The Journal of Open Source Software

VaMPy: An Automated and Objective Pipeline for Modeling Vascular Geometries

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DOI: 10.21105/joss.05278

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Submitted: 08 March 2023
Published: 19 May 2023

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Summary

In medical research, it has become increasingly common to use image-based computational fluid dynamics (CFD) to study vascular pathology. Hemodynamic forces, such as wall shear stress (WSS), are believed to play a crucial role in vessel wall adaptation and remodeling. However, measuring these forces directly is challenging due to limitations in current measurement techniques. Additionally, there is significant variability in CFD modeling choices and simulation results, which can make it difficult to compare and interpret findings across studies. To address this, we aim to create an automated CFD pipeline for modeling cardiovascular flows that is objective and consistent, where modeling choices are backed up by rigorous research. The Vascular Modeling Pypeline (`VaMPy`) is an entry-level high-performance CFD pipeline with a high-level Python interface that lets the user easily extend or modify the functionality.

Statement of Need

Simulation of the cardiovascular flows has become an indispensable research tool, which can potentially reveal fundamental properties of the cardiovascular system in both physiological and pathological states. More specifically, medical image-based CFD (Taylor & Steinman, 2010) has been used extensively in the investigation of disease initiation of, e.g., coronary artery disease (Taylor et al., 2013), carotid bifurcation (S. E. Lee et al., 2008), arteriovenous fistula (S.-W. Lee et al., 2005), and aneurysms (Steinman et al., 2003). Numerous scientific studies have been conducted to scrutinize and assess different components of a conventional image-based modeling process, with the objective of creating a genuinely "patient-specific" CFD model. As highlighted and examined in a review (Steinman & Pereira, 2019), particular emphasis has been placed on investigating the influence of medical imaging techniques, segmentation methods, flow velocities, and the impact of non-Newtonian rheology. However, recent challenge studies within aneurysm research have brought to light a significant inter-laboratory variability. When 26 research groups were provided with identical segmented surfaces and boundary conditions, the results showed large variability stemming from the various CFD solution strategies (Steinman et al., 2013). Furthermore, when provided with identical medical images and no guidelines – reflecting current research practice – results from 28 research groups showed significant variability in the predicted WSS (Valen-Sendstad et al., 2018). These results might point to a broader reproducibility issue. While modeling and simulating cardiovascular flow can provide valuable and additional insight to vascular remodeling, establishing local computational pipelines for medical image-based CFD remains a time-intensive process that is error-prone and a significant source of variability.

With this in mind, the objective was to devise a comprehensive and resilient open-source research code enabling reproducible science, with an emphasis on user-friendliness, geared towards students, educators, and researchers. By automating the process, we reduce the need for manual labor, which enables mass production of CFD results, and of equal importance, significantly reduces the variability. The latter is also ensured by making all aspects of the modeling choices based on state-of-the-art research shown to be the current gold-standard choices in aneurysm CFD modeling. Thus, VaMPy enables non-CFD-experts to perform objective and automated out-of-the-box CFD simulations, and to produce results of publication quality.

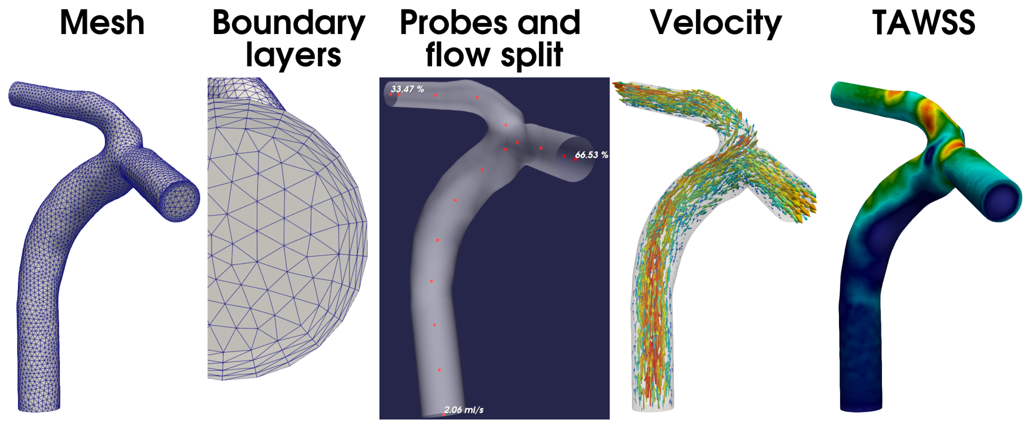

Figure 1: Illustration of the CFD pipeline for the `Artery.py` demo in VaMPy. From left to right: (1) volumetric mesh, (2) boundary layers, (3) boundary conditions (flow rate at the inlet and flow split at the outlets) and probe points along the computational domain for which the velocity and pressure is evaluated during the simulation, (4) instantaneous velocity field visualized with `Paraview` using glyphs, and (5) the resulting time averaged WSS.

Overview of features

The first feature of VaMPy is the pre-processing pipeline, which is built upon the methods introduced in `morphMan` (Kjeldsberg et al., 2019), a published framework for objective and automated manipulation of vascular morphologies. The pre-processing pipeline includes volumetric mesh generation, automated identification of inlets and outlets for boundary conditions, and generation of probe points for velocity and pressure measurements within the domain. Prior to meshing, the user may also add adjustable features such as flow extensions, surface smoothing, local refinement, and generation of boundary layers. The volumetric meshing may be set to uniform or variable mesh density, and in the two leftmost panels of Figure 1 we show a meshed artery model with boundary layers and flow extensions. Following the mesh generation, flow split boundary conditions are generated, and probe points are stored, visualized in the middle panel of Figure 1.

The second feature of VaMPy is the CFD simulation pipeline, based on the solver `Oasis` (Mortensen & Valen-Sendstad, 2015), which has been verified and validated against spectral element methods and experimental measurements (Bergersen et al., 2019; M. Khan et al., 2019). `Oasis` is an open-source, finite element-based segregated high-performance computing implementation of a space/time centered incremental pressure correction scheme. `Oasis` is formal second-order accurate in time that ensures a solution that preserves kinetic energy while minimizing numerical dispersion and diffusion errors (Karniadakis & Sherwin, 2005). A Womersley profile is prescribed at the inlet, where the inflow waveform was obtained from older adults (Hoi et al., 2010). We prescribe the flow rate according to the square law, which results in an average internal carotid artery flow rate of 245 mL/min for average sized arteries (Valen-Sendstad et al., 2015). At the outlets, we use a reduced order method to split the flow (Chnafa et al., 2017).

The third feature of VaMPy is post-processing, where we have scripts that compute the flow and simulation metrics, hemodynamic indices, probe point visualization, and velocity and pressure conversion. The flow metrics include parameters such as the friction velocity (and associated l^+ and t^+ values) (Valen-Sendstad et al., 2011), which allows the user to assess the relative resolution and simulation quality. The script also computes the Kolmogorov scales, kinetic energy, and turbulent kinetic energy, based on phase averaging multiple cardiac cycles. The script for computing hemodynamic indices includes the most commonly computed ones, including WSS, oscillatory shear index (OSI), and relative residence time (RRT), and to demonstrate we have shown the time averaged WSS (TAWSS) in the rightmost panel of Figure 1. The probe point visualization script creates a figure of velocity and pressure traces at predetermined points inside the domain. Finally, the conversion script creates viewable versions of the compact velocity and pressure solutions, and may be visualized in software such as `ParaView` (Ayachit, 2015) .

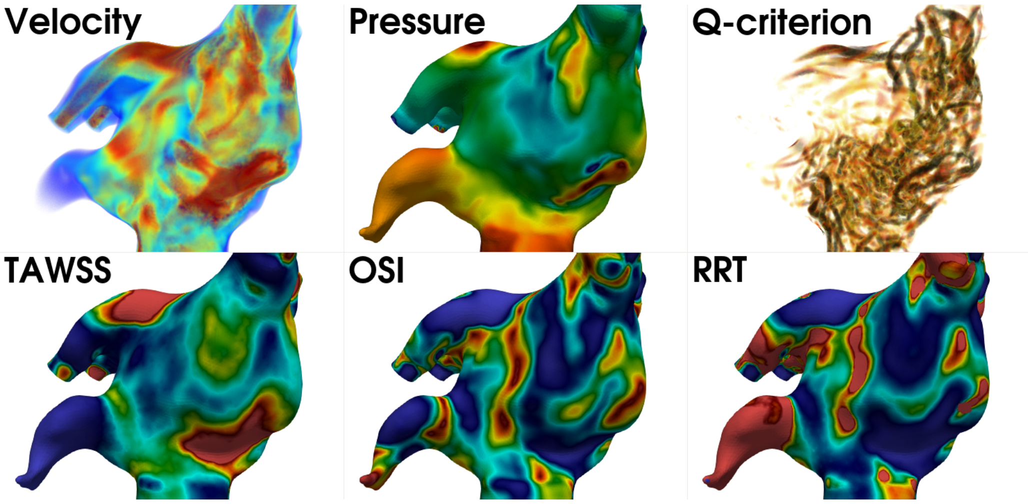

Figure 2: Example of an extension of `VaMPy` to cardiovascular flow in the left atrium and the associated hemodynamic stresses. From top left to bottom right: the volumetric rendering of velocity, the pressure field, volumetric rendering of the Q-criterion, TAWSS, OSI, and RRT.

Extension to cardiac flows

The pipeline is fully automated and has been demonstrated and tailored towards simulations of cerebrovascular flows. The demonstration shown in Figure 1 is configured to be run on a laptop within a reasonable time frame, but to perform simulations with adequate resolutions we refer to (M. O. Khan et al., 2015; Valen-Sendstad et al., 2014; Valen-Sendstad & Steinman, 2014). Beside cerebrovascular flows, `VaMPy` can easily be extended to also allow for simulation of other vascular territories. In Figure 2 we show the application to modeling of the left atrium. More specifically, from top left to bottom right the figure shows the instantaneous velocity magnitude, instantaneous pressure, vortex cores (Q-criterion), and the time averaged quantities WSS, OSI, and RRT, all of which are computed with the hemodynamics post-processing script.

Acknowledgements

This work was supported by the SimCardioTest project (Digital transformation in Health and Care SC1-DTH-06-2020) under grant agreement No. 101016496 and ERACoSysMed PARIS project under grant agreements No. 643271. The simulations were performed on the Saga cluster, with resources provided by UNINETT Sigma2 – the National Infrastructure for High Performance Computing and Data Storage in Norway, grant number nn9249k. We wish to thank Dr. Jørgen Dokken for technical assistance, and Dr. Christophe Chnafa for his contribution to the boundary condition methodology.

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