Modelling of blood flow and thrombus formation

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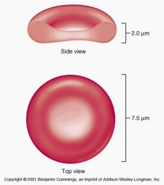
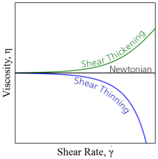
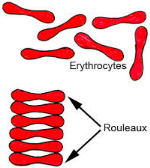
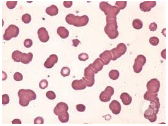
Outline



- elasticity because of membrane elasticity
- shear thinning viscosity because of rouleaux formation

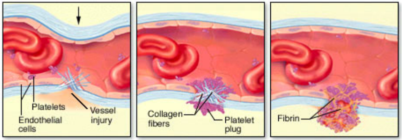




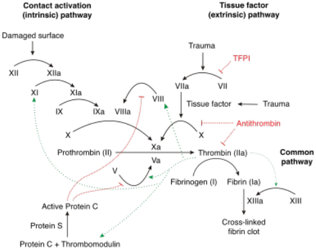


Introduction - hemostasis

- primary task of coagulation - hemostasis in order to seal the vessel wall injury

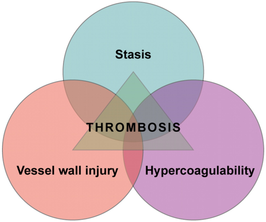


(a) Vasoconstriction (b) Platelet aggregation (c) Clot formation



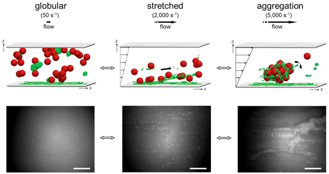
Two seemingly disparate trigger mechanisms of blood coagulation

- stasis flow conditions



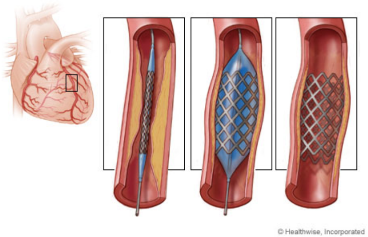
VS.

- high shear rate thrombosis



Material properties artificial surfaces - stents

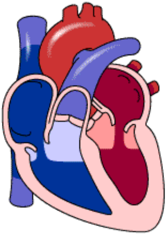
- angioplasty

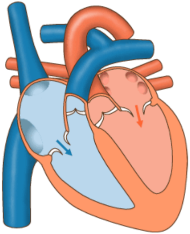


- restenosis can occur due to the reacting surface of stents
- how to choose the material and the shape of stents properly?

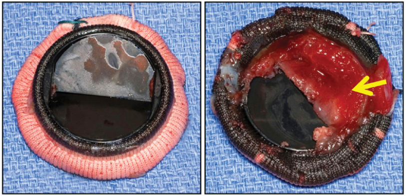
Material properties of artificial surfaces - artificial heart valves

- normally working heart valves





- heart valve prostheses



- how to choose the material and the shape of halves properly?

A microstructure based viscoelastic model of blood flow

- linear-momentum equations

$$Re\frac{D\mathbf{u}}{Dt} - 2\eta_s \nabla\cdot\mathbf{D} - \nabla\cdot\tau + \nabla p = 0,$$

$$\nabla\cdot\mathbf{u} = 0,$$

- reaction-convection equation for the size of average rouleaux size

$$\frac{D\hat{N}}{Dt} + \frac{1}{2}b(\dot{\gamma})(\hat{N} - \hat{N}_{st})(\hat{N} + \hat{N}_{st} - 1) = 0, \tag{1}$$

- equation for the development of the elastic part of the stress tensor

$$\tau + De(\dot{\gamma},\hat{N})(\left(\frac{\partial\tau}{\partial t} + (\mathbf{u}\cdot\nabla)\tau - \nabla\mathbf{u}\cdot\tau - \tau\cdot\nabla\mathbf{u}^T\right) = De(\dot{\gamma},\hat{N})\boldsymbol{D},$$

Re - Reynolds number
$\mathbf{D}(\mathbf{u})$ - symmetric velocity gradient
$\hat{N}$ - average rouleaux size $b(\dot{\gamma})$ - fragmentation rate of rouleaux dependent on the shear rate $\dot{\gamma}$
$\hat{N}_{st}(\dot{\gamma})$- the value of $\hat{N}$ given a steady simple shear flow with shear rate $\dot{\gamma}$
$De(\dot{\gamma},\hat{N})$ - Deborah number depending on the value of average rouleaux size $\hat{N}$

A phase-field model of blood clot

- linear-momentum equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot (\nu(c)\mathbf{D}(\mathbf{u})) + \mathbf{f} \quad \text{in} \quad \Omega$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega,$$

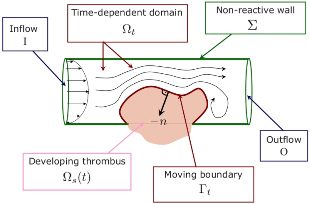
- phase-field equation

$$\frac{\partial c}{\partial t} - \nabla \cdot M \nabla \mu = kw|grad\varphi_\varepsilon|$$

$$\mu - \frac{1}{\varepsilon^2} W'(c) + \Delta c = 0,$$

- transport equation for platelets

$$\frac{\partial(\phi w)}{\partial t} - D\nabla \cdot (\phi \nabla w) + \nabla \cdot (\phi w \mathbf{u}) + \frac{1}{\varepsilon} B(\phi) kw = 0 \quad \text{in} \quad \Omega,$$



$\Omega = \Omega_t \cup \Omega_s(t)$
$\nu(c)$ - viscosity function dependent on the phase field c(supposed to be large in the area of the clot)
$\mathbf{D}(\mathbf{u})$ - symmetric velocity gradient
M - mobility constant
$k = k(s)$ -adhesion rate of platelets dependent on the wall shear rate s
ϕ - characteristic function of the time-dependent domain Ω_t
$B(\phi) = \phi^2(1-\phi)^2$ - function for handling of Neumann boundary condition

A splitting method for the linear-momentum equations and continuum equation

- the incompressible Navier-Stokes equations are a saddle point problem, its corresponding matrix (arising from FEM discretization) is indefinite $\rightarrow$ difficult to solve
- we use a projection method to avoid solving this problem
- we solve instead in each timestep a convection-diffusion equation for the velocity and a Poisson problem for the pressure
- we use incremental pressure correction scheme (IPCS):

For $k = 0 \dots N$

1. $$\frac{\mathbf{u}_*^{k+1} - \mathbf{u}^k}{\delta t} + N(\mathbf{u}_*^{k+1}) + \nabla p^k - L(\mathbf{u}_*^{k+1}) = 0$$
2. $$\Delta(p^{k+1} - p^k) = \frac{1}{\delta t} div \mathbf{u}_*^{k+1}$$
3. $$\mathbf{u}^{k+1} = \mathbf{u}_*^{k+1} - \delta t(\nabla p^{k+1} - \nabla p^k)$$

where

$$L(\mathbf{u}) = div(\nu \mathbf{D}) = div(2\nu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

and

$$N(\mathbf{u}) = [\nabla \mathbf{u}]\mathbf{u}$$

where the nonlinearity is resolved using Picard iteration

An heuristic adaptive time stepping method

- Our aim: reach the prescribed tolerance *TOL*: $\|u - u_{\Delta t}\| \approx TOL$

Local truncation error

- 1. $u_{\Delta t} = u + \Delta t^2 e(u) + \mathcal{O}(\Delta t^4)$
- 2. $u_{m\Delta t} = u + m^2 \Delta t^2 e(u) + \mathcal{O}(\Delta t^4)$

Estimate of the relative error

- $\|u - u_{\Delta t_*}\| \approx \left(\frac{\Delta t_*}{\Delta t}\right)^2 \frac{\|u_{\Delta t} - u_{m\Delta t}\|}{m^2 - 1} = TOL$

Heuristic error analysis

- $e(u) \approx \frac{u_{m\Delta t} - u_{\Delta t}}{\Delta t^2 (m^2 - 1)}$

Adaptive time stepping

$$(*) \quad \Delta t_*^2 = TOL \frac{\Delta t^2 (m^2 - 1)}{\|u_{\Delta t} - u_{m\Delta t}\|}$$

An heuristic adaptive time stepping method

Algorithm: Algorithm for one adaptive time step

Data: u^n
Result: u^{n+1}
Given the old solution u^n do:

begin

1. Make m small timesteps of size Δt to compute $u_{\Delta t}$
2. Make one large step of size of size $m\Delta t$ to compute $u_{m\Delta t}$
3. Evaluate the relative solution changes $\|u_{\Delta t} - u_{m\Delta t}\|$
4. Calculate the 'optimal' value Δt_* using (*) for the next time step
5. If $\Delta t_* << \Delta t$, reset the solution and go back to step 1, using Δt_* as new timestep
6. Set $u^{n+1} = u_{\Delta t}$

- different time scales of processes in the equations
  -> we take the minimum of the proposed times Δt_* from the previous algorithm,
  e.g.$\Delta t_{*FUTURE} = min\{\Delta t_{*NAVIERSTOKES}, \Delta t_{*PHASE}, \Delta t_{*TRANSPORT}\}$
- we solve equations as decoupled, however in reality they are coupled
  -> at the end of each time iteration we check the residual of the whole system and reiterate when necessary

Used tools

- deal.ii FEM library deal.II
  - C++11
  - (almost) dimension independent programming - dimension dependent on an integer C++ template parameter
  - enables fully distributed programming using MPI, wherein the mesh is not stored on any single core
  - support of threading from Threading Building Blocks
  - live open source community
  - support of automatic space adaptivity
- Trilinos and Petsc linear solvers, however Trilinos distributed solvers better integrate with deal.ii Trilinos

Some results

- Outlook
  - merge the viscoelastic model with the phase field model of blood clot
  - implement functional space adaptivity for the problem - finer mesh near the interface
  - find the proper configuration of iterative solvers with preconditioners for better scaling up
  - perform computations in realistic geometries - obtained from the medical imaging methods