

A Rosy e Wolmer

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Acronyms

AAA	Abdominal aortic aneurysm
BC	Boundary condition
BFGS	Broyden-Fletcher-Goldfarb-Shanno
CFD	Computational fluid dynamics
CMR	Coronary Magnetic Resonance
CN	Crank-Nicolson
FE	Finite Elements
GMRES	Generalized minimal residual method
IPCS	Incremental pressure correction scheme
MRI	Magnetic resonance imaging
NS	Navier Stokes
OSI	Oscillatory shear index
RE	Reynolds number
PDE	Partial differential equation
RMSE	Root Mean Squared Error
TAWSS	Time Averaged WSS
VarDA	Variational data assimilation
WSS	Wall shear stress

Chapter 1

Estimation of optimal inlet boundary conditions for blood flow assessment in abdominal aortic aneurysm using variational data assimilation

S. Paratico, R. Munafò, C. Trenti, P. Dyverfeldt, S. Saitta and E. Votta

Abstract

Blood fluid dynamics impacts vessel wall cells and tissue biomechanics, influencing thrombus formation and vessel wall remodeling. Accurate *in vivo* quantification can thus aid in understanding these mechanisms and patient stratification. Computational fluid dynamics (CFD) and 4D flow MRI are used for this purpose, but both have limitations: CFD involves assumptions and boundary condition simplifications, while 4D flow MRI suffers from low spatial resolution and noise. This study employs variational data assimilation (VarDA) to integrate CFD and 4D flow MRI, yielding a high-resolution, noise-free flow field closely aligned with 4D flow MRI velocity data. To enhance alignment, the optimal inlet velocity profile is determined iteratively via an incremental pressure correction scheme (IPCS). Previously tested in simple synthetic geometries and later in a complex patient-specific abdominal aortic aneurysm (AAA), this approach demonstrates improved reliability in patient-specific hemodynamic evaluation.

Introduction

Alterations in blood fluid dynamics often contribute to the onset or the progress of cardiovascular pathological conditions [Bappoo et al. (2021), Guzzardi et al. (2015)]. Hence, quantifying blood fluid dynamics on a patient-specific basis and non-invasively can support the understanding of pathological mechanisms or the stratification of patients based on the risk for adverse endpoints. To this aim, blood flow field can be reconstructed from clinical imaging, namely 4D flow MRI [Dyverfeldt et al. (2015)], or computed through patient-specific CFD models [Kheyfets et al. (2015)]. However, 4D flow MRI provides indirect and noisy velocity measure-

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ments with low spatio-temporal resolution, which often violate mass conservation. On the other hand, CFD models, which solve the discretized version of the Navier-Stokes (NS) equations to compute noise-free and well-resolved velocity fields, are not immune to numerical artefacts and typically rely on simplifying assumptions for boundary conditions (BCs), including inlet velocity BCs. Variational data assimilation (VarDA) combines physical governing equations with sparse, uncertain experimental data by optimizing initial or boundary conditions to minimize the misfit between simulation results and data. In cardiovascular fluid dynamics, VarDA merges CFD-based Navier-Stokes equations with in vivo 4D flow MRI velocity data, minimizing the misfit by optimizing the inlet velocity profile. A challenge is computing both the velocity and pressure gradient fields, particularly in large arteries with high velocities, requiring pressure-velocity coupling or correction schemes. However, noise in the velocity field, particularly from MRI data, can hinder proper pressure field correction in these schemes.

Related works

Several studies have explored VarDA in hemodynamics, ranging from 2D steady-state conditions to 3D transient conditions. D’Elia et al. (2012) showed that VarDA allows to reconstruct flow fields in geometrically complex 2D domains, such as the 2D representation of the aortic arch and carotid bifurcation, even with noisy velocity data. Subsequently, in D’Elia and Veneziani (2013), the same authors showed that, in 2D domains, noisy velocity data can be effectively managed by properly managing inlet BCs. In particular, they showed that the regularization of the inlet velocity profile through the use of a control variable also regularized the velocity field over the whole domain and allowed for successful pressure-velocity coupling. Tiago et al. (2017) extended VarDA to a 3D saccular aneurysm, demonstrating its flexibility with various BCs and optimization methods like gradient-based and genetic algorithms to improve accuracy. Koltukluolu and Blanco (2018) showed that VarDA, applied to 4D Flow MRI data, outperformed traditional CFD methods by dynamically adjusting boundary conditions in real-time to maintain flow congruence near inlets. Funke et al. (2019) demonstrated the effectiveness of 4D (3D space + time) VarDA in capturing transient blood flow in aneurysms using phase contrast-MRI data. Finally, Dokken et al. (2020) proposed a multimesh finite element (FE) method that enhanced stability and accuracy by allowing flexible BC management across multiple mesh domains, which is key for simulating complex hemodynamics in realistic geometries.

Aim of the work

This study aims to implementing a method to compute *in vivo* blood fluid dynamics on a patient-specific basis with high space-resolution without using simplifying hypotheses on the inlet BCs. To this aim, we leverage VarDA to estimate an optimal inlet BC for a CFD simulation, where the inlet BC initially consists in a noisy and uncertain 4D flow MRI-based velocity profile, and consistency between the CFD-computed velocity field and sparse 4D flow MRI-based data in the bulk flow region is enforced. We benchmarked the method on ideal 2D and 3D geometries and then applied it to a patient-specific abdominal aortic aneurysm (AAA) geometry.

Methods

Data Assimilation Method

The VarDA approach was formulated as an optimization problem constrained by the NS equations, using the *dolfin-adjoint* library for the adjoint problem. The process follows three steps: running a first numerical simulation with tentative inlet BCs (which we refer to as the *forward model* or *Tape*), solving the optimization problem to identify inlet BCs, and running a final numerical simulation yielding the refined velocity and pressure fields (Fig. 1.1).

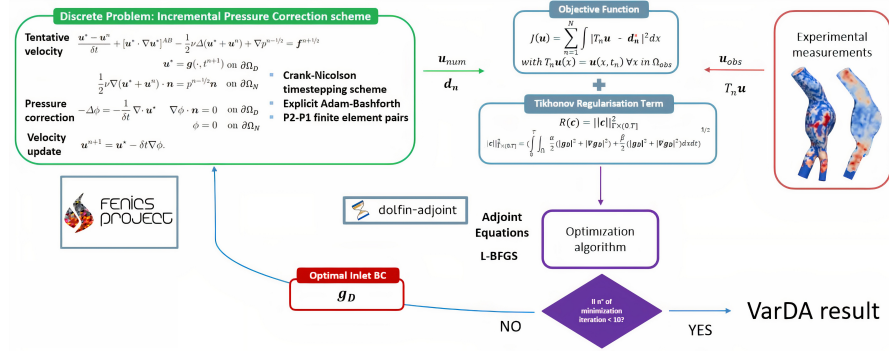


Fig. 1.1: **Top-left:** The finite element (FE) solver computes the Navier-Stokes (NS) equations with an initial guess for the inlet boundary conditions (BCs); **Top-right:** experimental velocity measurements are taken at discrete points in the domain; **Center:** discrepancy between the computational fluid dynamics (CFD) velocity field and experimental data is minimized by iteratively refining inlet velocity profile with a gradient-based method.

Forward problem definition

The weak and discretized form of NS equations for an incompressible fluid [?] was solved using the FE platform *FEniCS* [Alnaes et al. (2015)] to compute velocity field \mathbf{u} over a domain Ω given an initial condition $\mathbf{u} = \mathbf{u}_0$ on Ω at time t_0 , a zero pressure condition at the outlet section Ω_N and a Dirichlet boundary condition at the inlet section Ω_D in the form of a space- and time-dependent velocity profile \mathbf{g} . Through an in house Python script, 2D and 3D fluid domains Ω were discretized into triangular and tetrahedral elements, respectively, with 1-1.5 mm characteristic size and with linear and quadratic shape functions for nodal pressure and velocity, respectively. The semi-implicit Crank-Nicolson (CN) time-integration scheme was applied with a time increment of $\Delta t = 0.001$ s. The IPCS proposed in [Goda (1979)] was implemented. A generalized minimal residual method (GMRES) was chosen as linear solver, with tolerances of 1×10^{-4} for momentum and continuity equations.

Optimization Problem definition

The optimization problem (eq. (1.1)), constrained by the NS equations, aimed to minimize a functional $J(\mathbf{u})$ (eq. (1.2)), defined as the difference between the computed and observed velocities.

$$\begin{aligned} \min_{\mathbf{c}} J(\mathbf{u}) + R(\mathbf{c}) \quad \text{s.t.} \quad F(\mathbf{u}, \mathbf{c}) = 0 \\ J(\mathbf{u}) = \|\mathbf{u} - \mathbf{u}_{\text{obs}}\|_{L^2(\Omega)} \end{aligned} \quad (1.1)$$

To address the ill-posedness of the problem, a Tikhonov regularization term $R(\mathbf{c})$ was introduced, with respect to the controlled variable defined as c . It accounts for two terms that are scaled by parameters α and β , where β is set to 0 for steady-state conditions. This reformulation transforms the problem into an unconstrained optimization scenario, more suitable for gradient descent methods.

$$\begin{aligned} R(\mathbf{c}) &= \|\mathbf{c}\|_{L^2(\Omega)} \\ \text{where} \\ \|c\|_{\Gamma \times (0, T]} &= \left(\int_0^T \int_{\Omega} \frac{\alpha}{2} \left(|\mathbf{g}_D|^2 + |\nabla \mathbf{g}_D|^2 \right) + \frac{\beta}{2} \left(|\dot{\mathbf{g}}_D|^2 + |(\nabla \mathbf{g})_D|^2 \right) dx dt \right)^{\frac{1}{2}} \end{aligned} \quad (1.3)$$

The adjoint approach efficiently computes the total derivative of the functional, yielding the adjoint NS equations that facilitate optimization. The iterative Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm, in its L-BFGS variant [Liu and Nocedal (1989)], served as optimizer. The L-BFGS algorithm is already implemented in the SciPy library which is automatically called by *dolfin-adjoint* library. The SciPy library provides many user-friendly numerical routines, such as the routine for opti-

mization. Convergence was ensured through Wolfe conditions [Nocedal and Wright (2006)], with maximum number of iterations equal to 10 and the following tolerances' values: $\text{ftol} = 1 \times 10^{-9}$ and $\text{gtol} = 1 \times 10^{-12}$. The performances of the method were assessed by $J(\mathbf{u})$ value before and after optimization, Root Mean Squared Error (RMSE) between \mathbf{u} and \mathbf{u}_{obs} , and qualitative analysis of the effect on the velocity field through the software *Paraview*.

Benchmark Tests

Preliminary tests - First, preliminary tests were performed to compare the computational efficiency of IPCS versus the coupled scheme in a 2D straight conduit (which represents a case of 2D VarDA and can thus be addressed using the term I defined as *2DVar*). Simulations were run under laminar conditions at both low and high Reynolds numbers, in order to evaluate the method in laminar and transitionally unstable regimes. The conduit was a longitudinal section of a cylinder with a diameter of 41 mm and a length of 200 mm. Synthetic observations (\mathbf{u}_{obs}) were generated by an auxiliary CFD simulation, prescribing a parabolic velocity profile at the inlet with peak velocity $U_{\text{max}} = 600$ mm/s ($\text{Re} = 6649$) and with $U_{\text{max}} = 50$ mm/s ($\text{Re} = 554$) for turbulent and laminar conditions, respectively. In the Tape, the tentative inlet velocity profile was parabolic with $U_{\text{max}} = 800$ mm/s ($\text{Re} = 8865$) and $U_{\text{max}} = 100$ mm/s ($\text{Re} = 1108$). The iterative minimization of the discrepancy between \mathbf{u} and \mathbf{u}_{obs} was performed to determine the optimal velocity profile for CFD simulations, verifying if it matched the parabolic profile used to generate the synthetic observations.

Progressively demanding tests - Next, the method was benchmarked through three progressively more demanding tests:

1. 2D straight conduit in transient conditions (which represents a case of 2D VarDA also involving time and can thus be addressed using the term I defined as *2DVar+t* benchmark) - This benchmark shared the same domain of the 2DVar benchmark. However, both the auxiliary simulation for the generation of the experimental observations and Tape consisted in a sequence of two transient simulations: in the first simulation, velocity was initially equal to 0 mm/s everywhere in the domain, and at the inlet a parabolic velocity profile was imposed, whose peak velocity increased linearly from 0 to $\frac{U_{\text{max}}}{2}$ over 0.3 s; in the second simulation, the velocity field computed by the first one was used as IC and the inlet velocity parabolic profile was scaled by the time-dependent function $f(t)$:

$$f(t) = \begin{cases} \frac{U_{\text{max}}}{2} \cos\left(\frac{\pi}{T_s}\left(t - \frac{T_s}{2}\right)\right), & \text{if } t \leq T_s \\ \frac{U_{\text{max}}}{2}, & \text{if } T_s < t \leq T_d \end{cases} \quad (1.4)$$

where $T_s = 300$ ms and $T_d = 540$ ms are cardiac cycle's systolic and diastolic phases [Katz (1977)].

Besides determining the optimal velocity profile for CFD simulations, spatial and temporal regularization terms [eq. (1.3)] were incorporated into the optimization process and subjected to a sensitivity analysis.

2. 3D straight conduit in steady-state conditions (which represents a case of 3D VarDA and can thus be addressed using the term I defined as *3DVar* benchmark) - This benchmark evaluated the computational cost increase when transitioning from a 2D to a 3D problem. The fluid domain was a 3D cylinder with a radius of 30 mm and a length of 200 mm. IC and BCs, as well as the objective function, were identical to those in the 2DVar benchmark.
3. Patient-specific AAA geometry in steady-state conditions (which represents a case of 3DVar applied to a patient-specific AAA geometry and can thus be addressed using the term I defined as AAA benchmark) - This benchmark aimed to test VarDA in a complex 3D domain using real experimental observations. 4D flow imaging was acquired from an adult male with AAA using a 3T coronary magnetic resonance (CMR) system (Ingenia, Philips Healthcare, Netherlands) at Linkping University Hospital. The 4D flow data were processed with in-house Python [Saitta et al. (2024)] and CMR angiography was performed for 3D AAA geometry segmentation. Two tests were carried out with laminar flow in the AAA. In the first test, observations consisted in 4DFlow data acquired during early systole, corresponding to the third time frame (about 63 ms from the start of the cardiac cycle, with a 21 ms time step), while the Tape was generated by a CFD simulation fed by 4DFlow-based inlet velocity profiles. The second test assessed the method's robustness against noise, using an inlet velocity profile, scaled by 0.15, at peak systole to produce the Tape's output. Noisy observations were generated by processing the Tape's output according to medium noise setting of Saitta et al. (2024). In addition to already-mentioned metrics, wall shear stresses (WSSs) from final simulation we analyzed using custom Paraview filters.

The associated codes can be found at the following link: <https://github.com/saraparatico/proceedingsCodes/tree/main>.

Results

Computational costs

Numerical experiments were conducted on various setups: a workstation with 24 CPUs and 64 GB RAM for 2DVar and 3DVar and a high-performance computing system with 40 CPUs and 190 GB RAM for 2DVar+t and AAA benchmark. 2DVar took 30 minutes and 3DVar took 6 hours on 12 CPUs; on the other side, 6 hours were required for 2DVar+t and 17 hours for AAA benchmark.

Preliminary tests

In high Reynolds tests, IPCS optimization reduced RMSE from 142.60 mm/s to 6.70 mm/s, while the coupled scheme faced convergence issues. In low Reynolds conditions, IPCS proved to be five times faster than the coupled scheme and achieved a final RMSE of 1.76 mm/s compared to 4.22 mm/s for the coupled scheme.

Progressively Demanding Tests

2DVar + t benchmark - When a zero-velocity field was imposed as IC, the post-optimization velocity field showed inconsistencies with respect to the observations. In particular, a high-velocity region just downstream of the inlet section was obtained, while low velocity values were computed in the rest of the domain. Moreover, these tests did not yield improvements by changing α , and increasing β further worsened the performance (Fig. 1.2).

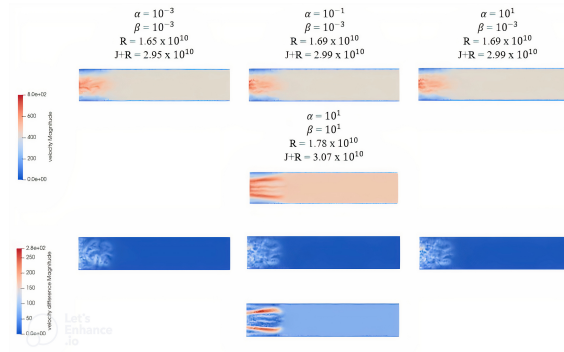


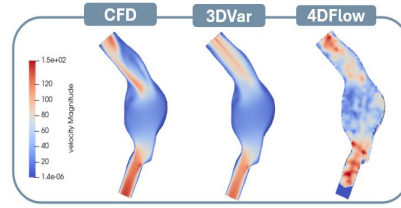
Fig. 1.2: Sensitivity analysis of regularization parameters at systolic peak. First row: 2DVar + t velocity magnitude for different α values (10^{-3} , 10^{-1} , 10^1), with $\beta = 10^{-3}$. Second row: test with $\beta = 10^1$ to assess time regularization. Third and fourth rows: velocity difference between reference and 3DVar results for each α and β .

When the initial velocity and pressure fields were set equal to those yielded by the previous post-optimization simulation, the results showed a more homogeneous flow better matching parabolic characteristics and with lower $J + R$ values.

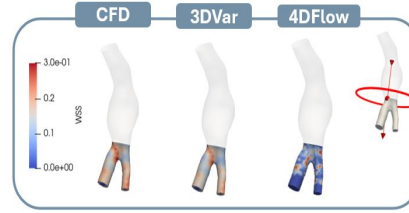
3DVar benchmark - VarDA was performed with spatial regularization terms set to $\alpha = 10^{-2}$, 10^1 , and 10^3 . The lowest value of $J + R$ was achieved with $\alpha = 10^{-2}$, but it did not correspond to the lowest RMSE. The velocity field exhibited a peak near the inlet, suggesting continuity loss. For $\alpha = 10^1$, the lowest RMSE was achieved,

and the post-optimization velocity field more accurately reflected the observed data. Increasing α to 10^3 resulted in significant deviations from the observations, with unexpected velocity behaviors and higher values of $J + R$ and RMSE. This suggests that lower α values improve RMSE, while higher α values lead to smoother solutions, but can introduce inaccuracies when too large.

AAA benchmark - In first tests, *RMSE* improved from 59.3 mm/s to 55.1 mm/s, indicating a better alignment with observations (Fig. 1.3a). Generating a Tape took



(a) AAA benchmark velocity magnitude maps.



(b) AAA benchmark WSS maps.

Fig. 1.3: (a) velocity and (b) wall shear stress (WSS) fields obtained on the abdominal aortic aneurysm (AAA) computed by computational fluid dynamics (CFD) (**left**), derived directly from 4DFlow MRI (**right**), and by data assimilation (**centre**).

about 25 minutes, while optimization required 17 hours with 80 Gb of memory. WSS distributions from Tape's output and 3DVar predictions were consistent, identifying regions with high shear stress (Fig. 1.3b). WSS distributions from Tape's output and 3DVar predictions were consistent in terms of location of high WSS regions. Moreover, while enforcing consistency with 4DFlow-based velocity measurements, the 3DVar method yielded a regular and realistic WSS distribution. This is a major difference as compared to the WSS distribution estimated directly from 4DFlow data, which was unrealistic owing to their poor space-resolution and to the impact of noise in the near-wall region.

In tests with noisy observations, 3DVar effectively reconstructed the velocity field, slightly reducing *RMSE* from 36.8 mm/s to 36.4 mm/s, while maintaining WSS predictions consistent with CFD results, particularly at the iliac bifurcation, which is

where the abdominal aorta splits into two smaller arteries, carrying blood to pelvis and legs.

Discussion

From 2DVar+t to 3DVar

The 2DVar+t reveals challenges due to inertial effects and short simulation durations, causing reconstruction defects from incomplete flow development. Extending simulation time for optimization is impractical due to high computational costs. A potential solution includes proper initialization of CFD simulations and implementing a checkpointing method to reduce computational costs by using only the last cardiac cycle for gradient calculations. Moreover, a key difference between 2DVar+t and 3DVar is the flow field's response to regularization. In 2DVar+t, increasing α has minimal effect due to dominant time-dependent effects, reducing spatial regularization's impact. Additionally, increasing β deteriorates the results, a challenge not present in 3DVar, emphasizing the difficulty of balancing temporal and spatial regularization in dynamic flows. Conversely, in 3DVar, moderate α values (10^1) significantly improve the velocity field, reducing inlet peaks and lowering *RMSE*. However, excessive regularization ($\alpha = 10^3$) causes unrealistic velocity patterns.

AAA benchmark

AAA benchmark effectively reconstructs the velocity field in AAA geometry, maintaining high consistency with data obtained from 4D flow imaging. It identifies high shear stress regions despite challenges due to lower resolution of 4D flow data near boundaries. The method remains robust against noise.

Conclusions

This study demonstrates the application of the VarDA method to estimate optimal inlet BC for CFD simulations using noisy 4D flow MRI data. The method minimizes mismatch between CFD solutions and in vivo velocity data, producing a resolved, noise-free velocity field aligned with experimental measurements. Benchmarked on 2D and 3D geometries and applied to a patient-specific AAA geometry, it shows potential for personalized hemodynamic simulations. The IPCS framework improves efficiency and accuracy in transient flow analyses. Despite challenges in transient simulations, the work paves the way for future VarDA advancements, with implications for cardiovascular medicine.

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Glossary

Abdominal aortic aneurysm Localized dilation of the abdominal aorta, which can lead to rupture and severe complications if untreated.

Boundary condition Condition that defines the values of variables in a physical system at the boundaries of a spatial domain to solve partial differential equations.

Broyden-Fletcher-Goldfarb-Shanno Numerical optimization algorithm used to solve unconstrained minimization problems.

Computational fluid dynamics Field that uses numerical methods to analyze and solve problems involving fluid flows.

Coronary Magnetic Resonance Medical imaging technique based on magnetic resonance to visualize coronary blood flow and heart tissue.

Crank-Nicolson Implicit numerical method used to solve parabolic and hyperbolic partial differential equations, often employed in CFD simulations.

Generalized minimal residual method Iterative method for solving non-symmetric linear systems, widely used in CFD and other scientific computing fields.

Incremental pressure correction scheme Numerical scheme for solving Navier-Stokes equations that separates velocity and pressure calculations into multiple steps.

Magnetic resonance imaging Non-invasive medical imaging technique that uses magnetic fields and radio waves to produce detailed images of tissues inside the body.

Navier-Stokes System of equations describing the motion of viscous fluids, fundamental in many fluid dynamics applications.

Oscillatory shear index Measure of the directional oscillation of shear stress on the walls of a blood vessel, often associated with vascular disease susceptibility.

Partial differential equation Equation involving partial derivatives of a function with respect to multiple variables, commonly used to model physical phenomena.

Root Mean Squared Error Statistical measure of the difference between predicted and observed values, used to evaluate the accuracy of a model.

Time Averaged Wall Shear Stress Time-averaged value of shear stress on vessel walls, relevant for studying hemodynamics.

Variational data assimilation Method that combines mathematical models and observational data to improve estimates of physical states, commonly used in fluid dynamics and meteorology.

Wall shear stress Stress exerted by a fluid on the wall of a vessel or conduit, crucial for analyzing hemodynamics and vascular diseases.