CIEM1110-1: FEM, lecture 2.2

FEM for the diffusion equation

Iuri Rocha, Martin Lesueur

TU Delft

Poisson equation

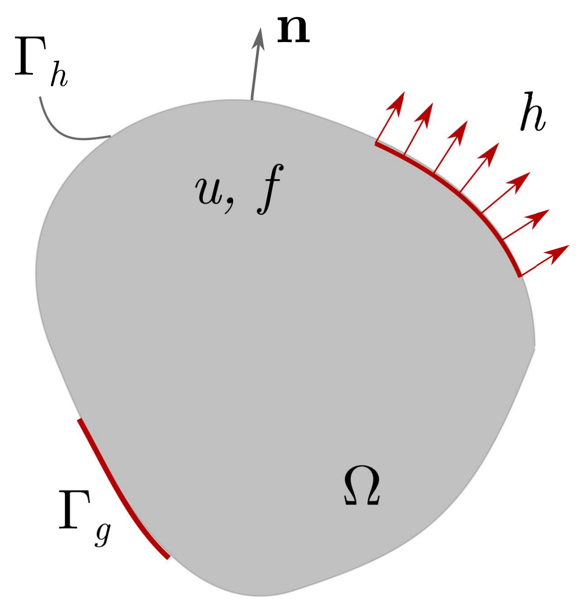
A relatively simple PDE with several practical applications:

- Steady-state heat conduction
- Steady-state flow or mass diffusion
- Electrostatic/gravitational force fields, etc

Poisson equation: strong form

As always, we start with the strong form:

$$
\begin{aligned}
-\nabla \cdot \mathbf{q} + f &= 0 && \text{in } \Omega && -q_{i,i} + f = 0 \\
u &= g && \text{at } \Gamma_g && u = g \\
-\mathbf{q} \cdot \mathbf{n} &= h && \text{at } \Gamma_h && -q_i n_i = h
\end{aligned}
$$



The flux $\mathbf{q}$ is related to the scalar field u through:

$$\mathbf{q} = -\boldsymbol{\kappa} \nabla u$$

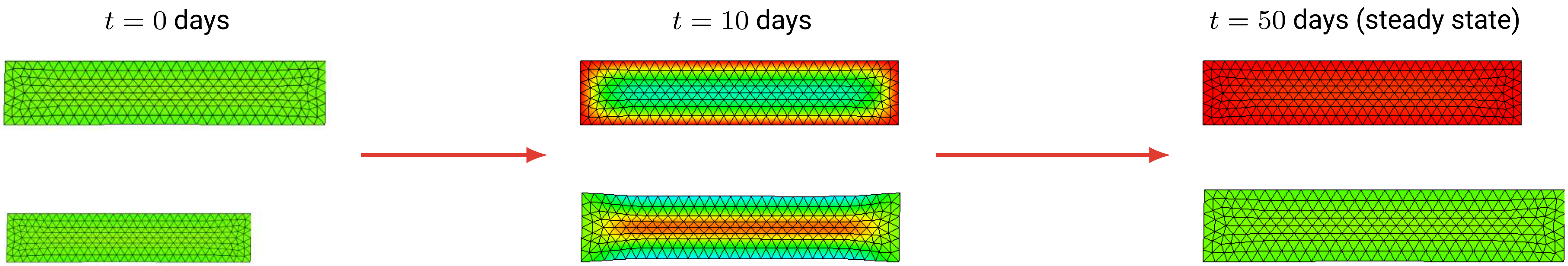
$$q_i = -\kappa_{ij} u_{,j}$$

- Heat conduction (Fourier's law): u is temperature, $\mathbf{q}$ is heat flux, f is heat source
- Water diffusion (Fick's law): u is water concentration, $\mathbf{q}$ is water flux, f is chemical source/sink
- Pressure diffusion (Darcy's law): u is hydraulic head, $\mathbf{q}$ is discharge rate, f is pressure source/sink

From Poisson equation to diffusion equation

The Poisson equation is only concerned with steady-state response. But why is time important?

Example of swelling phenomenon, showing the water concentration field in the row above and stress field below



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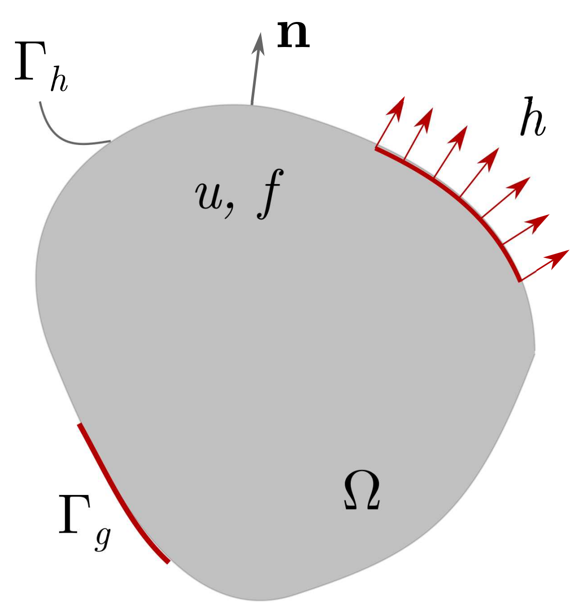
Diffusion equation: strong form

As always, we start with the strong form:

$-\nabla \cdot \mathbf{q} - \rho c \dot{u} + f = 0$	in Ω	$-q_{i,i} - \rho c \dot{u} + f = 0$
$u = g$	at Γ_g	$u = g$
$-\mathbf{q} \cdot \mathbf{n} = h$	at Γ_h	$-q_i n_i = h$
$u(\mathbf{x}, 0) = u_0(\mathbf{x})$	at $t = 0$	$u(x_i, 0) = u_0(x_i)$



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Diffusion equation: weak form

Building up the weak form requires pre-multiplication by w and integration over Ω:

$$-\nabla\cdot\mathbf{q} - \rho c\dot{u} + f = 0 \quad \Rightarrow \quad -\int_\Omega w\left(\nabla\cdot\mathbf{q}\right)\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega = 0, \quad \forall w\in\mathcal{V}$$

$$-q_{i,i} - \rho c\dot{u} + f = 0 \quad \Rightarrow \quad -\int_\Omega wq_{i,i}\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega = 0, \quad \forall w\in\mathcal{V}$$

Note that this is a mix between the two previously treated cases:

- the domain Ω can have more than one dimension (e.g. 2D, 3D)
- but the solution u is a scalar field, so w is also a scalar field

Removing derivatives of $\mathbf{q}$ – Integration by parts

Derivative of a scalar-vector product:

$$\int_{\Omega} \nabla \cdot (a\mathbf{b})\,\mathrm{d}\Omega = \int_{\Omega} \nabla a \cdot \mathbf{b}\mathrm{d}\Omega + \int_{\Omega} a\,(\nabla \cdot \mathbf{b})\,\mathrm{d}\Omega \qquad \int_{\Omega} (ab_i)_{,i}\,\mathrm{d}\Omega = \int_{\Omega} a_{,i}b_i\mathrm{d}\Omega + \int_{\Omega} ab_{i,i}\mathrm{d}\Omega$$

Removing derivatives of $\mathbf{q}$ – Integration by parts

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$$\int_\Omega (ab_i)_{,i}\, \mathrm{d}\Omega = \int_\Omega a_{,i} b_i \mathrm{d}\Omega + \int_\Omega a b_{i,i} \mathrm{d}\Omega$$

Divergence (Gauss) Theorem:

$$\int_\Omega \nabla \cdot (a\mathbf{b})\, \mathrm{d}\Omega = \int_\Gamma a\mathbf{b} \cdot \mathbf{n} \mathrm{d}\Gamma$$

$$\int_\Omega (ab_i)_{,i}\, \mathrm{d}\Omega = \int_\Gamma a b_i n_i \mathrm{d}\Gamma$$

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Substitute back and we are done:

$$\int_\Omega a\, (\nabla \cdot \mathbf{b})\, \mathrm{d}\Omega = -\int_\Omega \nabla a \cdot \mathbf{b} \mathrm{d}\Omega + \int_\Gamma a\mathbf{b} \cdot \mathbf{n} \mathrm{d}\Gamma \qquad \int_\Omega a b_{i,i} \mathrm{d}\Omega = -\int_\Omega a_{,i} b_i \mathrm{d}\Omega + \int_\Gamma a b_i n_i \mathrm{d}\Gamma$$

$$\int_\Omega w\, (\nabla \cdot \mathbf{q})\, \mathrm{d}\Omega = -\int_\Omega \nabla w \cdot \mathbf{q} \mathrm{d}\Omega + \int_\Gamma w\mathbf{q} \cdot \mathbf{n} \mathrm{d}\Gamma \qquad \int_\Omega w q_{i,i} \mathrm{d}\Omega = -\int_\Omega w_{,i} q_i \mathrm{d}\Omega + \int_\Gamma w q_i n_i \mathrm{d}\Gamma$$

Diffusion equation: weak form

We now use integration by parts to move ∇ from $\mathbf{q}$ to w:

$$-\int_\Omega w\left(\nabla\cdot\mathbf{q}\right)\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega = 0 \quad\Rightarrow\quad \int_\Omega \nabla w\cdot\mathbf{q}\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega - \int_{\Gamma_h} w\mathbf{q}\cdot\mathbf{n}\mathrm{d}\Gamma = 0$$

$$-\int_\Omega wq_{i,i}\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega = 0 \quad\Rightarrow\quad \int_\Omega w_{,i}q_i\mathrm{d}\Omega - \int_\Omega w\rho c\dot{u}\mathrm{d}\Omega + \int_\Omega wf\mathrm{d}\Omega - \int_{\Gamma_h} wq_in_i\mathrm{d}\Gamma = 0$$

Note that:

- the derivative of $\nabla\cdot\mathbf{q}$ is now gone!
- a new surface integral appears, but only where Neumann BCs are applied
- actually, the remaining surface vanishes because $w = 0$ at Γ_g and $\Gamma = \Gamma_g \cup \Gamma_h$
- we did not touch the time derivative

Diffusion equation: weak form

The final weak form is obtained by substituting the Neumann BC and the constitutive relation:

$$-\int_\Omega \nabla w \cdot \boldsymbol{\kappa} \nabla u \, \mathrm{d}\Omega - \int_\Omega w \rho c \dot{u} \, \mathrm{d}\Omega + \int_\Omega w f \, \mathrm{d}\Omega + \int_{\Gamma_h} w h \, \mathrm{d}\Gamma = 0 \quad \forall w \in \mathcal{V}$$

$$-\int_\Omega w_{,i} \kappa_{ij} u_{,j} \, \mathrm{d}\Omega - \int_\Omega w \rho c \dot{u} \, \mathrm{d}\Omega + \int_\Omega w f \, \mathrm{d}\Omega + \int_{\Gamma_h} w h \, \mathrm{d}\Gamma = 0 \quad \forall w \in \mathcal{V}$$

Note that:

- any solution to the weak form is still a valid and exact solution
- but this is only guaranteed because $\mathcal{V}$ is infinite dimensional
- weak solutions only obey the original PDE in a ”distribution” (integral) sense
- but now we get a whole new set of possible solutions with lower-order differentiability

Diffusion equation: semi-discretized form

We now introduce the actual approximation through the Galerkin Method:

- the infinite-dimensional function space $\mathcal{V}$ is reduced to a finite one $\mathcal{V}_h$
- by consequence, the set of possible solutions for u now moves from space $\mathcal{S}$ to space $\mathcal{S}_h$

More specifically, we introduce finite-dimensional function spaces based on shape functions:

$$u^h = \sum_{n}^{nn} N_n(\mathbf{x}) a_n, \qquad \dot{u}^h = \sum_{n}^{nn} N_n(\mathbf{x}) \dot{a}_n \qquad w^h = \sum_{n}^{nn} N_n(\mathbf{x}) c_n,$$

After which the weak form becomes:

$$-\int_\Omega \nabla w^h \cdot \boldsymbol{\kappa} \nabla u^h \mathrm{d}\Omega - \int_\Omega w^h \rho c \dot{u}^h \mathrm{d}\Omega + \int_\Omega w^h f \mathrm{d}\Omega + \int_{\Gamma_h} w^h h \mathrm{d}\Gamma = 0$$

$$-\int_\Omega w^h_{,i} \kappa_{ij} u^h_{,j} \mathrm{d}\Omega - \int_\Omega w^h \rho c \dot{u}^h \mathrm{d}\Omega + \int_\Omega w^h f \mathrm{d}\Omega + \int_{\Gamma_h} w^h h \mathrm{d}\Gamma = 0$$

Diffusion equation: semi-discretized form

We express summations over nodal values in matrix-vector form:

$$u^h = \mathbf{N}\mathbf{a}, \qquad \dot{u}^h = \mathbf{N}\dot{\mathbf{a}}, \qquad w^h = \mathbf{N}\mathbf{c}$$

$$u^h = N_n a_n, \quad \dot{u}^h = N_n \dot{a}_n, \quad w^h = N_m c_m$$

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$$u^h = N_n a_n, \quad \dot{u}^h = N_n \dot{a}_n, \quad w^h = N_m c_m$$

with

$$\mathbf{N} = \begin{bmatrix} N_1 & N_2 & \cdots & N_{nn} \end{bmatrix} \qquad \mathbf{a} = \begin{Bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{nn} \end{Bmatrix} \qquad \mathbf{c} = \begin{Bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{nn} \end{Bmatrix}$$

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and

$$\nabla u^h = \mathbf{B}\mathbf{a}, \qquad \nabla w^h = \mathbf{B}\mathbf{c}$$

$$u^h_{,j} = N_{n,j} a_n, \qquad w^h_{,i} = N_{m,i} c_m$$

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$$u^h_{,j} = N_{n,j} a_n, \qquad w^h_{,i} = N_{m,i} c_m$$

with

$$\mathbf{B} = \begin{bmatrix} N_{1,x} & N_{2,x} & \cdots & N_{nn,x} \\ N_{1,y} & N_{2,y} & \cdots & N_{nn,y} \end{bmatrix}$$

Diffusion equation: system of equations

Substituting these back into the discretized form, we have:

$$-\int_\Omega \nabla w^h \cdot \boldsymbol{\kappa} \nabla u^h \mathrm{d}\Omega - \int_\Omega w^h \rho c \dot{u}^h \mathrm{d}\Omega + \int_\Omega w^h f \mathrm{d}\Omega + \int_{\Gamma_h} w^h h \mathrm{d}\Gamma = 0, \quad \forall \mathbf{c} \quad \Rightarrow$$

$$\Rightarrow \quad -\int_\Omega (\mathbf{Bc})^\mathrm{T} \boldsymbol{\kappa} \mathbf{Ba} \mathrm{d}\Omega - \int_\Omega (\mathbf{Nc})^\mathrm{T} \rho c \mathbf{N} \dot{\mathbf{a}} \mathrm{d}\Omega + \int_\Omega (\mathbf{Nc})^\mathrm{T} f \mathrm{d}\Omega + \int_{\Gamma_h} (\mathbf{Nc})^\mathrm{T} h \mathrm{d}\Gamma = 0, \quad \forall \mathbf{c}$$

$$-\int_\Omega w^h_{,i} \kappa_{ij} u^h_{,j} \mathrm{d}\Omega - \int_\Omega w^h \rho c \dot{u}^h \mathrm{d}\Omega + \int_\Omega w^h f \mathrm{d}\Omega + \int_{\Gamma_h} w^h h \mathrm{d}\Gamma = 0, \quad \forall c_m \quad \Rightarrow$$

$$\Rightarrow \quad -\int_\Omega N_{m,i} c_m \kappa_{ij} N_{n,j} a_n \mathrm{d}\Omega - \int_\Omega N_m c_m \rho c N_n \dot{a}_n \mathrm{d}\Omega + \int_\Omega N_m c_m f \mathrm{d}\Omega + \int_{\Gamma_h} N_m c_m h \mathrm{d}\Gamma = 0, \quad \forall c_m$$

Diffusion equation: system of equations

Finally, taking $\mathbf{a}$ and $\mathbf{c}$ out of the integrals:

$$-\mathbf{c}^{\mathrm{T}}\left(\int_\Omega \mathbf{B}^{\mathrm{T}}\boldsymbol{\kappa}\mathbf{B}\,\mathrm{d}\Omega\right)\mathbf{a}-\mathbf{c}^{\mathrm{T}}\left(\int_\Omega \mathbf{N}^{\mathrm{T}}\rho c\mathbf{N}\,\mathrm{d}\Omega\right)\dot{\mathbf{a}}+\mathbf{c}^{\mathrm{T}}\left(\int_\Omega \mathbf{N}^{\mathrm{T}}f\,\mathrm{d}\Omega\right)+\mathbf{c}^{\mathrm{T}}\left(\int_{\Gamma_h} \mathbf{N}^{\mathrm{T}}h\,\mathrm{d}\Gamma\right)=0,\quad \forall\mathbf{c}$$

$$-c_m\left(\int_\Omega N_{m,i}\kappa_{ij}N_{n,j}\,\mathrm{d}\Omega\right)a_n-c_m\left(\int_\Omega N_m\rho cN_n\,\mathrm{d}\Omega\right)\dot{a}_n+c_m\left(\int_\Omega N_mf\,\mathrm{d}\Omega\right)+c_m\left(\int_{\Gamma_h} N_mh\,\mathrm{d}\Gamma\right)=0,\quad \forall c_m$$

Diffusion equation: final system of equations

The formulation ends by cancelling out $\mathbf{c}$ to arrive at:

$$\mathbf{K}\mathbf{a} + \mathbf{M}\dot{\mathbf{a}} = \mathbf{f} \qquad K_{mn}a_n + M_{mn}\dot{a}_n = f_m$$

where:

$$\mathbf{K} = \int_\Omega \mathbf{B}^\mathrm{T}\boldsymbol{\kappa}\mathbf{B}\,\mathrm{d}\Omega, \quad \mathbf{M} = \int_\Omega \mathbf{N}^\mathrm{T}\rho c\mathbf{N}\,\mathrm{d}\Omega, \quad \mathbf{f} = \int_\Omega \mathbf{N}^\mathrm{T} f\,\mathrm{d}\Omega + \int_{\Gamma_h} \mathbf{N}^\mathrm{T} h\,\mathrm{d}\Gamma$$

$$K_{mn} = \int_\Omega N_{m,i}\kappa_{ij}N_{n,j}\,\mathrm{d}\Omega, \quad M_{mn} = \int_\Omega N_m\rho c N_n\,\mathrm{d}\Omega, \quad f_m = \int_\Omega N_m f\,\mathrm{d}\Omega + \int_{\Gamma_h} N_m h\,\mathrm{d}\Gamma$$

Note that:

- in practice, we compute these integrals element by element and assemble the contributions
- isoparametric mapping and numerical integration carry over unchanged to this new problem
- in this case we do have a clean definition of $\mathbf{B}$ as $\mathbf{B} = \mathbf{J}^{-1}\begin{bmatrix} N_{1,\xi} & N_{2,\xi} & \cdots & N_{nn,\xi} \\ N_{1,\eta} & N_{2,\eta} & \cdots & N_{nn,\eta} \end{bmatrix}$

What to do about time?

This time we need to solve for both $\mathbf{a}$ and $\dot{\mathbf{a}}$. But how?

- No discretization in time assumed throughout the formulation
- Time-dependent shape functions would be an option, but are not used here
- Discretized form tacitly assumes we have access to either $\mathbf{a}$ or $\dot{\mathbf{a}}$

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The way out is to define a time stepper:

- Independent from original FEM formulation, so a range of schemes can be used
- Different strategies yield different accuracy and stability properties

A short detour — recap of MUDE week 1.5

Taylor expansion of an arbitrary function f around x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \cdots + \frac{h^n}{n!}f^{(n)}(x) + \mathcal{O}(h^{n+1})$$

- Of course we can also do this for time, just with $h = \Delta t$

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Using the Taylor approximation to define time steps for a transient problem:

$$u(t_0) = u_0, \quad u(t) = u_n, \quad u(t+\Delta t) = u_{n+1}$$

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- Forward Euler solver (explicit):

$$u_{n+1} = u_n + \Delta t \dot{u}_n$$

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- Backward Euler solver (implicit):

$$u_{n+1} = u_n + \Delta t \dot{u}_{n+1}$$

Forward Euler integration for the diffusion PDE

Forward Euler update:

$$\mathbf{a}_{n+1} = \mathbf{a}_n + \Delta t \dot{\mathbf{a}}_n$$

Forward Euler integration for the diffusion PDE

Forward Euler update:

$$\mathbf{a}_{n+1} = \mathbf{a}_n + \Delta t \dot{\mathbf{a}}_n$$

Substitute in the discretized form:

$$\mathbf{M}\dot{\mathbf{a}}_{n+1} + \mathbf{K}\left(\mathbf{a}_n + \Delta t \dot{\mathbf{a}}_n\right) = \mathbf{f}_{n+1}$$

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Solve for velocities at nodes:

$$\dot{\mathbf{a}}_{n+1} = \mathbf{M}^{-1}\hat{\mathbf{f}} \qquad \text{with} \qquad \hat{\mathbf{f}} = \mathbf{f}_{n+1} - \mathbf{K}\left(\mathbf{a}_n + \Delta t \dot{\mathbf{a}}_n\right)$$

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Store $\dot{\mathbf{a}}_{n+1}$ for the next step and advance in time

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Store $\dot{\mathbf{a}}_{n+1}$ for the next step and advance in time

- We solve for velocities, Dirichlet BCs should be consistent
- Solving can be accelerated by lumping the $\mathbf{M}$ matrix

Backward Euler integration for the diffusion PDE

Backward Euler update:

$$\mathbf{a}_{n+1} = \mathbf{a}_n + \Delta t \dot{\mathbf{a}}_{n+1} \quad \Rightarrow \quad \dot{\mathbf{a}}_{n+1} = \frac{\mathbf{a}_{n+1} - \mathbf{a}_n}{\Delta t}$$

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Substitute in the discretized form:

$$\mathbf{M}\left(\frac{\mathbf{a}_{n+1} - \mathbf{a}_n}{\Delta t}\right) + \mathbf{K}\mathbf{a}_{n+1} = \mathbf{f}_{n+1}$$

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Solve for the main field at the nodes:

$$\hat{\mathbf{K}}\mathbf{a}_{n+1} = \hat{\mathbf{f}} \qquad \text{with} \qquad \hat{\mathbf{K}} = \mathbf{K} + \frac{1}{\Delta t}\mathbf{M} \quad \hat{\mathbf{f}} = \mathbf{f}_{n+1} + \frac{1}{\Delta t}\mathbf{M}\mathbf{a}_n$$

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Store $\mathbf{a}_{n+1}$ and $\dot{\mathbf{a}}_{n+1}$ for the next step and advance in time

A range of time steppers — trapezoidal integration

Generalizing the two previous time steppers:

$$\mathbf{a}_{n+1} = \mathbf{a}_n + \Delta t\left((1-\theta)\dot{\mathbf{a}}_n + \theta\dot{\mathbf{a}}_{n+1}\right) \quad \Rightarrow \quad \dot{\mathbf{a}}_{n+1} = \frac{1}{\theta\Delta t}\left(\mathbf{a}_{n+1} - \mathbf{a}_n\right) - \frac{(1-\theta)}{\theta}\dot{\mathbf{a}}_n$$

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Substitute in the discretized form:

$$\mathbf{M}\left(\frac{1}{\theta\Delta t}\left(\mathbf{a}_{n+1} - \mathbf{a}_n\right) - \frac{(1-\theta)}{\theta}\dot{\mathbf{a}}_n\right) + \mathbf{K}\mathbf{a}_{n+1} = \mathbf{f}_{n+1}$$

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Solve for the main field at the nodes:

$$\hat{\mathbf{K}}\mathbf{a}_{n+1} = \hat{\mathbf{f}} \qquad \text{with} \qquad \hat{\mathbf{K}} = \frac{1}{\theta\Delta t}\mathbf{M} + \mathbf{K} \quad \hat{\mathbf{f}} = \mathbf{f}_{n+1} + \frac{1}{\theta\Delta t}\mathbf{M}\mathbf{a}_n + \frac{(1-\theta)}{\theta}\mathbf{M}\dot{\mathbf{a}}_n$$

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Store $\mathbf{a}_{n+1}$ and $\dot{\mathbf{a}}_{n+1}$ for the next step and advance in time

Outlook

Workshop tomorrow:

- Setting up and solving a diffusion problem in pyJive
- Investigating the stability and accuracy of the time steppers we have seen today

Next week:

- Introduction to nonlinear FEM
- Path-following techniques
- Nonlinear material models