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lifex-cfd: an open-source computational fluid dynamics solver for cardiovascular applications

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Abstract

Computational fluid dynamics (CFD) is an important tool for the simulation of the cardiovascular function and dysfunction. Due to the complexity of the anatomy, the transitional regime of blood flow in the heart, and the strong mutual influence between the flow and the physical processes involved in the heart function, the development of accurate and efficient CFD solvers for cardiovascular flows is still a challenging task. In this paper we present life^x-cfd, an open-source CFD solver for cardiovascular simulations based on the life^x finite element library, written in modern C++ and exploiting distributed memory parallelism. We model blood flow in both physiological and pathological conditions via the incompressible Navier-Stokes equations, accounting for moving cardiac valves, moving domains, and transition-to-turbulence regimes. In this paper, we provide an overview of the underlying mathematical formulation, numerical discretization, implementation details and instructions for use of life^x-cfd. The code has been verified through rigorous convergence analyses, and we show its almost ideal parallel speedup. We demonstrate the accuracy and reliability of the numerical methods implemented through a series of idealized and patient-specific vascular and cardiac simulations, in different physiological flow regimes. The life^x-cfd source code is available under the LGPLv3 license, to ensure its accessibility and transparency to the scientific community, and to facilitate collaboration and further developments.

Keywords: computational fluid dynamics, blood flow, cardiovascular modeling, high performance computing, open-source software, finite element method, numerical simulations

PROGRAM SUMMARY

Program Title: life^x-cfd

CPC Library link to program files: (to be added by Technical Editor)

Developer's repository link: https://gitlab.com/lifex/lifex-cfd

Code Ocean capsule: (to be added by Technical Editor)

Licensing provisions (please choose one): LGPLv3

Programming language: C++ (standard \geq 17)

Supplementary material: https://doi.org/10.5281/zenodo.7852089 contains the application executable in binary form, compatible with any recent enough x86-64 Linux system, assuming that glibc version \geq 2.28 is installed. Data and parameter files necessary to replicate the test cases described in this manuscript are also available.

Nature of problem: the program allows to run computational fluid dynamics simulations of cardiovascular blood flows in physiological and pathological conditions, modeled through incompressible Navier-Stokes equations, including moving cardiac valves, moving domains (such as contracting cardiac chambers) in the arbitrary Lagrangian-Eulerian framework, and transition-to-turbulence flow. Given the scale of the typical applications, the program is designed for parallel execution.

Solution method: the equations are discretized using the Finite Element method, on either tetrahedral or hexahedral meshes. The software builds on top of deal.II, implementing the mathematical models and numerical methods specific for CFD cardiovascular simulations. Parallel execution exploits the MPI paradigm. The software supports both Trilinos and PETSc as linear algebra backends.

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Additional comments including restrictions and unusual features: the program provides a general-purpose executable that can be used to run CFD simulations without having to access or modify the source code. The program allows to setup simulations through a user-friendly yet flexible interface, by means of readable and self-documenting parameter files. On top of that, more advanced users can modify the source code to implement more sophisticated test cases. $life^{x}-cfd$ supports checkpointing, i.e. simulations can be stopped and restarted at a later time.

1. Introduction

Computational Fluid Dynamics (CFD) simulations have emerged as a powerful tool for understanding the complex hemodynamics of the cardiovascular system and the mechanisms underlying pathological conditions [1-23]. Hemodynamics simulations can provide insights into complex flow patterns [12, 24-33], pressure distributions, and wall stresses [34, 35] that are difficult or impossible to measure in vivo. These insights can aid in the development of novel diagnostic tools and therapies [3, 36-39]. Indeed, cardiovascular diseases are a major global health concern, responsible for a significant number of deaths each year [40, 41].

However, despite the significant progress made in the computational modeling of the cardiovascular system, the development of accurate and efficient CFD solvers for cardiovascular applications remains a challenging task [42], due in part to the complex anatomy and physical processes involved, as well as to the need for high-performance computing resources required to capture the dynamics of thin structures (such as valves) [9, 43–46] and small turbulent scales [47, 48]. Indeed, most of the computational software libraries currently available on the market and open source only address some of these challenges, and there is room for enhancement in the development of a single comprehensive tool that provides, in a computationally efficient way, accurate results in terms of anatomical detail, flow kinematics, and stress reconstruction.

In this paper, we present life^x-cfd, an open-source CFD solver for cardiovascular applications in moving geometries with immersed structures. It is based on life^x [49], a flexible, high performance library for multiphysics, multiscale and multidomain finite element problems building on the deal.II [50] Finite Element (FE) core.

The scientific community has developed several open-source CFD software packages for cardiovascular simulations. The availability of the code under open-source licenses ensures accessibility and transparency to the wider scientific community, facilitating collaboration and further developments. Every available software package is characterized by the different needs it addresses and by its requirements, regarding the complexity of the simulation and the desired level of resolution, the size of the computational domain, and the availability of computational resources. Popular state-of-the-art methodologies for predictive simulation in cardiovascular health and disease are thoroughly reviewed in [9, 51]. FEBio provides rich capabilities for vascular flow simulations, differing from other CFD programs mainly by the use of fluid dilatation instead of pressure as a primary variable [52]. *CHeart* is a framework for multiphysics finite element simulations in biomedical research, including a CFD solver with advanced numerical features, an Arbitrary Lagrangian-Eulerian (ALE) formulation and the Streamline Upwind Petrov-Galerkin (SUPG) stabilization [53]. simVascular provides a complete computational framework, from the construction of an anatomic model to finite element simulation and postprocessing [42], with the possibility to solve the incompressible Navier-Stokes equations in an arbitrary domain and specifically designed for cardiovascular simulations. IBAMR is an adaptive and distributed-memory parallel implementation of the Immersed Boundary Method (IBM) has also been used in hemodynamics applications [54]. ExaDG is a high order Discontinuous Galerkin CFD solver based on deal.II, exploiting a matrix-free algorithm equipped with multigrid smoothers, with a focus on accuracy and extreme parallel performance [55]. Lethe allows to solve the incompressible Navier–Stokes equations using high-order continuous Galerkin formulations on quadrilateral and hexahedral adaptive meshes, leveraging the deal.II library [56]. General-purpose packages such as OpenFOAM [57–60] and FEniCS [61, 62] have also been used for cardiovascular simulations.

Compared to these alternatives, our $life^{x}-cfd$ solver offers several distinctive advantages, mostly inherited from the $life^{x}$ core structure [49]. It is designed to be user-friendly and easy to use, even for biomedical researchers without extensive experience in computational fluid dynamics, and comes with a clean and meticulously documented code base. The solver is implemented in C++ using modern programming paradigms and leverages MPI for distributed memory parallelism. Moreover, it supports arbitrary finite elements (among those available in deal.II), the possibility to import arbitrary meshes with either hexahedral or tetrahedral elements and several linear algebra backends (namely Trilinos [63], PETSc [64] and deal.II itself), ensuring a fine control over the numerical setting. The solver is also designed to be scalable, allowing it to efficiently simulate large-scale scenarios.In addition to the numerical and programming features stemming from its foundation on life^x, life^x-cfd can easily and efficiently solve differential problems with moving geometries, accounting for both moving domain boundaries and immersed surfaces. Furthermore, it supports several types of boundary conditions, all of which can be easily accessed and configured through the external parameter files and used without the need to access and modify the source code. To the best of our knowledge, none of the packages mentioned above exhibits similar features all together.

Besides the abovementioned programming features and numerical methods implemented, a paramount value proposition of life^{*}-cfd is the seamless integration with several other solvers for the cardiac function based on life^{*} [65], such as electrophysiology [66], mechanics [67–69], electromechanics [70–73], CFD [31, 74–80], fluid-structure interaction [81], electro-mechano-fluid interaction [82, 83] and myocardial perfusion [84, 85], which have been exploited ranging from single-chamber to whole-heart simulations.

The paper is organized as follows. In Sec. 2, we describe the underlying mathematical formulation and the corresponding numerical algorithms used in our solver, including its ability to handle complex geometries, enforce several kind of boundary conditions, and simulate both laminar and turbulent flows with efficient linear solvers and preconditioners. Implementation details and instructions on how to run $life^{x}-cfd$ simulations are described in Sec. 3. We verify our implementation by running convergence analyses and by assessing its parallel performance on the *Beltrami flow* benchmark [86]; we also demonstrate the code accuracy and reliability in reproducing different physiological flow regimes through a series of tests inspired by patient-specific vascular and cardiac applications of increasing complexity. All the numerical results are reported in Sec. 4. Finally, some conclusive remarks and the impact of $life^{x}-cfd$ are discussed in Sec. 5.

2. Mathematical and numerical methods

In the following sections, we introduce the mathematical models and numerical methods characterizing the life^x-cfd solver.

2.1. Mathematical models

In large vessels and heart chambers, blood can be regarded as a Newtonian incompressible fluid, in spite of the presence of small particles suspended and carried by the plasma. Therefore, we model it with the *incompressible Navier-Stokes equations* [87–90], using the ALE formulation [91–93] to account for the motion of vessels and heart chambers. Moving immersed valves are modeled by the Resistive Immersed Implicit Surface (RIIS) method [94, 95].

2.1.1. Domain displacement

Let (0,T) be the temporal domain, with T denoting the final time. Let $\Omega_t \subset \mathbb{R}^3$ be the spatial fluid domain at time $t \in (0,T)$, let $\Gamma_t = \partial \Omega_t$ be its boundary, and let \boldsymbol{n} be the outward-directed normal unit vector. To model the displacement of the domain over time, we introduce a fixed reference configuration $\widehat{\Omega} \subset \mathbb{R}^3$, such that the domain in current configuration Ω_t is defined at any $t \in (0,T)$ as

$$\Omega_t = \{ \boldsymbol{x} \in \mathbb{R}^3 : \, \boldsymbol{x} = \mathcal{A}_t(\widehat{\boldsymbol{x}}) = \widehat{\boldsymbol{x}} + \widehat{\boldsymbol{d}}(\widehat{\boldsymbol{x}}, t), \, \widehat{\boldsymbol{x}} \in \widehat{\Omega} \},\$$

where $\widehat{d}: \widehat{\Omega} \times (0,T) \to \mathbb{R}^3$ is the domain displacement. Throughout this paper, we assume that the displacement $\widehat{d}_{\widehat{\Gamma}^{\mathrm{D}}}: \widehat{\Gamma}^{\mathrm{D}} \times (0,T) \to \mathbb{R}^3$ is known on a Dirichlet boundary portion of $\partial \widehat{\Omega}$, that we denote by $\widehat{\Gamma}^{\mathrm{D}}$. We recover the displacement in the bulk domain by solving the following lifting problem:

$$\begin{cases} -\nabla \cdot \left(\alpha \, \sigma^{\mathrm{L}}(\widehat{d}) \right) = \mathbf{0} & \text{in } \widehat{\Omega} \times (0, T), \\ \widehat{d} = \widehat{d}_{\widehat{\Gamma}^{\mathrm{D}}} & \text{on } \widehat{\Gamma}^{\mathrm{D}} \times (0, T), \\ \sigma^{\mathrm{L}}(\widehat{d}) \widehat{n} = \mathbf{0} & \text{on } \partial \widehat{\Omega} \setminus \widehat{\Gamma}^{\mathrm{D}} \times (0, T). \end{cases}$$
(1)

Concerning the choice of $\sigma^{L}(\hat{d})$, life^x-cfd provides the following options:

- harmonic extension: $\sigma^L(\widehat{d}) = \nabla \widehat{d};$
- *linear elasticity*:

$$\sigma^{L}(\widehat{d}) = \frac{E}{1+\nu} \nabla^{S} \widehat{d} + \frac{E\nu}{(1+\nu)(1-2\nu)} \left(\nabla \cdot \widehat{d} \right) I,$$

where E and ν are the Young and Poisson moduli of a fictitious linear elastic material, and ∇^{S} denotes the symmetric gradient, defined as

$$oldsymbol{
abla}^S \widehat{oldsymbol{d}} = rac{1}{2} \left(oldsymbol{
abla} \widehat{oldsymbol{d}} + oldsymbol{
abla} \widehat{oldsymbol{d}}^T
ight) \; .$$

The coefficient $\alpha : \widehat{\Omega} \to \mathbb{R}$ in (1) is introduced to locally increase the stiffness in critical areas of the domain, to preserve the quality of mesh elements. life^x-cfd offers three options:

- no stiffening, i.e. $\alpha = 1$ in $\widehat{\Omega}$;
- Jacobian-based stiffening [96]:

$$\alpha(\widehat{\boldsymbol{x}}) = \left(\frac{J_0}{J(\widehat{\boldsymbol{x}})}\right)^{\chi}$$

where J_0 and χ are positive user-defined parameters, and $J(\hat{x})$ is the Jacobian of the map from the unit reference element to the one in $\widehat{\Omega}$; with this approach, elements that are small are made stiffer:

• boundary-based stiffening [97]:

$$\alpha(\widehat{\boldsymbol{x}}) = \max(d(\widehat{\boldsymbol{x}}), \beta)^{-\gamma}$$

where $d(\hat{x})$ is the distance from the boundary (or a portion of the boundary), and β and γ are two userdefined positive parameters; with this approach, the stiffness is increased in the elements that are close to the moving boundary.

Finally, the ALE velocity is computed by deriving the displacement w.r.t. time:

$$\boldsymbol{u}^{\text{ALE}} = \frac{\partial \boldsymbol{\hat{d}}}{\partial t} \circ \mathcal{A}_t^{-1} \quad \text{in } \Omega_t \times (0, T).$$
(2)

2.1.2. Navier-Stokes equations

We model blood as a fluid of constant density ρ and constant dynamic viscosity μ . Let $\boldsymbol{u}: \Omega_t \times (0,T) \to \mathbb{R}^3$ be the fluid's velocity and $p: \Omega \times (0,T) \to \mathbb{R}$ be its pressure. Their evolution is prescribed by incompressible Navier-Stokes equations in the ALE framework with RIIS modeling of cardiac values, that is:

$$\begin{cases} \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho((\boldsymbol{u} - \boldsymbol{u}^{\text{ALE}}) \cdot \boldsymbol{\nabla})\boldsymbol{u} + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\boldsymbol{u}, p) & \text{in } \Omega_t \times (0, T), \\ + \boldsymbol{\mathcal{R}}(\boldsymbol{u}, \boldsymbol{u}^{\text{ALE}}) = \boldsymbol{f} \end{cases}$$
(3a)

$$\mathbf{f} \cdot \boldsymbol{u} = 0$$
 in $\Omega_t \times (0, T),$ (3b)

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{u} &= 0 & \text{in } \Omega_t \times (0, T), & (3b) \\ \boldsymbol{u} &= \boldsymbol{u}_0 & \text{in } \Omega_0 \times \{0\}. & (3c) \end{aligned}$$

In the above, $\frac{\hat{\partial}}{\hat{\partial}t}$ denotes the time derivative in the ALE framework [92], $\boldsymbol{f}: \Omega_t \times (0,T) \to \mathbb{R}^3$ is a forcing term, and $\boldsymbol{u}_0: \Omega_0 \to \mathbb{R}^3$ is a suitable initial condition. The latter can either be zero, or be imported from clinical data or other simulation results. The tensor σ is the Cauchy stress tensor, defined for an incompressible, viscous and Newtonian fluid as

$$\sigma(\boldsymbol{u}, p) = -pI + 2\mu \boldsymbol{\nabla}^{S} \boldsymbol{u}.$$

The alternative definition $\sigma(\boldsymbol{u}, p) = -pI + \mu \nabla \boldsymbol{u}$ can also be considered: see (7) in Section 2.3. System (3) must be endowed with suitable boundary conditions, as described in Section 2.2.

The term $\mathcal{R}(u, u^{\text{ALE}})$ in (3a) is introduced to account for the presence of heart values in the fluid in cardiac simulations by means of the Resistive Immersed Implicit Surface (RIIS) method [94, 95]. The valves are represented by a set \mathcal{I}_{v} of immersed surfaces $\Sigma_{k}, k \in \mathcal{I}_{v}$. Each of them is characterized by a resistance coefficient $R_{\rm k}$ and a parameter $\varepsilon_{\rm k}$ representing the half thickness of the valve leaflets. To each valve we associate a signed distance function $\varphi_{\rm k}: \Omega_t \times (0,T) \to \mathbb{R}$. Then, $\mathcal{R}(\boldsymbol{u}, \boldsymbol{u}^{\rm ALE})$ is defined as [74, 82, 94, 95]

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{u}^{\text{ALE}}) = \sum_{\mathbf{k} \in \mathcal{I}_{\mathbf{v}}} \frac{R_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}} \delta_{\Sigma_{\mathbf{k}}, \varepsilon_{\mathbf{k}}}(\varphi_{\mathbf{k}}) \left(\boldsymbol{u} - \boldsymbol{u}^{\text{ALE}} - \boldsymbol{u}_{\Sigma_{\mathbf{k}}}\right).$$
(4)

This term weakly imposes the no-slip condition on the valve surfaces, by penalizing the difference between the relative fluid velocity $\boldsymbol{u} - \boldsymbol{u}^{\text{ALE}}$ and the relative velocity of the valves' leaflets $\boldsymbol{u}_{\Sigma_k}$. The term $\boldsymbol{\mathcal{R}}$ has support over a narrow layer around Σ_k defined through the following smoothed Dirac delta function:

$$\delta_{\Sigma_{\mathbf{k}},\varepsilon_{\mathbf{k}}}(\varphi_{\mathbf{k}}(\boldsymbol{x})) = \begin{cases} \frac{1 + \cos(\pi \varphi_{\mathbf{k}}(\boldsymbol{x})/\varepsilon_{\mathbf{k}}))}{2\varepsilon_{\mathbf{k}}} & \text{if } |\varphi_{\mathbf{k}}(\boldsymbol{x})| \le \varepsilon_{\mathbf{k}}, \\ 0 & \text{if } |\varphi_{\mathbf{k}}(\boldsymbol{x})| > \varepsilon_{\mathbf{k}}, \end{cases}$$

for all $k \in \mathcal{I}_v$.

2.2. Boundary conditions

life^x-cfd supports different types of boundary conditions, and for each type several options are available. In the following sections, we briefly describe each of the implemented options. All the boundary condition types discussed below can be combined seamlessly, by decomposing the boundary in an arbitrary number of subsets and selecting one of the following options for each subset. All the coefficients and parameters for the options that follow are easily customizable by the user without modifying the source code.

2.2.1. Dirichlet boundary conditions

Let $\Gamma_t^{\rm D} \subset \partial \Omega_t$ denote a subset of the domain boundary.life^x-cfd supports no-slip boundary conditions, i.e.

$$\boldsymbol{u} = \boldsymbol{u}^{\mathrm{ALE}} \quad \text{on } \Gamma^{\mathrm{D}}_t \times (0,T) ,$$

or u = 0 if the domain is not moving (i.e. if the ALE formulation is not enabled). Alternatively, it is possible to prescribe Dirichlet conditions in the form

$$\boldsymbol{u}(\mathbf{x},t) = \boldsymbol{g}(\mathbf{x},t) = \theta g(t) \boldsymbol{s}(\boldsymbol{x}) \quad \text{on } \Gamma_t^{\mathrm{D}} \times (0,T) ,$$

where the Dirichlet datum $\boldsymbol{g}: \Gamma_t^{\mathrm{D}} \times (0,T) \to \mathbb{R}^3$ is expressed by separation of variables, with $\boldsymbol{g}: (0,T) \to \mathbb{R}$ and $\boldsymbol{s}: \Gamma_t^{\mathrm{D}} \to \mathbb{R}^3$. The parameter $\theta > 0$ is a *repartition factor* that can be used to split total flow rate over multiple boundaries.

life^x-cfd offers several options for the function g(t):

• A constant function:

$$q(t) = \overline{q}$$
, for all $t \in (0, T)$.

• A sinusoidal *pulsatile function* from g_{\min} to g_{\max} , with period \mathcal{T} :

$$g(t) = g_{\min} + \left(g_{\max} - g_{\min}\right) \frac{1}{2} \left(1 - \cos\left(\frac{2\pi t}{\mathcal{T}}\right)\right)$$

• A sinusoidal ramp from g_0 to g_1 , starting at $t_0 > 0$ and lasting $t_L > 0$:

$$g(t) = \begin{cases} g_0 & \text{if } t < t_0, \\ g_0 + \frac{g_1 - g_0}{2} \left(1 - \cos\left(\frac{\pi(t - t_0)}{t_{\rm L}}\right) \right) & \text{if } t_0 \le t < t_0 + t_{\rm L} \\ g_1 & \text{if } t \ge t_0 + t_{\rm L}. \end{cases}$$

• Interpolation in time of prescribed flow rate or velocity data: the function g(t) is obtained by interpolating a given a set of pairs $\{(t_i, g_i)\}_{i=0}^{N_g}$. The interpolation can be a piecewise linear polynomial, a piecewise cubic spline, or a Fourier series interpolation [98].

For the space-dependent function s(x), the options below are available.

• A parabolic profile for a circular boundary of radius \tilde{R} :

$$oldsymbol{s}(oldsymbol{x}) = -2rac{\widetilde{R}^2 - r^2(oldsymbol{x})}{\pi \widetilde{R}^4}oldsymbol{n}(oldsymbol{x}),$$

where $r(\boldsymbol{x})$ is the distance of \boldsymbol{x} from the barycenter of Γ_t^{D} . A parabolic profile can be used for instance to prescribe a laminar inlet velocity profile [99].

• A uniform profile, i.e. a prescribed inflow velocity that is normal to the $\Gamma_t^{\rm D}$ and constant in space:

$$\boldsymbol{s}(\boldsymbol{x}) = -\boldsymbol{n}(\boldsymbol{x}).$$

A uniform profile can be used, for instance, to prescribe a turbulent inlet velocity profile [99].

• A Womersley profile [100] for a circular boundary of radius \tilde{R} , commonly used to describe a pulsatile flow in the cardiovascular system [88, 100]. This profile is computed by solving the inverse problem¹ described in [101]. The Womersley profile is only compatible with g(t) defined by interpolating given data using a Fourier series.

Remark 1. Parabolic and Womersley profiles have unit flow rate, so that the function g(t) represents flow rate over time. Conversely, the uniform profile has unit velocity, and the function g(t) is a velocity over time.

2.2.2. Periodic boundary conditions

Periodic boundary conditions are also available. Let $\Gamma^{A} \subset \partial \Omega$ and $\Gamma^{B} \subset \partial \Omega$ be two planar subsets of the boundary of the domain, mutually mapped through a translation $\phi_{AB} : \mathbb{R}^{3} \to \mathbb{R}^{3}$ such that $\Gamma^{B} = \phi_{AB}(\Gamma^{A})$. Then, periodic conditions are expressed as

$$\boldsymbol{u}(\boldsymbol{x},t) = \boldsymbol{u}(\boldsymbol{\phi}_{\mathrm{AB}}(\boldsymbol{x}),t) \quad \text{on } \Gamma^{\mathrm{A}} \times (0,T) .$$

Periodic conditions are only supported for hexahedral meshes. Moreover, the discretizations of Γ^{A} and Γ^{B} are required to be conforming (i.e. there must be a one-to-one correspondence between mesh elements on the two surfaces).

2.2.3. Neumann boundary conditions

life^x-cfd supports Neumann boundary conditions in the form

$$\sigma(\boldsymbol{u}, p)\boldsymbol{n} = -h(t)\boldsymbol{n} \qquad \text{on } \Gamma_t^{\mathsf{N}} \times (0, T) , \qquad (5)$$

where $\Gamma_t^{\mathbf{N}} \subset \partial \Omega_t$, \boldsymbol{n} is the outgoing normal to $\Gamma_t^{\mathbf{N}}$ (at a fixed time) and $h(t) : (0,T) \to \mathbb{R}$ is a time-dependent function representing the space-averaged pressure on the Neumann boundary. The same options introduced for g(t) (Section 2.2.1) are available for h(t).

Optionally, backflow instabilities can be prevented on Neumann boundaries by enabling *inertial backflow* stabilization [102-104], i.e. by modifying (5) as

$$\sigma(\boldsymbol{u},p)\boldsymbol{n} = -h(t)\boldsymbol{n} + \beta \frac{\rho}{2} |\boldsymbol{u} \cdot \boldsymbol{n}|_{-} \boldsymbol{u} \quad \text{on } \Gamma_{t}^{\mathrm{N}} \times (0,T) ,$$

where $|\mathbf{u} \cdot \mathbf{n}|_{-} = \min{\{\mathbf{u} \cdot \mathbf{n}, 0\}}$ and $\beta > 0$ is a user-defined stabilization parameter [102–104].

2.2.4. Resistance boundary conditions

Resistance boundary conditions [29, 105–107] are conditions of the form

$$\sigma(\boldsymbol{u}, p)\boldsymbol{n} = -\left(p_0(t) + C_{\mathrm{R}} \int_{\Gamma_t^{\mathrm{R}}} (\boldsymbol{u} - \boldsymbol{u}^{\mathrm{ALE}}) \cdot \boldsymbol{n} \, d\gamma\right) \boldsymbol{n} \qquad \text{on } \Gamma_t^{\mathrm{R}} \times (0, T) \;,$$

where $\gamma \subset \partial \Omega$, $p_0(t)$ is a baseline pressure, $C_{\rm R} > 0$ the resistance coefficient. The term $p_0(t)$ can be defined using the same temporal functions introduced for g(t).

2.2.5. Free-slip boundary conditions

Free-slip conditions, also known as symmetry conditions, are mixed Dirichlet-Neumann conditions of the form

$$\begin{split} \boldsymbol{u} \cdot \boldsymbol{n} &= 0 \qquad \text{on } \Gamma_t^{\mathrm{D}} \times (0, T) ,\\ (\sigma(\boldsymbol{u}, p) \boldsymbol{n}) \cdot \boldsymbol{t}_i &= 0 \qquad \text{on } \Gamma_t^{\mathrm{D}} \times (0, T) \qquad i \in \{1, 2\} \end{split}$$

where t_i , for $i \in \{1, 2\}$ are the tangent unit vectors to Γ_t^{D} .

¹This inverse problem is solved once and for all at the beginning of the simulation.

2.3. Numerical methods

We introduce the infinite-dimensional function spaces

$$\boldsymbol{\mathcal{V}}_{\boldsymbol{g}}^t := \left\{ \boldsymbol{v} \in [H^1(\Omega_t)]^3 : \boldsymbol{v} = \boldsymbol{g} \text{ on } \Gamma_t^{\mathrm{D}} \right\}, \quad \mathcal{Q}^t := L^2(\Omega_t).$$

For the spatial discretization of (3), we introduce a mesh \mathcal{T}^h over Ω_t , composed of either tetrahedra or hexahedra (life^x supports both types of meshes). We introduce the function space of *Finite Elements* (FE) with piecewise Lagrangian polynomials of degree $r \geq 1$ over \mathcal{T}^h as

$$X_r^h = \{ v_h \in C^0(\overline{\Omega}) : v_h |_K \in \mathbb{P}^r, \text{ for all } K \in \mathcal{T}^h \},\$$

wherein h is the diameter of the grid element $K \in \mathcal{T}^h$. We introduce the finite-dimensional spaces $\mathcal{V}_{g,h}^t =$ $\mathcal{V}_{g}^{t} \cap [X_{r}^{h}]^{3}$ and $\mathcal{Q}_{h}^{t} = \mathcal{Q}^{t} \cap X_{r}^{h}$, and denote by $u_{h} \in \mathcal{V}_{g,h}^{t}$, $p_{h} \in \mathcal{Q}_{h}^{t}$ the FE approximations of u and p, respectively. life^{*}-cfd supports polynomials of order 1 and 2 on tetrahedral meshes, and polynomials of arbitrary degree on hexahedral meshes.

Temporal discretization is carried out through Backward Differentiation Formulas (BDF) [98, 108] of order $\sigma_{\rm BDF} = 1, 2, 3$. We partition the time domain (0, T) into N_t subintervals of equal size $\Delta t = T/N_t$, and we denote with the subscript n quantities related to the time-step n, with $n = 0, \ldots, N_t$. The approximation of the velocity time derivative reads [98, 109]:

$$\left. \frac{\partial \boldsymbol{u}_h}{\partial t} \right|_{n+1} \approx \frac{\alpha_{\text{BDF}} \boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^{\text{BDF}}}{\Delta t} \quad \text{for } n = \sigma_{\text{BDF}} - 1, \dots, N_t - 1.$$

wherein α_{BDF} is a coefficient depending on the order σ_{BDF} of the method and u_h^{BDF} is a linear combination of

velocities at timesteps $n, n-1, \ldots, n-\sigma_{\rm BDF} + 1$. We also introduce an extrapolated velocity $\boldsymbol{u}_h^{\rm EXT}$ that approximates \boldsymbol{u}_h^{n+1} with accuracy order $\sigma_{\rm BDF}$ through a linear combination of velocities at timesteps $n, n-1, \ldots, n-\sigma_{\rm BDF} + 1$. We refer to [109] for the definition of $\alpha_{\rm BDF}, \boldsymbol{u}_h^{\rm BDF}$ and $\boldsymbol{u}_h^{\rm EXT}$.

The advection term in (3a) can be formulated in a *fully-implicit* or *semi-implicit* [109] way. For the sake of a compact notation, we denote the advection velocity by $\boldsymbol{u}_h^*,$ defined as

$$oldsymbol{u}_h^* = \left\{ egin{array}{ll} oldsymbol{u}_h^{n+1} - oldsymbol{u}_h^{ ext{ALE},n+1} & ext{(implicit formulation)}, \ oldsymbol{u}_h^{ ext{EXT}} - oldsymbol{u}_h^{ ext{ALE},n+1} & ext{(semi-implicit formulation)} \end{array}
ight.$$

The fully-discrete formulation of (3) reads: given $\boldsymbol{u}_h^n, \ldots, \boldsymbol{u}_h^{n+1-\sigma_{\text{BDF}}}$, for any $n = 0, \ldots, N_t - 1$, find $(\boldsymbol{u}_h^{n+1}, p_h^{n+1}) \in \boldsymbol{\mathcal{V}}_{\boldsymbol{g},h}^t \times \boldsymbol{\mathcal{Q}}_h^t$ such that, for all $(\boldsymbol{v}_h, q_h) \in \boldsymbol{\mathcal{V}}_{\boldsymbol{0}}^h \times \boldsymbol{\mathcal{Q}}_h^t$,

$$\left(\rho \frac{\alpha_{\text{BDF}} \boldsymbol{u}_{h}^{n+1}}{\Delta t}, \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} + \left(\rho \left(\boldsymbol{u}_{h}^{*} \cdot \boldsymbol{\nabla}\right) \boldsymbol{u}_{h}^{n+1}, \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} + \mathcal{D}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{v}_{h}) \\
- \left(p_{h}^{n+1}, \boldsymbol{\nabla} \cdot \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} + \left(\boldsymbol{\nabla} \cdot \boldsymbol{u}_{h}^{n+1}, q_{h}\right)_{\Omega_{n+1}} + \left(\boldsymbol{\mathcal{R}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{\text{ALE}, n+1}), \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} \\
+ \sum_{K \in \mathcal{T}_{h}} \mathcal{S}^{K}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, p_{h}^{\text{EXT}}, \boldsymbol{v}_{h}, q_{h})_{\Omega_{n+1}} \\
= \left(\boldsymbol{f}^{n+1}, \boldsymbol{v}_{h}\right) + \left(\boldsymbol{h}^{n+1}, \boldsymbol{v}_{h}\right)_{\Gamma_{n+1}^{N}} + \left(\rho \frac{\boldsymbol{u}_{h}^{\text{BDF}}}{\Delta t}, \boldsymbol{v}_{h}\right)_{\Omega_{n}}.$$
(6)

In the above, $(\cdot, \cdot)_X$ denotes the scalar product in $L^2(X)$. \mathcal{D} is the diffusion term, for which life^x-cfd offers the following formulations:

$$\mathcal{D}(\boldsymbol{u}_{h}^{n+1},\boldsymbol{v}_{h}) = \begin{cases} \left(\mu \nabla \boldsymbol{u}_{h}^{n+1}, \nabla \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} & (gradient - gradient) \\ \left(2\mu \nabla^{S} \boldsymbol{u}_{h}^{n+1}, \nabla \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} & (symmetric \ gradient - \ gradient) \\ \left(2\mu \nabla^{S} \boldsymbol{u}_{h}^{n+1}, \nabla^{S} \boldsymbol{v}_{h}\right)_{\Omega_{n+1}} & (symmetric \ gradient - \ symmetric \ gradient) \end{cases}$$
(7)

The formulation (6) includes terms \mathcal{S}^{K} that can be optionally enabled to stabilize the Galerkin formulation. life^x-cfd provides the Streamline Upwind Petrov Galerkin - Pressure Stabilizing Petrov Galerkin (SUPG-PSPG) [110] and the Variational Multiscale - Large Eddy Simulation (VMS-LES) [109, 111, 112] stabilization methods. Both methods stabilize the problem in terms of the *inf-sup* condition and stabilize possible advectiondominated regimes (typically occurring in cardiovascular hemodynamics) [113]. Furthermore, the VMS-LES acts also as a turbulence model, allowing to model the transition-to-turbulence regime characterizing the cardiovascular blood flow [12, 47, 48]. In a compact form, we define the stabilization terms as:

$$\mathcal{S}^{K}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, p_{h}^{\text{EXT}}, \boldsymbol{v}_{h}, q_{h}) = \begin{cases} \mathcal{S}^{K}_{\text{SUPG-PSPG}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, \boldsymbol{v}_{h}, q_{h}) & \text{if SUPG-PSPG} \\ \mathcal{S}^{K}_{\text{SUPG-PSPG}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, \boldsymbol{v}_{h}, q_{h}) & \\ + \mathcal{S}^{K}_{\text{VMS}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, \boldsymbol{v}_{h}) & \text{if VMS-LES} \\ + \mathcal{S}^{K}_{\text{LES}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, p_{h}^{\text{EXT}}, \boldsymbol{v}_{h}) & \end{cases}$$
(8)

with the SUPG-PSPG and VMS terms defined, respectively, as

$$\mathcal{S}_{\text{SUPG-PSPG}}^{K}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, p_{h}^{n+1}, \boldsymbol{v}_{h}, q_{h}) = \left(\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{n+1}, p_{h}^{n+1}), \rho\boldsymbol{u}_{h}^{*} \cdot \boldsymbol{\nabla}\boldsymbol{v}_{h} + \boldsymbol{\nabla}q_{h}\right)_{K} + \left(\tau_{\text{C}}(\boldsymbol{u}_{h}^{*})r_{\text{C}}(\boldsymbol{u}_{h}^{n+1}), \boldsymbol{\nabla}\cdot\boldsymbol{v}_{h}\right)_{K},$$

$$(9)$$

$$\mathcal{S}_{\text{Kace}}^{K}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{*}, \boldsymbol{v}_{h}^{n+1}, \boldsymbol{v}_{h}) = \left(\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{v}_{h}^{n+1}), \boldsymbol{\omega}\boldsymbol{u}_{h}^{*} \cdot (\boldsymbol{\nabla}\boldsymbol{v}_{h})^{T}\right)$$

$$(10)$$

$$\mathcal{S}_{\text{VMS}}^{K}(\boldsymbol{u}_{h}^{n+1},\boldsymbol{u}_{h}^{*},p_{h}^{n+1},\boldsymbol{v}_{h}) = \left(\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{n+1},p_{h}^{n+1}),\rho\boldsymbol{u}_{h}^{*}\cdot(\boldsymbol{\nabla}\boldsymbol{v}_{h})^{T}\right)_{K} .$$
(10)

The LES term – modeling the Reynolds stresses – is defined according to the implicit or semi-implicit formulation, as [109, 111]:

$$S_{\text{LES}}^{K}(\boldsymbol{u}_{h}^{n+1},\boldsymbol{u}_{h}^{*},p_{h}^{n+1},p_{h}^{\text{EXT}},\boldsymbol{v}_{h}) = \begin{cases} -(\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{n+1},p_{h}^{n+1})\otimes\tau_{\text{M}}(\boldsymbol{u}_{h}^{n+1},p_{h}^{n+1}),\rho\boldsymbol{\nabla}\boldsymbol{v}_{h})_{K} & \text{(implicit formulation),} \\ -(\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{\text{EXT}},p_{h}^{\text{EXT}})\otimes\tau_{\text{M}}(\boldsymbol{u}_{h}^{*})\boldsymbol{r}_{\text{M}}(\boldsymbol{u}_{h}^{n+1},p_{h}^{n+1}),\rho\boldsymbol{\nabla}\boldsymbol{v}_{h})_{K} & \text{(semi-implicit formulation).} \end{cases}$$
(11)

In the above, $r_{\rm M}$ and $r_{\rm C}$ are the strong residuals of the momentum balance (3a) and continuity (3b) equations, defined on each mesh element K as

$$\begin{split} \boldsymbol{r}_{\mathrm{M}}^{K}(\boldsymbol{u}_{h}^{n+1}, p_{h}^{n+1}) = & \rho \left(\frac{\alpha_{\mathrm{BDF}} \boldsymbol{u}_{h}^{n+1} - \boldsymbol{u}_{h}^{\mathrm{BDF}}}{\Delta t} + \boldsymbol{u}_{h}^{*} \cdot \boldsymbol{\nabla} \boldsymbol{u}_{h}^{n+1} \right) + \boldsymbol{\nabla} p_{h}^{n+1} - \mu \boldsymbol{\Delta} \boldsymbol{u}_{h}^{n+1} \\ & + \boldsymbol{\mathcal{R}}(\boldsymbol{u}_{h}^{n+1}, \boldsymbol{u}_{h}^{\mathrm{ALE}, n+1}) - \boldsymbol{f}^{n+1}, \\ r_{\mathrm{C}}^{K}(\boldsymbol{u}_{h}^{n+1}) = & \boldsymbol{\nabla} \cdot \boldsymbol{u}_{h}^{n+1}. \end{split}$$

The stabilization parameters are defined as [74, 109]

$$\begin{aligned} \tau_{\mathrm{M}}(\boldsymbol{u}_{h}^{*}) &= \left(\frac{\sigma_{\mathrm{BDF}}^{2}\rho^{2}}{\Delta t^{2}} + \rho^{2}\boldsymbol{u}_{h}^{*} \cdot \overline{G}\boldsymbol{u}_{h}^{*} + C_{r}\mu^{2}\overline{G} : \overline{G} + \sum_{\mathrm{k}\in\mathcal{I}_{\mathrm{v}}}\frac{R_{k}^{2}}{\varepsilon_{\mathrm{k}}^{2}}\delta_{\Sigma_{\mathrm{k}},\varepsilon_{\mathrm{k}}}^{2}(\varphi_{\mathrm{k}})\right)^{-\frac{1}{2}},\\ \tau_{\mathrm{C}}(\boldsymbol{u}_{h}^{*}) &= \left(\tau_{\mathrm{M}}(\boldsymbol{u}_{h}^{*})\overline{\boldsymbol{g}} \cdot \overline{\boldsymbol{g}}\right)^{-1}, \end{aligned}$$

where $\overline{G} = J^{-T}J^{-1}$ and $\overline{g} = J^{-T}\mathbf{1}$. are the metric tensor and the metric vector, respectively [111]. We remark that the definition of the stabilization terms has been modified with respect to the original formulation of [111] by accounting for the presence of immersed surfaces [74].

An analogous FE approximation is introduced for the quasi-static lifting problem (1), through which both the discrete displacement \hat{d}_h and the discrete ALE velocity u_h^{ALE} are defined.

2.4. Linear algebra

Following space and time discretizations, the lifting problem (1) leads to a symmetric, positive definite linear system, which we solve using either the GMRES or the conjugate gradient (CG) method [98, 114]. The system can be preconditioned using algebraic multigrid (AMG) [115], additive Schwarz [116] or a block Jacobi preconditioner.

The discretization of Navier-Stokes equations (6) leads to a block algebraic system, which can be linear or non-linear depending on the implicit or semi-implicit treatment of the advection term. It is linearized through Newton's method $[113]^2$, and the resulting block linear system is solved through the GMRES method [98, 114],

²In the linear case, only one Newton iteration is performed.

using the aSIMPLE preconditioner [117]. For further details on the algebraic form of the problem and its block structure, see [117]. The approximation of the velocity and Schur complement blocks is obtained through AMG, additive Schwarz or block Jacobi [114].

3. Implementation

life^x-cfd builds upon the core functionalities of life^x [49], which in turn relies on deal.II [50, 118] to provide general-purpose software facilities for finite elements. Specifically, life^x-cfd implements the mathematical models, numerical methods and utilities needed for CFD simulations in the cardiovascular setting. The linear algebra backend is offered either by Trilinos [63] or by PETSc [64, 119], as wrapped by deal.II. This includes the implementation of the linear solvers (CG and GMRES) and of the black-box preconditioners (AMG, additive Schwarz, block Jacobi) that life^x supports. Other dependencies include VTK [120], the Boost libraries [121] and general-purpose compilation tools such as CMake³ and GNU make. We provide a Docker⁴ image bundling all the dependencies, to facilitate the installation of life^x-cfd on new systems. We refer to the online documentation⁵ for further instructions on the download and installation procedures.

We exploit forward automatic differentiation [122] to assemble the linear system associated to (6). This is especially useful to deal with the large amount of the terms (8), associated to the SUPG-PSPG and VMS-LES stabilizations. In particular, this allows to easily implement the implicit VMS-LES formulation, in spite of the large amount of non-linear terms it involves.

We refer the interested reader to [49] for further details on the core functionalities of life^x. Below, we provide a quick-start guide on how to run simulations within life^x-cfd. More information can be found in the online documentation.

3.1. Running simulations in $life^{x}$ -cfd

A ready-to-run binary package is available for download at https://doi.org/10.5281/zenodo.7852089, compatible with any recent enough x86-64 Linux distribution, provided that glibc (https://www.gnu.org/software/libc/) version \geq 2.28 is installed. The binary file is shipped in AppImage (https://appimage.org/) format and is named lifex-cfd-1.5.0-x86_64.AppImage. For more detailed instructions on how to run the life^x-cfd binary, we refer the reader to [65].

Experienced users and those aiming at maximum computational efficiency on High Performance Computing (HPC) facilities and cloud platforms are recommended to compile life^x-cfd and its dependencies from source. Instructions are available in the online documentation, together with a manual for running simulations. Below we report a quick-start guide to use the solver, and refer the interested reader to the documentation for further information. All the commands hold also for the binary version, by simply replacing lifex_fluid_dynamics with lifex-cfd-1.5.0-x86_64.AppImage.

After compiling life^x-cfd, the main executable can be found within the compilation folder at apps/fluid_dynamics/lifex_fluid_dynamics. A brief description of its command line options can be obtained through

```
$ ./lifex_fluid_dynamics -h
```

The executable allows to run test cases with an arbitrary number of inlet and outlet boundaries. The configuration of the simulation is supplied through a parameter file. The user can generate a template parameter file using the following command:

wherein <boundary labels> is a list of the labels to be used for portions of the domain boundary where specific boundary conditions must be applied. In addition to the boundary condition specifications for each element of <boundary labels>, either no-slip or free-slip boundary conditions can be enforced on other boundaries: see Section 4.2 for a practical example.

³https://cmake.org/

⁴https://www.docker.com/

⁵https://lifex.gitlab.io/lifex-cfd/

The level of detail of the parameter files can be optionally reduced (by specifying the minimal option) or increased (by specifying the full option). The former is advised for an initial use of life^x-cfd, while the latter exposes advanced options such as parameter choices on the stabilization term and turbulence models, additional options for the ALE lifting and the RIIS method, the Jacobian-based or boundary-based stiffening of the lifting, detailed options on linear algebra and preconditioning, among others. If the user does not specify either option, an intermediate verbosity is selected by default. Parameters that are not present in the file retain their default value. We refer the reader to the documentation of the library for further information.

The parameters are written into a plain text file that provides a list of key-value pairs, grouped in subsections, that describe the configuration for the simulation to be run. Each parameter is supplied with a brief documentation (included in the parameter file itself) that explains its meaning. Once the user has edited the parameter file, the simulation can be started with:

```
$ ./lifex_fluid_dynamics [-b <boundary labels>...] \
        [-f parameter_file_name.prm] \
        [-o output_folder]
```

The boundary labels provided when executing must be the same as those used for generating the parameter file. A parallel simulation is started prepending the command with the mpirun or mpiexec wrapper (which may vary depending on the MPI implementation available), e.g.:

\$ mpirun -n N ./lifex_fluid_dynamics ...

where N is the desired number of parallel processes. The binary version supports parallel execution via MPICH (https://www.mpich.org/) version ≥ 4.0 , whereas there is in principle no restriction in the chosen MPI implementation when building life^x-cfd from source.

We point out that the parameter file also contains settings that allow to serialize the solution, so that the simulation can be stopped and restarted at a later time. Refer to the online documentation for additional details.

4. Illustrative numerical examples

In the following sections, we analyze the convergence and scalability properties of the solver, and propose some application examples to showcase the functionalities of $life^{x}-cfd$.

For the sake of reproducibility, all parameter files, meshes and auxiliary data associated with the test cases described below can be downloaded from https://doi.org/10.5281/zenodo.7852089.

4.1. Software verification and parallel performance (Test I)

For the purpose of software verification, we consider the *Beltrami flow* benchmark problem [86], which is a test case on a cubic domain for which an exact analytical solution exists (see Fig. 1 for a plot of the exact solution, and Appendix A for a detailed description). This test case is implemented in the life^x-cfd test fluid_dynamics_cube. The default parameter file lifex_test_fluid_dynamics_cube.prm for this test can be generated by

```
$ ./lifex_test_fluid_dynamics_cube -g
```

In all the tests in this section, we consider a hexahedral mesh and a second-order BDF scheme for temporal discretization. Moreover, we consider the *gradient-gradient* formulation of the diffusion term (see (7)). These settings (as well as others specified below for each test) can be encoded by modifying the file <code>lifex_test_fluid_dynamics_cube.pr</code> accordingly. The simulations can be run by

\$./lifex_test_fluid_dynamics_cube -f lifex_test_fluid_dynamics_cube.prm

We set $T = 10^{-5}$ s, $\Delta t = 10^{-6}$ s, and perform a convergence test in space for h = 0.17, 0.34, 0.68, 1.36 m (corresponding to a number of mesh refinements equal to 6, 5, 4, 3, respectively), with $\mathbb{Q}^2 - \mathbb{Q}^1$ finite elements and without any stabilization. Similarly, we set $T = 10^{-3}$ s and $\Delta t = 10^{-4}$ s and repeat the test for h = 0.85, 0.17, 0.34, 0.68, 1.36 m (corresponding to a number of mesh refinements equal to 7, 6, 5, 4, 3, respectively), with $\mathbb{Q}^1 - \mathbb{Q}^1$ finite elements and with the SUPG-PSPG stabilization. The results are reported in Figures 2a and 2b, from which we can observe that the expected convergence rates are observed for the L^2 and H^1 norms of the velocity error and for the L^2 norm of the pressure error, measured at the final time.

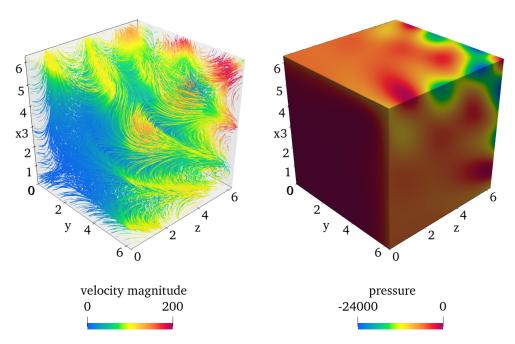


Figure 1: Test I. Solution of the Beltrami flow test case at time t = 0. Left: velocity streamlines. Right: pressure.

We perform a convergence test in time, fixing the mesh size to h = 0.17 m (corresponding to 6 mesh refinements, 262144 elements and 6714692 degrees of freedom) and progressively reducing the time step Δt by a factor 0.5, from $\Delta t = 2 \cdot 10^{-2} \text{ s to } \Delta t = 1.25 \cdot 10^{-3} \text{ s}$. We set $T = 10^{-1} \text{ s}$. The error, measured as in the previous test, tends to zero with the expected rate, as reported in Fig. 2c.

Finally, we perform a strong scalability study for this test case, by measuring the computational times associated to the assembly of the linear system and its solution with a varying number of parallel cores. The simulation is run with mesh size h = 0.085 m, corresponding to 2097152 elements and 53070468 degrees of freedom (and a number of mesh refinements equal to 7). The test was run on the GALILEO100 supercomputer provided by the CINECA supercomputing center, Italy⁶. The results, plotted in Fig. 3, show that the solver scales linearly up to 512 cores (corresponding to approximately 100 000 degrees of freedom per core), in agreement with [49, 117]. In particular, the assembly stage scales almost perfectly, whereas the performance of the linear solver deteriorates starting from around 512 cores. This is consistent with the observations of [117] on the performance of the aSIMPLE preconditioner.

4.2. Fluid dynamics in a cylinder (Test II)

We simulate the fluid dynamics in a compliant cylinder with a moving obstacle by using the $life^{x}-cfd$ app introduced in Section 3.1. A template parameter file for this setting (see also Section 3.1) can be obtained by running:

\$./lifex_fluid_dynamics -g -b "Inlet" "Outlet"

On the lateral wall of the cylinder, we prescribe no-slip boundary conditions. Therefore, we do not need to include it in the boundary label list (see below). We consider a cylinder of length L = 0.1 m and radius R = 0.01 m and the hexahedral mesh provided by the deal.II mesh generator with 5 refinements (see Table 1 for the details on the mesh obtained). The following parameters are set in the parameter file⁷:

subsection	Mesh and	space	discretization
<mark>set</mark> Mesl	n type		= Cylinder
set Eler	nent type		= Hex

⁶528 computing nodes each 2 x CPU Intel CascadeLake 8260, with 24 cores each, 2.4 GHz, 384GB RAM. See https://wiki.u-gov.it/confluence/display/SCAIUS/UG3.3%3A+GALILE0100+UserGuide for technical specifications.

⁷Each parameter is documented in the parameter file. In the paper, we omit the documentation for the sake of conciseness.

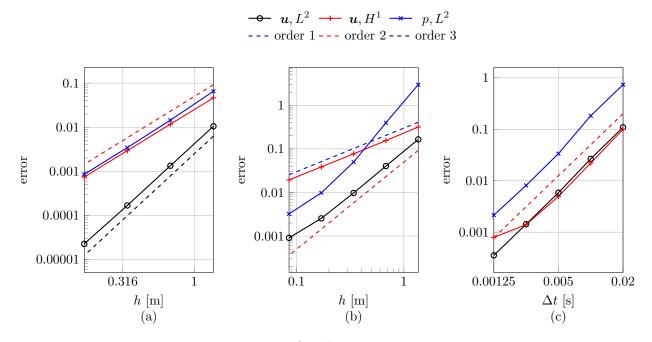


Figure 2: Test I. (a) Error against the mesh size h with $\mathbb{Q}^2 - \mathbb{Q}^1$ elements and without stabilization. (b) Error against the mesh size h with $\mathbb{Q}^1 - \mathbb{Q}^1$ elements with SUPG-PSPG stabilization. (c) Error against the time step size Δt with $\mathbb{Q}^2 - \mathbb{Q}^1$ elements and without stabilization. Dashed lines represent the expected convergence rates. Errors are measured at final time.

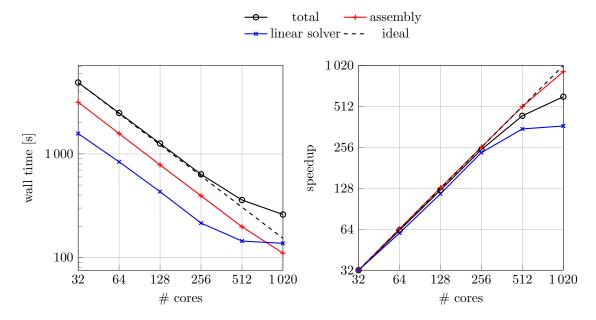


Figure 3: Test I. Strong scalability test. Wall times (left) and parallel speedup (right) varying the number of cores.

```
set Number of refinements = 5
# ...
subsection Cylinder
set Radius = 0.01
set Length = 0.1
# ...
end
# ...
end
```

We set a no-slip boundary condition on the wall (tag 0), a Dirichlet condition on the inlet section (tag 1), and a homogeneous Neumann condition on the outlet section (tag 2). For the inlet section, we prescribe a parabolic profile, with a pulsatile temporal function with $g_{\min} = 0 \text{ m}^3/\text{s}$, $g_{\max} = 2.5 \cdot 10^{-4} \text{ m}^3/\text{s}$ and period $\mathcal{T}_{\text{inlet}} = 0.8 \text{ s}$ (see Section 2.2.1).

```
subsection Boundary conditions
                    = 0
 set No-slip tags
 set Free-slip tags =
 # ...
 subsection Inlet
   set Tags
                                    = 1
   set Type of boundary condition = Dirichlet
    # ...
    subsection Dirichlet
      set Time evolution
                            = Pulsatile
      set Space distribution = Parabolic
      # ...
      subsection Pulsatile
        set Minimum value = 0.0
        set Maximum value = 2.5e-4
                      = 0.8
        set Period
      end
      # ...
    end
    # ...
 end
 subsection Outlet
   set Tags
                                    = 2
    set Type of boundary condition = Neumann
    # ...
    subsection Neumann
      set Time evolution = Constant
      # ...
      subsection Constant
       set Value = 0.0
      end
     # ...
    end
   # ...
 end
 # ...
end
```

The domain boundaries are moving according to a displacement read from a vtp file. This file contains the surface of the domain boundary and a sequence of 9 displacement fields, obtained as equispaced time samples (one every 0.1s) of the following displacement field:

$$\widehat{\boldsymbol{d}}^{\partial\Omega}(\widehat{\boldsymbol{x}},t) = C \, \frac{z(L-z)}{\sqrt{\widehat{x}^2 + \widehat{y}^2}} \, \sin\left(\frac{2\pi t}{T}\right) \left(\widehat{x},\,\widehat{y},\,0\right)^T,$$

with C = 0.015, $\hat{\boldsymbol{x}} = (\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}})^T$ and T = 0.8 s. These samples are interpolated in time by life^{*}-cfd with piecewise cubic splines.

Accordingly, the Navier-Stokes equations are solved in the ALE framework (3), in combination with a lifting problem (1) for the boundary displacement $\hat{d}^{\partial\Omega}$. We use the harmonic lifting, solved with the CG method with AMG preconditioning (see Section 2.1.1).

```
subsection Arbitrary Lagrangian Eulerian
 set Active
                                    = true
 set Import displacement from file = true
 # ...
 subsection Input file
   set Boundary displacements filename
                                             = displacement_cylinder.vtp
   set Boundary displacement field basename = d
    # ..
   set Time subintervals
                                              = 8
   set Time subinterval duration
                                              = 0.1
   # .
   set Interpolation mode
                                              = Splines
   # ...
 end
  subsection Lifting
   set Lifting operator = Harmonic
   set Tags Dirichlet = 0, 1, 2
    # ...
    subsection Linear solver
     # ...
     set Solver type = CG
     # ...
   end
   # ...
 end
 # ...
end
```

In the domain, a moving surface obstacle representing an idealized valve leaflet is immersed by the RIIS method. The closed configuration of the valve and its displacement field openingField are stored in a file cylinder_plane_closed.vtp. The parameters chosen for the RIIS method are $\varepsilon = 3 \text{ mm}, R = 10^4 \text{ kg/(m \cdot s)}$. The valve starts in closed configuration, opens for $t \in [0.15, 0.25]$ s, stays open for $t \in [0.25, 0.55]$ s, then closes during the interval $t \in [0.55, 0.65]$ s and stays closed from there on. The valve follows the displacement of the domain, whereas we use a quasi-static approach for its opening/closing, that is we set $\mathbf{u}_{\Sigma} \equiv \mathbf{0}$ in the RIIS term (4) [94, 95].

```
subsection Resistive Immersed Implicit Surface
 set Active
                                 = true
 set Use surface velocity
                                 = false
 set Surface labels
                                 = surface
 set Immersed surfaces basenames = cylinder_plane_closed
 set Move surfaces with ALE
                                 = true
 # ...
 set Displacement names
                                  = openingField
 # ...
 set Epsilons
                                  = 0.003
 set Resistances
                                  = 10000
  # ...
 subsection Displacement law
   set Displacement laws = Prescribed
    # ...
   subsection Prescribed
     set First ramp: start time = 0.15
      set First ramp: end time = 0.25
     set Second ramp: start time = 0.55
     set Second ramp: end time = 0.65
   end
 end
 # ...
end
```

For the solution of the problem, we use a semi-implicit treatment of the advection term, thus the problem is linear. To prescribe a single Newton iteration in the solution, the following parameters are used:

```
subsection Time solver
set BDF order = 1
set Non-linearity treatment = Semi-implicit
set Initial time = 0
```

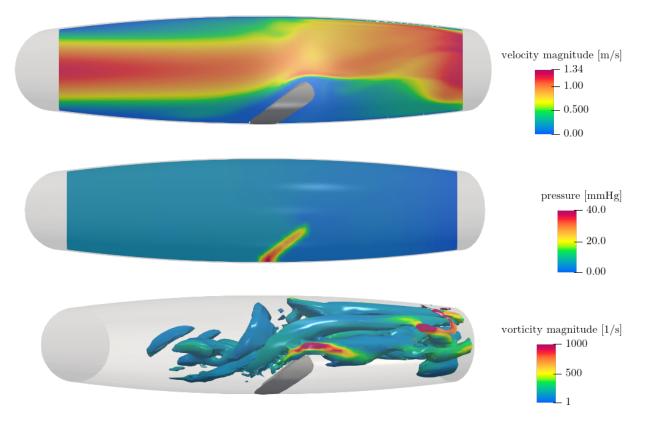


Figure 4: Test II. Flow results at t = 0.27 s: velocity magnitude (top) and pressure (center) distributions on a median slice, and Q-criterion contours (bottom, $Q = 1000/s^2$) colored by the vorticity magnitude. In grey, the region occupied by the valve.

```
set Final time = 0.8
set Time step = 2.5e-4
# ...
end
subsection Non-linear solver
set Linearized = true
# ...
end
```

Notice that the section Time solver also allows to setup the simulation to run from t = 0 s to T = 0.8 s, with $\Delta t = 2.5 \cdot 10^{-4}$ s, using a semi-implicit Euler time scheme (BDF1).

The results of the simulation at t = 0.27 s are displayed in Fig. 4. At this time, the value is in its open position: in the figure, we report in grey the support of the Dirac delta of the RIIS term:

$$\{ \boldsymbol{x} \in \Omega_t \colon |\varphi(\boldsymbol{x})| < \varepsilon \}.$$

The flow enters the domain from the left and is deviated by the valve, determining the generation of most of the coherent vorticity structures shown by the Q-criterion contours. In the pressure plot, the valve is not represented, so that one can notice that a high pressure jump is concentrated in the valve region, that acts as an obstacle to the flow.

4.3. Application to a vascular case (Test III)

We simulate the hemodynamics in a portion of aorta from a healthy 11-year-old male, also simulated in [123]. The mesh, shown in Fig. 5, and the associated boundary data were obtained from the Vascular Model Repository [124]. The domain does not move and no valves are present (i.e. ALE and RIIS are disabled). We impose Dirichlet boundary conditions on the inlet section Γ^{in} , with a parabolic velocity profile and a flow rate obtained by time interpolation of a given datum (see Section 2.2.1). On the outlet sections Γ^{out} , we impose

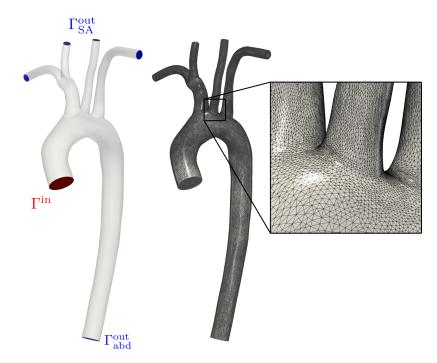


Figure 5: Test III. Computational domain and mesh, obtained from the Vascular Model Repository [124]

Test case	Mesh type	# elements	# vertices	$h_{ m min}$ [mm]	$h_{ m avg}$ [mm]	$h_{\rm max}$ [mm]
I (Beltrami flow, Section 4.1)	Hex	-	-	-	-	-
II (cylinder, Section 4.2)	Hex	81920	85345	1.64	1.75	1.91
III (aorta, Section 4.3)	Tet	2915690	543089	0.08	0.8	2.9
IV (left atrium, Section 4.4)	Tet	2438278	389484	0.28	0.8	1.3

Table 1: Mesh type (Hex: hexaedral, Tet: tetrahedral), number of mesh elements, number of mesh vertices and minimum, average and maximum mesh size for the test cases presented. Details on Test I are given in Section 4.1 since a mesh refinement study is carried out.

resistance boundary conditions (Section 2.2.4), setting $C_{\rm R} = 10^9 \, \text{kg}/(\text{s} \cdot \text{m}^4)$ on the supra-aortic outlets $\Gamma_{\rm SA}^{\rm out}$ and $C_{\rm R} = 3.5 \cdot 10^7 \, \text{kg}/(\text{s} \cdot \text{m}^4)$ on the abdominal outlet $\Gamma_{\rm abd}^{\rm out}$.

A template parameter file for this setting (see also Section 3.1) can be obtained by running:

```
$ ./lifex_fluid_dynamics -g \
    -b "Aortic root" "Right subclavian" \
        "Right common carotid" "Left common carotid" \
        "Left subclavian" "Abdominal aorta"
```

We simulate three heartbeats of period $t_{\rm hb} = 0.95 \,\mathrm{s}$ $(T = 3t_{\rm hb} = 3.8 \,\mathrm{s})$, with a time step $\Delta t = 0.001 \,\mathrm{s}$. We report in Table 1 details about the mesh used for this test case. We used $\mathbb{P}^1 - \mathbb{P}^1$ finite elements, with SUPG-PSPG stabilization, and the BDF1 time discretization method with the semi-implicit formulation for the advection term. The simulation was run on 92 parallel cores, endowed with Intel Xeon Platinum 8160 CPUs. The total wall time in this setting was 6.3 h. Figure 6 displays numerical results for this test case, which are in qualitative accordance with [123]. The solver can also be configured to compute post-processing quantities such as flow rate or average pressure on specific portions of the boundary. As an example, we report the average pressure and flow rate through $\Gamma_{\rm SA}^{\rm out}$ and $\Gamma_{\rm abd}^{\rm out}$ in Fig. 6a.

4.4. Application to a cardiac case (Test IV)

We simulate the hemodynamics in a patient-specific left atrium geometry. We consider the atrial geometry marked with ID 7 available in the public cohort [125, 126]. As we display in Figure 7a, the left atrium boundary

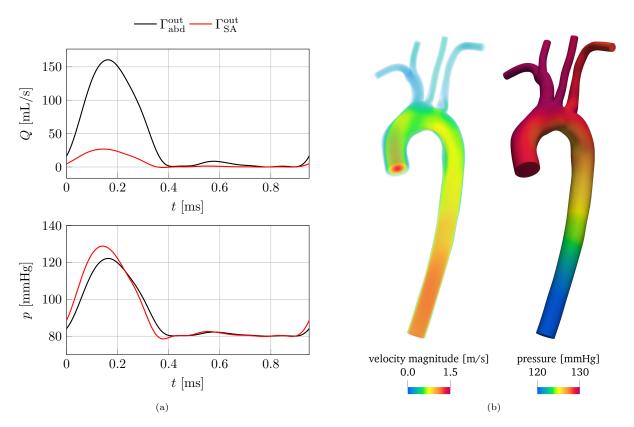


Figure 6: Test III. (a) Flowrate and average pressure on the supra-aortic and abdominal outlets during the last heartbeat of the simulation. (b) Volume rendering of the blood velocity magnitude and pressure at time t = 0.15 s of the last simulated cycle.

is made of four pulmonary veins inlet sections (Γ^{in}), an outlet section downstream of the mitral valve (Γ^{out}), and the endocardial wall (Γ^{wall}_t).

We generate the tetrahedral mesh of the left atrium in Figure 7b using vmtk [127] with the methods and tools discussed in [128]. The mesh is locally refined to capture the mitral valve leaflets as described by the RIIS method. Details on the mesh we used are provided in Table 1.

Since the patient-specific geometry of the mitral valve is not available, we generate an idealized valve geometry $\Sigma_{\rm mv}$, and the corresponding displacement, displayed in Figures 7a, 7c and 7d. We open and close the valve according to pressure jump conditions. Specifically, we monitor the pressures in control volumes located upstream and downstream the valve, as shown in Fig. 7c. The mitral valve opens when the atrial pressure overcomes the ventricular one. Viceversa, the valve closes when the pressure drop inverts its sign. Furthermore, we do not open and close the valve instantaneously, but we consider times coming from medical literature: the valve opens in 20 ms [129] and closes in 60 ms [130]. The opening and closing ramps follow the *cosinusoidal-exponential* law used in [82]. In Figures 8b and 8d, we report the pressure computed in the upstream and downstream control volumes and the opening coefficient of the mitral valve, respectively. Furthermore, we set a resistance coefficient $R_{\rm MV} = 10^4 \, {\rm kg}/({\rm m}\cdot{\rm s})$, such that the valve is sufficiently impervious, and we set $\varepsilon_{\rm MV} = 0.7 \, {\rm mm}$ by averaging the values of the mitral leaflet thicknesses reported in [131].

As boundary data, we prescribe Neumann boundary conditions on the inlet pulmonary veins sections and on the section downwind the mitral valve. We use the boundary data that we obtained in [31] by calibrating a 0D circulation model of the whole cardiovascular system [72]. On Γ^{in} , we prescribe the pulmonary venous pressure, whereas we set the left ventricular pressure on Γ^{out} . Inlet and outlet prescribed pressures are displayed in Figure 8c. On the endocardial wall, we set a no-slip condition by prescribing the displacement field that we computed in [31]. We refer the reader to [31] for additional details on the procedure we use to obtain boundary pressures and displacement.

We simulate 3 heartbeats of period $t_{\rm hb} = 1.0$ s ($T = 3t_{\rm hb} = 3.0$ s), with a time step size $\Delta t = 5 \cdot 10^{-4}$ s. We use \mathbb{P}^1 - \mathbb{P}^1 FE spaces, BDF1 as time integration scheme, semi-implicit treatment of nonlinearities, and the VMS-LES methods. Numerical simulations are run in parallel on the GALILEO100 supercomputer, using 240

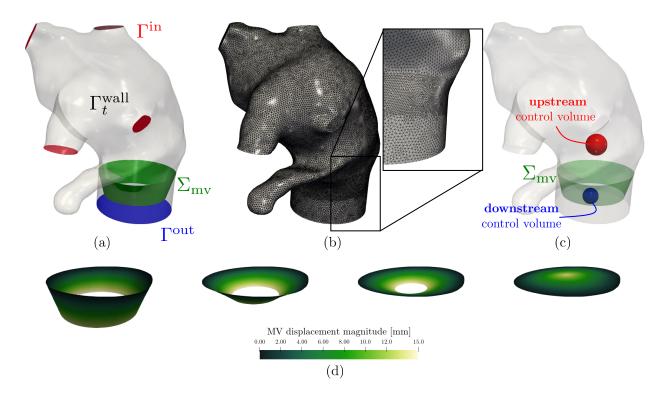


Figure 7: Test IV. (a): left atrium geometry, with boundary portions; (b) tethraedral mesh refined on the proximity of the mitral valve; (c) control volumes upstream the mitral valve; (d) mitral valve warped by its displacement (from open to closed configuration).

cores. The wall time for this simulation was about 22 h.

The simulation is carried out via the $life^{x}-cfd$ app. Since we are setting the same boundary condition on all the inlet sections, the parameter file for this setting (see also Section 3.1) can be obtained by running:

\$./lifex_fluid_dynamics -g -b "Pulmonary veins" "Mitral valve"

In Fig. 8, we report some representative output of a life^x-cfd CFD cardiac simulation. We highlight that all the reported quantities are directly computed in life^x-cfd and exported to a CSV file.

We report solutions on the last simulated heartbeat and shifted in the time domain $(0, t_{hb})$. For instance, we show the left atrial volume versus time in Fig. 8a. In Fig. 8e, we display the flow rates through each pulmonary vein and at the outlet section (i.e. downstream of the mitral valve), and Fig. 8f shows the kinetic energy against time.

Finally, in Fig. 9 we display some 3D representations of the CFD atrial simulation: we report the volume rendering of the velocity magnitude and the Q-criterion at the A-wave peak, when the incoming jets impact in the middle of the chamber, along with four ring vortices coming from the pulmonary veins.

We refer the interested reader to [74–77] for a more detailed assessment of the results provided by life^x-cfd in realistic and patient-specific settings.

5. Conclusions

We presented the open-source life^x-cfd solver aimed at cardiovascular CFD simulations. The solver employs an ALE formulation to solve the incompressible Navier-Stokes equations for both laminar and turbulent regimes. It incorporates the SUPG-PSPG and VMS-LES stabilization methods, with the latter also serving as a turbulence model. This enables the solver to accurately model the transition-to-turbulence regime present in cardiovascular blood flow. Cardiac valves can be included by means of the *Resistive Immersed Implicit Surface* method. Several types of flow and stress boundary conditions are also supported, and exposed to the user in a friendly and highly customizable way.

The numerical schemes incorporated into the code allow to discretize the equations in time using *Backward* Differentiation Formulas (BDF) of order $\sigma_{BDF} = 1, 2, 3$ and in space using Lagrangian Finite Elements (FE)

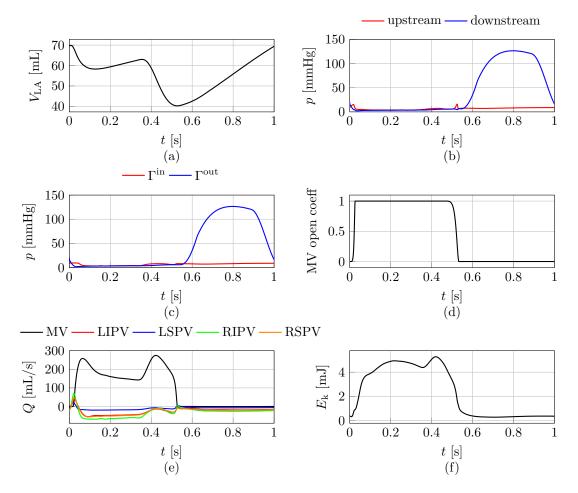


Figure 8: Test IV. Plots of left atrial CFD simulation results. (a) Left atrial volume versus time; (b) pressure in upstream and downstream control volumes (the control volumes are reported in Figure 7c); (c) prescribed pressure at inlet and outlet sections; (d) mitral valve opening coefficient; (e) flowrates at inlets and outlet sections versus time; (f) kinetic energy versus time.

of order 1 and 2 on tetrahedral meshes, and of arbitrary degree on hexahedral meshes. *Fully implicit* and *semi-implicit* formulations of the fluid dynamics problem are available. Thanks to automatic differentiation, the implementation of this complex and versatile formulation has become both effortless and efficient, making it an invaluable tool for new developers to further research. Furthermore, the user can also fine-tune parameters for the linear solvers and preconditioners.

We describe the $life^{x}$ -cfd implementation details and provide a step-by-step guide for running simulations, showcasing the solver's user-friendliness and versatility in simulating different cardiovascular applications. To demonstrate the capabilities of the solver, we present multiple representative examples, such as simulating vascular flow in an idealized cylinder, the hemodynamics in a patient-specific portion of the aorta, and the left atrial hemodynamics in a patient-specific geometry. The solver's accuracy is verified through convergence analyses on the Beltrami flow benchmark problem. We also demonstrate its parallel performance, achieving a nearly-ideal speedup up to $\approx 10^3$ processors. Overall, the tests and the results presented confirmed the effectiveness and efficiency of $life^{x}$ -cfd for simulating complex cardiovascular flow problems.

Our CFD solver is designed to be user-friendly, efficient, and accurate, while also providing a flexible and extensible platform for future development and research in cardiovascular modeling and simulation. The open-source nature of life^x-cfd allows for collaboration and contributions from the broader scientific community, and we hope that it will serve as a valuable companion for researchers and practitioners working in the field of cardiovascular fluid dynamics, ultimately leading to improved diagnosis and treatment of cardiovascular diseases.

The impact and wide applicability of life^x-cfd are demonstrated by the high number of journal articles [31, 74, 76–78, 81, 81, 82, 84] and preprints [75, 79, 80, 83, 85, 132] that have already used it in a diverse set of applications.

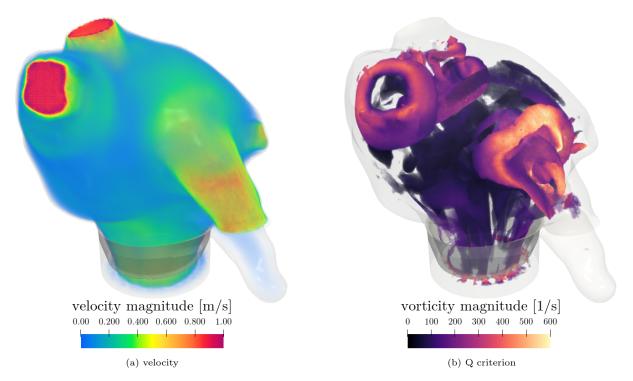


Figure 9: Test IV. 3D visualizations of left atrium simulation at the early-wave peak. (a) volume rendering of velocity magnitude; (b) volume rendering of Q criterion ($Q = 50/s^2$) coloured according to vorticity magnitude.

Future developments pursued regarding life^{*}-cfd include the coupling to external circulation models [74, 77], the extension to more sophisticated models for valve displacement [132, 133] and methods allowing the simulation of isovolumetric phases of the cardiac cycle [80, 134]. Moreover, we plan on introducing more advanced methods for the domain displacement, including non-linear lifting operators [82, 135, 136] and remeshing techniques [38]. Finally, the inclusion of scalar transport models [9, 27, 31] and non-Newtonian rheologies for blood [43, 137] will allow to better replicate several scenarios of clinical interest.

Author contributions

Pasquale Claudio Africa: conceptualization, methodology, software (development and maintenance), formal analysis, project administration, writing (original draft). Ivan Fumagalli: conceptualization, methodology, software (development and simulation), formal analysis, writing (original draft). Michele Bucelli: conceptualization, methodology, software (development, simulation and maintenance), visualization, formal analysis, project administration, writing (original draft). Alberto Zingaro: conceptualization, methodology, software (development and simulation), visualization, formal analysis, writing (original draft). Marco Fedele: methodology, software (development). Luca Dede': project administration, writing (review and editing), supervision. Alfio Quarteroni: funding acquisition, project administration, writing (review and editing), supervision.

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Appendix A. Beltrami flow

For the sake of reproducibility, we report the details of the test case with analytical solution considered in Section 4.1 and taken from [86]. We consider Navier-Stokes equations with the gradient-gradient formulation of the diffusion term (see (7)). The domain is the cube $\Omega = (0, 2\pi)^3$. The solution has the following analytical expression:

$$u_x(\boldsymbol{x},t) = -\frac{c(t)}{4} \left[\exp\left(\frac{\pi x}{4}\right) \cos\left(\frac{\pi(y+2z)}{4}\right) + \exp\left(\frac{\pi z}{4}\right) \cos\left(\frac{\pi(x+2y)}{4}\right) \right] ,$$
$$u_y(\boldsymbol{x},t) = -\frac{c(t)}{4} \left[\exp\left(\frac{\pi y}{4}\right) \cos\left(\frac{\pi(2x+z)}{4}\right) + \exp\left(\frac{\pi x}{4}\right) \cos\left(\frac{\pi(y+2z)}{4}\right) \right] ,$$
$$u_z(\boldsymbol{x},t) = -\frac{c(t)}{4} \left[\exp\left(\frac{\pi z}{4}\right) \cos\left(\frac{\pi(x+2y)}{4}\right) + \exp\left(\frac{\pi y}{4}\right) \cos\left(\frac{\pi(2x+z)}{4}\right) \right] ,$$

$$p(\boldsymbol{x},t) = -\frac{\rho\pi^2}{32} \exp\left(\frac{\pi^2 t\mu}{2\rho}\right) \left[\exp\left(\frac{\pi x}{2}\right) + \exp\left(\frac{\pi y}{2}\right) + \exp\left(\frac{\pi z}{2}\right) \\ + 2\exp\left(\frac{\pi(x+y)}{2}\right) \cos\left(\frac{\pi(y+2z)}{4}\right) \sin\left(\frac{\pi(2x+z)}{4}\right) \\ + 2\exp\left(\frac{\pi(x+z)}{2}\right) \cos\left(\frac{\pi(x+2y)}{4}\right) \sin\left(\frac{\pi(y+2z)}{4}\right) \\ + 2\exp\left(\frac{\pi(y+z)}{2}\right) \cos\left(\frac{\pi(2x+z)}{4}\right) \sin\left(\frac{\pi(x+2y)}{4}\right) \right]$$

wherein $\boldsymbol{u} = [u_x, u_y, u_z]^T$, $\boldsymbol{x} = [x, y, z]^T$ and

$$c(t) = \pi \exp\left(\frac{\pi^2 \mu t}{4\rho}\right)$$
.

The above functions satisfy Navier-Stokes equations with null forcing term (f = 0), no domain displacement and no resistive surfaces. We obtain the initial conditions by setting t = 0 in the above, and we set Dirichlet conditions on all sides of the cube except for the side $\{x = 0, y \in (0, 2\pi), z \in (0, 2\pi)\}$, where we impose Neumann conditions. All boundary conditions are derived from the exact solution. We set density $\rho = 1 \text{ kg/m}^3$ and viscosity $\mu = 10 \text{ Pa} \cdot \text{s}$.

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