Practical Course: Modeling, Simulation, Optimization

Week 4

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4.A Solutions Exercise Week 3

4.B 2-D Conservation laws

Recap: Conservation of mass in 1-D

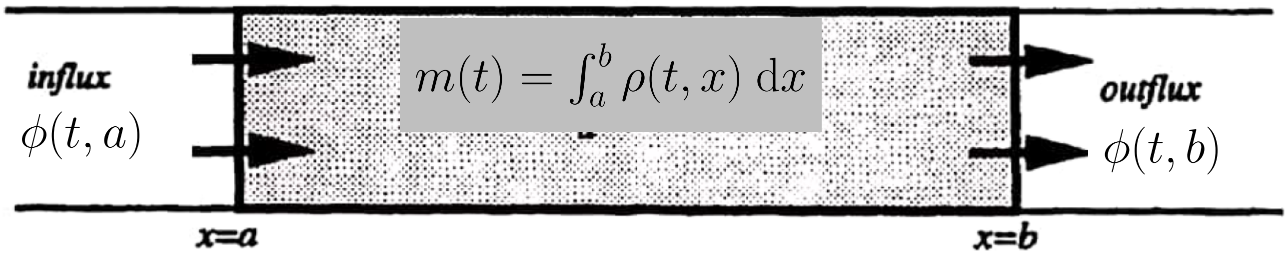


Figure: A slice of a 1-D continuum to investigate the conservation of mass (from [Roberts, 1994] but edited)

The mass $m(t)$ [kg] in $[a,b]$ changes only because of the mass fluxes $\phi(\cdot,a)$ and $\phi(\cdot,b)$ [kg/s]:

$$\frac{\partial m}{\partial t} = \phi(t,a) - \phi(t,b).$$

Using the fundamental theorem of calculus, we find

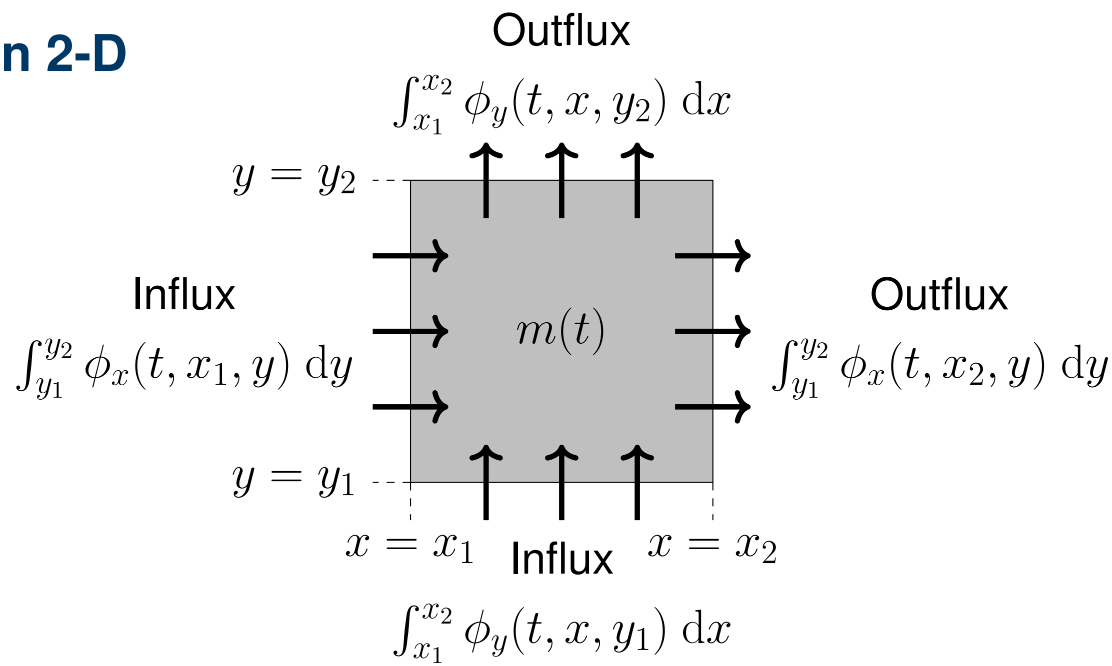
$$\int_a^b \frac{\partial \rho}{\partial t}(t,x)\,\mathrm{d}x = -\int_a^b \frac{\partial \phi}{\partial x}(t,x)\,\mathrm{d}x.$$

Because this holds for any interval $[a,b]$ in the domain $\Omega = [0,L]$:

Conservation of mass in 1-D

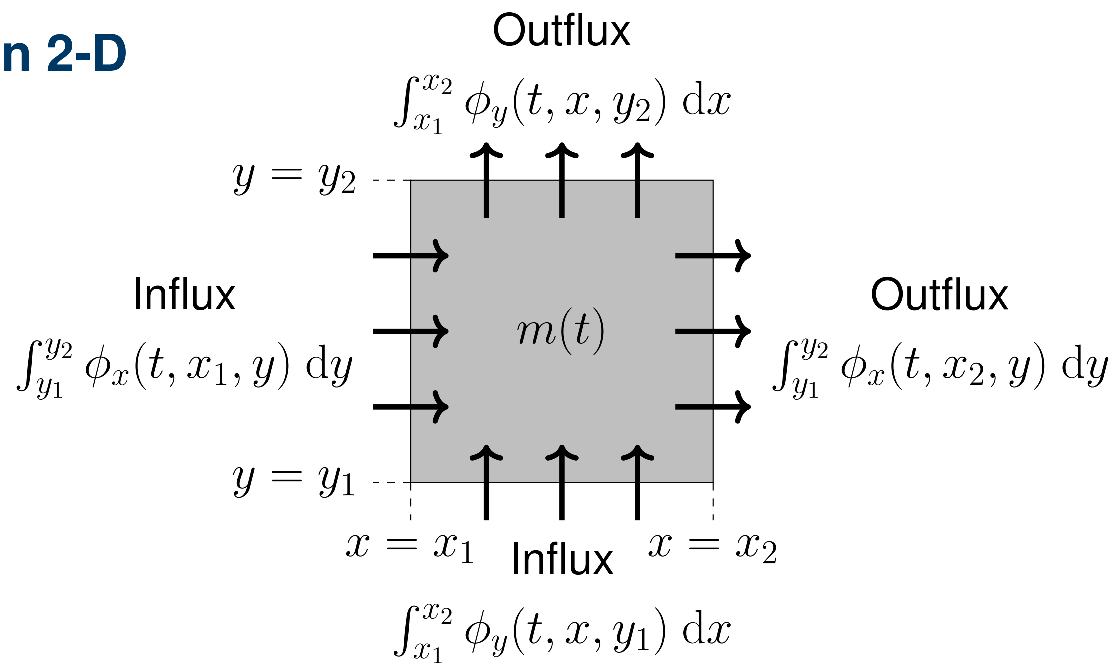
$$\frac{\partial \rho}{\partial t}(t,x) = -\frac{\partial \phi}{\partial x}(t,x).$$

Conservation of mass in 2-D



$$
\begin{aligned}
\frac{\partial m}{\partial t}(t,x,y) &= \int_{y_1}^{y_2} \left(\phi_x(t,x_1,y) - \phi_x(t,x_2,y)\right)\,\mathrm{d}y + \int_{x_1}^{x_2} \left(\phi_y(t,x,y_1) - \phi_y(t,x,y_2)\right)\,\mathrm{d}x \\
&= -\int_{y_1}^{y_2}\int_{x_1}^{x_2} \left(\frac{\partial \phi_x}{\partial x}(t,x,y) + \frac{\partial \phi_y}{\partial y}(t,x,y)\right)\,\mathrm{d}x\,\mathrm{d}y
\end{aligned}
$$

Conservation of mass in 2-D



$$\frac{\partial m}{\partial t}(t,x,y) = \int_{y_1}^{y_2} \left(\phi_x(t,x_1,y) - \phi_x(t,x_2,y)\right)\,\mathrm{d}y + \int_{x_1}^{x_2} \left(\phi_y(t,x,y_1) - \phi_y(t,x,y_2)\right)\,\mathrm{d}x$$
$$= -\int_{y_1}^{y_2}\int_{x_1}^{x_2} \left(\frac{\partial \phi_x}{\partial x}(t,x,y) + \frac{\partial \phi_y}{\partial y}(t,x,y)\right)\,\mathrm{d}x\,\mathrm{d}y$$

Because $m(t) = \int_{y_1}^{y_2}\int_{x_1}^{x_2} \rho(t,x,y)\,\mathrm{d}x\,\mathrm{d}y$ and $[x_1,x_2]\times[y_1,y_2]$ is arbitrary:

Conservation of mass in 2-D

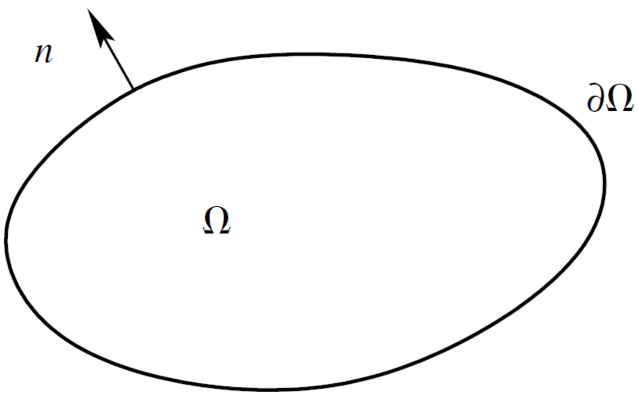
$$\frac{\partial \rho}{\partial t}(t,x,y) = -\frac{\partial \phi_x}{\partial x}(t,x,y) - \frac{\partial \phi_y}{\partial y}(t,x,y).$$

Another derivation

Mass flux vector $\boldsymbol{\phi} = [\phi_x, \phi_y]^\top$ [kg/m/s]
Outward pointing unit normal $n = [n_1, n_2]^\top$ [-]
Coordinate vector $\mathbf{x} = [x, y]^\top$ [m].

Mass flux through $\partial\Omega$ into Ω [kg/s]

$$-\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s$$



Another derivation

Mass flux vector $\boldsymbol{\phi} = [\phi_x, \phi_y]^\top$ [kg/m/s]
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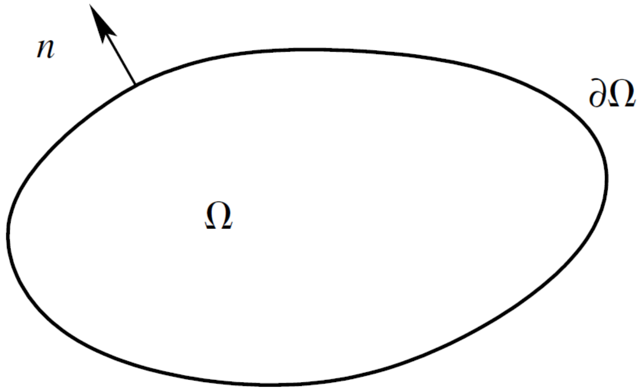

Mass flux through $\partial\Omega$ into Ω [kg/s]

$$-\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \,\mathrm{d}s$$

Conservation of mass in Ω and Gauss theorem:

$$\frac{\partial m}{\partial t} = -\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \,\mathrm{d}s = -\int_{\Omega} \nabla \cdot \boldsymbol{\phi} \,\mathrm{d}\mathbf{x}.$$

Because $m(t) = \int_\Omega \rho \,\mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Another derivation

Mass flux vector $\boldsymbol{\phi} = [\phi_x, \phi_y]^\top$ [kg/m/s]
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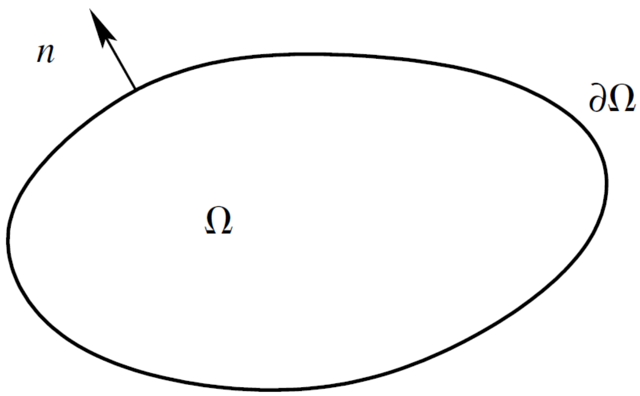


Mass flux through $\partial\Omega$ into Ω [kg/s]

$$-\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s$$

Conservation of mass in Ω and Gauss theorem:

$$\frac{\partial m}{\partial t} = -\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s = -\int_{\Omega} \nabla \cdot \boldsymbol{\phi} \, \mathrm{d}\mathbf{x}.$$

Because $m(t) = \int_\Omega \rho \, \mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Conservation of mass

$$\frac{\partial \rho}{\partial t}(t, \mathbf{x}) = -\nabla \cdot \boldsymbol{\phi}(t, \mathbf{x}).$$

Completing the model

$$\frac{\partial \rho}{\partial t}(t,\mathbf{x}) = -\nabla \cdot \boldsymbol{\phi}(t,\mathbf{x}) \qquad \left(\frac{\partial \rho}{\partial t}(t,x,y) = -\frac{\partial \phi_x}{\partial x}(t,x,y) - \frac{\partial \phi_y}{\partial y}(t,x,y) \right).$$

To complete the model, we need a *constitutive relation* that relates the mass flux $\boldsymbol{\phi}(t,\mathbf{x})$ to the mass density $\rho(t,\mathbf{x})$.

Two commonly used constitutive relations:

Fick's law

$$\boldsymbol{\phi}(t,\mathbf{x}) = -\kappa(t,\mathbf{x})\nabla\rho(t,\mathbf{x}) \qquad \left(\begin{bmatrix} \phi_x(t,x,y) \\ \phi_y(t,x,y) \end{bmatrix} = -\kappa(t,x,y) \begin{bmatrix} \frac{\partial \rho}{\partial x}(t,x,y) \\ \frac{\partial \rho}{\partial y}(t,x,y) \end{bmatrix} \right).$$

The coefficient $\kappa(t,\mathbf{x})$ [m^2/s] is called the diffusivity.
'Mass flows from locations with high concentrations to locations with low concentrations'

Advective transport

$$\boldsymbol{\phi}(t,\mathbf{x}) = \rho(t,\mathbf{x})\mathbf{v}(t,\mathbf{x}) \qquad \left(\begin{bmatrix} \phi_x(t,x,y) \\ \phi_y(t,x,y) \end{bmatrix} = \begin{bmatrix} \rho(t,x,y)v_x(t,x,y) \\ \rho(t,x,y)v_y(t,x,y) \end{bmatrix} \right).$$

The velocity field $\mathbf{v}(t,\mathbf{x})$ [m/s] is given.

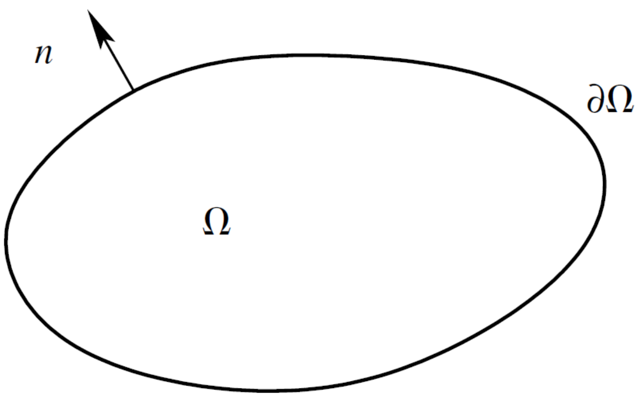
Energy conservation

Heat flux vector $\mathbf{q} = [q_x, q_y]^\top$ [W/m^2].
Outward pointing unit normal $n = [n_1, n_2]^\top$ [-].
Coordinate vector $\mathbf{x} = [x, y]^\top$ [m].

Heat flux through $\partial\Omega$ into Ω [W]

$$-H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s$$

Thickness H



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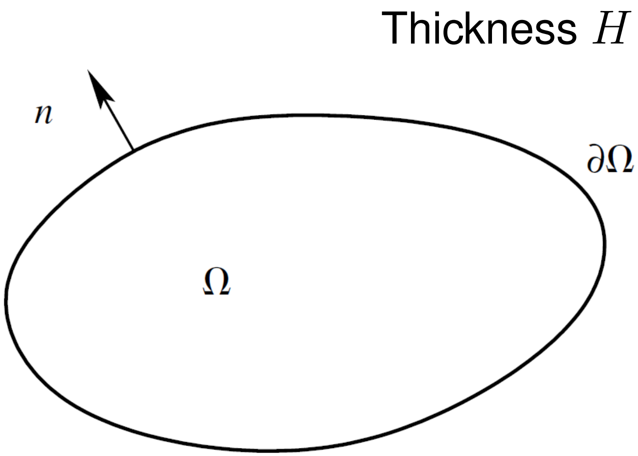


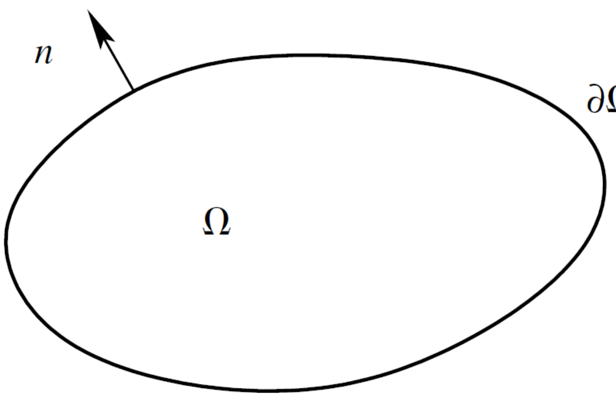
Heat flux through $\partial\Omega$ into Ω [W]

$$-H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s$$

Heat generated in Ω is $\int_\Omega Q(t, \mathbf{x}) \, \mathrm{d}\mathbf{x}$.
Conservation of energy in Ω and Gauss theorem:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \int_\Omega Q(t, \mathbf{x}) \, \mathrm{d}\mathbf{x} - H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s = \int_\Omega Q \, \mathrm{d}\mathbf{x} - H \int_\Omega \nabla \cdot \mathbf{q} \, \mathrm{d}\mathbf{x}.$$

Energy conservation



Heat flux vector $\mathbf{q} = [q_x, q_y]^\top$ [W/m^2].
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Because $U(t) = \int_\Omega \rho_u(t, \mathbf{x}) \, \mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Conservation of mass

$$\frac{\partial \rho_u}{\partial t}(t, \mathbf{x}) = -H \nabla \cdot \mathbf{q}(t, \mathbf{x}) + Q(t, \mathbf{x}).$$

Completing the model

$$\frac{\partial \rho_u}{\partial t}(t, \mathbf{x}) = -H\nabla \cdot \mathbf{q}(t, \mathbf{x}) + Q(t, \mathbf{x}).$$

We again need constitutive relations to complete the model.

Fourier's law of heat conduction in 2-D

$$\mathbf{q}(t, \mathbf{x}) = -k\nabla T(t, \mathbf{x}).$$

The coefficient k^* [W/m/K] is the thermal conductivity and $T(t, \mathbf{x})$ [K] is the temperature.
'Heat flows from locations with high temperatures to locations with low temperatures'

Internal energy in 2-D

$$\rho_u(t, \mathbf{x}) = cHT(t, \mathbf{x}).$$

The coefficient c [J/K/m^3] heat capacity per unit volume.

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4.C The weak form in 2-D

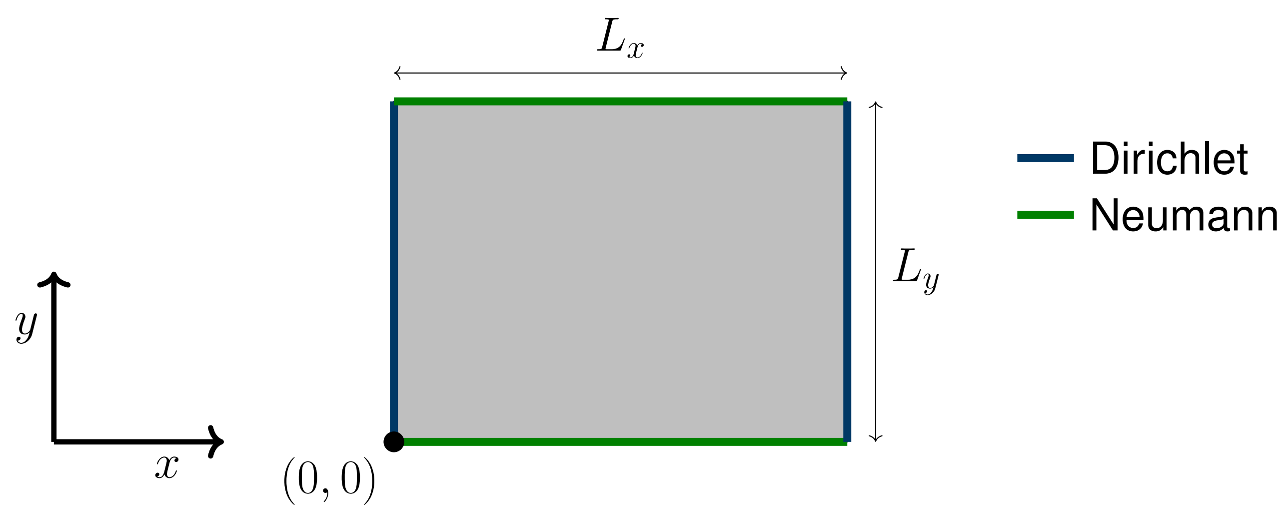
A sample problem

Consider the 2-D heat equation on $(x, y) \in [0, L_x] \times [0, L_y]$

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

$$u(t,0,y) = u(t,L_x,y) = 0, \qquad -\kappa \frac{\partial u}{\partial y}(t,x,0) = -\kappa \frac{\partial u}{\partial y}(t,x,L_y) = 0,$$

$$u(0,x,y) = u_0(x,y).$$



Integration by parts

Consider the 2-D heat equation on $(x, y) \in [0, L_x] \times [0, L_y]$

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

$$u(t,0,y) = u(t,L_x,y) = 0, \qquad -\kappa \frac{\partial u}{\partial y}(t,x,0) = -\kappa \frac{\partial u}{\partial y}(t,x,L_y) = 0,$$

$$u(0,x,y) = u_0(x,y).$$

Multiply by a test function $w(x, y)$ and integrate over $(x, y) \in [0, L_x] \times [0, L_y]$

- For the first term on the RHS, integration by parts over x shows that

$$\int_0^{L_y} \int_0^{L_x} w(x,y) \frac{\partial^2 u}{\partial x^2}(t,x,y) \, \mathrm{d}x \, \mathrm{d}y = \int_0^{L_y} w(x,y) \frac{\partial u}{\partial x}(t,x,y) \Big|_{x=0}^{L_x} \mathrm{d}y$$
$$- \int_0^{L_y} \int_0^{L_x} \frac{\partial w}{\partial x}(x,y) \frac{\partial u}{\partial x}(t,x,y) \, \mathrm{d}x \, \mathrm{d}y$$

- For the first term on the RHS, integration by parts over y shows that

$$\int_0^{L_y} \int_0^{L_x} w(x,y) \frac{\partial^2 u}{\partial y^2}(t,x,y) \, \mathrm{d}x \, \mathrm{d}y = \int_0^{L_x} w(x,y) \frac{\partial u}{\partial y}(t,x,y) \, \mathrm{d}x \, \Big|_{y=0}^{L_y}$$
$$- \int_0^{L_y} \int_0^{L_x} \frac{\partial w}{\partial y}(x,y) \frac{\partial u}{\partial y}(t,x,y) \, \mathrm{d}x \, \mathrm{d}y$$

The resulting weak form

Consider the 2-D heat equation on $(x,y) \in [0,L_x] \times [0,L_y]$

$$\begin{aligned}
&\frac{\partial u}{\partial t}(t,x,y) = \kappa \left(\frac{\partial^2 u}{\partial x^2}(t,x,y) + \frac{\partial^2 u}{\partial y^2}(t,x,y) \right) + f(t,x,y), \\
&u(t,0,y) = u(t,L_x,y) = 0, \qquad -\kappa \frac{\partial u}{\partial y}(t,x,0) = -\kappa \frac{\partial u}{\partial y}(t,x,L_y) = 0, \\
&u(0,x,y) = u_0(x,y).
\end{aligned}$$

A weak solution $u \in L^2([0,T],V)$ of the above problem satisfies

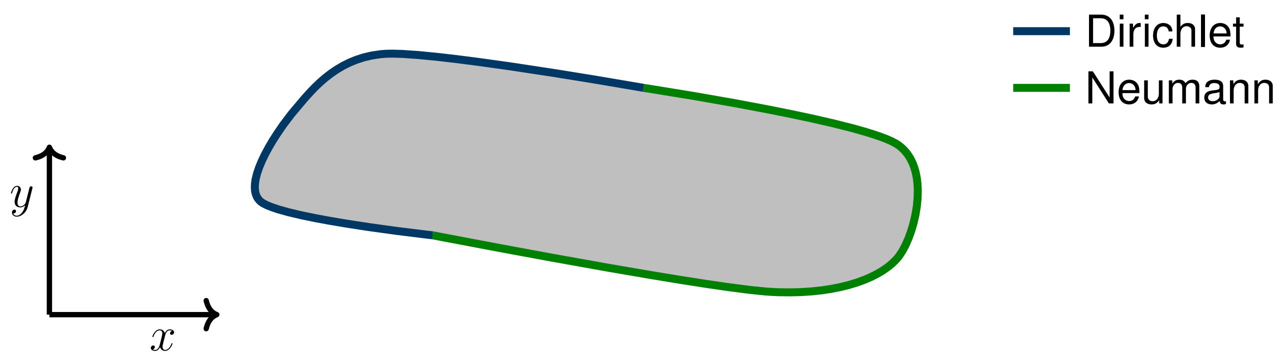
$$\begin{aligned}
\int_0^{L_y}\int_0^{L_x} w(x,y)\frac{\partial u}{\partial t}(t,x,y)\,\mathrm{d}x\,\mathrm{d}y &= -\kappa \int_0^{L_y}\int_0^{L_x} \frac{\partial w}{\partial x}(x,y)\frac{\partial u}{\partial x}(t,x,y)\,\mathrm{d}x\,\mathrm{d}y \\
&\quad - \kappa \int_0^{L_y}\int_0^{L_x} \frac{\partial w}{\partial y}(x,y)\frac{\partial u}{\partial y}(t,x,y)\,\mathrm{d}x\,\mathrm{d}y + \int_0^{L_y}\int_0^{L_x} w(x,y)f(t,x,y)\,\mathrm{d}x\,\mathrm{d}y \\
&\qquad u(0,x,y) = u_0(x,y),
\end{aligned}$$

for all $w \in V = \{w \in H^1([0,L_x] \times [0,L_y]) \mid w(0,\cdot) = w(L_x,\cdot) = 0\}$ and a.a. $t \in [0,T]$.

A more general setting

Consider the 2-D heat equation on $(x, y) \in \Omega \subset \mathbb{R}^2$

$$
\begin{aligned}
&\frac{\partial u}{\partial t} = \kappa \nabla^2 u + f, && (x, y) \in \Omega, t \in [0, T], \\
&u = 0, && (x, y) \in \partial\Omega_{\mathrm{D}}, t \in [0, T] \\
&-\kappa \nabla u \cdot \mathbf{n} = 0, && (x, y) \in \partial\Omega_{\mathrm{N}}, t \in [0, T], \\
&u(0) = u_0, && (x, y) \in \Omega.
\end{aligned}
$$



The resulting weak form

Consider the 2-D heat equation on $(x, y) \in \Omega \subset \mathbb{R}^2$

$$\begin{aligned}
&\frac{\partial u}{\partial t} = \kappa \nabla^2 u + f, && (x,y) \in \Omega, t \in [0,T], \\
&u = 0, && (x,y) \in \partial\Omega_{\mathrm{D}}, t \in [0,T] \\
&-\kappa \nabla u \cdot \mathbf{n} = 0, && (x,y) \in \partial\Omega_{\mathrm{N}}, t \in [0,T], \\
&u(0) = u_0, && (x,y) \in \Omega.
\end{aligned}$$

Multiply by a testfunction $w(x, y)$ and integrate over $(x, y) \in \Omega$.
For the first term on the RHS, we find using Green's first identity

$$\iint_\Omega w \nabla^2 u \,\mathrm{d}x\,\mathrm{d}y = \int_{\partial\Omega} w(\nabla u \cdot \mathbf{n}) \,\mathrm{d}S - \iint_\Omega \nabla w \cdot \nabla u \,\mathrm{d}x\,\mathrm{d}y.$$

A weak solution $u \in L^2([0, T], V)$ of the above problem satisfies

$$\iint_\Omega w \frac{\partial u}{\partial t} \,\mathrm{d}x\,\mathrm{d}y = -\kappa \iint_\Omega \nabla w \cdot \nabla u \,\mathrm{d}x\,\mathrm{d}y + \iint_\Omega w f \,\mathrm{d}x\,\mathrm{d}y, \qquad u(0) = u_0.$$

for all $w \in V = \{w \in H^1(\Omega) \mid w|_{\partial\Omega_{\mathrm{D}}} = 0\}$ and almost all $t \in [0, T]$.

4.D Galerkin discretization in 2-D

Galerkin discretization

We thus arrive at the weak formulation of our problem, for example

$$\iint_\Omega w \frac{\partial u}{\partial t} \,\mathrm{d}x\,\mathrm{d}y = -\kappa \iint_\Omega \nabla w \cdot \kappa \nabla u \,\mathrm{d}x\,\mathrm{d}y + \iint_\Omega w f \,\mathrm{d}x\,\mathrm{d}y$$

for all $w \in V = \{w \in H^1(\Omega) \mid w|_{\partial\Omega_\mathrm{D}} = 0\}$ and almost all $t \in [0, T]$.

The basic idea for a Galerkin discretization:
Replace the infinite dimensional space V by an N-dimensional subspace $V_N \subset V$.
Note: V_N must be a subspace of V.

This thus leads to a solution $u_N \in L^2(0, T; V_N)$ which satisfies

$$\iint_\Omega w_N \frac{\partial u_N}{\partial t} \,\mathrm{d}x\,\mathrm{d}y = -\kappa \iint_\Omega \nabla w_N \cdot \kappa \nabla u_N \,\mathrm{d}x\,\mathrm{d}y + \iint_\Omega w_N f \,\mathrm{d}x\,\mathrm{d}y, \qquad u(0) = u_0,$$

for all $w_N \in V_N$.

Galerkin approximation: a basis for V_N

We want to find the function $u_N \in L^2(0,T;V_N)$ which satisfies

$$\iint_\Omega w_N \frac{\partial u_N}{\partial t} \, \mathrm{d}x \, \mathrm{d}y = -\kappa \iint_\Omega \nabla w_N \cdot \kappa \nabla u_N \, \mathrm{d}x \, \mathrm{d}y + \iint_\Omega w_N f \, \mathrm{d}x \, \mathrm{d}y, \qquad u(0) = u_0,$$

for all $w_N \in V_N$.

Choose a basis $\{\mathbf{N}_1(x,y), \mathbf{N}_2(x,y), \dots, \mathbf{N}_N(x,y)\}$ for $V_N \subset V$ and define the row-vector

$$\mathbf{N}(x,y) = \begin{bmatrix} \mathbf{N}_1(x,y) & \mathbf{N}_2(x,y) & \cdots & \mathbf{N}_N(x,y) \end{bmatrix}.$$

Because $u_N \in L^2(0,T;V_N)$ and $w_N \in V_N$, we can write

$$u_N(t,x,y) = \sum_{n=1}^N \mathbf{N}_n(x,y) u_n(t) = \mathbf{N}(x,y)\mathbf{u}(t),$$

$$w_N(x,y) = \mathbf{N}(x,y)\mathbf{w} = \mathbf{w}^\top (\mathbf{N}(x,y))^\top,$$

where $\mathbf{u} \in L^2(0,T;\mathbb{R}^N)$ and $\mathbf{w} \in \mathbb{R}^N$ is a column vector.

Galerkin approximation: Mass and stiffness matrices

We want to find the function $\mathbf{u} \in L^2(0,T;V_N)$ which satisfies for all $\mathbf{w} \in \mathbb{R}^N$

$$\iint_\Omega w_N \frac{\partial u_N}{\partial t} \,\mathrm{d}x\,\mathrm{d}y = -\kappa \iint_\Omega \nabla w_N \cdot \kappa \nabla u_N \,\mathrm{d}x\,\mathrm{d}y + \iint_\Omega w_N f \,\mathrm{d}x\,\mathrm{d}y, \qquad u(0) = u_0,$$

$$u_N(t,x,y) = \mathbf{N}(x,y)\mathbf{u}(t), \qquad w_N(x,y) = \mathbf{w}^\top (\mathbf{N}(x,y))^\top,$$

Substitute the expressions for u_N and w_N into the above equation:

$$\iint_\Omega \mathbf{w}^\top \mathbf{N}^\top \mathbf{N} \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} \,\mathrm{d}x\,\mathrm{d}y = -\kappa \iint_\Omega \mathbf{w}^\top \nabla \mathbf{N}^\top \cdot \nabla \mathbf{N}\mathbf{u} \,\mathrm{d}x\,\mathrm{d}y + \iint_\Omega \mathbf{w}^\top \mathbf{N}^\top f \,\mathrm{d}x\,\mathrm{d}y,$$

Which can be rewritten as

$$\mathbf{w}^\top \mathbf{E} \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}(t) = \mathbf{w}^\top \mathbf{A}\mathbf{u}(t) + \mathbf{w}^\top \mathbf{f}(t), \qquad \mathbf{u}(0) = \mathbf{u}_0,$$

where

$$\mathbf{E} = \iint_\Omega \mathbf{N}^\top \mathbf{N} \,\mathrm{d}x\,\mathrm{d}y, \quad \mathbf{A} = -\kappa \iint_\Omega \nabla \mathbf{N}^\top \cdot \nabla \mathbf{N} \,\mathrm{d}x\,\mathrm{d}y, \quad \mathbf{f}(t) = \iint_\Omega \mathbf{N}^\top f(t) \,\mathrm{d}x\,\mathrm{d}y$$

Because this equation should be satisfied for all $\mathbf{w} \in \mathbb{R}^N$, we conclude

$$\mathbf{E} \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}(t) = \mathbf{A}\mathbf{u}(t) + \mathbf{f}(t), \qquad \mathbf{u}(0) = \mathbf{u}_0,$$

Question 1

We take $\Omega = [0,1] \times [0,1]$ and consider two shape functions:

$$\mathbf{N}(x,y) = \begin{bmatrix} x & y \end{bmatrix}.$$

Compute

$$\mathbf{E} = \iint_{\Omega} \mathbf{N}^{\top}\mathbf{N} \, \mathrm{d}x \, \mathrm{d}y.$$

A) $\mathbf{E} = \begin{bmatrix} \frac{1}{3} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{3} \end{bmatrix}$

B) $\mathbf{E} = \begin{bmatrix} \frac{1}{3} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} \end{bmatrix}$

C) $\mathbf{E} = \begin{bmatrix} \frac{1}{3} & 1 \\ 1 & \frac{1}{3} \end{bmatrix}$

D) $\mathbf{E} = \frac{2}{3}$

E) None of the above

Question 2

We take $\Omega = [0,1] \times [0,1]$ and consider two shape functions:

$$\mathbf{N}(x,y) = \begin{bmatrix} x & y \end{bmatrix}.$$

Compute

$$\mathbf{A} = \iint_\Omega \nabla\mathbf{N}^\top \nabla\mathbf{N} \, \mathrm{d}x \, \mathrm{d}y.$$

A) $\mathbf{A} = \begin{bmatrix} \frac{1}{3} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{3} \end{bmatrix}$

B) $\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

C) $\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

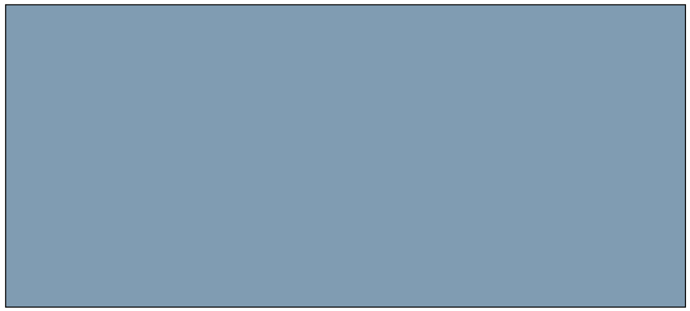
D) $\mathbf{A} = 2$

E) None of the above

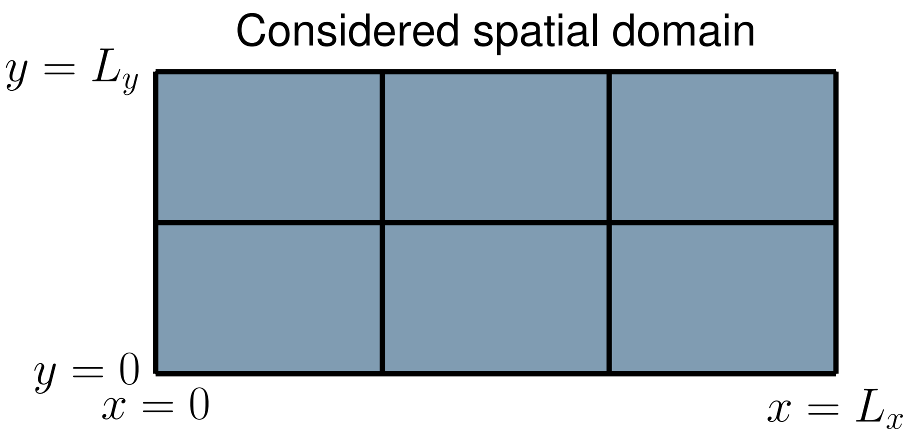
4.E Assembly procedure for 2-D Finite elements

2-D Finite Elements step-by-step

Considered spatial domain

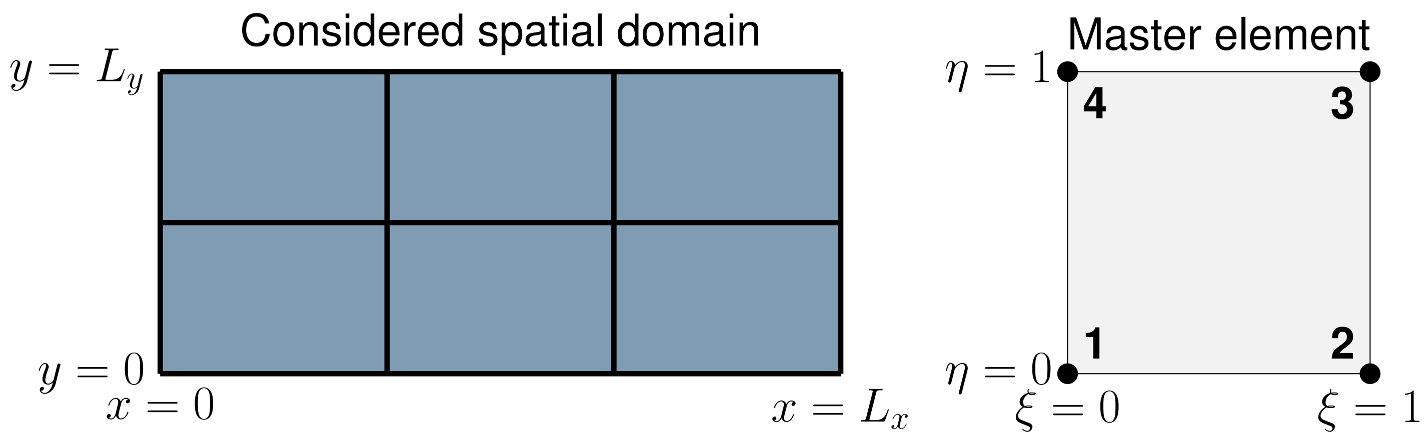


2-D Finite Elements step-by-step



STEP 1: Divide the domain $[0, L_x] \times [0, L_y]$ into M rectangular elements Ω^e.

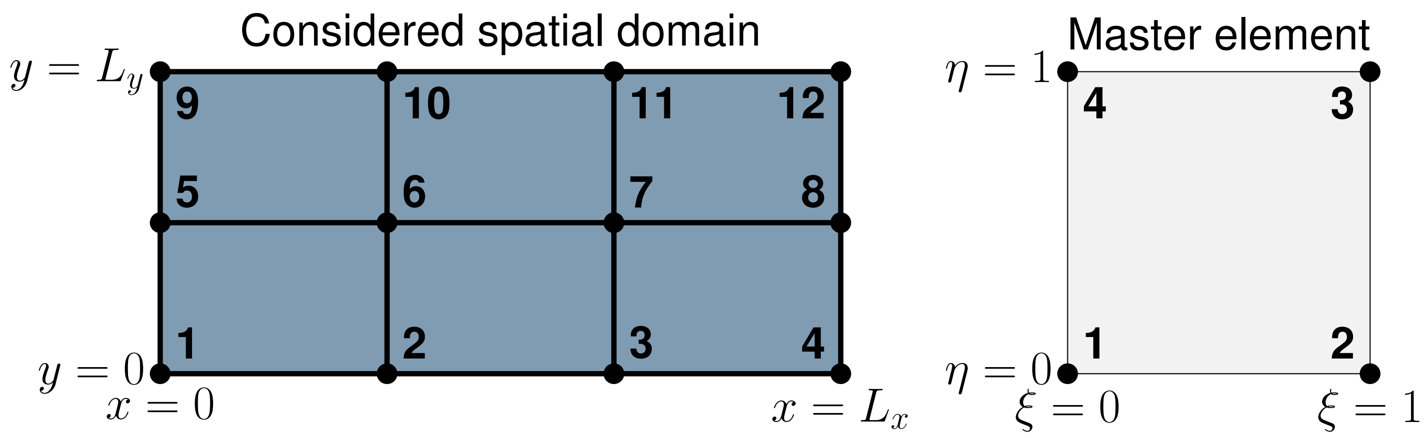
2-D Finite Elements step-by-step



STEP 1: Divide the domain $[0, L_x] \times [0, L_y]$ into M rectangular elements Ω^e.
STEP 2: Choose shape functions for the master element

$$\mathbf{N}^e(\xi, \eta) = \begin{bmatrix} (1-\xi)(1-\eta) & \xi(1-\eta) & \xi\eta & (1-\xi)\eta \end{bmatrix}.$$

2-D Finite Elements step-by-step



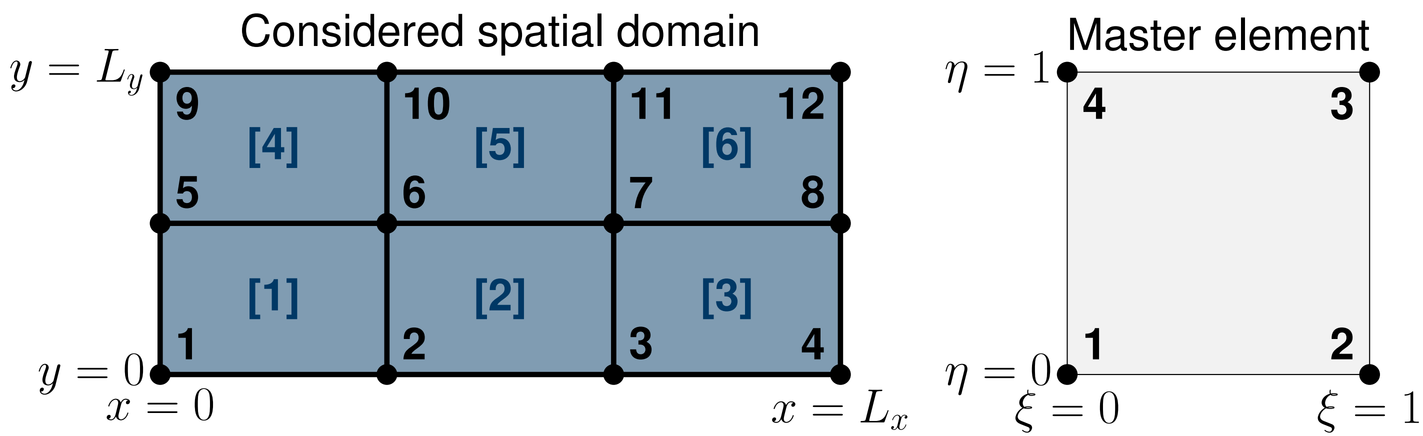
STEP 1: Divide the domain $[0, L_x] \times [0, L_y]$ into M rectangular elements Ω^e.
STEP 2: Choose shape functions for the master element

$$\mathbf{N}^e(\xi, \eta) = \begin{bmatrix} (1-\xi)(1-\eta) & \xi(1-\eta) & \xi\eta & (1-\xi)\eta \end{bmatrix}.$$

STEP 3: Define the nodes in the original domain based on the chosen master element. Assign a number to each node.

$$\texttt{node\_nmbrs} = \begin{bmatrix} 1 & 5 & 9 \\ 2 & 6 & 10 \\ 3 & 7 & 11 \\ 4 & 8 & 12 \end{bmatrix}.$$

The element list



STEP 4: Build the element list.
The element list contains the numbers of the nodes in each each element.
The order in which elements are stored also assigns a number to each element.

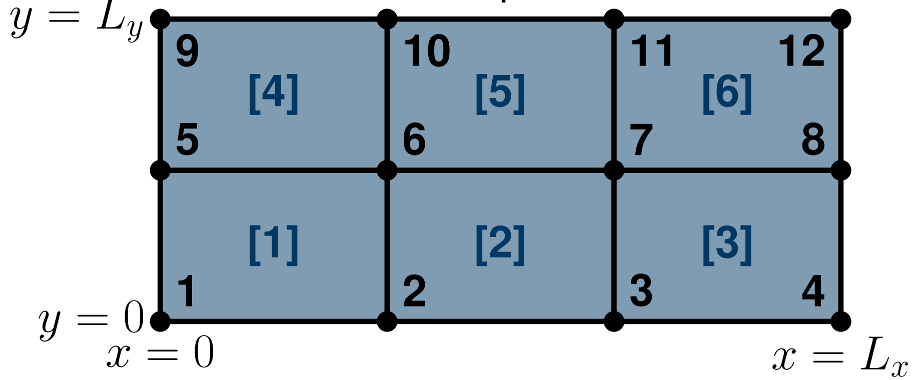
$$\texttt{elem\_list} = \begin{bmatrix} 1 & 2 & 6 & 5 \\ 2 & 3 & 7 & 6 \\ \vdots & \vdots & \vdots & \vdots \\ 7 & 8 & 12 & 11 \end{bmatrix}, \qquad \texttt{elem\_nmbrs} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}.$$

Note: the ordering of the node numbers should match with the master element!

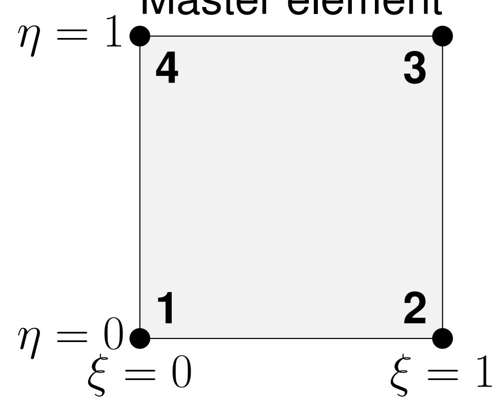
QUESTION 3: What is the fifth row in the matrix `elem_list`?

Element matrices (uniform mesh)

Considered spatial domain



Master element



STEP 5: when all elements are of the same size $L_{e,x} \times L_{e,y}$, we can compute the contributions of one element directly:

$$\tilde{\mathbf{E}}^e = \int_0^{L_{e,x}} \int_0^{L_{e,y}} \left(\mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})\right)^\top \mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}}) \,\mathrm{d}x\,\mathrm{d}y$$

$$\tilde{A}^e = \int_0^{L_{e,x}} \int_0^{L_{e,y}} \left(\frac{\partial \mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})}{\partial x}\right)^\top \frac{\mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})}{\partial x} + \left(\frac{\partial \mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})}{\partial y}\right)^\top \frac{\mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})}{\partial y} \,\mathrm{d}x\,\mathrm{d}y$$

$$\tilde{\mathbf{f}}^e = \int_0^{L_{e,x}} \int_0^{L_{e,y}} \left(\mathbf{N}^e(\tfrac{x}{L_{e,x}}, \tfrac{y}{L_{e,y}})\right)^\top \,\mathrm{d}x\,\mathrm{d}y$$

Note: these formulas depend on the size of the elements $L_{e,x} \times L_{e,y}$!

Remark: relation to the standard element

Using the change of variables

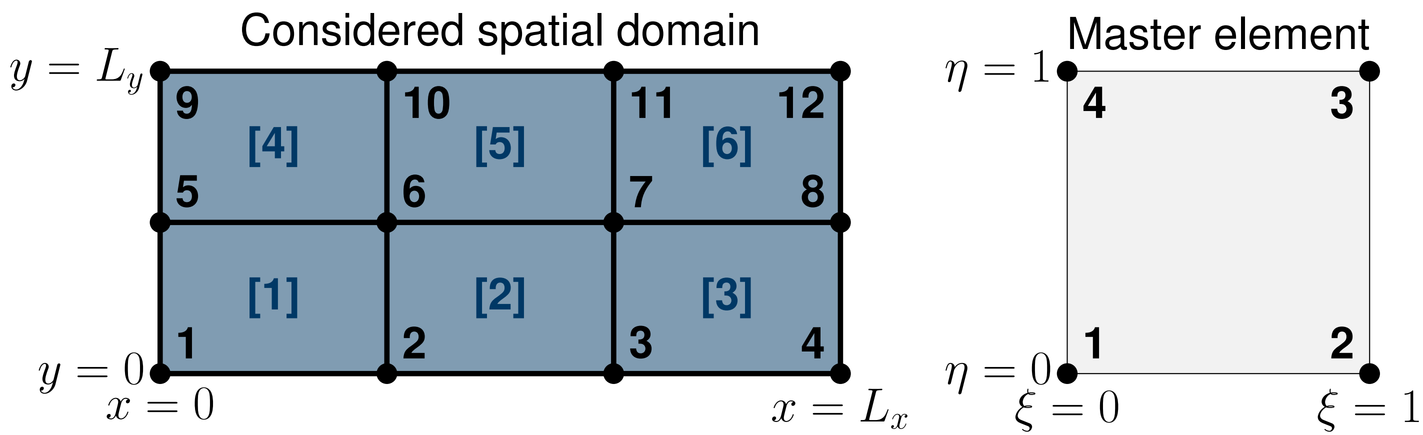
$$(\xi, \eta) = \left(\frac{x}{L_{e,x}}, \frac{y}{L_{e,y}} \right), \qquad (x, y) = (L_{e,x}\xi, L_{e,y}\eta),$$

we can relate the integrals from the previous slide to the standard element $[0, 1]^2$

$$\begin{aligned}
\tilde{\mathbf{E}}^e &= L_{e,x}L_{e,y} \int_0^1 \int_0^1 (\mathbf{N}^e(\xi,\eta))^\top \mathbf{N}^e(\xi,\eta)\, \mathrm{d}\xi\, \mathrm{d}\eta =: L_{e,x}L_{e,y}\mathbf{E}^e, \\
\tilde{\mathbf{A}}^e &= \frac{L_{e,y}}{L_{e,x}} \int_0^1 \int_0^1 \left(\frac{\partial \mathbf{N}^e(\xi,\eta)}{\partial \xi} \right)^\top \frac{\mathbf{N}^e(\xi,\eta)}{\partial \xi}\, \mathrm{d}\xi\, \mathrm{d}\eta \\
&\quad + \frac{L_{e,x}}{L_{e,y}} \int_0^1 \int_0^1 \left(\frac{\partial \mathbf{N}^e(\xi,\eta)}{\partial \eta} \right)^\top \frac{\mathbf{N}^e(\xi,\eta)}{\partial \eta}\, \mathrm{d}\xi\, \mathrm{d}\eta = \frac{L_{e,y}}{L_{e,x}}\mathbf{A}^e_{xx} + \frac{L_{e,x}}{L_{e,y}}\mathbf{A}^e_{yy}, \\
\tilde{\mathbf{f}}^e &= L_{e,x}L_{e,y} \int_0^1 \int_0^1 (\mathbf{N}^e(\xi,\eta))^\top\, \mathrm{d}\xi\, \mathrm{d}\eta =: L_{e,x}L_{e,y}\mathbf{f}^e.
\end{aligned}$$

Note: the two parts of $\tilde{\mathbf{A}}^e$ are scaled differently!

Assembly



STEP 6: Assemble the global mass and stiffness matrices $\mathbf{E}$ and $\mathbf{A}$ $(N \times N)$ and the global load vector $\mathbf{f}$ (length N) using the element list from STEP 4.

$$\texttt{elem\_list} = \begin{bmatrix} 1 & 2 & 6 & 5 \\ 2 & 3 & 7 & 6 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

Write the contribution of each element:

$$\mathbf{E}[[1,2,6,5],[1,2,6,5]] = \tilde{\mathbf{E}}^{e=1}, \qquad \mathbf{E}[[2,3,7,6],[2,3,7,6]] = \tilde{\mathbf{E}}^{e=2}, \qquad \dots$$

Boundary conditions

STEP 7: Include the contributions of Robin boundary conditions.
(See the example on the following slides)
STEP 8: Take into account (zero) Dirichlet boundary conditions by removing rows and columns corresponding to the constrained DOFs from $\mathbf{E}$, $\mathbf{A}$, and $\mathbf{f}$.

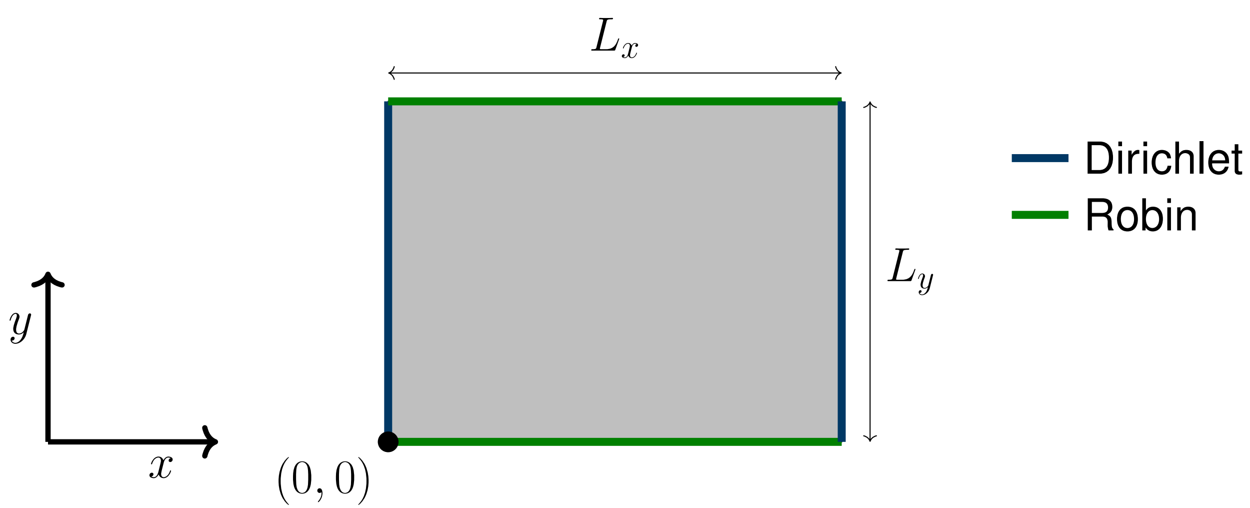
Example: boundary conditions

Consider the 2-D heat equation on $(x,y) \in [0, L_x] \times [0, L_y]$

$$0 = \kappa \left(\frac{\partial^2 u}{\partial x^2}(t,x,y) + \frac{\partial^2 u}{\partial y^2}(t,x,y) \right) + f(t,x,y),$$

$$u(t,0,y) = u(t,L_x,y) = 0, \qquad \kappa \frac{\partial u}{\partial y}(t,x,0) = hu(t,x,0), \qquad -\kappa \frac{\partial u}{\partial y}(t,x,L_y) = hu(t,x,L_y)$$

$$u(0,x,y) = u_0(x,y).$$



Example: boundary conditions

We obtain the following weak form:

$$0 = -h \int_0^{L_x} \left([vu]_{y=0} + [vu]_{y=L_y} \right) \, \mathrm{d}x \\ - \kappa \int_0^{L_x} \int_x^{L_y} \left(\frac{\partial v}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\frac{\partial u}{\partial y} \right) \, \mathrm{d}y \, \mathrm{d}x + \int_0^{L_x} \int_x^{L_y} vf \, \mathrm{d}y \, \mathrm{d}x.$$

To include the first two terms in the stiffness matrix $\mathbf{A}$, we need the element matrices

$$\tilde{\mathbf{E}}^e_{\text{bot}} = \int_0^{L_{e,x}} \left(\mathbf{N}^e(\tfrac{x}{L_{e,x}}, 0) \right)^\top \mathbf{N}^e(\tfrac{x}{L_{e,x}}, 0) \, \mathrm{d}x,$$

$$\tilde{\mathbf{E}}^e_{\text{top}} = \int_0^{L_{e,x}} \left(\mathbf{N}^e(\tfrac{x}{L_{e,x}}, 1) \right)^\top \mathbf{N}^e(\tfrac{x}{L_{e,x}}, 1) \, \mathrm{d}x.$$

For Robin BCs on the edges $x = 0$ and $x = L_{e,x}$ you would also need

$$\tilde{\mathbf{E}}^e_{\text{left}} = \int_0^{L_{e,y}} \left(\mathbf{N}^e(0, \tfrac{y}{L_{e,y}}) \right)^\top \mathbf{N}^e(0, \tfrac{y}{L_{e,y}}) \, \mathrm{d}y,$$

$$\tilde{\mathbf{E}}^e_{\text{right}} = \int_0^{L_{e,y}} \left(\mathbf{N}^e(1, \tfrac{y}{L_{e,y}}) \right)^\top \mathbf{N}^e(1, \tfrac{y}{L_{e,y}}) \, \mathrm{d}y.$$

Remark: relation to the standard element

Using the transformation

$$(\xi, \eta) = \left(\frac{x}{L_{e,x}}, \frac{y}{L_{e,y}} \right), \qquad (x, y) = (L_{e,x}\xi, L_{e,y}\eta),$$

we can relate the integrals from the previous slide to the standard element $[0,1]^2$

$$\begin{aligned}
\tilde{\mathbf{E}}^e_{\text{bot}} &= L_{e,x} \int_0^1 \left(\mathbf{N}^e(\xi, 0)\right)^\top \mathbf{N}^e(\xi, 0) \, \mathrm{d}\xi = L_{e,x}\mathbf{E}^e_{\text{bot}}, \\
\tilde{\mathbf{E}}^e_{\text{top}} &= L_{e,x} \int_0^1 \left(\mathbf{N}^e(\xi, 1)\right)^\top \mathbf{N}^e(\xi, 1) \, \mathrm{d}\xi = L_{e,x}\mathbf{E}^e_{\text{top}}, \\
\tilde{\mathbf{E}}^e_{\text{left}} &= L_{e,y} \int_0^1 \left(\mathbf{N}^e(0, \eta)\right)^\top \mathbf{N}^e(0, \eta) \, \mathrm{d}\eta = L_{e,y}\mathbf{E}^e_{\text{left}}, \\
\tilde{\mathbf{E}}^e_{\text{right}} &= L_{e,y} \int_0^1 \left(\mathbf{N}^e(1, \eta)\right)^\top \mathbf{N}^e(1, \eta) \, \mathrm{d}\eta = L_{e,y}\mathbf{E}^e_{\text{right}}.
\end{aligned}$$

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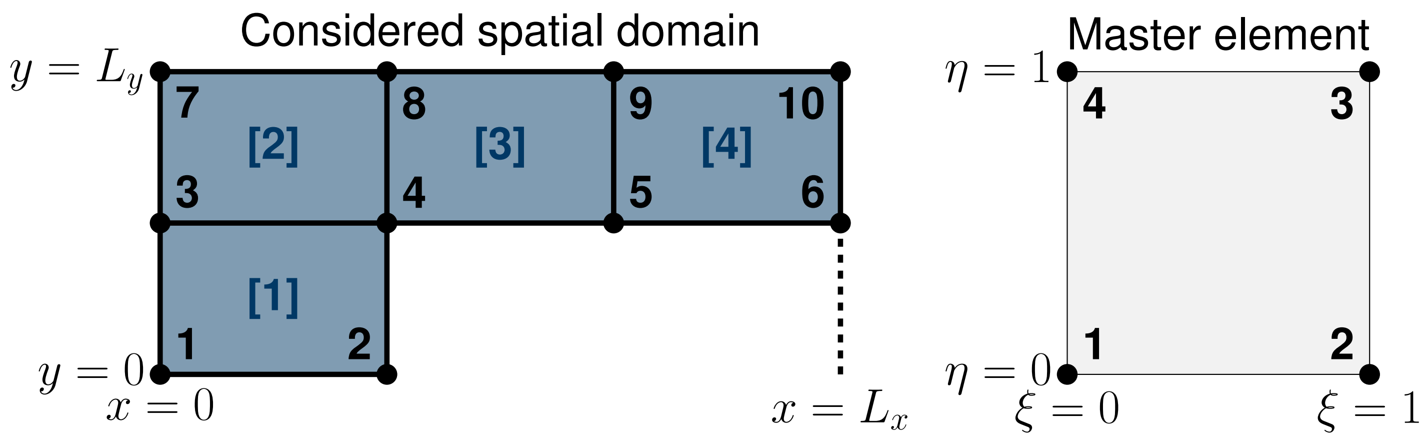
4.F Three final remarks

Remark 1/3: Domains that are not rectangular

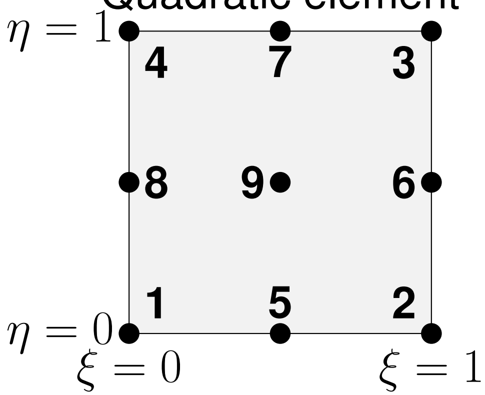


Only number the elements and nodes inside the considered domain.

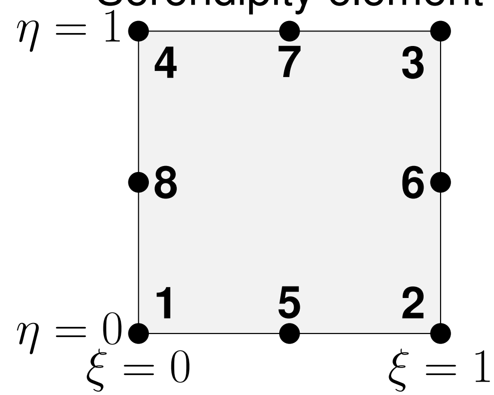
$$\texttt{node\_nmbrs} = \begin{bmatrix} 1 & 3 & 7 \\ 2 & 4 & 8 \\ 0 & 5 & 9 \\ 0 & 6 & 10 \end{bmatrix}, \qquad \texttt{elem\_list} = \begin{bmatrix} 1 & 2 & 4 & 3 \\ 3 & 4 & 8 & 7 \\ 4 & 5 & 9 & 8 \\ 5 & 6 & 10 & 9 \end{bmatrix}$$

Remark 2/3: Second order elements

Quadratic element



Serendipity element



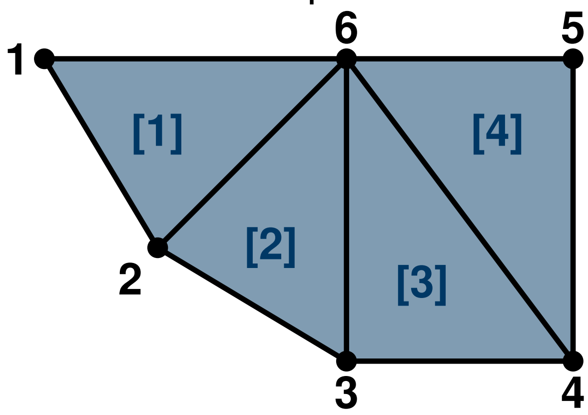
There are two commonly used quadratic shape functions on rectangular elements:

$$\mathbf{N}^e(\xi,\eta) = \begin{bmatrix} p_0(\xi)p_0(\eta) \\ p_1(\xi)p_0(\eta) \\ p_1(\xi)p_1(\eta) \\ p_0(\xi)p_1(\eta) \\ p_{1/2}(\xi)p_0(\eta) \\ p_1(\xi)p_{1/2}(\eta) \\ p_{1/2}(\xi)p_1(\eta) \\ p_0(\xi)p_{1/2}(\eta) \\ p_{1/2}(\xi)p_{1/2}(\eta) \end{bmatrix}^\top, \qquad \mathbf{N}^e(\xi,\eta) = \begin{bmatrix} p_0(\xi)p_0(\eta) \\ p_1(\xi)p_0(\eta) \\ p_1(\xi)p_1(\eta) \\ p_0(\xi)p_1(\eta) \\ p_{1/2}(\xi)p_0(\eta) \\ p_1(\xi)p_{1/2}(\eta) \\ p_{1/2}(\xi)p_1(\eta) \\ p_0(\xi)p_{1/2}(\eta) \end{bmatrix}^\top,$$

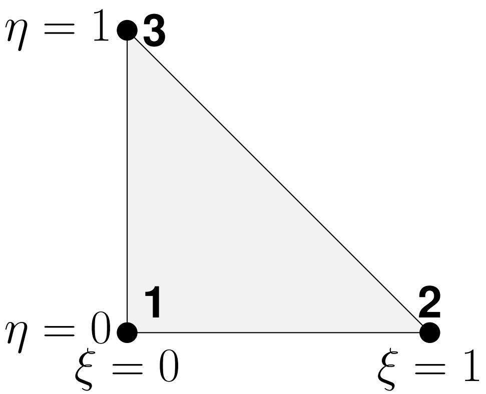
where $p_0(\xi) = (1-\xi)(1-2\xi)$, $p_{1/2}(\xi) = 4(1-\xi)\xi$, and $p_1(\xi) = (2\xi-1)\xi$.

Remark 3/3: Nonrectangular meshes

Considered spatial domain



Master element



We can no longer use the matrix `node_nmbrs` to assign numbers to the nodes. Instead we make a node list:

$$\texttt{node\_list} = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ x_4 & y_4 \\ x_5 & y_5 \\ x_6 & y_6 \end{bmatrix}, \qquad \texttt{elem\_list} = \begin{bmatrix} 1 & 2 & 6 \\ 2 & 3 & 6 \\ 3 & 4 & 6 \\ 4 & 5 & 6 \end{bmatrix},$$

where (x_i, y_i) is the position of node i.

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4.G Convergence analysis for finite elements

Stability: Cea's lemma

Original infinite dimensional problem:
find $u \in V$ such that

$$a(u, w) = b(w), \qquad \forall w \in V$$

Galerkin approximation:
find $u_N \in V_N \subset V$ such that

$$a(u_N, w_N) = b(w_N), \qquad \forall w_N \in V_N$$

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find $u_N \in V_N \subset V$ such that

$$a(u_N, w_N) = b(w_N), \qquad \forall w_N \in V_N$$

Assume that there are $m, M > 0$ such that for all $u, w \in V$

$$a(u, u) \geq m|u|^2, \qquad |a(u, w)| \leq M|u||w|.$$

Lemma (Cea)

$$|u - u_N| \leq \frac{M}{m} \inf_{v_N \in V_N} |u - v_N|$$

Proof: Because $w_N \in V_N$,

$$a(u - u_N, w_N) = a(u, w_N) - a(u_N, w_N) = b(w_N) - b(w_N) = 0.$$

Using this result, we can then compute

$$m|u - u_N|^2 \leq a(u - u_N, u - u_N) = a(u - u_N, u - v_N + \underbrace{v_N - u_N}_{\in V_N})$$

$$= a(u - u_N, u - v_N) \leq M|u - u_N||u - v_N|.$$

Consistency: convergence rates

Using Cea's lemma, we just need to compute

$$\inf_{w_N \in V_N} |u - w_N|.$$

Idea: we can choose a specific mapping $r_N : V \to V_N$ find a bound $|u - r_N u| \leq Ch^p$.
Using Cea's lemma, we then find that

$$|u - u_N| \leq \frac{M}{m} \inf_{w_N \in V_N} |u - w_N| \leq \frac{M}{m} |u - r_N u| \leq \frac{M}{m} Ch^p.$$

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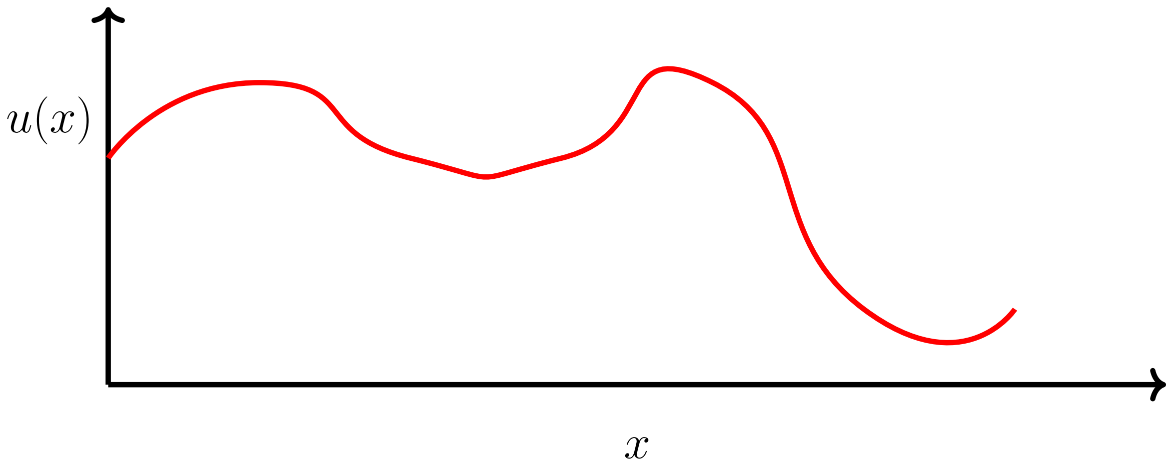
The operator r_N is typically chosen as the interpolation operator.



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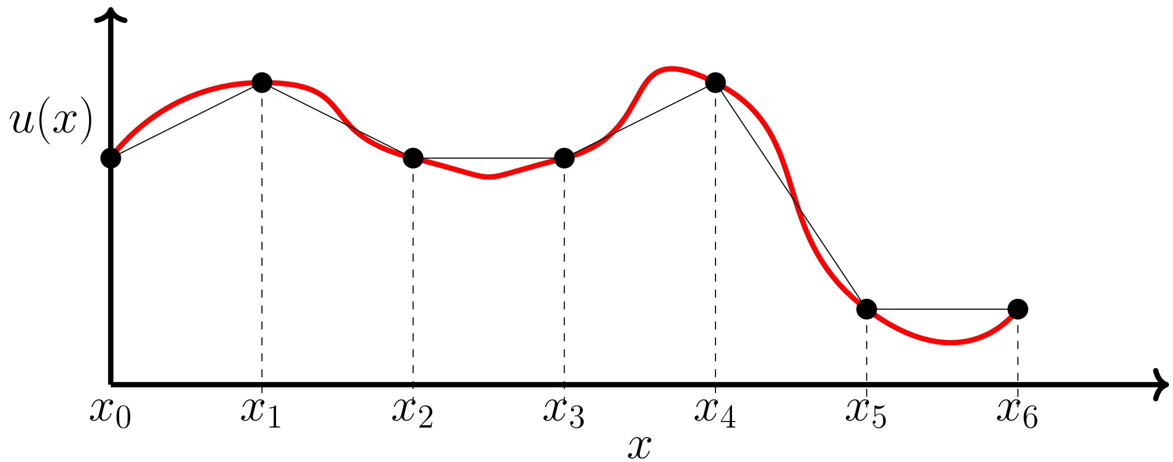

Deriving an error estimate for the interpolation operator in 1D (1/2)

Recall the **intermediate value theorem:**
for a differentiable function $f(x)$, there exists a $\xi \in [a, b]$ such that

$$f(b) - f(a) = (b - a)f'(\xi).$$

Take $f(x) = \int_a^x g(y)\,\mathrm{d}y$, then there exists a $\xi \in [a, b]$ such that

$$\int_a^b g(y)\,\mathrm{d}y = (b - a)g(\xi).$$

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$$\int_a^b g(y)\,\mathrm{d}y = (b-a)g(\xi).$$

Inside an element $[x_{e-1}, x_e]$, the interpolation operator gives an error

$$\begin{aligned}
\varepsilon_e(x) &= u(x) - \left(u(a) + \frac{x-a}{b-a}(u(b) - u(a)) \right) \\
&= \int_a^x u'(y)\,\mathrm{d}y - \frac{x-a}{b-a}\int_a^b u'(y)\,\mathrm{d}y \\
&= (x-a)u'(\xi_1) - \frac{x-a}{b-a}(b-a)u'(\xi_2), \qquad \xi_1, \xi_2 \in [a,b] \\
&= (x-a)(u'(\xi_1) - u'(\xi_2)) = (x-a)\int_{\xi_2}^{\xi_1} u''(y)\,\mathrm{d}y.
\end{aligned}$$

Deriving an error estimate for the interpolation operator in 1D (2/2)

Inside an element $[x_{e-1}, x_e]$, the interpolation operator gives an error

$$\varepsilon_e(x) = (x-a)\int_{\xi_2}^{\xi_1} u''(y)\,\mathrm{d}y.$$

Writing $h_e = x_e - x_{e-1}$, we obtain

$$\begin{aligned}(\varepsilon_e(x))^2 = (x-a)^2\left(\int_{\xi_2}^{\xi_1} u''(y)\,\mathrm{d}y\right)^2 &\leq (x-a)^2|\xi_1-\xi_2|\int_{\min\{\xi_1,\xi_2\}}^{\max\{\xi_1,\xi_2\}} (u''(y))^2\,\mathrm{d}y\\ &\leq h_e^3\int_{x_{e-1}}^{x_e}(u''(y))^2\,\mathrm{d}y.\end{aligned}$$

Integrating this bound over the element $[x_{e-1}, x_e]$ yields

$$\int_{x_{e-1}}^{x_e}(\varepsilon_e(x))^2\,\mathrm{d}x \leq h_e^4\int_{x_{e-1}}^{x_e}(u''(x))^2\,\mathrm{d}x.$$

Now considering all elements together, it follows that

$$|u - r_N u|_{L^2}^2 = \sum_{e=1}^{M}\int_{x_{e-1}}^{x_e}(\varepsilon_e(x))^2\,\mathrm{d}x \leq \sum_{e=1}^{M} h_e^4\int_{x_{e-1}}^{x_e}(u''(x))^2\,\mathrm{d}x \leq h^4|u''|_{L^2}.$$

Convergence rates for FE approximations

For **linear 1-D elements**, we have (see e.g. Allaire Lemma 6.2.10)

$$|u - u_N|_{L^2} \leq Ch^2 |u''|_{L^2}, \qquad |u' - u_N'|_{L^2} \leq Ch|u''|_{L^2}.$$

For **quadratic 1-D elements**, we have (see e.g. Allaire Theorem 6.2.14)

$$|u - u_N|_{H^1} \leq Ch^2 |u'''|_{L^2}.$$

More general, for $\mathbb{P}_k$ **rectangular elements**, we have (see e.g. Allaire Theorem 6.3.27)

$$|u - u_N|_{H^1} \leq Ch^k |u|_{H^{k+1}}.$$