GLOBAL FINAL EXAM

The use of computer is necessary. The solution of the problems has to be a unique file (pdf, word or something similar). The file has to include the solution, the codes used and the necessary explanations.

BLOCK 1

The natural logarithm function of a square matrix **A**, $\mathbf{F}(\mathbf{A}) = \log(\mathbf{I}+\mathbf{A})$, can be obtained by a Taylor expansion

$$\mathbf{F}(\mathbf{A}) = \log(\mathbf{I}+\mathbf{A}) = \sum_{n=1}^{\infty} \frac{1}{n}(-1)^{n+1}\mathbf{A}^n. \tag{1}$$

The series converges if $\|\mathbf{A}\| < 1$.

1. Implement a matlab function that for any square matrix **A** computes the matrix $\mathbf{F}(\mathbf{A})$ using the Taylor expansion.
   - The **inputs** have to be the matrix **A** and the tolerance (maximum error allowed for the truncation of the series)
   - The **outputs** have to be the value of the function $\mathbf{F}(\mathbf{A})$ and the number of iterations needed to achieve that tolerance
2. Use the function with the matrices, `A1=[0.1 0 0 ; 0 0.1 0; 0 0 0.1]` and `A2=[0.1 0.1 0.1; 0 0.1 0.1;0 0 0.1]` using a tolerance `tol=1E-16` and comment the results
3. Define a random matrix of size 3x3 and apply the function. Comment the results

iterations needed to achieve that tolerance

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BLOCK 1

1. The function is

```
function [Y n]=log1X(X,toler)
 error=1.;
 [nn nm]=size(X);
 Xn=eye(nn);
 Y=zeros(nn);
 n=0;
 while(error>toler)
  n=n+1;
  Xn=Xn*X;
  term=Xn*((-1)^(n+1))/n;
  Y=Y+term;
  error=norm(term);
 end
end
```

2. For matrix A1: [sol iter]=log1X([0.1 0 0;0 0.1 0;0 0 0.1],1E-6) and the solution takes 6 iterations and the matrix sol= [0.0953102 0 0; 0 0.0953102 0; 0 0 0.0953102]
   For the matrix A2: [sol iter]=log1X([0.1 0.1 0.1;0 0.1 0.1;0 0 0.1],1E-6) and the solution takes 7 iterations and the matrix sol= [0.0953102 0.0909091 0.0867769; 0 0.0953102 0.0909091; 0 0 0.0953102]
   Note that the first solution is equal to the logarithm of the diagonal terms [log(1.1) 0 0;0 log(1.1) 0;0 0 log(1.1)] while in the second case no.

3. Depending on the matrix it might work or not. If the norm(A) is less than 1 then it will converge, otherwise the algorithm will never stop or give an error.

BLOCK 2

The rate of a chemical reaction depends on the stoichiometric coefficients and the concentration of reactants. For instance, in a reaction such as

$3A + 2B \xrightarrow{k} C$, the rate would be $r = k[A]^3[B]^2$, where k is a constant.
The reaction of I_2 with H_2 in gas phase takes place as a chain reaction:

i) $I_2 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2I$

ii) $H_2 + 2I \xrightarrow{k_3} 2\ HI$

- Devise a Kinetic Monte Carlo algorithm to simulate this chain reaction
- Write below each event with its rate
- Run the code up to t= 0.03 s and plot the time evolution of all concentrations
- Calculate $[I_2]/[HI]$ for t=0.01 s and t=0.02 s
- Interpret and comment the results

Data
Initial concentrations: $[I_2] = 24000$, $[H_2] = 20000$, $[I] = 0$, $[HI] = 3000$
Constants: $k_1 = 100.0$, $k_2 = 200.0$, $k_3 = 1.0$

Do not forget to provide a copy of your code. Make sure that it is correctly indented.

- Interpret and comment the results

Data

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We can distinguish in this problem three events:

① $I_2 \rightarrow 2I$ (decomposition of the molecule into 2 atoms, with a constant k_1)

② $2I \rightarrow I_2$ (recombination of two atoms, with a constant k_2)

③ $H_2 + 2I \rightarrow 2HI$ (reaction of iodine atoms with a hydrogen molecule. Constant: k_3)

Each event is characterised by its rate:

① $r_1 = k_1[I_2]$; $k_1 = 100.0$

② $r_2 = k_2[I]^2$; $k_2 = 200.0$

③ $r_3 = k_3[H_2][I]^2$; $k_3 = 1.0$

Initial conditions:

$[I_2] = 24000$

$[H_2] = 20000$

$[I] = 0$

$[HI] = 3000$

Final time: 0.035

This data are to be inserted in a code such as 'nucllardecay.m'

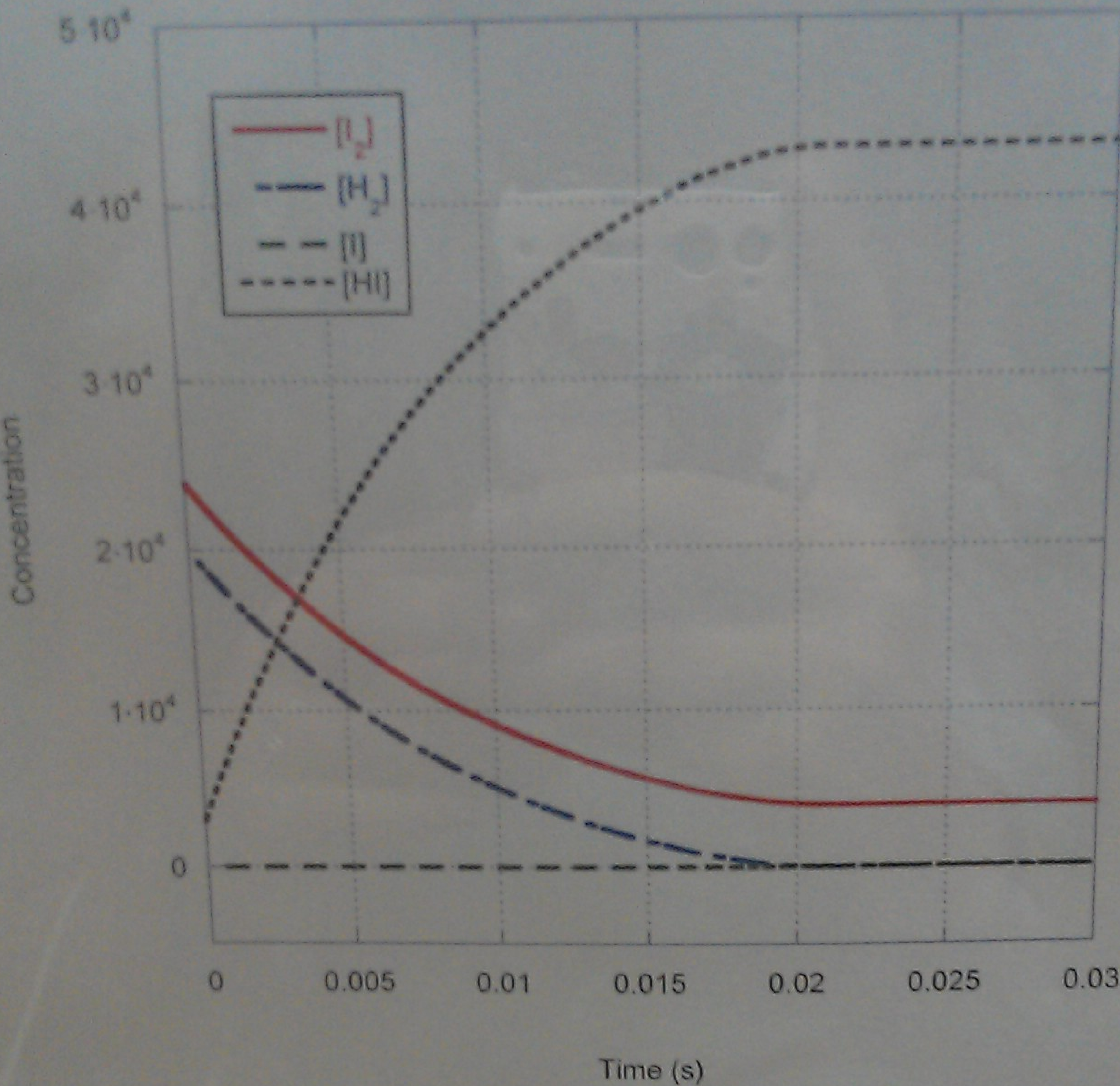
Don't forget to write the results to a file (e.g. 'concentrations.txt')

From the results:

$t = 0.01s \rightarrow \frac{[I_2]}{[HI]} \simeq \frac{9100}{32800} = 0,28$

$t = 0.02s \rightarrow \frac{[I_2]}{[HI]} \simeq \frac{4050}{42850} = 0,09$

[HI] 42850



Comment:

The concentration of both I_2 and H_2 molecules decreases exponentially with time, whereas the final product, HI, increases steadily. The high rate of the second reaction keeps the concentration of atomic iodine at very low levels. Finally, when molecular hydrogen gets exhausted, reaction 3 stops and the system reaches equilibrium.

BLOCK 3

A beam of length=5m, and a square section of 0.5x0.5m is fixed at both ends has to be dimensioned using a Finite Element model. The global force applied is 2MN homogeneously distributed in the upper surface of the beam (5×0.5 m^2). The finite element geometry definition is given in the FE code `FEM_planestress2D4N_exam`. The material of the beam is steal with $E = 200$GPa, $\nu = 0.2$ and yield stress $\sigma_Y = 200$MPa.

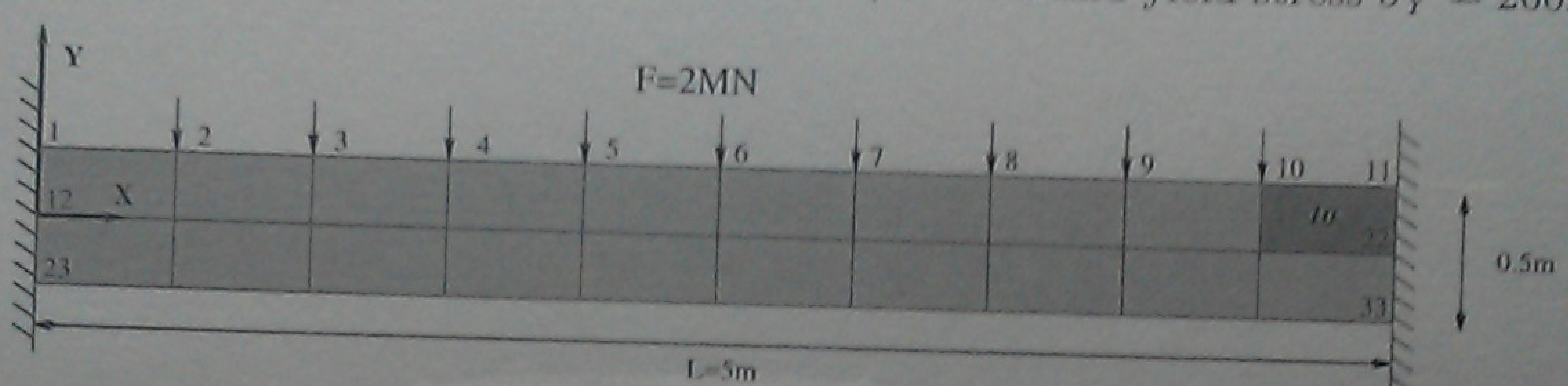


Figure 1: Double fixed beam with dimensions, coordinate systems and node definitions for boundary conditions. Element 10 is also highlighted

Complete the next points

1. Complete the FE code `FEM_planestress2D4N_exam` including boundary conditions and applied loads.
2. Plot the deformed mesh using the function `plot_deformed_2DMESH_mats.m` with a magnification of 10.
3. Compute the maximum deflection of the beam
4. The maximum stresses are located at the lower and upper edges of the fixed sections of the beam. Compute the stress tensor at one of those points, use for example $X = 5., Y = 0.25$ located at element 10
5. Obtain the horizontal and vertical reactions on the left fixed end.
6. The maximum stress in horizontal direction σ_{xx} (see point 4) is used to dimension the beam with a security factor of 1.3. Does the beam fulfills the design? If not, which is the maximum load that can be applied? (remember the problem is linear)

HELP:

- (3) and (5) For computing nodal forces or displacements, the global degrees of freedom that correspond to a given node of number n are $u_x = 2n-1$ and $u_y = 2n$.
- (4) and (6) To extract the stresses on an element use the function `element_output_xy.m` that computes the stresses at a given point of an element, defined by its natural coordinates $[\xi, \eta]$.
- (5) To compute the reactions, calculate the sum of the horizontal and vertical reactions of all the nodes on that fix end.

BLOCK 3:
The global load is 2MN on a surface 5x0.5. This load is distributed in the thickness F/e=2E6 N/0.5 m= 4E6 N/m and in 9 nodes (2,3,4,5,6,7,8,9,10)
being the nodal for

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1. The modified parts of the code are here:

```
%% HERE DEFINE elementMat
for ielem=1:numelements
  elementMat(ielem)=1
end

%% HERE DEFINE propMatlist
propMatlist(1).E=[200E9]
propMatlist(1).nu=[.2]

%% HERE ONLY BOUNDARY CONDITIONS=0  ARE DEFINED, ADD IMPOSED
DISPLACEMENTS OR LOADS
fkg=2e6
f=-(fkg/.5)/9
prescribedDispNodes=[1;1;12;12;23;23;11;11;22;22;33;33];
prescribedDispDof=[1;2;1;2;1;2;1;2;1;2;1;2];
prescribedForcNodes=[2;3;4;5;6;7;8;9;10]
prescribedForcDof=[2;2;2;2;2;2;2;2;2]

% 0.5.2 Applied Forces and displacements
forces=[f;f;f;f;f;f;f;f;f]
displacements =[0;0;0;0;0;0;0;0;0;0;0;0];
```

2. The deformed plot is obtained using the function given in the exam:

```
plot_deformed_2DMESH_mats(nodeCoordinates,elementNodes,displacement,10.,e
lementMat)
```

   where the deflection is pretty small but the symmetry of the deformation can be observed.

3. The maximum deflection is the vertical displacement of the central node (6), the corresponding global d.o.f is 6x2, so it is obtained using displacement(12)

```
Y=displacement(12)=-5.3112E-4
```

   Corresponding to 0.531 mm

4. To obtain the value of stresses at the point x=5, y=0.25 element 10 is selected and the function element_output_xy is used. The value of the natural coordinates of the element 10 where stresses should be obtained are xi=1, nu=1. This is because the element connectivity is 21 22 11 10 and in this case xi=1, nu=1 corresponds to the 3rd node (11), located at

4. To obtain the value of stresses at the point x=5, y=0.25 element 10 is selected and the function element_output_xy is used. The value of the natural coordinates of the element 10 where stresses should be obtained are xi=1, nu=1. This is because the element connectivity is 21 22 11 10 and in this case xi=1, nu=1 corresponds to the 3[rd] node (11), located at the position where stresses are asked (x=5,y=0.25).

```
element_output_xy(10,nodeCoordinates,elementNodes,displacement,propMat,
[ 1 1])
```

the output is the position in real space (5,0.25) and the strain and stress values, being the stress tensor terms sigma_x=23.10MPa; sigma_y=4.62MPa; tau=13.61MPa

5. The reactions can be obtained as the sum of the reaction forces of encastred nodes. If left side is chosen then the forces are the ones corresponding to nodes 1, 12 and 23. The horizontal forces are the sum of `force(1*2-1)+force(12*2-1)+force(23*2-1)`=4.1538E4 N/m. It can be observed that the corresponding values on the right side (nodes 11,22,33) have the same horizontal reaction with negative sign: `force(11*2-1)+force(22*2-1)+force(33*2-1)`=-4.1538E4 N/m. The vertical reactions in the left are the sum of `force(1*2)+force(12*2)+force(23*2)`=2E6 N, exactly the half of the total load F=4E6 N/m

6. Because 1.3*sigma_x=30.03 MPa < 200 MPa, so the beam fulfills the design requierements.