Finite Elements Project

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Abstract

This is the final project of the course **Numerical Methods**, given at Phelma in the Academic Year 2017/2018. In this project we will study a process of material elaboration involving heating by electrode. We 'll study the steady state of this process. The objective is to model the physical phenomena which take place in this process with *finite element method*.

1 Statement of the Problem

The study configuration is considered cylindrical. A scheme of the study geometry is given in Figure 1: The process is constituted by:

- a cylindrical crucible;
- the elaborated material; the geometry of the study domain occupied by the material is cylindrical;
- 2 electrodes.

The electrodes are in graphite. An electrical potential difference is applied between the top electrode and the bottom electrode included in the crucible: ΔU. This electrical potential difference is *continuous*. An electrical current pass through the material placed in the crucible. We suppose that the contact between the electrodes and elaborated material is perfect. **Joule effect heat the material**. The material of the crucible is an insulating material. The crucible is not model and will be replaced by an adapted boundary condition. Electrical problem has to be solved in the electrodes and in the elaborated material. The heat transfer has to be solved in the material only.

2 Equations of the physical phenomenon and Boundary Conditions

The objective of this part is to present the physical equations of the process in the steady state and boundary conditions. In this process two physical phenomena occur:

- electrical phenomenon;
- thermal phenomenon.

Figure 1: Problem Scheme

2.1 Presentation of the study domain

Describe the study domain. Precise where each phenomenon is solved.

The study domain is the one described in Figure 1, right part.

- We will solve the **thermal problem** only in the material only (yellow part), i.e. where $0.1 < r < 0.3$ and $0 < h < 0.3$.
- We will solve the **electrical problem** in the electrodes and in the elaborated material, i.e. for $0 \geq r < 0.3$ and $0 < h < 0.3$.

2.2 Electrical problem

Give the partial differential equation of the electrical problem. Give the boundary conditions of the electrical problem. Give the expression of the current density and of the Joule power density.

The Electrical problem can be modeled employing the fact that $E = -\nabla U$. We also now that the electrical flux is defined through $\vec{J} \cdot \vec{E}$. Using the fact that the divergence of the Electrical flux is 0 we obtain that:

$$\nabla \cdot (-\sigma \nabla U) = 0.$$

We focus now on the boundary conditions: we know that around the crucible there's insulator material, then we'll have that $\frac{\partial U}{\partial x} = 0$ on the boundary, i.e. $\nabla U \cdot \vec{n} = 0$. We can also take into consideration that ΔU is fixed and so we can write the final system as

$$\begin{cases} \nabla \cdot (-\sigma \nabla U) = 0, & 0 < x < 0.1,\ 0.02 < z < 0.42 \\ \nabla U \cdot \vec{n} = 0, & x \in \partial V \\ U = \Delta U, & 0 < x < 0.02,\ z = 0.4 \\ U = 0, & 0 < x < 0.04,\ z = 0. \end{cases}$$

2.3 Thermal problem

- Give the partial differential equation of the thermal problem.
- Give the boundary conditions of the thermal problem.

The Fourier Law tells us that:

$$q = -k \nabla T \tag{1}$$

where

q local heat flux density,

k material's conductivity,

∇T is the temperature gradient.

From the Gauss-Green theorem we know that

$$\iint_S q(x, y, z)\, dS = Q$$

where the first integral is all over the surface defined by $0.1 < r < 0.3$ and $0 < h < 0.3$ and Q is the heat generated by the Joule effect.

By the way, employing the divergence theorem, the left hand side of the equation can be rewritten as

$$\iiint \nabla \cdot q(x, y, z)\, dx\, dy\, dz = \iint_S q(x, y, z)\, dS$$

and then the following identity holds

$$\iiint \nabla \cdot q(x, y, z)\, dx\, dy\, dz = Q. \tag{2}$$

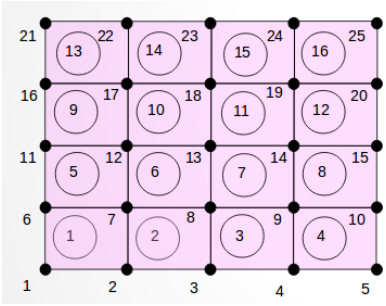

Figure 2: Discretization of the domain.

Using Fourier Law (1) and plugging it into the above equation we obtain

$$\nabla \cdot (-k\nabla T) = Q. \tag{3}$$

The final system of equation will be

$$\begin{cases} \nabla \cdot (-k\nabla T) = Q, \\ -\kappa \nabla T \cdot \vec{n} = h(T - T_r) \end{cases} \tag{4}$$

3 Principle of the Modeling

In this project, in a first step, each equation will be developed and test. In a second step, the model with the two coupling equations will be developed and test. For numerical modeling the finite element method is used. In this project, describe the steps of the calculation and the variables used. Take time to define how you will present your numerical results.

4 Numerical Modeling of Heat Transfer Problem with Finite Elements Method

4.1 Study Domain and Mesh

We want to discretize our domain in the same way described in figure 2.

The variable that we are going to use will be the *length and the height of the domain*, as well as the *number of the point* we want in our discretization.

A simple algorithm that takes care of that could be the one in Listing 1, where we have put in input of our function `mesh` the number of points in which we want to discretize our domain `nx,ny`.

Listing 1: Mesh

```
function [M,N] = points(lx,ly,nx,ny)
% M: matrix of [x,y] components of the point
% N: number of points generated

x=0, y=0; %initialize all the variables to zero
i=1; %set counter
dy=ly/ny; dx=lx/nx;
% use the loops for both x and y
for y=0:dy:ly
    for x=0:dx:lx
        M(i,:)= [x,y]; %save the point
        i=i+1; %update the counter
    end
end
N = i;
end
```

We stress the fact that in `for` loop we take care also of the fact that if the point considered is a boundary

point we have to come back and restart in *another line*.

The algorithm presented in Listing 2 takes care of numbering in a proper way the elements basis and the points we have generated with the alorithm `points`.

Listing 2: Build relationship for local point and overall point

```
function [E] = mesh(lx,ly,nx,ny,M)

for e=1:nx*(ny-1)
    if M(e,1)!=lx
       E(e,:)=(e,e+1,e+nx+1,e+nx);
end
end
```

In Listing **??** we give an algorithm for the mesh of the boundary elements.

Listing 3: Algorithm for boundary elements

```
function [b_Ele,N] = b_elements(lx,ly,nx,ny)
% M: matrix of [x,y] components of the point
% N: number of points generated

x=0, y=0; %initialize all the variables to zero
i=0; %set counter
dy=ly/ny; dx=lx/nx;

% bottom points
while x < lx
    i = i+1;
    b_Ele(i,:) = [i,i+1];
    x = x+dx;
    i = i+1;
end

% right-boundary point
while y < ly
    i = i+1;
    b_Ele(i,:) = [nx*i,(nx+1)*i];
    y = y+dy;
end

% top points
while x > 0
    i = i+1;
    b_Ele(i,:) = [i-1,i];
    x = x-dx;
end
```

4.2 Galerkin's Formulation of Heat Transfer Equation

4.2.1 Projection of the partial differential equation on an element of the basis of the functions α_i

We want to evaluate at this stage the projection of our unknown function T into the element basis β_i, i.e., $\forall i$ we want

$$\iiint_\Omega \beta_i \nabla \cdot (-\kappa \nabla T)\, d\Omega = \iiint_\Omega \beta_i Q\, d\Omega \tag{5}$$

Now we can identify the element basis β_i with the element basis α_i and so we can write

$$\iiint_\Omega \alpha_i \nabla \cdot (-\kappa \nabla T)\, d\Omega = \iiint_\Omega \alpha_i Q\, d\Omega$$

4.2.2 Give the weak formulation of the Galerkin's method. Introduce the boundary conditions in the formulation.

Using the differential identity

$$\nabla \cdot (-\alpha_i)\kappa\nabla T) = -\alpha_i \nabla \cdot (\kappa \nabla T) - \kappa \nabla \alpha_i \nabla T$$

we can plug the above equation into (5) obtaining

$$\iiint_\Omega \nabla \cdot (-\alpha_i)\kappa\nabla T \, d\Omega + \iiint_\Omega \kappa \nabla \alpha_i \nabla T \, d\Omega = \iiint_\Omega \alpha_i Q \, d\Omega$$

By the way, we have, thanks to the divergnece theorem, that

$$\iiint_\Omega \nabla \cdot (-\alpha_i)\kappa\nabla T \, d\Omega = -\iint_\Gamma \alpha_i \kappa \nabla T \cdot \vec{n} \, d\Gamma.$$

Then finally we have the **weak formulation of the problem** (5)

$$\iiint_\Omega \kappa \nabla \alpha_i \nabla T \, d\Omega - \iint_\Gamma \alpha_i \kappa \nabla T \cdot \vec{n} \, d\Gamma = \iiint_\Omega \alpha_i Q \, d\Omega.$$

Introducing the boundary conditions, see (4), we have

$$\begin{cases} -\kappa \nabla T \cdot \vec{n} = h(T - T_r), & \text{on the free surface} \\ -\kappa \nabla T \cdot \vec{n} = 0, & \text{on all the non-free surface} \end{cases}$$

and then

$$\forall i \iint_\Gamma \alpha_i h(T - T_r) \, d\Gamma + \iiint_\Omega \kappa \nabla \alpha_i \nabla T \, d\Omega = \iiint_\Omega \alpha_i Q \, d\Omega \tag{6}$$

4.2.3 Precise the expression of the elementary volume, the elementary surface for respectively the volume integral and surface integral.

The idea is to transform an integral all over the volume Ω in many sums all over the small elements e. The elements must be disjoint pairwise and the union of the small elements e must be give the original volume Ω. In symbols we have

$$\iiint_\Omega [\dots] \, d\Omega = \sum_e \iiint_{\omega_e} [\dots] \, d\Omega_e$$

Similarly we'll have that the integral all over the susface is made up by the sum by the sum of all the small surfaces:

$$\iint_\Gamma [\dots] \, d\Gamma = \sum_f \iint_{\gamma_f} [\dots] \, d\Gamma_f$$

We use the canonical change of variable, from cartesian to cylindrical, i.e.,

$$\begin{aligned} &(x, y, z) \to (r, \theta, z) \\ &(x, y, z) \mapsto (rcos(\theta), rsin(\theta), z) \end{aligned} \tag{7}$$

The change of variable given by Eq.7 gives as determinant of the Jacobian matrix the element r, in such a way that the integration must be performed changing $dx\, dy\, dz$ into $r\, dr\, d\theta\, dz$.

Then we have that

$$2\pi \iint_\Omega \kappa \nabla \alpha_i \nabla T \, r \, dr \, dz - 2\pi \int_\Gamma \alpha_i \kappa \nabla T \cdot \vec{n} \, dz = 2\pi \iint_\Omega \alpha_i Q \, r \, dr \, dz.$$

In particular we will perform this transformation

$$\iint_e f(x, y) \, dx \, dy = \int_{-1}^{1} \int_{-1}^{1} f(x(u, v), y(u, v)) det(Jac) \, du \, dv$$

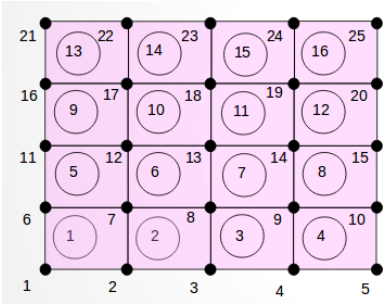

Figure 3: The boundary elements will have 3 boundaries or 2, depending on which one we are considering.

where

$$\begin{cases} x(u,v) = \sum_{i=1}^{N} \alpha_i(u,v) \cdot x_i \\ y(u,v) = \sum_{i=1}^{N} \alpha_i(u,v) \cdot y_i \end{cases} \quad \text{and} \quad \det(Jac) = \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial y}{\partial u} \\ \frac{\partial x}{\partial v} & \frac{\partial y}{\partial v} \end{vmatrix} = \begin{vmatrix} \sum_{i=1}^{N} \frac{\partial \alpha_i(u,v)}{\partial u} \cdot x_i & \sum_{i=1}^{N} \frac{\partial \alpha_i(u,v)}{\partial u} \cdot y_i \\ \sum_{i=1}^{N} \frac{\partial \alpha_i(u,v)}{\partial v} \cdot x_i & \sum_{i=1}^{N} \frac{\partial \alpha_i(u,v)}{\partial v} \cdot y_i \end{vmatrix}$$

and therefore the integral we have to evaluate become a summation with a suitable quadrature formula

$$\iint_e f(x,y)\,dx\,dy = \sum_{i \in \{nodes\}} f(x(u_i,y_i), y(u_i,y_i)) \det(J(u_i,y_i)) w_i$$

4.2.4 Give the expression of the integrals on the reference element

The expression for each element of the basis is then

$$\sum_j \iiint_e \nabla\alpha_i \nabla\alpha_j \xi \, d\xi \, d\eta.$$

Let's notice that we have

$$T = \sum_{j=1}^{N} \alpha_j(\xi,\eta,\zeta) \cdot T_j$$

and so the differential becomes

$$\nabla T = \sum_{j=1}^{N} \nabla\alpha_j(\xi,\eta,\zeta) \cdot T_j$$

where through elementary calculations we can see that

$$\nabla\alpha_j = \left[JacJ\right]^{-1} \begin{bmatrix} \frac{\partial\alpha}{\partial\xi} \\ \frac{\partial\alpha}{\partial\eta} \\ \frac{\partial\alpha}{\partial\zeta} \end{bmatrix}.$$

Then the final expression will be

$$\sum_e \iint_{\omega_e} \kappa\nabla\alpha_i \cdot \left(\sum_{j=1}^{N} \nabla\alpha_j T_j\right) \xi \, d\xi \, d\eta + \sum_f \int_\Gamma \alpha_i h \left(\sum_{j=1}^{N} \alpha_j T_j\right) d\eta = \sum_f \int_\Gamma \alpha_i h T_r \, d\eta + \sum_e \iiint_{\omega_e} \alpha_i Q \, \xi \, d\xi \, d\eta.$$

4.2.5 Detail the expression of the elementary matrix on an element e. Precise the size of each elementary matrix (sub matrix). Precise the expression of each integral and the principle of calculation. For each integral, precise the nature of the element e

The elementary matrix of an element e is given by the inner product $\nabla\alpha_i \nabla\alpha_j$. In particular we'll have a matrix A_{ij}^e in which we will have in position (i,j) the element $\nabla\alpha_i \nabla\alpha_j$.

The matrix A_{ij}^e is a 4×4 matrix, for each inner element. For the outer element it will be a 3×3 or 2×2 depending on the position.

4.3 Algorithm of the Finite Element Formulation of Heat Transfer Equation

The algorithm goes as follows:

- Discretize the domain and build the mesh.
- For each element e of the domain:
  - Construct the Jacobian matrix Jac with the functions α_i
  - Evaluate the Jacobian $\det(Jac)$
  - Evaluate all the 16 terms $\nabla\alpha_i \nabla\alpha_j$ with the help of the Gauss quadrature formula.

In the program we make use of the following functions:

- `jacobian(M, Elem, e)` where `M` is the coordinates matrix and `Elem` is the mesh matrix, while `e` is the global element taken into consideration.
- `alpha(xi,eta)` where `xi,eta` are the local coordinates.
- `update` for updating the global matrix with the 16 values obtained for each element e.
- The functions `points` and `mesh` as already stated in Section 4.1

4.4 Programming and calculation

4.4.1 Construct the program: main program and functions

Listing 4: main program

```
clc; clear all; close all;
% this is the main file

%% discretization of the domain and building of the mesh for the thermal part
% initialization of the variables lx, ly, nx, ny
% THESE VALUES MUST BE CHANGED!
[lx, ly, nx, ny] = [100, 100, 100, 100];

% creation of the points and of the mesh
[M, N_points] = points(lx,ly,nx,ny);
[Elem, N_elements] = mesh(lx,ly,nx,ny,M);
[b_Elem, N_b_elements] = b_elements(lx,ly,nx,ny,M);

%% initialization of the points for the gauss quadrature formula
w=[0.347855 0.652145 0.652145 0.347855];
u=[-0.861136 -0.339981 0.339981 0.861136];

%% creation of the big matrices
% this matrix has to be filled with all the terms of interactions between
% the internal elements
Interaction = zeros(N_points);

% this matrix must bel filled with the terms given by the boundary effects
Bound = zeros(N_points);

%% evaluation of the integral on the variuos elements of the basis
for e = 1:N_elements
    % creation of the Jacobian matrix
    [Jac] = jacobian(M, Elem, e);
    J = det(Jac); %jacobian
    A = zeros(4);
    for i = 1:4
        for j=1:4
            % evaluation of the 4x4 matrix
            % here we will need the gauss points
        end
    end
    % update the global matrix values; it will recollect the global number
```

```
    % from the local number and the element e
    Interaction = update(Interaction, Elem, e, A);

end

for f = 1:N_b_elements
    B = zeros(2);
    for i = 1:2
        for j=1:2
            % evaluation of the 2x2 matrix
            % here we will need the gauss points
        end
    end
    % update the global matrix values; it will recollect the global number
    % from the local number and the element e
    Bound = update(Bound, b_Elem, e, B);
end
```

Where we used the function `jacobian` and `alpha` listed below.

Listing 5: function for the creation of the jacobian matrix for each element

```
function [Jac] = jacobian(M, E, e)
% ———————— INPUT ————————————
% M: matrix of the points with x and y coordinates
% E: matrix of the mesh
% e: global number of the element we're considering
%
% ———————— OUTPUT ————————————
% Jac: 2x2 matrix with the values of the jacobian matrix

% we obtain the x and y coordinates of the points involved
x_i = M(E(e,:),1);
y_i = M(E(e,:),2);
% xi and eta points in which evaluate the functions
xi = [-1, 1, 1, -1];
eta = [-1, -1, 1, 1];

Jac = zeros(2);
for i = 1:4
    [alfa, dalfa_xi, dalfa_eta] = alpha(xi(i),eta(i))
    Jac(1,1) = Jac(1,1) +dalfa_xi(i)*x_i(i):
    Jac(1,2) = Jac(1,1) +dalfa_xi(i)*y_i(i);
    Jac(2,1) = Jac(1,1) +dalfa_eta(i)*x_i(i);
    Jac(2,2) = Jac(1,1) +dalfa_eta(i)*y_i(i);
end
```

Listing 6: Function for the creation of the alpha functions and the derivatives of the latter

```
function [alfa, dalfa_xi, dalfa_eta] = alpha(xi,eta)
% ———————— INPUT ————————————
% xi, eta: nodes in which the function must be evaluated
%
% ———————— OUTPUT ————————————
% alfa:      4x1 vector with the values of the four alfas evaluated at (xi,eta)
% dalfa_xi:  4x1 vector of the partial derivatives of alfas wrt xi evaluated
%            at (xi,eta)
% dalfa_eta: 4x1 vector of the partial derivatives of alfas wrt eta evaluated
%            at (xi,eta)

% alfa functions
alfa(1)=1/4*(1-xi).*(1-eta);
```

```
alfa(2)=1/4*(1+xi).*(1-eta);
alfa(3)=1/4*(1+xi).*(1+eta);
alfa(4)=1/4*(1-xi).*(1+eta);

% evaluation of the derivative respect to u
dalfa_xi(1)=-1/4.*(1-eta);
dalfa_xi(2)=1/4.*(1-eta);
dalfa_xi(3)=1/4.*(1+eta);
dalfa_xi(4)=-1/4.*(1+eta);

% evaluation of the derivative respect to v
dalfa_eta(1)=-1/4.*(1-xi);
dalfa_eta(2)=-1/4.*(1+xi);
dalfa_eta(3)=1/4.*(1+xi);
dalfa_eta(4)=1/4.*(1-xi);

end
```

Listing 7: Function for update the global matrix with the values obtained for the local element e

```
function [M] = update(M, Elements_matrix, e, A)
% --------- INPUT -------------
% Interaction    : matrix to be modified
% Elements_matrix: matrix of the mesh
% e              : number of the global element
% A              : matrix of the local contributions
%
% --------- OUTPUT ------------
% M: Matrix modified


for i=1:4
    for j=1:4
        M(Elements_matrix(e,i),Elements_matrix(e,j)) = M(Elements_matrix(e,i),
            Elements_matrix(e,j))+A(i,j);
    end
end
```

5 Model the Electrical Problem with the Finite Elements Method

5.1 Study Domain and Mesh

Since the domian of interest of the electric problem is larger than the thermal problem, we have to slightly modify our algorithm. We then have the algorithm in Listing 8, where we have put in input of our function `mesh electric` the number of points in which we want to discretize our domain.

Listing 8: Points

```
% point for the electric part
dx=0.01;  dy=0.01;  R=0.1;  L=0.3;
m=R/dx+1; n=L/dy +1;

% bottom electrod
for j=1:(nb-1)
    for i=1:mb
        N=N+1;
        Px(N)=dr*(i-1);
        Py(N)=dz*(j-1);
    end
end
 % material
```

```
for j=1:n1
    for i=1:m
        N=N+1;
        Px(N)=dr*(i-1);
        Py(N)=dz*(j-1)+0.02;
    end
end
No=N;

%top electrod points
for j=2:nt
    for i=1:mt
        N=N+1;
        Px(N)=dr*(i-1);
        Py(N)=dz*(j-1)+0.32;
    end
end
```

Listing 9: Build relationship for local point and overall point

```
% build the mesh for the electrical part
% bottom element
for j=1:(nb-1)
    for i=1:(mb-1)
        e=e+1;
        ele(e,1)=i+mb*(j-1);
        ele(e,2)=i+1+mb*(j-1);
        ele(e,3)=i+1+mb*j;
        ele(e,4)=i+mb*j;
    end
end
Nb=e;
% material element
for j=1:(n1-1)
    for i=1:(m-1)
        e=e+1;
        ele(e,1)=i+m*(j-1)+(nb-1)*mb;
        ele(e,2)=i+1+m*(j-1)+(nb-1)*mb;
        ele(e,3)=i+1+m*j+(nb-1)*mb;
        ele(e,4)=i+m*j+(nb-1)*mb;
    end
end
Nm=e;

for i=1:(mt-1)
    e=e+1;
    ele(e,1)=i+No-m;
    ele(e,2)=i+1+No-m;
    ele(e,3)=i+1+No;
    ele(e,4)=i+No;
end
% top element
for j=2:(nt-1)
    for i=1:(mt-1)
        e=e+1;
        ele(e,1)=i+No+mt*(j-2);
        ele(e,2)=i+1+No+mt*(j-2);
        ele(e,3)=i+1+mt*(j-1)+No;
        ele(e,4)=i+mt*(j-1)+No;
    end
end
```

5.2 Galerkin's Formulation of the Electrical Equation

The projection of the partial differential equation on a basis element is

$$\iiint_{\omega} \alpha_i \nabla \cdot (-\sigma \nabla U)\, d\Omega = 0, \quad \forall i$$

and then the **weak formulation for the electric part** becomes

$$\iiint_{\omega} \sigma \alpha_i \cdot \nabla U\, d\Omega = 0, \quad \forall i. \tag{8}$$

The boundary conditions given can be modelized in the following fashion

$$\begin{cases} U = 0, & \text{on the top of the crucible,} \\ U = U_0, & \text{on the bottom of the crucible,} \\ J \cdot n = 0, & \text{on all the other surfaces.} \end{cases}$$

As before, the elementary element of surface and volume are given by the canonical change of variables, from cartesian to cylindrical, i.e.,

$$\begin{aligned} &(x, y, z) \rightarrow (r, \theta, z) \\ &(x, y, z) \mapsto (rcos(\theta), rsin(\theta), z) \end{aligned} \tag{9}$$

The change of variable given by Eq.9 gives as determinant of the Jacobian matrix the element r, in such a way that the integration must be performed changing $dx\, dy\, dz$ into $r\, dr\, d\theta\, dz$.

The second change of variables will be

$$\begin{aligned} &(r, \theta, z) \rightarrow (\xi, \eta) \\ &(r, \theta, z) \mapsto (\xi(r, z), \eta(r, z) \end{aligned} \tag{10}$$

and we will have $dxdydz = det(Jac)d\xi d\eta$.