Finite Elements for Fluids

Final Assignment

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Introduction

Actin plays an important role in cells motility. Lately, different models have been proposed to predict the concentration of actin monomers and filaments and their interaction with the mechanics of cell cortex and cytosol. Here, we will try to solve a simplified model for density of actin filaments and monomers coupled with the cortex's mechanics.

In this assignment we have 3 main problems that will have to be treated differently. In a first instance we have a Transport problem; this one will be treated as an Unsteady Convection in 2D. The second part of the assignment is a Stokes problem; in this case we are going to use the code Stokes provided and adapt the boundary conditions and parameters to our case. Finally, a coupled problem is proposed to account for the interaction of the actin filaments and the cortex.

The domain considered for this problem is the following:

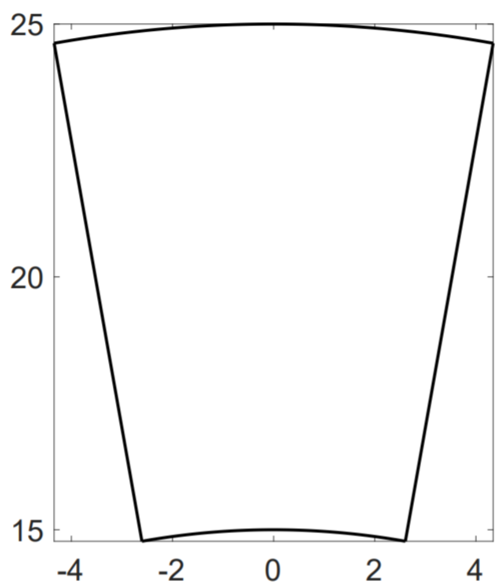


Figure 1 Proposed domain

Transport Problem

In this first problem, we have the actin filaments and monomers densities (F and G) that are modeled by the following equations:

$$\begin{cases} \dfrac{\partial F}{\partial t} = -\boldsymbol{u} \cdot \boldsymbol{\nabla} F + D_F \nabla^2 F - \sigma_F F & \text{in } (0, T) \times \Omega \\ \dfrac{\partial G}{\partial t} = D_G \nabla^2 G - \sigma_G G + \hat{\sigma}_{GF} F & \text{in } (0, T) \times \Omega \end{cases}$$

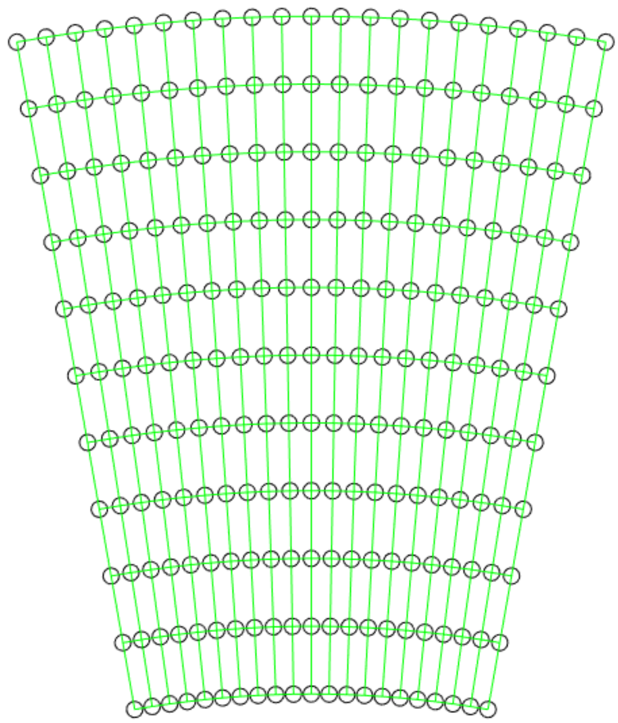
and the material parameters along the problem are:

$$D_F = 5\ \mu\text{m/s} \qquad \sigma_F = 0.25\ \text{s}^{-1}$$
$$D_G = 15\ \mu\text{m/s} \quad \sigma_G = 2\ \text{s}^{-1} \qquad \hat{\sigma}_{GF} = 0.5\ \text{s}^{-1}$$

And we will consider a velocity field u(x, y) = −1/1500 (rx, ry) µm/s, where (x, y) are the points coordinates and r = p x 2 + y 2.
To solve this problem, we can use part of the code used during the course from the 2D Unsteady Convection Diffusion.

Mesh

The mesh selected for this problem is formed by 20x10 quadrilateral elements in the vertical and horizontal direction respectively as seen in the figure below:



Time Discretization (Crank Nicolson, theta family)

In this part we are going to develop the time discretization of the equation given by the statement. As we wanted a good accuracy for the problem and a scheme that was always stable, we chose and implicit 2nd order discretization scheme from the theta family: Crank Nicolson (theta=0.5).

$$\frac{\Delta F}{\Delta t}+0.5\left[\underline{u}\cdot\underline{\nabla}-D_F\nabla^2+\sigma_F\right]\Delta F=-\left[\underline{u}\cdot\underline{\nabla}-D_F\nabla^2+\sigma_F\right]F^n$$

Once we have discretized in time for F, we do the same exact thing for G such as:

$$\frac{\Delta G}{\Delta t}+0.5\left[-D_G\nabla^2+\sigma_G\right]\Delta G-0.5\sigma_{FG}\Delta F=-\left[-D_G\nabla^2+\sigma_G\right]G^n+\sigma_{FG}F^n$$

As we can see above, the time discretization for both equations using Crank Nicolson is done, the next stage is apply a spatial discretization.

Spatial Discretization (Galerkin)

The following formulas show the equation after applying the time and space discretization cited above. As we can see, we are going to define

$$(w,\sigma_F\Delta F)=\sigma_F\int_{\Omega} w\Delta F d\Omega$$

$$c(\underline{u};w,\Delta F)=\int_{\Omega^e} w(\underline{u}\cdot\underline{\nabla}\Delta F)d\Omega$$

$$a(w,D_F\,\Delta F)=D_F\int_{\Omega^e}\underline{\nabla}w\cdot\underline{\nabla}\Delta F d\Omega$$

So, the equations have taken the following look:

$$(w,\frac{\Delta F}{\Delta t})+0.5\left[c(\underline{u};w,\Delta F)+a(w,D_F\,\Delta F)+(w,\sigma_F\Delta F)\right]=-\left[c(\underline{u};w,F^n)+a(w,D_F\,F^n)+(w,\sigma_F F^n)\right]$$

$$(w,\frac{\Delta G}{\Delta t})+0.5\left[a(w,D_G\,\Delta G)+(w,\sigma_G\Delta G)\right]+0.5(w,\sigma_{FG}\Delta F)=-\left[a(w,D_G\,G^n)+(w,\sigma_G G^n)\right]+(w,\sigma_{FG}F^n)$$

The next step is using the shape functions in order to construct the system of equations that wil be solved with MATLAB. We obtain the following equations:

$$\frac{1}{\Delta t}\overline{M}\Delta F+0.5\left[\overline{C}+D_F\overline{K}+\sigma_F\overline{M}\right]\Delta F=-\left[\overline{C}+D_F\overline{K}+\sigma_F\overline{M}\right]F^n$$

$$\frac{1}{\Delta t}\overline{M}\Delta G+0.5\left[D_G\overline{K}+\sigma_G\overline{M}\right]\Delta F+0.5\sigma_{FG}\Delta F=-\left[D_G\overline{K}+\sigma_G\overline{M}\right]G^n-\sigma_{FG}F^n$$

Taking into consideration that:

$$\overline{M}=\sum_e\int_{\Omega^e}N^T N d\Omega$$

$$\overline{C}=\sum_e\int_{\Omega^e}N^T(\underline{u}\cdot\underline{\nabla}N)d\Omega$$

$$\overline{K}=\sum_e\int_{\Omega^e}\underline{\nabla}N^T\cdot\underline{\nabla}N d\Omega$$

As we can see, the problem is all set and ready to code and solve.

MATLAB Analysis

In this part we are going to analyse the different results obtained after solving for F and G. The parameters used for this computation are the following:

- Number of Time-steps: 150
- Total Time: 10s
- $\Delta t = 0.06667$ s

The MATLAB function surf was used to plot the densities F and G as we can see right below:

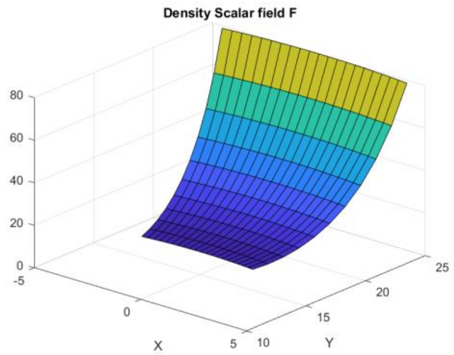


Figure 2 Density Scalar field F

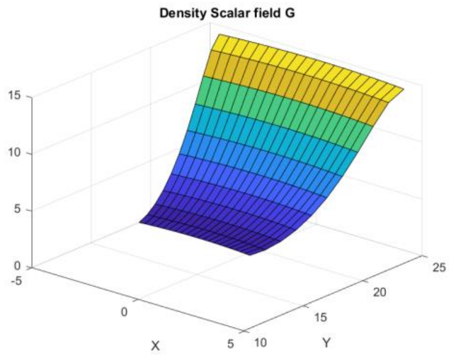


Figure 3 Density Scalar field G

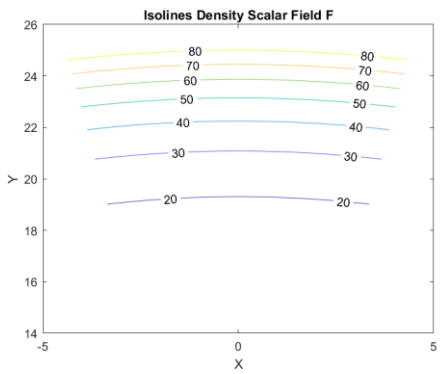


Figure 4 Isolines Density Scalar Field F

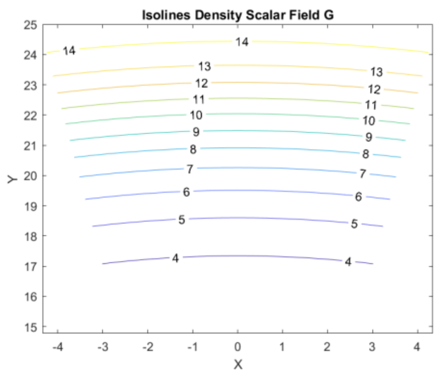


Figure 5 Isolines Density Scalar Field G

As we can see above in figure 4, the boundary conditions (Dirichlet B.C.) applied on the upper boundary show that the density is the same along the border. This is due to the imposition of a constant density (80) along the computation.

We want to know at what moment in time the densities reach the steady regime. To do this, we are going to follow 2 nodes during the computation.

The figure right below shows the density evolution in time of 2 nodes from the mesh. We see that the F density reaches the steady regime before G due to the big difference in the diffusion coefficient of both densities. F reaches stability before since is diffusion velocity is lower (0.25) compared to the diffusion velocity of G (2). The reason behind this is due to the difference of dimensions of both components (Actin filaments and monomers).

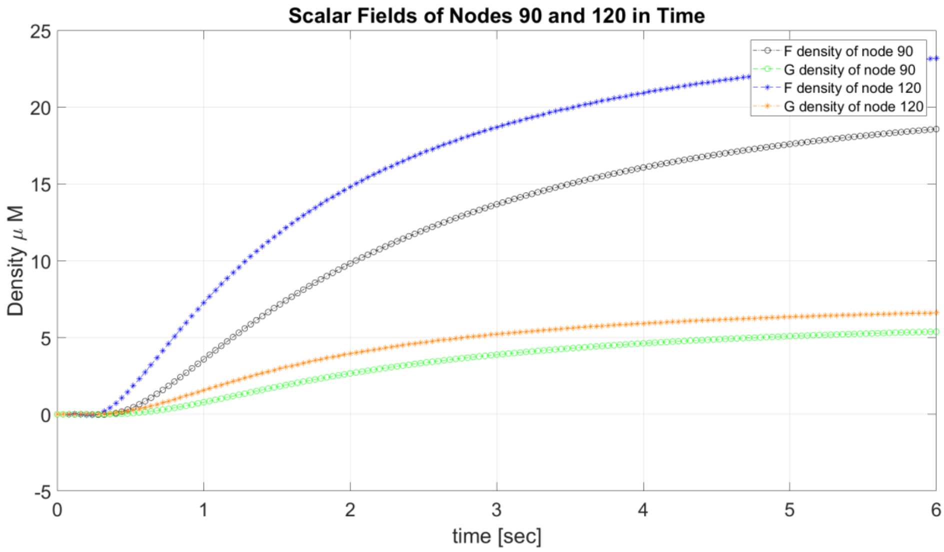


Figure 6 Scalar Field of Nodes 90 and 120 in Time

Stokes Problem

In this part of the assignment we are going to solve the following equation:

$$\begin{cases} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \mathbf{0} & \text{in } \Omega \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 & \text{in } \Omega \end{cases}$$

The velocities are prescribed at r=15 and r=25 such as:

$$u_r(r=15) = -0.15, \; u_\theta(r=15) = 0$$
$$u_r(r=25) = -0.30, \; u_\theta(r=25) = 0$$

We will also consider zero traction of the straight sides of the boundary as well as the following viscosity:

$$\nu = 10^3 \text{ pN} \cdot \text{s}/\mu\text{m}$$

Mesh

For this problem, we are going to use a Q2Q1 mesh with 20x10 elements in the vertical and horizontal directions respectively such as:

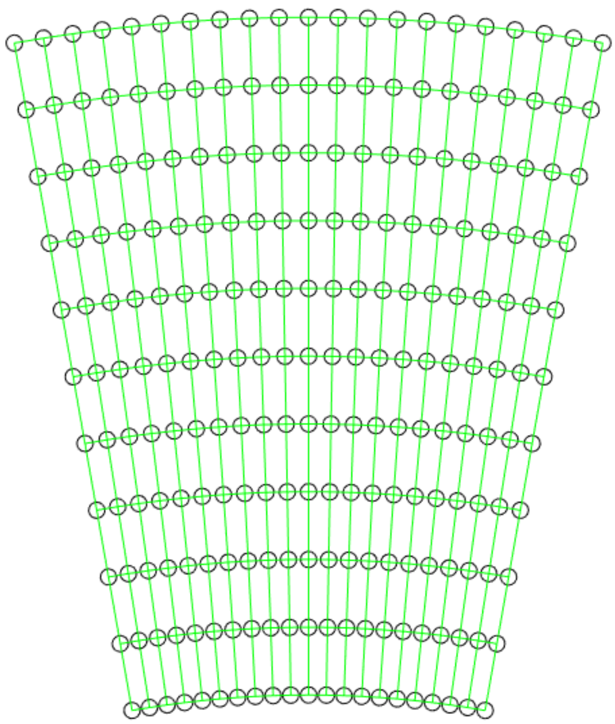


Figure 7 Mesh Q2Q1 Stokes

The difference with the mesh used in the previous part is the central node. The reason why this mesh was chosen is because it had to meet the LBB condition.

Time and spatial Discretization

In order to be able to solve the problem we are going to express the equation such as:

$$\underline{\nabla} \cdot (\underline{\underline{S}}(\underline{v})) - \underline{\nabla} p = \underline{0}$$

This is necessary because we will need to have the equation in terms of the velocity and pressure. To do so, the Stokes' Law has been applied:

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + \underline{\underline{S}}(\underline{v})$$

$\underline{S}(\underline{v})$ being the deviatoric part of sigma.

Once this is done, we can integrate by parts and apply the divergence theorem. The weak form of the problem reads:

$$\begin{aligned} &a(\underline{w},\underline{u}) + b(\underline{w},p) = \underline{0} \\ &b(\underline{u},q) = 0 \end{aligned}$$

Taking a($\underline{w}$,$\underline{u}$) and b($\underline{w}$,p) as:

$$a(\underline{w},\underline{u}) = \int_{\Omega} \underline{\nabla}\underline{w} : \underline{\underline{\underline{\underline{C}}}}_{\upsilon} : \underline{\nabla}\underline{u}\, d\Omega$$

$$b(\underline{w},p) = -\int_{\Omega} p \underline{\nabla} \cdot \underline{w}\, d\Omega \;\text{ and }\; b(q,\underline{u}) = -\int_{\Omega} q \underline{\nabla} \cdot \underline{u}\, d\Omega$$

The next step is applying Galerkin. The goal is find $\underline{u}^h \in V^h$ and $p^h \in Q^h$.

$$\begin{aligned} &a(\underline{w}^h,\underline{u}^h) + b(\underline{w}^h,p^h) = \underline{0} \\ &b(\underline{u}^h,q^h) = 0 \end{aligned}$$

Now it's time to use the Shape functions and place our problem as the following system of equations:

$$\begin{matrix} K & G \\ G^T & 0 \end{matrix} \quad \begin{matrix} u \\ p \end{matrix} = \begin{matrix} 0 \\ 0 \end{matrix}$$

Using:

$$K = \sum_e \int_{\Omega^e} B^T C_{\upsilon} B\, d\Omega$$

$$G = -\sum_e \int_{\Omega^e} N_p^{\,T} (\underline{\nabla} \cdot \underline{N})\, d\Omega$$

$$G^T = -\sum_e \int_{\Omega^e} N_q^{\,T} (\underline{\nabla} \cdot \underline{N})\, d\Omega$$

MATLAB Analysis

In this part we are going to analyze the results obtained using MATLAB. We have computed the pressure and velocity fields as well as the components of the X and Y velocities in different plots to see how they behave.

In the figures below we can see both the velocity and pressure fields. As it is remarkable, the velocity field shows the direction of the velocity on each node of the mesh. This was done using "quiver" in MATLAB.

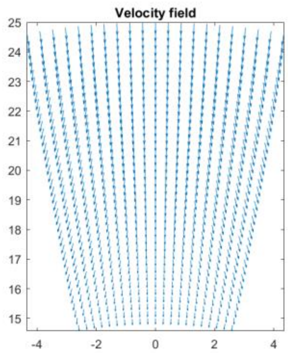


Figure 8 velocity Field

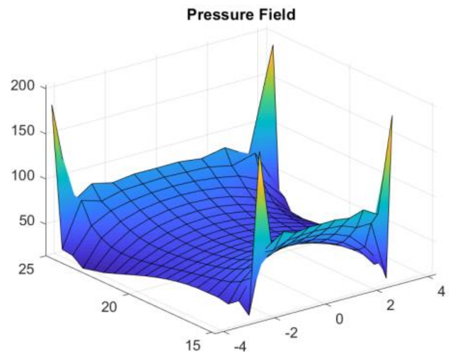


Figure 9 Pressure Field

As we can see above, the pressure field shows 4 horns on the corners which coincide with the boundaries. Since the imposed boundary conditions and problem statement is in agreement with the zero pressure on the sides and high pressure on the corners, the plot shown above looks this way. A low pressure level is observed throughout the domain.

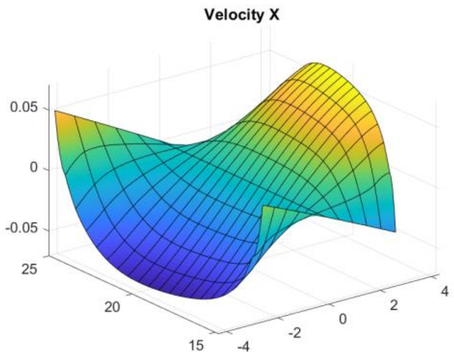


Figure 10 Velocity X

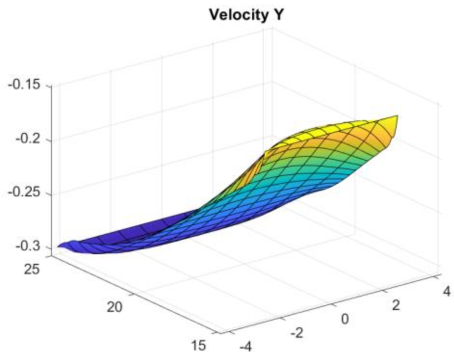


Figure 11 Velocity Y

As we can see in the figures below, the velocities in the X and Y components are in agreement with the BC, since the velocities are prescribed in the lower boundary as 0.15 and 0.3 in the upper, we can perfectly see in the right plot (Velocity Y) that the statement is satisfied.

Coupled Problem

The equation describing the evolution of monomers densities G does not involve any convective transport and, therefore, only the fluid around the fibers has to be considered.
This fluid is modeled using the equations of a quasi-steady viscous fluid. Moreover, due to the presence of actin fibers, the incompressibility constrain is dropped and pressure is neglected. Then, the equations governing the coupled problem can be written as:

$$\begin{cases} \nu \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}^s \boldsymbol{u}) + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_m(F) + \mathbf{T}_m(\boldsymbol{u}) = \mathbf{0} & \text{in } (0,T) \times \Omega \\ \dfrac{\partial F}{\partial t} = -\boldsymbol{u} \cdot \boldsymbol{\nabla} F + D_F \nabla^2 F - \sigma_F F & \text{in } (0,T) \times \Omega \\ \dfrac{\partial G}{\partial t} = D_G \nabla^2 G - \sigma_G G + \hat{\sigma}_{GF} F & \text{in } (0,T) \times \Omega \end{cases}$$

Where $\nabla \cdot \sigma_m$ and T_m are surface forces on the leading edge.

The boundary conditions for this problem will be the same as the ones we had in the first problem. Those are:

$$D_F = 5\ \mu\text{m/s} \qquad \sigma_F = 0.25\ \text{s}^{-1}$$

$$D_G = 15\ \mu\text{m/s} \quad \sigma_G = 2\ \text{s}^{-1} \qquad \hat{\sigma}_{GF} = 0.5\ \text{s}^{-1}$$

And we will consider a velocity field u(x, y) = −1/1500 (rx, ry) µm/s, where (x, y) are the points coordinates and r = p x 2 + y 2.

Mesh

The mesh used for this problem is the exact same as the one used in the first problem. Linear quadrilateral elements ranged as 20x10 in the vertical and horizontal direction such as:

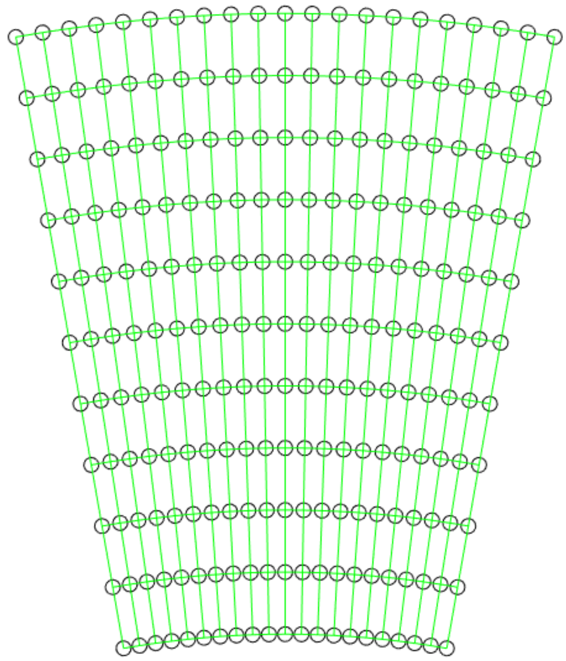


Figure 12 Mesh

Time Discretization (Crank Nicolson, theta family)

In this part we are going to develop the time discretization of the equation given by the statement. As we wanted a good accuracy for the problem and a scheme that was always stable, we chose and implicit 2nd order discretization scheme from the theta family: Crank Nicolson (theta=0.5).

The first equation is going to take the following look:

$$\frac{\Delta F}{\Delta t}+0.5\left[\underline{u}\cdot\underline{\nabla}-D_F\nabla^2+\sigma_F\right]\Delta F=-\left[\underline{u}\cdot\underline{\nabla}-D_F\nabla^2+\sigma_F\right]F^n$$

We do the exact same for the second equation and we obtain:

$$\frac{\Delta G}{\Delta t}+0.5\left[-D_G\nabla^2+\sigma_G\right]\Delta G-0.5\sigma_{FG}\Delta F=-\left[-D_G\nabla^2+\sigma_G\right]G^n+\sigma_{FG}F^n$$

Spatial Discretization (Galerkin)

In order to obtain the weak form by using Galerkin weighted residuals we will need to multiply all the terms by a weighting function w and integrate the terms.

$$\left(\underline{w}, \upsilon\underline{\nabla}\cdot\left(\underline{\nabla}^{s}\underline{u}\right)\right)+\left(\underline{w}, \underline{\nabla}\cdot\underline{\underline{\sigma_m}}(F)\right)+\left(\underline{w}, T_m(\underline{u})\right)=0$$

We will need to integrate by parts as well as apply the Divergence's theorem.
After doing so, we obtain the following equation which is the weak form of the problem:

$$a(\underline{\nabla}\underline{w}, \upsilon\underline{\nabla}^{s}\underline{u})+\left(\underline{w}, \underline{\nabla}\cdot\underline{\underline{\sigma_m}}(F)\right)+\left(\underline{w}, T_m(\underline{u})\right)=0$$

The next step will be computing the following system of equations(knowing that T_f and T_u come from the discretization of $(\underline{w}, T_m(\underline{u}))$ + $(\underline{w}, \underline{\nabla}\cdot\underline{\sigma_m}(F))$:

$$\overline{K}u+\overline{T_f}F+\overline{T_u}u=0$$

Taking:

$$\frac{1}{\Delta t}\overline{M}\Delta F+0.5\left[\overline{C}+D_F\overline{K}+\sigma_F\overline{M}\right]\Delta F=-\left[\overline{C}+D_F\overline{K}+\sigma_F\overline{M}\right]F^{n}$$

For the first equation and

$$\frac{1}{\Delta t}\overline{M}\Delta G+0.5\left[D_G\overline{K}+\sigma_G\overline{M}\right]\Delta F+0.5\sigma_{FG}\Delta F=-\left[D_G\overline{K}+\sigma_G\overline{M}\right]G^{n}-\sigma_{FG}F^{n}$$

for the second one.

MATLAB Analysis

In this part we are going to analyze the results obtained after coding in MATLAB.
As we can see below, we can see represented the F and G densities scalar fields, as it is not unusual, their plots look alike the ones obtained in the first Transport Problem.

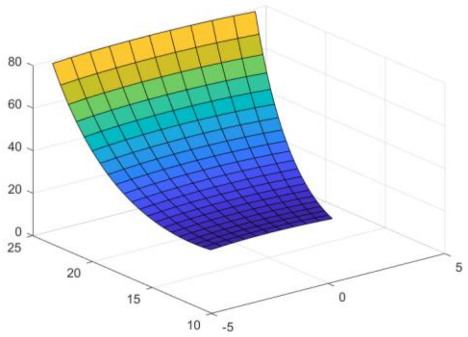


Figure 13 Density Scalar Field F

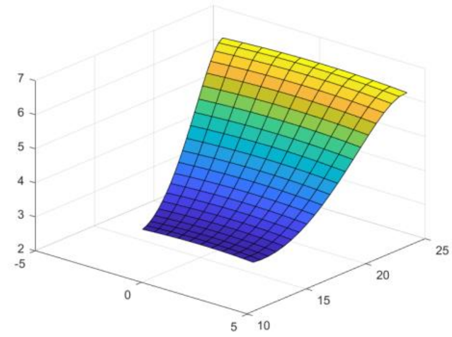


Figure 14 Density Scalar Field G

Since the diffusion coefficients haven't changed from the Transport Problem the F densities go to steady regime long after G, since the coefficients are very different. (0.25 and 2 respectively).

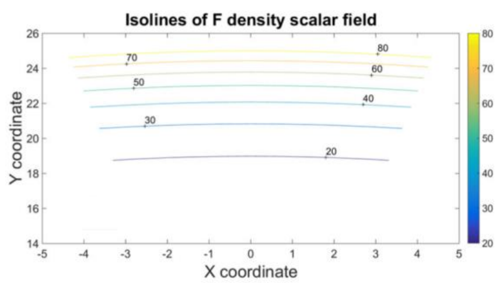


Figure 15 Isolines Density Scalar Field F

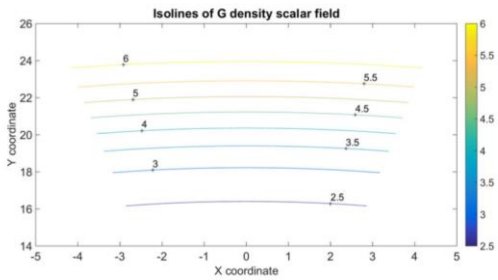


Figure 16 Isolines Density Scalar Field G

If we take a look at the isolines of F and G we see that what they show is similar at the ones we had in the 1st problem. Since the density is prescribed at the boundary, at the upper part it is constant. We still see the difference between the diffusion velocities.

We can also point out that since the boundary conditions are applied on the upper border, for the velocity following the Y component, a big jump occurs due to the change of values of the velocities in the nodes which are constrained to the BC. Once the velocity is computed in the following nodes, the velocity takes a much different form as we can see right below. The same thing happens for the velocity in the X component.

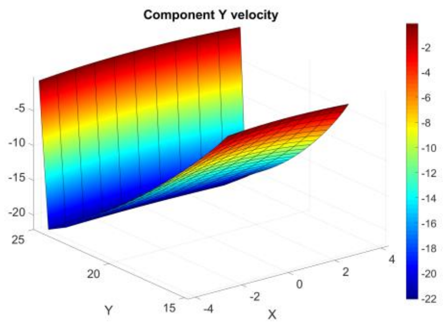


Figure 17 Vel Y

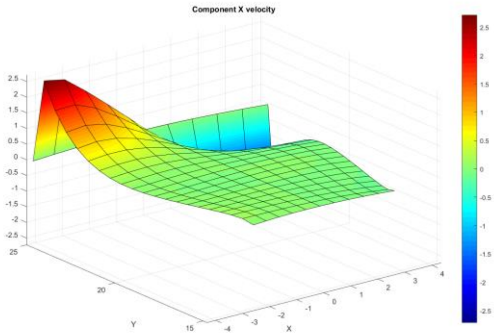
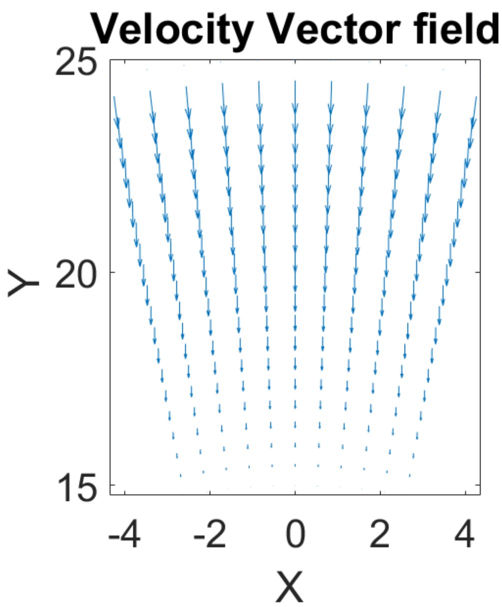


Figure 18 Vel X

Finally, we can appreciate how the velocity vector field looks alike the first problem, however, we need to point out that the velocity follows at all moments the direction of the radius.



Conclusion

In this assignment we had the opportunity to work on the different concepts taught during the semester, as well as, practicing on the different codes provided.
The major problem found during this assignment was coding the last part of the exercise, since the coupled problem was the most complicated thing to understand in the whole process.