$WS \ 11/12$ To be submitted in the lecture on 11.01.2012

Numerische Mathematik für Ingenieure II Homework 8

Programming exercise 11: (20 points)

Consider the following Dirichlet boundary value problem: find $u: \overline{\Omega} \to \mathbb{R}$ such that

$$-\Delta u + cu = f$$
 in $\Omega \subset \mathbb{R}^3$ and $u = g$ on $\Gamma := \partial \Omega$

with a constant c > 0, a right hand side $f: \Omega \to \mathbb{R}$ and a boundary value function $g: \Gamma \to \mathbb{R}$. In this exercise, the solution to this problem is approximated with the Galerkin finite element method using a tetrahedral mesh and element-wise linear basis functions. To describe tetrahedrons and triangles we define the convex hull of the points $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^3$:

$$conv(x^{(1)}, \dots, x^{(n)}) := \Big\{ \sum_{k=1}^{n} \lambda_k x^{(k)} \mid \lambda_k \ge 0, \ \sum_{k=1}^{n} \lambda_k = 1 \Big\}.$$

The domain Ω and its boundary Γ are defined by three matrices:

- $p \in \mathbb{R}^{3,np}$ describes a set of points: $p(:,i) \in \mathbb{R}^{3,1}$ are the coordinates of the i-th point $(i \in \{1,...,np\})$.
- $t \in \mathbb{N}^{4,nt}$ is an index matrix describing the elements that make up the domain Ω : for $j \in \{1, ..., nt\}$ the columns of the matrix $pt := p(:, t(:, j)) \in \mathbb{R}^{3,4}$ are the vertices of the j-th element (a tetrahedron):

$$\Omega_i := \operatorname{conv}(\operatorname{pt}(:,1),\ldots,\operatorname{pt}(:,4)).$$

The whole domain is $\overline{\Omega} := \bigcup_{j=1}^{\mathtt{nt}} \Omega_j$ and for $i, j \in \{1, \ldots, \mathtt{nt}\}$ with $i \neq j$ the tetrahedrons Ω_i and Ω_j may only share a face, a edge or a vertex.

• $e \in \mathbb{N}^{3,ne}$ is an index matrix describing the faces belonging to the boundary Γ : for $j \in \{1, ..., ne\}$ the columns of the matrix $pe := p(:, e(:, j)) \in \mathbb{R}^{3,3}$ are the vertices of the j-th boundary face (a triangle):

$$\Gamma_i := \text{conv}(\text{pe}(:,1),\text{pe}(:,2),\text{pe}(:,3)).$$

The whole boundary is $\Gamma := \bigcup_{j=1}^{ne} \Gamma_j$ and for $i, j \in \{1, ..., nt\}$ with $i \neq j$ the triangles Γ_i and Γ_j may only share a edge or a vertex.

For $i \in \{1, ..., np\}$ the global basis function $w_i : \overline{\Omega} \to \mathbb{R}$ is defined by the following conditions:

- w_i restricted to Ω_i is a linear polynomial for all $j \in \{1, \dots, nt\}$.
- $w_i(p(:,j)) = \delta_{ij}$ for all $j \in \{1,\ldots,np\}$.

The local basis functions $\widehat{w}_i: \widehat{\Omega} \to \mathbb{R}$ on the reference element $\widehat{\Omega} := \text{conv}(0, e_1, e_2, e_3)$ are given for $\widehat{x} = [\widehat{x}_1, \widehat{x}_2, \widehat{x}_3]^\mathsf{T} \in \widehat{\Omega}$ by

$$\widehat{w}_1(\widehat{x}) := 1 - \widehat{x}_1 - \widehat{x}_2 - \widehat{x}_3, \qquad \widehat{w}_2(\widehat{x}) := \widehat{x}_1, \qquad \widehat{w}_3(\widehat{x}) := \widehat{x}_2, \qquad \widehat{w}_4(\widehat{x}) := \widehat{x}_3.$$

The local and global basis functions are related by t: for $j \in \{1, ..., nt\}$ the relation is

$$w_{\mathsf{t}(i,j)}(F_i(\widehat{x})) = \widehat{w}_i(\widehat{x}) \quad \forall \widehat{x} \in \widehat{\Omega} \text{ and } i \in \{1,2,3,4\},$$

where $F_j: \widehat{\Omega} \to \Omega_j$ is the transformation defined by $F_j(\widehat{x}) := \mathtt{pt}(:,1) + G_j \widehat{x}$ for all $\widehat{x} \in \widehat{\Omega}$ with \mathtt{pt} as defined above and $G_j := [\mathtt{pt}(:,2) - \mathtt{pt}(:,1), \mathtt{pt}(:,3) - \mathtt{pt}(:,1), \mathtt{pt}(:,4) - \mathtt{pt}(:,1)] \in \mathbb{R}^{3,3}$.

(a) Implement a function b=p11getBoundD0Fs(p,e) that returns a column vector $b \in \mathbb{R}^{np,1}$ such that for $i \in \{1, ..., np\}$ the following holds:

$$b(i) = \begin{cases} 1 & \text{if } p(:,i) \in \Gamma \\ 0 & \text{else.} \end{cases}$$

- (b) Write a function [elS,elM,elfh]=p11getLoc(pt,c,f) that computes the local contributions from an element $k \in \{1, ..., nt\}$ that is given by its points pt=p(:,t(:,k)). As shown in the tutorial the following quantities have to be computed for all $i, j \in \{1, ..., 4\}$:
 - (a) element "stiffness matrix": $els(i,j) = \int_{\widehat{\Omega}} (\nabla \widehat{w}_j(\widehat{x}))^{\mathsf{T}} (G_k^{\mathsf{T}} G_k)^{-1} \nabla \widehat{w}_i(\widehat{x}) |\det G_k| d\widehat{x}.$
 - (b) element "mass matrix": $elM(i,j) = c \int_{\widehat{\Omega}} \widehat{w}_j(\widehat{x}) \widehat{w}_i(\widehat{x}) |\det G_k| d\widehat{x}$.
 - (c) element right hand side: $\mathsf{elfh}(i) = \int_{\widehat{O}} \mathsf{f}(F_k(\widehat{x})) \widehat{w}_i(\widehat{x}) |\det G_k| d\widehat{x}.$

Thus elS and elM are both $\mathbb{R}^{4,4}$ matrices and elfh should be a $\mathbb{R}^{4,1}$ column vector. Use the quadrature formula

$$\int_{\widehat{\Omega}} h(\widehat{x}) d\widehat{x} \; \approx \; \frac{1}{6} \; h\Big(\begin{bmatrix} 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} \Big)$$

for integrals that cannot be computed explicitly.

(c) Write a function [S,M,D,fh]=p11getLS(p,e,t,c,f,g) that uses b=p11getBoundD0Fs(p,e) and p11getLoc to construct the linear system $(S+M+D)\alpha=fh$, where $u_h=\sum_{i=1}^{np}\alpha_iw_i$ is the globally defined approximate solution. As it will be shown in the tutorial on 16.12.2011, the matrices and right hand side have to be adapted to incorporate the Dirichlet boundary conditions. For $i,j\in\{1,\ldots,np\}$ the following should hold:

(a)
$$S(i,j) = \begin{cases} \int_{\Omega} \nabla w_j(x) \cdot \nabla w_i(x) dx & \text{if } p(:,i) \notin \Gamma, \\ 0 & \text{else.} \end{cases}$$

(b)
$$M(i,j) = \begin{cases} c \int_{\Omega} w_j(x)w_i(x)dx & \text{if } p(:,i) \notin \Gamma, \\ 0 & \text{else.} \end{cases}$$

(c)
$$D(i,j) = \begin{cases} 0 & \text{if } p(:,i) \notin \Gamma, \\ \delta_{ij} & \text{else.} \end{cases}$$

(d)
$$fh(i) = \begin{cases} \int_{\Omega} f(x)w_i(x)dx & \text{if } p(:,i) \notin \Gamma, \\ g(p(:,i)) & \text{else.} \end{cases}$$

(Here and in the following $x = [x_1, x_2, x_3]^{\mathsf{T}} \in \overline{\Omega}$.) Thus S, M and D should be *sparse* $\mathbb{R}^{\mathsf{np},\mathsf{np}}$ matrices and fh is a $\mathbb{R}^{\mathsf{np},1}$ column vector.

(d) Test and verify your implementation with $\overline{\Omega} = [0,1]^3$, $c = \frac{1}{2}$, the right hand side function

$$f(x) = \sin(2\pi x_1)\sin(2\pi x_2)\left(\frac{5}{2} + 8\pi^2 x_3(1 - x_3)\right) + x_1 x_2 x_3$$

and the Dirichlet boundary value function

$$g(x) = \exp\left(\frac{x_3}{\sqrt{2}}\right) + x_1 x_2 x_3.$$

The exact solution then is

$$u(x) = \sin(2\pi x_1)\sin(2\pi x_2)x_3(1 - x_3) + \exp\left(\frac{x_3}{\sqrt{2}}\right) + x_1x_2x_3.$$

Write a function [err,eoc]=p11eoc() that computes the approximate solution u_r for a uniform tetrahedral mesh with mesh size $h_r = 1/2^r$ for $r \in \{1, 2, 3, 4\}$. The output should be 2 column vectors with

$$\begin{split} & \texttt{err(r)} = \max_{i \in \{1, \dots, np\}} |u(\texttt{p(:,i)}) - u_r(\texttt{p(:,i)})| & \text{for } r \in \{1, 2, 3, 4\} \\ & \texttt{eoc(r)} = \frac{\log(\texttt{err(r)/err(r-1)})}{\log(h_r/h_{r-1})} & \text{for } r \in \{2, 3, 4\}. \end{split}$$

A uniform mesh for the unit cube $\overline{\Omega}$ with mesh size $h_r = 1/2^r$ can be generated with the provided function [p,e,t]=p11mshUnit(3, $2^r - 1$). The linear systems should be solved with the backslash operator. Verify that the EOC converges to 2.

Some notes for further experiments:

- An approximate solution given by a coefficient vector alpha can be written to a VTK (visualization toolkit) file (.vtu) with the provided function p11vtkWrite(filename, p,e,t,alpha). The VTK files can then be plotted and post-processed by several tools, for example ParaView (free software).
- You can generate your own meshes with the tool *gmsh* (also free software). Use the provided function [p,e,t]=p11mshRead(filename,3) to read a *gmsh* mesh from a .msh file. Feel free to conduct experiments with your own geometry!



Level surfaces and corresponding part of the mesh for an approximation to the solution u visualized with ParaView (with the Contour filter).