NUCLEAR ENGINEERING, UC BERKELEY

ME 280A Finite Element Analysis HOMEWORK 3: Potential and efficient solution techniques

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1 INTRODUCTION

The objective of this project is to solve a 1-D differential equation using linear elements.

$$\begin{aligned} \frac{d}{dx}(A_1(x)\frac{du}{dx}) &= f(x) \\ f(x) &= 256sin(\frac{3\pi kx}{4})cos(16\pi x) \\ A_1(x) &= piecewise \\ L &= 1 \\ u(0) &= 0 \\ A1(L)\frac{du}{dx}(L) &= 1 \end{aligned} \tag{1}$$

A_1 is a piece wise function, defined as bellow:

$$\begin{aligned} For \quad 0.0 \le x < 0.1: \quad A_1 = 2.0 \\ For \quad 0.1 \le x < 0.2: \quad A_1 = 2.5 \\ For \quad 0.2 \le x < 0.3: \quad A_1 = 1.25 \\ For \quad 0.3 \le x < 0.4: \quad A_1 = 0.25 \\ For \quad 0.4 \le x < 0.5: \quad A_1 = 4.0 \\ For \quad 0.5 \le x < 0.6: \quad A_1 = 1.75 \\ For \quad 0.6 \le x < 0.7: \quad A_1 = 0.5 \\ For \quad 0.7 \le x < 0.8: \quad A_1 = 0.75 \\ For \quad 0.8 \le x < 0.9: \quad A_1 = 3.25 \\ For \quad 0.9 \le x \le 1.0: \quad A_1 = 1.0 \end{aligned} \tag{2}$$

2 ANALYTICAL SOLUTION

The general solution for this equation on every segment can be found after two integrations:

$$\begin{aligned} A_1(x)\frac{du}{dx} &= \int 256sin(\frac{3\pi kx}{4})cos(16\pi x)dx \\ &= \int 128[sin(\frac{67\pi x}{4}) - sin(\frac{61\pi x}{4})] \\ &= \frac{512(67cos(\frac{61\pi x}{4}) - 61cos(\frac{67\pi x}{4}))}{4087\pi} + C1 \end{aligned} \tag{3}$$

$$\frac{du}{dx} = \frac{1}{A_1(x)}\left(\frac{512(67cos(\frac{61\pi x}{4}) - 61cos(\frac{67\pi x}{4}))}{4087\pi} + C1\right) \tag{4}$$

Integrating $\frac{du}{dx}$, we obtain the analytical solution for the differencial equation:

$$u(x) = \frac{1}{A1(x)}\frac{\frac{137216sin(\frac{61\pi x}{4})}{61\pi} - \frac{124928sin(\frac{67\pi x}{4}))}{67\pi}}{4087\pi} + \frac{C1x}{A_1(x)} + C2 \tag{5}$$

where C1 and C2 are piecewise constants that can be calculated using the boundary conditions and interface conditions.

At the interface between segments x_N (N=1,...,10), the function u and its derivation is continuous, i.e.,

$$\begin{aligned} u(x_N^+) &= u(x_N^-) \\ A1(x_N^+)\frac{du}{dx}(x_N^+) &= A1(x_N^-)\frac{du}{dx}(x_N^-) \end{aligned} \tag{6}$$

In particular, at the left endpoint, $u(0) = u_0 = 0$ and at the right end point, $A1(L)\frac{du}{dx}(L) = 1$.

Applying the boundary conditions and continuation conditions at the interfaces, we can solve the equation system and obtain the analytical solution:

$$\begin{aligned} For \quad & 0.0 \le x < 0.1: \quad C_1 = 1.1692 \\ For \quad & 0.1 \le x < 0.2: \quad C_1 = 1.1692 \\ For \quad & 0.2 \le x < 0.3: \quad C_1 = 1.1692 \\ For \quad & 0.3 \le x < 0.4: \quad C_1 = 1.1692 \\ For \quad & 0.4 \le x < 0.5: \quad C_1 = 1.1692 \\ For \quad & 0.5 \le x < 0.6: \quad C_1 = 1.1692 \\ For \quad & 0.6 \le x < 0.7: \quad C_1 = 1.1692 \\ For \quad & 0.7 \le x < 0.8: \quad C_1 = 1.1692 \\ For \quad & 0.8 \le x < 0.9: \quad C_1 = 1.1692 \\ For \quad & 0.9 \le x \le 1.0: \quad C_1 = 1.1692 \end{aligned} \tag{7}$$

$$
\begin{aligned}
For \quad & 0.0 \le x < 0.1: \quad C_2 = 0 \\
For \quad & 0.1 \le x < 0.2: \quad C_2 = 0.0101 \\
For \quad & 0.2 \le x < 0.3: \quad C_2 = -0.0964 \\
For \quad & 0.3 \le x < 0.4: \quad C_2 == 1.4040 \\
For \quad & 0.4 \le x < 0.5: \quad C_2 = 0.2742 \\
For \quad & 0.5 \le x < 0.6: \quad C_2 = 0.1166 \\
For \quad & 0.6 \le x < 0.7: \quad C_2 = -0.8391 \\
For \quad & 0.7 \le x < 0.8: \quad C_2 = -0.2384 \\
For \quad & 0.8 \le x < 0.9: \quad C_2 = 0.7997 \\
For \quad & 0.9 \le x \le 1.0: \quad C_2 = 0.0931
\end{aligned} \tag{8}
$$

3 Finite Element Method

3.1 Weak form

The first step of FEM is to derive the weak form of the differential equation:

$$
\begin{gathered}
\text{Find u, u}|\Gamma \text{ u =d, such that } \forall \text{ v, v}|\Gamma \text{ u =0} \\
\int_\Omega \frac{dv}{dx} A_1(x) \frac{du}{dx} dx = \int_\Omega f v dx + t v\,|_{\Gamma t}
\end{gathered} \tag{9}
$$

We approximate the real solution u by

$$
u(x) = \sum_{j=1}^{N} a_j \phi_j(x) \tag{10}
$$

and we choose the test function v with the same approximation functions

$$
v(x) = \sum_{i=1}^{N} b_i \phi_i(x) \tag{11}
$$

where N is the number of degree of freedom(number of nodes).

Then the equation becomes:

$$\int_\Omega \frac{d}{dx}(\sum_{j=1}^{N+1} a_j\phi_j(x))A_1(x)\frac{d}{dx}(\sum_{i=1}^{N+1} b_i\phi_i(x))dx = \int_\Omega f(\sum_{i=1}^{N+1} b_i\phi_i(x))dx + (\sum_{i=1}^{N+1} b_i\phi_i(x)t)\,|_{\Gamma t}, \forall b_i \quad (12)$$

We can regroup the terms into:

$$\sum_{i=1}^{N+1} b_i \int_\Omega (\sum_{j=1}^{N+1} a_j \frac{d}{dx}\phi_j(x)A_1(x)\frac{d}{dx}\phi_i(x))dx = \sum_{i=1}^{N+1} b_i \int_\Omega f\phi_i(x)dx + \sum_{i=1}^{N+1} b_i(\phi_i(x)t)\,|_{\Gamma t} \quad (13)$$

As the equation should be valid for any b_i, we obtain the matrix system to solve:

$$\begin{aligned} K_{ij} &= \int_\Omega \frac{d}{dx}\phi_j(x)A_1(x)\frac{d}{dx}\phi_i(x)dx \\ R_i &= \int_\Omega f\phi_i(x)dx + \phi_i(x)t\,|_{\Gamma t} \\ Ka &= R \end{aligned} \quad (14)$$

Linear shape functions are defined as:

$$\begin{aligned} \hat{\phi}_1 &= \frac{1-\xi}{2} \\ \hat{\phi}_2 &= \frac{1+\xi}{2} \end{aligned} \quad (15)$$

and

$$\begin{aligned} \frac{d\hat{\phi}_1}{d\xi} &= -\frac{1}{2} \\ \frac{d\hat{\phi}_2}{d\xi} &= \frac{1}{2} \end{aligned} \quad (16)$$

Corresponding global coordinate x can be calculate x from ξ:

$$x = \sum \chi_i \hat{\phi}_i \quad (17)$$

where χ_i are the coordinates of the nodes in the global element.

3.2 DATA STRUCTURE

Matrix K is assembled from symmetric 2x2 element matrices. KE table is used to store only the three elements in Ke: Ke(1, 1), Ke(1, 2) and Ke(2, 2). The connectivity table stores the endpoints of each mesh element, in the case of 1D meshing, the connectivity table is:

$$connectivity = \begin{pmatrix} 1,2 \\ 2,3 \\ 3,4 \\ \vdots \end{pmatrix} \tag{18}$$

$$KE_{table} = \begin{pmatrix} K_{11}^1 & K_{12}^1 & K_{22}^1 \\ K_{11}^2 & K_{12}^2 & K_{22}^2 \\ & \dots & \\ K_{11}^{Ne} & K_{12}^{Ne} & K_{22}^{Ne} \end{pmatrix} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ & \dots & \\ K_{N1} & K_{N2} & K_{N3} \end{pmatrix} \tag{19}$$

The multiplication operation of KE table and an array Q (y=KE table * Q)is

$$\begin{aligned} &\text{Loop through e:} \\ Ke &= KEtable[e] \\ Qe &= Q(connectivity[e]) \\ y_e &= Ke * Qe \\ y(connectivity[e]) &+= y_e \end{aligned} \tag{20}$$

And the operation of $T^T * K * T$ is:

$$T^T * K * T = \begin{pmatrix} K_{11}T_1T_1 & K_{12}T_1T_2 & K_{13}T_1T_3 \\ K_{21}T_2T_1 & K_{22}T_2T_2 & K_{23}T_2T_3 \\ & \cdots & \\ K_{N1}T_NT_1 & K_{N2}T_NT_2 & K_{N3}T_NT_3 \end{pmatrix} \tag{21}$$

3.3 APPLYING BOUNDARY CONDITION TO KE TABLE AND R

As discussed in the previous homeworks, for Dirichlet BC on u(0):

$$\begin{aligned} K(1,1) &= & 1, K(1,2) = 0 \\ R(1) &= & u(0) \end{aligned}$$

in the form of KE table:

$$\begin{aligned} R(1) &= & u(0) \\ R(2) &= & R(2) - KE_{table}(1,2) * u(0) \\ KE_{table}(1,1) &= & 1, KE_{table}(1,2) = 0 \end{aligned}$$

For Dirichlet BC on u(L):

$$\begin{aligned} K(N,N) &= & 1, K(N,1:N-1) = 0 \\ R(N) &= & u(L) \end{aligned}$$

in the form of KE table:

$$\begin{aligned} R(N) &= & u(L) \\ R(N-1) &= & R(N-1) - KE_{table}(N-1,2) * u(L) \\ KE_{table}(N-1,3) &= & 1, KE_{table}(N-1,2) = 0 \end{aligned}$$

Neumann boundary condition gives the value of traction $A1(x)\frac{du}{dx}$ on an end point. The implementation doesn't change if KE table is used.

For Neumann BC on x=0:

$R(1) = R(1) + A_1 \frac{du}{dx}[x = 0]$

For Neumann BC on x=L:

$R(N) = R(N) + A_1 \frac{du}{dx}[x = L]$

4 PRECONDITIONED CONJUGATE-GRADIENT SOLVER

There are two approaches to solve the equation for [K]a = R, direct and iterative. The number of operations in direct solvers are $O(N^3)$. They are employed when the number of unknowns are not very large, and there are multiple load vectors. Iterative solver are prefered when the systems are very large. Conjugate gradient type iterative techniques need only $O(N^2)$ operations.

We define a potential(eq23) whose derivative is the residual of the equation to solve. So the minimizer of the potential Π is the solution to the equation.

$$\bigtriangledown \Pi = [K]\{a\} - \{R\} \tag{22}$$

$$\Pi = \frac{1}{2}\{a\}^T[K]\{a\} - \{a\}^T\{R\} \tag{23}$$

$$\begin{aligned} \{r\}^i &= -\bigtriangledown \Pi = \{R\} - [K]\{a\}^i \\ \{a\}^{i+1} &= \{a\}^i + \lambda^i\{r\}^i \end{aligned} \tag{24}$$

The idea of steepest descent is to find this minimizer of potential by going to the direction of the gradiant of the potential, i.e. $\{a\}^{i+1} = \{a\}^i + \lambda^i\{z\}^i$, where $\{z\}^i = \{r\}^i + \theta^i\{z\}^{i-1}$. The coefficient θ is chosen so that z is [K] conjugate to $\{z\}^{i-1}$, i.e.,

$$\begin{aligned} \{z\}^{T,i}[K]\{z\}^{i-1} &= 0 \\ \theta^i &= -\frac{\{r\}^{T,i}[K]\{z\}^{i-1}}{\{z\}^{T,i-1}[K]\{z\}^{i-1}} \end{aligned} \tag{25}$$

Looking for λ to minimize the potential, we force $\frac{\partial \Pi}{\partial \lambda^i} = 0$ and solve for λ:

$$\lambda^i = \frac{\{z\}^{T,i}\{r\}^i}{\{z\}^{T,i}[K]\{z\}^i} \tag{26}$$

4.1 PRECONDITIONING OF [K]

The rate of convergence of the CG method is related to the condition number

$$\|\{a\} - \{a\}^i\|_K \leq (\frac{\sqrt{C([K])-1}}{\sqrt{C([K])+1}})^i \|\{a\} - \{a\}^1\|_K \tag{27}$$

To reduce the condition number, preconditioning of [K] is done by forming the transformation of variables:

$$\begin{aligned} T^T K T[T^{-1}A] &= [T^T R] \\ [\bar{K}] &= [T]^T[K][T] \\ \bar{R} &= T^T R \\ [\bar{K}]a &= \bar{R} \\ A &= aT \end{aligned} \tag{28}$$

Diagonal preconditioning is an inexpensive widely used, where [T] is defined from the diaganol of [K] as:

$$T_{ij} = \frac{1}{\sqrt{K_{ij}}}, i, j = 1, ...ndof \tag{29}$$

Note that in order to use this preconditioner, the diagonal of K has to be positive, as in our case.

4.2 ITERATION

Starting from an initial guess for $\{a\}^0$, we can calculate the residual defined as in equation 30.

$$\begin{aligned} \{r\}^0 &= -\bigtriangledown \Pi = \{R\} - [K]\{a\}^0 \\ \{z\}^0 &= \{r\}^0 \\ \lambda^0 &= \frac{\{z\}^{T,0}\{r\}^0}{\{z\}^{T,0}[K]\{z\}^0} \\ \{a\}^1 &= \{a\}^0 + \lambda^0\{z\}^0 \end{aligned} \tag{30}$$

For iteration i >0,

$$\begin{aligned} \{r\}^i &= \{R\} - [K]\{a\}^i \\ \theta^i &= -\frac{\{r\}^{T,i}[K]\{z\}^{i-1}}{\{z\}^{T,i-1}[K]\{z\}^{i-1}} \\ \{z\} &= \{r\}^i + \theta^i\{z\}^{i-1} \\ \lambda^i &= \frac{\{z\}^{T,i}\{r\}^i}{\{z\}^{T,i}[K]\{z\}^i} \\ \{a\}^{i+1} &= \{a\}^i + \lambda^i\{z\}^i \end{aligned} \tag{31}$$

and compute the error for each iteration as:

$$e^i = \frac{\|\{a\}^i - \{a\}^i\|_K}{\|\{a\}^i\|_k} = \frac{|\lambda^i| \, \|\{z\}\|_K}{\|\{a\}^i_K\|} \tag{32}$$

If $e^i < \tau$ stop, otherwise reiterate.

5 Error Calculations

The error is defined as

$$
\begin{aligned}
e^N &= \frac{\|u-u^N\|_{A_1(\Omega)}}{\|u\|_{A_1(\Omega)}} \\
\|u\|_{A_1(\Omega)} &= \sqrt{\int_\Omega \frac{du}{dx} A_1 \frac{du}{dx} dx} = \sqrt{\int_\Omega A_1 (\frac{du}{dx})^2 dx} \\
\|u-u^N\|_{A_1(\Omega)} &= \sqrt{\int_\Omega A_1 (\frac{d(u-u^N)}{dx})^2 dx}
\end{aligned} \tag{33}
$$

To compute the error numerically, we calculate the two following quantities element by element, and then assemble them to obtain the overall error:

$$
\begin{aligned}
\|u\|^2_{A_1(x)(\Omega)} &= \int_\Omega A_1(x) (\frac{du}{dx})^2 dx \\
\|u-u^N\|^2_{A_1(x)(\Omega)} &= \int_\Omega A_1(x) (\frac{d(u-u^N)}{dx})^2 dx \\
&= A_1(x) \int_\Omega (\frac{du}{dx} - \frac{du_N}{dx})^2 dx \\
&= A_1(x) \sum_{e=1}^{N_e} \int_{x_e}^{x_{e+1}} (\frac{du}{dx} - \frac{du_N}{dx})^2 dx \\
&= A_1(x) \sum_{e=1}^{N_e} \int_{-1}^{1} (\frac{du}{d\xi} - \frac{du_N}{d\xi})^2 J d\xi
\end{aligned} \tag{34}
$$

6 Potential energy

The potential energy is defined as:

$$
J(u) = \frac{1}{2} B(u,u) - F(u) = \frac{1}{2} \int_\Omega \frac{du}{dx} E \frac{du}{dx} - \int_\Omega f u dx - t u|_{\Gamma t} \tag{35}
$$

7 Results

The numerical solution for N = 100, 1000 and 10000 are plotted in figure

P	Ne_{opt}	$N_{opt} = Ne_{Opt} * P + 1$
1	1348	1349
2	94	189
3	34	103

Table 1: Minimum number of nodes needed for the error criteria

Minimum number of elements and number of nodes to achieve to error criteria for different order of elements are tabulated bellow. N_{Opt} drops dramatically with the order of the elements.

The numerical solution and the analytical solution are compared in figure **??**.

7.1 Relationship between the error and the element size

Error estimate for FEM is:

$$e^N \leq Ch^{\gamma=min(r-1,P)} \tag{36}$$

r is smoothness, and P is the polynomial order.

8 Conclusion

This homework extends the previous one to higher order of element. Having higher order element shape functions can reduce the number of degree of freedom needed for solving the problem by better capturing the fluctuations in the solution.