Adjoint Optimization for Applications in Hemodynamics

Adjoint-based Optimization under Uncertainties on FSI Systems for Applications in Hemodynamics.

***G. Bletsos, T. Rung**, Institute for Fluid Dynamics and Ship Theory, Hamburg University of Technology (TUHH)*

In Short

- Biomedical devices must be optimized to ensure good bio-compatibility.
- Adjoint methods enable a computationally efficient shape optimization.
- Fluid-Structure Interaction (FSI) is required to efficiently capture hemodynamics in blood vessels due to strong coupling between the blood flow and the vessels.
- Shape optimization of artificial blood vessels can ensure complete and successful treatment after surgery.
- The sensitive nature of the applications requires an extension of the optimization methods to consider potential uncertainties.

Biomedical devices, such as blood pumps, in which large velocity gradients are found, may damage the treated blood. Therefore, this project targets to optimize the shape of such devices so that to minimize the potential blood-damage induction. To this extent, an adjoint-based methodology is introduced to facilitate the efficient realization of such a task. Furthermore, this project targets to deal with problems arising from vascular surgery. Very often artificial materials are used to restore and control a regular blood flow. Despite, however, all the advances in medicine and material science there are still restrictions in the anastomosis area, such as restenosis, leading to restricted blood flow. Restenosis usually arises due to intimal hyperplasia, which has been associated with hemodynamic parameters. Crucial to this is a substantial change of the (wall) shear stress due to possibly unnatural flow patterns originating from the implants. This change of the wall shear stress influences the deformable vessel walls, therefore resulting in a direct interaction between the fluid flow and the solid material. Motivated by this, the project targets on the shape optimization of artificial blood vessels through adjoint-based FSI simulations. The above scenarios are potentially subject to uncertainties, that must be taken into account due to the sensitive nature of the applications.

The project is part of the "SENSUS" (Simulationsbasierte Entwurfsoptimierung Dynamischer Systeme unter Unsicherheit) research training centre at the interface between applied mathematics and computational engineering. The research centre involves 6 teams from mathematics as well as fluid dynamics and structural engineering from three Hamburg universities and is funded by a Landesexzellenzinitiative of Hamburg. For the purposes of the project, the (RANS/LES) Navier-Stokes FreSCo^{+} code is to be used and further developed (for the fluid part of the FSI system). It is an efficient and parallelizable code, developed at the Institute for Fluid Dynamics and Ship Theory of TUHH, which employs the finite volume method (FVM) for the numerical solution of the primal and dual (adjoint) equations of laminar or turbulent flows. For the FSI simulations, the procedure is coupled with the high-order finite element code, AdhoC together with the coupling tool, comana [2,3]. This work is primarily concerned with the application of gradient-based shape optimization for hemodynamic systems, e.g. artificial arteries, including FSI coupling. Several objective functions are considered, such as hemolysis, dissipated power and shear-stress. Due to the highly expensive nature of FSI problems, attention is also given to efficiency aspects. In particular, methods for the acceleration of the gradient process as part of the partitioned approach are also investigated.

Standardization of computational fluid dynamics (CFD) techniques used to evaluate performance and blood damage safety in medical devices has not yet been widely achieved. This led to a U.S. Food and Drug Administration (FDA) initiative towards that direction [4]. Through that initiative, the absence of widely accepted and credible blood damage models was noted. At the same time, however, a widely agreed blood-damage model which relates a damage index (DI) with the shear stress τ and exposure time t^*, is frequently used. Such an expression can be cast into a residual form and facilitate the development of an appropriate adjoint system targeting to minimize flow-induced blood damage. In the first stage of the project, the primal and dual problem for minimizing hemolysis (red blood cell damage) was theoretically built and incorporated in FreSCo^{+}. The method was then verified, validated and subsequently applied on an FDA-proposed nozzle geometry, shown in Fig. 1, in which a reduction of hemolysis induction by up to $\sim 25\%$ was achieved [1].

In the second stage, the adjoint-based shape opti-

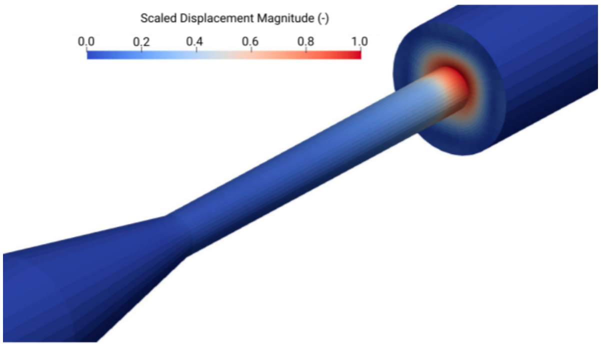

Figure 1: *Displacement magnitude field on an FDA-proposed nozzle geometry, computed after the successive solution of primal and adjoint equation systems targeting to minimize flow-induced hemolysis.*

mization method is extended towards including non-Newtonian properties of the fluid, which have been shown to be more suitable at describing blood in low shear-rate conditions. In specific, three prominent viscosity models, namely the Power-Law, modified Casson and Carreau models are considered. It has been shown that considering "*frozen*" viscosity in the adjoint problem can lead to an incorrect estimation of shape sensitivities. Additionally, deviations between hemodynamic quantities computed in a purely CFD and FSI manner have been investigated. The consideration of FSI is crucial to the objective of the simulation-based research. We showed that between a flow simulation through rigid material and a coupled FSI simulation, differences of up to 51% in wall shear-stress metrics can occur.

In a later stage, adjoint-based shape optimizations of arterial bypass-grafts, cf. Fig. 2, are to be performed, including considerations of non-Newtonian properties. Furthermore, additional FSI simulations on grafts are intended to investigate the impact of different inflow paths on relevant hemodynamics. The

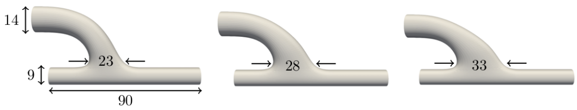

Figure 2: *Sketch of the investigated idealized bypass-graft anastomoses. All dimensions shown in [mm].*

above mentioned numerical simulations can be significantly expensive due to the inherently unsteady nature of the problem as well as instabilities that may arise in the numerical solution of a partitioned coupling. For this reason, attention is to be given to efficiency aspects. Once the most significant hemodynamic quantities have been identified for applications related to vascular surgery, an adjoint-based optimization method is to be built. This method will target the proposal of feasible shapes and would assist medical clinicians on performing an effective surgery.

Ultimately, the project targets to combine the above mentioned investigated aspects into producing a partitioned approach to adjoint shape optimization of coupled FSI problems. Finally, consideration will be given to uncertainties that may arise from inflow or/and material properties.

WWW

http://www.tuhh.de/fds
https://www.tuhh.de/sensus

More Information

[1] Bletsos, G., Kühl, N., Rung, T. Adjoint-based shape optimization for the minimization of flow-induced hemolysis in biomedical applications. *Engineering Applications of Computational Fluid Mechanics* (2021) 15, pp. 1095 – 1112 doi:10.1080/19942060.2021.1943532

[2] Radtke, L. A partitioned solution approach for fluid-structure interaction problems in the arterial system. PhD thesis, Hamburg University of Technology, 2020

[3] Heners, J., Radtke, L., Hinze, M., Düster, A. Adjoint Shape Optimization for Fluid-Structure Interaction of Ducted Flows. *Computational Mechanics* (2018) 61, pp. 259 – 276 doi: 10.1007/s00466-017-1465-5

[4] Stewart, S., Paterson, E., Burgreen, G., Hariharan, P., Giarra, M., Reddy, V., Day, S., Manning, K., Deutsch, S., Berman, M., Myers, M., Malinauskas, R. Assessment of CFD Performance in Simulations of an Idealized Medical Device: Results of FDA's First Computational Interlaboratory Study. *Cardiovascular Engineering and Technology* (2012) 3, pp. 139 – 160 doi: 10.1007/s13239-012-0087-5

Project Partners

TUHH, Ship Structural Design and Analysis
TUHH, Structural Optimization for Lightweight Design
TUHH, Mechanics and Ocean Engineering
U. Hamburg, Mathematics - Center for Optimization and Approximation
Helmut-Schmidt-Univ. Hamburg, Mathematics for Civil Engineering

Funding

Landesforschungsförderung LFF- GK11

DFG Subject Area

404-04 Fluid Mechanics