Introduction into Finite Elements FEM for Convection-Diffusion Problems

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Transport phenomena: Convection

Convection (alias **advection**) is the transport of a conserved quantity of interest by a vector field, e.g., the velocity field.

Injection of tracer particles in a moving fluid.





Transport phenomena: Diffusion

Diffusion is the transport of a conserved quantity from a region of high concentration to a region of low concentration, e.g., due to Brownian random molecular motion or heat conduction.

Transport of particles due to random molecular motion.





Examples of transport phenomena

- Flow processes in our body (blood flow, drug delivery)
- Heating and air conditioning in rooms, cars, aircrafts
- Transport of pollutants in air (with turbulent effects)





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Governing equations

Transient convection-diffusion equation in conservative form

 $\partial_t u + \partial_x (vu) - \partial_x (d\partial_x u) = f$

with

- transient term $\partial_t u = \partial_t u(x, t)$
- velocity field v = v(x, t)
- diffusion coefficient $d = d(x) \ge 0$
- load vector f = f(x, t)

Simplification for constant uniform diffusion coefficient d

$$\partial_t u + \partial_x (vu) - d\partial_{xx} u = f$$



Governing equations, cont'd

Application of the chain rule to the convective term yields

 $\partial_x(vu) = v(\partial_x u) + (\partial_x v)u$

In case of a so-called divergence-free velocity field

div
$$\mathbf{v} = \partial_x v^x + \partial_y v^y + \dots = 0$$

 $\partial_x v = 0 \quad \Leftrightarrow \quad v = \text{const} \quad \text{in 1D}$

this leads to the non-conservative form

$$\partial_t u + v \partial_x u - d \partial_{xx} u = f$$



Model problems

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Time-dependent convection-diffusion problem

$$\partial_t u + \partial_x (vu) - \partial_x (d\partial_x u) = f$$
 in $[a, b]$

is complemented by initial conditions at time t = 0

$$u = u_0$$
 in $[a, b]$

and boundary conditions at a = x and x = b:

- Dirichlet bc's: $u = u_D$ Neumann bc's: $u' = g_N$
- Flux bc's: $(vu d\partial_x u)' = g_F$

Model problems, cont'd

Time-dependent convection problem (hyperbolic)

$$\partial_t u + \partial_x (vu) = f$$
 in $[a, b]$

is complemented by initial conditions at time t = 0

$$u = u_0$$
 in $[a, b]$

and boundary conditions at x = a and/or x = b if and only if the (normal) flow velocity is directed into the domain

Example: If $v \equiv \text{const} > 0$ ($\hat{=}$ translation of u_0 to the right) then $u(x = a) = u_D$ is prescribed at the inflow boundary part at x = a but no boundary condition is imposed at the outflow part at x = b.



Steady convection-diffusion problem

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Boundary value problem: Given v and d > 0 find u

s.t.
$$\begin{cases} \partial_x (vu) - \partial_x (d\partial_x u) &= f & \text{ in } [a, b] \\ u &= u_a & \text{ at } x = a \\ u &= u_b & \text{ at } x = b \end{cases}$$

Weak form: Find $u \in S = \{u \in H^1 : u(a) = u_a \land u(b) = u_b\}$

s.t.
$$\int_{a}^{b} w \left[\partial_{x}(vu) - \partial_{x}(d\partial_{x}u)\right] dx = \int_{a}^{b} wf dx$$
$$\Leftrightarrow \int_{a}^{b} w \partial_{x}(vu) + \partial_{x}w(d\partial_{x}u) dx - \underbrace{w(d\partial_{x}u)}_{=0}^{b} = \int_{a}^{b} wf dx$$

for all
$$w\in W=\{u\in H^1:w(a)=0\wedge w(b)=0\}$$



Steady convection-diffusion problem, cont'd

Boundary value problem: Given v and d > 0 find u

s.t.
$$\begin{cases} \partial_x (vu) - \partial_x (d\partial_x u) &= f & \text{ in } [a, b] \\ u &= u_a & \text{ at } x = a \\ u' &= g_b & \text{ at } x = b \end{cases}$$

Weak form: Find $u \in S = \{u \in H^1 : u(a) = u_a\}$

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s.t.
$$\int_{a}^{b} w \left[\partial_{x}(vu) - \partial_{x}(d\partial_{x}u)\right] dx = \int_{a}^{b} wf dx$$
$$\Leftrightarrow \int_{a}^{b} w \partial_{x}(vu) + \partial_{x}w(d\partial_{x}u) dx - \underbrace{w(b)}_{\neq 0}(dg_{b}) = \int_{a}^{b} wf dx$$

for all
$$w \in W = \{u \in H^1 : w(a) = 0\}$$

Steady convection-diffusion problem, cont'd

Boundary value problem: Given v and d > 0 find u

s.t.
$$\begin{cases} \partial_x (vu) - \partial_x (d\partial_x u) &= f & \text{ in } [a, b] \\ u &= u_a & \text{ at } x = a \\ (vu - d\partial_x u)' &= g_b & \text{ at } x = b \end{cases}$$

Weak form: Find $u \in S = \{u \in H^1 : u(a) = u_a\}$

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s.t.
$$\int_{a}^{b} w \left[\partial_{x} (vu) - \partial_{x} (d\partial_{x} u) \right] dx = \int_{a}^{b} wf dx$$

$$\stackrel{\text{i.b.p.}}{\Leftrightarrow} \int_{a}^{b} -\partial_{x} w \left[vu - d\partial_{x} u \right] dx + \underbrace{w(b)}_{\neq 0} \underbrace{g_{b}}_{\neq 0} = \int_{a}^{b} wf dx$$

for all
$$w \in W = \{u \in H^1 : w(a) = 0\}$$

Galerkin finite element method

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Generic weak form for the problem at hand

Find
$$u \in S$$
: $a(u, w) = b(w)$ for all $w \in W$

with non-symmetric bilinear form (i.e. $a(u, w) \neq a(w, u)$)

$$a(u, w) = \int_{a}^{b} w \partial_{x}(vu) + \partial_{x} w(d\partial_{x} u) dx$$

or
$$a(u, w) = \int_{a}^{b} -\partial_{x} w(vu - d\partial_{x} u) dx$$

and linear form with or without boundary contributions

$$b(w) = \int_a^b wf + w(b)(dg_b) dx \quad \text{or} \quad b(w) = \int_a^b wf dx - w(b)g_b$$

Introduction into Finite Elements

Galerkin finite element method, cont'd

Approximate trial and test spaces by finite approximations

$$u_{h} = \sum_{j=1}^{N} \varphi_{j} u_{j} \in S_{h} = \operatorname{span} \langle \varphi_{1}, \dots, \varphi_{N} \rangle \subset S$$
$$w_{h} = \sum_{i=1}^{N} \phi_{i} w_{i} \in W_{h} = \operatorname{span} \langle \phi_{1}, \dots, \phi_{N} \rangle \subset W$$

and solve the discrete problem

$$\mathsf{Find} \ u_h \in \mathcal{S}_h: \quad \mathsf{a}(u_h, w_h) = \mathsf{b}(w_h) \quad \mathsf{for \ all} \ w_h \in \mathcal{W}_h$$



Image: A matrix A

Galerkin finite element method, cont'd

Assemble the system matrix A and the right-hand side vector b

$$A = \begin{pmatrix} a(\varphi_1, \phi_1) & \dots & a(\varphi_N, \phi_1) \\ \vdots & \ddots & \vdots \\ a(\varphi_1, \phi_N) & \dots & a(\varphi_N, \phi_N) \end{pmatrix} \qquad b = \begin{pmatrix} b(\phi_1) \\ \vdots \\ b(\phi_N) \end{pmatrix}$$

and impose Dirichlet boundary conditions, e.g. $u(x = a) = u_a$

$$A = \begin{pmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ a(\varphi_1, \phi_N) & \dots & a(\varphi_N, \phi_N) \end{pmatrix} \qquad b = \begin{pmatrix} u_a \\ \vdots \\ b(\phi_N) \end{pmatrix}$$

Solve the linear system Au = b for the vector of unknowns

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Numerical example

Boundary value problem: Given v and d > 0 find u

s.t.
$$\begin{cases} v\partial_x u - d\partial_{xx} u = 1 & \text{in } [0,1] \\ u = 0 & \text{at } x = 0 \text{ and } x = 1 \end{cases}$$

with known exact solution

$$u_{\mathrm{ex}}(x) = rac{1}{v}\left(x - rac{1 - e^{\gamma x}}{1 - e^{\gamma}}
ight)$$

where $\gamma = \frac{v}{d}$. If $\gamma \gg 1$ the problem is termed convectiondominated. Numerical methods have problems in resolving the boundary layer at x = b.

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Let $\varphi_j = \phi_j, j = 1, \dots, N$ and choose linear finite elements



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Resulting system matrix and right-hand side vector

$$A = \begin{pmatrix} 1 & 0 & \dots & \dots & \dots & 0 \\ -\frac{v}{2} - \frac{d}{h} & \frac{2d}{h} & \frac{v}{2} - \frac{d}{h} & & & \\ & -\frac{v}{2} - \frac{d}{h} & \frac{2d}{h} & \frac{v}{2} - \frac{d}{h} & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{v}{2} - \frac{d}{h} & \frac{2d}{h} & \frac{v}{2} - \frac{d}{h} \\ 0 & \dots & \dots & \dots & 0 & 1 \end{pmatrix}$$
$$b = \begin{pmatrix} 0 & h & \dots & \dots & h & 0 \end{pmatrix}^{T}$$

Galerkin FEM for an internal node i ($\hat{=}$ central FD scheme)

$$v\frac{u_{i+1}-u_{i-1}}{2h}-d\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}=1$$



FEM yields good approximations for $\gamma = 2$.



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FEM yields poor approximations for $\gamma = 20$ unless *h* is small.



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FEM yields oscillatory approximation for $\gamma = 100$ even for small *h*.



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Analysis of the discrete problem

Observation: oscillatory behavior depends on the size of γ and on the mesh width *h*. A useful measure is the mesh Péclet number

$$\mathsf{Pe} = \frac{\gamma h}{2} = \frac{vh}{2d}$$

Galerkin FEM for an internal node *i* in terms of Pe reads

$$v \frac{u_{i+1} - u_{i-1}}{2h} - d \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 1$$

$$\Leftrightarrow \quad \left(\frac{v}{2h} - \frac{d}{h^2}\right) u_{i+1} + \frac{2d}{h^2}u_i - \left(\frac{v}{2h} + \frac{d}{h^2}\right)u_{i-1} = 1$$

$$\Leftrightarrow \quad \frac{v}{2h}\left(\frac{\operatorname{Pe} - 1}{\operatorname{Pe}}u_{i+1} + \frac{2}{\operatorname{Pe}}u_i - \frac{\operatorname{Pe} + 1}{\operatorname{Pe}}u_{i-1}\right) = 1$$



Analysis of the discrete problem, cont'd

Aim: to construct an alternative three-point formula

$$\alpha_1 u_{i-1} + \alpha_2 u_i + \alpha_3 u_{i+1} = 1$$

which reproduces the exact solution at the mesh nodes

$$u_{i-1} = \frac{1}{\nu} \left(x_i - h - \frac{1 - e^{\gamma x_i} e^{-2\mathsf{Pe}}}{1 - e^{\gamma}} \right)$$
$$u_i = \frac{1}{\nu} \left(x_i - \frac{1 - e^{\gamma x_i}}{1 - e^{\gamma}} \right)$$
$$u_{i+1} = \frac{1}{\nu} \left(x_i + h - \frac{1 - e^{\gamma x_i} e^{2\mathsf{Pe}}}{1 - e^{\gamma}} \right)$$



Image: A matrix A

Analysis of the discrete problem, cont'd

Substitute expressions for u_i and $u_{i\pm 1}$ into three-point formula and derive sufficient conditions for the unknown coefficients

$$\underbrace{(\alpha_1 + \alpha_2 + \alpha_3)}_{=0} x_i \underbrace{-(\alpha_1 - \alpha_3)}_{v/h} h - \underbrace{(\alpha_1 e^{-2\mathsf{Pe}} + \alpha_2 + \alpha_3 e^{2\mathsf{Pe}})}_{=0} \frac{1 - e^{\gamma x_i}}{1 - e^{\gamma}} = v$$

Solution of the 3 \times 3 system for the coefficients $\alpha_1,\alpha_2,\alpha_3$ yields

$$\alpha_1 = -v \frac{1 + \text{cothPe}}{2h}, \quad \alpha_2 = v \frac{\text{cothPe}}{h}, \quad \alpha_3 = v \frac{1 - \text{cothPe}}{2h}$$



Analysis of the discrete problem, cont'd

Conclusion: given $\gamma = v/d$ and *h* the exact solution at the nodes is reproduced by the alternative discrete method

$$rac{v}{2h}\left((1- ext{cothPe})u_{i+1}+(2 ext{cothPe})u_i-(1+ ext{cothPe})u_{i-1}
ight)=1$$

$$\Leftrightarrow \quad v \frac{u_{i+1} - u_{i-1}}{2h} - (d + \hat{d}) \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 1$$

with stabilizing artificial/numerical diffusion

$$\hat{d} = eta rac{vh}{2} = eta d \operatorname{Pe}, \quad eta = \operatorname{cothPe} - rac{1}{\operatorname{Pe}}$$



Conclusions on Galerkin FEM

Galerkin FEM tends to produce oscillations if $Pe \gg 1$ but it can be stabilized by adding artificial diffusion, e.g.

$$v\frac{u_{i+1}-u_{i-1}}{2h}-(d+\hat{d})\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}=1$$

 Galerkin FEM without stabilization produces nodally exact solution to the modified equation

$$v\partial_x u - d\left(1 - \beta \frac{\sinh^2}{\operatorname{Pe}}\right)\partial_{xx} u = 1$$

with $\underline{\text{negative}}$ net diffusion for Pe>1

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Systematic approach towards stabilization for FEM

Given the residual of the original PDE, e.g.,

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$$\mathcal{R}[u] = \partial_{\mathsf{X}}(\mathsf{v} u) - \partial_{\mathsf{X}}(\mathsf{d} \partial_{\mathsf{X}} u) - \mathsf{f}$$

an element-wise contribution is added to the standard weak form

$$\int_{a}^{b} w \mathcal{R}[u] dx + \sum_{k=1}^{N-1} \int_{x_{k}}^{x_{k+1}} \tau_{k} \mathcal{P}[w] \mathcal{R}[u] dx = 0$$

$$\Leftrightarrow \sum_{k=1}^{N-1} \int_{x_{k}}^{x_{k+1}} (w + \tau_{k} \mathcal{P}[w]) \mathcal{R}[u] dx = 0 \quad \forall w \in W$$

This stabilization is *consistent*, that is, all terms on the left-hand side vanish if u equals the exact solution since $\mathcal{R}[u_{ex}] \equiv 0$

Making it work in practice

Stabilization parameter τ_k may be defined per element

$$\tau_k = \beta \frac{h_k}{|\mathbf{v}|}, \quad h_k = x_{k+1} - x_k$$

Streamline-Upwind Petrov-Galerkin (SUPG) method

 $\mathcal{P}[w] = v(\partial_x w)$

Galerkin Least-Squares (GLS)/Subgrid Scale (SGS) method

 $\mathcal{P}[w] = v(\partial_x w) \mp \partial_x (d\partial_x w) \pm (\partial_x v) w$

Since i.b.p is not performed for the stabilizing term the second-order derivative vanishes for linear finite elements



Working out the (bi-)linear forms

Definition of bilinear and linear forms with SUPG-stabilization, e.g.,

$$a(u,w) = \sum_{k=1}^{N-1} a_k(u,w), \quad b(w) = w(b)(dg_b) + \sum_{k=1}^{N-1} b_k(w)$$

with element-wise counterparts defined as follows

$$a_{k}(u,w) = \int_{x_{k}}^{x_{k+1}} w \partial_{x}(vu) + \partial_{x}w(d\partial_{x}u) + \tau_{k}(v\partial_{x}w)(\partial_{x}(vu) + \partial_{x}(d\partial_{x}u)) dx$$

$$b_k(w) = \int_{x_k}^{x_{k+1}} wf + \tau_k(v\partial_x w)f \,\mathrm{d}x$$



Shock capturing methods

Observation: *linear* stabilization methods such as SUPG, GLS, and SGS may fail ti suppress oscillations in the vicinity of steep gradients or discontinuities (e.g., shock waves)

Remedy: replace $\mathcal{P}[w]$ by a *nonlinear* stabilization operator

$$\int_{a}^{b} w \mathcal{R}[u] \, \mathrm{d}x + \sum_{k=1}^{N-1} \int_{x_{k}}^{x_{k+1}} \tau_{k} \hat{\mathcal{P}}[u, w] \mathcal{R}[u] \, \mathrm{d}x = 0$$

where

$$\hat{\mathcal{P}}[u,w] = \left\{ egin{array}{cc} \hat{v}\partial_x w & ext{if } |u|
eq 0 \ 0 & ext{otherwise} \end{array}
ight.$$
 and $\hat{v} = \left(rac{\mathcal{R}[u]}{|\partial_x u|^2}
ight) \partial_x u$



Extension to time-dependent problems

Redefine the residual of the PDE to include the transient term

 $\mathcal{R}[u] = \partial_t u + v \partial_x u - d \partial_{xx} u - f$

Redefine the stabilization operator

SUPG: $\mathcal{P}[w] = v\partial_x w$ GLS/SGS: $\mathcal{P}[w] = \pm \frac{w}{\Delta t} + v(\partial_x w) \mp \partial_x (d\partial_x w) \pm (\partial_x v) w$

and work out the (bi-)linear forms so that the weak problem reads

$$\int_a^b w \frac{du}{dt} \, \mathrm{d} x + a(u,w) = b(w) \quad \text{for all } w \in W$$



Extension to time-dependent problems, cont'd

Discretization in space by FEM yields the semi-discrete problem

$$M\frac{\mathrm{d}u}{\mathrm{d}t} + Au = b$$

Application of the θ -scheme yields the fully discrete problem

$$M\frac{u^{n+1}-u^n}{\Delta t}+\theta Au^{n+1}+(1-\theta)Au^n=\theta b^{n+1}+(1-\theta)b^n$$

• $\theta = 0$: explicit forward Euler method

- $\theta = \frac{1}{2}$: implicit Crank-Nicolson method
- $\theta = 1$: implicit backward Euler method

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