Introduction into Finite Elements FEM for Convection-Diffusion Problems

Matthias Möller, DIAM TU Delft November 21, 2013

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 $d = d(x) > 0$
- 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

$$
\begin{aligned}\n\text{div}\mathbf{v} &= \partial_x v^x + \partial_y v^y + \dots = 0 \\
\partial_x v &= 0 \quad \Leftrightarrow \quad v = \text{const} \quad \text{in} \quad 1D\n\end{aligned}
$$

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

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

is complemented by initial conditions at time $t = 0$

$$
u = u_0 \quad \text{in} \quad [a, b]
$$

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

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

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Model problems, cont'd

Time-dependent convection problem (hyperbolic)

$$
\partial_t u + \partial_x (vu) = f \qquad \text{in} \quad [a, b]
$$

is complemented by initial conditions at time $t = 0$

$$
u = u_0 \quad \text{in} \quad [a, b]
$$

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 $v \equiv \text{const} > 0$ (\cong 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.
$$
\begin{cases} \frac{\partial_x (vu) - \partial_x (d\partial_x u)}{u} = f & \text{in [a, b]} \\ u = u_a & \text{at } x = a \\ u = u_b & \text{at } x = b \end{cases}
$$

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

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

\n
$$
\stackrel{\text{i.b.p}}{\leftrightarrow} \int_{a}^{b} w \partial_{x}(vu) + \partial_{x}w(d\partial_{x}u) dx - \underbrace{w(d\partial_{x}u)|_{a}^{b}}_{=0} = \int_{a}^{b} wf dx
$$

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

Steady convection-diffusion problem, cont'd

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

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

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

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

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

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

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Steady convection-diffusion problem, cont'd

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

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

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

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

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

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

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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

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

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Galerkin finite element method, cont'd

Approximate trial and test spaces by finite approximations

$$
u_h = \sum_{j=1}^N \varphi_j u_j \in S_h = \text{span}\langle \varphi_1, \dots, \varphi_N \rangle \subset S
$$

$$
w_h = \sum_{i=1}^N \phi_i w_i \in W_h = \text{span}\langle \phi_1, \dots, \phi_N \rangle \subset W
$$

and solve the discrete problem

Find
$$
u_h \in S_h
$$
: $a(u_h, w_h) = b(w_h)$ for all $w_h \in W_h$

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Galerkin finite element method, cont'd

Assemble the system matrix \vec{A} and the right-hand side vector \vec{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. $u(x = a) = u_a$

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

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

$$
u_{\rm ex}(x) = \frac{1}{v} \left(x - \frac{1 - e^{\gamma x}}{1 - e^{\gamma}} \right)
$$

where $\gamma = \frac{v}{g}$ $\frac{v}{d}$. If $\gamma \gg 1$ the problem is termed convectiondominated. Numerical methods have problems in resolving the boundary layer at $x = b$. $\frac{6}{9}$ 0.2 0.4 0.6 0.8

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

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Resulting system matrix and right-hand side vector

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

$$
b = \begin{pmatrix} 0 & h & \dots & \dots & h & 0 \end{pmatrix}^T
$$

Galerkin FEM for an internal node $i \in \mathbb{C}$ central FD scheme)

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

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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_1 . 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

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

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

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

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

$$
u_{i-1} = \frac{1}{v} \left(x_i - h - \frac{1 - e^{\gamma x_i} e^{-2\text{Pe}}}{1 - e^{\gamma}} \right)
$$

$$
u_i = \frac{1}{v} \left(x_i - \frac{1 - e^{\gamma x_i}}{1 - e^{\gamma}} \right)
$$

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

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Analysis of the discrete problem, cont'd

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

$$
\underbrace{(\alpha_1+\alpha_2+\alpha_3)}_{=0}x_i\underbrace{-(\alpha_1-\alpha_3)}_{v/h}h-\underbrace{(\alpha_1e^{-2Pe}+\alpha_2+\alpha_3e^{2Pe})}_{=0}\frac{1-e^{\gamma x_i}}{1-e^{\gamma}}=v
$$

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

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

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

$$
\frac{v}{2h}((1-\coth \text{Pe})u_{i+1}+(2\coth \text{Pe})u_i-(1+\coth \text{Pe})u_{i-1})=1
$$

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

with stabilizing artificial/numerical diffusion

$$
\hat{d} = \beta \frac{vh}{2} = \beta d \text{ Pe}, \quad \beta = \text{cothPe} - \frac{1}{\text{Pe}}
$$

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

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

with 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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$$
\mathcal{R}[u] = \partial_x (vu) - \partial_x (d\partial_x u) - f
$$

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 $\mathcal{R}[u_{\text{ex}}] \equiv 0$

Making it work in practice

Stabilization parameter τ_k may be defined per element

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

■ Streamline-Upwind Petrov-Galerkin (SUPG) method

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

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

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

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

$$
a_k(u, w) = \int_{x_k}^{x_{k+1}} w \partial_x(vu) + \partial_x w(d\partial_x u)
$$

+ $\tau_k(v \partial_x w)(\partial_x(vu) + \partial_x(d\partial_x u)) dx$

$$
b_k(w) = \int_{x_k}^{x_{k+1}} w f + \tau_k(v \partial_x w) f dx
$$

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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

$$
\int_a^b w \mathcal{R}[u] dx + \sum_{k=1}^{N-1} \int_{x_k}^{x_{k+1}} \tau_k \hat{\mathcal{P}}[u, w] \mathcal{R}[u] dx = 0
$$

where

$$
\hat{\mathcal{P}}[u, w] = \left\{ \begin{array}{ll} \hat{v} \partial_x w & \text{if } |u| \neq 0 \\ 0 & \text{otherwise} \end{array} \right. \quad \text{and} \quad \hat{v} = \left(\frac{\mathcal{R}[u]}{|\partial_x u|^2} \right) \partial_x u
$$

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

$$
\int_{a}^{b} w \frac{du}{dt} dx + a(u, w) = b(w) \text{ for all } w \in W
$$

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

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

 $\theta = 0$: explicit forward Euler method

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

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