FEF Final Assignment

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1. Transport Problem

① Introduction

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

$$\frac{\partial F}{\partial t} = -\boldsymbol{u} \cdot \nabla F + D_F \nabla^2 F - \sigma_F F \qquad in\ (0,T) \times \Omega$$

$$\frac{\partial G}{\partial t} = D_G \nabla^2 G - \sigma_G G + \hat{\sigma}_{GF} F \qquad in\ (0,T) \times \Omega$$

Where $\boldsymbol{u}$ is the fluid velocity and the following material parameters are used:

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

Boundary conditions:

a. The filament density is constant at the upper boundary: $F(r = 25) = 80\mu M$
b. No flux boundary conditions are considered for F everywhere else and for G on the entire boundary

Velocity field:

Consider a velocity field, where $\boldsymbol{u}(x,y) = -\frac{1}{1500}(rx, ry)\ \mu m/s$, where (x,y) are the points coordinates and

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

Initial conditions:

$$F(x,y)|_{t=0} = 80\mu M \quad in\ \Omega$$
$$G(x,y)|_{t=0} = 0 \quad in\ \Omega$$

From above equations, we can find that the procedures for solving this problem should be:
Solving the unsteady convection diffusion reaction problem about F. Then turn to solving the G by using the result of F.

② Derivation and Implementation

In this problem, we can find that both equations are time dependent, so finding appropriate time scheme is essential for getting the precise results. As a result, I have chosen the Crank-Nicolson method, which is unconditionally stable and has second order accuracy. Because the results are stable and no oscillations happened here, so the stabilization technics have not been implemented.

The discretized time schemes are as following:

$$\frac{\Delta F}{\Delta t}+\frac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{\nabla}-D_F\boldsymbol{\nabla}^2+\sigma_F)\Delta F=-(\boldsymbol{u}\cdot\boldsymbol{\nabla}-D_F\boldsymbol{\nabla}^2+\sigma_F)F^n$$
$$\frac{\Delta G}{\Delta t}+\frac{1}{2}(D_G\boldsymbol{\nabla}^2+\sigma_G)\Delta G=\frac{1}{2}(s^{n+1}+s^n)-(D_G\boldsymbol{\nabla}^2+\sigma_G)G^n$$
$$s=\hat{\sigma}_{GF}F$$

For spatial discretization, we can apply Galerkin method:

For F:

$$\int\omega\cdot\frac{\Delta F}{\Delta t}+\frac{1}{2}\int\omega(\boldsymbol{u}\cdot\boldsymbol{\nabla})(\Delta F)+\frac{1}{2}D_F\int\boldsymbol{\nabla}\omega\cdot\boldsymbol{\nabla}(\Delta F)+\frac{1}{2}\int\omega\,\sigma_F\Delta F$$
$$=-\int\omega(\boldsymbol{u}\cdot\boldsymbol{\nabla})(F^n)-D_F\int\boldsymbol{\nabla}\omega\cdot\boldsymbol{\nabla}(F^n)-\int\omega\,\sigma_F F^n\ ,\ in\ \Omega\quad\text{and}\ \omega=0\ on\ \partial\Omega$$

For G:

$$\int v\cdot\frac{\Delta G}{\Delta t}+\frac{1}{2}D_G\int\boldsymbol{\nabla}v\cdot\boldsymbol{\nabla}(\Delta G)+\frac{1}{2}\int v\,\sigma_G\Delta G$$
$$=\frac{1}{2}\int v(s^{n+1}+s^n)-D_G\int\boldsymbol{\nabla}v\cdot\boldsymbol{\nabla}(G^n)-\int v\,\sigma_G G^n\ ,\ in\ \Omega\quad\text{and}\ v=0\ on\ \partial\Omega$$

The results:

I have chosen end time $t=1s$.

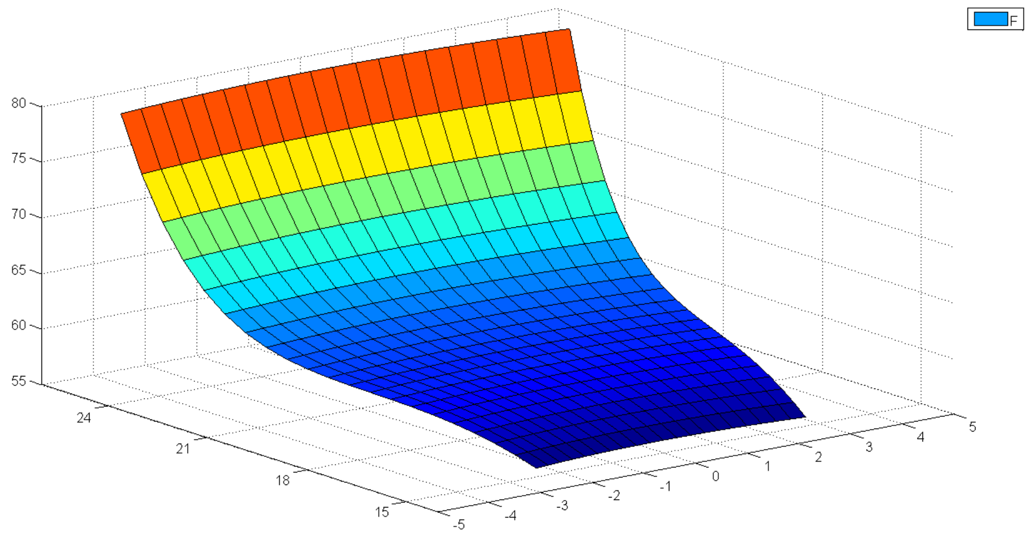

Figure 1. The filaments density field

The figure 1 presents the actin filaments density. On the boundary $r=25$, we can find that the values are fixed, which is equal to $80\mu M$. When r decreases, the filaments density also decreases accordingly. On the boundary $r=15$, the filaments densities are about $55\mu M$.

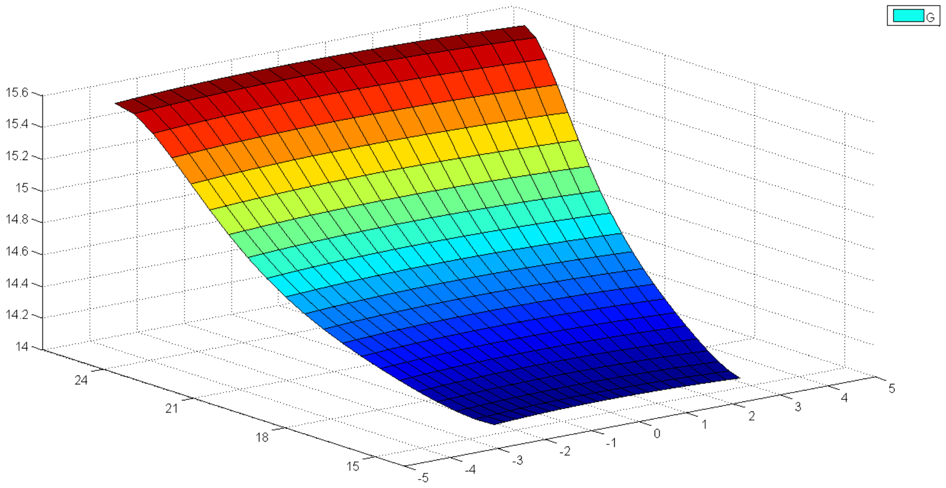

Figure 2. The monomers density field

③ Conclusion

For unsteady convection problem, we need to choose the appropriate time scheme to consider the information transport along the characteristic lines.

2. Stokes Problem

① Introduction

In this part, we need to solve the following stokes equations:

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} &= 0 \quad in\ \Omega \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} &= 0 \quad in\ \Omega \\ \boldsymbol{u} &= \boldsymbol{u}_D \quad on\ \Gamma_D \end{aligned}$$

Boundary conditions:

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

And zero traction on the straight sides of the boundary.
Consider a viscosity $\nu = 10^3 pN \cdot s/\mu m$.

This is a steady stokes problem without source term. We have several difficulties in this problem to get the precise solution:
First, this is a nonlinear system in which the velocity and pressure are coupled. Then, the selection of elements for velocity and pressure will also influence the results. Because the elements should satisfy the LBB condition

such that the problem has unique solution. If we don't choose the LBB elements, what we need to do is that applying stabilization technics here to get the solution.

② Derivation and Implementation

In order to get the weak form of the stokes equations, we firstly need to use the constitutive equation, Cauchy stress $\boldsymbol{\sigma}$**,** which is related to velocity and pressure like Stokes law:

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\mu\boldsymbol{\nabla}^s\boldsymbol{u}$$

We replace the $\boldsymbol{\sigma}$ in the stokes equations, then get:

$$\begin{gathered} -\nu\boldsymbol{\nabla}^2\boldsymbol{u} + \boldsymbol{\nabla}p = 0 \qquad in\ \Omega \\ \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \quad in\ \Omega \\ \boldsymbol{u} = \boldsymbol{u}_D \qquad on\ \Gamma_D \end{gathered}$$

Neumann boundary condition is not considered in this problem.
Multiplying the velocity test function $\boldsymbol{\omega}$ and the pressure test function q, we can get:

$$\begin{gathered} \int \nu\nabla\boldsymbol{\omega}:\nabla\boldsymbol{u} + \int \boldsymbol{\omega}\cdot\nabla p = 0 \quad in\ \Omega, \qquad \forall\boldsymbol{\omega} \in H^1_{\Gamma_D}(\Omega) \\ \int q\ \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \quad in\ \Omega, \quad \forall q \in L_2(\Omega) \\ \boldsymbol{u} = \boldsymbol{u}_D \qquad on\ \Gamma_D \end{gathered}$$

Where:

$$H^1_{\Gamma_D}(\Omega) = \{\boldsymbol{v} \in H^1(\Omega) |\ \boldsymbol{v} = 0\ on\ \Gamma_D\}$$

After discretization, we can get the following system:

$$\begin{bmatrix} \boldsymbol{K} & \boldsymbol{G}^T \\ \boldsymbol{G} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = [\boldsymbol{0}]$$

Where

$$\begin{gathered} \boldsymbol{K}: \int \nu\nabla\boldsymbol{\omega_h}:\nabla\boldsymbol{u_h} \\ \boldsymbol{G}: \int q_h\ \boldsymbol{\nabla}\cdot\boldsymbol{u_h} \end{gathered}$$

This problem has unique solution if $ker(\boldsymbol{G}) = 0$, or $\boldsymbol{G}^T\boldsymbol{K}^{-1}\boldsymbol{G}$. The condition $ker(\boldsymbol{G}) = 0$ holds when the spaces chosen for the velocity and pressure satisfy the LBB condition.
Where LBB condition is as following:

$$\forall q^h \in \mathcal{F}^h \quad \exists\omega^h \in \mathcal{M}^h, \omega^h \neq 0: (q^h, \boldsymbol{\nabla}\cdot\omega^h) \geq \alpha \parallel q^h \parallel_0 \parallel \omega^h \parallel_1$$

If the LBB condition is not satisfied, we need to use stabilization techniques.

The result:

a. The results without stabilization

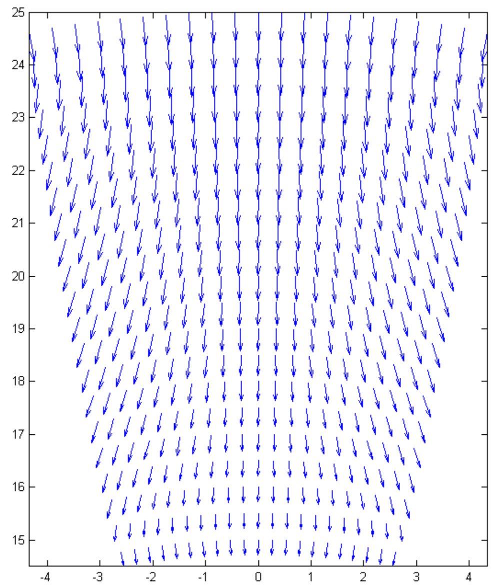

Figure 3. The stream line of the stokes problem without GLS

Figure shows the stream line of this problem. The velocity field on the boundaries $r = 15$ and $r = 25$ satisfy the boundary conditions.

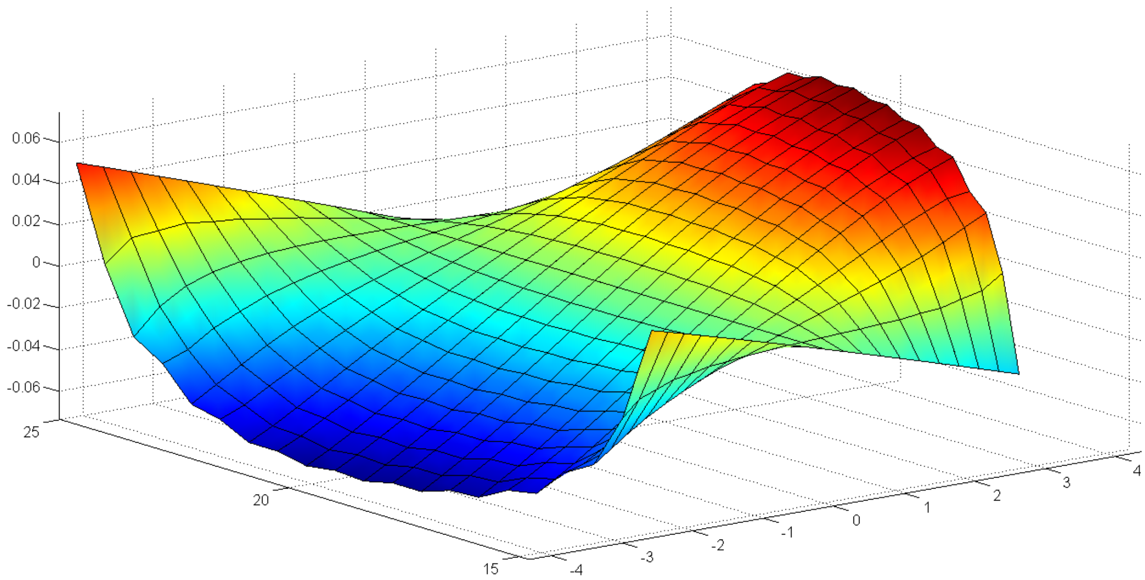

Figure 4. The velocity field on X direction of the stokes problem without GLS

Figure shows the velocity field on horizontal direction. The highest value happens on the middle areas of the vertical boundaries. However, the velocity solution on horizontal direction is not stable.

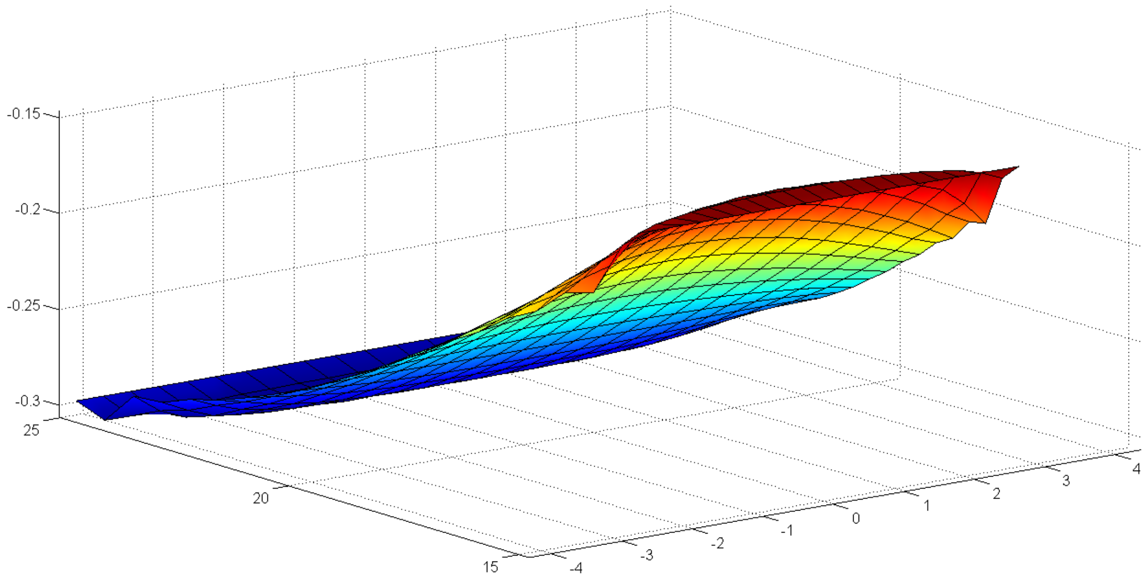

Figure 5. The velocity field on Y direction of the stokes problem without GLS

Figure shows the velocity field on vertical direction. The highest value happens on the boundary $r = 25$. Like the solution on the horizontal direction, the velocity solution on the vertical direction is also not stable.

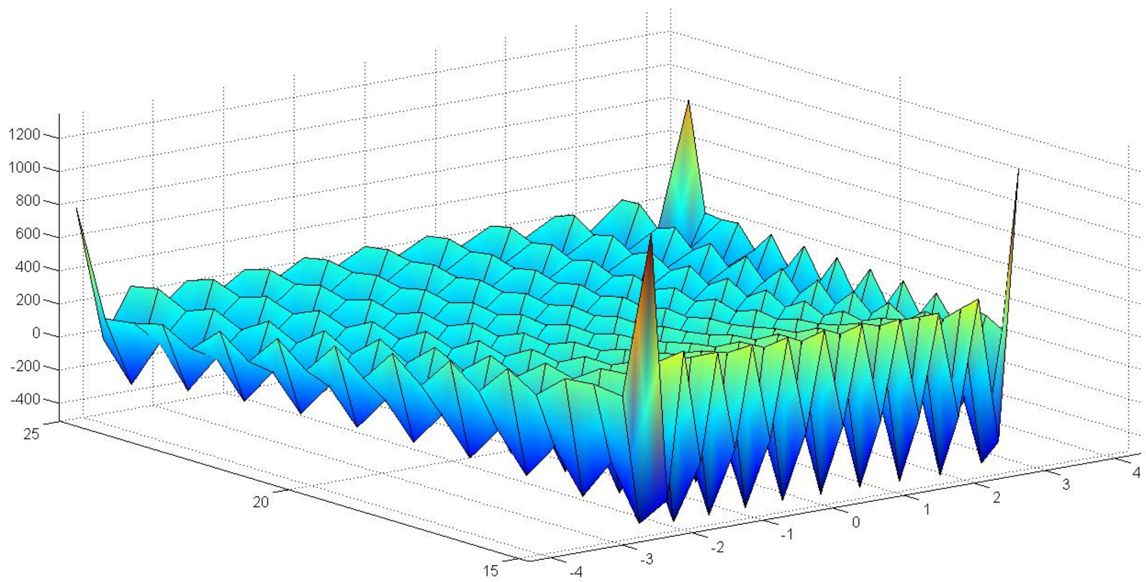

Figure 6. The pressure field of the stokes problem without GLS

From above figure, it's clear that the pressure field result is not stable and the oscillations happen in the whole domain.

The reason why the instabilities happen in both velocity and pressure fields is that I have used Q1Q1 element which is not satisfying the LBB condition, meaning that the stabilization is needed here. In next part, I have implemented the GLS stabilization method.

b. The results with GLS method

i. The GLS method used in stokes equations

According to the lecture of professor Ramon Codina, the GLS method here can be expressed as:

$$\nu(\nabla \boldsymbol{u}_h, \nabla \boldsymbol{\omega}_h) + (\boldsymbol{\omega}, \nabla p_h) + (q_h, \nabla \cdot \boldsymbol{u}_h) + \sum_K \int_K \tau_1(-\nu \boldsymbol{\Delta \omega}_h + \nabla q_h)(-\nu \boldsymbol{\Delta} u_h + \nabla p_h)$$

$$+ \sum_K \int_K \tau_2 \, (\nabla \cdot \boldsymbol{\omega}_h)(\nabla \cdot \boldsymbol{u}_h) = 0$$

Because we have used the linear element and we assume that $\tau_2 = 0$, so we get:

$$\boldsymbol{\Delta \omega}_h = 0, \boldsymbol{\Delta} u_h = 0 \ \ and \ \ \tau_2 = 0$$

So the equation becomes:

$$\nu(\nabla \boldsymbol{u}_h, \nabla \boldsymbol{\omega}_h) + (\boldsymbol{\omega}, \nabla p_h) = 0$$

$$(q_h, \nabla \cdot \boldsymbol{u}_h) + \sum_K \int_K \tau_1 \nabla q_h \cdot \nabla p_h = 0$$

Then we get the following stabilized system:

$$\begin{bmatrix} \boldsymbol{K} & \boldsymbol{G}^T \\ \boldsymbol{G} & \boldsymbol{L} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = [\boldsymbol{0}]$$

Where the $\boldsymbol{L}$ represents the GLS stabilization.

b. The results

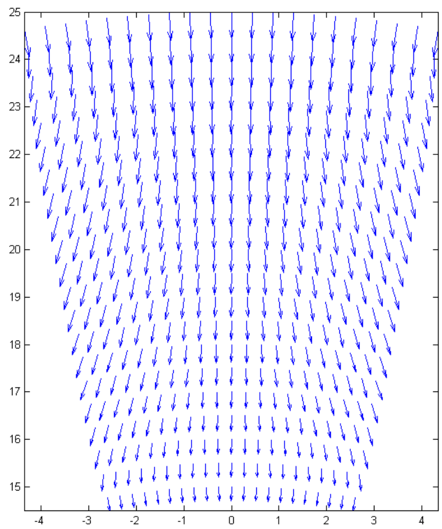

Figure 7. The stream line of the stokes problem with GLS

Figure shows the stream line of this problem. The velocity field on the boundaries $r = 15$ and $r = 25$ satisfy the boundary conditions.

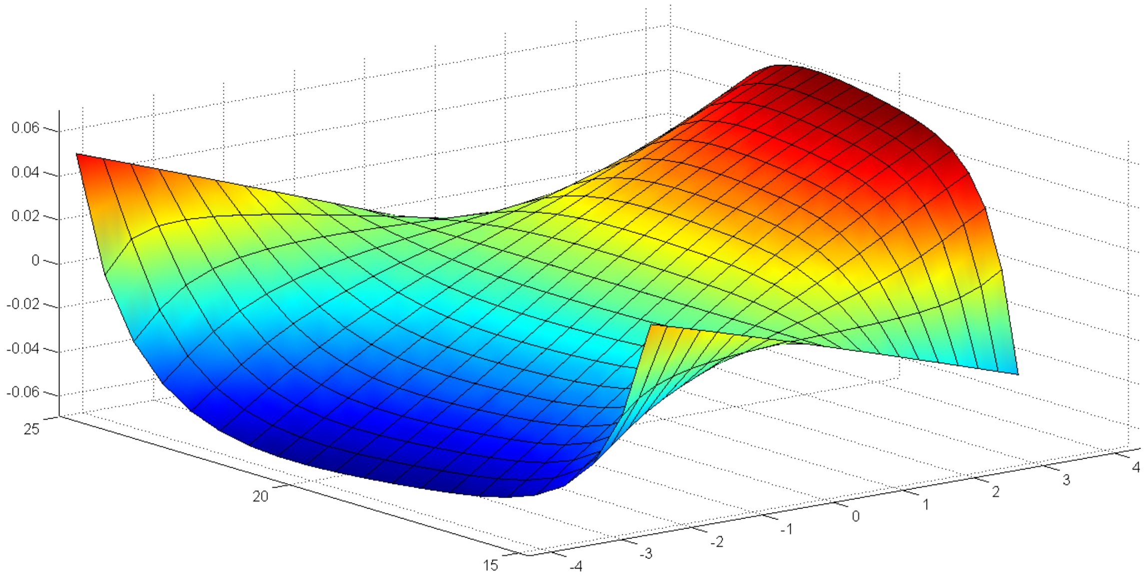

Figure 8. The velocity field on X direction of the stokes problem with GLS

Figure shows the velocity field on horizontal direction. The highest value happens on the middle areas of the vertical boundaries. And the instability disappears after implementing the stabilization method.

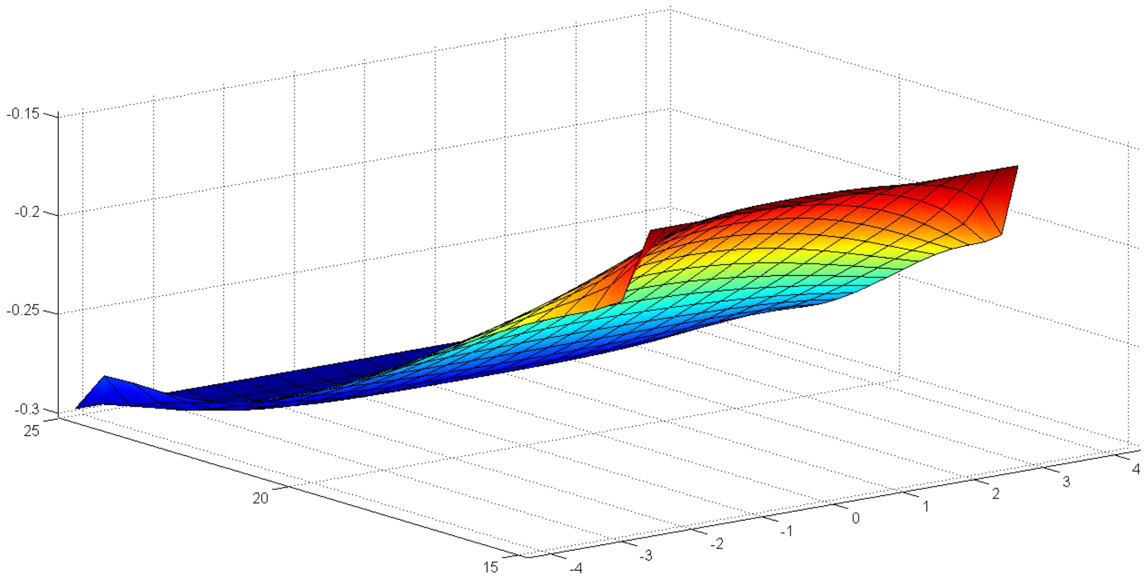

Figure 9. The velocity field on Y direction of the stokes problem with GLS

Figure shows the velocity field on vertical direction. The highest value happens on the boundary $r = 25$ and result becomes stable.

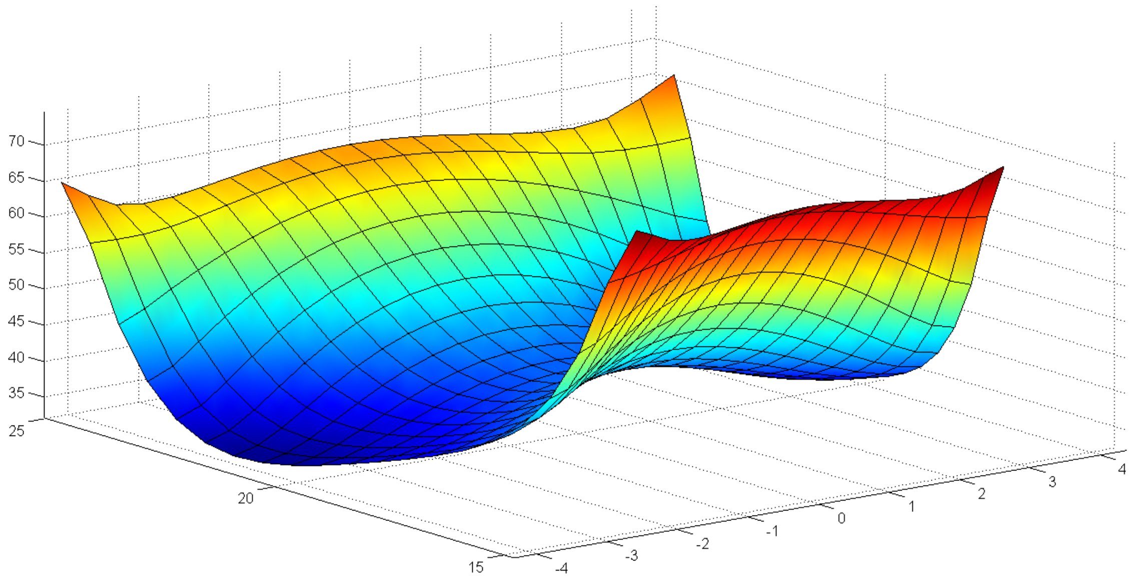

Figure 10. The pressure field of the stokes problem with GLS

As we can see, applying the GLS stabilization technique has successfully solved the oscillation of pressure field. And the highest value of pressure happens on the middle areas of the boundaries $r = 15$ and $r = 25$.

③ Conclusion

For stokes problem, the velocity and the pressure are coupled, which brings us the difficulties. Choosing the appropriate elements here is an essential task that we need to consider carefully. The element which is not satisfying the LBB condition like Q1Q1 we have used above might be easy to implement, but the stabilization techniques should be applied. Another choice is that we can use the element satisfying the LBB condition, like Q2Q1.

3. The coupled problem

① Introduction

The third problem can be expressed as following equations:

$$\nu \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}^s \boldsymbol{u}) + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma_m}(F) + \boldsymbol{T_m}(\boldsymbol{u}) = \boldsymbol{0} \qquad in\ (0, T) \times \Omega$$

$$\frac{\partial F}{\partial t} = -\boldsymbol{u} \cdot \boldsymbol{\nabla} F + D_F \boldsymbol{\nabla}^2 F - \sigma_F F \qquad in\ (0, T) \times \Omega$$

$$\frac{\partial G}{\partial t} = D_G \boldsymbol{\nabla}^2 G - \sigma_G G + \hat{\sigma}_{GF} F \qquad in\ (0, T) \times \Omega$$

Where $\boldsymbol{\sigma_m}$ and $\boldsymbol{T_m}$ are surface forces on the leading edge. These two terms can be gotten from the function **boundaryMatrices.m**. The parameters are same to the first problem.

② Derivation and Implementation

In the first equation, the term is equal to:

$$\boldsymbol{\nabla}^{s}\boldsymbol{u} = \frac{1}{2}(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^{\boldsymbol{T}})$$

After multiplying the test function and integration by parts, we finally get:

First equation:

$$\frac{1}{2}\nu \ \left(\int \boldsymbol{\nabla}\boldsymbol{\omega}\cdot\boldsymbol{\nabla}\boldsymbol{u} + \int (\boldsymbol{\nabla}\cdot\boldsymbol{\omega})(\boldsymbol{\nabla}\cdot\boldsymbol{u})\right) + \int \boldsymbol{\omega}\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_{\boldsymbol{m}}(F) + \int \boldsymbol{\omega}\,\boldsymbol{T}_{\boldsymbol{m}}(\boldsymbol{u}) = \boldsymbol{0}\ , \qquad \forall\boldsymbol{\omega} \in H^{1}_{\Gamma_D}(\Omega)$$

$$H^{1}_{\Gamma_D}(\Omega) = \{\boldsymbol{v} \in H^{1}(\Omega)|\ \boldsymbol{v} = 0\ on\ \Gamma_D\}$$

For $\boldsymbol{F}$:

$$\int \omega\cdot\frac{\Delta F}{\Delta t} + \frac{1}{2}\int \omega(\boldsymbol{u}\cdot\boldsymbol{\nabla})(\Delta F) + \frac{1}{2}D_F\int \boldsymbol{\nabla}\omega\cdot\boldsymbol{\nabla}(\Delta F) + \frac{1}{2}\int \omega\,\sigma_F\Delta F$$
$$= -\int \omega(\boldsymbol{u}\cdot\boldsymbol{\nabla})(F^{n}) - D_F\int \boldsymbol{\nabla}\omega\cdot\boldsymbol{\nabla}(F^{n}) - \int \omega\,\sigma_F F^{n}\ \ ,\ in\ \Omega\ \ \text{and}\ \omega = 0\ on\ \ \partial\Omega$$

For $\boldsymbol{G}$:

$$\int v\cdot\frac{\Delta G}{\Delta t} + \frac{1}{2}D_G\int \boldsymbol{\nabla}v\cdot\boldsymbol{\nabla}(\Delta G) + \frac{1}{2}\int v\,\sigma_G\Delta G$$
$$= \frac{1}{2}\int v(s^{n+1} + s^{n}) - D_G\int \boldsymbol{\nabla}v\cdot\boldsymbol{\nabla}(G^{n}) - \int v\,\sigma_G G^{n}\ \ ,\ in\ \Omega\ \ \text{and}\ v = 0\ on\ \ \partial\Omega$$

As we can see, the F and $\boldsymbol{u}$ are coupled in the first and second equations. Here I have considered two ways to solve it. One is using serial scheme, meaning that we solve F and $\boldsymbol{u}$ serially. Another method is using the method we have implemented in stokes equation. The situation is similar, because in stokes equations the velocity and pressure are coupled.

a.Serial method

The step is: we use $\boldsymbol{u}^{i}$ to compute F_1^{i+1} using the second equation, then we can apply iterative method in each time step, using F_j^{i+1} to get $\boldsymbol{u}_j^{i+1}$ until we get the satisfied results.

The results:

I have chosen end time $t = 1s$.

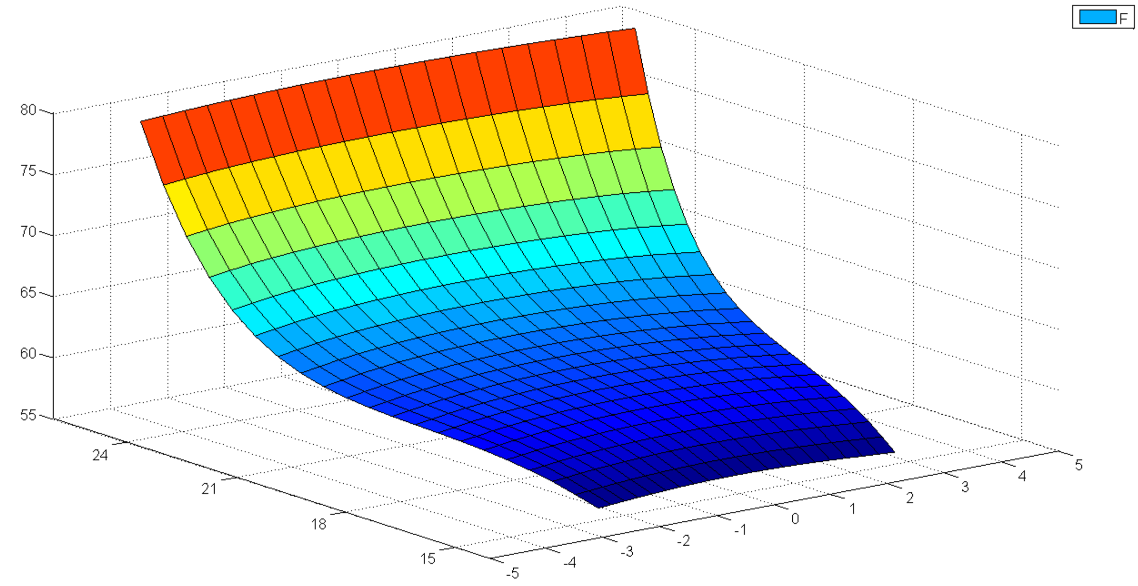

Figure 11. The filaments density field of coupled problem (first application)

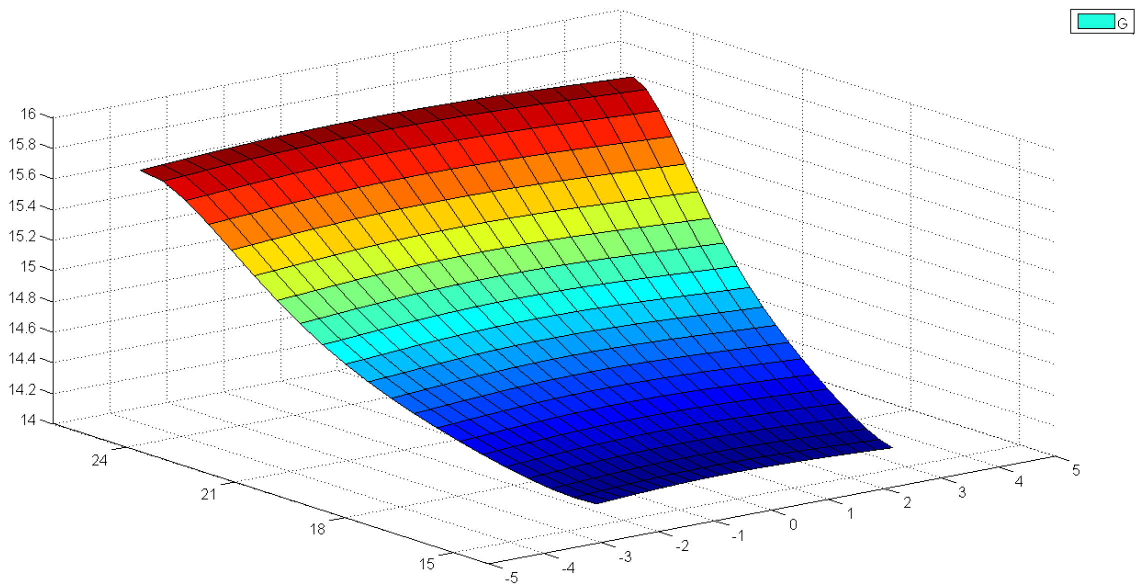

Figure 12. The monomers density field of coupled problem (first application)

But this method is totally wrong. I find that the velocity in each step doesn't change. This is because that, in my application, once we calculate the ΔF from $\boldsymbol{u}$ using the second equation, the results will automatically satisfy the first equation. Then, the circulation will appear. As a result, we get the results of using the same velocity field.

I applied the second way, then the results are like following:

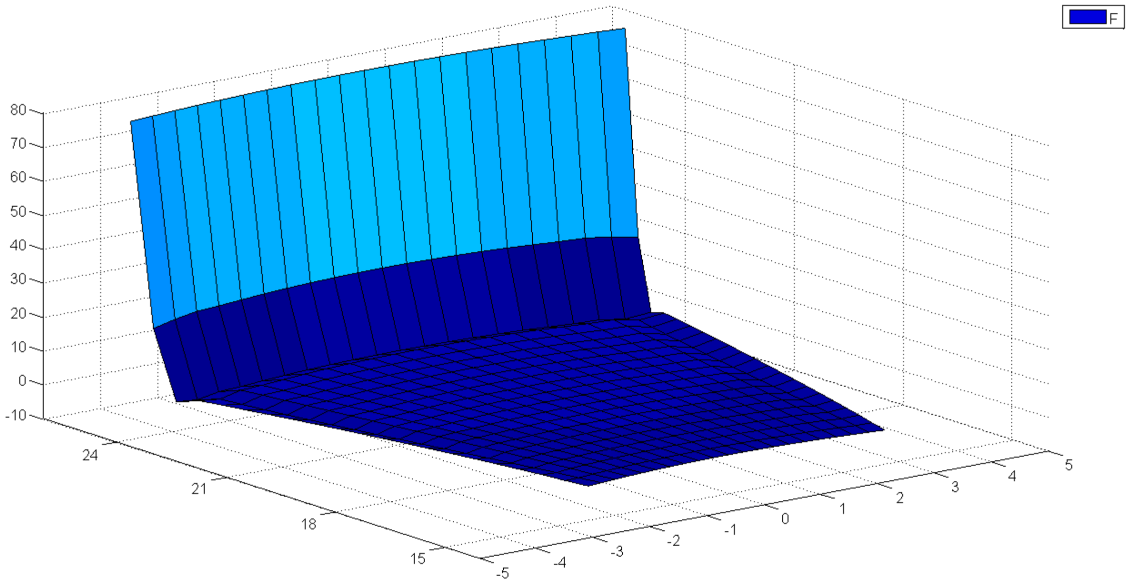

Figure 13. The filaments density field of coupled problem (second application)

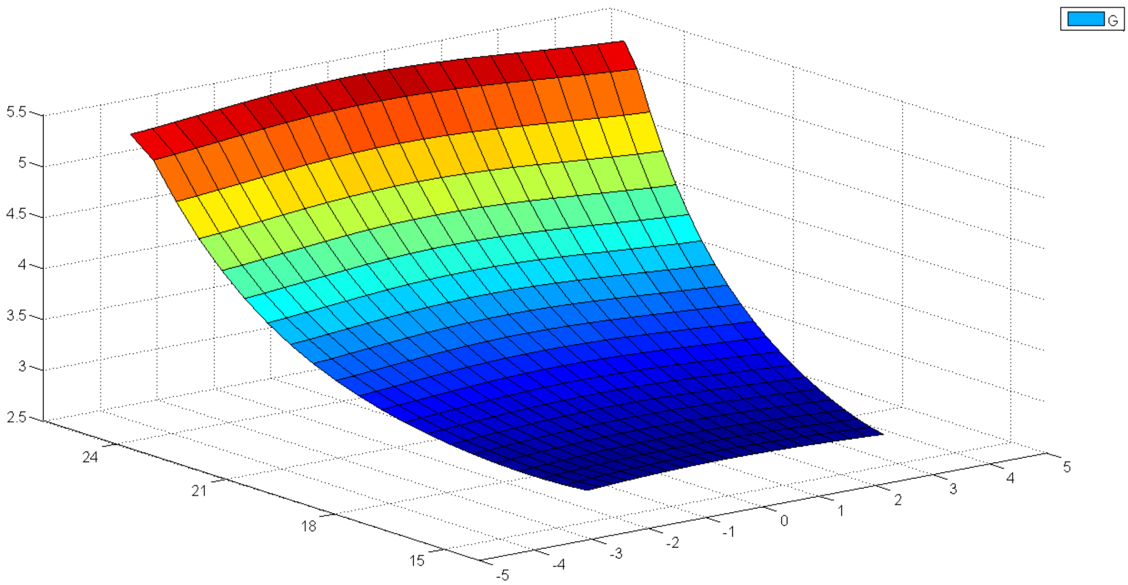

Figure 14. The monomers density field of coupled problem (second application)

As we can see, the results are not very well, especially for F.

b.Picard Method

Still working on it.