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A coupling procedure for the convection-diffusion problem and the stokes problem

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1 Introduction

Many physical phenomena are governed by PDEs and these equations can be approximated by finite element (FE) methods, which results in a sparse linear system of equations to be solved via numerical linear algebra. The ever-increasing demand of reality in the simulation of the complex scientific and engineering problems faced nowadays involves the solution of coupled problems.

Coupled convection-diffusion and stokes problems are very common in industrial application. One classical application is in the transport of air contaminants. In some circumstances, the stokes problem that model the convective part of the problem is conditioned by the amount of contaminants and, in the other way around, contaminants are convected by the underlying (Navier-)Stokes problem. Another application of the coupled (Navier-)Stokes and convectiondiffusion problems is in the medical industry which focuses on solving problems relevant to bioscience and biology. The proteins (actin filament in cells and hemoglobin in bloods) or monomers (amino acid and polysaccharides) exist in living body maintaining the vital signs. Here we are trying to model this kind of fluid with the goal to provide some numerical point of view for medical industry.

This report first provide the fractional-step method for solving Navier-Stokes equations numerically, and then explain the model to be solved numerically, and finally show some results.

Consider the general Navier-Stokes equations prescribed a purely Dirichlet boundary condition:

$$\begin{cases} \mathbf{u}_t - \nu \nabla^2 \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \mathbf{b} & in \quad \Omega \times]0, T[\\ \nabla \cdot \mathbf{u} = 0 & in \quad \Omega \times]0, T[\\ \mathbf{u} = \mathbf{u}_D & on \quad \Gamma_D \times]0, T[\\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) & in \quad \Omega \end{cases}$$
(1)

Solving equation 1 shows mainly two difficulties:

- Incompressibility constraint. The unknowns, velocity and pressure, cannot be discretized anyhow.Solution is guaranteed if interpolation spaces verify a stability condition known as inf-sup or LBB condition.
- Transient problem. The unknowns should advance in each time step which is similar to unsteady-convection-convection equation.

An effective method to solve the Navier-Stokes equations is the projection method computing the velocity field and pressure field separately by the computation of an intermediate velocity which is then projected onto the subspace of the solenoidal vector function. Basic to the derivation of the projection method is a theorem of orthogonal decomposition due to Ladyzhenskaya(1969), which is based on the Helmholtz decomposition principle. This theorem implies that any vector field \mathbf{v} defined on a simply connected domain can be uniquely decomposed into a divergence-free(solenoidal) part \mathbf{v}_{sol} and an irrotational part \mathbf{v}_{irrot} . Thus,

$$\mathbf{v} = \mathbf{v}_{sol} + \mathbf{v}_{irrot} = \mathbf{v}_{sol} + \nabla\phi \tag{2}$$

Since $\nabla \times \nabla \phi = 0$ for some scalar function, ϕ . Taking the divergence of equation 2,

$$\nabla \cdot \mathbf{v} = \nabla^2 \phi \quad with \quad \nabla \cdot \mathbf{v}_{sol} = 0 \tag{3}$$

So we obtain a Poisson equation for the scalar function ϕ . If the vector field **v** is obtained first, the above equation 3 would help solve for the scalar function ϕ and the divergence-free part of **v** can extracted,

$$\mathbf{v}_{sol} = \mathbf{v} - \nabla\phi \tag{4}$$

Equation 4 is the key point and principle of solenoidal projection method for solving incompressible Navier-Stokes equations.

1.1 Fractional-step method for Navier-Stokes equations

Here we use the Chorin's projection method which is member of fractional methods. The typical algorithm for solving time-discretized equations of the projection method consists of two consecutive steps. First given previous time-step velocity field \mathbf{u}^n , an intermediate velocity field \mathbf{u}_{int}^{n+1} is computed with the pressure term omitted, not satisfying the condition of incompressibility, shown as equation 5:

$$\begin{cases} \frac{\mathbf{u}_{int}^{n+1} - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^* \cdot \nabla) \mathbf{u}^{**} - \nu \nabla^2 \mathbf{u}^{**} = \mathbf{b}^{n+1} \\ \mathbf{u}_{int}^{n+1} = \mathbf{u}_D^{n+1} \quad on \quad \Gamma_D \end{cases}$$
(5)

for the treatment of the nonlinear convective term, there are three choices of velocities \mathbf{v}^* and \mathbf{v}^{**} ,

for the explicit Euler method, conditionally stable:

$$\mathbf{v}^* = \mathbf{v}^{**} = \mathbf{v}^n$$

for a semi-implicit method, unconditionally stable:

$$\mathbf{v}^* = \mathbf{v}^n \quad \mathbf{v}^{**} = \mathbf{v}_{int}^{n+1}$$

for the implicit Euler method, unconditionally stable:

$$\mathbf{v}^* = \mathbf{v}^{**} = \mathbf{v}_{int}^{n+1}$$

It is now necessary to derive a weak form of equation 5 to construct a finite element version for the first step. The goal for the current problem is to find the intermediate velocity $\mathbf{u}_{int}^{n+1} \in \mathcal{S}_{int}$, such that for all $\omega \in \mathcal{V}_{int}$,

$$(\mathbf{w}, \frac{\mathbf{u}_{int}^{n+1} - \mathbf{u}^n}{\Delta t}) + c(\mathbf{u}^*; \mathbf{w}, \mathbf{u}^{**}) + a(\mathbf{w}, \mathbf{u}^{**}) = (\mathbf{w}, \mathbf{b}^{n+1})$$

where the trilinear and bilinear forms have the same definition as before. And the functional spaces S_{int} and \mathcal{V}_{int} completely fulfill the Dirichlet boundary conditions, namely $\mathbf{u}_{int}^{n+1} = \mathbf{u}_D^{n+1}$ on Γ .

For semi-implicit and fully implicit method, the discretized algebraic system resulting from Galerkin method is shown in equation 6

$$\mathbf{M}_{1}\left(\frac{\mathbf{u}_{int}^{n+1} - \mathbf{u}^{n}}{\Delta t}\right) + (\mathbf{C}(\mathbf{u}^{*}) + \mathbf{K})\mathbf{u}_{int}^{n+1} = \mathbf{f}^{n+1}$$
(6)

where \mathbf{M}_1 is the consistent mass matrix, \mathbf{C} is the convection matrix, \mathbf{K} is the viscosity matrix, and vector \mathbf{f}^{n+1} includes the applied body force \mathbf{b} and Dirichlet boundary conditions.

In terms of the computational complexity, the fully implicit option, $\mathbf{v}^* = \mathbf{v}_{int}^{n+1}$, requires the times integration to repeat computations of the inverse of the nonlinear and non-symmetric matrix $\mathbf{M}_1 + \Delta t(\mathbf{C}(\mathbf{u}_{int}^{n+1}) + K)$. Predictor-corrector methods are usually implemented in this

case. For the semi-implicit methods, $\mathbf{v}^* = \mathbf{v}^n$, a modified convective term is adopted to maintain unconditional stability.

The *second step* of Chorin's projection is to determine the velocity \mathbf{v}^{n+1} and pressure p^{n+1} solving equation 7

$$\begin{cases} \frac{\mathbf{u}^{n+1} - \mathbf{u}_{int}^{n+1}}{\Delta t} + \nabla p^{n+1} = 0 & in \quad \Omega\\ \nabla \cdot \mathbf{u}^{n+1} = 0 & in \quad \Omega\\ \mathbf{n} \cdot \mathbf{u}^{n+1} = \mathbf{n} \cdot \mathbf{u}_D^{n+1} & on \quad \Gamma \end{cases}$$
(7)

Note that the last step involves the remaining term (pressure) and condition (incompressibility) of the Navier-Stokes equations. However, the boundary condition only prescribes the normal component of the velocity, not the tangential components. This is an key aspect of the method: the tangential components of the velocity cannot be controlled on the boundary according to Helmholtz decomposition principle, where a condition on the normal component can be prescribed only. In accordance with equation 4, the first of equation 7 can be rewritten as

$$\mathbf{u}^{n+1} = \mathbf{u}_{int}^{n+1} - \triangle t \nabla p^{n+1}$$

Now, the weak form of the second step equation 7 is: find the end-of-step velocity $\mathbf{u}^{n+1} \in \mathcal{S}$ and the pressure $p^{n+1} \in \mathcal{Q}$, such that, $\forall (\mathbf{w}, q) \in \mathcal{V} \times \mathcal{Q}$,

$$\begin{cases} (\mathbf{w}, \frac{\mathbf{u}^{n+1} - \mathbf{u}_{int}^{n+1}}{\Delta t}) + b(\mathbf{w}, p^{n+1}) = 0\\ b(\mathbf{u}^{n+1}, q) = 0 \end{cases}$$
(8)

where the function space S and V verify the prescribed boundary condition, $\mathbf{n} \cdot \mathbf{u}^{n+1} = \mathbf{n} \cdot \mathbf{u}_D^{n+1}$ on Γ . Similarly, the discretized formulation of equation 8 is,

$$\begin{cases} \mathbf{M}_{2}(\frac{\mathbf{u}^{n+1}-\mathbf{u}_{int}^{n+1}}{\Delta t}) + \mathbf{G}\mathbf{p}^{n+1} = 0\\ \mathbf{G}^{T}\mathbf{u}^{n+1} = 0 \end{cases}$$
(9)

or equivalently,

$$\begin{pmatrix} \mathbf{M}_2/\Delta t & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}^{n+1} \\ \mathbf{p}^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{M}_2 \mathbf{u}_{int}^{n+1}/\Delta t \\ \mathbf{0} \end{pmatrix}$$
(10)

1.2 Viscosity splitting fractional-step method

Although it is enough to solve to the Navier-Stokes equation through Chorin's projection method, the difficult regarding the imposition of Dirichlet boundary condition in the second step still exists. To alleviate this problem, Balsco, Codina and Huerta(1997;1998) introduced a viscosity splitting fractional-step method where the projection idea is avoided in the second step. They add a new diffusion term in the momentum equation in the second step, which thus loses its inviscid property for preventing control of the prescribed tangential component of the velocity at the boundary, as shown in equation 11:

$$\begin{cases} \frac{\mathbf{u}^{n+1} - \mathbf{u}_{int}^{n+1}}{\Delta t} - \nu \nabla^2 (\mathbf{u}^{n+1} - \mathbf{u}_{int}^{n+1}) + \nabla p^{n+1} = 0 \quad in \quad \Omega\\ \nabla \cdot \mathbf{u}^{n+1} = 0 \quad in \quad \Omega\\ \mathbf{u}^{n+1} = \mathbf{u}_D^{n+1} \quad on \quad \Gamma \end{cases}$$
(11)

Combined with equation 5 of the first step in Chorin's projection method, this formulation allow us to impose the original Dirichlet boundary conditions directly in both step, although the LBB condition is required to make it solvable.

1.3 Spatial discretization

The weak formulation can be obtained by projection equation 1 onto a space of weighting function $\mathbf{w}_1 \in \mathcal{V}$ for the momentum equation and $q \in \mathcal{Q}$ for the incompressibility condition. The following variational problem is thus the result: given \mathbf{b}, \mathbf{u}_D and \mathbf{u}_0 , find $\mathbf{u}(\mathbf{x}, t) \in \mathcal{S} \times]0, T[$ and $p(\mathbf{x}, t) \in \mathcal{Q} \times]0, T[$, such that, $\forall (\mathbf{w}_1, q) \in \mathcal{V} \times \mathcal{Q}$,

$$\begin{cases} (\mathbf{w}_1, \mathbf{u}_t) + a(\mathbf{w}_1, \mathbf{u}) + c(\mathbf{u}; \mathbf{w}_1, \mathbf{u}) + b(\mathbf{w}_1, p) = 0\\ b(\mathbf{u}, q) = 0 \end{cases}$$
(12)

In a matrix form

$$\begin{cases} \mathbf{M}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u} + \mathbf{G}p(t) = \mathbf{f}(t, \mathbf{v}(t)) \\ \mathbf{G}^{T}\mathbf{u}(t) = \mathbf{h}(t) \end{cases}$$
(13)

Let us denote some node indexes with superscripts a, b and the space indexes with subscripts i,j.Let N_u^a be the standard shape function associated to the velocity node a and N_p^c the standard shape function associated to be pressure node c. In general, the velocity and pressure interpolation may be different. So previous matrices in equation 13 are:

$$\begin{split} \mathbf{M}_{ij}^{ab} &= (\mathbf{N}_u^a, \mathbf{N}_u^b) \delta_{ij} \quad G_j^{cb} = -(\mathbf{N}_p^c, \partial_j \mathbf{N}_u^b) \\ \mathbf{K}_{ij}^{ab} &= (\mathbf{N}_u^a, \mathbf{u}^{n+\alpha} \cdot \nabla \mathbf{N}_u^b) \delta_{ij} + \nu (\nabla \mathbf{N}_u^a, \nabla \mathbf{N}_u^b) \delta_{ij} \\ \mathbf{h}(t) &= -(\mathbf{v}_d(t), \mathbf{N}_p) \quad \mathbf{f}(t, \mathbf{v}(t)) = -\mathbf{K}^{ab} \mathbf{v}_d(t) \end{split}$$

where δ_{ij} is the Kronecker δ .

1.4 Time discretization

Here we have to solve equation 13, a transient-diffusion Navier-Stokes equation. The technique used for unsteady-transportation-diffusion equation which updates the solution in each time step can also be applied to the current case. However, we could adopt *Chorin-Temam projection method*, where we compute the velocity and pressure fields through the computation of an intermediate velocity, which is then projected onto the subspace of the solenoidal vector function.

The *first step* includes the viscous and convective terms in the Navier-Stokes equation. Luckly we do not have convective terms here, thereby making $\mathbf{C}(\mathbf{u}^*) = 0$ in equation 6 to satisfy the current problem,

$$\mathbf{M}_{1}\left(\frac{\mathbf{u}_{int}^{n+1} - \mathbf{u}^{n}}{\Delta t}\right) + \mathbf{K}\mathbf{u}_{int}^{n+1} = \mathbf{f}^{n+1}$$
(14)

where $u^{**} = u_{int}^{n+1}$ for implicit Euler method. Rewrite equation 14 in terms of computation, the complete matrix form of first step for equation 1 is,

$$(\mathbf{M}_1 + \Delta t \mathbf{K}) \mathbf{u}_{int}^{n+1} = \mathbf{M}_1 \mathbf{u}^n + \Delta t \mathbf{f}^{n+1}$$
(15)

The second step of the projection method determines the end-of-step velocity \mathbf{u}^{n+1} and pressure p^{n+1} . Instead of the original projection method in the second step,here we adopt the viscosity splitting fractional-step method as equation 11, which helps alleviate the difficulties regards the imposition of Dirichlet boundary conditions in the original method. The problem now is to translate equation 11 from strong form to a final matrix form,

$$\begin{bmatrix} \frac{\mathbf{M}_2}{\Delta t} + \mathbf{K} & \mathbf{G} \\ \mathbf{G}^{\mathbf{T}} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u}^{\mathbf{n}+\mathbf{1}} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \frac{\mathbf{M}_2 \mathbf{u}_{int}^{n+1}}{\Delta t} + \mathbf{K} \mathbf{u}_{int}^{n+1} \\ \mathbf{0} \end{bmatrix}$$
(16)

The final projection method has been applied to construct the matrix formulation for equation 1 into two consecutive, equation 15 and 16.

2 Coupled convection-diffusion and stokes model

2.1 Physical background

We are going to propose a model which describes one kind of fluid which are compressible and convected with neglected dynamic internal pressure, which exist in many life entities. In the computational biology community, there are many mathematical models trying to simulate the vital movement such as blood circulation and cell migration which play important roles in medical industry ,for example, actin dynamics in cell motility, cancer or embryogenesis.

The actin flow acts as an engine for the effective motion of motile cells by means of protrusive and retractile mechanisms conditioned also by myosin motors. Different mathematical and numerical models have appeared in literature to model the action flow. Generally, these equations include a force balance of the action-myosin network modeled by Stokes flow and mass conservation law modeled by transient-convection-diffusion equation.

2.2 Mass conservation and stress generation

According to the conservation law, we have the mass conservations in following forms,

$$\frac{dm}{dt} = \frac{\partial m}{\partial t} + \nabla \cdot (\mathbf{u}\rho) = 0 \tag{17}$$

It is worthy note that equation 17 considers only the physical transport of a substance in a velocity field, where there is no chemical reaction. Once the chemical reaction is involved, we shall consider a well-mixed system consisting of an active form, A, and an inactive form, B, of the same materials but in different status,

$$B \rightleftharpoons A$$
 (18)

In biology, the reaction rate are governed by Hill function[2] which provide the following kinetic function with maximal rate γ and saturation parameter K,

$$f(a,b) = b(k_0 + \frac{\gamma a^2}{K^2 + a^2}) - \delta a$$
(19)

where k_0 is the basal conversion rate, δ is reverse reaction rate.

In cell migration, the myosin is governed by a transient convection-diffusion-reaction equation,

$$\frac{\partial \rho_{m1}}{\partial t} = \nabla \cdot (D_{m1} \nabla \rho_{m1}) - \nabla \cdot (\mathbf{u} \rho_{m1}) + f_m(\rho_{m1}, \rho_{m0})$$
(20)

$$\frac{\partial \rho_{m0}}{\partial t} = \nabla \cdot \left(D_{m0} \nabla \rho_{m0} \right) - \nabla \cdot \left(\mathbf{u} \rho_{m0} \right) - f_m(\rho_{m1}, \rho_{m0}) \tag{21}$$

where f_m is the mass-conserved kinetic function with form like in equation 19; ρ_{m1} and ρ_{m0} are the myosin either associated with or dissociated from F-actin network. The total amount of myosin is conserved. On the other hand, the actin in cell migration is also mass conserved,

$$\frac{\partial \rho_{a1}}{\partial t} = \nabla \cdot (D_{a1} \nabla \rho_{a1}) - \nabla \cdot (\mathbf{u} \rho_{a1}) + f_a(\rho_{a1}, \rho_{a0})$$
(22)

$$\frac{\partial \rho_{a0}}{\partial t} = \nabla \cdot (D_{a0} \nabla \rho_{a0}) - \nabla \cdot (\mathbf{u} \rho_{a0}) - f_a(\rho_{a1}, \rho_{a0})$$
(23)

where ρ_{a1} is the concentration of actin filament and ρ_{a1} is the concentration of actin monomers.

2.3 Force balance of the actin-myosin network

Several studies have proposed different hyperbolic model describing the actin-myosin network. One of these model is as the following formulation[1],

$$\rho_{a1}(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \nu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \nabla \cdot \tau^{myo} + \mathbf{F}$$
(24)

Where **u** is the local flow velocity in the coordinate system; ρ_{a1} is the density of the fluids. The right-hand side describes the local forces: p is pressure; the second term is the stress generated by strain deformation; the last term is responsible for other kind of forces for example in cell migration this term would include the stress generated by myosin contractile stress, τ^{myo} , and some effective viscous drag, \mathbf{F}_{adh} .

$$\rho_{a1}\frac{\partial \mathbf{u}}{\partial t} = \nu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \nabla \cdot \tau^{myo} + \mathbf{F}$$
(25)

In medical industry for solving fluid problems, they are usually fluids of low Reynolds numbers especially in cell biology, so we can drop the nonlinear term $(\mathbf{u} \cdot \nabla)\mathbf{u}$. Also, we can drop the pressure terms because this terms originates from the incompressibility of the combined polymer/fluid system. However, in biology, the polymers are usually compressible. So the final force equation is shown in equation 25

3 Results and analysis

The proposed PDEs (Eq.20, 21, 22, 23 and 25) model is solved numerically, and we are going to show the results with different initial conditions. As boundary conditions, we implemented zero-flux boundary in order to keep the quantity conserved in the who domain. The results are shown below with different initial conditions,

3.1 Uniform initial condition

In this case, the initial condition is constant for each equations,

$$\rho_{m1}(t=0) = 1, \quad \rho_{m0}(t=0) = 0$$
$$\rho_{a1}(t=0) = 1, \quad \rho_{a0}(t=0) = 0$$
$$\mathbf{u}_x(t=0) = 0, \quad \mathbf{u}_y(t=0) = 0$$



Figure 1: Numerical solution with uniform initial condition

This initial condition mean at the beginning, there is no non-active myosin, and action monomers in the system, all the polymers or monomers are uniformly distributed in the system with constant concentration, and besides, the fluid is static velocity.

This case is a preliminary test for further complicated test. Here we can see from figure 1a that the activated actin which is consistent with our initial condition that everywhere is 1. However, due to the reaction relationship shown in equation 18, the activated form of actin is transformed into its product, i.e., component monomers or non-active forms, so we can see that the solution at time t = 100 becomes smaller than 1 (figure 1b) while its product rising from 0 (figure 1d) to the solution larger than 0 as shown in figure 1d

3.2 Non-uniform initial condition

Initial conditions in biology system are usually mot constant, and they are usually distributed nonlinearly with respect to the coordinate, here we test the following initial conditions,

$$\rho_{m1}(t=0) = \sin(x) + 1, \quad \rho_{m0}(t=0) = \sin(x+\pi) + 1$$
$$\rho_{a1}(t=0) = \sin(x+\pi) + 1, \quad \rho_{a0}(t=0) = \sin(x) + 1$$
$$\mathbf{u}_x(t=0) = 0, \quad \mathbf{u}_y(t=0) = 0$$

This group of initial condition has the following physical means: In the system the actin and myosin is distributed as trigonometric function from its back to the front with zero initial velocity field.the mixed chemical reaction process is well defined using the periodicity of the function, the maximal quantity of one substance is usually accompanied with minimal corresponding product.

We can see from figure 2a and figure 2c that the initial condition is distributed non-uniformly with respect to the coordinates, so the activated and non-activated can be transformed to each other through the relationship defined in equation 18. After some times (1000s), the substance convected by the velocity but the distribution of active actin become smooth as shown in figure 2b and similar trend is shown also for its product in figure 2d.

Besides, we show the velocity field at different time stages. Initially, because we set velocity field zero, so we do not get the velocity field in figure 3a. Later, we have the velocity field in figure 3b, figure 3c and figure 3d. It is interesting that the velocity point from left to the right which means the flows moves to the right. This is not always this case that the direction of the velocity field remains constant, initial condition affecting the directions is not trivial.



Figure 2: Numerical solution with non-uniform initial condition



Figure 3: Numerical solution of non-uniform initial condition

4 Conclusions

In this project, we studied the projections method for solving general transient (Navier-)Stokes equations, and based on this method, the coupled algorithm for transient convection-diffusion equations and Stokes equations becomes easier to implemented in with time integration scheme. Additionally, we apply this method and try to model the physical phenomena exist in reality. Results are well explained according to the boundary conditions and initial conditions. However, this work reported here also suggests that more work is needed to carry out systematic numerical experiment on more complicated initial conditions which would affect the behavior of the velocity field. This work is important because in real life entities they should have a consistent status where the mass is conserved, the force is balanced.

5 Appendix

The code is available at my Github

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