MATH0024 – Modeling with PDEs

Variational formulation and finite element method with applications to Laplace/Poisson equation

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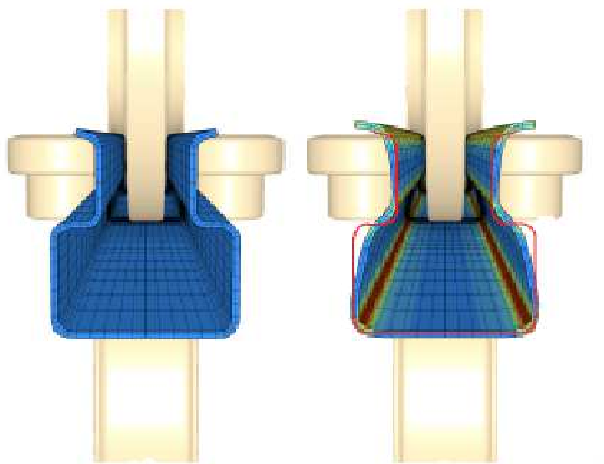
Introduction

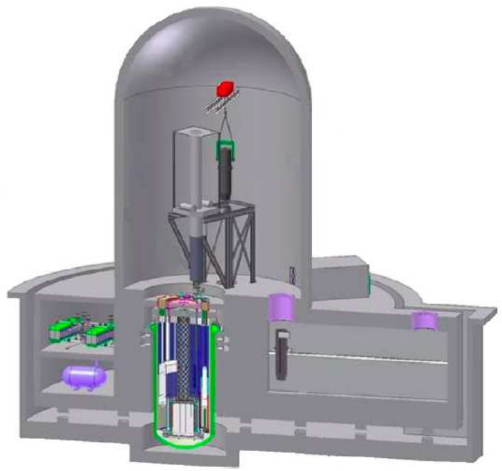
Introduction

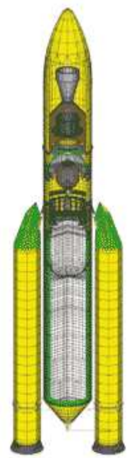
Motivation behind variational formulation from mathematical point of view

- A variational formulation provides a notion of generalized solution, whose existence, uniqueness, and stability can be studied by using **functional analysis** or **optimization theory** or both.
- Thus, the theory of variational formulations provides a useful bridge between PDEs, functional analysis, optimization theory, and other related mathematical fields.

Motivation behind variational formulation from numerical point of view







- The theory of variational formulations is the foundation for the **finite element method**, a numerical method for solving PDEs used in all areas of science and engineering.

Variational formulation of Laplace/Poisson equation

Introduction

- Let us consider the following BVP:

$$\begin{cases} -\dfrac{d^2u}{dx^2}(x) = f(x) & \text{for } 0 < x < 1, \\ + \text{ BCs} & \text{at } x = 0 \text{ and } x = 1. \end{cases}$$

- Multiplying the PDE with a function v, which is often called **test function** in the context of a variational formulation, and integrating over the domain $]0,1[$, we obtain

$$-\int_0^1 \frac{d^2u}{dx^2} v dx = \int_0^1 f v dx.$$

- Integrating by parts in the term on the left-hand side, we obtain the following **integral equation**

$$\int_0^1 \frac{du}{dx}\frac{dv}{dx} dx - \left[\frac{du}{dx} v\right]_0^1 = \int_0^1 f v dx,$$

which will be at the heart of the variational formulation of the BVP, as we will describe later.

Introduction (continued)

- We can observe that the partial integration moves one derivative of the exact solution u onto the test function v and introduces boundary terms which must be evaluated at the edge points.

- Further, we can observe that if Neumann boundary conditions (BCs) were specified at the edge points, then these Neumann BCs could be used when evaluating the boundary terms.

- By contrast, if Dirichlet BCs were specified at the edge points, there would be no obvious way of accounting for these Dirichlet BCs in the integral equation itself.

- Finally, we can observe that if the test function v vanished at the edge points, that is, $v(0) = v(1) = 0$, then the boundary terms would disappear.

Introduction (continued)

- To evaluate when the integral equation makes sense, we will use the following property:

  For two square-integrable functions v and w from $]0,1[$ into $\mathbb{R}$, we have

  $$\left|\int_0^1 vw dx\right| \leq \sqrt{\int_0^1 v^2 dx}\sqrt{\int_0^1 w^2 dx}.$$

  This property is proved as follows. Let λ be any real scalar. Then, we have

  $$\int_0^1 (v+\lambda w)^2 dx \geq 0, \quad \lambda \in \mathbb{R};$$

  hence, owing to the linearity of the integral, we have

  $$\int_0^1 v^2 dx + 2\lambda \int_0^1 vw dx + \lambda^2 \int_0^1 w^2 dx \geq 0, \quad \lambda \in \mathbb{R}.$$

  This quadratic expression for λ on the left-hand side being positive, its discriminant must satisfy

  $$\left(2\int_0^1 vw dx\right)^2 - 4\int_0^1 v^2 dx \int_0^1 w^2 dx \leq 0, \quad \text{as asserted.}$$

Introduction (continued)

- It follows that if $\int_0^1 \left(\frac{du}{dx}\right)^2 < +\infty$ and $\int_0^1 \left(\frac{dv}{dx}\right)^2 < +\infty$, the left-hand-side integral in the aforementioned integral equation makes sense:

$$\left|\int_0^1 \frac{du}{dx}\frac{dv}{dx}dx\right| \leq \sqrt{\int_0^1 \left(\frac{du}{dx}\right)^2 dx}\sqrt{\int_0^1 \left(\frac{dv}{dx}\right)^2 dx} < +\infty.$$

- And if $\int_0^1 f^2 dx < +\infty$ and $\int_0^1 v^2 dx < +\infty$, the right-hand-side integral in the aforementioned integral equation makes sense:

$$\left|\int_0^1 fv dx\right| \leq \sqrt{\int_0^1 f^2 dx}\sqrt{\int_0^1 v^2 dx} < +\infty.$$

- In Lecture 1 Part C, we saw that for a PDE of order k, a solution is said to be a classical solution if it is at least k times continuously differentiable. Thus, in the classical theory of PDEs, regularity properties of functions are gauged in terms of the continuity of derivatives.

  By contrast, we can observe that for a variational formulation, it is more natural to gauge regularity properties of functions in terms of the square-integrability of derivatives.

Notations for function spaces

- Let us recall from Lecture 1 Part B that the notation L^2 is often used to refer to a space of square-integrable functions. For example, when considering functions from $]0,1[$ into $\mathbb{R}$, we have

$$L^2(]0,1[) = \left\{ \text{functions } v \text{ from }]0,1[\text{ into } \mathbb{R} \text{ such that } \|v\|_{L^2}^2 = \int_0^1 |v|^2 dx < +\infty \right\}.$$

- In the context of the theory of variational formulations, the notation H^1 is often used to refer to a space of square-integrable functions whose first-order partial derivatives are also square-integrable functions. For example, when considering functions from $]0,1[$ into $\mathbb{R}$, we have

$$H^1(]0,1[) = \left\{ \text{functions } v \text{ from }]0,1[\text{ into } \mathbb{R} \text{ such that } \|v\|_{H^1}^2 = \|v\|_{L^2}^2 + \left\| \frac{dv}{dx} \right\|_{L^2}^2 < +\infty \right\}.$$

  Please note that for the theory to be mathematically fully rigorous in the following, the derivative $\frac{dv}{dx}$ must be defined in the sense of the distributions here.

  Further, please note that in applications in mechanics and physics, the contributions $\|v\|_{L^2}^2$ and $\left\| \frac{dv}{dx} \right\|_{L^2}^2$ are sometimes weighted by appropriate constants, thus ensuring compatibility of units.

Variational formulation of Dirichlet problem

- Let us consider the Dirichlet problem

$$\begin{cases} -\dfrac{d^2u}{dx^2}(x) = f(x) & \text{for } 0 < x < 1 \quad \text{(governing PDE)}, \\ u(0) = u_0 & \text{at } x = 0 \quad \text{(Dirichlet BC)}, \\ u(1) = u_1 & \text{at } x = 1 \quad \text{(Dirichlet BC)}. \end{cases}$$

- A variational formulation of this Dirichlet problem:

Given f in $L^2(]0,1[)$, find a function u in $H^1(]0,1[)$ with $u(0) = u_0$ and $u(1) = u_1$ such that

$$\int_0^1 \frac{du}{dx}\frac{dv}{dx}dx = \int_0^1 fv dx$$

for all test functions v in $H^1(]0,1[)$ with $v(0) = 0$ and $v(1) = 0$.

Variational formulation of Dirichlet problem (continued)

- We can observe that the solution u is sought among the functions that are in $H^1(]0,1[)$ and satisfy the Dirichlet BCs ($u(0) = u_0$ and $u(1) = u_1$).

  Further, we can observe that the integral equation is required to hold for all test functions v that are in $H^1(]0,1[)$ and satisfy homogeneous Dirichlet BCs ($v(0) = 0$ and $v(1) = 0$) wherever the solution is required to satisfy Dirichlet BCs ($u(0) = u_0$ and $u(1) = u_1$).

- By requiring that the solution u and the test functions v be sufficiently regular, specifically, that they be in $H^1(]0,1[)$, the **integrals in the integral equation are ensured to make sense**.

- Because there is no obvious way of accounting for Dirichlet BCs in the integral equation, the **Dirichlet BCs** ($u(0) = u_0$ and $u(1) = u_1$) are **imposed explicitly on the solution**.

- By requiring the test functions v to satisfy homogeneous Dirichlet BCs ($v(0) = 0$ and $v(1) = 0$) wherever the solution is required to satisfy Dirichlet BCs ($u(0) = u_0$ and $u(1) = u_1$), the corresponding boundary terms that result from the integration by parts disappear.

Variational formulation of mixed problem

- What happens if we change the boundary conditions? Let us consider the mixed problem

$$\begin{cases} -\dfrac{d^2u}{dx^2}(x) = f(x) & \text{for } 0 < x < 1 \quad \text{governing PDE,} \\ u(0) = u_0 & \text{at } x = 0 \quad \text{Dirichlet BC,} \\ \dfrac{du}{dx}(1) = g_1 & \text{at } x = 1 \quad \text{Neumann BC.} \end{cases}$$

- A variational formulation of this mixed problem:

Given f in $L^2(]0,1[)$, find a function u in $H^1(]0,1[)$ with $u(0) = u_0$ such that

$$\int_0^1 \frac{du}{dx}\frac{dv}{dx}dx - g_1 v(1) = \int_0^1 fv dx$$

for all test functions v in $H^1(]0,1[)$ with $v(0) = 0$.

- Because there is no obvious way of accounting for Dirichlet BCs in the integral equation, the Dirichlet BC ($u(0) = u_0$) is imposed explicitly on the solution.

- The **Neumann BC** ($\frac{du}{dx}(1) = g_1$) is **taken into account in the integral equation**, specifically, in the evaluation of the corresponding boundary term.

- By requiring the test functions v to satisfy a homogeneous Dirichlet BC ($v(0) = 0$) wherever the solution must satisfy a Dirichlet BC ($u(0) = u_0$), the corresponding boundary term disappears.

More generally...

- A variational formulation of a boundary value problem can be expected to take the following form

Given * in *, find a function * in * with * such that
$$*$$
for all test functions * in * with *.

- The solution and the test functions must be required to be sufficiently regular to ensure that the integrals in the integral equation make sense.

- Because there is no obvious way of accounting for Dirichlet BCs in the integral equation, Dirichlet BCs must be imposed explicitly on the solution.

- Neumann BCs are taken into account in the integral equation, specifically, in the evaluation of the corresponding boundary terms.

- By requiring the test function to satisfy homogeneous Dirichlet BCs wherever the solution is required to satisfy Dirichlet BCs, the corresponding boundary terms disappear from the integral equation.

Relationship between classical solution and solution to variational formulation

- Let us examine the relationship between a classical solution to the aforementioned Dirichlet problem and a solution to the aforementioned variational formulation of this Dirichlet problem.

- A classical solution is also a solution to the variational formulation.
  - For u to be a classical solution, u must be at least 2 times continuously differentiable on $[0, 1]$.

    For u to solve the variational formulation, u and $\frac{du}{dx}$ must be square-integrable over $]0, 1[$.

    Thus, because u being at least 2 times continuously differentiable on $[0, 1]$ implies that u and $\frac{du}{dx}$ are square-integrable over $]0, 1[$, the regularity property required for u to be a classical solution is stronger than that required for u to solve the variational formulation.

  - Further, if u is at least 2 times continuously differentiable on $[0, 1]$ and v and $\frac{dv}{dx}$ are square-integrable over $]0, 1[$, then the integrals in $-\int_0^1 \frac{d^2u}{dx^2} v dx = \int_0^1 f v dx$ make sense, and it follows from the integration by parts of the left-hand-side integral that $\int_0^1 \frac{du}{dx}\frac{dv}{dx} dx = \int_0^1 f v dx$ for all functions v such that v and $\frac{dv}{dx}$ are square-integrable over $]0, 1[$ and $v(0) = v(1) = 0$.

Relationship between classical solution and solution to variational formulation (continued)

- By contrast, the variational formulation may have a solution even in cases wherein there does not exist a classical solution (for example, when f is discontinuous).
  - Indeed, as we have already mentioned, the regularity property required for u to be a classical solution is stronger than that required for u to solve the variational formulation.

- More generally. . .
  - A classical solution to a boundary value problem can be expected to also satisfy a variational formulation of this boundary value problem.
  - However, a variational formulation of a boundary value problem may have a solution even in cases wherein this boundary value problem does not have a classical solution. In such circumstances, we speak of a generalized solution.

Mathematics of variational formulations in a nutshell

- A classical solution to a boundary value problem will also satisfy a variational formulation of this boundary value problem.
- However, a variational formulation of a boundary value problem may have a solution even in cases wherein this boundary value problem does not have a classical solution. In such circumstances, we speak of a generalized solution.
- The existence, uniqueness, and stability of a solution to a variational formulation can be studied by using the theory of functional analysis, which provides many useful results, such as the Lax-Milgram lemma, the Riesz representation theorem, and the Fredholm alternative.
- It is often easier to prove the well-posedness of a variational formulation of a boundary value problem than to prove the well-posedness of a classical solution of this boundary value problem.
- Once the existence, uniqueness, and stability of a solution to a variational formulation have been established, one can study conditions under which this solution is in fact sufficiently many times continuously differentiable to also be a classical solution.
- This leads to analyses of regularity of generalized solutions, which are often very complicated.
- A variational formulation is not unique. For a given boundary value problem, different types of variational formulation can in general be considered, which can differ in their mathematical properties, as well as in the type of finite element method that they can facilitate.

Equivalence between variational formulation and optimization problem

- Certain variational formulations can be written equivalently as optimization problems. However, let us emphasize that not every variational formulation is equivalent to an optimization problem.

- For example, if the Dirichlet BCs are homogeneous in the aforementioned Dirichlet problem, that is, $u(0) = 0$ and $u(1) = 0$, its variational formulation

> Given f in $L^2(]0,1[)$, find a function u in $H^1(]0,1[)$ with $u(0) = 0$ and $u(1) = 0$ such that
> $$\int_0^1 \frac{du}{dx}\frac{dv}{dx}dx = \int_0^1 fv dx$$
> for all test functions v in $H^1(]0,1[)$ with $v(0) = 0$ and $v(1) = 0$.

is equivalent to the following optimization problem:

> Given f in $L^2(]0,1[)$, find a function u in $H^1(]0,1[)$ with $u(0) = 0$ and $u(1) = 0$ such that
> $$\mathcal{J}(u) = \min_{\substack{v \text{ in } H^1(]0,1[) \\ \text{with } v(0)=v(1)=0}} \mathcal{J}(v), \quad \text{where} \quad \mathcal{J}(v) = \frac{1}{2}\int_0^1 \left(\frac{dv}{dx}\right)^2 dx - \int_0^1 fv dx.$$

Equivalence between variational formulation and optimization problem (continued)

- In fact, if u is a solution to the optimization problem, then we have

$$\underbrace{\lim_{\lambda\to 0}\frac{\mathcal{J}(u+\lambda v)-\mathcal{J}(u)}{\lambda}}_{\text{directional derivative of } \mathcal{J} \text{ at } u \text{ in direction } v} = 0 \quad \text{for all } v \text{ in } H^1(]0,1[) \text{ with } v(0)=v(1)=0.$$

Elaborating the term $\mathcal{J}(u+\lambda v)$ as follows:

$$\begin{aligned}\mathcal{J}(u+\lambda v) &= \frac{1}{2}\int_0^1 \left(\frac{du}{dx}+\lambda\frac{dv}{dx}\right)^2 dx - \int_0^1 f(u+\lambda v)dx \\ &= \frac{1}{2}\int_0^1 \left(\left(\frac{du}{dx}\right)^2 + 2\lambda\frac{du}{dx}\frac{dv}{dx} + \lambda^2\left(\frac{dv}{dx}\right)^2\right) dx - \int_0^1 fu dx - \int_0^1 f\lambda v dx,\end{aligned}$$

we obtain

$$\frac{\mathcal{J}(u+\lambda v)-\mathcal{J}(u)}{\lambda} = \frac{1}{2}\int_0^1 \left(2\frac{du}{dx}\frac{dv}{dx} + \lambda\left(\frac{dv}{dx}\right)^2\right) dx - \int_0^1 f v dx,$$

and therefore

$$\lim_{\lambda\to 0}\frac{\mathcal{J}(u+\lambda v)-\mathcal{J}(u)}{\lambda} = \int_0^1 \frac{du}{dx}\frac{dv}{dx}dx - \int_0^1 f v dx = 0 \text{ for all } v \text{ in } H^1(]0,1[) \text{ with } v(0)=v(1)=0.$$

Hence, if u solves the optimization problem, then u solves the variational formulation.

Equivalence between variational formulation and optimization problem (continued)

- Conversely, if u is a solution to the variational formulation, then we have

$$\mathcal{J}(u+v) = \frac{1}{2}\int_0^1 \left(\frac{d(u+v)}{dx}\right)^2 dx - \int_0^1 f(u+v)dx$$
$$= \underbrace{\frac{1}{2}\int_0^1 \left(\frac{du}{dx}\right)^2 dx - \int_0^1 fudx}_{=\mathcal{J}(u)} + \underbrace{\int_0^1 \left(\frac{du}{dx}\frac{dv}{dx}\right) dx - \int_0^1 fvdx}_{=0 \text{ because } u \text{ solves var. for.}} + \underbrace{\frac{1}{2}\int_0^1 \left(\frac{dv}{dx}\right)^2 dx}_{\geq 0}.$$

It follows that:

$$\mathcal{J}(u) \leq \mathcal{J}(u+v), \qquad \forall v \in H^1(]0,1[) \text{ with } v(0)=0 \text{ and } v(1)=0.$$

Hence, if u solves the variational formulation, then u is a minimum of the optimization problem.

3D electrostatics

- Let us consider the following boundary value problem:

$$\begin{cases} -\triangle_{\boldsymbol{x}}\Phi = \rho/\epsilon_0 & \text{in } \Omega \quad \text{(Gauss's law)}, \\ \Phi = 0 & \text{on } \partial\Omega \quad \text{(potential B.C.)}, \end{cases}$$

where Φ is the electrical potential, ρ the charge density, and ϵ_0 the electrical permittivity.

- Multiplying the PDE with a test function Ψ and integrating over the domain Ω, we obtain

$$-\int_\Omega \triangle_{\boldsymbol{x}}\Phi\,\Psi dV = \int_\Omega \rho/\epsilon_0 \Psi dV.$$

"Integrating by parts," that is, using the definition $\triangle_{\boldsymbol{x}}\varphi = \text{div}_{\boldsymbol{x}}\boldsymbol{\nabla}_{\boldsymbol{x}}\varphi$ and the property $\text{div}_{\boldsymbol{x}}(\varphi\boldsymbol{a}) = \boldsymbol{a}\cdot\boldsymbol{\nabla}_{\boldsymbol{x}}\varphi + \varphi\text{div}_{\boldsymbol{x}}\boldsymbol{a}$, which we recalled in Lecture 1 Part B,

$$\int_\Omega \boldsymbol{\nabla}_{\boldsymbol{x}}\Phi\cdot\boldsymbol{\nabla}_{\boldsymbol{x}}\Psi dV - \int_\Omega \text{div}_{\boldsymbol{x}}(\Psi\boldsymbol{\nabla}_{\boldsymbol{x}}\Phi)dV = \int_\Omega \rho/\epsilon_0\Psi dV,$$

and using Stokes's theorem for a volume, $\int_\Omega \text{div}_{\boldsymbol{x}}\boldsymbol{a}dV = \int_{\partial\Omega}\boldsymbol{a}\cdot d\boldsymbol{S}$, which we also recalled in Lecture 1 Part B, we obtain,

$$\int_\Omega \boldsymbol{\nabla}_{\boldsymbol{x}}\Phi\cdot\boldsymbol{\nabla}_{\boldsymbol{x}}\Psi dV - \int_{\partial\Omega}\Psi\boldsymbol{\nabla}_{\boldsymbol{x}}\Phi\cdot d\boldsymbol{S} = \int_\Omega \rho/\epsilon_0\Psi dV.$$

3D electrostatics (continued)

- A variational formulation of this boundary value problem:

Given ρ/ϵ_0 in $L^2(\Omega)$, find a function Φ in $H^1(\Omega)$ with $\Phi = 0$ on $\partial\Omega$ such that

$$\int_\Omega \boldsymbol{\nabla}_{\boldsymbol{x}}\Phi \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}\Psi dV = \int_\Omega \rho/\epsilon_0 \Psi dV$$

for all test functions Ψ in $H^1(\Omega)$ with $\Psi = 0$ on $\partial\Omega$.

- This variational formulation is equivalent to the optimization problem:

Given ρ/ϵ_0 in $L^2(\Omega)$, find a function Φ in $H^1(\Omega)$ with $\Phi = 0$ on $\partial\Omega$ such that

$$\mathcal{J}(\Phi) = \min_{\substack{\Psi \text{ in } H^1(\Omega) \\ \text{with } \Psi = 0 \text{ on } \partial\Omega}} \mathcal{J}(\Psi), \quad \text{where} \quad \mathcal{J}(\Psi) = \frac{1}{2}\int_\Omega \|\boldsymbol{\nabla}_{\boldsymbol{x}}\Psi\|^2 dV - \int_\Omega \rho/\epsilon_0 \Psi dV.$$

3D elasticity

- Let us consider the following boundary value problem:

$$\begin{cases} \textbf{div}_{\boldsymbol{x}}\boldsymbol{\sigma} + \boldsymbol{f}_{\mathsf{V}} = \boldsymbol{0} & \text{in } \Omega & \text{(equilibrium equation)}, \\ \boldsymbol{\sigma} = \boldsymbol{C}(\boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{u}) & \text{in } \Omega & \text{(constitutive equation)}, \\ \boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{u} = 1/2\big(\mathbf{D}_{\boldsymbol{x}}\boldsymbol{u} + \mathbf{D}_{\boldsymbol{x}}\boldsymbol{u}^{\mathrm{T}}\big) & \text{in } \Omega & \text{(strain-displacement relationship)}, \\ \boldsymbol{u} = \boldsymbol{0} & \text{on } \partial\Omega_{\mathsf{D}} & \text{(displacement B.C.)}, \\ \boldsymbol{\sigma}(\boldsymbol{n}) = \boldsymbol{f}_{\mathsf{s}} & \text{on } \partial\Omega_{\mathsf{N}} & \text{(traction B.C.)}, \end{cases}$$

- Multiplying the equilibrium equation with a test function $\boldsymbol{v}$ and integrating over Ω, we obtain

$$\int_\Omega \textbf{div}_{\boldsymbol{x}}\boldsymbol{\sigma} \cdot \boldsymbol{v} dV + \int_\Omega \boldsymbol{f}_{\mathsf{V}} \cdot \boldsymbol{v} dV = 0.$$

"Integrating by parts," that is, using the property $\mathrm{div}_{\boldsymbol{x}}\big(\boldsymbol{A}^{\mathrm{T}}(\boldsymbol{a})\big) = \boldsymbol{A} : \mathbf{D}_{\boldsymbol{x}}\boldsymbol{a} + \boldsymbol{a} \cdot \textbf{div}_{\boldsymbol{x}}\boldsymbol{A}$,

$$-\int_\Omega \boldsymbol{\sigma} : \mathbf{D}_{\boldsymbol{x}}\boldsymbol{v} dV + \int_\Omega \mathrm{div}_{\boldsymbol{x}}\big(\boldsymbol{\sigma}^{\mathrm{T}}(\boldsymbol{v})\big) dV + \int_\Omega \boldsymbol{f}_{\mathsf{V}} \cdot \boldsymbol{v} dV = 0,$$

where, owing of the symmetry of $\boldsymbol{\sigma}$, we have $\mathrm{div}_{\boldsymbol{x}}\big(\boldsymbol{\sigma}^{\mathrm{T}}(\boldsymbol{v})\big) = \mathrm{div}_{\boldsymbol{x}}\big(\boldsymbol{\sigma}(\boldsymbol{v})\big)$ and $\boldsymbol{\sigma} : \mathbf{D}_{\boldsymbol{x}}\boldsymbol{v} = \boldsymbol{\sigma} : \boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{v}$, and using Stokes's theorem for a volume, we obtain,

$$-\int_\Omega \boldsymbol{\sigma} : \boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{v} dV + \int_{\partial\Omega} \boldsymbol{\sigma}(\boldsymbol{n}) \cdot \boldsymbol{v} dS + \int_\Omega \boldsymbol{f}_{\mathsf{V}} \cdot \boldsymbol{v} dV = 0.$$

3D elasticity (continued)

- A variational formulation of this boundary value problem:

Given $\boldsymbol{f}_{\mathsf{V}}$ in $\left(L^2(\Omega)\right)^3$ and $\boldsymbol{f}_{\mathsf{S}}$ in $\left(L^2(\partial\Omega_{\mathsf{N}})\right)^3$, find $\boldsymbol{u}$ in $\left(H^1(\Omega)\right)^3$ with $\boldsymbol{u} = \mathbf{0}$ on $\partial\Omega_{\mathsf{D}}$ s.t.

$$\int_\Omega \boldsymbol{C}(\boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{u}) : \boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{v} dV = \int_\Omega \boldsymbol{f}_{\mathsf{V}} \cdot \boldsymbol{v} dV + \int_{\partial\Omega_{\mathsf{N}}} \boldsymbol{f}_{\mathsf{S}} \cdot \boldsymbol{v} dS$$

for all test functions $\boldsymbol{v}$ in $\left(H^1(\Omega)\right)^3$ with $\boldsymbol{v} = \mathbf{0}$ on $\partial\Omega_{\mathsf{D}}$.

In mechanics, this is also known as the principle of virtual work.

- This variational formulation is equivalent to the optimization problem:

Given $\boldsymbol{f}_{\mathsf{V}}$ in $\left(L^2(\Omega)\right)^3$ and $\boldsymbol{f}_{\mathsf{S}}$ in $\left(L^2(\partial\Omega_{\mathsf{N}})\right)^3$, find $\boldsymbol{u}$ in $\left(H^1(\Omega)\right)^3$ with $\boldsymbol{u} = \mathbf{0}$ on $\partial\Omega_{\mathsf{D}}$ s.t.

$$\mathcal{J}(\boldsymbol{u}) = \min_{\substack{\boldsymbol{v} \text{ in } \left(H^1(\Omega)\right)^3 \\ \text{with } \boldsymbol{v} = \mathbf{0} \text{ on } \partial\Omega_{\mathsf{D}}}} \mathcal{J}(\boldsymbol{v}), \text{ where } \mathcal{J}(\boldsymbol{v}) = \frac{1}{2}\int_\Omega \boldsymbol{C}(\boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{v}) : \boldsymbol{\epsilon}_{\boldsymbol{x}}\boldsymbol{v} dV - \int_\Omega \boldsymbol{f}_{\mathsf{V}} \cdot \boldsymbol{v} dV - \int_{\partial\Omega_{\mathsf{N}}} \boldsymbol{f}_{\mathsf{S}} \cdot \boldsymbol{v} dS.$$

In mechanics, this is also known as the principle of minimum potential energy.

Finite element method for Laplace/Poisson equation

Notion of Galerkin approximation

- The **Galerkin approximation** is a method for constructing an approximate solution to a variational formulation. Stated abstractly, this approximate solution is obtained by restricting the variational formulation to a finite-dimensional function space.
- Stated more concretely, the Galerkin approximation constructs an approximate solution in the form of a linear combination of a finite number of given **basis functions**. The coefficients in this linear combination are determined by requiring the integral equation in the variational formulation to be fulfilled for all test functions that, likewise, are linear combinations of the given basis functions.

Galerkin approximation to Dirichlet problem

- Let us consider the following Dirichlet problem with homogeneous Dirichlet BCs:

$$\begin{cases} -\dfrac{d^2u}{dx^2}(x) = f(x) & \text{for } 0 < x < 1, \\ u(0) = u(1) = 0 & \text{at } x = 0 \text{ and } x = 1. \end{cases}$$

- And let us consider the following variational formulation of this Dirichlet problem:

> Given f in $L^2(]0,1[)$, find a function u in $H^1(]0,1[)$ with $u(0) = 0$ and $u(1) = 0$ such that
> $$\int_0^1 \frac{du}{dx}\frac{dv}{dx}dx = \int_0^1 fv dx$$
> for all test functions v in $H^1(]0,1[)$ with $v(0) = 0$ and $v(1) = 0$.

Galerkin approximation to Dirichlet problem (continued)

- Let a finite number μ_h of basis functions $\varphi_1, \ldots, \varphi_{\mu_h}$ be given. Let each φ_j be a function from $[0,1]$ into $\mathbb{R}$ that is square-integrable over $]0,1[$, whose derivative is square-integrable over $]0,1[$, and such that $\varphi_j(0) = \varphi_j(1) = 0$.
- Then, the Galerkin approximation leads to the construction of an approximate solution u^h in the form of a linear combination of the basis functions, that is,

$$u^h(x) = \sum_{j=1}^{\mu_h} u_j \varphi_j(x), \quad u_1, \ldots, u_{\mu_h} \in \mathbb{R}.$$

- The coefficients $u_1, \ldots, u_{\mu_h}$ are determined by requiring the integral equation in the variational formulation to be fulfilled for all test functions that are linear combinations of the basis functions,

$$v^h(x) = \sum_{j=1}^{\mu_h} v_j \varphi_j(x), \quad v_1, \ldots, v_{\mu_h} \in \mathbb{R}.$$

- Thus, the Galerkin approximate problem takes the following form:

> Given f in $L^2(]0,1[)$, find a function $u^h = \sum_{j=1}^{\mu_h} u_j \varphi_j$ such that
>
> $$\int_0^1 \frac{du^h}{dx} \frac{dv^h}{dx} dx = \int_0^1 f v^h dx$$
>
> for all test functions $v^h = \sum_{j=1}^{\mu_h} v_j \varphi_j$ with $v_1, \ldots, v_{\mu_h}$ in $\mathbb{R}$.

Galerkin approximation to Dirichlet problem (continued)

- By linearity, for the integral equation in the variational formulation to be fulfilled for all test functions $v^h = \sum_{j=1}^{\mu_h} v_j \varphi_j$ with $v_1, \ldots, v_{\mu_h}$ in $\mathbb{R}$, it suffices that it is fulfilled for every basis function:

$$\int_0^1 \sum_{j=1}^{\mu_h} u_j \frac{d\varphi_j}{dx} \frac{d\varphi_1}{dx} dx = \int_0^1 f \varphi_1 dx,$$

$$\vdots$$

$$\int_0^1 \sum_{j=1}^{\mu_h} u_j \frac{d\varphi_j}{dx} \frac{d\varphi_{\mu_h}}{dx} dx = \int_0^1 f \varphi_{nh} dx.$$

- This system of equations can be written equivalently in the following matrix-vector form:

$$\begin{bmatrix} \int_0^1 \frac{d\varphi_1}{dx} \frac{d\varphi_1}{dx} dx & \ldots & \int_0^1 \frac{d\varphi_{\mu_h}}{dx} \frac{d\varphi_1}{dx} dx \\ \vdots & & \vdots \\ \int_0^1 \frac{d\varphi_{\mu_h}}{dx} \frac{d\varphi_1}{dx} dx & \ldots & \int_0^1 \frac{d\varphi_{\mu_h}}{dx} \frac{d\varphi_{\mu_h}}{dx} dx \end{bmatrix} \begin{bmatrix} u_1 \\ \ldots \\ u_{\mu_h} \end{bmatrix} = \begin{bmatrix} \int_0^1 f \varphi_1 dx \\ \ldots \\ \int_0^1 f \varphi_{\mu_h} dx \end{bmatrix};$$

hence, more compactly, the Galerkin approximate problem takes the form of the linear problem

$$[K]\boldsymbol{u} = \boldsymbol{f},$$

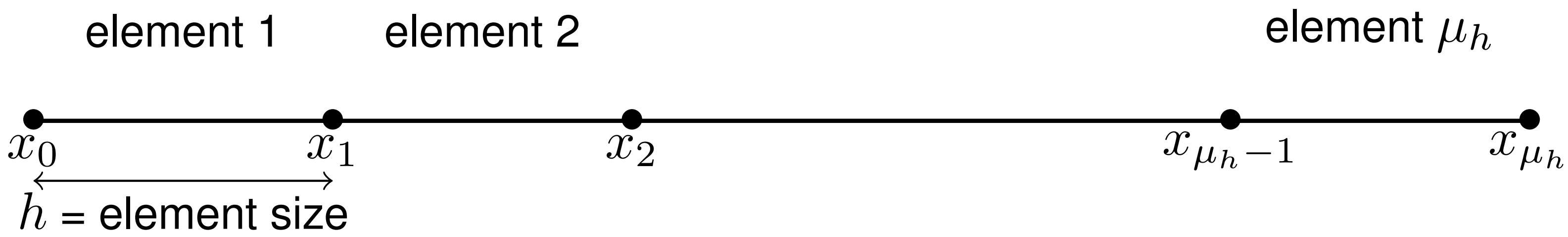
where $[K]$ is the square μ_h-dimensional matrix such that $K_{ij} = \int_0^1 \frac{d\varphi_i}{dx} \frac{d\varphi_j}{dx} dx$ for $1 \leq i, j \leq \mu_h$ and $\boldsymbol{f}$ the μ_h-dimensional vector such that $f_j = \int_0^1 f \varphi_j dx$ for $1 \leq j \leq \mu_h$.

Notion of finite element method

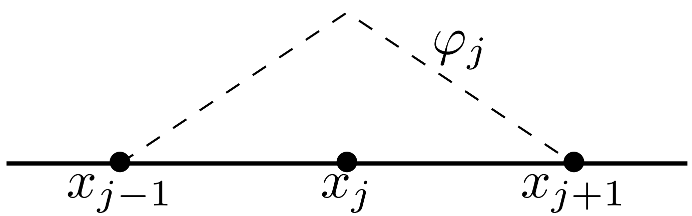
- The **finite element method** is essentially a method for constructing basis functions for use in the Galerkin approximation. First, the domain is partitioned into a finite number of subdomains ("elements"); then, the basis functions are constructed as elementwise low-degree polynomials.

A simple finite element method for aforementioned Dirichlet problem

- Let the domain be meshed as follows:



- Basis functions can then be obtained, for example, by associating to each node x_j a corresponding basis function φ_j that is elementwise linear and equal to one at x_j and zero at the other nodes:



$$\varphi_j(x) = \begin{cases} \dfrac{x - x_{j-1}}{x_j - x_{j-1}} & \text{for } x_{j-1} \leq x \leq x_j, \\ \dfrac{x_{j+1} - x}{x_{j+1} - x_j} & \text{for } x_j \leq x \leq x_{j+1}, \\ 0 & \text{otherwise.} \end{cases}$$

A simple finite element method for aforementioned Dirichlet problem (continued)

- For this choice of basis functions, the Galerkin approximation leads to the linear system

$$\begin{bmatrix} \int_0^1 \frac{d\varphi_1}{dx}\frac{d\varphi_1}{dx}dx & \dots & \int_0^1 \frac{d\varphi_{\mu_h}}{dx}\frac{d\varphi_1}{dx}dx \\ \vdots & & \vdots \\ \int_0^1 \frac{d\varphi_{\mu_h}}{dx}\frac{d\varphi_1}{dx}dx & \dots & \int_0^1 \frac{d\varphi_{\mu_h}}{dx}\frac{d\varphi_{\mu_h}}{dx}dx \end{bmatrix} \begin{bmatrix} u_1 \\ \dots \\ u_{\mu_h} \end{bmatrix} = \begin{bmatrix} \int_0^1 f\varphi_1 dx \\ \dots \\ \int_0^1 f\varphi_{\mu_h} dx \end{bmatrix};$$

  Because the support of each basis function is limited to only a small portion of the domain, many entries of the system matrix vanish. In fact, calculating these entries of the system matrix and accounting for the support of each basis function in the right-hand side, we obtain

$$\frac{1}{h}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{\mu_h-2} \\ u_{\mu_h-1} \end{bmatrix} = \begin{bmatrix} \int_{x_0}^{x_2} f\varphi_1 dx \\ \int_{x_1}^{x_3} f\varphi_2 dx \\ \vdots \\ \int_{x_{\mu_h-3}}^{x_{\mu_h-1}} f\varphi_{\mu_h-2} dx \\ \int_{x_{\mu_h-2}}^{x_{\mu_h}} f\varphi_{\mu_h-1} dx \end{bmatrix}$$

- We can observe that the system matrix is sparse, symmetric, and positive definite. Further, especially if h is small, it can be expected to be large and ill-conditioned. As in Lecture 3, we refer to INFO0939 “High- performance scientific computing” and MATH0471 “Multiphysics integrated computational project” (R. Boman and C. Geuzaine) for details on storage and solution algorithms.

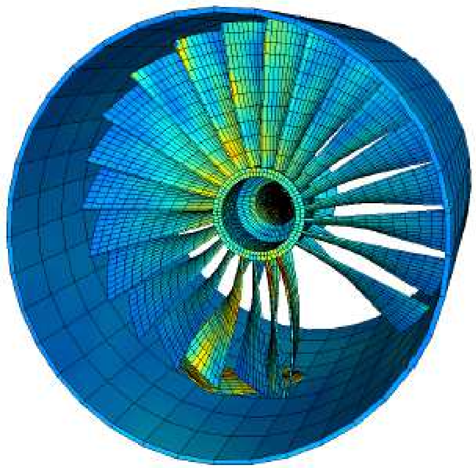
Convergence of finite element method

- As the mesh is refined, that is, as $h \to 0$, more and more functions become representable as a linear combination of basis functions. Hence, intuitively, we can expect that as the mesh is refined, the Galerkin approximate problem will approximate better and better the variational formulation, so that the approximate solution u^h will converge to the exact solution u to this variational formulation.
- Fully rigorous convergence analyses of finite element methods typically combine results from functional analysis (such as the Poincaré inequality and the Céa lemma) with results from real analysis (such as polynomial approximation theory). If interested, you can find an accessible example of such a convergence analysis, for example, in Chapter 2 in [Quarteroni, 2009].

Outlook

- There are many interesting aspects and challenges.

  Meshing. Polynomial degree of basis functions. Efficient computation of integrals by quadrature. Efficient assembly and storage of system matrices. Efficient solution algorithms. Pre- and post-processing of results. Modeling expertise. Application area specificities. Usage of commercial finite element software. . . .



- MECA0036 “Finite element method” (J.-P. Ponthot; 2ième quadri).

Summary and conclusion

- To obtain a variational formulation, typically, we proceed as follows:
  - We multiply the governing PDE with a test function, integrate over the domain, and carry out an integration by parts, thus obtaining an integral equation.
  - We obtain a variational formulation by seeking, from among the functions that make sense, a solution that satisfies the integral equation for all test functions that, likewise, make sense, while accounting in an appropriate way for the BCs. Dirichlet BCs are imposed explicitly on the solution. Neumann BCs are taken into account in the integral equation. By requiring the test function to satisfy homogeneous Dirichlet BCs wherever the solution is required to satisfy Dirichlet BCs, the corresponding boundary terms disappear from the integral equation.
- A variational formulation provides a notion of generalized solution, whose existence, uniqueness, and stability can be studied by using functional analysis or optimization theory or both.
- A variational formulation is the foundation for the finite element method. In fact, the finite element method is a particular instance of the Galerkin approximation:
  - In the Galerkin approximation, an approximate solution to a variational formulation is constructed in the form of a linear combination of a finite number of given basis functions by requiring the integral equation in this variational formulation to be fulfilled for all test functions that, likewise, are linear combinations of the given basis functions.
  - The finite element method provides basis functions for use in the Galerkin approximation.

References

Suggested reading material:

- P. Olver. Introduction to Partial Differential Equations. Chapter 10.

Additional references also consulted to prepare this lecture:

- D. Aubry. Mécanique des milieux continus. Ecole Centrale Paris. Lecture notes.
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- A. Quarteroni. Numerical models for differential problems. Springer, 2009.
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