# HPC-based uncertainty quantification for fluid-structure coupling in medical engineering

Jonas Kratzke
Engineering Mathematics and Computing Lab (EMCL)
IWR, Heidelberg University
Heidelberg, Germany
jonas.kratzke@iwr.uni-heidelberg.de

Vincent Heuveline
Engineering Mathematics and Computing Lab (EMCL)
IWR, Heidelberg University
Heidelberg, Germany

***Abstract*—In recent decades biomedical studies with living probands (in vivo) and artificial experiments (in vitro) have been complemented more and more by computation and simulation (in silico). In silico techniques for medical engineering can give for example enhanced information for the diagnosis and risk stratification of cardiovascular disease, one of the most occurring causes of death in the developed countries. Other use cases for in silico methods are given by virtual prototyping and the simulation of possible surgery outcomes. High reliability is a requirement for cardiovascular diagnosis and risk stratification methods especially with surgical decision-making. Given uncertainties in the input data of a simulation, this implies a necessity to quantify the uncertainties in simulation results. Uncertainties can be propagated within a numerical simulation by methods of Uncertainty Quantification (UQ).**

**For many cardiovascular applications, such as the simulation of blood flow through the aorta, the physiological understanding and mathematical modeling has still challenging aspects. Modeling the biomechanics of aortic blood flow by means of a three-dimensional fluid-structure interaction (FSI) problem, the simulation becomes computationally highly expensive. UQ usually multiplies the computational costs even further. We present an approach to compute patient-specific aortic FSI simulations incorporating UQ based on parallel computing. The coupled fluid- and elasto-mechanical problem is computed with a monolithic finite element (FEM) solver. The quantification of uncertainties is realized by a collocation method based on polynomial chaos (PC).**

**For validation purposes we consider an in vitro prototypical silicon phantom experiment and compare the simulation results with flow magnetic resonance images (MRI) of the phantom. Flow MRI is capable of visualizing the velocity field of the fluid flow. Taking the uncertainty into account, the simulation results are in well accordance with the MRI-measured velocity field. Furthermore, we present a patient-specific simulation method for simulating blood flow through the aortic bow based on high performance computing. Possible risk parameters can be evaluated in consideration of the uncertainty in the input data.**

***Keywords—Uncertainty Quantification, Fluid-Structure Interaction, Numerical Simulation, Blood Flow***

## I. Introduction

Cardiovascular diseases are one of the most occurring causes of death in the developed countries. Investigating the physiology of the cardiovascular system and the pathogenesis of its diseases leverages medical diagnosis and therapeutic possibilities. Greater knowledge can be acquired from medical studies with living patients and probands in vivo. Furthermore, investigations with artificial, i.e. in vitro experiments have been complemented more and more with virtual, so called in silico methods by means of computations and simulations. Overviews on the application of numerical simulations for investigating cardiovascular dynamics are given by [1,2,3]. For example, dynamics that are hard to be assessed non-invasively can be simulated supplementing pre-operative risk parameters. The outcome of different surgical procedures can be evaluated beforehand by means of simulations.

For the verification of cardiovascular numerical simulations, aortic phantom experiments can be used. In [4] a prototypical aortic phantom is presented. Fully consisting of non-metallic materials, the three-dimensional flow field can be measured in time by phase contrast magnetic resonance imaging (MRI) and compared to simulations of the same. Using a silicon material, the movement of the elastic vessel wall can also be observed in the phantom. As to the aorta, the elasticity of the complex vessel wall structure is crucial for damping the pressure waves induced by each heart beat. Though the layers of vessel wall soft tissue have been examined with respect to their biomechanics [5], it remains a challenging effort to simulate blood flow in elastic vessels in detail. One factor is given by the lack of non-invasive measurability of structural material parameters of a specific patient. The arising uncertainty in the soft tissue structure can be modeled by Uncertainty Quantification (UQ). In particular, UQ can provide a measure of the reliability of simulation results.

An overview on the modeling and numerical simulation of blood flow is given in [6]. Methods of UQ for flow simulations are reviewed in [7]. This work describes new developments in the simulation of blood flow coupled with elastic vessel wall movement by means of fluid-structure interaction (FSI) taking the uncertainty of input parameters into account. The presented framework is verified by means of MRI measurements of an aortic phantom experiment.

The paper is structured as follows: First, the underlying mathematical model is described. Section III gives an overview on the discretization and the utilized numerical methods. The simulation results for the phantom and a patient-specific aortic bow are presented in section IV. The conclusion gives a summary and an outlook to future work.

## II. Mathematical Modeling

Figure 1 gives an overview on the considered prototypical aortic phantom. The general configuration is in accordance with a human aorta except for the presence of branching vessels and the complexity of the soft tissue structure.

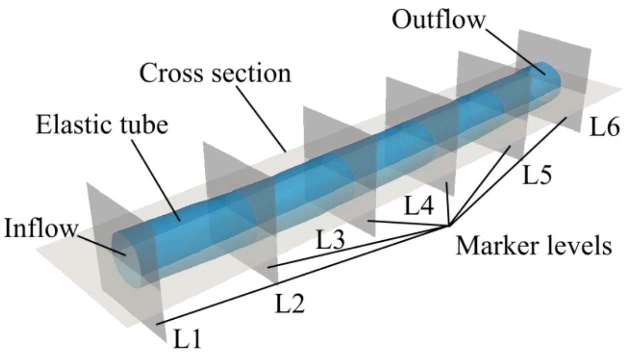



Fig. 1: Schematic overview on the aortic phantom used in [4]. A pulsatile flow is pumped through the inflow of the elastic vessel tube. The outflow is followed by a flow resistor. The flow was measured by phase contrast MRI at the cross-sectional planes of the marker levels.

### A. Fluid flow

The flow dynamics of the glycerin-water mixture as used in the phantom experiment can be modeled by the incompressible Navier Stokes equations (NSE) for a Newtonian fluid. The NSE can also be used for modeling blood flow in large arteries, in which the shear-thinning influence of the red blood cells is relatively small.

$$\partial_t v + ( v \cdot \nabla )v - \nu\nabla \cdot ( \nabla v + \nabla v^T ) + 1/\rho\nabla p = 0, \qquad (1)$$
$$v \cdot \nabla = 0. \qquad (2)$$

Equation (1) refers to the momentum conservation in the three-dimensional velocity and the one-dimensional pressure field v and p, respectively. (2) is derived from the conservation of mass. The glycerin (40%) to water (60%) proportions were chosen, such that the density $\rho$ and kinematic viscosity $\nu$ is similar to blood. The inflow velocity of the simulation is set by means of a Dirichlet Poisseuille boundary condition scaled by the pulsatile flow rate measured at the marker plane L1. The inflow rate is modeled as an uncertain parameter of a uniform distribution with a maximal deviation of 15% from the measured value.

### B. Elastic vessel wall structure

Aortic vessel wall soft tissue consists of three layers of cellular structures with different anisotropic biomechanical behavior. The phantom, however, can be modeled as a homogeneous hyperelastic Saint-Venant Kirchhoff material given by:

$$\rho\partial_{tt}u - \nabla \cdot ( \lambda \mathrm{tr}( E ) I + 2\mu E ) = 0, \qquad (3) \qquad \text{with } E = 0.5( \nabla u^T \nabla u + \nabla u^T + \nabla u ). \quad (4)$$

The conservation of momentum, equation (3), governs the strain tensor E of the material which is defined by the three-dimensional displacement field u. Compressibility and stiffness are determined by the Poisson ratio $\gamma$ and Young's modulus Y, respectively. They define the Lamé-constants $\lambda = Y\gamma(1 + \gamma)^{-1} (1 - 2\gamma)^{-1}$ and $\mu = 0.5Y(1 + \gamma)^{-1}$. The trace operator is denoted by tr and I is the identity matrix. To address the uncertainty in the generally hard to measure stiffness of vessel wall material, we model the Young's modulus Y as uncertain parameter of a uniform distribution with a maximal deviation of 30%.

### C. Coupling of fluid flow and wall elasticity

In the mathematical problem formulation, coupling conditions model the interaction between fluid flow and vessel wall elasticity. At the interface, the displacement and the tension forces are assumed to coincide. The flow equations (1,2) are stated in the Eulerian frame of reference and the elasticity equations (3,4) in the Lagrangian frame of reference. A standard approach to couple these two perspectives is given by the Arbitrary Lagrangian-Eulerian (ALE) method. The ALE method introduces a mapping of the fluid domain from a reference state to the current configuration in time [8].

## III. HPC Simulation

In order to numerically solve a complex stochastical boundary value problem as stated in section II, computationally efficient and parallel scalable methods have to be utilized. The large number of discrete unknowns requires the computation on high performance computing (HPC) clusters.

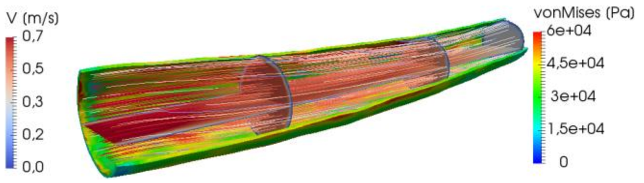
The FSI problem is solved in a monolithic way, resulting in a strong coupling of the fluid flow and vessel wall elasticity. The non-linearities in the mathematical problem are linearized by exact Newton-linearization. Finite elements of Taylor-Hood type discretize the spatial dimensions. The time steps are allocated by the one-step-$\theta$-scheme. See for example [9] for details on the numerical methods. For the quantification of uncertainties, we use the generalized polynomial chaos expansion [10] with Legendre polynomials as a basis for the stochastic space. As a collocation method we use the Gauss-Legendre quadrature [11]. Each collocation point represents a single deterministic simulation run. This way, the code for the deterministic simulation does not have to be altered for the UQ study.

To numerically solve the discretized systems of equations, the open-source FEM framework HiFlow³ [12] is utilized on the HPC bwForCluster MLS&WISO production. Sufficient numerical accuracy is obtained with a polynomial chaos expansion degree of 3 resulting in 36 collocation points. Each collocation point is given by a number of approximately 1.6m FEM degrees of freedom for the aortic phantom and 1500 time steps. With a wall time of 32 hours on 64 CPU cores for each deterministic simulation, this leads to an overall computational demand of approximately 74k core hours.

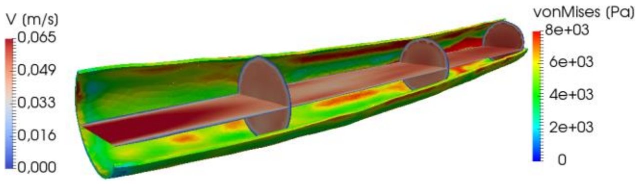
## IV. Numerical Results

### A. Prototypical aortic phantom

Figure 2 shows a visualization of the aortic phantom simulation results. One can say that, with high standard deviation, the uncertainty of the results is highest at the time and location of maximal flow. The load stress in the vessel wall can be indicated by the von Mises stress as a comparative scalar field [13].




(a) Mean value.




(b) Standard deviation.

Fig. 2: Visualization of the aortic phantom simulation at the time step of highest inflow. The flow field is illustrated by streamlines and at cross-sectional planes. The vessel wall displacement is shown by the resulting von Mises stress.

The flow mean values in the cross-sectional planes indicated in figure 1 are compared to the MRI measurement in figure 3. The flow amplitude decreases with the distance to the inflow, which is an effect of the elasticity of the vessel wall. This effect cannot be observed in pure flow simulations with a rigid wall assumption, c.f. [14].

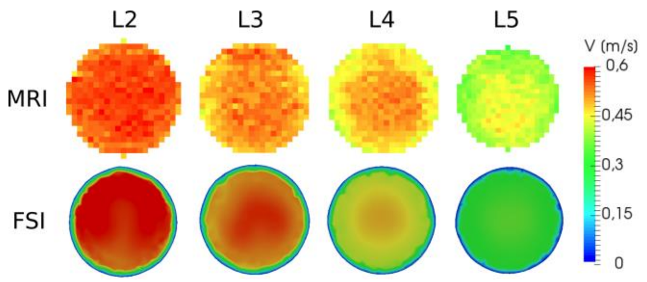



Fig. 3: Visualization of the flow through the cross-sectional planes at the marker levels depicted in figure 1 at the time of highest inflow. The corresponding MRI measurements and FSI simulation results are shown for comparison.

With regards to the volume flow rates through the cross-sectional planes, the simulation is in well accordance with the MRI measurement as can be seen in Figure 4.

### B. Patient-specific aortic bow

We developed the framework for the simulation of an aortic phantom in a generic way, such that it can be directly applied to patient-specific geometries. Figure 5 shows a simulation result for the aortic bow of a healthy proband. Though the material models have to be adapted to human blood and to an

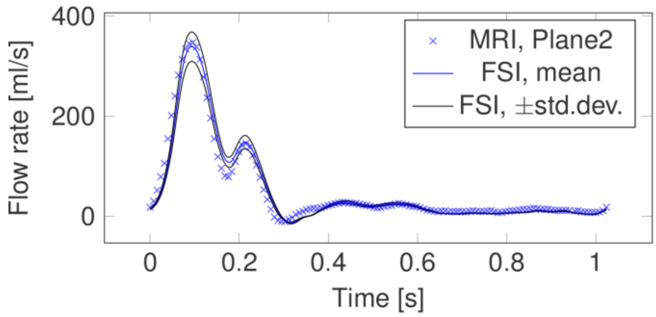


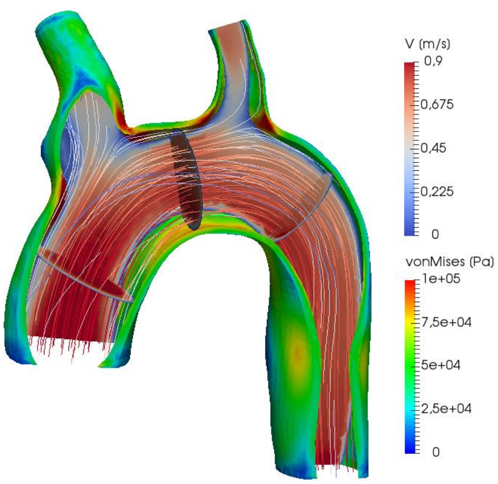

Fig. 4: MRI-measured volume flow rate through marker level 2 together with the simulated mean and standard deviation from the mean.

approximation of the complex structure of the vessel wall, the results reveal the feasibility and potential of uncertainty quantification for cardiovascular simulations. Hereby, the discrete geometry leads to 1.8m FEM degrees of freedom. The computational demand for a UQ simulation was 147k core hours.

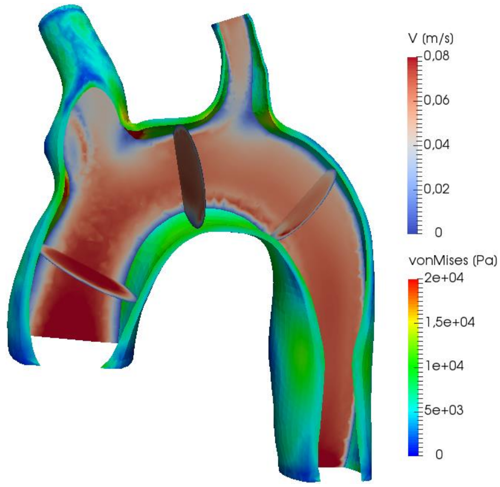
## V. Conclusion

This work presents a numerical framework for the patient-specific simulation of the fluid-structure interaction dynamics of aortic blood flow. The framework is verified by means of phase contrast MRI measurements of the flow field in a prototypical aortic phantom. Taking uncertainties into account, the simulation results obtain a measure of reliability, which is crucial for clinical decision-making.

Future work can concentrate on the incorporation of more realistic material properties of blood and vessel walls. Modeling the soft tissue as inhomogeneous structure, methods can be developed to include a spatially varying stochastic distribution of the material parameters. Furthermore the MRI-based flow measurements can be used not only to define boundary conditions but also to be assimilated by the simulation in order to utilize the simulation as enhancement of the medical imaging modality. The developed framework could finally be used in clinical trials to investigate risk factors for aortic diseases such as aortic stenosis, aneurysm development and vessel rupture.




(a) Mean value.




(b) Standard deviation.

Fig. 5: Visualization of the FSI simulation of an human aortic bow at mid-systole. The flow field is illustrated by streamlines and at cross-sectional planes. The vessel wall displacement is shown by the resulting von Mises stress.

## Acknowledgment

This work is being supported by the German government in the BMBF-project 'Ein integriertes Herz-Modell – Kopplung von Elektrophysiologie, Elastomechanik, Fluss und Kreislauf'. The authors acknowledge support by the state of Baden-Württemberg through bwHPC and the German Research Foundation (DFG) through grant INST 35/1134-1 FUGG. The authors gratefully acknowledge the data storage service SDS@hd supported by the Ministry of Science, Research and the Arts Baden-Württemberg (MWK) and the German Research Foundation (DFG) through grant INST 35/1314-1 FUGG.

## References

[1] B. Chung, and J. Cebral, "CFD for evaluation and treatment planning of aneurysms: Review of proposed clinical uses and their challenges," Annals of Biomedical Engineering, vol. 43(1), pp. 122-138, 2015.

[2] J. B. Freund, "Numerical simulation of flowing blood cells," Annual review of fluid mechanics, vol. 46, pp. 67-95, 2014.

[3] A. L. Marsden, "Optimization in cardiovascular modeling," Annual review of fluid mechanics, vol. 46, pp. 519–546, 2014.

[4] M. Delles, F. Rengier, S. Ley, H. von Tengg-Kobligk, H. Kauczor, R. Unterhinninghofen, R. Dillmann, "Influence of imaging quality on magnetic resonance-based pressure gradient measurements," Proc. SPIE 7626, Medical Imaging 2010: Biomedical Applications in Molecular, Structural, and Functional Imaging, 762624, March 2010.

[5] G. A. Holzapfel, "Microstructure and mechanics of human aortas in health and disease," in Biomechanics: Trends in Modeling and Simulation, G. A. Holzapfel, and R. W. Ogden, Eds. Springer International Publishing, 2017, pp. 157-192.

[6] L. Formaggia, A. Quarteroni, and A. Veneziani, "Cardiovascular mathematics: Modeling and simulation of the circulatory system," vol. 1. Springer Science & Business Media, 2010.

[7] H. N. Najm, "Uncertainty quantification and polynomial chaos techniques in computational fluid dynamics," Annual review of fluid mechanics, vol. 41, pp. 35-52, 2009.

[8] J. Hron and S. Turek, "A monolithic fem/multigrid solver for an ale formulation of fluid-structure interaction with applications in biomechanics," in Fluid-structure interaction, H. Bungartz and M. Schäfer, Eds. Springer, 2006, pp. 146–170.

[9] G. P. Galdi, R. Rannacher, A. M. Robertson, and S. Turek, "Hemodynamical flows," Birkhäuser Basel, 2008.

[10] D. Xiu, and G. E. Karniadakis, "The Wiener-Askey polynomial chaos for stochastic differential equations," SIAM journal on scientific computing vol. 24(2), pp. 619-644, 2002.

[11] F. Nobile, R. Tempone, and C. G. Webster, "A Sparse Grid Stochastic Collocation Method for Partial Differential Equations with Random Input Data," SIAM Journal on Numerical Analysis, vol. 46(5), pp. 2309-2345, 2008.

[12] S. Gawlok, P. Gerstner, S. Haupt, V. Heuveline, J. Kratzke, P. Lösel, K. Mang, M. Schmidtobreick, N. Schoch, N. Schween, J. Schwegler, C. Song and M. Wlotzka, "HiFlow$^3$ – Technical Report on Release 2.0", Preprint Series of the Engineering Mathematics and Computing Lab, vol. 06, 2017.

[13] A. Valencia, P. Burdiles, M. Ignat, et al., "Fluid Structural Analysis of Human Cerebral Aneurysm Using Their Own Wall Mechanical Properties", Computational and Mathematical Methods in Medicine, vol. 2013, Article ID 293128, 2013.

[14] J. Kratzke, F. Rengier, C. Weis, C. Beller, and V. Heuveline, "In vitro flow assessment: From PC-MRI to computational fluid dynamics including fluid-structure interaction," Proc. SPIE 9783, Medical Imaging 2016: Physics of Medical Imaging, 97835C, April 2016.