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Improving Numerical Stability of a Tensor-Based Blood Damage Model using the Log-Conformation Formulation

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Micro Abstract
Computational Hemodynamics enables the prediction of hydraulic properties and biocompatibility of new Ventricular Assist Devices (VADs). For hemolysis predictions, we use a tensor-based morphology model that accounts for the physiological behavior of red blood cells in blood flow. It resembles the viscoelastic Oldroyd-B equation and shows similar difficulties in numerical stability. Therefore, we apply the log-conformation formulation to the morphology model and show its enhanced stability.

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Introduction

Heart failure is the main cause of death in developed countries; heart transplants often being the only permanent medical treatment. However, the number of donor hearts is significantly lower than the number of patients in need of a transplant. Therefore, artificial blood pumps, such as Ventricular Assist Devices (VADs), are often the only alternative. State-of-the-art devices can support the failing heart for more than 5 years and can therefore function as a bridge-to-transplant or even as a permanent medical treatment and a bridge-to-recovery.

Computational Fluid Dynamics (CFD) has become an important development tool for new VADs. It is possible to predict both the hydraulic performance and the biocompatibility with computational simulations. Hemolysis, the release of hemoglobin from red blood cells (RBCs) to the blood plasma, can be increased in the non-physiological flow conditions in artificial organs leading to multiple organ failure in severe cases [1]. Hence, a prediction of the hemolysis produced is important for the assessment of the biocompatibility of such a device. Most research groups use a stress-based approach for these predictions; the shear stresses in the pump are calculated from the precomputed flow field and are used in a power-law model fitted to experimental data of blood tests in simple shearing devices. This approach assumes an instantaneous deformation of the RBCs according to the flow stresses. It cannot account for the complex behavior of RBCs in blood flow.

At low shear rates, bi-concave shaped RBCs form coin-like stacks, called rouleaux; with increasing shear, the individual RBCs move in the blood flow; at shear stresses above 1 Pa, the RBC gets deformed to an ellipsoidal shape and starts to tumble and rotate; a further increase in shear lets the surface of the RBCs rotate around the enclosed cytoplasm; pores can form on the surface of the RBC due to the deformation through which hemoglobin can leak to the blood plasma; the deformations up to this point are reversible and the RBCs can relax to their biconcave shape; but ultimately, at shear stresses above 150 Pa, the RBCs start to rupture, leading to fatal hemolysis. In order to account for this complex behavior, Arora et al. [2] modified a droplet model that can describe the RBCs relaxation, elongation and rotation in the blood flow. This model is used to estimate an effective shear rate acting on the RBCs. In this strain-based model, the effective shear rate can then be used in the power-law model to estimate the produced hemolysis [3, 4].

1 Tensor-Based Blood Damage Model

The RBCs in the aforementioned model are described by a 3×3 symmetric, positive definite tensor $\boldsymbol{S}$, that represents the ellipsoidal shape. The eigenvalues of the tensor $\boldsymbol{S}$ are related to the three semi-axes of the ellipsoid. The resting shape without any shear stresses is assumed to be the sphere. The governing equation—the so called morphology equation—for the behavior of $\boldsymbol{S}$ in a flow $\boldsymbol{u}$ becomes

$$\frac{\partial \boldsymbol{S}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\, \boldsymbol{S} = -\underbrace{f_1 \left(\boldsymbol{S} - g(\boldsymbol{S})\boldsymbol{I}\right)}_{relaxation} + \underbrace{f_2 \left(\boldsymbol{E}\boldsymbol{S} + \boldsymbol{S}\boldsymbol{E}\right)}_{elongation} + \underbrace{f_3 \left(\boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W}\right)}_{rotation}, \tag{1}$$

where $\boldsymbol{I}$ is the identity tensor, $\boldsymbol{E} = \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)/2$ is the strain-rate tensor and $\boldsymbol{W} = \left(\nabla \boldsymbol{u} - \nabla \boldsymbol{u}^T\right)/2$ is the vorticity tensor. The scalar $g(\boldsymbol{S})$ ensures the volume conservation of the RBCs and can be derived with the second invariant, $II_{\boldsymbol{S}}$, and third invariant, $III_{\boldsymbol{S}}$, of the tensor $\boldsymbol{S}$ as

$$g(\boldsymbol{S}) = \frac{3 III_{\boldsymbol{S}}}{II_{\boldsymbol{S}}}. \tag{2}$$

The solution of this equation is a deformed ellipsoid for which we can quantify the deformation by a scalar $D = {}^{(L-B)}/_{(L+B)}$, with L, the longest and B, shortest semiaxes of the ellipsoid computed with the eigenvalues of $\boldsymbol{S}$. The distortion D can be used to compute an effective shear rate acting on the deformed RBC by

$$G_{\mathit{eff}} = \frac{2 f_1 D}{f_2 \left(1 - D^2\right)}. \tag{3}$$

Equation (3) is derived from an analytical solution for a simple shear flow and generalised to arbitrary flow deformations.

We discretize the morphology equation using a stabilised finite element approach and use a pre-calculated blood flow $\boldsymbol{u}$, governed with the incompressible Navier-Stokes equations, to solve for $\boldsymbol{S}$. This means that we assume no backcoupling from the morphology equation to the blood flow. The positive definiteness of $\boldsymbol{S}$ has to be fulfilled in order to describe a physical state. However, solving the discretized equations for complex flows can lead to negative eigenvalues of $\boldsymbol{S}$, causing the simulation to fail. This can be circumvented by introducing a logarithmic transformation to the morphology equation.

2 Logarithmic Transformation of the Morphology Equation

The morphology equation introduced in the last section resembles the viscoelastic Oldroyd-B equation. In the Oldroyd-B equation, the conformation tensor has to be positive definite, which might be violated when solving the discretized equations. Fattal and Kupferman [5] introduced a transformation to the Oldroyd-B equation that ensures the positive definiteness of the conformation tensor naturally and Knechtges et al. [6, 7] derived a constitutive equation for this transformed variable, called the log-conformation or log-conf equation. They showed that a transformed solution of this new log-conf equation is also a solution to the original equation.

2.1 Constitutive Equation

The same transformation as in Knechtges et al. [6], i.e. $\boldsymbol{S} = \exp(\boldsymbol{\Psi})$, can be introduced to the morphology equation and the corresponding constitutive equation, the so-called log-morph equation, is given by

$$\begin{aligned} \frac{\partial \boldsymbol{\Psi}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\, \boldsymbol{\Psi} = &- f_1 \left(\boldsymbol{I} - g\left(\boldsymbol{\Psi}\right) \exp(-\boldsymbol{\Psi})\right) + f_3 \left(\boldsymbol{W}\boldsymbol{\Psi} - \boldsymbol{\Psi}\boldsymbol{W}\right) \\ &+ f_2 \frac{1}{(2\pi i)^2} \int_\Gamma \int_\Gamma f(z - z') \frac{1}{z - \boldsymbol{\Psi}} \boldsymbol{E} \frac{1}{z' - \boldsymbol{\Psi}} dz dz', \end{aligned} \tag{4}$$

with the function $f(x) = {}^{x}/_{\tanh(x/2)}$. The double integral on the rght-hand side (RHS) is a Cauchy's integral on the complex plane with a suitable contour Γ (please refer to Knechtges [7] for more details). The volume conservation constant can be derived for this transformed equation as

$$g\left(\mathbf{\Psi}\right) = \frac{3}{\mathrm{tr}(\exp(-\mathbf{\Psi}))}. \tag{5}$$

The differences to the Oldroyd-B equation are the prefactors of the RHS terms and the volume conservation term. Nevertheless, the argument of Knechtges et al. [6, 7] can still be applied and, hence, a solution of the log-morph eq. (4) transformed back to the original variables is also a solution of the morphology eq. (1).

2.2 Numerical Discretization

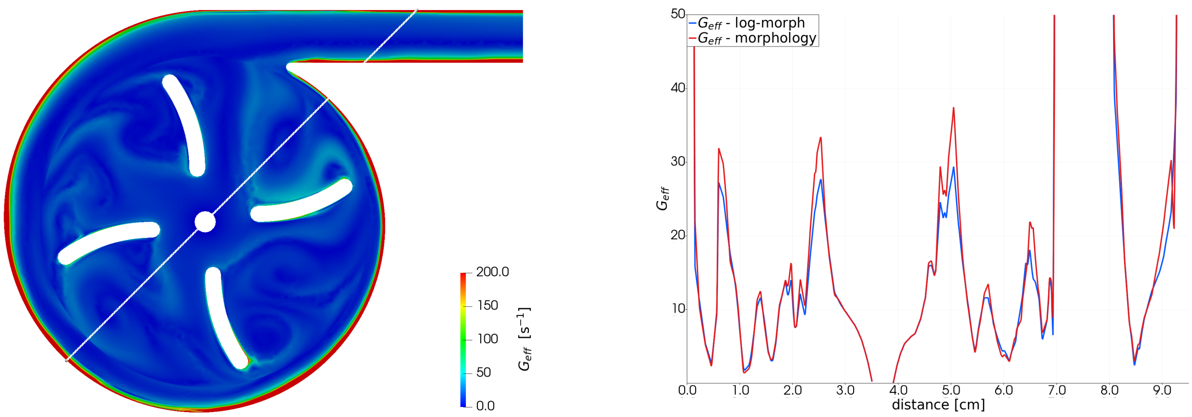
The major part of the numerical finite element discretization and linearization can be done in the same way as described by Knechtges [7]. Special attention has to be given to the volume conservation term $g(\mathbf{\Psi}) = {}^{3}/_{\mathrm{tr}(\exp(-\mathbf{\Psi}))}$. For the RHS of the discretized equations, one can use the computed eigenvalues of $\mathbf{\Psi}$ to compute $g(\mathbf{\Psi})$. For the linearized LHS, one has to derive its directional derivative

$$\begin{aligned} \frac{\partial}{\partial\xi}\frac{3}{\mathrm{tr}(\exp(-\mathbf{\Psi}-\xi\delta\mathbf{\Psi}))}\bigg|_{\xi=0} &= -\frac{3}{\mathrm{tr}(\exp(-\mathbf{\Psi}))^2}\,\frac{\partial}{\partial\xi}\mathrm{tr}(\exp(-\mathbf{\Psi}-\xi\delta\mathbf{\Psi}))\bigg|_{\xi=0} \\ &= -\frac{3}{\mathrm{tr}(\exp(-\mathbf{\Psi}))^2}\mathrm{tr}\left(\frac{\partial}{\partial\xi}\exp(-\mathbf{\Psi}-\xi\delta\mathbf{\Psi})\bigg|_{\xi=0}\right). \end{aligned} \tag{6}$$

This term can then be evaluated with the methods presented in [7].

3 Results for a 2D Pump Test Case

We investigate the behavior of the new log-morph equation for a simple 2D pump test case. The log-morph equation and the untransformed morphology equation for a precomputed flow should predict the same deformation of the RBCs. Fig. 1(b) shows a good agreement of both results on a line plot through the pump domain.



(a) Effective shear rate computed with the log-morph approach and scaled to $200\,\mathrm{s}^{-1}$ (maximum $G_{eff} = 7751\,\mathrm{s}^{-1}$).

(b) Comparison of the morphology (red) and log-morph approach (blue) on a line depicted in Fig. 1(a).

Figure 1. Effective shear rate for a 2D pump testcase.

The enhanced numerical stability of the log-morph implementation allows the simulation to run with a significantly larger time step size. We could increase the time step size by one order of magnitude from 0.001 s to 0.01 s already for this simple 2D pump test case. For complex 3D geometries, we could even increase the time step size by two or three orders of magnitude, if the untransformed equation was able to give a result at all.

As an additional positive effect, we realized an enhanced volume conservation in the log-morph simulations. The volume conservation can be quantified by $\det(\boldsymbol{S})$, which is proportional to the RBC's volume. Since the shape of an RBC at rest is approximated with the unit sphere, the determinant of $\boldsymbol{S}$ should always be close to 1. The maximal deviation from $\det(\boldsymbol{S}) = 1$ for the 2D pump test case for the solution of the morphology equation is $3.89 \cdot 10^{-3}$ and the error for all nodes i is $\varepsilon = \sqrt{\sum_i (\det(\boldsymbol{S}_i) - 1)^2} = 1.71 \cdot 10^{-2}$, while it is much better for the log-morph solution with a maximal deviation of only $2.37 \cdot 10^{-6}$ and an error of $\varepsilon = 1.34 \cdot 10^{-5}$.

Conclusions

We successfully applied a fully-implicit logarithmic transformation for a strain-based hemolysis estimation in medical devices. The newly-derived, discretized set of equations shows an increased numerical stability and is applicable to complex geometries. Furthermore, we were able to significantly increase the time step sizes in our simulations, leading to shorter overall simulation times.

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