Finite Element in Fluids

Final Assignment

By

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Master in numerical method in engineering

1. 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.

2. Goal

Here, we will try to solve a simplified model for density of actin filaments and monomers coupled with the cortex's mechanics. First, we will propose to solve a transport problem to obtain the actin densities. Then, we solve a Stokes problem to obtain the velocity and pressure distribution of the fluid surrounding the actin filaments and monomers. Finally, a coupled problem is proposed to account for the interaction of the actin filaments and the cortex.

3. Domain

All problems will be solved in the domain Ω shown in the figure below.

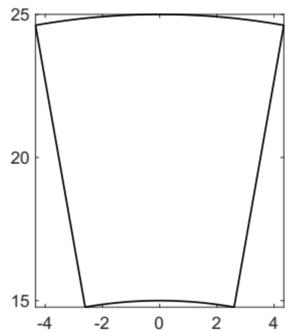

Figure 1: Domain.

4. Meshes

In ***Figure 2*** can be observed the different meshes used for the different problems to be solved.

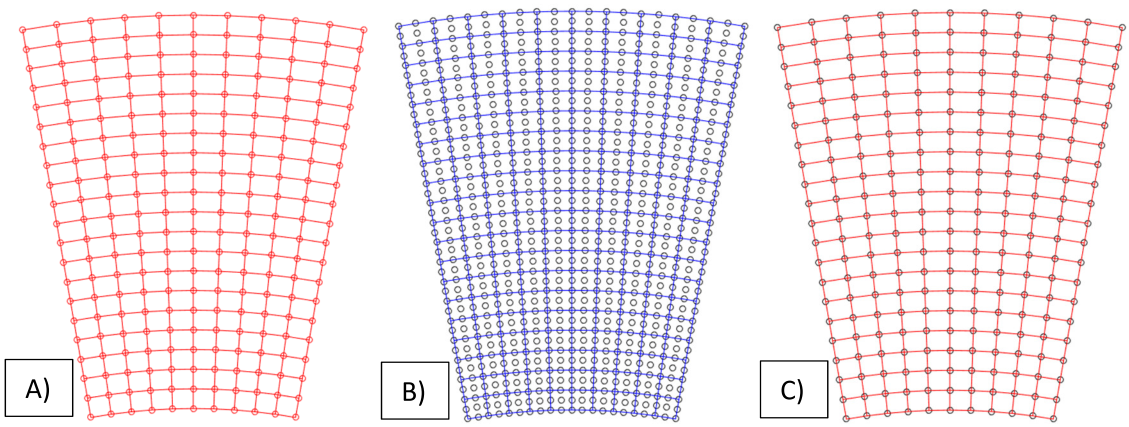

Figure 2: Different meshes used in different problems. A) and C) Mesh made with Quad4 (Q1) elements, B) Mesh made with Quad9 (Q2).

Q1 mesh is shown in Figure 2 A) was used in the problem number 1 and 3 in order to compute the densities scalar fields F and G and the velocity vector field u. On the other hand, Meshes B (Q2) and C (Q1) were used, in problem number 2, in order to compute the velocity vector field and the pressure scalar field respectively.

Q1Q1 elements were used in the problem number 1 and 3, and Q2P1 elements were used in order to avoid to use stabilization methods.

5. Problems

In this section will be shown different problems to be solved. The first problem corresponds to a couple transport system, the second one is related with a Stokes problem and the last one is a couple problem.

5.1. Transport problem

The actin filaments and monomers densities (F and G) are modelled by the following coupled system of partial differential equations.

$$\frac{\partial F}{\partial t} = -\underline{u} \cdot \underline{\nabla} F + D_F \nabla^2 F - \sigma_F F$$
$$\frac{\partial G}{\partial t} = D_G \nabla^2 F - \sigma_G G + \sigma_{GF} F$$

Where $\mathbf{u}$ is the fluid velocity and it was considered following the next expression.

$$\underline{u}(x,y) = \frac{-1}{1500}(rx, ry)\mu m/s$$

Where:

$$r = \sqrt{x^2 + y^2}$$

And the other parameters are:

$$D_F = 5\mu m/s \; D_G = 15\mu m/s \; \sigma_F = 0.25 s^{-1} \; \sigma_G = 2s^{-1} \; \sigma_{FG} = 0.5 s^{-1}$$

It was considered the following boundary conditions:

F (r=25) = 80 µM, the filament density is constant at the upper boundary. No Neuman bc were considered.

Time discretization: The theta method

It was considered a theta method in order to discretize in time. Crank-Nicholson scheme (θ=0.5) was used in order to get a second order of accuracy and an unconditionally stable method.

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

Space discretization: Galerkin formulation of theta method

The variational form associated with the theta family method, in particularly, Crank-Nicholson is:

$V := H^1_{\Gamma_D}(\Omega) = \{w \in H^1(\Omega) \,|\, w=0 \text{ on } \Gamma_D\}$

$$\left(w, \frac{\Delta F}{\Delta t}\right) - \left(\left(w, \theta\left(-u.\nabla(\Delta F)\right)\right) + \left(w, \theta D_F \nabla^2(\Delta F)\right) - \left(w, \theta\sigma_F(\Delta F)\right)\right) = (w, -u.\nabla F^n) + (w, D_F \nabla^2 F^n) - (w, \sigma_F F^n)$$

$$\left(w,\frac{\Delta G}{\Delta t}\right)-\left(\left(w,\theta D_G\nabla^2(\Delta G)\right)-\left(w,\theta\sigma_G(\Delta G)\right)+\left(w,\theta\hat{\sigma}_{GF}(\Delta F)\right)\right)=(w,D_G\nabla^2G^n)-(w,\sigma_G G^n)+(w,\hat{\sigma}_{GF}F^n)$$

Using the divergence theorem, the diffusion term that contains the second derivative of the variable can be broken down into two first order derivative

$$\left(w,\frac{\Delta F}{\Delta t}\right)-\left(\left(w,\theta\left(-u.\nabla(\Delta F)\right)\right)-\left(\nabla w,\theta D_F\nabla(\Delta F)\right)-\left(w,\theta\sigma_F(\Delta F)\right)\right)=(w,-u.\nabla F^n)-(\nabla w,D_F\nabla F^n)-(w,\sigma_F F^n)$$

$$\left(w,\frac{\Delta G}{\Delta t}\right)-\left(-\left(\nabla w,\theta D_G\nabla(\Delta G)\right)-\left(w,\theta\sigma_G(\Delta G)\right)+\left(w,\theta\hat{\sigma}_{GF}(\Delta F)\right)\right)=-(\nabla w,D_G\nabla G^n)-(w,\sigma_G G^n)+(w,\hat{\sigma}_{GF}F^n)$$

Afterwards, with the definition of u^h and w^h the discrete weak form is obtained.

$$F^h(x,t)=\sum_{A\in\eta/\eta_D} N_A(x)F_A(t)+\sum_{A\in\eta_D} N_A(x)F_D(x_A,t)$$

The same routine is taken for G.

$$w^h\in V^h:=\text{span}\{N_A\}$$

$$M_{ab}=\int_\Omega N_a N_b \, d\,\Omega$$

$$C_{ab}=\int_\Omega N_a(u.\nabla N_b) \, d\,\Omega$$

$$K_{ab}=\int_\Omega \nabla N_a(v\nabla N_b) \, d\,\Omega$$

Finally, the equations in matrix form are obtained as the following:

$$(M+\theta C\Delta t+\theta D_F K\Delta t+\theta\sigma_F M\Delta t)\dot{F}-(C\Delta t+D_F K\Delta t+\sigma_F M\Delta t)F=0$$

$$(M+\theta D_G K\Delta t+\theta\sigma_G M\Delta t)\dot{G}-(D_G K\Delta t+\sigma_G M\Delta t)G=\hat{\sigma}_{GF}M\Delta t(\theta\dot{F}+F)$$

Results

In order to obtain different results for F and G, were used the following time parameters:
Time end = 10 seconds.
Number of time steps = 120
Time increment = t_end/nstep = 0.0833

Figure 3 shows the F and G densities surface plot, and F and G isolines.

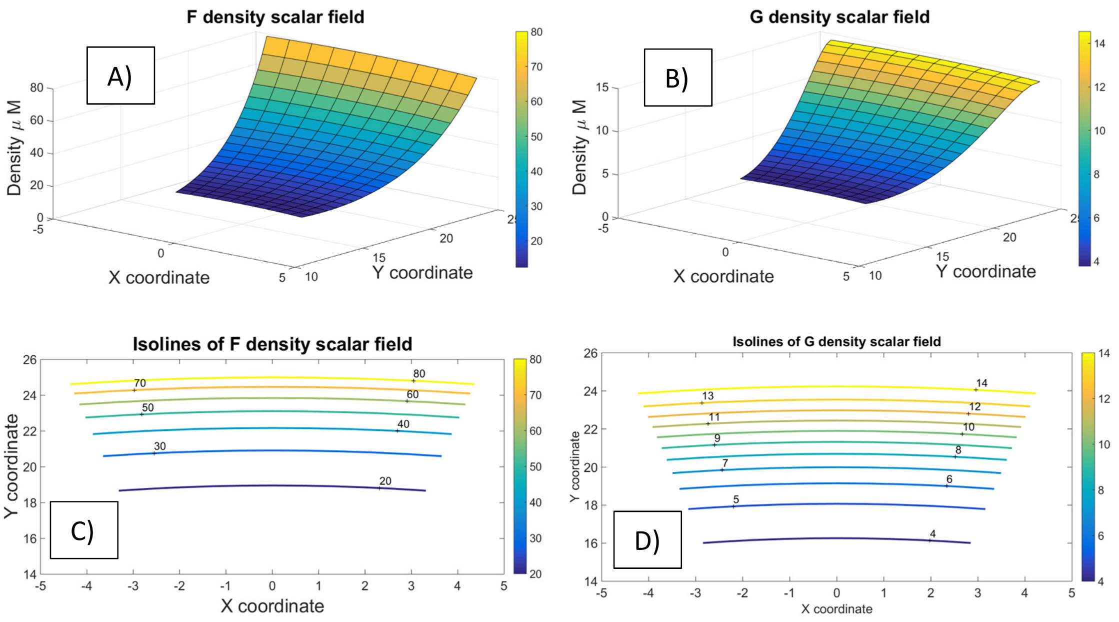

Figure 3: Results at t = 10 sec. A) F density scalar field, B) G density scalar field, C) Isoline of F density, D) Isoline of G density.

In Figure 3 C can be observed that the filament density remained constant at the upper boundary along the time and equal to 80. This is in accordance with the Dirichlet boundary condition applied.

According to the time and space discretization methods used, the solution for both F and G densities remained stable along the time and independently to the mesh size. Second accuracy in time and first accuracy in space were reached.

Were chosen two different nodes in order to plot the temporal evolution of the densities. In figure bellow can be seen that the G density starts reaching a steady regimen at t = 3 sec, while F density starts reaching a steady regimen at t = 6 sec.

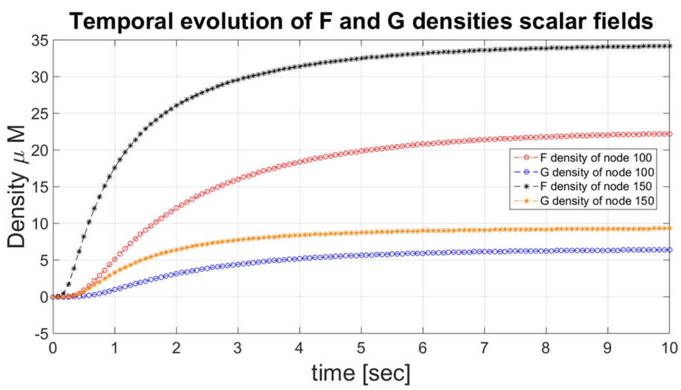

Figure 4: Temporal evolution of F and G densities using two different nodes.

The remark written above could be related to the fact that the diffusion velocity of G Acting (D_G) is greater than the diffusion velocity of F Acting (D_F), so, the diffusion of the G Acting density reaches a steady condition much faster than the F Acting density. This observation is related to the fact that G Acting (monomer) is smaller than F Acting (polymer made with monomers of G Acting).

5.2. Stokes problem

The stokes system of equation to be solved is:

$$\underline{\nabla} \cdot \underline{\underline{\sigma}} = \underline{0}$$
$$\underline{\nabla}.\underline{u} = 0$$

With the following boundary conditions:

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

Zero traction on the straight sides of the boundary.

It was considered kinematic viscosity $\upsilon = 10^3 pN \cdot s / \mu m$.

Space discretization

Before starting to discretize the Strokes equation, it was necessary to express this equation in terms of pressure and velocity using the following expression so-called Stokes' law.

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + \underline{\underline{S}}(\underline{v}) = -p\underline{\underline{I}} + \upsilon \nabla^s \underline{u}$$

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

So, the Stokes equation will be:

$$\underline{\nabla} \cdot (\nabla^s \underline{u}) - \underline{\nabla} p = \underline{0}$$
$$\underline{\nabla}.\underline{u} = 0$$

Multiplying with vector function w and scalar function q, we obtain:

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

$(w, \underline{\nabla}.\underline{u}) = 0$

After using integration by part and divergence theorem, the weak formulation of Stokes problem will be: find ($\underline{u}$, p) $\in SxQ$, such that:

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

Where:

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

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

Now, invoking Galerkin formulation of the Stokes problem, may then be stated as follow:

Find $\underline{u}^h \in V^h$ and $p^h \in Q^h$, both velocity and pressure respectively, such that:

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

And using shape functions for velocity and pressure, then, the weak form of the problem becomes in a matrix problem.

$$K\underline{u} + Gp = \underline{0}$$
$$G^T \underline{u} = 0$$

Where:

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

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

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

Results

Next figure shows different results obtained for this problem. It can be observed, the pressure scalar field, components of velocity and its modulus.

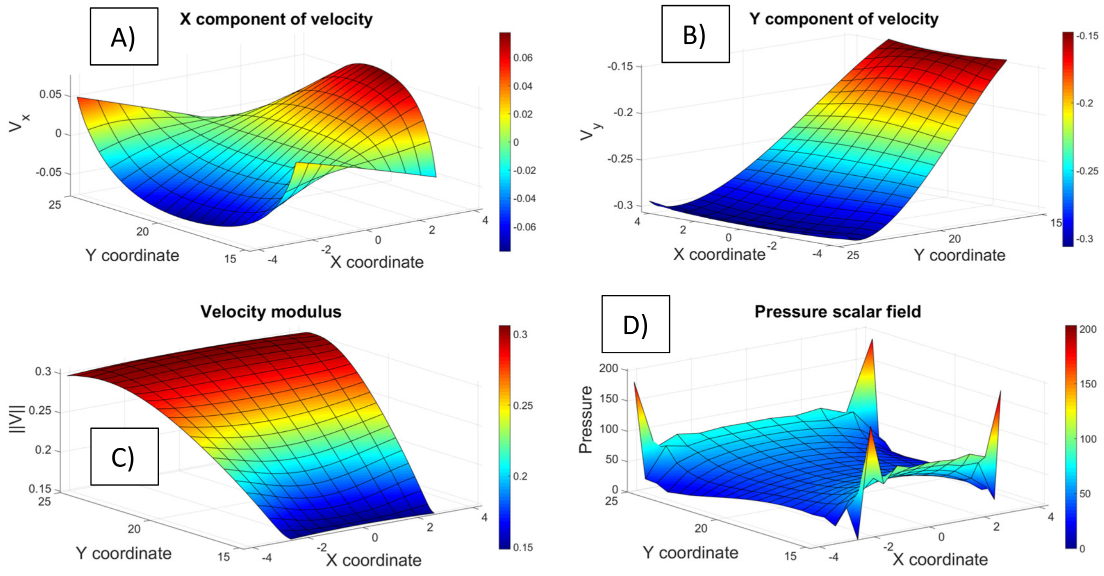

Figure 5: Results. A) X component of Vel., B) Y component of Vel., C) Velocity modulus, D) Pressure.

Several remarks can be said. Firs of all, how it expected, Q2P1 elements have given a stable solution without numerical oscillations. Second, it can be seen, in Figure 5 C, Dirichlet boundary conditions on the upper boundary and equal to 0.30 and on the lower boundary and equal to 0.15, both values expressed in absolute value. Third, Y component of velocity (V_y) became dominant in the whole domain, in comparation whit X component of velocity (V_x), this remark can be observed in Figure 5 A and B. Finally, zero pressure was observed on the straight sides of the boundary. On the other hand, it was observed a high-pressure level at each corner of the domain.

5.3. 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 modelled using the equations of a quasi-steady viscous fluid. Moreover, due to the presence of actin fibres, the incompressibility constrain is dropped and pressure is neglected. Then, the equations governing the coupled problem can be written as

$$1)\ \upsilon \underline{\nabla}\cdot\left(\underline{\nabla}^{s}\underline{u}\right)+\underline{\nabla}\cdot\underline{\underline{\sigma}}_{m}(F)+T_{m}(u)=0$$

$$2)\ \frac{\partial F}{\partial t}=-\underline{u}\cdot\underline{\nabla}F+D_{F}\nabla^{2}F-\sigma_{F}F$$

$$3)\ \frac{\partial G}{\partial t}=D_{G}\nabla^{2}F-\sigma_{G}G+\sigma_{GF}F$$

Were considered the same boundary conditions used in the previous problems:

F (r=25) = 80 µM, the filament density is constant at the upper boundary. No Neuman bc were considered.

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

Zero traction on the straight sides of the boundary.

It was considered kinematic viscosity $\upsilon=10^3 pN\cdot s/\mu m$, and the following time parameters were used:

Time end = 10 seconds.

Number of time steps = 120

Time increment = t_end/nstep = 0.0833

Discretization

Equation 2 and 3 were discretized using the discretization written in the first problem. Equation 1 was only discretized in space.

Time discretization: The theta method

It was considered a theta method in order to discretize in time. Crank-Nicholson scheme (θ=0.5) was used in order to get a second order of accuracy and an unconditionally stable method.

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

Space discretization: Galerkin formulation of theta method

The variational form associated with the theta family method, in particularly, Crank-Nicholson is:

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

Space discretization: Galerkin formulation of Stokes equation

Here, we will use some equation used in previous problems.

First of all, in order to obtain a weak form of the equation, integration by parts will be applied in the first term. The Identity written bellow will be used in order to obtain the weak form of the equation.

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

$$\underline{\nabla}\cdot\left(\underline{w}\cdot\upsilon\underline{\nabla}^s\underline{u}\right)=\underline{\nabla}\underline{w}:\left(\upsilon\underline{\nabla}^s\underline{u}\right)+\underline{w}\cdot\upsilon\underline{\nabla}\cdot(\underline{\nabla}^s\underline{u})$$

Using divergence's theorem and rewrite some terms,

$$\cancel{\int_\Gamma\underline{w}\cdot\upsilon\underline{\nabla}^s\underline{u}\cdot\underline{n}d\Gamma}-\int_\Omega\underline{\nabla}\underline{w}:\left(\upsilon\underline{\nabla}^s\underline{u}\right)d\Omega+\int_\Omega\underline{w}\cdot\underline{\nabla}\cdot\underline{\underline{\sigma_m}}(F)\int_\Omega\underline{w}\cdot\underline{T_m}d\Omega=0$$

Finally, the equation is:

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

At the end, the system of equation to be solved is:

$$\bar{K}u+\bar{T}_f F+\bar{T}_u u=0$$

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

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

Remark: T_f and T_u: These two matrices arising from the discretisation of $\left(\underline{w},\underline{\nabla}\cdot\underline{\underline{\sigma}}_m(F)\right)+\left(\underline{w},T_m(\underline{u})\right)$ respectively.

<u>Results</u>

In Figure 6 can be observed different results obtained.

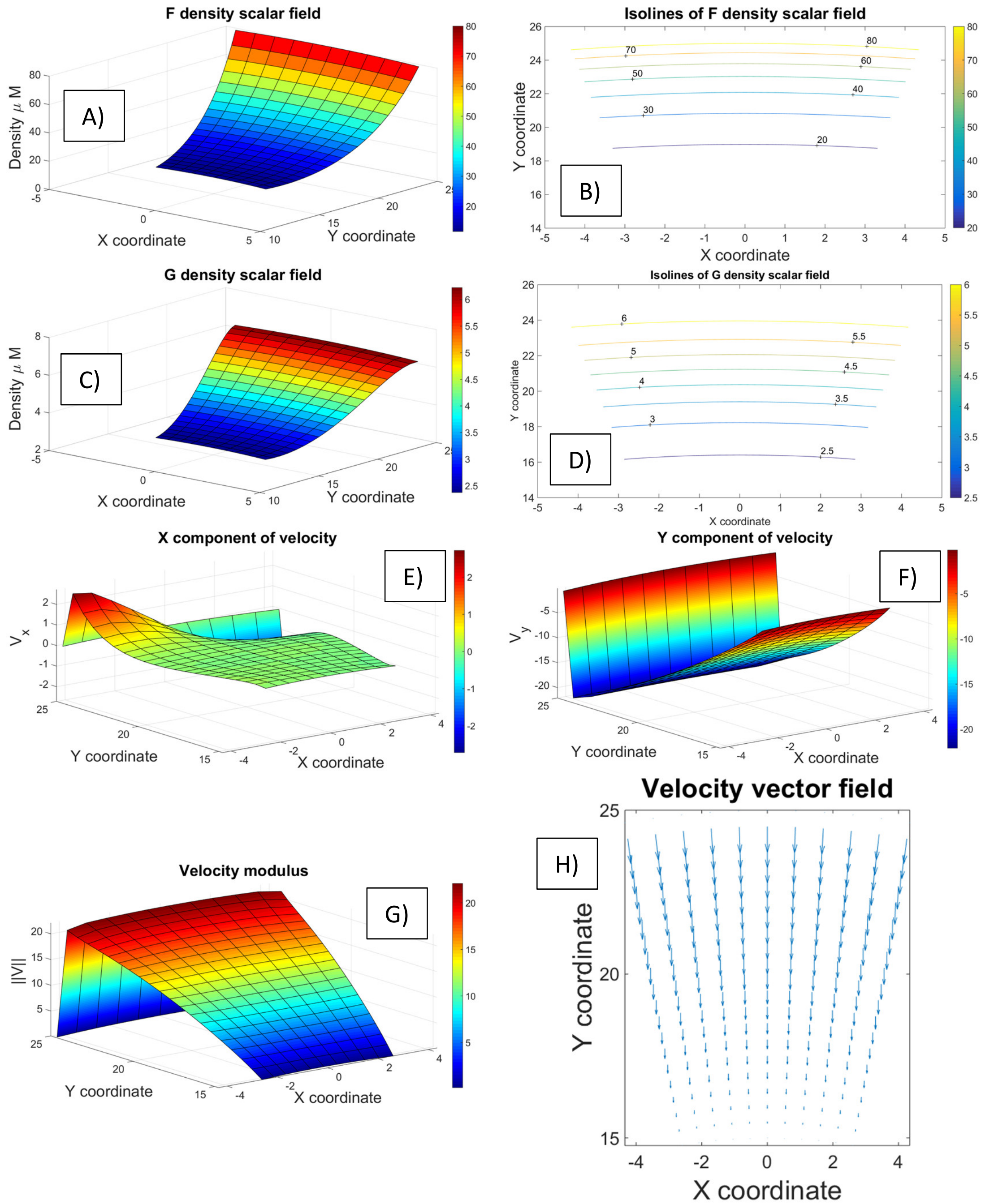

Figure 6: Results. A) F density scalar field, B) Isoline of F density, C) G density scalar field, D) Isoline of G density E) X component of Vel., F) Y component of Vel., G) Velocity modulus, H) Velocity vector field.

As was expected, numerical oscillations were not observed. In order to prove if the Dirichlet boundary conditions were applied properly, in Figure 6 A y G can be observed the Dirichlet boundary condition value applied on the upper and lower boundaries. An important remark, in Figure 6 G the Dirichlet boundary values were expressed in absolute value.

In Figure 6 H can be seen the velocity direction. As it expected the velocity direction on upper and lower boundary is on radial direction. On the other hand, it can be seen the velocity goes out to the domain.

As equal to the second problem, Y component of the velocity became dominant in the whole domain. It can be observed, in Figure 6 F, a jump from nodes belong to the upper boundary to next nodes. This drastically change in velocity could be associated to a boundary layer presence.