ESS101- Modeling and Simulation
Lecture 21

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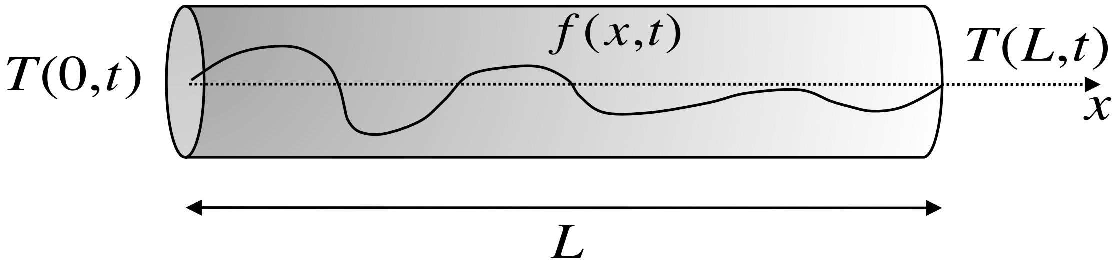
Today*

- ☞ Introductory example.
  - ☞ The heat conduction problem
  - ☞ The finite differences method
- ☞ Finite elements method

*Claes Johnson, *Numerical solution of partial differential equations by the finite element method*, Studentlitteratur

Example. Heat conduction

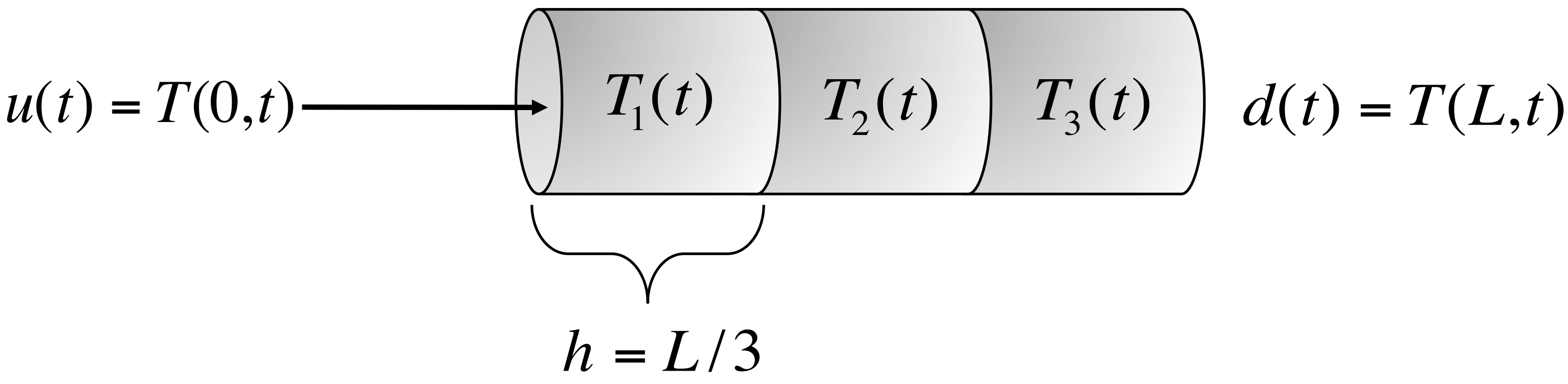


Fourier's law (1D) and energy conservation

$$\frac{\partial}{\partial t}T(x,t) = k\frac{\partial^2}{\partial x^2}T(x,t) + f(x,t)$$

- x longitudinal coordinate [m]
- t time [s]
- T temperature [K]
- k thermal diffusivity [m^2/s]

Example. Heat conduction



Assumption of *temperature homogeneity* in each part

$$T(x,t) = T_1(t),\ \forall x \in [0,h[$$
$$T(x,t) = T_2(t),\ \forall x \in [h,2h[$$
$$T(x,t) = T_3(t),\ \forall x \in [2h,3h[$$

Example. Heat conduction

Approximate the partial derivatives with finite differences

First order *backward* difference

$$\left.\frac{\partial}{\partial x}T(x,t)\right|_{x\in[(i-1)h,ih]} \cong \frac{\partial T_i(t)}{\partial x} \cong \frac{T_i(t)-T_{i-1}(t)}{h},$$

Second order *central* difference

$$\left.\frac{\partial^2}{\partial x^2}T(x,t)\right|_{x\in[(i-1)h,ih]} \cong \frac{T_{i+1}(t)-2T_i(t)+T_{i-1}(t)}{h^2}$$

For our 3rd order approximation, define

$$x_i(t) = \left.T(x,t)\right|_{x\in[(i-1)dx,idx]}$$

$$u(t) = \left.k\frac{\partial}{\partial x}T(x,t)\right|_{x=0} \qquad \text{and} \qquad f(x,t)=0,\ \forall x,\ t$$

Example. Heat conduction

$$\frac{\partial}{\partial t}T(x,t) = k\frac{\partial^2}{\partial x^2}T(x,t) + f(x,t)$$

Rewrite the approximation for each element with $f(x,t)=0$ and $dx=h$

$$\dot{x}_1(t) = \frac{k}{h^2}\left(x_2(t) - 2x_1(t) + u(t)\right)$$

$$\dot{x}_2(t) = \frac{k}{h^2}\left(x_3(t) - 2x_2(t) + x_1(t)\right)$$

$$\dot{x}_3(t) = \frac{k}{h^2}\left(d(t) - 2x_3(t) + x_2(t)\right)$$

Example. Heat conduction

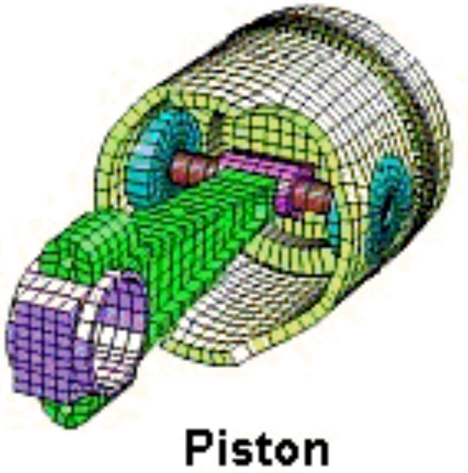
In a more compact form

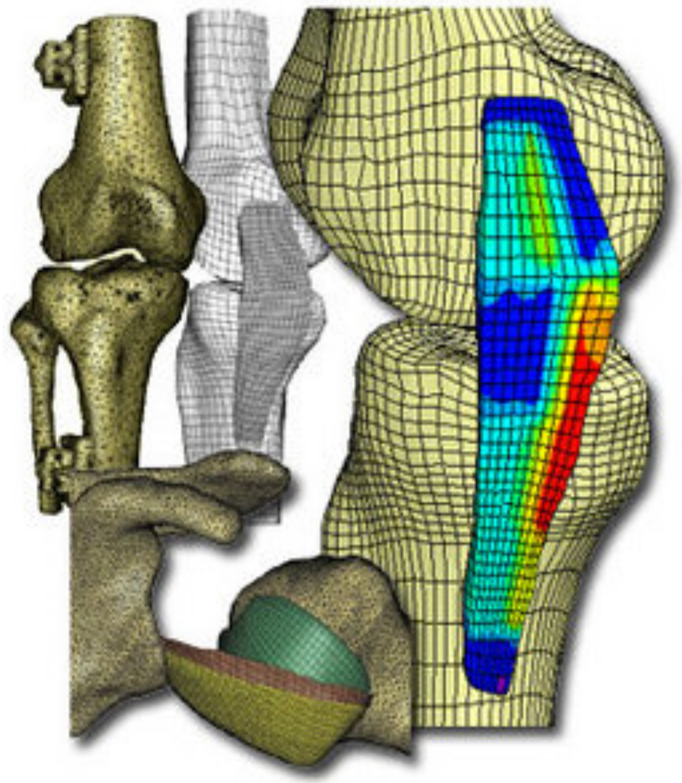
$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \end{bmatrix} = \underbrace{\begin{pmatrix} -2\frac{k}{h^2} & \frac{k}{h^2} & 0 \\ \frac{k}{h^2} & -2\frac{k}{h^2} & \frac{k}{h^2} \\ 0 & \frac{k}{h^2} & -2\frac{k}{h^2} \end{pmatrix}}_{A} \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} + \underbrace{\begin{pmatrix} \frac{k}{h^2} \\ 0 \\ 0 \end{pmatrix}}_{B} u(t) + \underbrace{\begin{pmatrix} 0 \\ 0 \\ \frac{k}{h^2} \end{pmatrix}}_{E} d(t)$$

Exercise. Derive a state space model for $h=L/5$. Simulate the two models with $k=1\ Km^2/s$, $u(t)=sin0.2t$ and $d(t)=5$ and compare the temperatures at $x=L/4$.

More complicated problems

How complex would the problem be for such systems?





Finite differences method *inefficient* and *not flexible* for complex geometries and materials.

Finite element methods

In this course we will cover

- Steady state simulations
- One-dimensional problems

This lecture will ***not*** cover

- Transient simulations*
- Higher-dimensional problems*
- Computational aspects*

*Covered in the Comsol tutorial

Boundary value problem formulation

Consider the following second order partial differential equation

$$-u''(x) = \underbrace{f(x)}_{\text{Continuous function}}, \qquad 0 < x < 1$$
$$\underbrace{u(0) = u(1) = 0}_{\text{Boundary conditions}}$$

We will solve the following

Problem D. To find a solution *u(x)* of the PDE

Notation

We introduce the functionals

$$(v,w) = \int_0^1 v(x)w(x)dx$$

and

$$F : V \rightarrow R$$

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

where the function space V is defined as

$$V = \left\{ \begin{array}{l} v : v \text{ continuous in } [0,1],\ v' \text{ piecewise} \\ \text{continuous and bounded and } v(0) = v(1) = 0 \end{array} \right\}$$

Auxiliary problems

We formulate the following minimization

Problem M (Principle of minimum potential energy). To find a function $u \in V$ such that

$$F(u) \leq F(v) \quad \forall v \in V$$

and the following variational

Problem V (Principle of virtual work). To find a function $u \in V$ such that

$$(u', v') = (f, v) \quad \forall v \in V$$

In summary

Problem D. To find a solution *u(x)* of the PDE

$$-u''(x) = f(x), \quad 0 < x < 1$$
$$u(0) = u(1) = 0$$

Problem M. To find a function $u \in V$ such that

$$F(u) \leq F(v) \quad \forall v \in V$$

Problem V. To find a function $u \in V$ such that

$$(\mathrm{u}', \mathrm{v}') = (\mathrm{f}, \mathrm{v}) \quad \forall v \in V$$

Fundamental results

Theorem 1. If $u \in V$ is a solution of the problem ***(D)***, then it is also a solution of the problem ***(V)***.

Theorem 2. The problems ***(V)*** and ***(M)*** have the same solutions.

Corollary. If $u \in V$ is a solution of the problem ***(D)***, then it is also a solution of the problems ***(V)*** and ***(M)***.

Moreover, if u'' is continuous, the converse is also true

Conclusion

The solution of the original problem ***(D)*** can be found by solving either the auxiliary problem ***(V)*** or ***(M)***.

In this course we will show how to find a solution of ***(D)*** by solving ***(V)*** (***Galerkin's method***).

Actually we will solve a "*discrete*" version of ***(V)***.

Galerkin's method

Problem D. To find a solution *u(x)* of the PDE

$$-u''(x) = f(x), \quad 0 < x < 1$$
$$u(0) = u(1) = 0$$

Problem V. To find a function $u \in V$ such that

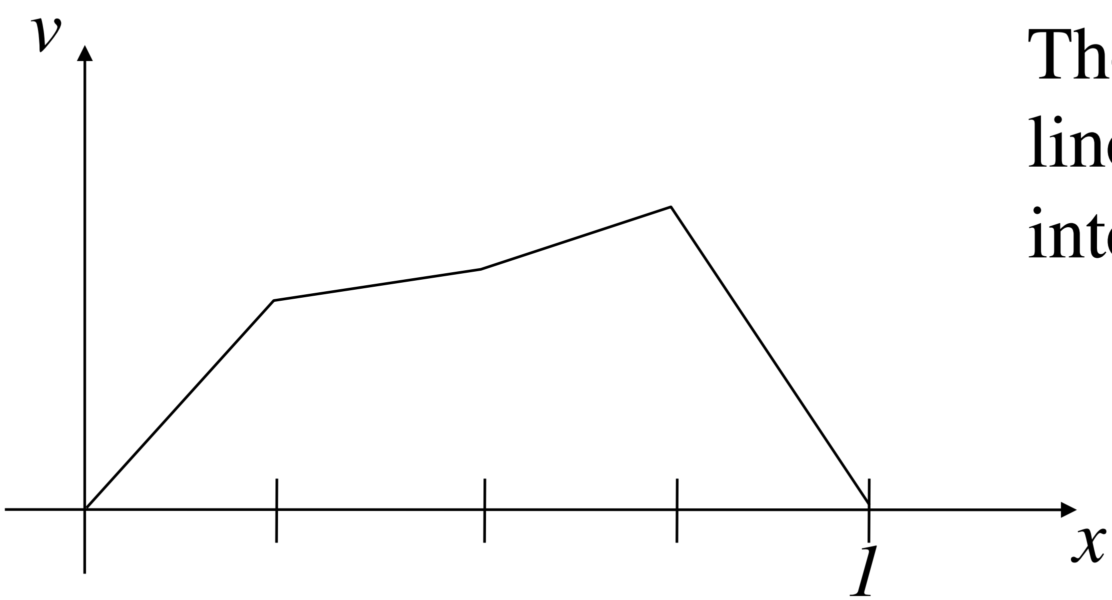
$$(\mathrm{u}',\mathrm{v}') = (\mathrm{f},\mathrm{v}) \quad \forall v \in V$$

Recall that $(u,v) = \int_0^1 u(x)v(x)dx$

Formulation of the Finite Element Problem

First step. Define the function space V

In this lecture, for simplicity, we will consider the space of *piecewise linear functions*, that is, we'll consider u, $v \in V$ of the following type



The function is linear in each interval

Formulation of the Finite Element Problem

Partition the domain of the function v, i.e., (0,1) as

$$0 = x_0 < x_1 < \ldots < x_M < x_{M+1} = 1$$

and set

$$h_j = x_j - x_{j-1} \qquad\qquad h = \max h_j$$

Denote by V_h the set of functions v which are linear on each subinterval

$$I_j = \left(x_{j-1}, x_j\right)$$

Formulation of the Finite Element Problem

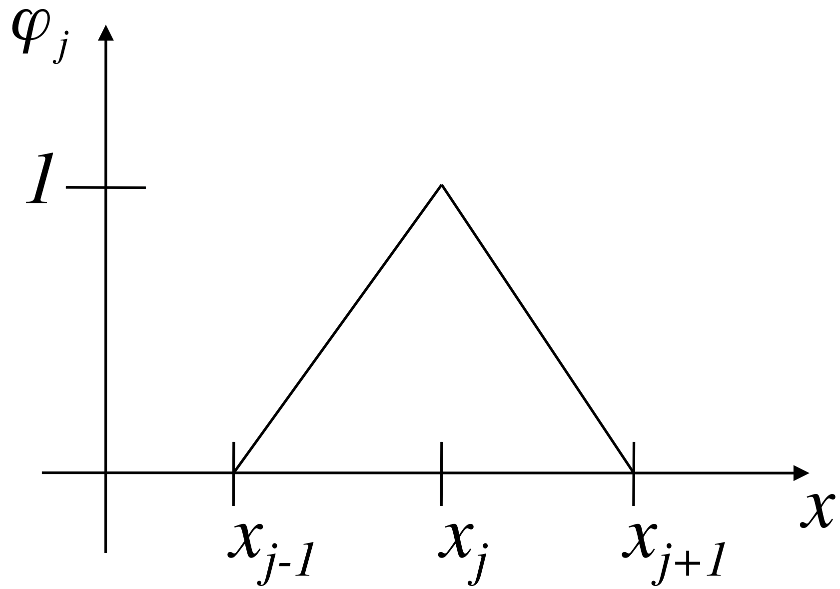
A function $v \in V_h$ can be expressed as

$$v(x) = \sum_{i=1}^{M} \eta_i \varphi_i(x), \quad x \in [0,1]$$

where $\eta_i = v(x_i)$ and $\varphi_j(x_i)$ ***basis functions***

Example (of basis function)

$$\varphi_j(x_i) = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$



Formulation of the Finite Element Problem

We can solve the problem ***(D)*** by equivalently formulating and solving the problem

Problem V_h. To find a function $u_h \in V_h$ such that

$$\left(u_h', v'\right) = \left(f, v\right) \quad \forall v \in V_h$$

$$v(x) = \sum_{i=1}^{M} \eta_i \varphi_i(x), \quad x \in [0,1]$$

$$u_h(x) = \sum_{i=1}^{M} \xi_i \varphi_i(x), \quad x \in [0,1]$$

Solution of the variational problem (V_h)

Problem V_h. To find a function $u_h \in V_h$ such that

$$(\mathrm{u}'_\mathrm{h}, \mathrm{v}') = (\mathrm{f}, \mathrm{v}) \quad \forall v \in V_h$$

Note that if $u_h \in V_h$

$$(\mathrm{u}'_\mathrm{h}, \mathrm{v}') = (\mathrm{f}, \mathrm{v}) \Rightarrow \left(\mathrm{u}'_\mathrm{h}, \sum_{\mathrm{i}=1}^{M} \eta_i \varphi'_\mathrm{i}\right) = \left(\mathrm{f}, \sum_{\mathrm{i}=1}^{\mathrm{M}} \eta_i \varphi_i\right)$$

$$\Rightarrow \sum_{\mathrm{i}=1}^{M} \eta_i (\mathrm{u}'_\mathrm{h}, \varphi'_\mathrm{i}) = \sum_{\mathrm{i}=1}^{M} \eta_i (\mathrm{f}, \varphi_i)$$

$$\Rightarrow (\mathrm{u}'_\mathrm{h}, \varphi'_\mathrm{i}) = (\mathrm{f}, \varphi_i), \quad i = 1, \ldots, M, \ \forall \mathrm{v} \in \mathrm{V}_\mathrm{h}$$

Solution of the variational problem (V_h)

Problem $\boldsymbol{V_h}$. To find a function $u_h \in V_h$ such that

$$\left(\mathrm{u}'_\mathrm{h}, \mathrm{v}'\right) = \left(\mathrm{f}, \mathrm{v}\right) \quad \forall v \in V_h$$

Moreover if $\left(\mathrm{u}'_\mathrm{h}, \varphi'_\mathrm{i}\right) = \left(\mathrm{f}, \varphi_i\right),\ i = 1, \ldots, M$ by taking linear combinations

$$\sum_{\mathrm{i}=1}^{M} \eta_i \left(\mathrm{u}'_\mathrm{h}, \varphi'_\mathrm{i}\right) = \sum_{\mathrm{i}=1}^{M} \eta_i \left(\mathrm{f}, \varphi_i\right) \Rightarrow \left(\mathrm{u}'_\mathrm{h}, \sum_{\mathrm{i}=1}^{M} \eta_i \varphi'_\mathrm{i}\right) = \left(\mathrm{f}, \sum_{\mathrm{i}=1}^{\mathrm{M}} \eta_i \varphi_i\right)$$

$$\Rightarrow \left(\mathrm{u}'_\mathrm{h}, \mathrm{v}'\right) = \left(\mathrm{f}, \mathrm{v}\right)$$

Hence, $\left(\mathrm{u}'_\mathrm{h}, \mathrm{v}'\right) = \left(\mathrm{f}, \mathrm{v}\right) \Leftrightarrow \left(\mathrm{u}'_\mathrm{h}, \varphi'_\mathrm{i}\right) = \left(\mathrm{f}, \varphi_i\right),\ i = 1, \ldots, M,\ \forall v \in V_h$

Solution of the variational problem (V_h)

Reformulate the problem (V_h) as

Problem V_h. To find a function $u_h \in V_h$ such that

$$\left(u_h', \varphi_i'\right) = \left(f, \varphi_i\right), \quad i = 1, \ldots, M$$

Since $u_h \in V_h$ then

$$u_h(x) = \sum_{i=1}^{M} \xi_i \varphi_i(x), \quad x \in [0,1]$$

Problem V_h reduces to the problem of finding ξ_i such that

$$\left(u_h', \varphi_i'\right) = \left(f, \varphi_i\right), \quad i = 1, \ldots, M$$

Solution of the variational problem (V_h)

Rewrite $\left(\mathrm{u}_\mathrm{h}', \varphi_\mathrm{i}'\right) = \left(\mathrm{f}, \varphi_i\right), \quad i = 1, \ldots, M$ as

$$\sum_{j=1}^{M} \xi_j \left(\varphi_\mathrm{j}', \varphi_\mathrm{i}'\right) = \left(\mathrm{f}, \varphi_i\right), \quad i = 1, \ldots, M$$

This system of equations can be compactly written as

$$A\xi = b$$

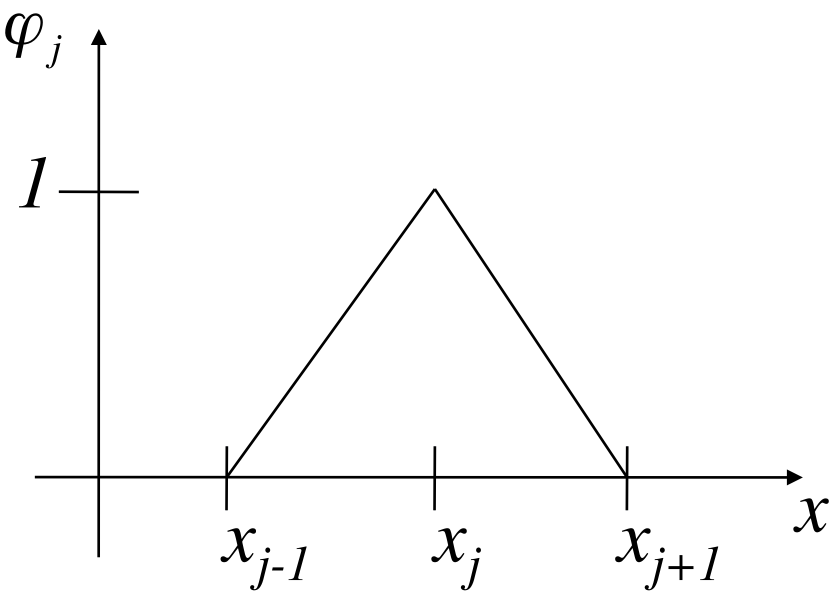
with

$$A = \begin{pmatrix} \left(\varphi_1', \varphi_1'\right) & \cdots & \left(\varphi_1', \varphi_M'\right) \\ \vdots & \ddots & \vdots \\ \left(\varphi_M', \varphi_1'\right) & \cdots & \left(\varphi_M', \varphi_M'\right) \end{pmatrix} \quad \xi = \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_M \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ \vdots \\ b_M \end{bmatrix} = \begin{bmatrix} \left(f, \varphi_1\right) \\ \vdots \\ \left(f, \varphi_M\right) \end{bmatrix}$$

Solution of the variational problem (V_h)

Assume

$$\varphi_j(x_i) = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$



We have

$$\left(\varphi_i', \varphi_i'\right) = \int_{x_{i-1}}^{x_i} \frac{1}{h_i^2}\,dx + \int_{x_i}^{x_{i+1}} \frac{1}{h_{i+1}^2}\,dx = \frac{1}{h_i} + \frac{1}{h_{i+1}}$$

$$\left(\varphi_i', \varphi_{i-1}'\right) = \left(\varphi_{i-1}', \varphi_i'\right) = -\int_{x_{i-1}}^{x_i} \frac{1}{h_i^2}\,dx = -\frac{1}{h_i}$$

Solution of the variational problem (V_h)

Moreover, A is ***symmetric*** since

$$\left(\varphi_i',\varphi_j'\right)=\left(\varphi_j',\varphi_i'\right)$$

and ***positive definite*** since

$$\begin{bmatrix}\eta_1 & \cdots & \eta_M\end{bmatrix} A \begin{bmatrix}\eta_1\\ \vdots \\ \eta_M\end{bmatrix} = \sum_{j=1}^{M}\left(\sum_{i=1}^{M}\left(\varphi_j',\varphi_i'\right)\eta_i\right)\eta_j$$

$$= \left(\sum_{i=1}^{M}\eta_i\varphi_i', \sum_{j=1}^{M}\eta_j\varphi_j'\right) = \left(v',v'\right)\geq 0$$

with $\left(v',v'\right)\geq 0 \Leftrightarrow v'=0 \Leftrightarrow v=0$

Finite element methods

In this course we will cover

- Steady state simulations
- One-dimensional problems

This lecture will ***not*** cover

- **Transient simulations***
- **Higher-dimensional problems***
- Computational aspects*

*Covered in the Comsol tutorial

Transient simulations

$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t) + f(x,t)$$

In this case, we define V_h such that $u_h \in V_h$

$$u_h(x,t) = \sum_{i=1}^{M} \xi_i(t)\varphi_i(x), \quad x \in [0,1]$$

Moreover, we need to provide initial conditions

$$u_h(x,t) = u_h^0(x), \;\; x \in [0,1]$$

Applying the Galerkin method lead to a system of ODE to calculate the unknown functions $\xi_i = \xi_i(t), \;\; i = 1,\ldots,M$