general we have $L_p(\Omega)$ with $\|v\|_{L_p(\Omega)} = \left(\int_\Omega v^p dx \right)^{1/p}$

  and k denotes up to which order the weak derivatives of v are from $L_p(\Omega)$ space

  these space can be made complete resulting in Banach spaces

  but only for $p=2$ we get Hilbert spaces

  with the norm corresponding to the inner product

Example: Let us consider a problem

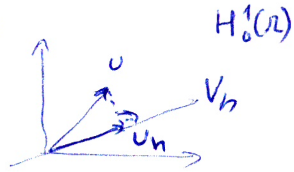
(D) $\quad -\Delta u + u = f$ on Ω and $u = 0$ on Γ

we get the weak formulation

(W) $\quad (u, v)_{H^1_0(\Omega)} = (f, v)$ for all $v \in H^1_0(\Omega)$

or
$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, dx + \int_\Omega u v \, dx = \int_\Omega f v \, dx = (f,v)$$
here the bilinear form $a(u,v)$ is directly the inner product of $H^1_0(\Omega)$

if we would use a finite subspace $V_h \in H^1_0(\Omega)$ and try to solve the problem on this subspace
$$(u_h, v)_{H^1_0(\Omega)} = (f, v) \text{ for all } v \in V_h$$
we get (subtracting (W))
$$(\underbrace{u - u_h}, v)_{H^1_0(\Omega)} = 0 \text{ for } \forall\, v \in V_h$$



i.e. the error e_h is perpendicular to V_h with respect to $(\cdot,\cdot)_{H^1_0(\Omega)}$

or in this case the FEM solution is a projection of u on V_h using $(\cdot,\cdot)_{H^1_0(\Omega)}$

and in this sense it is the closest $v \in V_h$ to the actual solution

- this is the basic idea of „geometrical interpretation" of FEM but in general the discussion is more complicated

- <u>other boundary conditions</u>
  - <u>Dirichlet boundary conditions</u> $u = u_0$ on Γ, it can be shown that the weak formulation is

    Find $u \in V(u_0) = \{v \in H^1(\Omega) : v = u_0 \text{ on } \Gamma\}$ such that $a(u,v) = (f,v)$ for all $v \in H^1_0(\Omega)$

    i.e. the testing functions v can be taken with zero boundary condition

    here boundary conditions modify the space $\Rightarrow$ <u>substantial boundary condition</u> (essential)

  - <u>von Neumann boundary condition</u> $\frac{\partial u}{\partial n} = g$ on Γ $\left(\frac{\partial u}{\partial n} = \frac{\partial u}{\partial x_1} n_1 + \dots + \frac{\partial u}{\partial x_d} n_d\right)$

    Find $u \in H^1(\Omega)$ such that $a(u,v) = (f,v) + \langle g, v\rangle$ for all $v \in H^1(\Omega)$

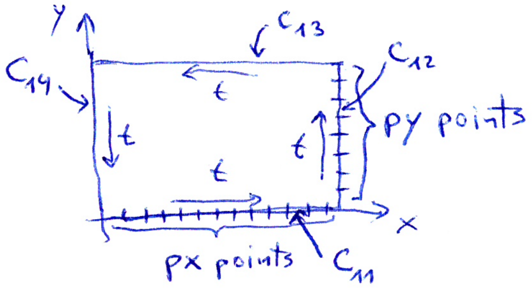
    where $\langle g, v\rangle = \int_\Gamma g \cdot v \, ds$ (because using the Green identity we cannot get rid of the boundary term)

    here boundary conditions are in the weak form. $\Rightarrow$ <u>natural boundary condition</u> (in FEM it is satisfied only approximately)

Notes on FreeFEM++

- FreeFEM++ is one of ~~many~~ many software packages which solve PDEs using the finite element method; see e.g. List of finite element software packages on Wikipedia
- I chose FreeFEM++ for its simple language and use

Problem 1: 2D Poisson equation on a rectangle or an ellipse



we would like to solve

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y) \qquad (*)$$

where

$$f(x,y) = 2(x-a)x + 2(y-b)y$$

with the boundary condition

$$u(C_1) = 0$$

the complete boundary is

$$C_1 = C_{11} + C_{12} + C_{13} + C_{14}$$

- the right-hand side was chosen to have the solution in the close form $u(x,y) = (x-a)x(y-b)y$ for an easier determination of the error and test of convergence rate
- in FreeFEM++, the boundary is described parametrically (see the example code), finite elements are then generated automatically using Delaunay-Voronoi algorithm from an initial number of points along the boundary
- the weak formulation of $(*)$

$$-\int_{\Box} \left(\frac{\partial u}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial u}{\partial y} \right) dx\,dy = \int_{\Box} f \cdot v \, dx\,dy$$

where $v(x,y)$ are testing functions from a space where we solve the problem

corresponds to the FreeFEM++ notation

```
problem Poisson(u,v) = -int2d(Th)(dx(u)*dx(v) + dy(u)*dy(v))
                       - int2D(Th)(f*v) + on(C1, u=0);
```

where Th is of type `mesh Th = buildmesh(C11(px)+...+C14(py));`

and u and v are of type `fespace Vh(Th,P1); Vh u,v;`

- in FreeFEM++, there are various bases implemented for scalar and vector functions (see documentation for details)

  in fespace we can use directly P1 (linear functions, $\mathcal{O}(h^2)$)

  or P2 (quadratic, $\mathcal{O}(h^3)$)

  or using load "Element_P3" also P3 (cubic, $\mathcal{O}(h^4)$)

- if we know the exact solution we can determine the error

  e.g. by $$e(h) = \left(\int_{\Box} (u - u_{exact})^2 \, dx\, dy \right)^{1/2}$$

  or in FreeFEM++ language

  L2error = sqrt(int2d(Th)((u-uexact)^2));

  after, of course, we solve the problem using

  solve Poisson (u,v);

  with u, we can deal almost as a normal function

  i.e. we can call directly u(x,y) to get its value

  at a specific point or, as above, we can integrate it over Th

- from the error for h and 2h (setting e.g. px=200, py=100 or px=100, py=50)

  we can determine the order of convergence using

  (assuming h is sufficiently small to be in the region where the error behaves as assumed)

$$\left.\begin{aligned} e(2h) &= c(2h)^\alpha \\ e(h) &= c h^\alpha \end{aligned}\right\} \Rightarrow \frac{e(2h)}{e(h)} = 2^\alpha \quad \text{or} \quad \alpha = \frac{\log\left(\frac{e(2h)}{e(h)}\right)}{\log 2}$$

  - change ~~the~~ the basis in the example from P1 to P2 to P3

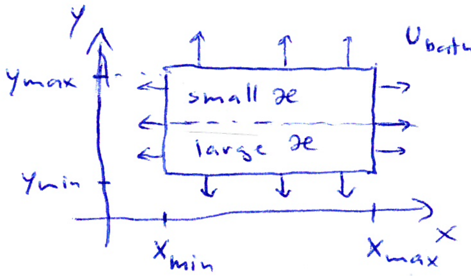
    to see that α is ~ 2, ~ 3, and ~ 4 respectively

- to change the rectangle to ellipse is rather straightforward

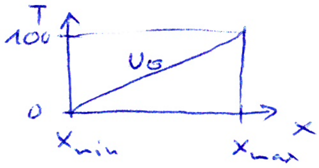
  - now we can use just one boundary

  - see PoissonEllipse.edp

Problem 2: 2D heat equation



initial temperature (constant in y)



we solve (thermal conductivity)

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(\varkappa(x,y) \cdot \nabla u \right)$$

with the initial condition

$$u_0 = u(t=0,x,y) = 0 + 100 \frac{(x - x_{min})}{(x_{max} - x_{min})}$$

and boundary condition

$$\varkappa(x,y) \frac{\partial u}{\partial n} + \alpha (u - u_{bath}) = 0$$

where
$$\varkappa(x,y) = \begin{cases} 0{,}1 & \text{for } y > \frac{y_{max}+y_{min}}{2} \\ 2{,}0 & \text{for } y < \frac{y_{max}+y_{min}}{2} \end{cases}$$

and $\alpha = 0{,}25$

- for stability reasons, we use the Euler implicit method for time propagation, i.e.

we apply $\int_\square v \, dxdy$ to get

$$\left.\frac{\partial u}{\partial t}\right|_{t_n} \approx \frac{u_n - u_{n-1}}{dt} = \nabla \cdot (\varkappa \nabla u_n)$$

using Green's theorem (identity)

or in the weak form

$$\int_\square \frac{u_n \cdot v}{dt} dxdy + \int_\square (\nabla u_n) \varkappa \nabla v \, dxdy \underbrace{- \int_\square \nabla \cdot (v \varkappa \nabla u_n) dxdy}_{\text{using Gauss} \to \,\shortparallel} - \int_\square \frac{u_{n-1} v}{dt} dxdy = 0$$

normal derivative

$$- \int_\Gamma v \varkappa \underbrace{(n \cdot \nabla u_n)}_{= \frac{\partial u_n}{\partial n}} dl = \int_\Gamma v \alpha (u - u_{bath}) dl$$

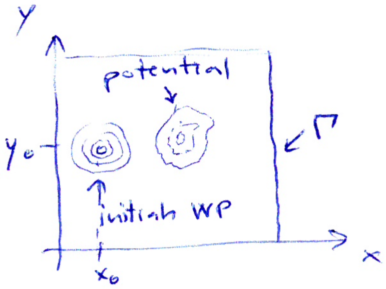
from the boundary condition

- in FreeFEM++, it is necessary to seperate the integrals with the unknow function u and v and the integrals with (already) known functions ($u_{n-1} = u_{old}$ and v)
- note that here the boundary condition is a part of the weak formulation, finally we get

problem thermic (u,v) = int2d(Th)$\left(\frac{u*v}{dt} + \varkappa \left(dx(u)dx(v) + dy(u)dy(v) \right) \right)$ +

+ $\underbrace{\text{int1d(Th)}}_{\text{integral over boundary}}(\alpha*u*v)$ $\underbrace{-\text{int1d(Th)}(\alpha*u\text{bath}*v) - \text{int2d(Th)}(\text{uold}*v/dt)}_{\text{these two must be separated}}$

Problem 3: 2D time-dependent Schrödinger equation



we solve „scattering" problem in 2D

i.e.

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2m}\Delta\psi + V(x,y)\,\psi = H\psi$$

with the initial condition

$$\psi(t=0,x,y) = \frac{1}{\sqrt{2\pi\sigma_x\sigma_y}}\, e^{-\frac{(x-x_0)^2}{4\sigma_x^2}+ip_x x}\, e^{-\frac{(y-y_0)^2}{4\sigma_y^2}+ip_y y}$$

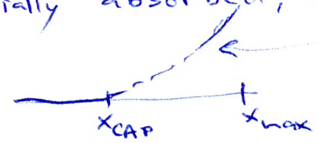
and boundary conditions

$\psi(\Gamma)=0$ for sufficiently small t and large Γ

(otherwise there would be reflections from the boundary

(or with the complex absorbing potential we can propagate to larger t, because the wave packet (WP) is then at least partially absorbed, e.g.

$$V_{CAP} = \begin{cases} -ic\,(x-x_{CAP})^{\alpha} & \text{for } x > x_{CAP} \\ 0 & \text{for } x < x_{CAP} \end{cases}$$)



- here we will use a more accurate Crank-Nicolson method for time propagation (centered difference and averaging of $H\psi$)

$$i\frac{\partial\psi}{\partial t} \approx i\,\frac{\psi_n-\psi_{n-1}}{dt} = \frac{1}{2}\left(H\psi_n + H\psi_{n-1}\right)$$

or

$$\left(1+\frac{i\,dt}{2}H\right)\psi_n = \left(1-\frac{i\,dt}{2}H\right)\psi_{n-1}$$

- in FreeFEM++, we can use Vh<complex> (for ψ psi and testing φ phi)

(note that conjugation φ^* of testing functions in the weak formulation is not necessary, they are just testing functions)

the weak formulation in the FreeFEM++ language is

problem SchEq =

$$= \text{int2d}(Th)\Big(\psi*\varphi + \frac{1i*dt}{4*m}*\big(dx(\psi)*dx(\varphi)+dy(\psi)*dy(\varphi)\big) + 0.5*1i*dt*\psi*V*\varphi\Big)$$

$$-\,\text{int2d}(Th)\Big(\psi_{old}*\varphi - \frac{1i*dt}{4*m}*\big(dx(\psi_{old})*dx(\varphi)+dy(\psi_{old})*dy(\varphi)\big) - 0.5*1i*dt*\psi_{old}*V*\varphi\Big)$$

$$+\,\text{on}(\Gamma,\psi=0)$$