Technische Universität München
Lehrstuhl für Informatik V
Dr. T. Neckel
M.Sc. D. Jarema

WS 2013/14
Sheet 12
22.01.2014

Scientific Computing

Finite Element Methods

Exercise 27: Convection-Diffusion Equations

Consider the convection-diffusion equation for temperature transport in a fluid which moves at constant velocity $v \in \mathbb{R}$:

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x} = D\frac{\partial^2 T}{\partial x^2} \tag{1}$$

where $D \in \mathbb{R}^+$ denotes the diffusion constant of the fluid. The problem shall be solved on the unit interval with homogeneous Dirichlet conditions.

(a) Derive the weak formulation of the equation. Discretise space by piecewise linear hat functions. Derive the semi-discrete set of equations and compute all coefficients. How can we categorise this set of equations?

(b) Perform mass-lumping to facilitate the time discretisation. Therefore, approximate the mass matrix $M_{ij} := \int \varphi_i \varphi_j dx$ by a diagonal matrix $\tilde{M}_{ij}$,

$$\tilde{M}_{ij} := \begin{cases} \sum\limits_j M_{ij} & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

Use the explicit Euler method to subsequently discretise the problem in time.

(c) Solve the problem with maple for $D = 1.0$, $v = 1.0$, a mesh size $h = 1/10$ and a time step $\tau = 0.002, 0.02$. Use initial conditions $T = 1$ inside the domain (and homogeneous Dirichlet conditions at the boundaries).

Solution:

(a) Multiplying Eq. (1) by the test function $\varphi_i(x)$ and integrating in space yields:

$$\int_0^1 \frac{\partial T}{\partial t}\varphi_i(x)dx + v\int_0^1 \frac{\partial T}{\partial x}\varphi_i(x)dx = D\int_0^1 \frac{\partial^2 T}{\partial x^2}\varphi_i(x)dx \qquad \forall i \tag{3}$$

The right hand side can be transformed via integration by parts:

$$\int_0^1 \frac{\partial^2 T}{\partial x^2}\varphi_i(x)dx = \underbrace{\left[\int_0^1 \frac{\partial T}{\partial x}\varphi_i(x)\right]}_{=0} - \int_0^1 \frac{\partial T}{\partial x}\frac{\partial \varphi_i}{\partial x}dx \tag{4}$$

The discrete solution of the temperature is written as linear combination of the basis functions, $T = \sum_j a_j(t)\varphi_j(x)$. The basis functions are chosen to discretise space whereas the evolution over time is achieved via the coefficients $a_j(t)$. The arising finite element system of equations reads:

$$\sum_j \frac{\partial a_j(t)}{\partial t} \int_0^1 \varphi_i(x)\varphi_j(x)dx + v \cdot \sum_j a_j(t) \int_0^1 \frac{\partial \varphi_j(x)}{\partial x}\varphi_i(x)dx = -D\sum_j a_j(t)\int_0^1 \frac{\partial \varphi_j(x)}{\partial x}\frac{\partial \varphi_i(x)}{\partial x}dx \quad \forall i \tag{5}$$

To simplify the writing, we define the mass matrix M, the stiffness matrix A and the convective transport matrix C:

$$\begin{aligned} M_{ij} &:= \int_0^1 \varphi_i(x)\varphi_j(x)dx \\ A_{ij} &:= \int_0^1 \frac{\partial \varphi_j(x)}{\partial x}\frac{\partial \varphi_i(x)}{\partial x}dx \\ C_{ij} &:= \int_0^1 \frac{\partial \varphi_j(x)}{\partial x}\varphi_i(x)dx \end{aligned} \tag{6}$$

Our problem thus reads:

$$\sum_j M_{ij}\frac{\partial a_j(t)}{\partial t} + v \cdot \sum_j C_{ij}a_j(t) = -D\sum_j A_{ij}a_j(t) \quad \forall i \tag{7}$$

Now, we can insert the piecewise linear hat functions $\varphi_i(x)$ and evaluate the coefficients M_{ij}, A_{ij} and C_{ij}. Let h denote the mesh size of our one-dimensional grid. Integration of the local hat functions yields:

$$M_{ij} := \begin{cases} \frac{1}{6}h & |i-j| = 1 \\ \frac{2}{3}h \quad \text{if} & i = j \\ 0 & \text{otherwise} \end{cases}, A_{ij} := \begin{cases} -\frac{1}{h} & |i-j| = 1 \\ \frac{2}{h} \quad \text{if} & i = j \\ 0 & \text{otherwise} \end{cases}, C_{ij} := \begin{cases} \frac{1}{2} & j = i+1 \\ -\frac{1}{2} \quad \text{if} & j = i-1 \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

The set of equations from Eq. (7) is a *coupled system of ODEs*. As we can see from the form of the mass matrix M, a coupling of the time derivatives for the coefficients $a_{i-1}(t)$, $a_i(t)$ and $a_{i+1}(t)$ is currently enforced. This automatically does not allow for explicit time-stepping.

(b) We apply the mass-lumping and so reduce the tridiagonal structure of the mass matrix to a diagonal matrix. We collect all contributions of a single row of the mass matrix M and store their sum in a diagonal matrix $\tilde{M}$:

$$\tilde{M}_{ii} = \sum_j M_{ij}, \quad \tilde{M}_{ij} = 0 \quad \text{for } i \neq j. \tag{9}$$

This procedure conserves the overall weight of a single matrix row and is therefore known as *mass-lumping*. However, there is no coupling of basis functions included anymore. With respect to momentum or energy conservation, this implies that linear momentum or kinetic energy is conserved whereas angular momentum may not be preserved[1]. Considering the matrix M from the part (a), we obtain $\tilde{M}_{ii} = \sum_j M_{ij} = \frac{1}{6}h + \frac{2}{3}h + \frac{1}{6}h = h$. Inserting all matrix expressions including the mass-lumping approach into Eq. (7) yields:

$$\begin{aligned}
\tilde{M}_{ii}\tfrac{\partial a_i(t)}{\partial t} &= -v \cdot \sum_j C_{ij}a_j(t) - D\sum_j A_{ij}a_j(t) && \forall i \\
\Leftrightarrow \quad h\tfrac{\partial a_i(t)}{\partial t} &= -\tfrac{v}{2}(a_{i+1}(t) - a_{i-1}(t)) - \tfrac{D}{h}(-a_{i-1}(t) + 2a_i(t) - a_{i+1}(t)) && \forall i \\
\Leftrightarrow \quad \tfrac{\partial a_i(t)}{\partial t} &= -\tfrac{v}{2h}(a_{i+1}(t) - a_{i-1}(t)) - \tfrac{D}{h^2}(-a_{i-1}(t) + 2a_i(t) - a_{i+1}(t)) && \forall i
\end{aligned} \tag{10}$$

Remark: we already dealt with convection-diffusion problems before, cf. Exercise 17. If we compare the right hand side of the equation above with the discrete version of the steady-state problem from Exercise 17(a), we can observe great similarity between both formulations in this special case (for $D = 1$).
Similar to previous discrete formulations for time-space partial differential equations, we obtained a (simplified) system of ordinary equations that can now be solved by any time-stepping method. We use the explicit Euler method and a time step τ:

$$\frac{\partial a_i(t)}{\partial t} = f(t) \to \frac{a_i(t+\tau) - a_i(t)}{\tau} = f(t) \leftrightarrow a_i(t+\tau) = a_i(t) + \tau f(t) \tag{11}$$

Inserting the explicit Euler method into Eq. (10) results in:

$$\begin{aligned}
a_i(t+\tau) &= a_i(t) - \tfrac{v\tau}{2h}(a_{i+1}(t) - a_{i-1}(t)) - \tfrac{D\tau}{h^2}(-a_{i-1}(t) + 2a_i(t) - a_{i+1}(t)) \\
a_i(t+\tau) &= \left(\tfrac{v\tau}{2h} + \tfrac{D\tau}{h^2}\right)a_{i-1}(t) + \left(1 - \tfrac{2D\tau}{h^2}\right)a_i(t) + \left(-\tfrac{v\tau}{2h} + \tfrac{D\tau}{h^2}\right)a_{i+1}(t)
\end{aligned} \tag{12}$$

(c) See ws13_27c.mw. For the large time step, instabilities occur. Several sources for these instabilities can be stated: first, the explicit Euler method yields restrictions onto the time step. This can be resolved by implicit time stepping schemes. Second, the central difference expression for the convective term further reduces the stability interval of the method. Changing the finite element discretisation to obtain upwind-like expressions for the convective term can reduce this issue to a certain extent.

Exercise 28: Reference Elements

In the following, we want to compute the mapping from an arbitrary triangle E onto a reference triangle E_{ref}, cf. Fig. 1. This can be useful in several contexts, for example to simplify the integration procedures in the FE method or to prove error estimates for the respective finite elements and their basis functions.

(a) Define a transformation $\chi(\xi)$ which maps the coordinates ξ within the reference triangle E_{ref} (triangle on the right in Fig. 1) onto the triangle E (triangle on the left in Fig. 1). Use arbitrary coordinates P_0, P_1, $P_2 \in \mathbb{R}^2$ to define the transformation.

[1]For further information on mass-lumping and properties of the arising matrices, you may check out Chapter 32 of http://www.colorado.edu/engineering/CAS/courses.d/IFEM.d/.

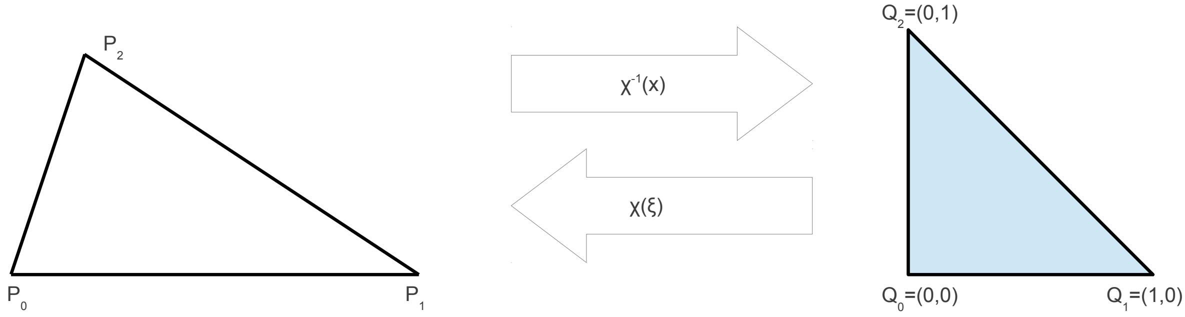

Figure 1: Coordinate mapping between a triangle of arbitrary shape (left) and a reference triangle (right).

(b) Denote the corners of the reference triangle by $Q_0 = (0,0)^\top, Q_1 = (1,0)^\top, Q_2 = (0,1)^\top$. Define linear functions $\Phi_i(\xi), i = 0,1,2$, on the reference triangle such that $\Phi_i(Q_j) = \delta_{ij}$, that is

$$\Phi_i(Q_j) := \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j. \end{cases} \tag{13}$$

Compute the mass matrix $A_{ij}^{\text{ref}} := \int_{E_{\text{ref}}} \Phi_i(\xi)\Phi_j(\xi)d\xi$ of the reference element; you may use maple for this purpose.

(c) Use the u-substitution to derive a formula which evaluates the mass matrix $A_{ij} = \int_E \phi_i(x)\phi_j(x)dx$ for an arbitrary triangle and its respective basis functions $\phi_i(x)$. The formula may only make use of the transformation $\chi(\xi)$ and the mass matrix A^{ref} of the reference triangle.

(d) Validate your formula from task (c) by computing the mass matrix of the reference element from Exercise 26. You may use maple for this purpose.

Solution:

(a) Let $\xi \in E_{\text{ref}}$ denote a point inside the reference triangle. Then, we can define the mapping $\chi(\xi)$ as

$$\chi(\xi) := P_0 + B \cdot \xi, \quad B := (P_1 - P_0, P_2 - P_0) \in \mathbb{R}^{2\times 2}. \tag{14}$$

For $Q_0 = (0,0)^\top, Q_1 = (1,0)^\top, Q_2 = (0,1)^\top$, we thus obtain $\chi(Q_i) = P_i, i = 0,1,2$.

(b) The linear functions are given by

$$\begin{aligned} \Phi_0(\xi) &:= 1 - \xi_1 - \xi_2 \\ \Phi_1(\xi) &:= \xi_1 \\ \Phi_2(\xi) &:= \xi_2. \end{aligned} \tag{15}$$

The mass matrix evolves at

$$A^{\text{ref}} := \begin{pmatrix} \frac{1}{12} & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{12} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & \frac{1}{12} \end{pmatrix}, \tag{16}$$

see also massmatrix.mw.

(c) Let $\phi_i(x)$ denote the linear functions on the general triangle E. By construction, these functions satisfy $\phi_i(P_j) = \delta_{ij}$. Now, we want to compute $A_{ij} = \int_E \phi_i(x)\phi_j(x)dx$. Using u-substitution, we can write the integral as

$$A_{ij} = \int_E \phi_i(x)\phi_j(x)dx = \int_{E_{\text{ref}}} \phi_i(\chi(\xi))\phi_j(\chi(\xi))\det(\mathcal{J}(\xi))d\xi \tag{17}$$

where $\mathcal{J}(\xi)$ denotes the Jacobi matrix of χ. The Jacobian $\mathcal{J}$ of a function $f(x) : \mathbb{R}^N \to \mathbb{R}^M$ is defined as

$$\mathcal{J} := \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{pmatrix}. \tag{18}$$

Considering the linear mapping $\chi(\xi) := P_0 + B \cdot \xi$, we see that the Jacobian is given by $\mathcal{J}(\xi) = B$. On the current element E, the determinant $\det(B)$ is a constant, arising from

$$\det(B) = \begin{vmatrix} P_{1_1} - P_{0_1} & P_{2_1} - P_{0_1} \\ P_{1_2} - P_{0_2} & P_{2_2} - P_{0_2} \end{vmatrix} = (P_{1_1} - P_{0_1})(P_{2_2} - P_{0_2}) - (P_{2_1} - P_{0_1})(P_{1_2} - P_{0_2}). \tag{19}$$

We can hence move the determinant to the front of the integral expression:

$$A_{ij} = \int_{E_{\text{ref}}} \phi_i(\chi(\xi))\phi_j(\chi(\xi))\det(B)d\xi = \det(B)\int_{E_{\text{ref}}} \phi_i(\chi(\xi))\phi_j(\chi(\xi))d\xi \tag{20}$$

Consider the function $\phi_i(\chi(\xi))$ in more detail. If we insert Q_j, we see that

$$\phi_i(\chi(Q_j)) = \phi_i(P_0 + B \cdot Q_j) = \phi_i(P_j) = \delta_{ij}. \tag{21}$$

From this, we observe that the functions $\phi_i(\chi(\xi))$ and $\Phi_i(\xi)$ deliver the same results for all Q_j, $j = 0, 1, 2$. Since both functions are linear, they are further uniquely defined via these three points. As a result, both expressions must be identical,

$$\phi_i(\chi(\xi)) = \Phi_i(\xi). \tag{22}$$

The mass matrix for the general element E can hence be written as follows:

$$A_{ij} = \det(B)\int_{E_{\text{ref}}} \phi_i(\chi(\xi))\phi_j(\chi(\xi))d\xi = \det(B)\int_{E_{\text{ref}}} \Phi_i(\xi)\Phi_j(\xi)d\xi = \det(B)A_{ij}^{\text{ref}}. \tag{23}$$

(d) Computing the mass matrix for the linear basis functions on the reference element of Exercise 26 yields the matrix

$$A := \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix} \tag{24}$$

We can further evaluate the determinant of the matrix B of this triangle:

$$\det(B) := |(P_2 - P_1 \quad P_3 - P_1)| = \left| \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix} \right| = 2 \tag{25}$$

where P_i, $i = 1, 2, 3$ are the points illustrated in the respective figure of Exercise 26. Evaluating the formula from Eq. (23) shows the validity of our derivations:

$$A_{ij} = \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix} = 2 \cdot \begin{pmatrix} \frac{1}{12} & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{12} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & \frac{1}{12} \end{pmatrix} = \det(B) \cdot A_{ij}^{\text{ref}} \tag{26}$$