FINITE ELEMENT METHODS IN FLUIDS (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 are solving a simplified model for density of actin filaments and monomers coupled with the cortex's mechanics. First, we 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 solved to account for the interaction of the actin filaments and the cortex.
All the problems are solved in the domain Ω shown in the figure below.

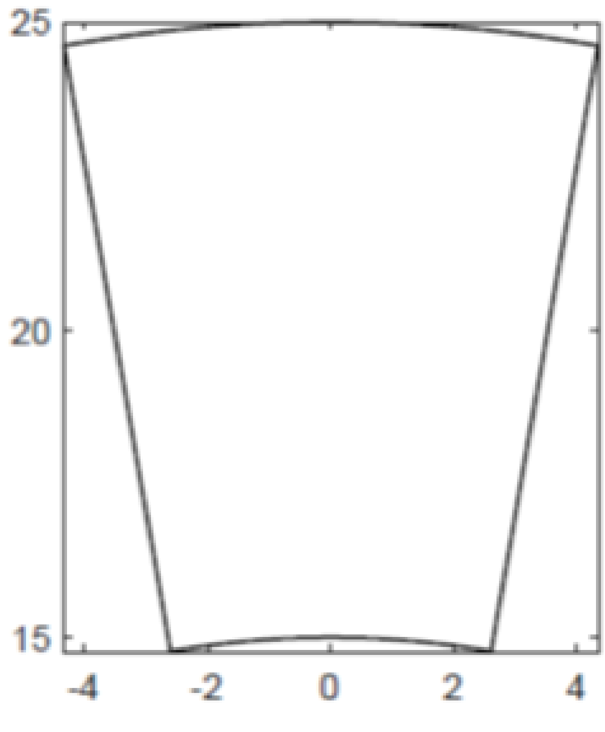

Figure 1: The domain

For each one of the three problems (we have solved),we state the method we have chosen to solve it,and we present the weak form of the governing equations we solve and mention solution procedures. We have depicted the obtained results lucidly and finally, we analyse the obtained solutions.

1.**TRANSPORT PROBLEM**:

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

$$F_t = \frac{\partial F}{\partial t} = -\mathbf{u}.\boldsymbol{\nabla} F + D_F \boldsymbol{\nabla}^2 F - \sigma_F F \qquad in\ (0,T) \times \Omega \tag{1}$$

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

where $\mathbf{u}$ 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:

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

Implemented initial Conditions:
$F(\mathbf{x}, t = 0) = 80\ \mu M$, and $G(\mathbf{x}, t = 0) = 0\ \mu M$, where $\mathbf{x} \in \Omega$ has been considered.

A given velocity profile $\mathbf{u}(x, y) = \frac{-1}{1500}(rx, ry)\ \mu m/s$ is considered; where $r = \sqrt{x^2 + y^2}$ and (x,y) are the points coordinates.

Method:

The most popular methods for parabolic problems (transient) are the θ family of methods. It can be noted that the second derivatives of F and G are present due to the diffusion operator in both of the given governing equations (in strong form). Among the θ family methods, it is known that the Crank-Nicolson, $\theta = 1/2$, is the only second-order accurate method. As to solve the given true transient problems where the time accuracy is important, the Crank-Nicolson scheme is preferred.

Crank-Nicolson scheme:($\theta = \frac{1}{2}$)**:**

Using the θ method, the above two equations can be discretized as follows:

$$\frac{F(t^{n+1}) - F(t^n)}{\triangle\ t} = \theta F_t(t^{n+1}) + (1-\theta) F_t(t^n) + \mathcal{O}((\frac{1}{2} - \theta) \triangle\ t, \triangle\ t^2)$$

$$\frac{G(t^{n+1}) - G(t^n)}{\triangle\ t} = \theta G_t(t^{n+1}) + (1-\theta) G_t(t^n) + \mathcal{O}((\frac{1}{2} - \theta) \triangle\ t, \triangle\ t^2)$$

As in the CN scheme ($\theta = \frac{1}{2}$), the above equations can be written as:

$$\frac{F(t^{n+1}) - F(t^n)}{\triangle\ t} = \frac{1}{2} F_t(t^{n+1}) + \frac{1}{2} F_t(t^n) + \mathcal{O}(\triangle\ t^2)$$

$$\frac{G(t^{n+1}) - G(t^n)}{\triangle\ t} = \frac{1}{2} G_t(t^{n+1}) + \frac{1}{2} G_t(t^n) + \mathcal{O}(\triangle\ t^2)$$

By substituting the given F_t *and* G_t values mentioned in the equations (1) and (2) in to the above two equations respectively, and neglecting the temporal truncation error,we obtain :

Equation 1:

$$\frac{F(t^{n+1})-F(t^n)}{\triangle\ t}=\frac{1}{2}(-\mathbf{u}.\boldsymbol{\nabla}F^{n+1}+D_F\boldsymbol{\nabla}^2F^{n+1}-\sigma_F F^{n+1})+\frac{1}{2}(-\mathbf{u}.\boldsymbol{\nabla}F^{n}+D_F\boldsymbol{\nabla}^2F^{n}-\sigma_F F^{n})\Rightarrow$$

$$\tfrac{F(t^{n+1})-F(t^n)}{\triangle t}-\tfrac{1}{2}(-\mathbf{u}.\boldsymbol{\nabla}F^{n+1}+D_F\boldsymbol{\nabla}^2F^{n+1}-\sigma_F F^{n+1})+\tfrac{1}{2}(-\mathbf{u}.\boldsymbol{\nabla}F^{n}+D_F\boldsymbol{\nabla}^2F^{n}-\sigma_F F^{n})$$

$$=(-\mathbf{u}.\boldsymbol{\nabla}F^{n}+D_F\boldsymbol{\nabla}^2F^{n}-\sigma_F F^{n})$$

Implementing the notation, $\triangle\ F=F^{n+1}-F^n\ and\ \ \triangle\ F_t=F_t^{n+1}-F_t^n$,neglecting the temporal truncation error,we obtain

$$\frac{\triangle\ F}{\triangle\ t}-\frac{1}{2}(-\mathbf{u}.\boldsymbol{\nabla}\triangle\ F+D_F\boldsymbol{\nabla}^2\triangle\ F-\sigma_F\triangle\ F)=(-\mathbf{u}.\boldsymbol{\nabla}F^{n}+D_F\boldsymbol{\nabla}^2F^{n}-\sigma_F F^{n})\tag{3}$$

Equation 2:

$$\tfrac{G(t^{n+1})-G(t^n)}{\triangle t}=\tfrac{1}{2}(D_G\boldsymbol{\nabla}^2G^{n+1}-\sigma_G G^{n+1}+\hat{\sigma}_{GF}F^{n+1})+\tfrac{1}{2}(D_G\boldsymbol{\nabla}^2G^{n}-\sigma_G G^{n}+\hat{\sigma}_{GF}F^{n})\Rightarrow$$

$$\tfrac{G(t^{n+1})-G(t^n)}{\triangle t}-\tfrac{1}{2}(D_G\boldsymbol{\nabla}^2G^{n+1}-\sigma_G G^{n+1}+\hat{\sigma}_{GF}F^{n+1})+\tfrac{1}{2}(D_G\boldsymbol{\nabla}^2G^{n}-\sigma_G G^{n}+\hat{\sigma}_{GF}F^{n})=$$

$$(D_G\boldsymbol{\nabla}^2G^{n}-\sigma_G G^{n}+\hat{\sigma}_{GF}F^{n})$$

Implementing the notation, $\triangle\ G=G^{n+1}-G^n\ and\ \ \triangle\ G_t=G_t^{n+1}-G_t^n$,we obtain

$$\frac{\triangle\ G}{\triangle\ t}-\frac{1}{2}(D_G\boldsymbol{\nabla}^2\triangle\ G-\sigma_G\triangle\ G)=(D_G\boldsymbol{\nabla}^2G^{n}-\sigma_G G^{n})+\frac{1}{2}\hat{\sigma}_{GF}F^n+\frac{1}{2}\hat{\sigma}_{GF}F^{n+1}\tag{4}$$

If we compare the equation 3 with a general form

$$\frac{\triangle\ F}{\triangle\ t}-WF_t^{n+1}=w\ F_t^n$$

we can obtain $W=\frac{1}{2}$ and w=1.

Weak Form:

Here, we present the Galerkin formulation associated with the strong form of the equations 3 and 4. The space of weighting functions denoted by $\mathcal{V}$ satisfies the dirichlet boundary conditions on Γ_D The functions, w, in $\mathcal{V}$ do not depend on time.$\mathcal{V}=\{w\in H^1(\Omega)|w=0\ on\ \Gamma_D\}$. The time dependency of the approximate solution F can be translated to the trial space $\mathcal{S}_t$, which varies as a function of time, $\mathcal{S}_t=\{F|F(.,t)\in\mathcal{H}^1(\Omega),t\in[0,T]\ and\ F(\mathbf{x},t)=F_D\ for\ \mathbf{x}\in\Gamma_D\}$. The same can be generalised for G. The weak form is obtained multiplying the equations (3 and 4) by the test function w, the result integrated over the computational domain Ω, and following this, integrating by parts the term involving $\boldsymbol{\nabla}^2$, thereby generating the natural boundary condition on F and G on Γ_N.After which the given boundary conditions are applied. The obtained results have been delineated below.For equation 3,we obtain:

$$(w,\frac{\triangle\ F}{\triangle\ t})+\frac{1}{2}[\mathbf{C}(\mathbf{u};w,\triangle\ F)+\mathbf{a}(w,\triangle\ F)+(w,\sigma_F\triangle\ F)]=-[\mathbf{C}(\mathbf{u};w,F^n)+\mathbf{a}(w,F^n)+(w,\sigma_F F^n)]$$

For equation 4,we obtain:

$$(w,\frac{\triangle\ G}{\triangle\ t})+\frac{1}{2}[\mathbf{a}(w,\triangle\ G)+(w,\sigma_G\triangle\ G)]=-[\mathbf{a}(w,G^n)+(w,\sigma_G G^n)]+(w,\frac{1}{2}\hat{\sigma}_{GF}F^n)+(w,\frac{1}{2}\hat{\sigma}_{GF}F^{n+1})$$

The numerical solutions to be obtained are represented as :

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

$$G^h(\mathbf{x},t) = \sum_{A\in\eta\neq\eta_D} N_A(\mathbf{x})G_A(t) + \sum_{A\in\eta=\eta_D} N_A(\mathbf{x})G_D(\mathbf{x}_A,t)$$

where, η is the set of global node numbers in the finite element mesh and $\eta_D \in \eta$, the subset of nodes belonging to the Dirichlet portion of the boundary,Γ_D.The shape function, $N_A(\mathbf{x})$, is the standard bilinear shape functions for quadrilaterals in 2D and is independent of time. The dirichilet boundary conditions are implemented using the Lagrange multiplier method.The matrices $\mathbf{M},\mathbf{C},\mathbf{a}$ are defines as:

$M_{ab}{}^e = \int_{\Omega^e} N_a\ N_b\ \ d\Omega; \quad \mathbf{C}(\mathbf{u};w,F) = \int_{\Omega} w\ (\mathbf{u}.\nabla F)\ \ d\Omega$

$\mathbf{a}(w,F) = \int_{\Omega} \nabla w.\ (D_F\ \nabla F)\ \ d\Omega\ ; \quad (w,\sigma_F F) = \int_{\Omega} w.\ (\sigma_F\ F)\ \ d\Omega$

These can be generalised for G too. The matrices $\mathbf{M},\mathbf{C},\mathbf{a}$ are obtained, as usual, from the assembly of element contributions.

Solution:

Using the above mentioned procedures the given transport problem has been solved. The Matlab code for this case has been uploaded on the virtual center with the folder name Q1. To obtain the solution, A uniform mesh of 20*10 elements have been selected in the directions of r and θ respectively. Time step size has been set as 0.01 s. Final time has been chosen as sufficiently high (20 seconds), such that the solution reaches the steady state by the final time step. The obtained distribution of the actin filament's density,F, over the computational domain at the final time step has been delineated in the Figure 2. The contour of the actin filament's density,F , obtained at the final time step has been shown in the Figure 3.

For the first case, an unsteady convection- diffusion -reaction equation is solved. Also it is investigated that the mesh Peclet's (Pe) is low for the considered case. So, convection does not dominate the diffusion. Therefore, Galerkin method provides better results. Also the implemented Crank Nicolson method is always stable. We have considered a very small time step , it results in a small courant number for the considered mesh size. So we can conclude that we obtain more improved(more accurate) solutions. From the obtained solution it can be observed that, the actin filament's density, F is 80 at the upper boundary of the computational domain, where the dirichilet boundary conditions were implemented. With time it reaches a minimum of 21.98 when the steady state prevails, at the final time step, in the computational domain due to the combined effect of convection-diffusion-reaction.

In the second case, an unsteady diffusion-reaction has been solved. So, due to the absence of the convection term, the Galarkin method behaves well.The obtained distribution of the Monomer's density,G,at the final time-step, over the computational domain has been delineated in the Figure 4. The contour of the Monomer's density,G , obtained at the final time step has been shown in the Figure 5. As for the observed case we have considered the CN method to solve the equation, we can conclude that we obtain reasonably accurate solutions for the considered parameters. To obtain the solution of G, at the n+1 th time step, it uses the solution values of the F in its source term, which were obtained corresponding to the n and n+1 time steps. For the considered parameters, it is observed that the obtained solution decreases from a maximum value of $G = 14.1$ to a minimum value of $G = 7.31$ due to the combined effects of the diffusion and reaction when the steady state prevails. The observations have been made at the end of the final time step.

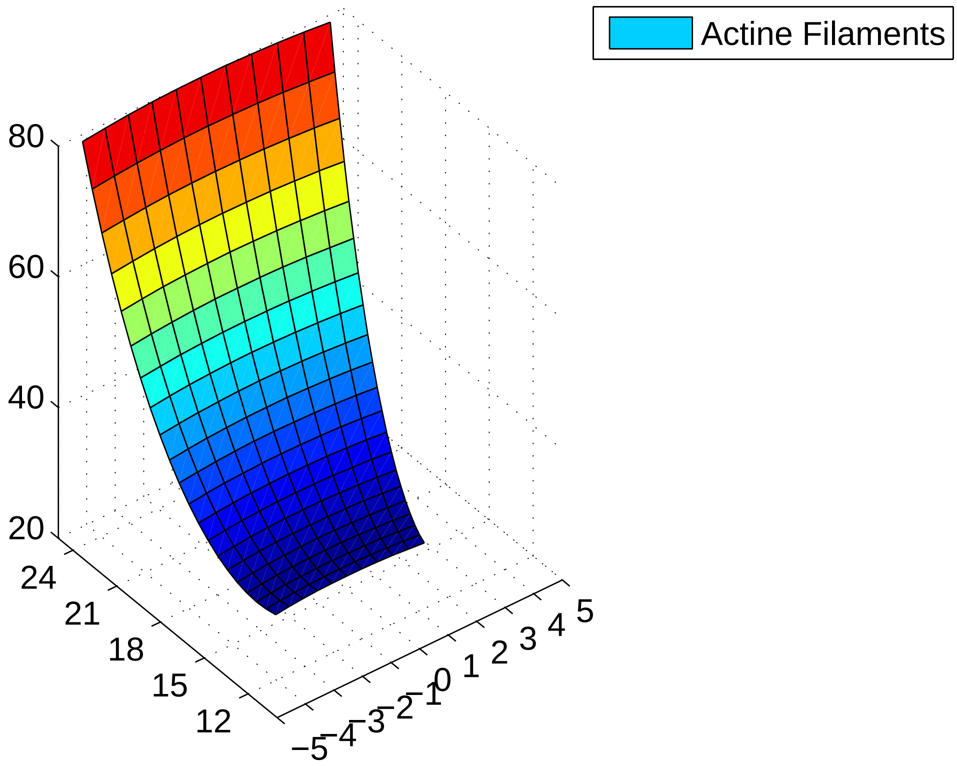

Figure 2: Distribution of the actin Filament's density,F over the computational domain

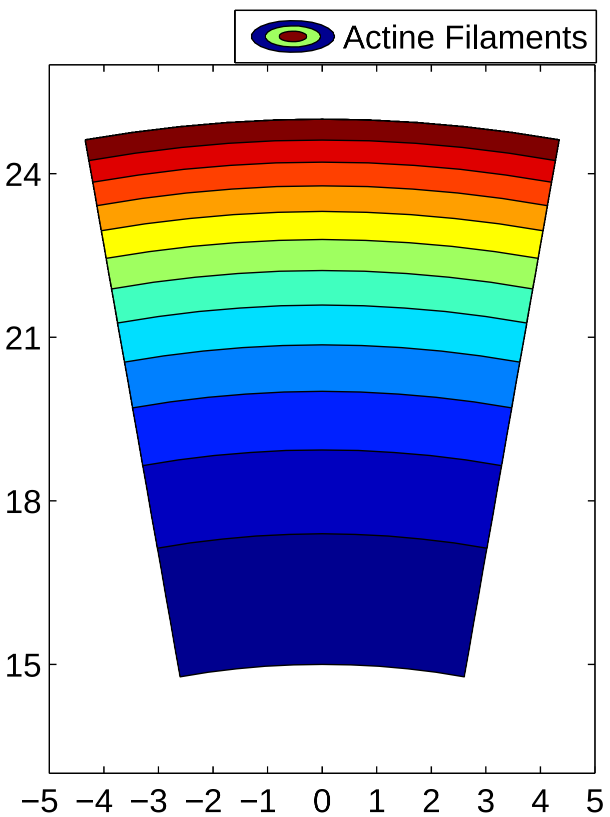

Figure 3: Contour of the actin Filament's density,F over the computational domain

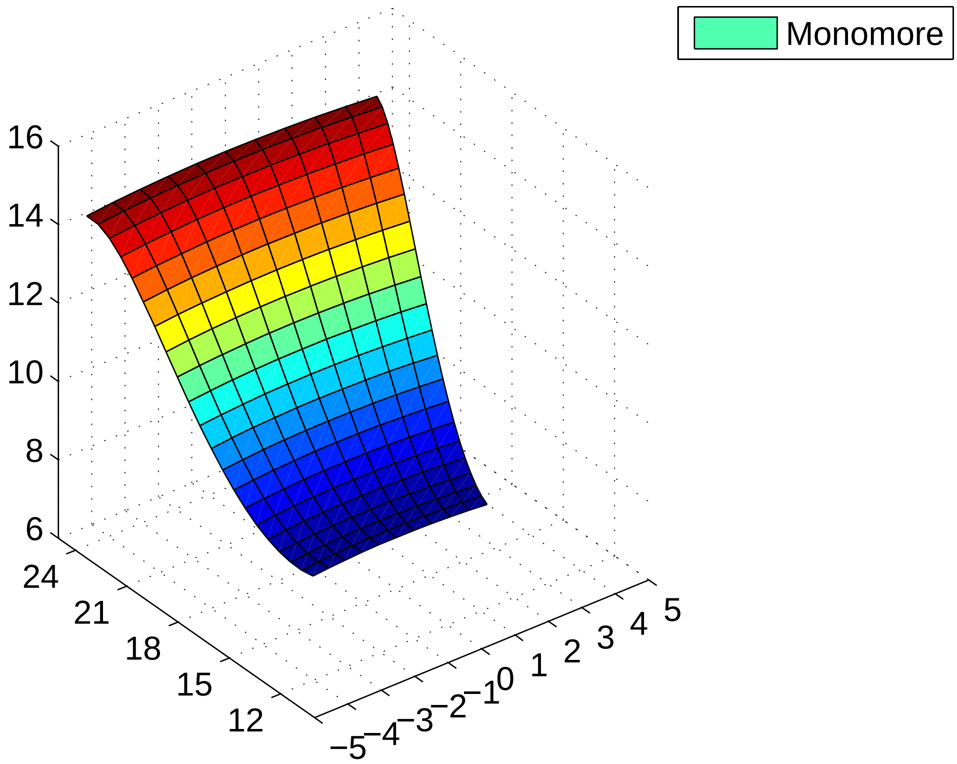

Figure 4: Distribution of the Monomer's density,G over the computational domain

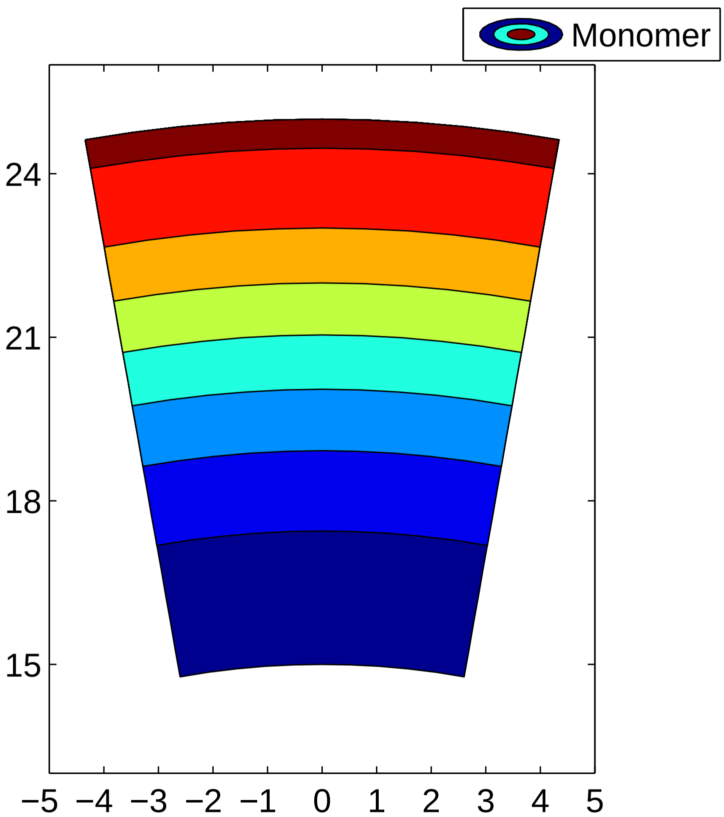

Figure 5: Contour of the Monomer's density,G over the computational domain

2. STOKES PROBLEM:

Problem statement:

In differential form, a steady Stokes problem is stated as follows in terms of Cauchy stress: given the body force as zero, prescribed velocities $\mathbf{u}_D$ on portion Γ_D of the boundary and imposed boundary tractions,$\mathbf{t} = 0$ on the remaining portion, we need to determine the velocity field $\mathbf{u}$ and the pressure field p in the given domain such that:

$$\boldsymbol{\nabla}.\boldsymbol{\sigma} = 0 \tag{5}$$

$$\boldsymbol{\nabla}.\mathbf{u} = 0 \tag{6}$$

Given Essential Boundary conditions:
$u_r(r = 15) = -0.15, u_\theta(r = 15) = 0$
$u_r(r = 25) = -0.30, u_\theta(r = 25) = 0$
Modified Implemented Boundary Conditions:

We know that $u = u_r \cos(\theta) - u_\theta \sin(\theta)$ $\;$ *and* $\;$ $v = u_r \sin(\theta) + u_\theta \cos(\theta) \Rightarrow$
$u = u_r \cos(\theta)$ $\;$ *and* $\;$ $v = u_r \sin(\theta)$ $\;$ *as* $u_\theta = 0$
$u(r = 15) = -0.15 \cos(\theta); v(r = 15) = -0.15 \sin(\theta)$
$u(r = 25) = -0.3 \cos(\theta); v(r = 25) = -0.3 \sin(\theta)$

A viscosity to be considered as $\gamma = 10^3 pN.s/\mu m.$ It can be noted that a constitutive equation is needed to close the problem. That is, the Cauchy stress,σ, must be related to velocity, $\mathbf{u}$, and pressure, p, that is $\boldsymbol{\sigma} = \boldsymbol{\sigma}(p, \mathbf{u})$, for instance by the linear Stokes' law $\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\boldsymbol{\nabla}^s\mathbf{u}$.

The Stokes equations define a constrained equilibrium problem. Among many other solution methods, here, the Lagrange multiplier method is used to solve the Stokes problem. In this method, the minimization of an objective function (the total potential energy) subject to constraints (the incompressibility) corresponds to the stationary points of the sum of the objective function and the constraints weighted by the Lagrange multipliers.

The weak form is obtained multiplying the equation of motion (5) by the velocity test function $\mathbf{w}$ and integrating by parts the stress term, thereby generating the natural boundary condition (but, given $\mathbf{t} = 0$) on Γ_N.Similarly, the incompressibility condition (6) is multiplied by the pressure test function q and the result integrated over the computational domain Ω.Thus the weak form of Stokes problem becomes: given $\mathbf{b}$=0,$\boldsymbol{u}_D$and the boundary traction $\mathbf{t} = 0$, find the velocity field $\mathbf{u} \in \mathcal{S}$ and the pressure field $p \in \mathbb{Q}$, such that for all velocity test functions $\mathbf{w} \in \boldsymbol{\mathcal{V}}$ and all pressure test functions $q \in \mathbb{Q}$,where The trial solution space $\mathcal{S}$ containing the approximating functions for the velocity is thus characterized as follow $\mathcal{S} = \{\boldsymbol{u} \in H^1(\Omega) | \boldsymbol{u} = \boldsymbol{u}_D \; on \; \Gamma_D\}$. The weighting functions of the velocity, $\mathbf{w}$, belong to $\mathcal{V}$. Functions in this class have the same characteristics as those in class $\mathcal{S}$, except that the weighting functions are required to vanish on Γ_D where the velocity is prescribed. $\mathcal{V} = \{\boldsymbol{w} \in H^1(\Omega) | \boldsymbol{w} = 0 \; on \; \Gamma_D\}$. Finally, a space of functions, denoted as $\mathbb{Q}$, for the pressure is considered. As we see, spatial derivatives of pressure do not appear in the weak form of the (Stokes) problem; thus functions in $\mathbb{Q}$ are simply required to be square-integrable. Moreover, since there are no explicit boundary conditions on pressure, the space $\mathbb{Q}$,$\mathbb{Q} = \mathcal{L}_2(\Omega)$ (pressure space), suffices as the trial solution space and as the weighting function space. This case, the flow is not confined. When the linear Stokes' law can be invoked, it is preferable to start from a strong form of written in terms of velocity and pressure because in this form the velocity components are uncoupled. The strong form now becomes:

$$-\nu\boldsymbol{\nabla}^2\mathbf{u} + \boldsymbol{\nabla}p = 0 \;\; in \;\; \Omega \quad (equilibrium), \tag{7}$$

$$\boldsymbol{\nabla}.\mathbf{u} = 0 \;\; in \;\; \Omega \quad (Incompressibility \;\; condition), \tag{8}$$

$$\mathbf{u} = \mathbf{u}_D \;\; on \;\; \Gamma_D \quad (Dirichilet \;\; b.c.), \tag{9}$$

$$-p\mathbf{n} + \nu(\mathbf{n}.\boldsymbol{\nabla})\mathbf{u} = \mathbf{t} = 0 \quad on \;\; \Gamma_N \;\;\; (Neumann B.C.) \tag{10}$$

The weak formulation of Stokes problem can be written as:

$$-\nu \int_{\Gamma_N+\Gamma_D} \mathbf{w}.(\boldsymbol{\nabla}\mathbf{u}).\mathbf{n} \;\; d\Gamma \;\; + \nu \int_{\Omega} \boldsymbol{\nabla}\mathbf{w} : \boldsymbol{\nabla}\mathbf{u} \;\; d\Omega + \int_{\Gamma_N+\Gamma_D} p \; \mathbf{w}.\boldsymbol{n} \;\; d\Gamma \;\; - \int_{\Omega} p \; \boldsymbol{\nabla}.\mathbf{w} \;\; d\Omega = 0 \Rightarrow$$

As $\mathbf{t} = -p\mathbf{n} + \nu(\mathbf{n}.\boldsymbol{\nabla})\mathbf{u} = 0 \; on \; \Gamma_N$ and $\boldsymbol{w} = 0 \; on \; \Gamma_D$, So we obtain,

$$\nu \int_{\Omega} \boldsymbol{\nabla}\mathbf{w} : \boldsymbol{\nabla}\mathbf{u} \;\; d\Omega - \int_{\Omega} p \; \boldsymbol{\nabla}.\mathbf{w} \;\; d\Omega = 0 \quad \forall \mathbf{u} \in \mathcal{V} \tag{11}$$

$$\int_{\Omega} q \; \boldsymbol{\nabla}.\mathbf{u} \;\; d\Omega = 0 \qquad \forall q \in \mathcal{Q} \tag{12}$$

The above two equations can be written as:

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

$$a(\mathbf{w}, \mathbf{u}) = \nu \int_{\Omega} \boldsymbol{\nabla}\mathbf{w} : \boldsymbol{\nabla}\mathbf{u} \;\; d\Omega$$
$$b(\mathbf{w}, p) = -\int_{\Omega} p \; \boldsymbol{\nabla}.\mathbf{w} \;\; d\Omega$$
$$b(\mathbf{w}, q) = -\int_{\Omega} q \; \boldsymbol{\nabla}.\mathbf{w} \;\; d\Omega$$

To derive the matrix problem governing Stokes flow in the Galerkin formulation, we can introduce the above explained concepts for the trial and weighting functions into the Galerkin form. This results in the following set of nodal equations for the unknown components of the velocity field: for each $A \in \eta \backslash \eta_{D_i} \; and \; 1 \leq i \leq n_{sd}$

$$\sum_{j=1}^{n_{sd}} \left\{ \sum_{B \in \eta \backslash \eta_{D_j}} a(N_A e_i, N_B \; e_j) u_{jB} \right\} + \sum_{\hat{A} \in \hat{\eta}} b(N_A \; e_i, \hat{N}_{\hat{A}}) p_{\hat{A}} = -\sum_{j=1}^{n_{sd}} \left\{ \sum_{B \in \eta_{D_j}} a(N_A e_i, N_B \; e_j) u_{D_j} \right\}$$

Similarly, the following set of discrete equations corresponding to the incompressibility condition is obtained for $\hat{A} \in \hat{\eta}$:

$$\sum_{j=1}^{n_{sd}} \left\{ \sum_{B \in \eta \backslash \eta_{D_j}} b(N_B e_i, \hat{N}_{\hat{A}}) u_{iB} \right\} = -\sum_{i=1}^{n_{sd}} \left\{ \sum_{B \in \eta_{D_i}} (N_B e_i, \hat{N}_{\hat{A}}) u_{D_i} \right\}$$

From these equations it is found that the matrix system which governs the discrete Stokes problem assumes the following partitioned form:

$$\begin{pmatrix} \boldsymbol{K} & \boldsymbol{G} \\ \boldsymbol{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{h} \end{pmatrix} \tag{13}$$

Matrix $\mathbf{K}$ is the viscosity matrix and results from the discretization of $a(.,.)$. It is obtained, as usual, from the assembly of element contributions.Matrix $\mathbf{G}$ is the discrete gradient operator, and $\boldsymbol{G}^T$is the discrete divergence operator. Matrix $\mathbf{G}$ arises from the discretization of the term $b(\mathbf{w}, p)$ in the Galerkin variational form.Vectors $\mathbf{f}$ and $\mathbf{h}$ incorporate the effect of the velocity $\mathbf{u}_D$ prescribed on the Dirichlet portion Γ_D of the boundary. Vector $\mathbf{f}$ also includes the contributions emanating from the applied body force $\mathbf{b}$ and the prescribed traction $\mathbf{t}$ on the Neumann portion of the boundary. They are obtained, as usual, from the assembly of the corresponding element contributions.

Solvability condition and solution procedure:
It has been previously investigated that, provided the kernel (null space) of matrix **G** is zero, the global matrix (eq. 13) is non-singular, that is **u** and p are uniquely defined. If this is not the case, a stable and convergent velocity field might be obtained, but the pressure field is likely to present spurious and oscillatory results.The kernel of $n_{eq} \times \hat{n}_{eq}$matrix **G** is the set of all vectors **q** ($\hat{n}_{eq}$ components) such that $\mathbf{Gq} = 0$, namely
$ker(\mathbf{G}) := \{q \mid q \in R^{\hat{n}_{eq}} \; and \; \mathbf{Gq} = 0\}$, where n_{eq} is the number of velocity unknowns, and $\hat{n}_{eq}$ is the number of pressure unknowns, $\hat{n}_{eq} = dim(\mathcal{Q}^h)$. It is known that, to have $ker(\mathbf{G}) = 0$, the velocity and pressure interpolations must satisfy a compatibility condition, called the LBB condition. The LBB condition states that velocity and pressure spaces cannot be chosen arbitrarily, a link between them is necessary.
The given problem has been basically solved in the following two ways:

- Considering Continuous biquadratic velocity, Continuous bilinear pressure (Q2Q1 elements).
- Considering Continuous bilinear velocity, Continuous bilinear pressure (Q1Q1 elements).

Case 1::(Q2Q1 elements)

The Q2Q1 element method satisfies LBB condition, and Quadratic convergence is achieved. So using these elements, we can confirm that we obtain more accurate results. The given createMesh.m has been modified in order to become able to generate Q2Q1 mesh. Elements are numbered in the clock-wise direction. The code for this method has been uploaded on the virtual center with the folder name, Q2-CW-Q2Q1. The given boundary conditions were implemented. The obtained velocity profile in the computational domain has been shown in the Figure 7. The pressure distribution has been presented in the Figure 9. For this observation 10 elements have been considered in the r direction and 20 are considered in the theta direction.The obtained mesh for velocity and pressure for the considered case has been shown in the Figure 6. It can be observed that the velocity profile is radial in the negative direction and symmetric about $\theta = 0$. It has a higher value (-0.3)in the negative r direction near the upper edge of the boundary (r=25), and it has a lower value (-0.15), in the negative r direction near the lower edge (r=15) of the domain. The zero traction condition on the straight side of the boundary is reflected in the obtained figures. More accurate pressure results are obtained with this considered case.

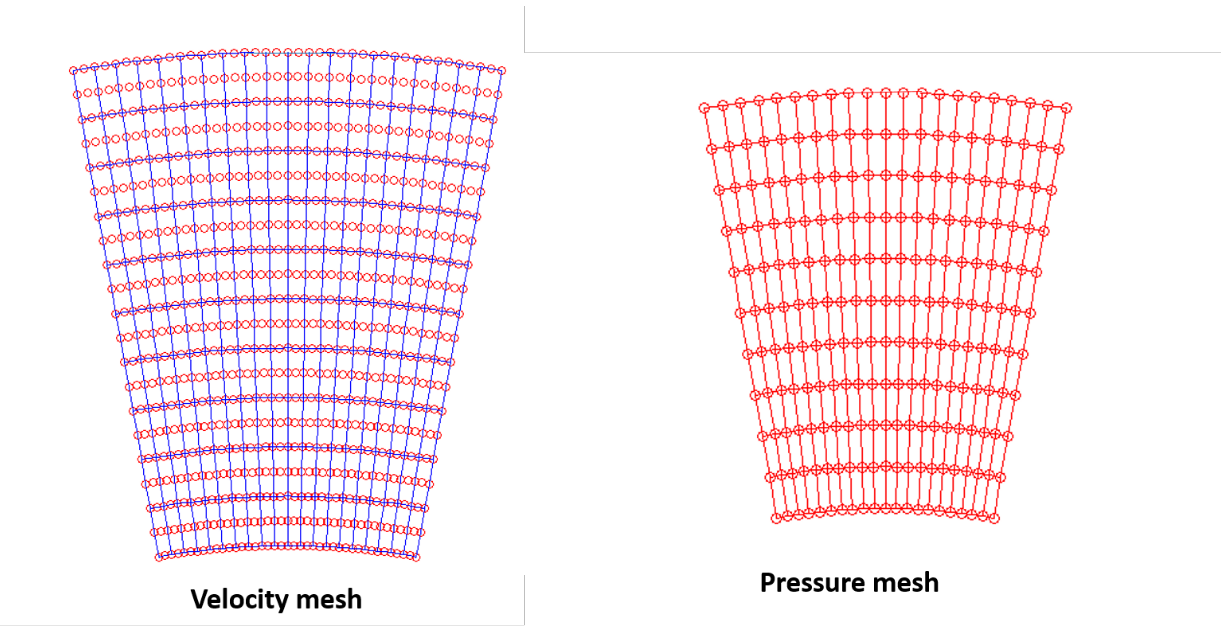

Figure 6: Q2Q1 10*20 mesh for velocity and pressure

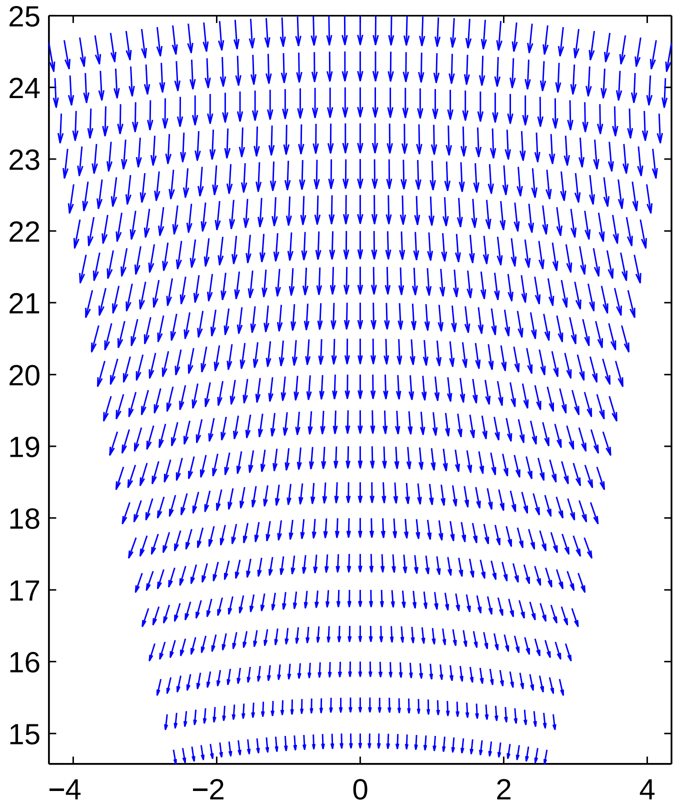

Figure 7: Velocity profile with Q2Q1 elements(10*20 mesh)

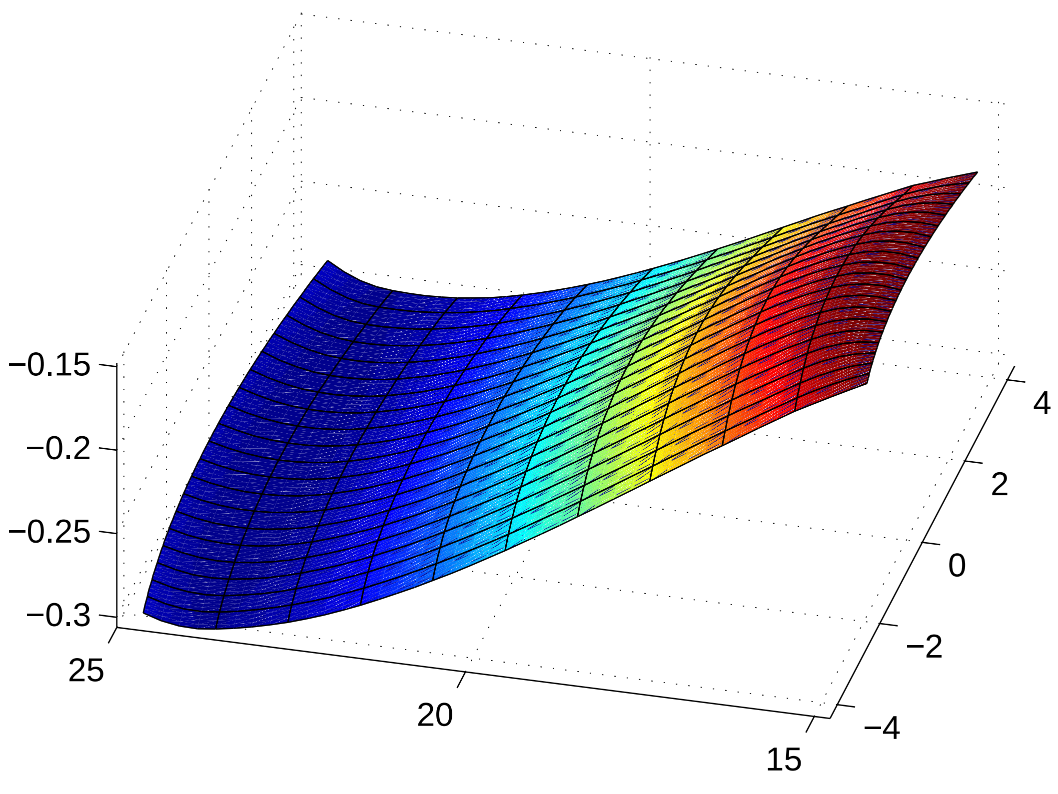

Figure 8: Contour of the velocity over the computational domain(10*20 mesh)

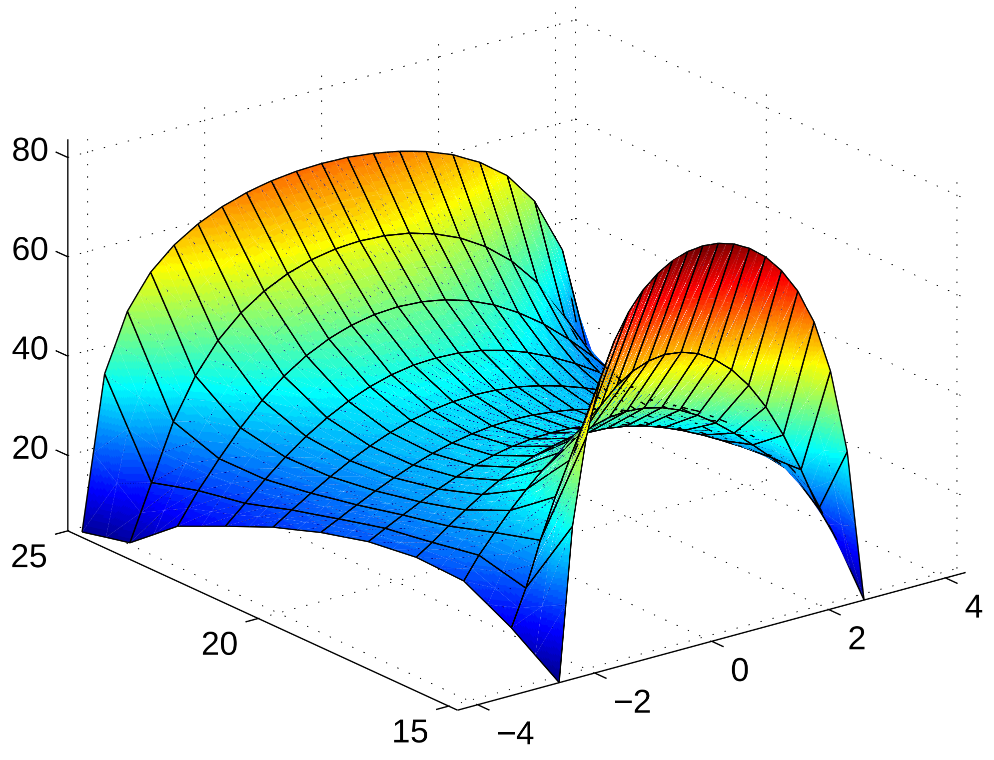

Figure 9: Pressure distribution with Q2Q1 elements (10*20 mesh)

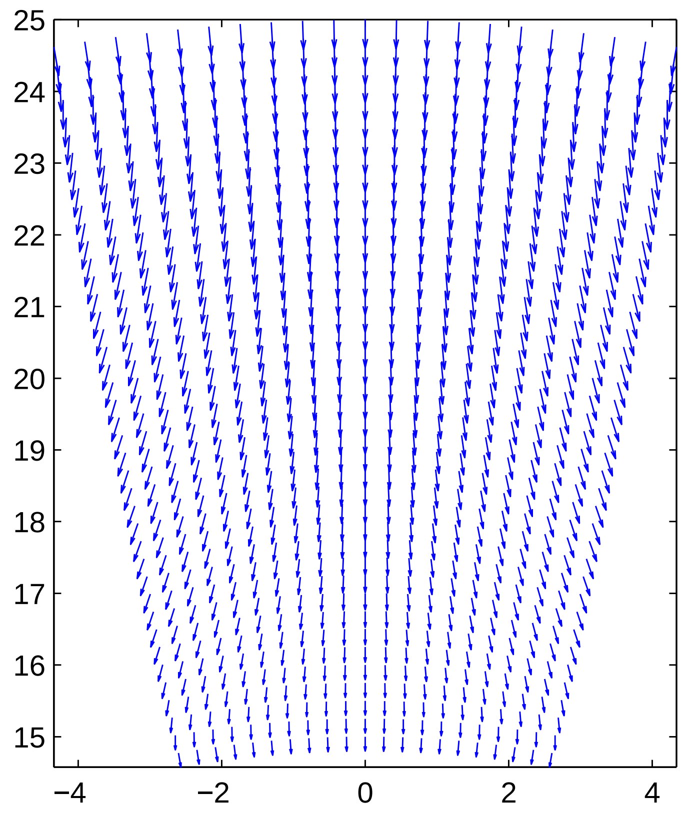

Figure 10: velocity profile with Q2Q1 elements (20*10 mesh)

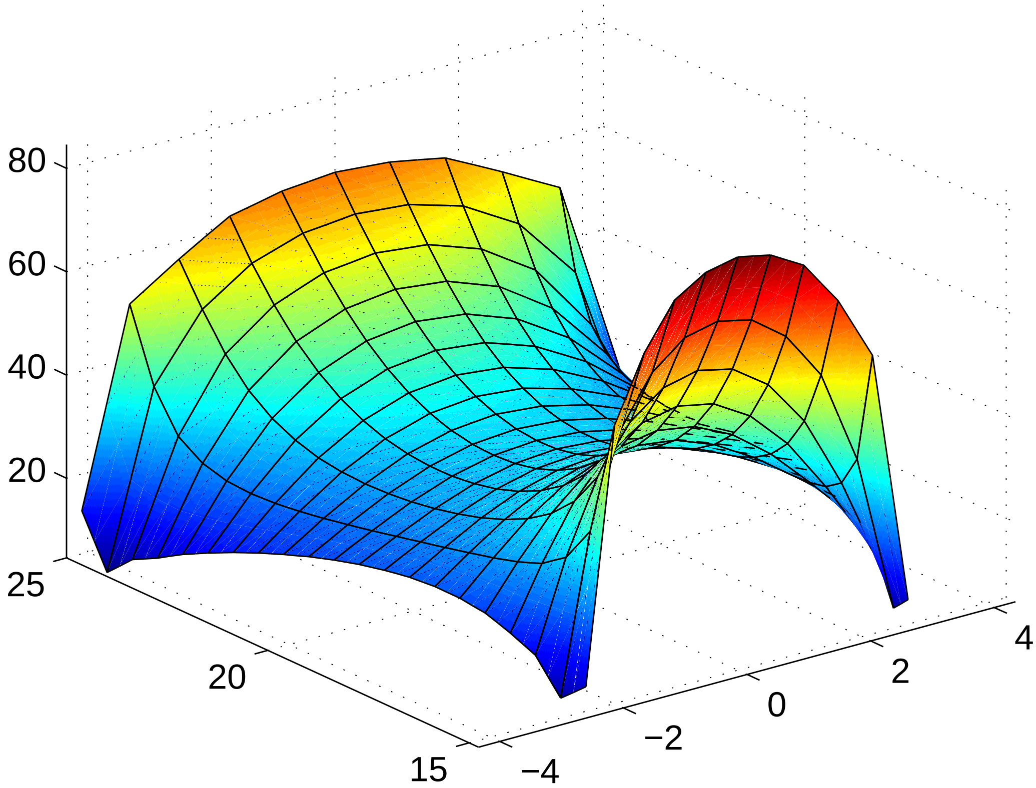

Figure 11: Pressure distribution with Q2Q1 elements (20*10 mesh)

Case 2:Using Q1Q1 elements:

The Q1Q1 element, (Continuous bilinear velocity, Continuous bilinear pressure),does not satisfy the LBB condition. Therefore, in this case stable and convergent velocity field might be obtained, but the pressure field is likely to present spurious and oscillatory results. So, a Stabilized formulation(GLS) of the Stokes problem has been used. The basic idea behind stabilization procedures is to enforce the positive definiteness of matrix $\begin{pmatrix} \boldsymbol{K} & \boldsymbol{G} \\ \boldsymbol{G}^T & \mathbf{0} \end{pmatrix}$.This can, for instance, be accomplished through a modification of the weak form of the incompressibility condition in order to render non-zero the diagonal term resulting from the incompressibility condition.The stabilization of the Stokes problem is obtained by adding to the Galerkin weak form (eq. 12,13) the previous equations emanating from the least-squares form. This entails a modification of both the momentum and the continuity equations. To avoid additional continuity requirements due to the presence of second spatial derivatives, the terms added to the Galerkin weak form act on the element interiors only. These terms depend on the residual of the momentum equation and therefore ensure the consistency of the stabilized formulation.The stabilized discrete problem is then formulated as

$$\mathbf{a}(\mathbf{w}^h, \mathbf{u}) + \mathbf{b}(\mathbf{w}^h, p^h) + \sum_{e=1}^{n_{el}} \tau_e(-\nu\ \boldsymbol{\nabla}^2 \mathbf{w}^h, -\nu\ \boldsymbol{\nabla}^2 \mathbf{u} + \boldsymbol{\nabla} p^h - \mathbf{b}^h)_{\Omega^e} = (\mathbf{w}^h, \mathbf{b}^h) + (\mathbf{w}^h, \mathbf{t}^h)_{\Gamma_N}$$

$$\mathbf{b}(\mathbf{u}, q^h) - \sum_{e=1}^{n_{el}} \tau_e(\boldsymbol{\nabla} q^h, -\nu\ \boldsymbol{\nabla}^2 \mathbf{u} + \boldsymbol{\nabla} p^h - \mathbf{b}^h)_{\Omega^e} = 0$$

$\mathbf{u} = \mathbf{u}^h + \mathbf{u}^h_D, \quad \mathcal{S}^h \subset \mathcal{S}, \quad \mathcal{V}^h \subset \mathcal{V}$

where τ_e is the stabilization parameter. It can be noted that due to the presence in the second equation of the term $(\nabla q^h, \nabla p^h)$ introduces a non-zero diagonal term in the partitioned matrix resulting from the spatial discretization of the above GLS weak form. This produces the desired stabilization of the pressure field.For linear elements the GLS stabilization does not affect the weak form of the momentum equation because the terms involving the second derivatives of the weighting function **w** vanish. So, for the given problem, the GLS formulation can be written as *find* $\mathbf{u}^h \in \mathcal{S}^h$ *and* $p^h \in \mathcal{Q}^h$, *such that* $,\forall\ (\mathbf{w}^h, q^h) \in \mathcal{V}^h \times \mathcal{Q}^h$,

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

$$\mathbf{b}(\mathbf{u}, q^h) - \sum_{e=1}^{n_{el}} \tau_e (\nabla q^h, \nabla p^h)_{\Omega^e} = 0$$

An interesting consequence of the GLS stabilization of the Stokes problem is that elements with equal order interpolations, which are unstable in the Galerkin formulation, now become stable. The stabilisation parameter τ_e is chosen as $\tau_e = \frac{\alpha_0 h_e^2}{4\nu}$, $\alpha_0 = 1/3$. The code for this implementation has been uploaded on the virtual center with the folder name Q2-ACW-Q1Q1-STABILIZED. Here all nodes are numbered in the anti clockwise direction. The obtained results for the velocity profile has been shown in the Figure 11. The obtained pressure distribution with the GLS stabilisation method has been shown in the Figure 13. It can be compared with the spurious pressure distribution obtained without using any stabilization techniques, presented in Figure 14. Spurious pressure solutions are observed in that Figure, associated with the Q1Q1 elements without the implementation of any stabilisation techniques(due to the reason that they do not satisfy the LBB condition). For this observation 10 elements have been considered in the r direction and 20 are considered in the theta direction.It can be observed that the velocity profile is radial in the negative direction and symmetric about $\theta = 0$. It has a higher value (-0.3)in the negative r direction near the upper edge (r=25), and it has a lower value (-0.15), in the negative r direction at the lower edge(r=15). The zero traction condition on the straight side of the boundary is reflected in the obtained figures.

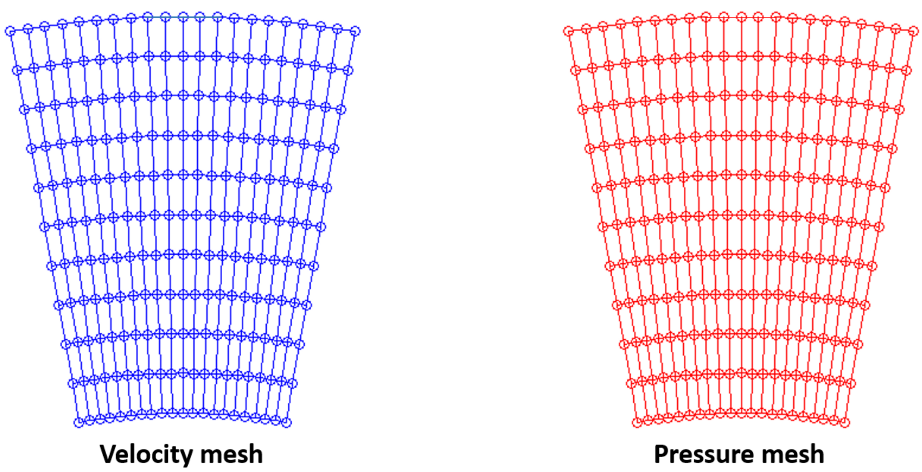

Figure 12: Q1Q1 10*20 mesh for velocity and pressure

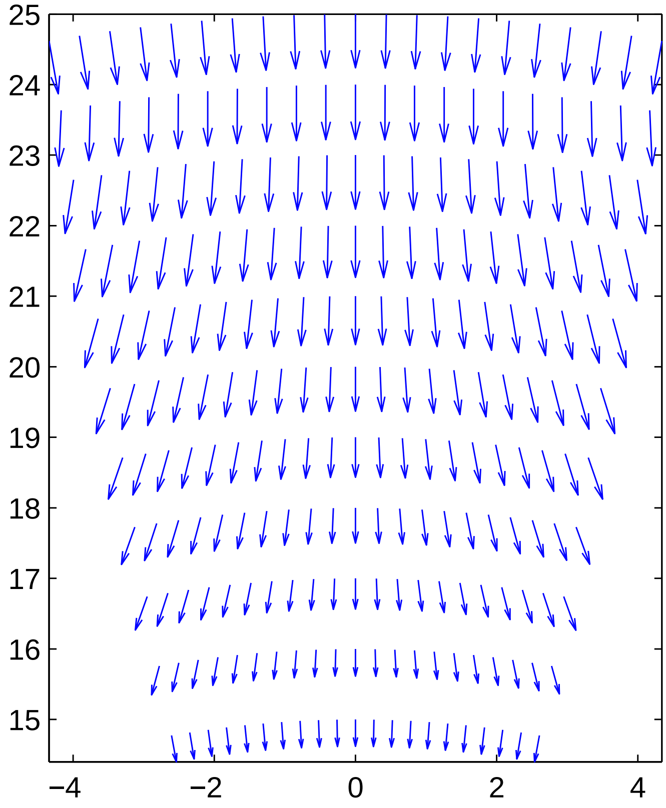

Figure 13: Velocity profile with Q1Q1 elements with GLS stabilisation(10*20 mesh)

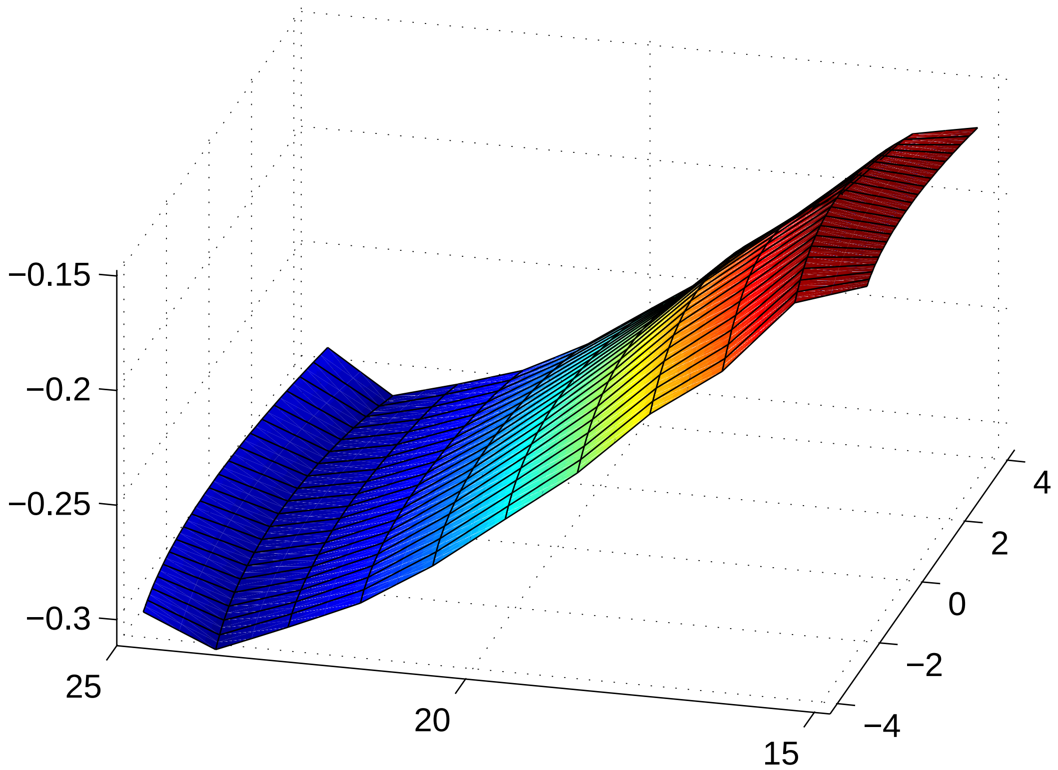

Figure 14: Contour of the velocity over the computational domain(10*20 mesh)

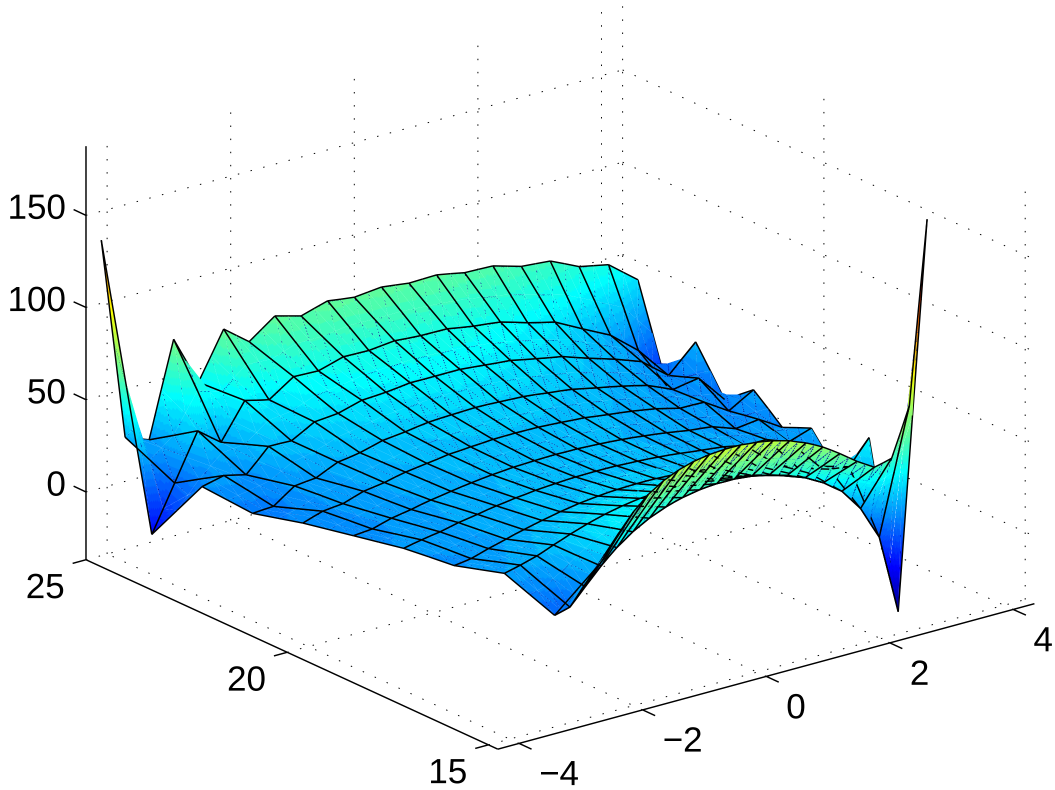

Figure 15: Pressure distribution, Q1Q1 elements with GLS stabilisation(10*20 mesh)

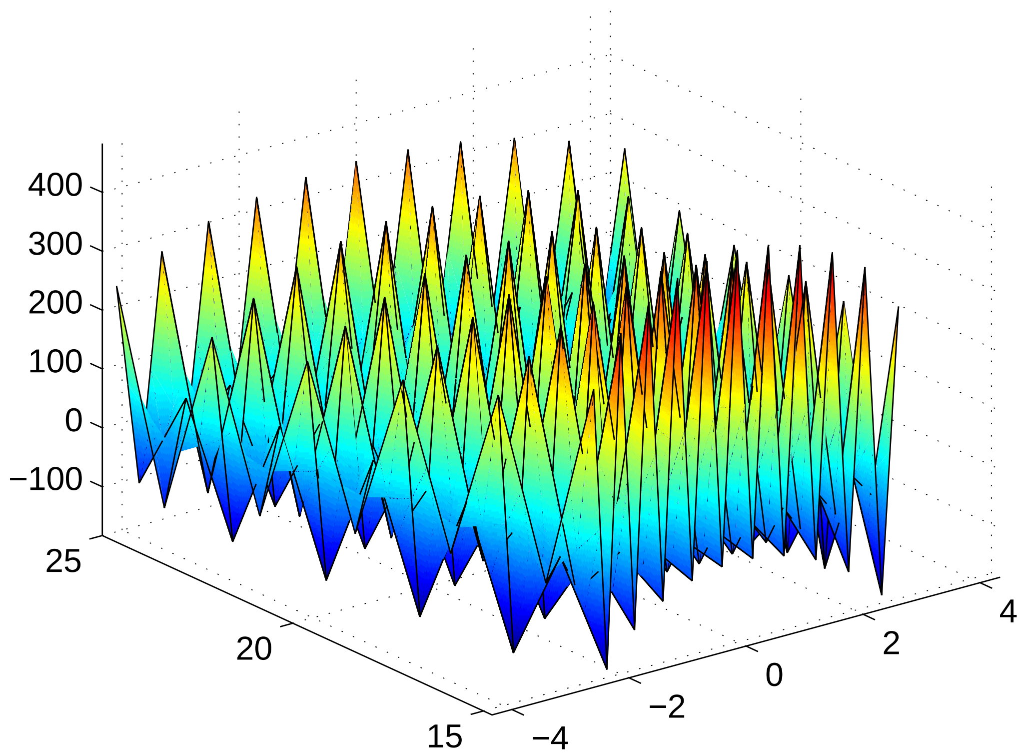

Figure 16: Spurious Pressure distribution, Q1Q1 elements without any stabilisation(10*20 mesh)

3.COUPLED PROBLEM:

Problem Statement:
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 fibers, the incompressibility constrain is dropped and pressure is neglected. Then, the equations governing the coupled problem can be written as:

$$\nu \boldsymbol{\nabla}.(\boldsymbol{\nabla}^s \boldsymbol{u}) + \boldsymbol{\nabla}.\boldsymbol{\sigma}_m(F) + \boldsymbol{T}_m(\boldsymbol{u}) = 0 \quad in\ (0,T)\times\Omega \tag{14}$$

$$F_t = \frac{\partial F}{\partial t} = -\mathbf{u}.\boldsymbol{\nabla} F + D_F \boldsymbol{\nabla}^2 F - \sigma_F F \qquad in\ (0,T)\times\Omega \tag{15}$$

$$G_t = \frac{\partial G}{\partial t} = D_G \boldsymbol{\nabla}^2 G - \sigma_G G + \hat{\sigma}_{GF} F \qquad in\ (0,T)\times\Omega \tag{16}$$

Where, $\boldsymbol{\nabla}.\boldsymbol{\sigma}_m$ and $\boldsymbol{T}_m$ are the surface forces on the leading edge. $\mathbf{u}$ is the fluid velocity and the following material parameters are used:
$D_F = 5\ \mu m/s, \sigma_F = 0.25s^{-1}, D_G = 15\ \mu m/s, \sigma_G = 2s^{-1}, \hat{\sigma}_{GF} = 0.5s^{-1}$

Boundary conditions:

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

Implemented initial Conditions:
$\mathbf{u}_0 = 0$
$F(\mathbf{x}, t=0) = 0\ \mu M$, and $G(\mathbf{x}, t=0) = 0\ \mu M$, where $\mathbf{x} \in \Omega$ has been considered.

Given Essential Boundary conditions for u:
$u_r(r=15) = -0.15, u_\theta(r=15) = 0$
$u_r(r=25) = -0.30, u_\theta(r=25) = 0$
Modified Implemented Boundary Conditions for u:

We know that $u = u_r\cos(\theta) - u_\theta\sin(\theta)\ \ and\ \ v = u_r\sin(\theta) + u_\theta\cos(\theta) \Rightarrow$
$u = u_r\cos(\theta)\ \ and\ \ v = u_r\sin(\theta)\ \ as\ u_\theta = 0$
$u(r=15) = -0.15\cos(\theta); v(r=15) = -0.15\sin(\theta)$
$u(r=25) = -0.3\cos(\theta); v(r=25) = -0.3\sin(\theta)$

A viscosity to be considered as $\nu = 10^3 pN.s/\mu m$.

Procedures: First, the coupled equations 14 and 15 are solved to obtain values of the **u** and F in the computational domain at each time step. The obtained solutions for F are used later in the equation 16 to solve for the values of G at each time time step in the given computational domain with respect to the above mentioned initial and boundary conditions. The equation 14 is written at the n+1 th time step, and the crank nicolson method is used to discretise the equation 15 and 16. The corresponding weak form is written to solve the equations 14 and 15 first, which are coupled together. Later similar to the question 1, the equation 16 is solved using the previously solved values of F for each time step.

The weak formulation is obtained, as usual like in the above questions, by projection of the equation (14) onto a space of weighting functions $\boldsymbol{w} \in \boldsymbol{\mathcal{V}}$,for the equation 14.For the equations 15 and 16, the test function w is similar to that we chose while solving the transport problem. The end result is the following variational problem:
given $\mathbf{b}$,$\mathbf{u}_D$, F_D,t and $\mathbf{u}_0$,find $\mathbf{u}(\mathbf{x},t) \in \boldsymbol{\mathcal{S}}\times]0,T[$ and $F(\mathbf{x},t) \in \mathcal{Q}\times]0,T[$, such that, $\forall(\boldsymbol{w}, w) \in \boldsymbol{\mathcal{V}} \times \mathcal{Q}$,

$$\nu\boldsymbol{\nabla}.(\boldsymbol{\nabla}^s\boldsymbol{u}^{n+1}) + \boldsymbol{\nabla}.\boldsymbol{\sigma}_m(F^{n+1}) + \boldsymbol{T}_m(\boldsymbol{u}^{n+1}) = 0 \Rightarrow$$
$$(\boldsymbol{w}, \nu\boldsymbol{\nabla}.(\boldsymbol{\nabla}^s\boldsymbol{u}^{n+1})) + (\boldsymbol{w}, \boldsymbol{\nabla}.\boldsymbol{\sigma}_m(F^{n+1})) + (\boldsymbol{w}, \boldsymbol{T}_m(\boldsymbol{u}^{n+1})) = 0 \Rightarrow$$
$$(\boldsymbol{w}, \nu\boldsymbol{\nabla}.(\boldsymbol{\nabla}^s\boldsymbol{u}^{n+1})) + \boldsymbol{T}_f F^{n+1} + \boldsymbol{T}_{\mathbf{u}}\mathbf{u}^{n+1} = 0$$

Integrating by parts the first term, and applying $\mathbf{w} = 0$ *on* Γ_D and neglecting other terms, we get

$$\int_\Omega \boldsymbol{\nabla}\mathbf{w} : \boldsymbol{\nabla}^s\mathbf{u}^{n+1} \quad d\Omega + \boldsymbol{T}_f F^{n+1} + \boldsymbol{T}_{\mathbf{u}}\mathbf{u}^{n+1} = 0 \tag{17}$$

Where $\boldsymbol{T}_u$ and $\boldsymbol{T}_f$ are matrices arising from the discretization of the terms on the boundary. $\boldsymbol{T}_u$ is a given matrix of dimension $(n_{ud}) \times (n_{ud})$ and $\boldsymbol{T}_f$ is a given matrix of dimension $(n_{ud}) \times (n_{fd})$. Where n_{ud} is the number of velocity degrees of freedom and n_{fd} is the number of degrees of freedom of the actin fiber. The above equation can be written as :

$$\mathbf{K}_s\mathbf{u}^{n+1} + \boldsymbol{T}_f F^{n+1} + \boldsymbol{T}_{\mathbf{u}}\mathbf{u}^{n+1} = 0 \tag{18}$$

For the equation 15, it is discretized in the similar manner using the Crank Nicolson scheme like we performed while solving the Transport problem. It is written like :

$$\frac{F(t^{n+1}) - F(t^n)}{\triangle\ t} - \frac{1}{2}(-\mathbf{u}^{n+1}.\boldsymbol{\nabla}F^{n+1} + D_F\boldsymbol{\nabla}^2F^{n+1} - \sigma_F F^{n+1}) = \frac{1}{2}(-\mathbf{u}^n.\boldsymbol{\nabla}F^n + D_F\boldsymbol{\nabla}^2F^n - \sigma_F F^n) \Rightarrow$$
$$\frac{F(t^{n+1})}{\triangle\ t} + \frac{1}{2}\mathbf{u}^{n+1}.\boldsymbol{\nabla}F^{n+1} - \frac{1}{2}D_F\boldsymbol{\nabla}^2F^{n+1} + \frac{1}{2}\sigma_F F^{n+1} = \frac{F(t^n)}{\triangle\ t} - \frac{1}{2}\mathbf{u}^n.\boldsymbol{\nabla}F^n + \frac{1}{2}D_F\boldsymbol{\nabla}^2F^n - \frac{1}{2}\sigma_F F^n \tag{19}$$

In the weak form it can be written as :

$$\left[\frac{\boldsymbol{M}}{\triangle\ t} + \frac{1}{2}\boldsymbol{C}(\mathbf{u}^{n+1}, F^{n+1}) + \frac{1}{2}D_F\boldsymbol{K}_F + \frac{1}{2}\sigma_F\ \boldsymbol{M}\right] F^{n+1} = \left[\frac{\boldsymbol{M}}{\triangle\ t} - \frac{1}{2}\boldsymbol{C}(\mathbf{u}^n, F^n) - \frac{1}{2}D_F\boldsymbol{K}_F - \frac{1}{2}\sigma_F\ \boldsymbol{M}\right] F^n \tag{20}$$

In the matrix form the above two coupled equations can be written as

$$\begin{pmatrix} \boldsymbol{K}_s + \boldsymbol{T}_u & \boldsymbol{T}_f \\ \mathbf{0} & \frac{\boldsymbol{M}}{\triangle t} + \frac{1}{2}\boldsymbol{C}(\mathbf{u}^{n+1}, F^{n+1}) + \frac{1}{2}D_F\boldsymbol{K}_F + \frac{1}{2}\sigma_F\boldsymbol{M} \end{pmatrix} \begin{pmatrix} \boldsymbol{u}^{n+1} \\ \boldsymbol{F}^{n+1} \end{pmatrix} =$$
$$\begin{pmatrix} \mathbf{0} \\ \left[\frac{\boldsymbol{M}}{\triangle t} - \frac{1}{2}\boldsymbol{C}(\mathbf{u}^n, F^n) - \frac{1}{2}D_F\boldsymbol{K}_F - \frac{1}{2}\sigma_F\ \boldsymbol{M}\right] F^n \end{pmatrix}$$

It is considered that $\boldsymbol{u} = \boldsymbol{u}^h + \boldsymbol{u}^D;\ F = F^h + F^D$. The previously mentioned boundary conditions for both F *and* $\mathbf{u}$ are implemented using the lagrange's multiplier method.

For the equation 15, it is discretized in the similar manner using the Crank Nicolson scheme like we performed while solving the Transport problem. It is written like :

$$\frac{G(t^{n+1}) - G(t^n)}{\triangle t} - \frac{1}{2}(D_G\boldsymbol{\nabla}^2G^{n+1} - \sigma_G G^{n+1} + \hat{\sigma}_{GF}F^{n+1}) + \frac{1}{2}(D_G\boldsymbol{\nabla}^2G^n - \sigma_G G^n + \hat{\sigma}_{GF}F^n) =$$

$$(D_G\boldsymbol{\nabla}^2G^n - \sigma_G G^n + \hat{\sigma}_{GF}F^n)$$

The weak form is obtained in the similar manner as we obtained in the question 1:

$$(w, \frac{\triangle\ G}{\triangle\ t}) + \frac{1}{2}[\mathbf{a}(w, \triangle\ G) + (w, \sigma_G \triangle\ G)] = -[\mathbf{a}(w, G^n) + (w, \sigma_G G^n)] + (w, \frac{1}{2}\hat{\sigma}_{GF}F^n) + (w, \frac{1}{2}\hat{\sigma}_{GF}F^{n+1}) \tag{21}$$

Where $\triangle\ G = G^{n+1} - G^n$

In order to treat the matrix $\boldsymbol{C}(\mathbf{u}^{n+1}, F^{n+1})$, which arises from the weak form of the term $(-\mathbf{u}^{n+1}.\boldsymbol{\nabla} F^{n+1})$, we use the Picard's iteration method.

At the first step : $\boldsymbol{C}({}^{k}\mathbf{u}^{n+1}, F^{n+1})$ is evaluated.${}^{k}\mathbf{u}^{n+1}$ can be considered as $\mathbf{u}^{n}$. After that the following system of equations are solved for $({}^{k+1}\mathbf{u}^{n+1})$.

$$\begin{pmatrix} \boldsymbol{K}_s + \boldsymbol{T}_u & \boldsymbol{T}_f \\ \mathbf{0} & \frac{\boldsymbol{M}}{\triangle t} + \frac{1}{2}\boldsymbol{C}({}^{k}\mathbf{u}^{n+1}, F^{n+1}) + \frac{1}{2}D_F\boldsymbol{K}_F + \frac{1}{2}\sigma_F\boldsymbol{M} \end{pmatrix} \begin{pmatrix} {}^{k+1}\boldsymbol{u}^{n+1} \\ \boldsymbol{F}^{n+1} \end{pmatrix} =$$

$$\begin{pmatrix} \mathbf{0} \\ \left[\frac{\boldsymbol{M}}{\triangle t} - \frac{1}{2}\boldsymbol{C}(\mathbf{u}^{n}, F^{n}) - \frac{1}{2}D_F\boldsymbol{K}_F - \frac{1}{2}\sigma_F\ \boldsymbol{M}\right] F^{n} \end{pmatrix}$$

After that we iterate k till the convergence is achieved for that time step.

Solution:

The given problem is solved using a Q1Q1 mesh of 20×10 elements. The time step has been chosen as 0.01 s. The final time has been selected as 15 s, such that by the final time step, the solution reaches the steady state. The code for this implementation has been uploaded on the virtual center with the file name HWQ3.The obtained velocity profile, the density of the actin filament (F), the density of the monomer(G),at the final time step, has been delineated in the Figures 17,18, and 19 respectively. In side the computational domain when the steady state prevails,at the final time step, the maximum value of F is observed as 80, and it achieves a minimum value of 72.3554. A maximum value of 0.198 and a minimum value of 0.1797 are observed for the monomer density,G, at the final time step, inside the computational domain.

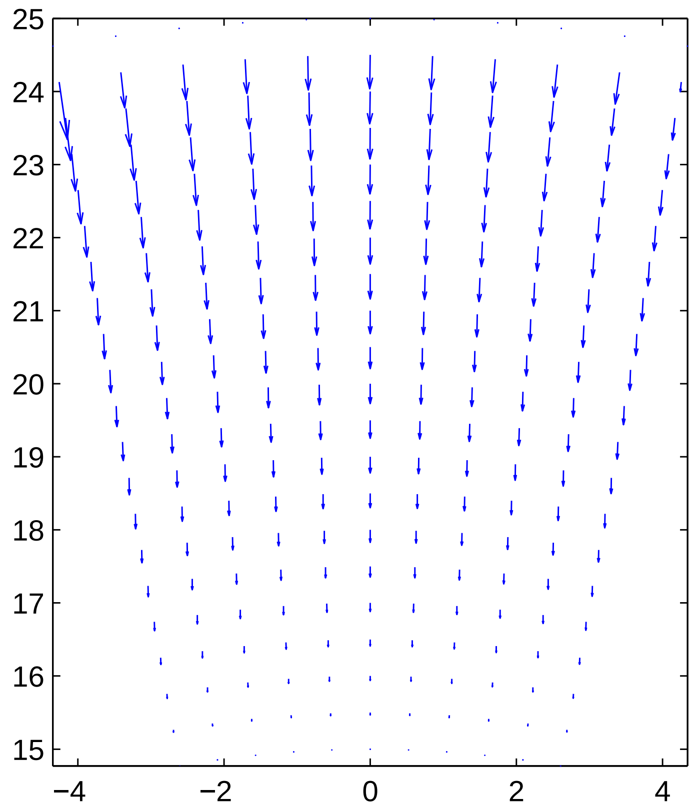

Figure 17: Velocity profile with Q1Q1 elements (20*10 mesh)

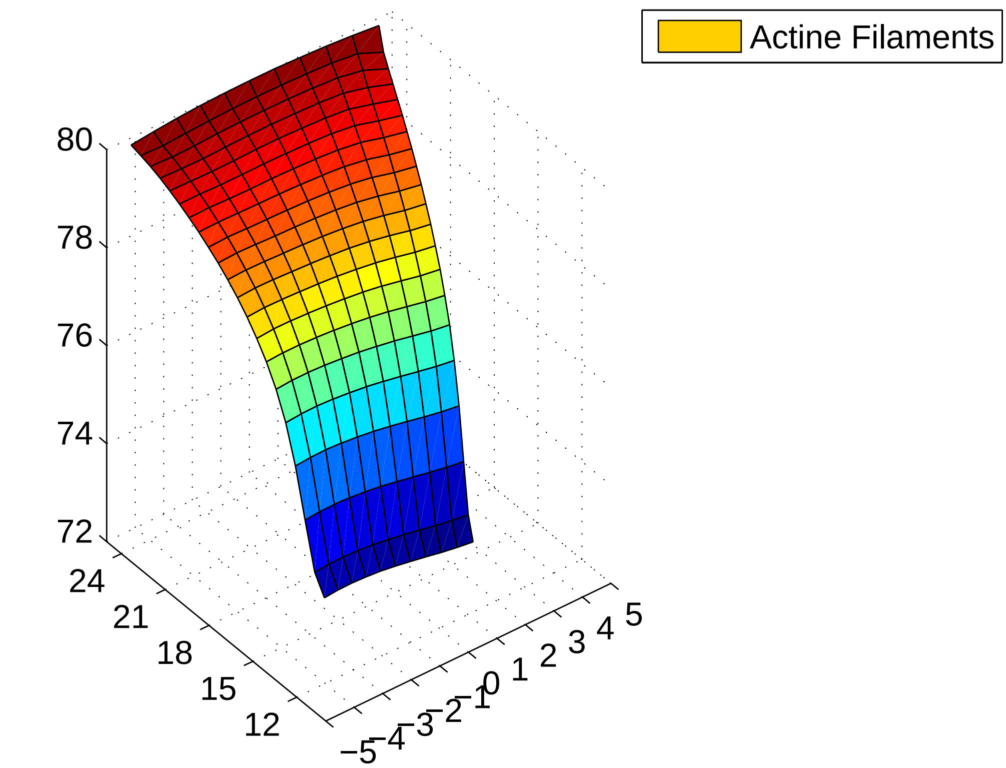

Figure 18: Actin filament density distribution,F(20*10 mesh)

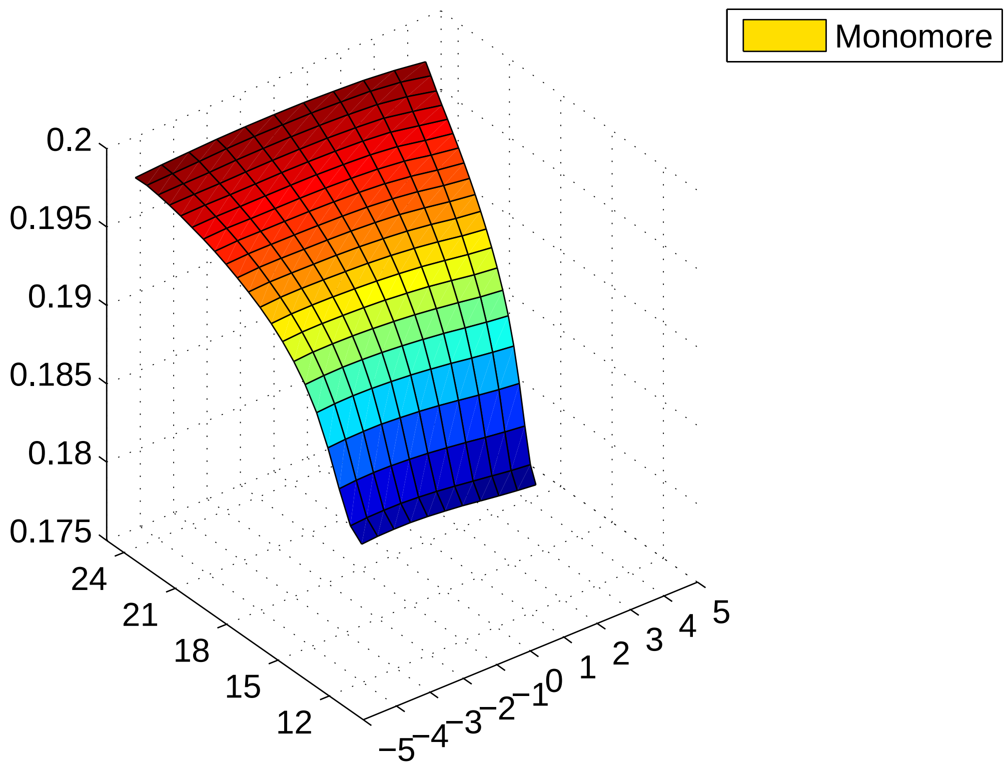

Figure 19: Monomer density distribution,G with Q1Q1 elements (20*10 mesh)