

UNIVERSIDAD POLITÉCNICA DE MADRID
Escuela Técnica Superior de Ingeniería Aeronáutica y del Espacio



**Advanced Computational Modeling and
Innovative Data-Driven Analysis of Left
Ventricular Hemodynamics**

DOCTORAL THESIS

Submitted for the degree of Doctor by:

Eneko Lazpita Suinaga
Máster en Matemática Industrial

Madrid, 2025



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Doctoral Degree in Aerospace Engineering

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Under the supervision of:

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*“Rejection is a part of any man’s life.
If you can’t accept and move past rejection,
or at least use it as writing material,
you’re not a real man.”*
Jiraiya – Naruto

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While the present Doctoral Thesis is fully written in English, some paragraphs will be written in different languages depending on the person for whom the message is intended.

Lehenik eta behin, hasieratik hasi beharko gea, hasieratik nirekin daudenekin. Ama, eskerrik asko beti nere apoyua izatearren, momentu onetan pozten eta ospatzen erakutsi didazulako, eta txarretan, gehien behar izan dudanean, alboan euki zaitudalako. Telefono dei batekin badakizulako zeoze gertatzen zaiten eta hortik pare bat ordura asteburua Madrilen pasatzeko busa hartzeko prest zaudelako. Aita, nere ingeniero erreferentea, bizitza akademikua hasteko Madril bertara ekarri ninduzula iada 9 urte pasa dia. Beti nere erabakiak aurrera eramaten lagundu didazulako, neregana sinisten eta konfiatzen erakutsi didazulako, bakarrik sentitu naizenean beti neri zaintzen norbait daukadalako, mila esker. Zuengatik ez balitzake, enintzen hemen egongo, naizena izango eta lortu dudana lortuko. Nire bizitza akademiko luze honetan, ehun bat irakasle eukiko nituen eta hala ere, zuek izan zarete nere irakasle onenak; maitatzen, amore ez ematen, enpatia eukitzen, neregana eta nere baloreengan sinisten, erori ondoren altzatzen, eta beste mila gauza erakutsi didazue. Maite zaituztet, bihotz-bihotzez.

Hala ere, txikitatik ez dira nire alboan egon diren bakarrak. Gorka, jaio nintzenetik hor zaude, batzutan hobeto, bestetan okerro, baña beti zuri jarraitzen ibili naiz, zuregandik ikasten. Gaur naizen frikia zuri esker da. Tontakeri bat emango du, baña aurrera joaten lagundu didan nere bizitzako parte handi bat hori da, eta zuri esker existitzen da. Elur eta Gaizka, beranduago agertu zinen zuek biok. Neregana jartzen duzuen konfiantza, partekatzen ditugun esperientzi eta gustuak, horiek denak lagundu didate hona iristen. Eman didazuen segurtasuna, lasaitasuna eta maitasunagatik, pila maite zaituztet hiruroi.

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Abstract

Understanding blood flow in the left ventricle (LV) is essential for assessing cardiac performance and detecting pathological conditions. This doctoral thesis investigates intraventricular flow using computational simulations and modal decomposition techniques, with the aim of identifying dominant flow patterns and developing efficient predictive models for potential clinical applications.

A robust numerical framework was developed to simulate the transient LV flow, incorporating wall motion and physiologically realistic boundary conditions. Two idealized LV geometries were employed to assess how morphological features influence the formation and evolution of the diastolic vortex ring, a key marker of cardiac fluid dynamics.

A dedicated postprocessing pipeline was implemented to extract meaningful physical insights from the simulation data. Modal decomposition techniques such as proper orthogonal decomposition (POD) and higher order dynamic mode decomposition (HODMD) were applied to identify coherent structures, track their temporal behavior, and associate dominant modes with characteristic system frequencies. POD captures dominant spatial features, and combining it with FFT links them to characteristic frequencies. HODMD improves this analysis by offering more accurate spectral separation and clearer representation of dynamic events like vortex ring breakdown.

The potential of HODMD for reduced-order modeling (ROM) was also explored. Using limited training data, predictive models that accurately forecast flow evolution at a much lower computational cost than full simulations were implemented. However, a trade-off between accuracy and efficiency was observed depending on the size and diversity of the training set.

Overall, this thesis contributes to the development of efficient and interpretable computational tools for the analysis of cardiac flows, paving the way toward real-time, data-driven cardiovascular modeling.

Resumen

Comprender el flujo sanguíneo en el ventrículo izquierdo (VI) es fundamental para evaluar el funcionamiento cardíaco y detectar posibles patologías. Esta tesis doctoral estudia el flujo intraventricular mediante simulaciones computacionales y técnicas de descomposición modal, con el objetivo de identificar patrones dominantes de flujo y desarrollar modelos predictivos eficientes con potencial aplicación clínica.

Se ha desarrollado un marco numérico robusto para simular el flujo transitorio en el VI, incorporando el movimiento de la pared ventricular y condiciones de contorno fisiológicamente realistas. Se emplearon dos geometrías idealizadas del VI para analizar cómo las características morfológicas influyen en la formación y evolución del anillo vortical durante la diástole, una estructura clave en la dinámica del flujo cardíaco.

Para extraer información física relevante de los campos simulados, se implementó un proceso de postprocesado dedicado. Se aplicaron técnicas de descomposición modal como la descomposición ortogonal propia (POD) y la descomposición modal dinámica de orden superior (HODMD), permitiendo identificar estructuras coherentes, analizar su evolución temporal y asociar modos dominantes con frecuencias características del sistema. La POD permite capturar las estructuras espaciales dominantes, y al combinarla con transformada rápida de Fourier (FFT), se pueden relacionar con las frecuencias del flujo. La HODMD mejora este análisis, ofreciendo una separación espectral más precisa y una descripción más clara de fenómenos dinámicos como la ruptura del anillo vortical.

También se exploró el potencial de la HODMD para construir modelos de orden reducido (ROM). A partir de conjuntos de entrenamiento limitados, se construyeron modelos predictivos capaces de anticipar la evolución del flujo con alta fidelidad y a un coste computacional mucho menor que las simulaciones completas. No obstante, se observó un compromiso entre precisión y eficiencia en función del tamaño y la diversidad del conjunto de entrenamiento.

En conjunto, esta tesis contribuye al desarrollo de herramientas computacionales eficientes e interpretables para el análisis de flujos cardíacos, avanzando hacia una modelización cardiovascular en tiempo real basada en datos.

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Abbreviations and acronyms

0D	Zero-Dimensional
1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
4D	Four-Dimensional
ANN	A rtificial N eural N etwork
BC	B oundary C ondition
CAD	C omputer- A ided D esign
CFD	C omputational F luid D ynamics
CFL	C ourant- F riedrichs- L ewy
CNIC	C entro N acional de I nvestigaciones C ardiovasculares
CNN	C onvolutional N eural N etwork
CPU	C entral P rocessing U nit
CT	C omputed T omography
CVD	C ardio V ascular D isease
DICOM	D igital I maging and C ommunications in M edicine
DMD	D ynamic M ode D ecomposition
DNS	D irect N umerical S imulation
DRL	D eep R einforcement L earning
EDV	E nd- D iastrolic V olume
ESV	E nd- S ystolic V olume
EU	E uropean U nion
FDA	F ood and D rug A dministration
FEM	F inite E lement M ethod

FFT	F ourier F ast T ransform
FVM	F inite V olume M ethod
HODMD	H igher O rders D ynamic M ode D ecomposition
HOSVD	H igher O rders S ingular V alue D ecomposition
IBM	I mmersed B oundary M ethod
KTH	K unliga T ekniska H ögskolan
LAX	L ong A xis
LES	L arge E ddy S imulation
LV	L eft V entricle
mdHODMD	m ulti d imensional H igher O rders D ynamic M ode D ecomposition
MRI	M agnetic R esonance I maging
NS	N avier S tokes
ODE	O rdinary D ifferential E quation
OpenFOAM	O pen S ource F ield O peration and M anipulation
PhD	D octor of P hilosophy
PISO	P ressure- I mplicit with S plitting of O perators
PIV	P article I mage V elocimetry
POD	P roper O rthogonal D ecomposition
PSD	P ower S pectral D ensity
RANS	R eynolds- A veraged N avier S tokes
Re	R eynolds number
ROM	R educed O rders M odel
RRMSE	R elative R oot M ean S quare E rror
SAX	S hort A xis
SciML	S cientific M achine L earning
SPOD	S pectral P roper O rthogonal D ecomposition
St	S trouhal number

STL **S**tereolithography
SVD **S**ingular **V**alue **D**ecomposition
TAC **T**ransverse **A**ortic **C**onstriction
UCD **U**nicode **C**haracter **D**atabase
UDF **U**ser-**D**efined **F**unction
UPM **U**niversidad **P**olitécnica de **M**adrid
UPV **U**niversitat **P**olitècnica de **V**alencia
VR **V**ortex **R**ing

Chapter 1

Introduction

1.1 Background in intracardiac flows

The heart is a central organ in the circulatory system, responsible for maintaining the continuous flow of blood that is essential for delivering oxygen and nutrients to tissues and organs. Cardiovascular health is of paramount importance, as heart-related diseases remain among the leading causes of morbidity and mortality worldwide. In 2019 alone, an estimated 17.9 million people died from cardiovascular diseases (CVDs), accounting for 32% of all global deaths. Of these, 85% were due to heart attacks and strokes (World Health Organization, [2024](#)). Gaining insight into the internal flow dynamics of the heart is crucial for the diagnosis, monitoring, and treatment of such conditions.

The heart comprises four chambers as represented in Fig. 1.1: the left and right atria, and the left and right ventricles, each with distinct flow characteristics that are critical for efficient blood circulation. The left side of the heart, which handles oxygenated blood, plays a key role in systemic circulation. During diastole, the left atrium transfers blood to the left ventricle through the mitral valve, a process characterized by the formation of vortices that optimize filling efficiency (Kilner et al., [2000](#)). In systole, the left ventricle ejects blood into the aorta, delivering it to the body. These processes involve three-dimensional and highly complex flow patterns, which are sensitive to changes in heart function and geometry.

In particular, the analysis of blood flow within the left ventricle (LV) is essential for assessing cardiac pumping efficiency and identifying potential functional abnormalities (Pedrizzetti and Domenichini, [2005](#)). During early diastole, the inflow through the mitral valve forms a vortex ring (VR) that travels toward the apex. This vortex ring not only facilitates efficient ventricular filling but also aids systolic ejection by conserving angular momentum. Its formation, evolution, and stability are governed by anatomical and physiological conditions, and its characterization is considered a potential indicator of cardiac health (Pedrizzetti et al., [2014](#)).

From a medical perspective, the study of intracardiac flows has advanced significantly through imaging techniques that provide insight into cardiac function and hemodynamics. Doppler echocardiography, a widely used non-invasive tool, enables clinicians to visualize blood

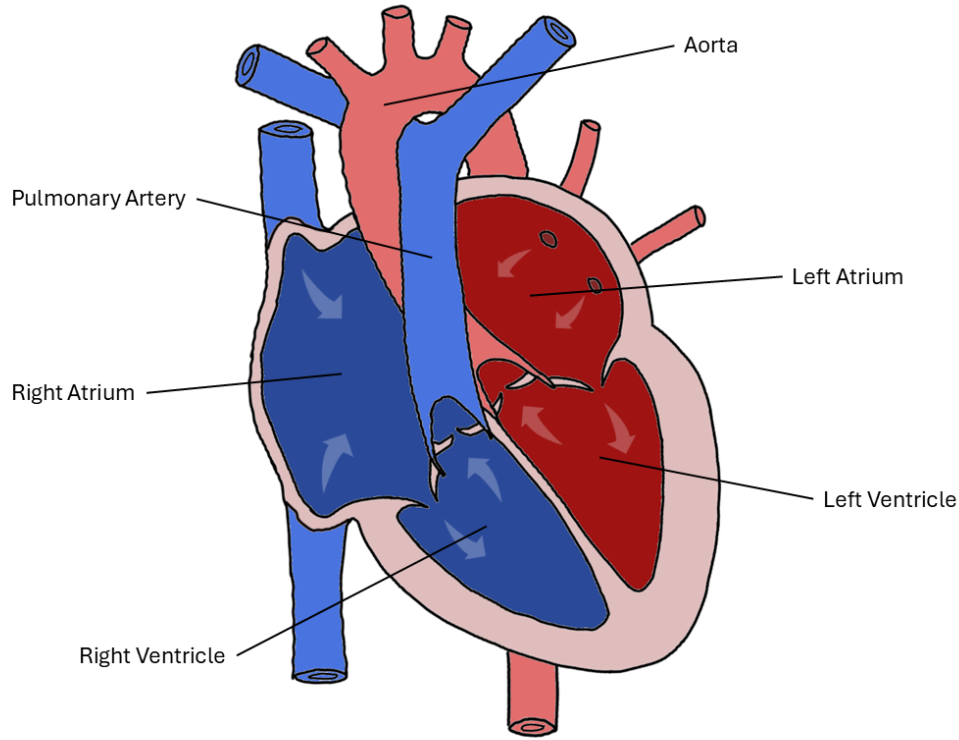


Figure 1.1: General scheme of the heart chambers.

flow velocities and detect abnormalities in real time (Nagueh et al., 2016; Otto, 2007). It applies the Doppler effect to ultrasound waves to measure the direction and velocity of blood flow within the heart and vessels, providing key insights into cardiac function and valvular pathologies. It is particularly effective in identifying valvular dysfunctions, intracardiac shunts, and regions of abnormal flow. However, its spatial resolution is limited and often requires skilled interpretation.

Magnetic resonance imaging (MRI) has further enriched the understanding of intracardiac flows, with four-dimensional (4D) flow MRI emerging as a state-of-the-art technique (Markl et al., 2012). This method captures three-dimensional flow fields over time, allowing for a detailed analysis of velocity profiles, vortex structures, and wall shear stress distributions. These insights are invaluable in assessing conditions such as left ventricular dysfunction, hypertrophic cardiomyopathy, and valvular diseases. In addition, computed tomography (CT) and nuclear imaging are used to evaluate cardiac anatomy and perfusion, respectively, providing complementary diagnostic information (Niemeyer et al., 1995; Pontone et al., 2022).

Despite advances in imaging technology, limitations persist. High-resolution techniques, such as 4D flow MRI, are demanding in terms of resources and not universally accessible. Furthermore, these methods frequently capture flow patterns indirectly, relying on mathematical models and assumptions to reconstruct flow dynamics. This calls for the development of supplementary approaches to facilitate a more comprehensive understanding of the underlying physics of intracardiac flows.

Beyond clinical imaging, experimental methods have been developed to mimic and study heart function in controlled environments. Silicone heart models, for instance, are widely used in experimental studies to replicate the geometry and mechanical properties of the heart (Colebank and Chesler, 2022; Korn et al., 2020). These models can be coupled with pulsatile flow systems to simulate cardiac cycles, enabling detailed investigations of flow dynamics under various conditions. Advanced fabrication techniques, such as 3D printing, have further improved the anatomical accuracy of these models, making them useful for validating computational simulations and testing medical devices.

Particle image velocimetry (PIV) is another experimental approach that has been applied to study intracardiac flows in physical models (Kilner et al., 2000; Querzoli et al., 2010). By seeding a fluid with tracer particles and using high-speed cameras to track their motion, PIV provides high-resolution velocity fields that reveal intricate flow patterns, such as vortex formation and jet dynamics. These experiments offer a complementary perspective to medical imaging, as they can isolate specific factors and provide insights that are challenging to obtain *in vivo*.

In summary, the study of intracardiac flows relies on a combination of medical imaging, experimental techniques, and computational tools. However, significant challenges remain in this field. Clinical imaging techniques, though advanced, are often limited by resolution, cost, and accessibility, making it difficult to capture fine-scale flow structures in routine practice. Experimental approaches, while valuable for controlled studies, face difficulties in replicating the full complexity of physiological conditions, including tissue compliance and dynamic boundary interactions. Additionally, integrating data from these diverse methods into cohesive frameworks for understanding and predicting intracardiac flow behavior remains an open problem. To address these challenges, CFD has been increasingly applied to study intracardiac flows.

1.2 CFD Simulation in Cardiac Flows

The use of CFD to simulate intracardiac flows has become a fundamental method in the study of cardiac hemodynamics. CFD facilitates a detailed exploration of blood flow within the heart, providing critical insights that are essential for understanding both normal physiology and pathological conditions. The progression of computational models, from simplified representations to sophisticated patient-specific simulations, reflects the continuous effort to achieve a comprehensive and clinically relevant representation of cardiac flows.

Computational modeling of the cardiovascular system often begins with simplified representations that trade spatial resolution for computational efficiency. Zero-dimensional (0D) or lumped parameter models describe the circulation as a set of interconnected compartments characterized by averaged quantities such as pressure, flow, resistance, and compliance. These models are widely used for studying global hemodynamics, ventricular-arterial coupling, and for prescribing boundary conditions (BCs) to higher-dimensional simulations (Shi et al., 2011). One-dimensional (1D) models extend this framework by incorporating spatial variation along vascular segments, enabling the simulation of pulse wave propagation and reflection phenomena. Seminal work by Stergiopoulos et al., 1992, highlighted the capability of 1D

models to analyze pressure dynamics in pathologies like aortic stenosis. Together, 0D and 1D models serve as essential tools for multiscale cardiovascular simulations, offering a balance between physiological fidelity and computational cost. While 0D and 1D models are efficient and useful for global hemodynamic studies, they are inherently limited in their ability to capture local flow features, such as the formation of intraventricular vortices or valve-level dynamics. These phenomena require a fully three-dimensional description of cardiac geometry and motion. Therefore, to capture accurately the full complexity of blood flow within the heart chambers, three-dimensional (3D) models are necessary. These models can be broadly classified into two categories: idealized and patient-specific geometries.

The use of simplified geometries provides a valuable framework for studying fundamental hemodynamic phenomena, such as vortex ring dynamics and jet-wall interactions, under controlled and reproducible conditions. Zheng et al., 2012, employed an idealized left ventricular model to investigate intraventricular flow features, highlighting the influence of geometry on vortex formation. A similar approach was followed by Vedula et al., 2014, who validated numerical results against experimental data using a simplified left ventricular setup to enhance understanding of diastolic filling. Additionally, Spandan et al., 2017, proposed a high-fidelity fluid–structure interaction framework by combining a parallel interaction potential method with the immersed boundary method (IBM), enabling fully resolved simulations of deformable cardiac structures such as ventricular walls and valves. Although idealized models facilitate fundamental studies, their simplified anatomy and boundary conditions limit their clinical relevance. As such, the extent to which these models generalize to patient-specific cases remains an open question, one that this thesis seeks to address.

In recent years, the application of CFD to cardiac modeling of patient-specific geometries has experienced a significant increase. Reconstructed from medical imaging data, patient-specific models allow for personalized simulations that account for individual anatomical variations and pathological conditions. For instance, Grünwald et al., 2022, introduced a methodology for simulating patient-specific right ventricular geometries, highlighting impaired washout and reduced vortex formation in single ventricle cases. Similarly, Korte et al., 2023, adopted a comparable approach to investigate left ventricular function under rest and exercise conditions, focusing on the impact of mitral insufficiency on intraventricular flow dynamics.

As mentioned before, 0D/1D models can be coupled with higher order simulations to study global hemodynamics. Fedele et al., 2023, present a comprehensive electromechanical model of the human heart including accurate geometry, myocardial fiber orientation, active force generation models, and coupled with a zero-dimensional closed-loop lumped parameters circulatory system model. An even more advanced multiphysics and multiscale geometric framework was developed by Zingaro et al., 2024, enabling detailed modeling of full-heart electromechanics and hemodynamics.

Despite increasing use of patient-specific CFD, several challenges remain. Wall motion is often approximated or static, inlet conditions are empirically prescribed, and postprocessing remains qualitative. Moreover, the computational cost of full-cycle CFD remains prohibitive for clinical use, motivating the search for reduced-order, interpretable alternatives.

1.3 Machine Learning in Cardiac Flows

The CFD data generated from intraventricular simulations is typically high-dimensional and time-resolved, posing challenges for interpretation and analysis. Traditional flow visualization techniques, such as streamlines, velocity contour plots, or the Q-criterion, are commonly used to identify coherent structures and qualitatively analyze flow behavior during the cardiac cycle (Colorado-Cervantes et al., 2022; Nguyen et al., 2015; Schenkel et al., 2009). These methods are often complemented with experimental validation techniques such as PIV (Di Labbio et al., 2022; Fortini et al., 2013).

However, these qualitative tools often fall short of revealing the intrinsic mechanisms driving flow evolution, frequencies, and flow instabilities associated to the vortex breakdown. To address this, modal decomposition techniques such as proper orthogonal decomposition (POD, Lumley, 1967) and dynamic mode decomposition (DMD, Schmid, 2010) have been increasingly applied to cardiovascular flows, particularly in arteries and veins, to extract coherent structures and dominant flow features (Habibi et al., 2020; Kazemi et al., 2022).

Nevertheless, the use of modal decomposition techniques in left ventricular applications remains relatively limited. In a recent study, Wu et al., 2023, combined Shake-the-Box (an advanced Lagrangian particle tracking algorithm that reconstructs dense, time-resolved 3D velocity fields from particle images) with POD to capture the complex, three-dimensional, and time-resolved nature of intraventricular flows. Likewise, M. G. Borja et al., 2024, applied POD to patient-specific simulations, identifying characteristic flow patterns and quantifying the energy content of each mode. While insightful, these studies mainly focused on spatially energetic structures and did not fully explore their temporal evolution.

Efforts to include temporal dynamics are beginning to emerge through the use of DMD. For example, M. Borja et al., 2016, and Mikhail et al., 2017, applied DMD to extract coherent flow structures and proposed modal biomarkers for characterizing cardiac function and disease. In a more recent contribution, Di Labbio and Kadem, 2019, combined POD and DMD to construct a reduced-order model of left ventricular flow under aortic regurgitation. These studies illustrate the potential of modal decomposition techniques to uncover both spatial and temporal features in intraventricular hemodynamics, although their application remains relatively unexplored.

Moreover, the use of these techniques has grown significantly in recent years for the analysis of medical data. In the work by Groun et al., 2022a, higher order dynamic mode decomposition (HODMD) was employed to analyze medical imaging and identify flow patterns associated with cardiovascular diseases. This information was subsequently integrated with deep learning techniques to develop an automatic classification system, which achieved substantially higher accuracy than models relying solely on image-based features Bell-Navas et al., 2025. This shows the effectiveness to identify flow patterns in cardiac flows.

The present study is, to the best of the authors' knowledge, the first to combine POD and HODMD for intraventricular flow analysis, enabling both the extraction of coherent structures and the characterization of their temporal behavior. HODMD offers a crucial advantage over POD by enabling the extraction of coherent structures associated with specific frequencies,

thereby providing a more physically interpretable decomposition of unsteady flow phenomena. This is particularly relevant for capturing the interplay between the main and secondary vortex rings and understanding the mechanisms behind vortex breakdown, features that are not readily separable using purely energy-based methods like POD. By comparing two idealized ventricular geometries, this study highlights how geometric variations influence vortex dynamics, offering valuable insight for the selection of modeling strategies in future studies, particularly when investigating pathological conditions.

1.4 Research Trajectory and Project Contributions

Throughout my academic journey, I have developed a strong and sustained interest in fluid dynamics, with a particular focus on its modeling and analysis. This interest emerged during my undergraduate studies in Aerospace Engineering, where I first encountered the fundamental principles governing fluid flow. My bachelor's thesis marked the beginning of my integration of traditional fluid mechanics with emerging computational techniques, as I applied machine learning algorithms to analyze urban fluid flow data. This early experience highlighted the potential of combining data-driven methods with physical modeling to study complex systems.

Motivated by the desire to deepen my understanding of mathematical modeling across a broader range of physical phenomena, I pursued a Master's degree in Industrial Mathematics. This program reinforced my analytical foundation and exposed me to diverse applications, including biomedicine, combustion, and fluid mechanics. It was during this stage that I was introduced to modal decomposition techniques, such as proper orthogonal decomposition (POD) and dynamic mode decomposition (DMD), which provided rigorous tools for extracting coherent structures and dominant patterns from high-dimensional datasets.

The convergence of these interests materialized during my doctoral work through my involvement in the *DigitHEART* and *CardioAging* research projects. These initiatives focus on the simulation and analysis of blood flow in the left ventricle using computational fluid dynamics (CFD) and data-driven tools. They offered an ideal setting to apply and refine my expertise in both fluid dynamics and advanced analysis techniques, particularly in a biomedical context where understanding intraventricular flow patterns has direct clinical relevance. This thesis represents the culmination of this trajectory, aiming to contribute to the field of hemodynamics through a combined approach of high-fidelity simulations and reduced-order modeling techniques.

1.4.1 Group and Projects

The ModelFLOWS research group (ModelFLOWS, [2023a](#)), under the leadership of Soledad Le Clainche, operates within the Department of Applied Mathematics at the School of Aerospace Engineering at the Universidad Politécnica de Madrid (UPM). The group's area of expertise lies in the development and application of data-driven methodologies, including modal decomposition, machine learning architectures, and data assimilation techniques (A. Hetherington et al., [2024](#)). These methodologies are employed to construct hybrid ROMs that are based on physical principles. These models are characterized by their robustness

and strong generalization capabilities, making them well-suited for the study of nonlinear dynamical systems, the reconstruction and repair of incomplete datasets, and temporal forecasting. The ModelFLOWs group has successfully applied these tools across a range of applications, including complex turbulent and reactive flows, as well as diverse nonlinear systems (A. I. Hetherington et al., 2024).

The data-driven methods developed within the group have been successfully applied to a wide range of problems. Notable applications include the analysis of urban fluid dynamics (Lazpita et al., 2022; Martínez-Sánchez et al., 2023), flow control (Corrochano and Le Clainche, 2022), heat transfer optimization (Lazpita et al., 2024a), and the diagnosis and prognosis of cardiac function (Bell-Navas et al., 2025; Groun et al., 2022b), among others.

Before the start of this doctoral thesis, I was actively involved in two independent research lines that laid the foundation for my training in data analysis techniques. The first focused on urban flow analysis, a field of growing importance due to its implications for pollutant dispersion, air quality, and the response to high-impact events. In collaboration with the Universitat Politècnica de València (UPV) and the Kungliga Tekniska Högskolan (KTH), I contributed to the study of flow behavior around simplified urban geometries. This work resulted in two peer-reviewed publications (Lazpita et al., 2022; Martínez-Sánchez et al., 2023), in which I analyzed coherent structures and dominant flow patterns in urban environments. These studies ultimately helped initiate the European project MODELAIR, 2023–2026.

In parallel, I participated in a second research line on thermal management in engineering systems. In collaboration with Purdue University and supported by the Office of Naval Research (Grant No. N00014-19-1-2433), I developed and applied a data-driven strategy for flow control aimed at enhancing convective cooling in aircraft engine components. This work was published in Lazpita et al., 2024a.

These early research experiences marked the beginning of my training in data analysis and model reduction methods. The techniques developed and applied in these contexts were later extended and adapted to the study of intraventricular blood flows within the scope of this doctoral thesis.

Within the cardiovascular domain, this transition materialized through my incorporation into the *ModelFLOWs-Cardiac* subgroup (ModelFLOWs, 2023b), created to investigate flow dynamics in the heart. This research line was initiated through the *DigitHEART* and *CardioAging* projects, two national initiatives that integrate clinical data and computational modeling for the early detection and monitoring of cardiovascular diseases. These projects are developed in collaboration with the Hospital Universitario Puerta de Hierro and the Centro Nacional de Investigaciones Cardiovasculares (CNIC), facilitating the integration of patient-specific imaging data and clinical expertise.

The research conducted under ModelFLOWs-Cardiac is divided into two main modules: The first module involves the analysis of medical data, while the second focuses on the obtention and analysis of CFD simulations.

The medical data module focuses on processing and analyzing clinical imaging datasets, such as echocardiography and MRI, to detect patterns, classify cardiac conditions, and predict

their outcomes. Two types of data have been employed for it:

- Echocardiography data: Long-axis (LAX) and short-axis (SAX) video loops from mice with varying cardiac conditions were analyzed: healthy, diabetic cardiomyopathy, myocardial infarction, obesity, and transverse aortic constriction (TAC) hypertrophy. Each video consists of approximately 120 frames, offering rich temporal data for analysis.
- MRI data: The MRI datasets comprise 10 slices of the heart, each represented by 20 snapshots with a resolution of 128×128 . These datasets are used to explore cardiac dynamics across multiple cycles.

Advances in data science have had a considerable impact on the field of medical imaging. Specifically, tools such as the HODMD have been adapted to analyze echocardiography images, extracting key patterns related to various cardiac conditions. The use of HODMD allows for the identification of dominant features, such as heart and respiratory rates, and the visualization of modes that capture structural variations between healthy and diseased hearts (Groun et al., 2022a, 2022b).

A hybrid approach that combines HODMD with convolutional neural networks (CNNs) was developed to classify five distinct cardiac conditions (see Bell-Navas et al., 2025). The incorporation of DMD modes into echocardiography images has been shown to enhance classification accuracy by up to 22%, underscoring the potential of the combination of physics-based decomposition and machine learning methodologies.

More recently, a new study by Groun et al., 2025, was published where an innovative tool based on a well recognized method known as the eigenfaces approach was used to classify cardiac diseases.

The second module of the *ModelFLOWs-Cardiac* initiative focuses on the generation and analysis of CFD simulations of left ventricular flows (Lazpita et al., 2024b; Nagargoje et al., 2025). Within this framework, I was responsible for the complete CFD pipeline: designing the simulation strategy, generating and refining the computational meshes, setting up the solver configurations, and validating the results against clinical benchmarks. I also developed open-source scripts for data preprocessing and postprocessing, along with a set of public tutorials to standardize practices and support knowledge transfer within and outside the group. This thesis centers on this simulation-based module, employing CFD tools to generate high-fidelity intraventricular flow datasets and applying advanced data analysis techniques to study key flow features, such as vortex ring dynamics.

1.4.2 Peer-reviewed journal articles

The journal articles and conference proceedings which were published during the Doctoral Thesis are the following:

- 2025 Nagargoje, M. S., **Lazpita, E.**, Garicano-Mena, J., & Le Clainche, S. (2025). A review on vortex dynamics in the healthy and dilated left ventricles and its application to heart health. *Flow*, 5, E10.

 <https://doi.org/10.1017/flo.2025.6>

- 2024 **Lazpita, E.**, Mares, A., Quintero, P., Garicano-Mena, J., & Le Clainche, S. (2024). Modeling heart flow dynamics using numerical simulations to identify the vortex ring: a practical guide. *Results in Engineering*, 24, 103644.
 <https://doi.org/10.1016/j.rineng.2024.103644>
- 2024 **Lazpita, E.**, Nagargoje, M.S., Le Clainche, S., & Garicano-Mena, J. (2024). On The Numerical Simulation Of Left Ventricle Models. In *ECCOMAS Congress 2024 - 9th European Congress on Computational Methods in Applied Sciences and Engineering*.
 <https://www.scipedia.com/public/Lazpita-et-al-2024a>
- 2024 Hetherington, A., Corrochano, A., Abadía-Heredia, R., **Lazpita, E.**, Muñoz, E., Díaz, P., Maiora, E., López-Martín, M. & Le Clainche, S. (2024). ModelFLOWS-app: data-driven post-processing and reduced order modelling tools. *Computer Physics Communications*, 301, p.109217.
 <https://doi.org/10.1016/j.cpc.2024.109217>
- 2024 **Lazpita, E.**, Garicano-Mena, J., Paniagua, G., Le Clainche, S., & Valero, E. (2024). A data-driven sensibility tool for flow control based on resolvent analysis. *Results in Engineering*, 22, 102070.
 <https://doi.org/10.1016/j.rineng.2024.102070>
- 2023 Martínez-Sánchez, Á., **Lazpita, E.**, Corrochano, A., Le Clainche, S., Hoyas, S., & Vinuesa, R. (2023). Data-driven assessment of arch vortices in simplified urban flows. *International Journal of Heat and Fluid Flow*, 100, 109101.
 <https://doi.org/10.1016/j.ijheatfluidflow.2022.109101>
- 2022 **Lazpita, E.**, Begiashvili, B., Garicano, J., Le Clainche, S., & Valero, E. (2022). Efficient Data-Driven Algorithms to Identify Patterns in Aeronautical Industrial Problems. In *ISUDEF: International Symposium on Unmanned Systems and The Defense Industry*, pp. 201-206.
 <https://doi.org/10.1007/978-3-031-37160-8-31>
- 2022 **Lazpita, E.**, Martínez-Sánchez, Á., Corrochano, A., Hoyas, S., Le Clainche, S., & Vinuesa, R. (2022). On the generation and destruction mechanisms of arch vortices in urban fluid flows. *Physics of Fluids*, 34(5).
 <https://doi.org/10.1063/5.0088305>

1.4.3 Conference presentations

The underlined author is the speaker.

- 2025 **Lazpita, E.**, Garicano-Mena, J., & Le Clainche, S. (Jun. 2025). Integrating machine learning and CFD for the study of intraventricular blood flow. In *3rd Spanish Fluid Mechanics Conference*, Malaga, Spain (**upcoming**).
- 2024 **Lazpita, E.**, Koumoutsakos, P., Garicano-Mena, J., & Le Clainche, S. (Sep. 2024). Integrating CFD and deep learning for enhanced hemodynamic predictions in the left ventricle. In *50th European Society for Artificial Organs Congress*, Aachen, Germany.

- 2024 **Lazpita, E.**, Nagargoje, M.S., Mares, A., Quintero, P., Neidlin, M., Lara-Pezzi, E., Villalba-Orero, M., Garicano-Mena, J., & Le Clainche, S. (Jul. 2024). Code-to-code comparison: an assessment of commercial cfd tools for left ventricle model geometries. In *29th Congress of the European Society of Biomechanics*, Edinburgh, Scotland.
- 2024 **Lazpita, E.**, Nagargoje, M.S., Le Clainche, S., & Garicano-Mena, J. (Jun. 2024). On the numerical simulation of left ventricle models. In *9th European Congress on Computational Methods in Applied Sciences and Engineering*, Lisbon, Portugal.
- 2023 **Lazpita, E.**, Nagargoje, M.S., Garicano-Mena, J., Valero, E., Villalba-Orero, M., Lara-Pezzi, E., & Le Clainche, S. (Sep. 2023). Flow patterns in turbulent cardiac flows using computational fluid dynamics and classical analysis tools. In *18th European Turbulence Conference*, Valencia, Spain.
- 2023 **Lazpita, E.**, Martínez-Sánchez, A., Hoyas, S., Vinuesa, V., & Le Clainche, S. (Jul. 2023). Unraveling the generation and destruction mechanisms of arch vortices in urban fluid flows: a comprehensive analysis. In *2nd Spanish Fluid Mechanics Conference*, Barcelona, Spain.
- 2023 **Lazpita, E.**, Garicano-Mena, J., Paniagua, G., Valero, E., & Le Clainche, S. (Jun. 2023). Advanced data-driven tools for flow control in aeronautical applications. In *1st International Conference Math 2 Product*, Taormina, Italy.
- 2022 **Lazpita E.**, Hoyas, S., Valero, E., Vinuesa, R., & Le Clainche, S. (Jul. 2022). Data-driven tools to solve industrial problems. In *1st Spanish Fluid Mechanics Conference*, Cádiz, Spain.
- 2022 **Lazpita E.**, Begiashvili, B., Garicano-Mena, J., Le Clainche, S. & Valero, E. (Jun. 2022). Efficient data-driven algorithms to identify patterns in aeronautical industrial problems. In *International Symposium on Unmanned Systems and the Defense Industry*, Online.

1.5 Objectives of the Thesis

The main objective of this thesis is to advance the understanding and modeling of intra-ventricular flow dynamics, with the broader goal of supporting cardiovascular diagnosis and treatment. To this end, we aim to develop a robust computational framework that combines high-fidelity CFD simulations with advanced data-driven analysis techniques.

The first step involves constructing a flexible pipeline for generating left ventricular geometries, both idealized and patient-specific, incorporating physiological wall motion and appropriate boundary conditions to replicate realistic flow scenarios. This raises several open questions: how to introduce wall kinematics efficiently into CFD solvers; how to generalize geometry generation tools to handle diverse datasets; and how to ensure numerical stability across models.

A key focus is placed on evaluating how anatomical variability influences intraventricular flow, particularly the formation and evolution of the diastolic vortex ring, a recognized indicator of

cardiac efficiency. We investigate whether simplified geometries can replicate essential flow features and how structural differences affect vortex dynamics and energy distribution.

Once simulations are performed, the objective shifts toward systematic postprocessing. This includes the application of modal decomposition techniques, such as POD, FFT, and HODMD, to extract dominant spatial and temporal patterns from the flow. These methods are used to provide quantitative insights that go beyond classical visualization.

Finally, we explore whether reduced-order models based on the extracted dynamics can offer reliable, computationally efficient predictions over future cardiac cycles. These models are evaluated in terms of reconstruction accuracy and suitability for practical applications.

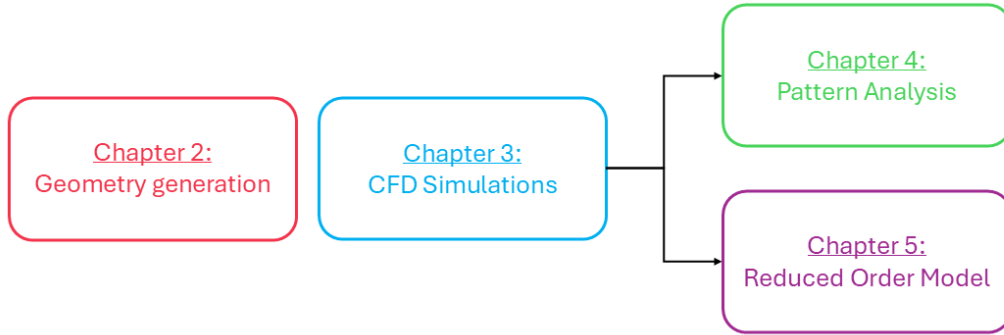


Figure 1.2: Schematic summary of the main objectives of the present Doctoral Thesis.

1.6 Thesis Outline

This thesis is organized into seven chapters, following a progression from methodological development to applied analysis and modeling of cardiac flows.

Chapter 2 details the construction of left ventricular models and the development of a fully scripted pipeline for CFD simulations. This includes geometry generation, mesh creation, boundary condition setup, solver configuration, and the integration of dynamic wall motion. The chapter also introduces the scientific machine learning tools used in later analysis.

Chapter 3 presents the CFD results for idealized geometries, with emphasis on the characterization of the diastolic vortex ring. Chapter 4 extends this analysis by applying modal decomposition techniques to identify dominant flow patterns and spectral features across different geometries.

Chapter 5 introduces the reduced-order model based on HODMD. It demonstrates the ability of the model to reconstruct and forecast intraventricular flow fields with high accuracy and significantly reduced computational cost.

Chapter 6 discusses the key findings, integrating insights from both flow analysis and the ROM. It also addresses the limitations of the current work and outlines future research directions. Finally, Chapter 7 concludes the thesis by summarizing its main contributions to the development of efficient CFD tools and data-driven analysis frameworks for cardiac flows.

Chapter 2

Methodology

2.1 Geometry Preprocessing

Designing a left ventricle model requires addressing several key aspects to ensure a faithful and relevant representation of cardiac function.

First, the model can be either idealized or patient-specific. Idealized models simplify the geometry to facilitate analysis and reduce computational cost, while patient-specific models are reconstructed from medical images and better capture anatomical variability.

Second, the model can be static or dynamic. Static models represent a fixed instant of the cardiac cycle, typically end-diastole or end-systole. In contrast, dynamic models incorporate ventricular motion, which must be either imposed from a known motion profile or generated algorithmically. The choice between these options depends on the required physiological fidelity, computational constraints, and the availability of patient data.

In this chapter, two idealized models are presented. The first one is based on an analytical description of the ventricular motion, allowing full control of its deformation. The second model is derived from an experimental setup and approximates a simplified physiological geometry. These models are used to study the impact of geometry and motion on intraventricular flow patterns.

2.1.1 Geometry Generation

An idealized model represents a simplified geometric approximation of the LV chamber, facilitating its creation and manipulation. These geometries are commonly generated using computer-aided design (CAD) tools or similar computational programs, given their relatively straightforward definition. In this study, we employ two distinct idealized models: the first, denoted as **Ideal 1**, is a semi-ellipsoid with an inlet and an outlet tube, originally proposed by Zheng et al., 2012. The second, referred to as **Ideal 2**, corresponds to a more complex structure adapted from Vedula et al., 2014. Both geometries are depicted in Fig. 2.1. These idealized models have served as the basis for several recent investigations. Some studies favor simplified ellipsoidal geometries (Dedè et al., 2021; Khalafvand et al., 2018), while others

adopt more anatomically inspired configurations, such as the one used in **Ideal 2** (Kjeldsberg et al., 2023). By employing both types of geometries in this work, we aim to investigate how the specific shape and associated wall motion influence vortex ring formation and breakdown during the filling phase.

A patient-specific model provides a detailed and anatomically accurate representation of the LV, capturing the unique morphology of an individual heart. These geometries are typically reconstructed from medical imaging techniques such as MRI, CT, or echocardiography, allowing for a precise depiction of the ventricular structure. The process involves segmentation of the imaging data, followed by surface reconstruction.

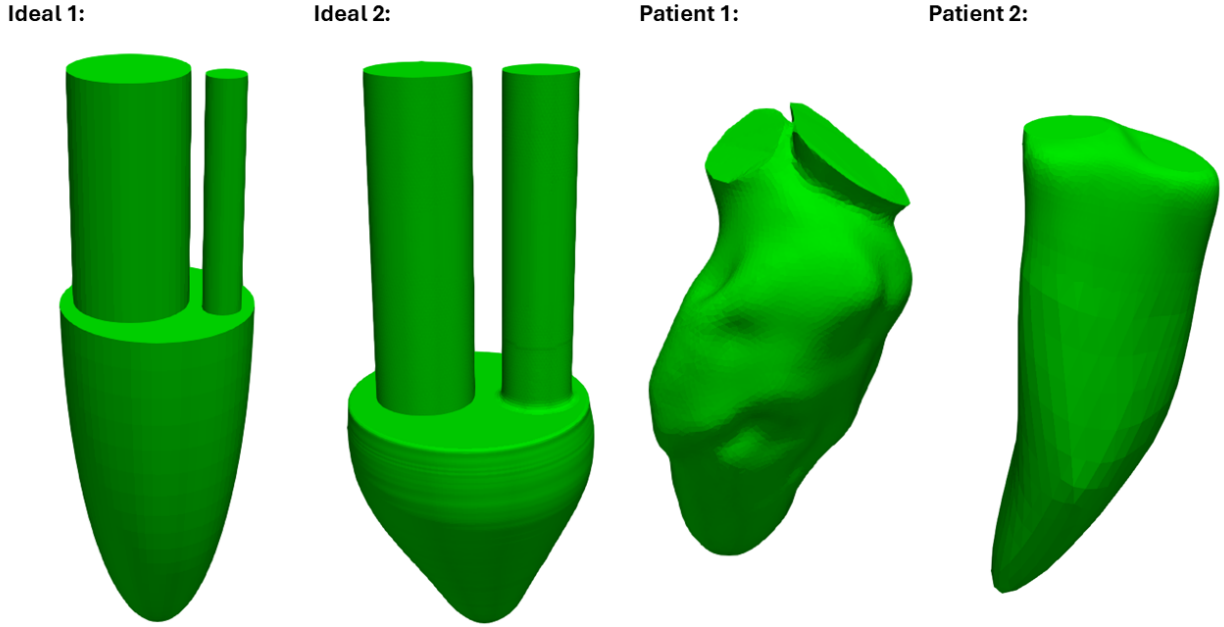


Figure 2.1: Representation of left ventricle models: (left) **Ideal 1** extracted from Zheng et al., 2012, (center-left) **Ideal 2** extracted from Vedula et al., 2014, (center-right) **Patient 1** segmented from CT scans (Karim et al., 2018), and (right) **Ideal 2** extracted from Grünwald et al., 2022

Ideal 1: A Simplified Semi-Ellipsoidal Model

The **Ideal 1** geometry consists of a semi-ellipsoidal chamber representing the left ventricle, to which two cylindrical tubes are connected at the top to emulate the mitral and aortic valves.

The base model is defined with a short semiaxis of $a = 20$ mm and a long semiaxis of $b = 80$ mm, resulting in a semiaxis ratio of $k = a/b = 1/4$. The inlet tube has a diameter of $D = 1.2a = 24$ mm, while the outlet tube has a smaller diameter of $d = 0.4a = 8$ mm. Both tubes extend vertically by the same height H , and their centers are offset laterally from the main axis of the ellipsoid: the inlet by $C = 0.275a = 5.5$ mm, and the outlet by $c = 0.675a = 13.5$ mm.

A schematic depiction of this configuration is shown in Fig. 2.2, which also introduces two reference cross-sections used throughout the analysis: the symmetry plane A–A' (X–Z plane at $y/a = 0$) and the orthogonal section B–B' (Y–Z plane aligned with the inlet direction). The coordinate system is oriented such that velocity and vorticity components are expressed with respect to the X, Y, and Z axes. For instance, v_x denotes the velocity in the X direction, and ω_y the vorticity around the Y axis.

Also included in the sketch are two probe points located on plane A–A' and used in the analysis of flow dynamics. Point P1 is placed at $\mathbf{x} = [0.35a, 0, 0.17a] = [7, 0, 3.4]$ mm, and point P2 at $\mathbf{x} = [0, 0, 1.38a] = [0, 0, 27.6]$ mm.

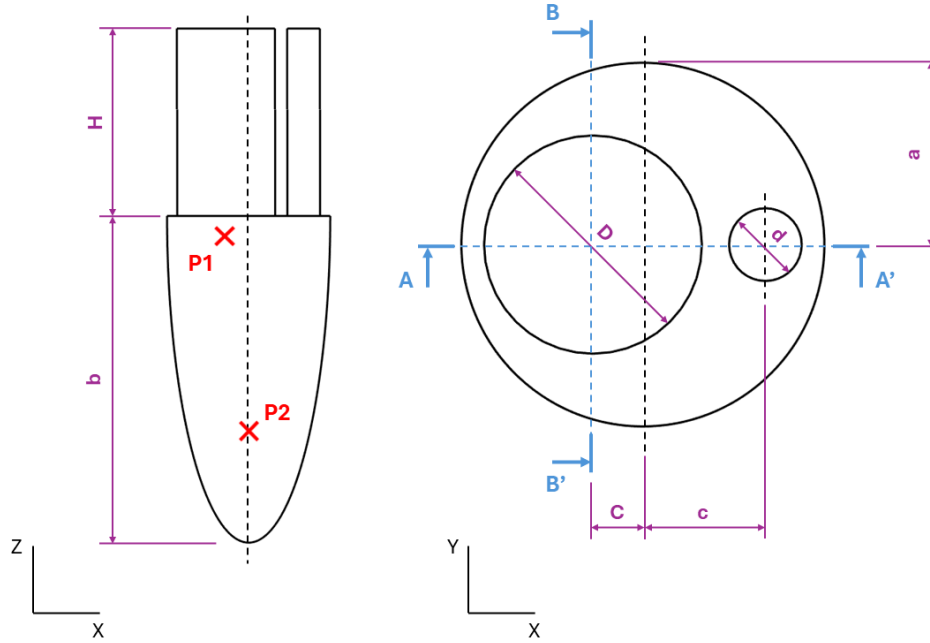


Figure 2.2: Geometrical scheme of the model *Ideal 1*

Given these dimensions, the end-systolic volume (ESV) of the model, excluding the contribution of the inlet and outlet tubes, can be determined using the volume formula for a semi-ellipsoid with a circular base:

$$ESV = \frac{2}{3}\pi a^2 b \quad (2.1)$$

This selection of geometrical dimensions ensures that the model maintains physiologically relevant volume conditions, closely aligning with expected clinical ESV values for a healthy human left ventricle ($ESV = 67$ mL). This volume typically ranges from 25 to 70 mL, depending on factors such as age, sex, and overall cardiac function.

Ideal 2: Experimental Model

The **Ideal 2** model incorporates inlet and outlet conduits to represent the mitral and aortic valves, similar to the **Ideal 1** configuration. However, the ventricular chamber here does not follow a simple semi-ellipsoidal profile. Instead, it is based on a model derived from an experimental setup developed by Vedula et al., 2014. In that study, the geometry of the left ventricle was reconstructed from biplanar imaging, where the myocardial wall was captured from two orthogonal views and subsequently processed to obtain a three-dimensional surface. The resulting chamber exhibits a broader and more rounded morphology compared to the simplified ideal model.

For the purposes of this work, the digital reconstruction from Vedula et al., 2014 was directly integrated into the CFD pipeline. To preserve interpretability and enable direct comparisons with the previous idealized configuration, certain geometric characteristics were retained. A schematic of the model is shown in Fig. 2.3, where all relevant geometrical parameters are presented. The chamber base radius is approximately $a = 2.9$ cm and extends vertically with a height-to-base ratio of $k = a/b = 0.45$, resulting in a total length of approximately 6.38 cm. The diameters of the inlet and outlet tubes are $D = 0.85a \approx 24.7$ mm and $d = 0.6a \approx 17.4$ mm, respectively, while both tubes share the same vertical extent of $H = 2.7a \approx 7.83$ cm. Laterally, the centers of the tubes are offset from the main axis by $C = 0.35a \approx 10.2$ mm (inlet) and $c = 0.6a \approx 17.4$ mm (outlet).

The same spatial references introduced for **Ideal 1** are used to define the analysis planes: the central X-Z symmetry plane at $y/a = 0$ (plane A-A') and the orthogonal Y-Z plane aligned with the inlet (plane B-B'). These planes are consistently employed throughout the study to present and interpret velocity and vorticity data. In addition, two probe points located within plane A-A' are defined for comparative analysis in the results. The first point (P1) is placed at coordinates $\mathbf{x} = [0.35a, 0, 0.17a] \approx [10.15, 0, 4.93]$ mm, and the second (P2) at $\mathbf{x} = [0, 0, 1.38a] \approx [0, 0, 40.0]$ mm.

This configuration corresponds to the end-systolic phase of the cardiac cycle, where the left ventricle is at its minimum volume. The total enclosed volume in this state is estimated at approximately 108 mL, aligning well with physiological values and ensuring a realistic representation of cardiac conditions for subsequent flow analysis.

Patient 1: Computed Tomography Model

When working with patient-specific data, the preprocessing of the geometry becomes significantly more complex and requires multiple steps to ensure an accurate and high-quality representation of the LV. It is a crucial process that extracts the anatomical region of interest from the medical images and prepares it for later use in our CFD solver. The preprocessing includes:

1. *Segmentation*: We use 3D Slicer (Fedorov et al., 2012), an open-source software designed for the visualization, processing, segmentation, registration, and analysis of medical data. The CT scan data, stored in Digital Imaging and Communications in Medicine (DICOM) format, is imported into the software, allowing us to examine the heart from multiple perspectives. The segmentation process involves selecting the regions to be

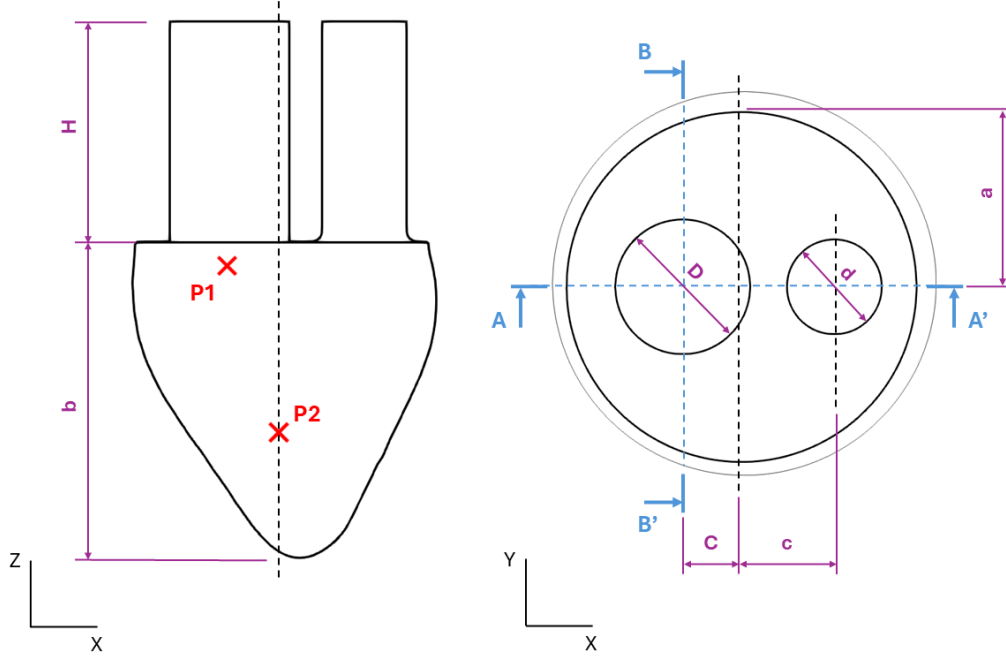


Figure 2.3: Geometrical scheme of the model *Ideal 2*

extracted as a three-dimensional surface representation. In our case, we define the LV along with the left atrium and the aortic arch, ensuring that the inlet and outlet regions are appropriately captured.

2. *Smoothing and Cleaning:* Remove noise and irregularities from the segmented surface to ensure a more accurate representation of the ventricular chamber.
3. *Exporting the Surface:* The refined geometry is saved as a stereolithography (STL) file, a common format for 3D surface representation.
4. *Cutting and Remeshing:* Unnecessary parts of the heart are removed, and any gaps or holes in the surface are closed to obtain a well-defined LV chamber. The surface is also remeshed to prevent irregularities and improve element quality.
5. *Rescaling and Alignment:* The ventricle is adjusted to match physiological dimensions, ensuring consistency with patient-specific measurements. Additionally, the geometry is reoriented to align with a preferred coordinate system, facilitating subsequent analysis and simulation.

This workflow, from medical image segmentation to final surface processing, is depicted in Fig. 2.4.

The dataset for this model was obtained from Karim et al., [2018](#), which provides CT scans of a human heart. The imaging was acquired during mid-atrial diastole, near the end of ventricular diastole. This implies that the extracted left ventricular volume closely corresponds to the end-diastolic volume (EDV). The estimated EDV for this dataset is approximately 152 mL.

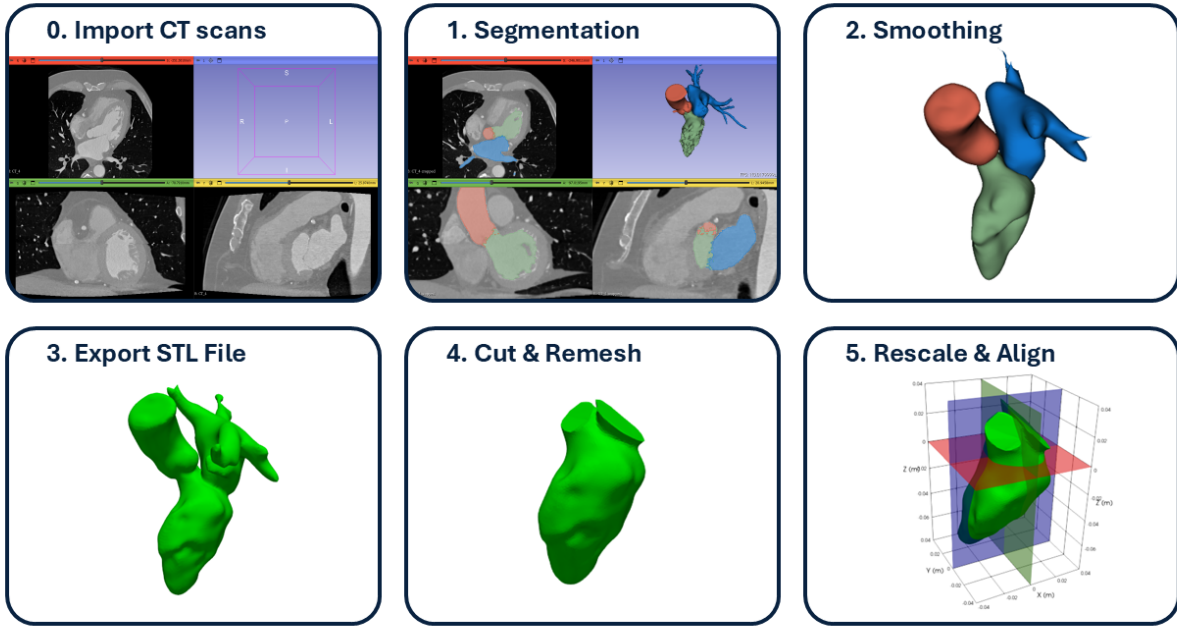


Figure 2.4: Workflow of extracting Patient 1 model from CT scans.

Patient 2: Real-Time 3D-Echocardiography Model

The dataset for the Patient 2 model was provided in STL format by Neidlin, 2023, allowing straightforward integration into the CFD simulations without the need for additional pre-processing. However, the segmentation and preprocessing workflow utilized in Grünwald et al., 2022, for these data is closely aligned with the approach described for the Patient 1 model (as seen in Fig. 2.4). In their study, the geometric data obtained from echocardiography was converted to a Unicode Character Database (UCD) format using ImageArena software (TOMTEC Imaging Systems, Unterschleißheim, Germany) before further processing. The initial volume of this geometry is approximately 10 mL, reflecting the smaller scale of a child's heart compared to adult models.

2.1.2 Wall Motion

The incorporation of myocardial wall motion is imperative for accurate simulation of left ventricular dynamics, as it plays a fundamental role in capturing the main features of efficient cardiac pumping. In this study, we adopt a fluid dynamics-based simulation approach, where wall motion is translated as mesh movement. This enables the periodic contraction and expansion of the ventricle, thereby mimicking physiological heart function through the periodic inflow and outflow of blood.

However, implementing this movement is not a straightforward task. Several key factors must be considered:

- The mesh motion must accurately follow the flow rate or volume change evolution

observed in a physiological heart cycle to ensure realistic pumping behavior.

- The STL surface mesh must maintain element number and connectivity throughout the deformation process. Although dynamic meshing techniques can be applied during the simulation, the initial setup must ensure mesh connectivity.
- The prescribed motion must be compatible with the boundary conditions imposed at the inlet and outlet, ensuring continuity between wall kinematics and the simulated blood flow.

To address these challenges, we implemented two distinct approaches for modeling wall motion depending on the data available: a synthetic motion derived from flow rate or volume change data and the motion extracted from experimental or medical imaging data. Each approach presents its own advantages, with the first offering controlled and customizable wall motion dynamics, while the second ensures high anatomical and physiological fidelity when data is available.

Synthetic Motion

This method, developed within our research group, prescribes wall displacement based on predefined ventricular flow rate evolution curves. This ensures a controlled and physiologically realistic contraction-expansion cycle in both idealized and patient-specific models.

Before detailing the methodology, it is essential to understand the ventricular motion throughout the cardiac cycle. The left ventricle undergoes a coordinated sequence of contraction and relaxation to ensure effective blood circulation. This cycle consists of two main phases: diastole, when the ventricle fills with blood, and systole, when it ejects blood into the aorta. These phases can be identified in the flow rate curve shown in Fig. 2.5, where characteristic features such as the E-wave and A-wave appear.

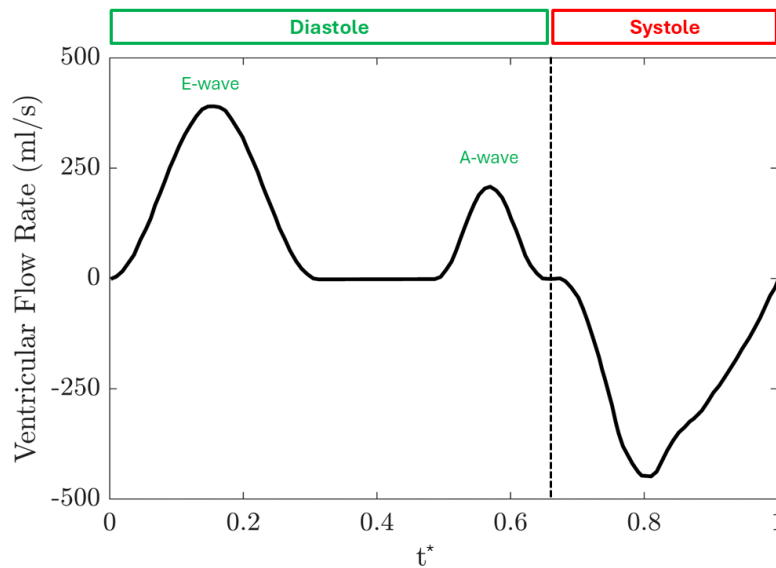


Figure 2.5: Detailed flow rate chart of the *Ideal 1* model of the left ventricle.

Diastole begins with the relaxation of the ventricle, causing a decrease in pressure inside the ventricle. Once this pressure falls below that of the left atrium, the mitral valve opens, allowing blood to enter. The resulting sudden inflow of blood generates the E-wave, which corresponds to the peak filling velocity. As the ventricle continues to fill, the flow rate gradually decreases until atrial contraction occurs. This contraction increases atrial pressure, which in turn drives additional blood into the ventricle, resulting in the generation of the A-wave, a secondary peak in the flow rate curve. The end of diastole is marked by the closure of the mitral valve, as the ventricle prepares for contraction.

Once diastole ends, the ventricle contracts, increasing internal pressure until it exceeds aortic pressure. At this point, the aortic valve opens, initiating systole and allowing blood to be ejected. The ventricular volume decreases progressively until most of the blood is expelled, at which point the pressure drops again, causing the aortic valve to close. This marks the transition back to diastole, completing the heart cycle.

To replicate this physiological motion in computational simulations, we developed a methodology with the following steps:

1. *Load data:* The initial ventricle geometry is loaded from an STL file, extracting point coordinates and connectivity data while applying appropriate scaling if needed (e.g., converting to meters). Additionally, face normals are computed to assist in displacement calculations.
2. *Classify vertices:* Before applying motion, the geometry is classified to distinguish static and moving regions. For example, in the idealized models, the inlet and outlet tubes remain fixed, whereas in patient-specific models, motion is more pronounced near the apex and less near the mitral annulus.
3. *Process flow rate data:* If real flow rate measurements are available, they are loaded; otherwise, a synthetic profile is generated using Fourier-based approximations, combining sine and cosine functions. The resulting flow rate curve is discretized to match the chosen temporal resolution. To maintain physiological consistency, the total volume entering the ventricle during diastole must equal the volume ejected during systole, ensuring that the initial and final ventricular volumes remain unchanged.
4. *Calculate volume change:* The flow rate curve is integrated numerically to obtain the volume variation at each time step. If directly volume evolution data is available, this integration step and the previous one are unnecessary.
5. *Generate STL files:* Using the computed volume variation, displacement factors are determined for each point in the mesh. The displacement is applied iteratively, with a bisection optimization algorithm adjusting the deformation until the desired volume change is achieved. This process ensures that each deformed geometry accurately follows the prescribed flow rate curve while preserving mesh connectivity. At each time step, the updated geometry is saved as an STL file for further use in CFD simulations.
6. *Inlet and outlet profile computation:* Finally, the corresponding inlet and outlet flow rate profiles are computed to match the volume evolution. Since the mitral valve remains closed during systole and the aortic valve is closed during diastole, these boundary

conditions are enforced to ensure realistic flow dynamics.

This methodology is illustrated in Fig. 2.6 for the **Ideal 1** model, where the stepwise deformation process and its effect on ventricular geometry are shown.

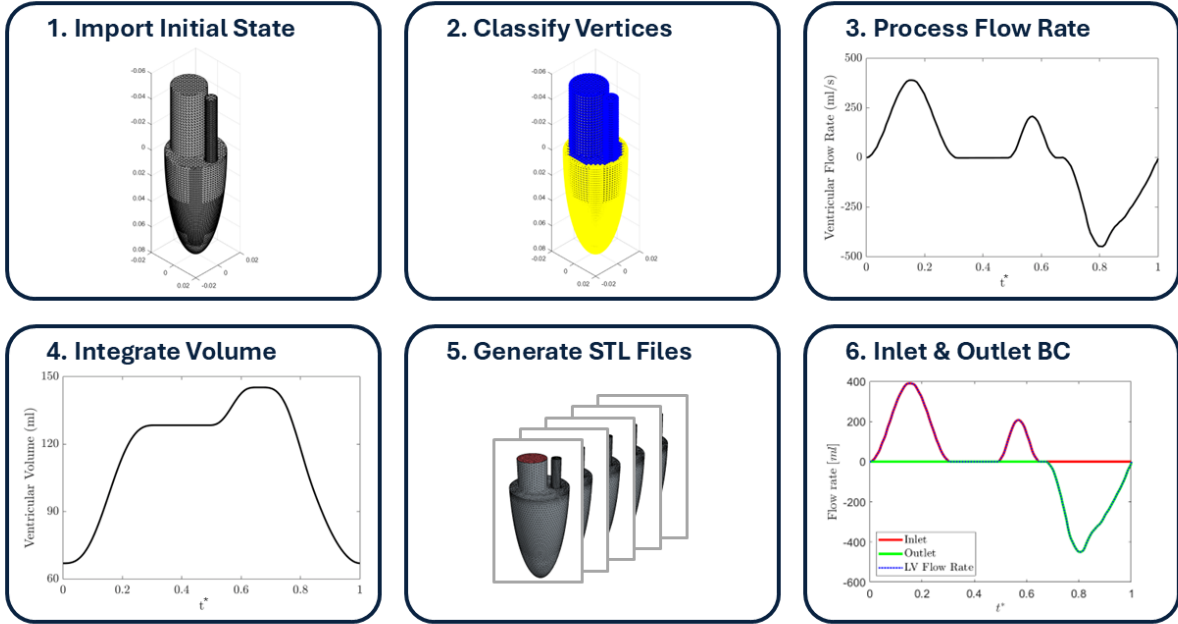


Figure 2.6: Detailed flow rate chart of the **Ideal 1** model of the left ventricle.

In the case of simplified models, such as **Ideal 1**, the methodology can be made more efficient because geometric parameters can be directly controlled to achieve the desired volume evolution. In this case, the surface can be computed explicitly using Equation 2.1, which provides the semiaxis evolution:

$$\begin{aligned} b(t) &= \left(\frac{3k^2}{2\pi} V_{LV}(t) \right)^{1/3} \\ a(t) &= k b(t) \end{aligned} \quad (2.2)$$

where $V_{LV}(t)$ corresponds to the temporal evolution of the left ventricular volume. This approach eliminates the need for iterative optimization, as the surface of the ellipsoid can be computed directly from the volume change data.

The proposed methodology enables the creation of a synthetic left ventricle evolution using only an initial state or, if desired, can be adapted to incorporate other time-instant data. Although this approach serves as a proof of concept, assuming uniform volumetric expansion for idealized models, it remains a valuable tool. Literature suggests that uniform expansion provides a reasonable approximation of LV wall motion, though it remains a simplification of physiological behaviour (Rankin and Olsen, 1980). In patient-specific cases, achieving highly

accurate motion tracking remains a challenge, as the heart does not always move strictly in the normal direction, showing complex deformations.

Nonetheless, this method provides a practical solution in contexts where high-quality medical imaging data is scarce, an issue that is even more pronounced when working with publicly available datasets. By offering this approximation of ventricular motion, the framework enables the generation of synthetic data. This data can then be used in the development of robust simulation pipelines, contributing to the advancement of computational cardiac modeling.

Extracted Motion

In scenarios where time-resolved surface deformations are accessible, the reconstruction of myocardial wall motion can be achieved through direct methods, such as experimental marker tracking or medical image segmentation. This data-driven approach offers a more precise depiction of ventricular dynamics, capturing realistic deformation patterns that reflect actual physiological processes.

The methodology for extracting the surface is determined by the nature of the available data. In the case of the **Ideal 2** geometry, the ventricular surface is reconstructed using biplanar images captured in two perpendicular directions (Vedula et al., 2014). Following the enhancement of the images through filtering and thresholding, the ventricular edges are detected. The subsequent generation of a 3D surface is achieved through the implementation of a surface fitting process.

For the **Patient 2** model, the available medical data required a segmentation process similar to that illustrated in Fig. 2.4, but in this case, the segmentation had to be performed for each time frame. Various tools facilitate this process by propagating the segmentation from an initial state to the subsequent time frames in the sequence, ensuring temporal consistency.

Following the extraction of the temporal evolution of the surfaces, a shared mesh must be defined and interpolated onto these surfaces to maintain mesh element correspondence and connectivity across all time instants. This step is essential for ensuring numerical stability in subsequent CFD simulations.

For our study, this preprocessing was not required, as the data was already provided as a fully processed mesh with ensured connectivity, ready for direct integration into our CFD solvers. The datasets were made available by external collaborators: the **Ideal 2** model was provided by Vedula et al., 2014, while the **Patient 2** model was shared by Neidlin, 2023.

2.2 Computational Fluid Dynamics

In order to comprehend the dynamics of blood flow within the left ventricle, it is necessary to solve the governing equations of fluid motion under conditions that are relevant to physiology. CFD provides a robust framework for simulating these flows, enabling detailed analysis of intraventricular transport and vortex formation. Given the density and viscosity of blood and assuming it behaves as a Newtonian fluid within the large-scale ventricular flow, the

incompressible Navier-Stokes equations are solved. The energy equation is not considered.

The governing equations leading the hemodynamics inside the left ventricle are the following:

- The conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (2.3)$$

where ρ is the density of the fluid.

- The conservation of momentum:

$$\frac{D(\rho \mathbf{v})}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}, \quad (2.4)$$

where p is the pressure, $\mathbf{g}$ is the gravity and $\boldsymbol{\tau}$ is the fluid stress tensor. This tensor is calculated as:

$$\boldsymbol{\tau} = -\mu \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^\top \right) + \left(\frac{2}{3}\mu - \kappa \right) (\nabla \cdot \mathbf{v}) \mathbb{I}, \quad (2.5)$$

where μ is the viscosity of the mixture and κ is the mixture dilatational viscosity. The identity matrix is denoted by $\mathbb{I}$ and the superscript $()^\top$ refers to a matrix transpose.

CFD enables the numerical solution of the governing equations of fluid motion, providing detailed insights into complex flow phenomena. The numerical solution of these equations requires discretization methods that transform the continuous differential equations into a system of algebraic equations, solvable using iterative or direct numerical techniques.

2.2.1 Solver

For our simulations, we employed Ansys Fluent 2024R2 (Ansys, 2024), a widely used CFD solver built on the finite volume method (FVM). This method is particularly well-suited for fluid flow problems due to its inherent conservation properties, robustness in handling complex geometries, and flexibility in meshing strategies. Ansys Fluent discretizes the governing equations using a control volume approach, where the integral form of the Navier-Stokes equations is solved within each computational cell, ensuring mass and momentum conservation at a local level.

To enhance numerical accuracy and stability, the solver offers a variety of spatial and temporal discretization schemes, allowing for higher-order accuracy when needed. Additionally, Fluent provides multiple turbulence modeling options, including laminar flow, RANS, LES, and hybrid models, ensuring adaptability across different flow regimes. Pressure-velocity coupling is handled through several algorithmic approaches, such as SIMPLE, PISO, and Coupled schemes, which optimize convergence depending on the simulation requirements.

A key reason for selecting Ansys Fluent for our LV simulations was its extensive customization capabilities. The solver supports user-defined functions (UDFs), enabling precise implementa-

tion of physiological boundary conditions, time-dependent flow profiles, and post-processing routines tailored to our study. Furthermore, its compatibility with structured, unstructured, and hybrid meshes grants flexibility in adapting to ideal and patient-specific geometries alike.

Beyond its technical capabilities, Ansys Fluent’s intuitive user interface and comprehensive documentation were instrumental in streamlining our workflow. These features not only facilitated a structured simulation process but also allowed us to develop a well-documented and accessible tutorial on left ventricle blood flow simulation, ensuring reproducibility for future studies.

For validation and comparative purposes, we have also employed STAR-CCM+ (Siemens, 2023), another widely used CFD tool that similarly relies on the finite volume approach. This solver is another industry-standard CFD solver, developed by Siemens, that also employs the FVM.

While both Ansys Fluent and STAR-CCM+ rely on the finite volume method, it is useful to compare this approach with the finite element method (FEM), another common discretization technique in computational fluid dynamics. While FEM-based solvers (such as those used in COMSOL Multiphysics or Abaqus CFD) offer greater flexibility in certain engineering applications, they are generally more computationally expensive for fluid flow simulations. The FVM remains the preferred choice for CFD due to its balance between accuracy, computational efficiency, and simpler implementation on arbitrary geometries.

Given the nature of our study, which focuses on ventricular blood flow simulations, Ansys Fluent was selected to perform the simulations in our LV models. However, Star-CCM+ was also employed to validate our results and assess solver-dependent discrepancies. In our results, we present the validation and comparative analysis of the two solvers for **Ideal 1** model, evaluating key hemodynamic indicators such as vortex ring formation and evolution, and kinetic energy evolution throughout the cardiac cycle. By leveraging both solvers, we aim to enhance the robustness of our findings and ensure that the numerical approach remains consistent across different computational frameworks.

2.2.2 Flow Modelling

Accurately defining the fluid properties and governing parameters is crucial for obtaining meaningful simulation results in hemodynamic studies. Blood is commonly modeled as an incompressible Newtonian fluid at the macroscopic scale, an assumption supported by various studies in the field (Bucelli et al., 2023; Fedele et al., 2023; He et al., 2022). While blood exhibits shear-thinning properties at lower shear rates, within the LV and under physiological conditions, treating it as Newtonian is a reasonable simplification. Based on previous works (Korte et al., 2023), we adopt a constant density of $\rho = 1060 \text{ kg/m}^3$ and a dynamic viscosity of $\mu = 0.004 \text{ Pa} \cdot \text{s}$.

To characterize the flow regime, we compute the Reynolds number (Re), which represents the ratio of inertial to viscous forces. Using the inlet tube diameter, D , as the characteristic length and the peak inlet velocity V_{max} of the cardiac cycle, the Reynolds number is estimated

as:

$$\text{Re} = \frac{\rho V_{\max} D}{\mu} \quad (2.6)$$

Both models run at a similar Reynolds number, approximately 5000. This value suggests that the flow operates in a transitional regime, where laminar and turbulent structures coexist.

Another critical non-dimensional parameter in cardiovascular fluid dynamics is the Womersley number (α), which characterizes the pulsatile nature of blood flow by comparing transient inertial effects to viscous forces. It is defined as:

$$\alpha = D \left(\frac{\omega \rho}{\mu} \right)^{1/2} \approx 31, \quad (2.7)$$

where ω represents the angular frequency of the heart cycle, taken here as 2π . This relatively high Womersley number indicates that inertial effects dominate over viscosity, leading to the development of complex flow structures that evolve over the cardiac cycle.

Despite the potential for turbulent flow inside the LV, numerous studies have successfully analyzed vortex ring dynamics using laminar assumptions, arguing that turbulence plays a secondary role in this specific phenomenon (He et al., 2022; Tagliabue et al., 2017). Consequently, our simulations adopt a laminar model, as our primary goal is to capture the formation and evolution of the intraventricular vortex ring. The accuracy of this approach is later assessed in the validation section, where we compare our results against literature and experimental data.

It is important to note that to model the full spectrum of ventricular flow dynamics, including smaller-scale turbulent structures and their interactions, requires more advanced turbulence models. Some studies have addressed this challenge using techniques such as large eddy simulation (LES) (Bennati et al., 2023; Bucelli et al., 2023) or Reynolds-averaged Navier-Stokes (RANS) models (Grünwald et al., 2022; Korte et al., 2023), which allow for a more detailed representation of flow fluctuations. For instance, the study by

For our study, we prioritize computational efficiency while ensuring that the primary flow features of interest, the formation and progression of the vortex ring, are well captured. The effects of this choice are discussed more in detail in the validation section, where we demonstrate that our laminar model provides an accurate representation of the key intraventricular flow characteristics.

2.2.3 Meshing

Meshing plays a crucial role in our simulations, particularly given the complex dynamics of fluid flow within the left ventricle. The presence of multiple spatial and temporal scales necessitates a carefully designed mesh to accurately capture key flow features.

To construct the computational mesh, a base element size is first defined, setting the standard resolution across the domain. This base size typically ranges from 10^{-3} to 10^{-4} . The mesh is then refined adaptively near the walls, striking a balance between numerical accuracy and computational efficiency.

The meshing strategy adopts a hybrid approach: an unstructured tetrahedral core mesh supported by a "Patch Conforming Method" is combined with refined regions close to the boundaries. A volumetric growth rate, set to 1.3, is applied to gradually increase mesh size away from the wall. This refinement near surfaces is essential for resolving near-wall flow features and enhancing accuracy in wall-bounded regions. Mesh generation is carried out through an automated, iterative refinement procedure to ensure element quality and conformity throughout the domain.

To illustrate the resulting mesh structure, Fig. 2.7 presents the volumetric mesh of the *Ideal 2* model at a medium resolution with a base size of 7.5×10^{-4} m.

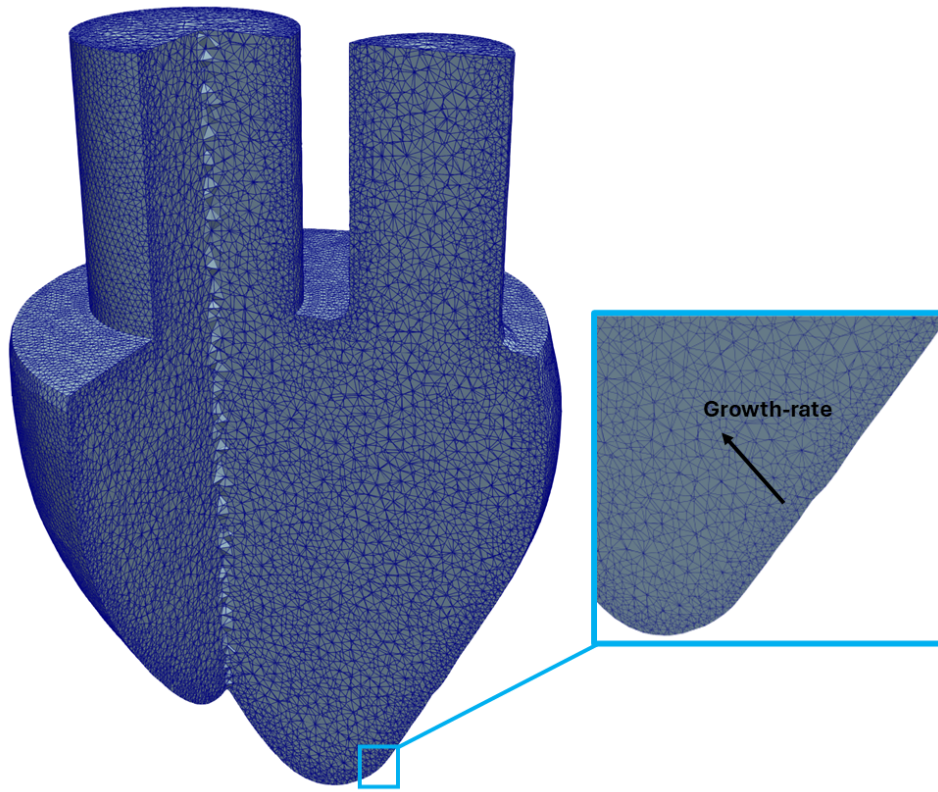


Figure 2.7: Illustration of the mesh for a base size of 7.5×10^{-4} m.

In contrast to the availability of literature on other aspects of computational simulations, meshing details are often scarce. This lack of information poses a significant challenge in reproducing published results. To address this gap in the literature, our website (ModelFLOWS, 2023b) offers a comprehensive methodology for tuning and optimizing meshes (<https://modelflows.github.io/modelflowsapp/cardiacpathologydetection/#tutorials>).

This rigorous meshing approach ensures an accurate representation of wall-bounded flow, while also enabling the integration of wall motion and mesh deformation techniques critical for simulating physiological dynamics.

2.2.4 Boundary Conditions

In our study, we consider three primary boundaries: the ventricular wall, the inlet, and the outlet. Each boundary plays a pivotal role in accurately representing the physiological processes of the heart, necessitating precise definitions to ensure the realism and success of our simulations.

In the study of LV hemodynamics, the selection of wall boundary conditions requires careful consideration. The decision to employ fixed walls or periodically moving walls, which more closely reflect the dynamic nature of the heart, is of critical importance yet introduces varying degrees of complexity in implementation and analysis. Initially, the walls were considered fixed throughout the cardiac cycle, aiming to approximate inflow and outflow rates to match idealized or physiological data. However, our initial tests showed that fixed walls could not accurately model the flow dynamics within the ventricle. Key features such as the vortex ring evolution and recirculation to the apex were not captured, highlighting the limitations of the fixed-wall configuration in representing intricate flow patterns within the ventricular chamber.

In order to address the need for capturing precise dynamics, we have implemented moving walls. To this end, we used the methodology introduced in Section 2.1.2 to obtain wall movement via a synthetic generator.

In the solver, Ansys Fluent (Ansys, 2024), the evolution of the ventricular volume at each time instant must be provided as STL files with shared mesh connectivity, either created using the synthetic generator or extracted from medical or experimental data. A Python script then converts and interpolates these files into a format readable by Fluent (.asc) with the final desired time step. Finally, each mesh file is loaded, and the wall location is updated at each time step using the dynamic mesh tool and UDFs.

For validation in Star-CCM+ (Siemens, 2023), the methodology is more complex. First, we preprocess the volume change data by normalizing it between 0 (ESV) and 1 (EDV) to use the data in the morphing tool as incremental displacements. The process begins by importing the model at its minimum volume instant, then defining its maximum volume state and extracting the total displacement from the minimum to maximum volumes using the preprocessed mesh states. Finally, the incremental displacements between each time step are introduced as a morphing wall boundary condition to guide the morphing process and match the volume change to the flow rate graph.

These implementations enable the simulation of ventricular wall movement in a manner that closely approximates physiological reality.

Next, we consider the inlet and outlet boundaries, which model the mitral and aortic valves, respectively. Our study examines two configurations:

1. *Flow rate-based configuration* (BC1), where the flow rate of blood entering and exiting each valve is imposed.
2. *Pressure-based configuration* (BC2), where blood enters and exits based on pressure gradients generated in the LV due to wall movement.

The pressure-based configuration more accurately represents physiology, as heart movement

drives blood flow. The mitral valve opens during ventricular expansion, allowing blood inflow due to the pressure difference between the LA and LV during the E-wave, followed by additional inflow during the A-wave when the LA contracts. The aortic valve opens when the ventricle contracts, expelling blood into the aorta. A key challenge of this method is the need for dynamic events to switch boundaries: the outlet behaves as a wall during diastole while the inlet remains open as a pressure inlet, and in systole, this reverses, with the inlet closing (becoming a wall) and the outlet opening (becoming a pressure outlet). This methodology was straightforward to implement in Ansys Fluent using dynamic events, but Star-CCM+ lacks an equivalent built-in function. Additionally, pressure-based boundaries create abrupt valve openings and closings, that could potentially cause numerical instabilities.

The flow rate-based configuration mitigates these difficulties. This method extracts inlet and outlet flow rates from the volumetric flow rate chart generated by the synthetic wall motion methodology. Since the flow is considered incompressible, the LV's volumetric expansion matches the inlet flow rate, and its contraction corresponds to the outlet flow rate. This configuration smooths valve transitions (as zero flow is gradually imposed at valve closures) and improves convergence. However, incorrect matching of flow rate and volume change can introduce compressibility effects, reducing simulation accuracy. Additionally, spatial velocity profiles (parabolic or hyperbolic) can be imposed to refine incoming flow behavior. This method is straightforward to implement in both Ansys Fluent and Star-CCM+.

For solver validation, we use the flow rate-based configuration, as it is easy to implement and ensures fast convergence. For Ansys Fluent specific cases, we use the pressure-based configuration, as it better mimics physiological heart behavior.

2.2.5 Numerical Schemes

Since the simulation is transient, an implicit time-stepping scheme was chosen to enhance numerical stability while allowing for larger time steps compared to explicit methods. This approach ensures that the solution remains stable even at relatively high Courant-Friedrichs-Lewy (CFL) numbers, which were adjusted dynamically based on flow characteristics.

For temporal discretization, a second-order scheme was employed to improve accuracy in capturing time-dependent phenomena, reducing errors associated with temporal approximations. Gradient calculations were performed using the least-squares method, which provides a reliable approximation of flow variable gradients, particularly on unstructured meshes where accuracy can be compromised by irregular element distribution.

To discretize the advection terms, the Second-Order Upwind scheme was used. This method offers a balance between numerical stability and accuracy, minimizing numerical diffusion while ensuring that strong velocity and pressure gradients are well captured.

For pressure-velocity coupling, the Pressure-Implicit with Splitting of Operators (PISO) algorithm was implemented. This scheme is particularly effective for transient simulations as it enhances convergence and stability, particularly when dealing with rapidly evolving flow fields.

The simulation was run with a time step size of $\delta t = 5 \times 10^{-4}$ seconds, with 30 internal

iterations per time step to ensure proper convergence at each iteration. Finally, wall treatment was handled using the Implicit Tree method, which was chosen for its robustness in resolving boundary layer effects while maintaining computational efficiency.

2.3 Scientific Machine Learning

Scientific Machine Learning (SciML) combines data-driven techniques with physics-based modeling to enhance the analysis, interpretation, and prediction of complex dynamical systems. In the context of cardiovascular flow studies, SciML enables the extraction of meaningful patterns from high-dimensional, time-resolved data, facilitating a deeper understanding of flow structures and their evolution.

Machine learning methodologies can generally be classified into supervised and unsupervised learning, each serving distinct purposes depending on the nature of the data and the goals of the analysis. In supervised learning, models are trained using labeled data, where each input is associated with a known output. The goal is to learn a mapping from inputs to outputs so that the trained model can make accurate predictions on new, unseen data.

On the other hand, unsupervised learning deals with unlabeled data, aiming to extract meaningful patterns, structures, or representations without explicit output labels. Instead of learning direct input-output relationships, unsupervised methods identify dominant features in the data, allowing for dimensionality reduction, clustering, or pattern discovery. This is particularly useful in analyzing large-scale fluid flow datasets, where extracting underlying flow structures can lead to a deeper understanding of key physical mechanisms. The present study primarily focuses on unsupervised learning techniques to identify dominant flow patterns and reconstruct essential features of the intracardiac flow field.

Within this scope, we explore modal decomposition methods, which offer reduced-order representations of complex unsteady flows by extracting coherent structures that dominate the system's dynamics. In this study, we employ POD and HODMD. To the best of our knowledge, these techniques have not been previously applied to analyze the formation and breakdown of the intraventricular vortex ring in idealized LV models. Their application enables a deeper understanding of the spatiotemporal organization of the flow and the key mechanisms governing vortex evolution. This insight is particularly relevant given the established link between vortex dynamics and cardiac efficiency. In the long term, such knowledge could contribute to the early detection or prevention of cardiovascular diseases by identifying altered flow patterns associated with pathological conditions.

2.3.1 Tensorial Formulation

To apply data-driven algorithms, we first preprocess the simulation data and transform it into a structured format. Specifically, we represent our 4D dataset as a tensor by organizing the unstructured simulation data onto a structured grid. The tensor construction follows this scheme:

- The first dimension (J_1) stores different flow variables (e.g., pressure, velocity compo-

nents, vorticity).

- The next three dimensions (J_2, J_3, J_4) represent the spatial grid.
- The last dimension (K) corresponds to the temporal snapshots.

Thus, the dataset is arranged into a 5D tensor ($\mathbf{A}$) of dimensions $J_1 \times J_2 \times J_3 \times J_4 \times K$.

A major challenge arises from the dynamic nature of the left ventricle, whose volume changes throughout the cardiac cycle. This complicates the construction of a structured tensor suitable for data-driven analysis. To address this, a fixed control volume is defined as a bounding box enclosing the ventricle at maximum expansion. The unstructured CFD data at each time step is then interpolated onto a regular Cartesian grid using linear scattered interpolation without extrapolation, as implemented via MATLAB's `scatteredInterpolant` with the `linear/none` option. This avoids artificial values outside the original domain.

To mitigate numerical diffusion near the ventricular wall, a masking strategy is applied: STL surface files representing the endocardial geometry at each time step are used to identify grid points of the structured domain outside the ventricular cavity. These regions are excluded from the interpolation and subsequently set to zero in the tensor, preventing spurious blending across solid-fluid interfaces. This is illustrated in Fig. 2.8.

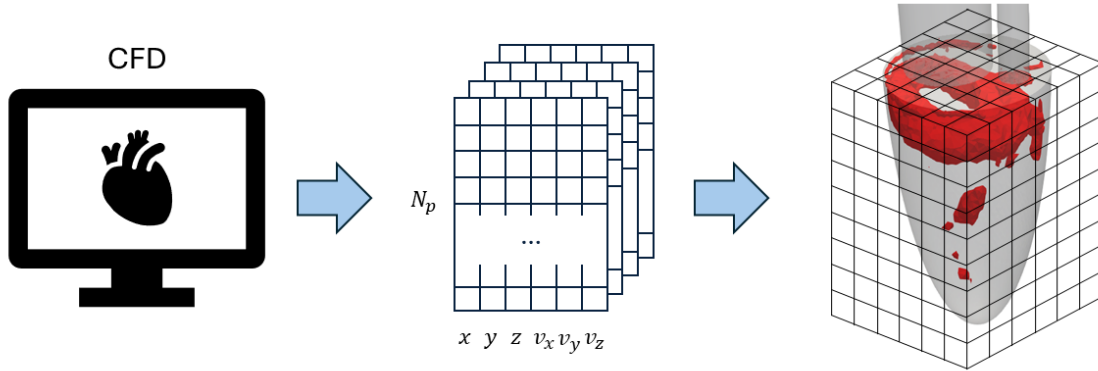


Figure 2.8: Illustration of the tensorization process.

For some low-order algorithms, such as, singular value decomposition (SVD), we need to rearrange the tensor and convert it into a snapshot matrix $\mathbf{V}_1^K$. This transformation involves concatenating all spatial variables and grid points into a single dimension while keeping the temporal snapshots as a separate dimension. Thus, we construct a snapshot matrix of dimensions $J \times K$, where $J \equiv J_1 \times J_2 \times J_3 \times J_4$ represents the total number of spatial degrees of freedom, and K remains the number of temporal snapshots.

2.3.2 Proper Orthogonal Decomposition

POD (Lumley, 1967) is a widely used method for data-driven dimensionality reduction and pattern extraction in complex fluid dynamics problems. In the literature, this term is interchangeable with the SVD term since it is one of the two ways of extracting the POD

modes. The method relies on SVD (Sirovich, 1987) to extract the most energetic structures from spatiotemporal data, allowing for an efficient representation of the system with a reduced number of modes.

The data is stored in the snapshot matrix $\mathbf{V} = \{\mathbf{v}_1, \dots, \mathbf{v}_K\}$, where each column represents a state of the system at a given time. Given the typically large values of J (e.g., $\mathcal{O}(10^6)$), direct processing is computationally expensive, necessitating dimensionality reduction.

In SVD, we decompose it as follows:

$$\mathbf{V}_1^K = \mathbf{U}\mathbf{\Sigma}\mathbf{T}^T = \sum_{n=1}^N \sigma_n \mathbf{u}_n \cdot \mathbf{t}_n^T, \quad (2.8)$$

where $\mathbf{U} = \{\mathbf{u}_1, \dots, \mathbf{u}_N\}$ contains the spatial modes (POD modes), $\mathbf{\Sigma}$ is a diagonal matrix of singular values $\sigma_1, \dots, \sigma_N$, and $\mathbf{T} = \{\mathbf{t}_1, \dots, \mathbf{t}_N\}$ contains the temporal coefficients. The tolerance ε_1 determines the number of retained modes N_r , ensuring that $\sigma_{N_r+1}/\sigma_1 \leq \varepsilon_1$. The reduced snapshot matrix is then reconstructed using Eq. 2.8 and the reduced matrices. This reduction retains only the most significant energetic structures while filtering out noise and spatial redundancies.

The extracted POD modes $\mathbf{U}$ enable the visualization of the dominant features in the spatiotemporal database, providing insight into the underlying physics of the problem. A schematic representation of this method is shown in Fig. 2.9, illustrating the decomposition of the snapshot matrix and identifying the POD modes along with the temporal matrix, which will be utilized in the next section.

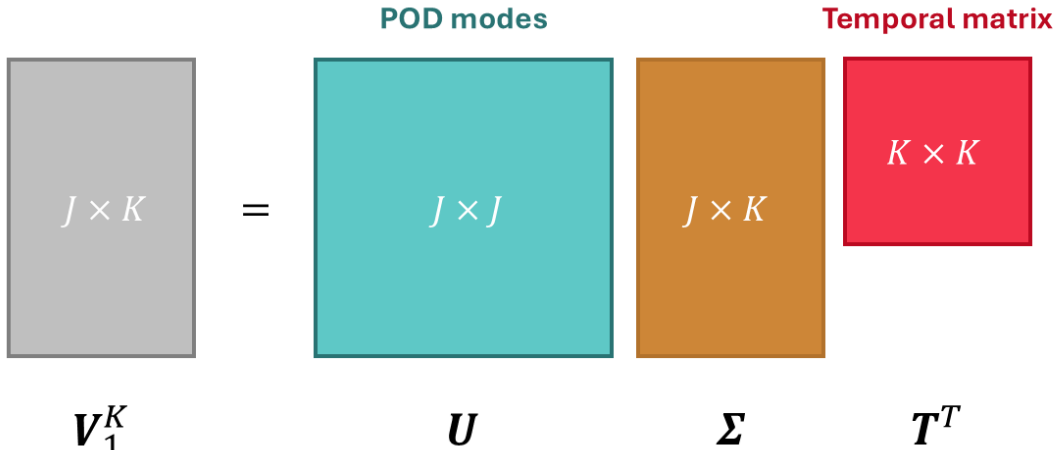


Figure 2.9: Schematic illustration of the POD modes extraction.

When analyzing the singular values obtained from the SVD algorithm, we aim to evaluate the energy contribution of each mode to the overall system dynamics. To this end, we compute the normalized modal energy decay, which assesses how much of the system's total energy is captured by each individual mode. The energy associated with the n -th mode is given by:

$$e_n = \frac{\sigma_n^2}{\sum_{n=1}^N \sigma_n^2} \cdot 100. \quad (2.9)$$

Moreover, we analyze the temporal evolution of the extracted modes to identify the dominant frequencies present in the system. Given the temporal coefficients associated with each POD mode n , namely $\mathbf{T}_n(t)$, we apply the fast fourier transform (FFT) to decompose these signals into their frequency components, f :

$$\tilde{\mathbf{T}}_n(f) = \int_{-\infty}^{\infty} \mathbf{T}_n(t) e^{-i2\pi ft} dt. \quad (2.10)$$

This transformation provides the spectral content of each POD mode, enabling the identification of the fundamental frequencies and their harmonics. The power spectral density (PSD) of each mode can then be computed as $\mathbf{P}_n(f) = |\tilde{\mathbf{T}}_n(f)|^2$, which quantifies the contribution of different frequency components to each mode. The dominant peaks in the spectra correspond to the most significant oscillatory features in the flow field.

2.3.3 Higher Order Dynamic Mode Decomposition

Dynamic Mode Decomposition (DMD) (introduced by Schmid, 2010) is a powerful tool for extracting the temporal dynamics of spatiotemporal data, decomposing it as an expansion of M DMD modes. This expansion of the snapshot matrix $\mathbf{V}_{j_1}(x, y, z, t_k)$, where $j_1 = 1, \dots, 3$ indexes the velocity components, is defined as:

$$\mathbf{V}^{(j_1)}(x, y, z, t_k) \simeq \sum_{m=1}^M a_m \mathbf{u}_m(x, y, z) e^{(\delta_m + i\omega_m)t_k} \quad \text{for } k = 1, \dots, K, \quad (2.11)$$

where $\mathbf{u}_m$ are the extracted modes, each with an associated amplitude a_m . These modes evolve according to a growth rate δ_m and oscillate at frequency ω_m , providing a modal representation of the system's dynamics.

To compute this expansion, we relate each snapshot to the preceding one using a linear operator:

$$\mathbf{V}_2^K \simeq \mathbf{R} \mathbf{V}_1^{K-1}. \quad (2.12)$$

However, fluid flow datasets are often large, making this operation computationally expensive. To mitigate this issue, an alternative methodology can be developed to reduce the computational burden (Tu, 2013). First, we apply SVD to the snapshot matrix $\mathbf{V}_1^K$, reducing the problem's dimensionality as described in the previous section. The reduced temporal matrix, defined as $\hat{\mathbf{T}}_1^K = \mathbf{\Sigma} \mathbf{T}^T$, serves as the input for the DMD algorithm. The evolution of snapshots is then modeled using the Koopman operator $\hat{\mathbf{R}}$ as:

$$\hat{\mathbf{T}}_2^K \simeq \hat{\mathbf{R}} \hat{\mathbf{T}}_1^{K-1}. \quad (2.13)$$

Higher order dynamic mode decomposition (HODMD) (Le Clainche and Vega, 2017a; Tucker et al., 1964) extends standard DMD, enhancing its robustness and accuracy, particularly for complex fluid flow problems. In this study, we employ the multi-dimensional higher order dynamic mode decomposition (mdHODMD) (Le Clainche et al., 2017), which further improves the method by preserving its tensorial formulation.

To achieve this, mdHODMD first applies high order singular value decomposition (HOSVD) (Le Clainche and Vega, 2017a) to the 5D data tensor $\mathbf{A}$, expressed as:

$$\mathbf{A}_{j_1 j_2 j_3 j_4 k} = \sum_{p_1=1}^{P_1} \sum_{p_2=1}^{P_2} \sum_{p_3=1}^{P_3} \sum_{p_4=1}^{P_4} \sum_{n=1}^N \mathbf{S}_{p_1 p_2 p_3 p_4 n} \mathbf{W}_{j_1 p_1}^{(v)} \mathbf{W}_{j_2 p_2}^{(x)} \mathbf{W}_{j_3 p_3}^{(y)} \mathbf{W}_{j_4 p_4}^{(z)} \mathbf{T}_{kn}, \quad (2.14)$$

where $\mathbf{S}_{p_1 p_2 p_3 p_4 n}$ is the core tensor, and the columns of the matrices $\mathbf{W}^{(v)}$, $\mathbf{W}^{(x)}$, $\mathbf{W}^{(y)}$, $\mathbf{W}^{(z)}$, and $\mathbf{T}$ represent the SVD modes for each tensor dimension. As in standard SVD, the number of retained modes N_r is determined based on the tunable tolerance ε_1 . The temporal matrix $\mathbf{T}$, with dimensions $N_r \times K$, is then used as input for the DMD-d algorithm, which incorporates a higher-order Koopman assumption:

$$\hat{\mathbf{T}}_{d+1}^K \simeq \hat{\mathbf{R}}_1 \hat{\mathbf{T}}_1^{K-d} + \hat{\mathbf{R}}_2 \hat{\mathbf{T}}_2^{K-d+1} + \dots + \hat{\mathbf{R}}_d \hat{\mathbf{T}}_d^{K-1}. \quad (2.15)$$

This formulation links each snapshot to d time-delayed snapshots, capturing more intricate temporal dynamics compared to standard DMD. The Koopman matrix $\hat{\mathbf{R}}$ is then computed to extract the DMD modes and obtain the expansion of them as in Eq. 2.11.

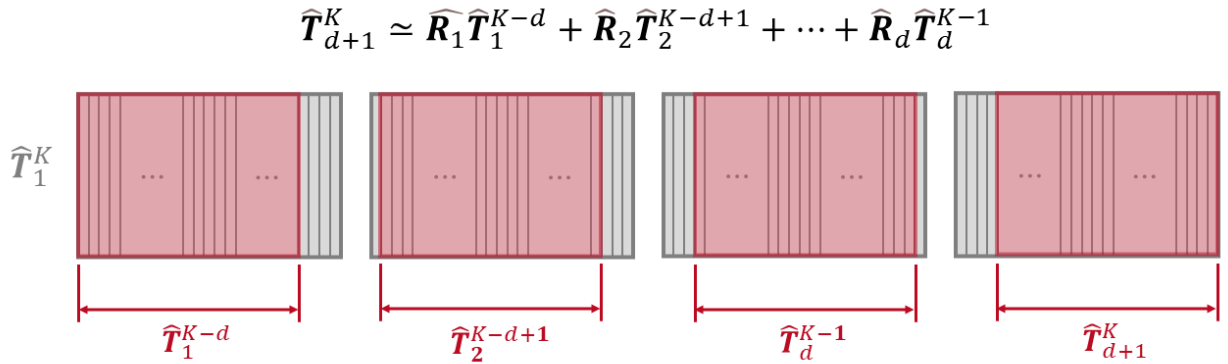


Figure 2.10: Scheme of the windowing process of the mdHODMD.

This method has been widely used to achieve a wide variety of objectives:

- Pattern analysis (Le Clainche et al., 2020, Lazpita et al., 2022, Martínez-Sánchez et al., 2023).
- Classification via feature extraction (Groun et al., 2022a, Mekhaël et al., 2024).
- Reconstruction (Corrochano et al., 2023, Pérez et al., 2020).
- Clustering (Corrochano et al., 2024).
- Flow control (Corrochano and Le Clainche, 2022).
- Prediction (Le Clainche and Ferrer, 2018, Jones and Utyuzhnikov, 2024).

2.3.4 Reduced Order Model based on HODMD

Once the data is decomposed into DMD modes, future-state predictions are obtained by evaluating Eq. (2.11) at time instants beyond the training window $t > t_K$. Specifically, the model is constructed using data within the interval $t \in [0, pT]$, where T is the period of the cardiac cycle and p is the number of cycles employed for training. The resulting reduced-order model is then used to predict the flow dynamics in a later interval, namely $t \in [10T, 20T]$, allowing us to assess the long-term predictive capabilities of the method.

The way modes are selected plays a crucial role in ensuring prediction accuracy and stability in the model. Depending on the calibration of the algorithm, spurious modes unrelated to the underlying physics may be captured, typically associated with noise or numerical artifacts. As a result, using all computed M DMD modes can degrade the quality of the extrapolated prediction. To address this difficulty, we adopt a filtering strategy in which only those modes with growth rate lower than a certain threshold are deemed physically relevant and retained for prediction. This threshold is set with a tunable growth rate value δ_{tune} . Almost all of the selected modes correspond to frequencies associated with the dominant dynamics of the system.

Furthermore, when working with transient simulation data, certain modes, although physically relevant, may exhibit highly negative growth rates, leading to their rapid attenuation over time. This offers the potential to enhance the temporal stability of the model predictions, we also construct an alternative formulation in which we enforce $\delta_m = 0$, thereby eliminating exponential decay. This modification prevents excessive damping of key flow structures and enables more reliable long-term forecasts of the intraventricular dynamics.

To assess the accuracy of the ROM, we analyze the absolute error distribution over the entire dataset by computing the histogram of the normalized absolute error, defined as:

$$E(\%) = \frac{|\mathbf{v} - \mathbf{v}_{pred}|}{\max |\mathbf{v} - \mathbf{v}_{pred}|} \cdot 100, \quad (2.16)$$

where $\mathbf{v}$ denotes the reference simulation data and $\mathbf{v}_{pred}$ is the reconstructed prediction. The normalization factor corresponds to the maximum absolute error computed independently for each velocity component, considering all spatial locations and time steps in the domain.

The number of bins in the histogram is determined using Sturges's formula, applied to the spatial grid:

$$N_{bins} = 1 + \log_2(N_{grid}), \quad (2.17)$$

where $N_{grid} = N_x \times N_y \times N_z$ represents the total number of spatial points. In our case, this results in approximately 20 bins, allowing for an intuitive interpretation: the first bin represents the relative frequency of errors within range 0–5%, the second within 5–10%, and so forth.

A key advantage of the ROM is its drastic reduction in computational cost. In this study, this increase in computational efficiency is quantified using the speed-up factor (SUF), defined as:

$$SUF = \frac{t_{CFD} \times N_{CPU}}{t_{ROM}} \quad (2.18)$$

where t_{CFD} is the runtime of the full-order CFD simulation, N_{CPU} is the number of processors used, and t_{ROM} is the time required for the ROM prediction.

Chapter 3

CFD simulations of left ventricles

Having introduced the computational tools and methodologies used and developed in this thesis, we now present the results of the CFD simulations performed to analyze intraventricular blood flow. Specifically, we have simulated the flow inside the two different idealized LV models introduced previously.

By accurately resolving the formation and breakdown of the main VR, we can gain insight into the efficiency of LV filling and potential deviations linked to pathological conditions.

In this work, the temporal evolution of the flow is described using the dimensionless time variable $t^* = t/T$, where T represents the duration of a full cardiac cycle. A constant heart rate of 60 beats per minute is assumed, corresponding to $T = 1$ s. For the **Ideal 1** geometry, the simulated cardiac cycle is split into a diastolic phase spanning $t^* \in [0, 0.67]$, and a systolic phase occupying $t^* \in [0.67, 1]$. Meanwhile, the **Ideal 2** case exhibits an extended diastole over $t^* \in [0, 0.8]$, followed by a comparatively brief systolic interval from $t^* = 0.8$ to $t^* = 1$.

3.1 Validation

This section validates the CFD simulations described in Sec. 2.2 by analyzing mesh convergence, comparing results between solvers, and benchmarking against existing literature.

Mesh convergence is assessed using the relative root mean square error (RRMSE), calculated with respect to the finest mesh solution:

$$RRMSE = \frac{\|\mathbf{L} - \mathbf{L}_{\text{true}}\|}{\|\mathbf{L}_{\text{true}}\|} \cdot 100, \quad (3.1)$$

where $\mathbf{L}_{\text{true}}$ is the solution from the finest mesh and $\mathbf{L}$ the corresponding value from a coarser resolution.

Additionally, the total kinetic energy (TKE) is used as a key metric to evaluate the dynamic behavior of the flow. It represents the integrated kinetic content of the velocity field at each non-dimensional time t^* and is defined as:

$$\text{TKE}(t^*) = \int_{V(t^*)} \frac{1}{2} \rho \mathbf{v}^2 dV, \quad (3.2)$$

where $V(t^*)$ is the ventricular volume at time t^* , ρ is the fluid density, and $\mathbf{v}$ the velocity vector. This quantity provides a global measure of flow intensity and energy throughout the cardiac cycle.

3.1.1 Ideal 1: Geometry based on a semi-ellipsoid.

We begin the analysis with the **Ideal 1** configuration, a simplified LV geometry modeled as a semi-ellipsoid. This benchmark case is used to verify the consistency and robustness of the CFD approach developed throughout this thesis. Particular attention is given to the formation and evolution of the intraventricular vortex ring, which is widely recognized as a marker of filling efficiency.

To ensure numerical reliability, simulations were performed using two commercial solvers: Ansys Fluent and Simcenter STAR-CCM+. This comparison aimed to quantify the sensitivity of the results to differences in numerical implementation, meshing tools, and boundary handling.

Initially, identical geometry and BCs were employed, including a time-varying velocity profile at the inlet and a mass flow rate at the outlet, hereafter referred to as BC1. The wall motion was prescribed using the synthetic deformation model detailed in Section 2.2.4.

Despite maintaining consistent input data, variations appeared due to each solver's specific meshing algorithm and treatment of dynamic meshes. To evaluate the influence of mesh resolution, three levels of refinement were tested in both solvers: coarse (~ 0.3 million elements), medium (~ 1 million elements), and fine (~ 1.6 million for Fluent, ~ 1.2 million for STAR-CCM+).

The primary metric for validation was the TKE within the LV cavity, excluding the inlet and outlet regions. Figure 3.1 shows the TKE evolution over a cardiac cycle, averaged across four cycles. The results demonstrate consistent trends between solvers and across mesh levels, with minor differences in peak magnitude.

To evaluate the consistency of the selected BCs, an additional configuration with pressure boundaries (without imposed profiles) was also tested, which will be denoted as BC2 in the following. Comparing the results of this setup with the constrained boundaries, we can see that the matching during systole is quite perfect. However, for the peak velocity in diastole phase corresponding to the E-wave, the pressure BC implementation captures higher velocities.

Table 3.1 presents the RRMSE values obtained from mesh convergence studies and solver comparisons. A clear reduction in error is observed as the mesh is refined, with the medium meshes already showing a significant improvement over the coarse ones. For both STAR-CCM+ and Fluent under BC1, the RRMSE drops from approximately 6 to below 2 when moving from coarse to medium mesh, indicating satisfactory mesh convergence. Comparing the most converged configurations, the RRMSE between STAR-CCM+ and Fluent is lower than

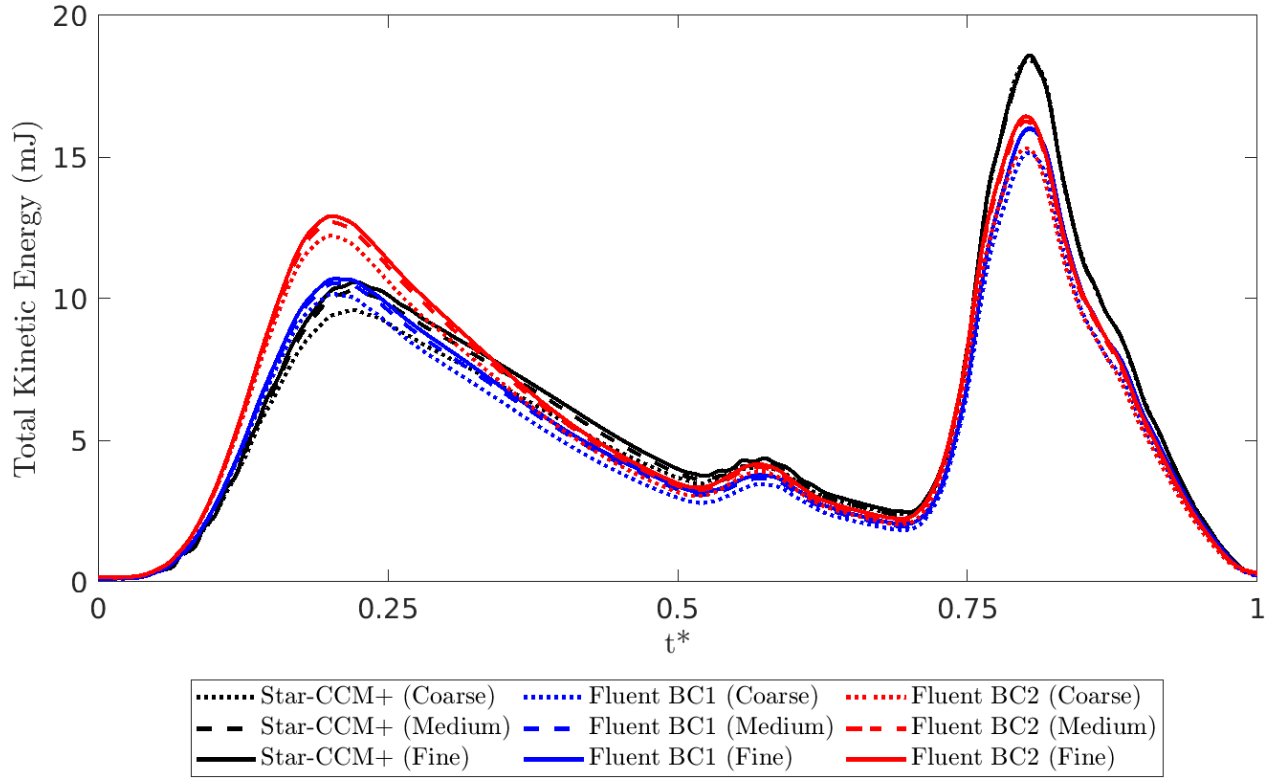


Figure 3.1: Comparison of the total kinetic energy evolution over a heart cycle, averaged across four cycles, for STAR-CCM+ (black), Fluent with constrained BC (blue) and Fluent with pressure BC (red) using different mesh resolutions.

Configuration	RRMSE (%)		
	Coarse	Medium	Fine
Star-CCM+ (BC1)	6.00	1.95	–
Fluent (BC1)	5.80	1.65	–
Fluent (BC2)	6.05	1.75	–
Star-CCM+ vs Fluent	7.95	5.90	5.80
BC1 vs BC2	8.25	7.90	7.80

Table 3.1: RRMSE comparison for different solver configurations. BC1: Constrained; BC2: Pressure.

6%, confirming consistency across solvers. Additionally, Fluent simulations under different boundary conditions (BC1 and BC2) shows notably higher discrepancies. Still, the RRMSE values are consistent and lower than 8%, supporting the robustness of the boundary setup.

This validation exercise confirms the robustness of the simulation framework across different grid resolutions, numerical solvers and boundary conditions. The good agreement between the high-resolution cases suggests that the main intraventricular flow features, such as the generation and development of the vortex ring, are reliably captured with the adopted modeling strategy.

3.1.2 Ideal 2: Geometry based on experimental setup.

The second idealized configuration, **Ideal 2**, is adapted from the model presented by Vedula et al., 2014. This case has been extensively studied in the literature and serves here as a reference for validating our numerical methodology. Unlike **Ideal 1**, wall motion is directly extracted from experimental imaging data, as detailed in Sec. 2.1.2, removing the need for synthetic deformation models.

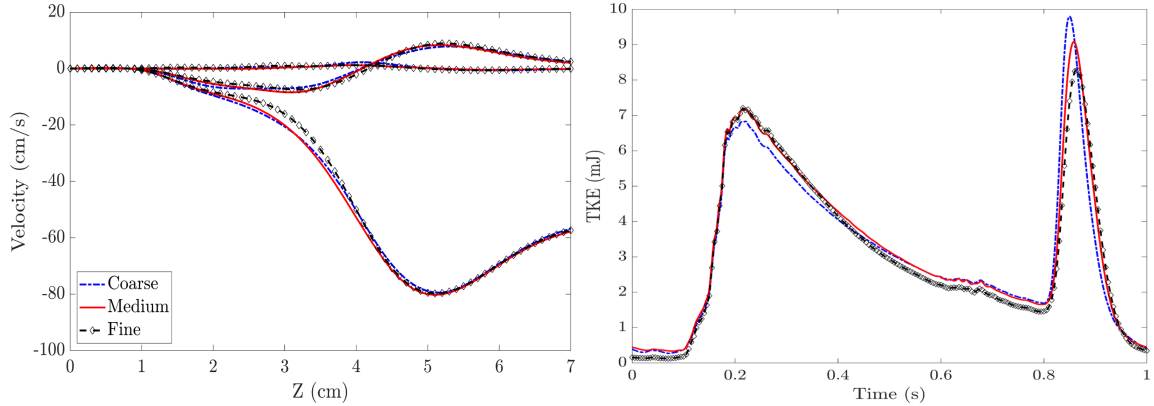


Figure 3.2: Mesh convergence results for **Ideal 2**: (left) velocity along the mitral orifice centerline at $t^* = 0.22$; (right) TKE evolution during one cardiac cycle.

Mesh	Elements	$RRMSE(v_x)$	$RRMSE(v_y)$	$RRMSE(v_z)$	$RRMSE(TKE)$
Coarse	0.6M	32.75%	5.65%	0.85%	27.65%
Medium	1.1M	24.70%	4.40%	0.25%	3.50%

Table 3.2: RRMSE values of the medium and coarse meshes relative to the fine mesh for the **Ideal 2** case.

To reproduce the original setup as closely as possible, pressure-based boundary conditions are imposed at the inlet and outlet. Valve dynamics are approximated by converting these boundaries into rigid walls at the corresponding closing times.

Mesh size	Estimated Average Mesh Density [$\times 10^{-4}$ mL/ele]m]		
	Vedula et al., 2014	Current Study (ESV)	Current Study (EDV)
Coarse	3.05	2.65	3.65
Medium	1.30	1.35	1.90
Fine	0.20	0.80	1.10

Table 3.3: Estimated mesh densities in our simulations and in Vedula et al., 2014, reported at end-systolic volume (ESV) and end-diastolic volume (EDV).

To assess mesh independence, simulations were performed with coarse (~ 0.6 million elements), medium (~ 1.1 million elements), and fine (~ 1.8 million elements) grids. Figure 3.2 displays the axial velocity profile at $t^* = 0.22$ and the TKE over the cardiac cycle. The coarse mesh underestimates key features, especially during systole. In contrast, medium and fine meshes yield similar results.

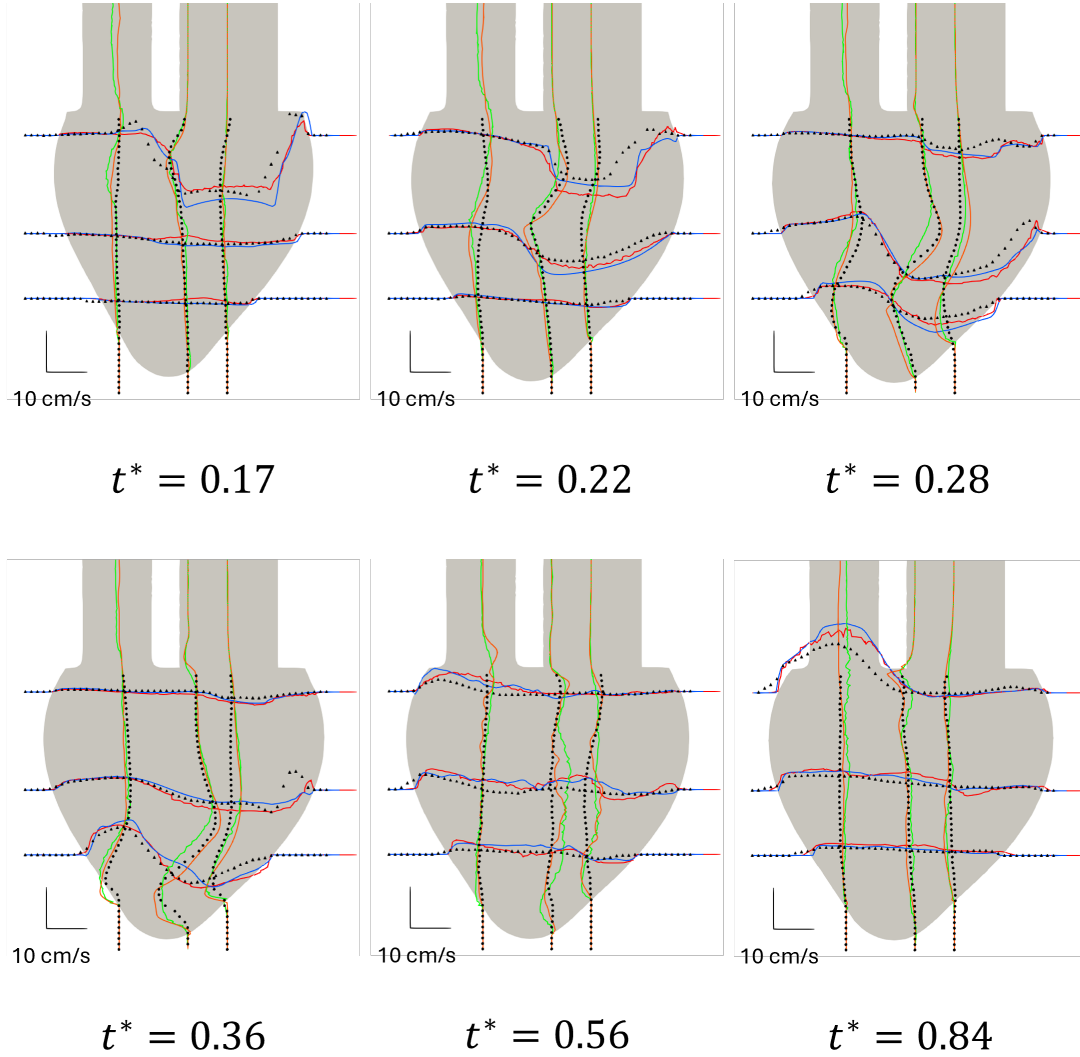


Figure 3.3: Velocity profiles along six lines in the A–A' plane at several time instants, compared with Fig. 6 from Vedula et al., 2014. Reference experiments: v_z (—▲—), v_x (—●—); Reference simulations: v_z (—), v_x (—); Present study: v_z (—), v_x (—).

Table 3.2 summarizes the errors of each configuration using again Eq. 3.1. The medium mesh achieves RRMSE values below 5% across all relevant quantities, offering a suitable balance between resolution and computational cost.

A direct comparison with the mesh strategy in Vedula et al., 2014, is not straightforward. Their model embeds the LV in a Cartesian mesh, whereas in our case, the cavity defines the control volume. To establish a consistent reference, we define the estimated average mesh density ψ as the volume of the ventricle (in mL) divided by the number of elements.

In our case, the ventricular volume varies with time due to wall motion, so mesh density is reported at ESV and EDV. As shown in Table 3.3, values at ESV are comparable to those in the reference. At EDV, the mesh appears coarser due to the increased volume, particularly in the fine mesh. The finest mesh in Vedula et al., 2014, comprises over 33 million elements,

yielding $\psi = 0.20 \times 10^{-4}$ mL/elem. In contrast, our fine mesh results in $\psi = 0.80 \times 10^{-4}$ at ESV and 1.10×10^{-4} at EDV. Overall, the meshes employed are of comparable resolution.

Despite the mesh resolution differences, our simulations show excellent agreement with both the experimental and numerical results from Vedula et al., 2014 - Fig.6. Figure 3.3 compares velocity profiles across six lines in the A-A' symmetry plane at selected time points. Early in the cycle, strong inflow creates vertically aligned profiles. As the vortex ring forms and tilts, the flow structure becomes more complex, particularly around $t^* = 0.22$. During systole, the profiles realign vertically due to ventricular contraction. The agreement across datasets confirms the robustness of the computational setup and the adequacy of the selected mesh resolution.

3.2 Intraventricular flow dynamics

Before presenting the numerical results, we first discuss the fundamental dynamics of the vortex ring. The formation and evolution of intraventricular VR has been extensively investigated through both experiments and simulations (Le et al., 2012; Töger et al., 2012). These structures play a crucial role in enhancing diastolic filling efficiency by reducing energy loss and supporting effective blood transport within the LV. A schematic overview of this process is shown in Fig. 3.4.

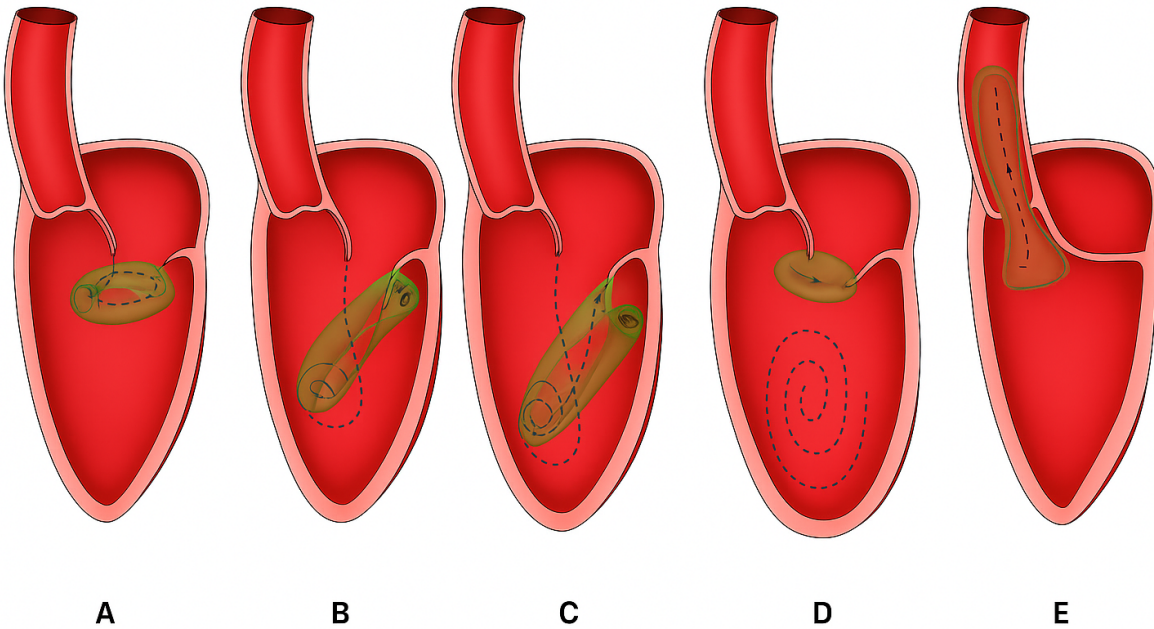


Figure 3.4: Qualitative schematic of vortex ring dynamics during the cardiac cycle: (A) early diastole, (B) peak E-wave velocity, (C) velocity deceleration, (D) A-wave inflow, and (E) systolic ejection.

At the beginning of diastole (A), the mitral valve opens and initiates blood inflow into the LV. This inflow reaches a peak velocity during the E-wave phase (B), which triggers the formation of a circular vortex ring near the mitral annulus. The ring then propagates toward the apex.

As it advances, the interaction with the ventricular walls alters its shape, gradually stretching it into an elliptical form.

Later in diastole (C), the primary ring comes into proximity with the surrounding walls, which leads to the development of secondary vortex structures that wrap around it. These interactions destabilize the vortex core, contributing to the eventual disintegration of the main ring into smaller vortical elements.

A secondary vortex ring forms during the A-wave (D), generated by a second, weaker mitral inflow. This secondary structure carries less energy due to the reduced flow rate and volume, and consequently, its propagation is more limited.

Finally, during systole (E), ventricular contraction increases the internal pressure, opening the aortic valve and pushing blood into the systemic circulation. This completes the cardiac cycle with a strong outflow phase.

In this work, the described vortex mechanisms are examined in detail for two LV geometries. Analyzing the formation, development, and decay of the main vortex ring is essential for understanding intraventricular flow and evaluating ventricular performance. Alterations in these dynamics may reflect compromised cardiac function.

For the following analysis, to visualize the vorticity field we will make use of the **Q -criterion**, a scalar quantity that enables the identification of vortical structures by comparing the relative magnitude of rotation to strain in the velocity gradient tensor. It is defined as:

$$Q = \frac{1}{2} \left(\|\boldsymbol{\Omega}\|^2 - \|\mathbf{S}\|^2 \right), \quad (3.3)$$

where $\mathbf{S} = \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top \right)$ is the symmetric part of the velocity gradient tensor (*i.e.* strain rate tensor), and $\boldsymbol{\Omega} = \frac{1}{2} \left(\nabla \mathbf{u} - (\nabla \mathbf{u})^\top \right)$ is the antisymmetric part (vorticity tensor). Positive values of Q indicate regions where the rotational effects dominate over the strain, making it a valuable tool to visualize coherent vortex structures, such as the vortex ring.

3.2.1 Ideal 1: Geometry based on a semi-ellipsoid.

Figure 3.5 represents the Q -Criterion isosurfaces at a threshold of 1000 for the **Ideal 1** geometry. Each panel captures a distinct phase of the cardiac cycle. At $t^* = 0.15$, during early diastole, the vortex ring begins to form at the mitral orifice as blood enters the ventricle. Initially, the ring is nearly circular. As it travels toward the apex, the ring encounters the ventricular wall and experiences a decrease in inflow velocity. By $t^* = 0.20$, these effects induce tilting and distortion into an elliptical shape. At $t^* = 0.25$, secondary vortex filaments begin to appear, generated by interactions with the ventricular boundaries. These structures continue to grow and encircle the main ring, which becomes increasingly unstable. By $t^* = 0.40$, the vortex is destabilized, and at $t^* = 0.60$, it has fully dissipated. At this point, a secondary ring forms due to the weaker A-wave inflow. During late systole ($t^* = 0.80$), the ventricle contracts, leading to a strong aortic outflow. Both solvers produce similar vortex dynamics and show close agreement with the reference results in Zheng et al., 2012.

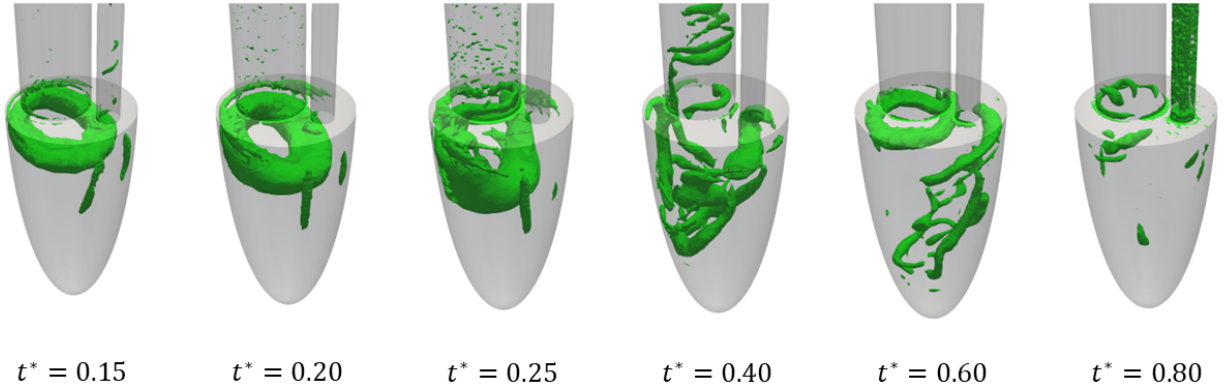


Figure 3.5: Three-dimensional representation of the Q-Criterion isosurfaces within the left ventricle across six time instants.

To further assess the flow structures, we examine two-dimensional contours of plane-normal vorticity. Figure 3.6 (bottom) shows the component ω_y in the symmetry plane (A-A'), where the ring's asymmetry and tilt are evident during the early stages. Later instants display residual recirculation patterns and the emergence of the A-wave-induced vortex. Additionally, Figure 3.6 (bottom) presents ω_x contours in the B-B' plane along the inlet axis. These visualizations confirm the ring's initial symmetry and track its deformation and eventual dissipation.

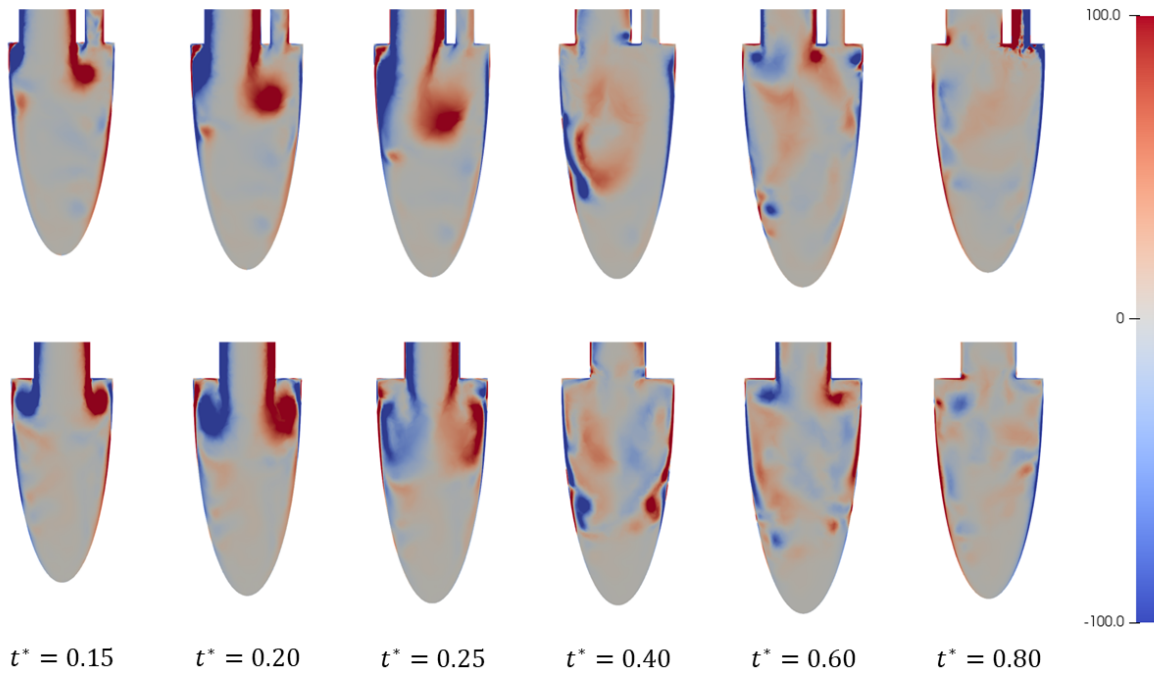


Figure 3.6: Plane-normal vorticity contours for the *Ideal 1* model. Top: ω_x in the A-A' plane. Bottom: ω_y in the cross-sectional B-B' plane.

In this simplified geometry, the narrow ventricular chamber enhances wall influence on the vortex ring. The structure impinges early during diastole, promoting rapid tilting and instability development. Consequently, the primary ring dissipates before reaching the apex, and residual flow structures are comparatively weak. The secondary ring, generated during the A-wave, undergoes slower breakdown due to reduced interaction with remnants of the earlier vortex.

3.2.2 Ideal 2: Geometry based on experimental setup.

As with *Ideal 1*, the intraventricular flow structures are analyzed using Q-Criterion isosurfaces and plane-normal vorticity contours. Figure 3.7 shows the time evolution of the vortex ring using a Q-Criterion threshold of 2000.

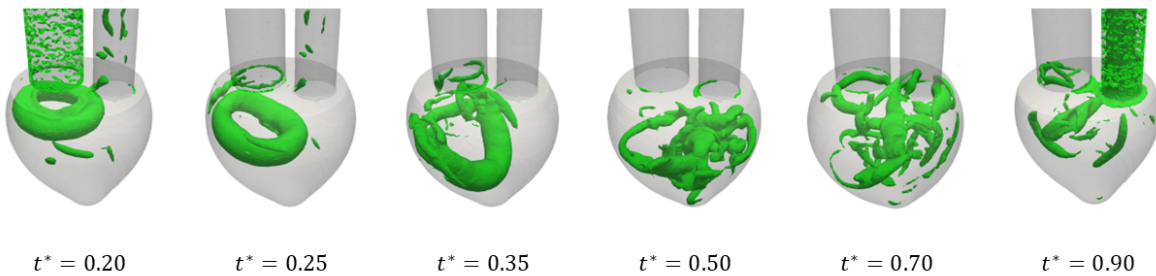


Figure 3.7: Counterpart of Fig. 3.5 for the *Ideal 2* model.

At $t^* = 0.20$, the vortex ring forms near the mitral orifice during the early E-wave. The ring initially exhibits a circular shape, but asymmetry quickly develops due to the proximity of one side to the ventricular wall. This asymmetry induces differential advection, causing the structure to elongate. As the ring progresses toward the apex, secondary trailing vortices appear along the wall by $t^* = 0.35$, contributing to the destabilization and dissipation of the primary ring. A second, weaker vortex ring is generated during the A-wave but dissipates rapidly due to limited energy and interaction with residual flow structures. By $t^* = 0.80$, the ventricle begins systolic contraction, opening the aortic valve and initiating the ejection phase.

Further insight into flow development is obtained from the plane-normal vorticity contours in Figure 3.8. The top row displays ω_x contours in the Y-Z symmetry plane. The ring forms symmetrically but undergoes tilting and stretching as it travels through the cavity. The bottom row shows X-Z cross-sections through the inlet axis, highlighting the preservation of symmetry along the transverse direction.

The observed vortex dynamics are consistent with both experimental and numerical findings reported in Vedula et al., 2014, particularly, Figures 5, 7, and 8 of that study. This agreement further confirms the accuracy and reliability of the present computational model in capturing physiologically relevant intraventricular flow features.

In contrast to the narrower cavity of *Ideal 1* (Sec. 3.2.1), the wider chamber in *Ideal 2* reduces the intensity of vortex-wall interactions. As a result, the primary vortex ring propagates further and reaches the apex before breaking down. However, this delayed

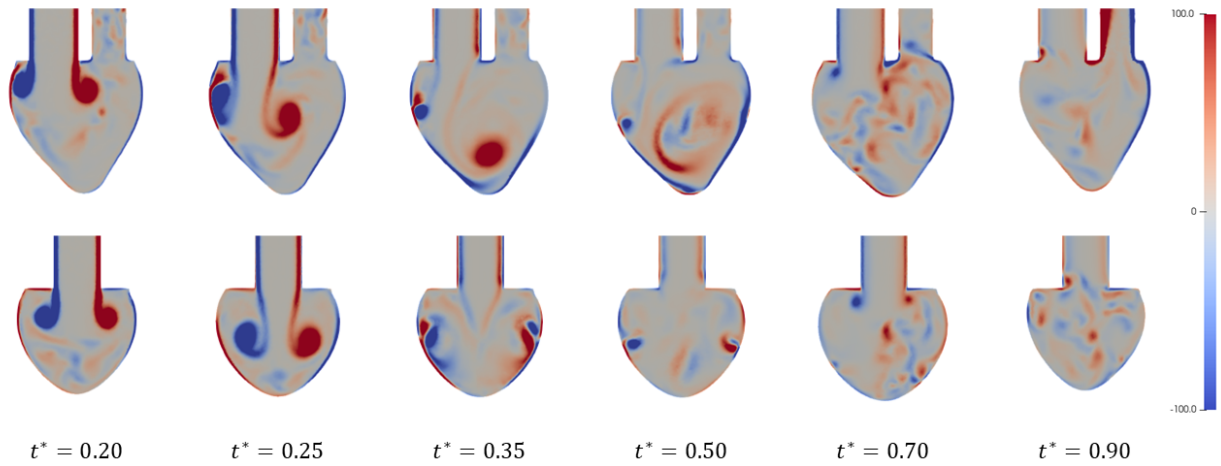


Figure 3.8: Counterpart of Fig. 3.6 for the `Ideal 2` model.

dissipation enhances the interaction between the primary and secondary rings, causing the latter—formed during the A-wave—to dissipate more rapidly due to its collision with stronger residual structures.

Chapter 4

Characterization of LV main features

In this study, we apply these modal decomposition techniques to analyze the underlying physics of the LV simulation datasets. We begin by presenting results for the **Ideal 1** case, which exhibits more complex dynamics and a faster vortex breakdown process. In contrast, the **Ideal 2** model features clearer flow dynamics, allowing for an alternative analysis of vortex breakdown.

The analysis of both simulations has been performed on the velocity field. For each case, a spatiotemporal database was extracted using the most converged part of the simulation, corresponding to cycles 10 through 20. The data were interpolated onto a structured spatial grid of dimensions $64 \times 64 \times 128$, with 20 snapshots acquired per cardiac cycle at temporal intervals of $\Delta t = 0.05$.

4.1 Ideal 1: Geometry based on a semi-ellipsoid.

As outlined earlier, both POD and HODMD are applied to extract characteristic modes that capture key features of the vortex ring inside the left ventricle.

The POD decomposition produces a set of orthogonal modes sorted by energy. The normalized singular value spectrum, shown in Fig. 4.1, exhibits a steep decline, with the first 15 modes retaining most of the relevant flow features. Notably, the first 10 modes ($\sum_{n=1}^{10} e_n$) account for 99% of the total kinetic energy, as defined in Eq. 2.9.

Despite the periodic nature of the simulation, the singular values do not appear in energy-balanced pairs, which is commonly observed in strictly periodic systems (Begiashvili et al., 2023). This deviation indicates a higher level of complexity in the flow evolution, a point that will be reinforced by subsequent analysis.

Given that the simulation period is defined as $T = 2\pi/f$, the main intraventricular flow phenomena unfold at the fundamental frequency $f = 2\pi$: the generation of the primary vortex ring, its subsequent tilting and dissipation, the emergence of secondary vortices, and the final ejection phase. However, the cardiac cycle also includes two distinct inflow events, the E-wave and A-wave, which occur roughly every $T/2$. This leads to the emergence of an additional

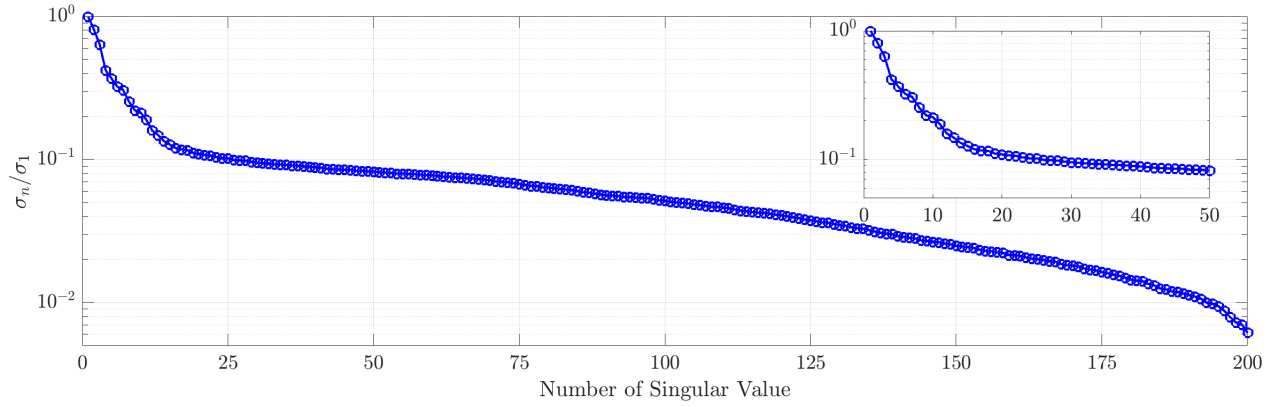


Figure 4.1: Normalized singular value decay for the **Ideal 1** dataset.

characteristic frequency, $f = 4\pi$, associated with the double-pulsed inflow pattern.

Figure 4.2 shows the FFT spectra of the temporal coefficient matrix $\mathbf{T}(t)$ for the six most energetic POD modes. Clear spectral peaks appear at 2π and its harmonics (4π , 6π , etc.), consistent with the periodic forcing of the system. The dominant peak at 2π reflects the overall cardiac rhythm, while the secondary peak at 4π is attributed to the dual inflow structure of the cycle, specifically linked to the E- and A-wave phases.

The spectral content of individual modes reveals distinct patterns. The first mode (Fig. 4.2 (a)), which carries the highest energy, shows a dominant peak at the fundamental frequency 2π , accompanied by a secondary peak at 4π and a smaller contribution at 6π . This suggests that the mode primarily captures the main vortex ring dynamics, while also reflecting double-pulsing effects and mild nonlinear interactions.

The first mode (Fig. 4.2 (b)) displays a similar spectrum, though the 2π component is less prominent. In this case, the peak at 4π becomes dominant, with a residual contribution from 6π , indicating stronger sensitivity to the dual inflow pattern.

The third mode is mostly governed by the 4π frequency but still contains moderate energy at 2π and weaker peaks at higher harmonics such as 6π , 8π , and 10π .

Modes with lower energy are dominated by higher-frequency content and exhibit broader spectral distributions, highlighting nonlinear couplings and interactions among multiple harmonics.

Figure 4.3 shows the normalized spatial distribution (scaled between -1 and 1) of the nine most energetic POD modes for the **Ideal 1** case. The top row corresponds to the v_x velocity component on the X-Z symmetry plane (A-A'), and the bottom row to the v_y component on the Y-Z inlet plane (B-B').

Mode 1 presents a coherent structure aligned with the primary vortex ring, consistent with the dominant 2π frequency identified in the spectral analysis. Mode 3, mainly associated with the 4π frequency, shows the emergence of a secondary vortex near the inlet and a decaying ring toward the apex. Mode 2 reflects a combination of both features, with energy contributions from the fundamental and secondary frequencies.

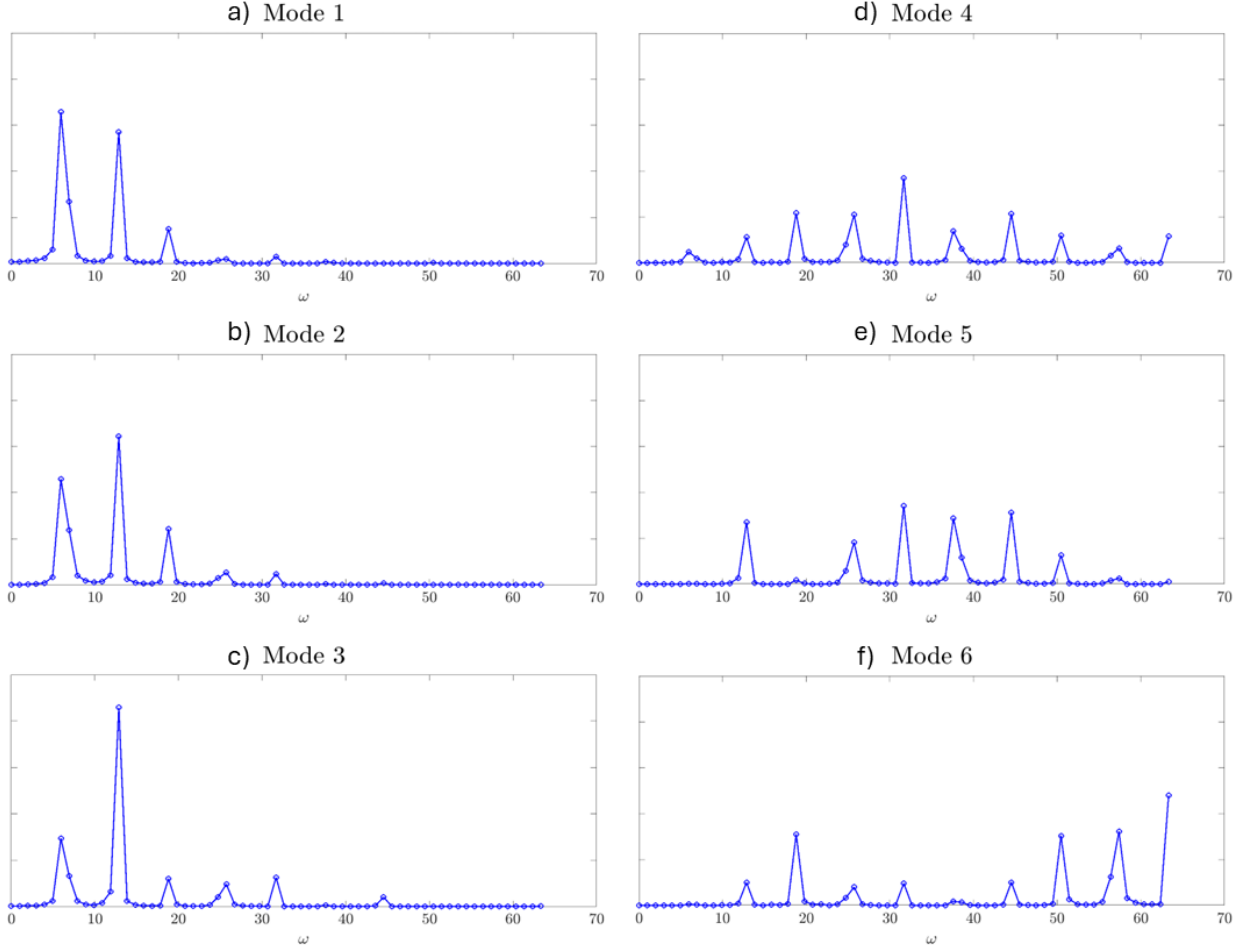


Figure 4.2: Normalized FFT spectra of the first six most energetic modes for the *Ideal 1* dataset.

Higher-order modes, carrying less energy, reveal finer structures linked to nonlinear dynamics and energy transfer. These effects are particularly visible in the B-B' plane, where an evident reduction in the size of spatial features correlates with the increasing presence of high-frequency components.

The three-dimensional Q-criterion isocontours presented in Fig. 4.4 reinforce the previous observations. Mode 1 (panel a) shows a strong recirculation pattern surrounding the main vortex ring, particularly highlighting the initial tilting phase. In Mode 2 (panel b), the shift in dominant frequency is evident. The corresponding isosurface reveals both the formation of the ring near the inlet and its propagation along the ventricle.

As discussed earlier, Mode 3 is strongly influenced by the 4π frequency. This is reflected in its Q-criterion structure, which captures coherent vortical patterns near both the inlet and distal regions, with extensions reaching toward the apex. The visualized motion indicates that the vortex ring advances through the geometry before dissipating. These dynamics underscore the role of higher harmonics, as vortex breakdown arises from nonlinear interactions between multiple frequency components and other flow instabilities.

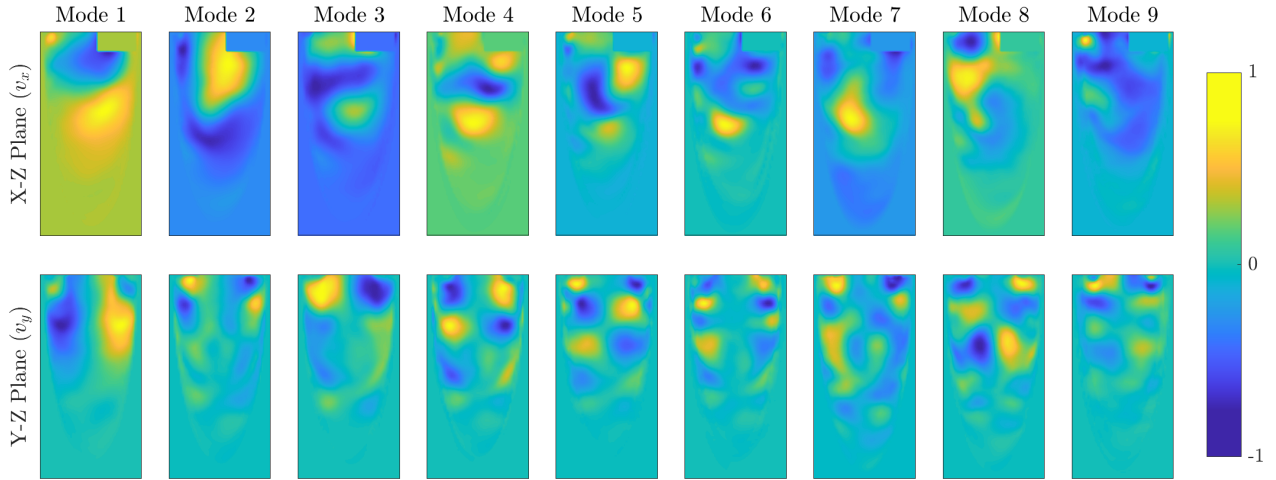


Figure 4.3: Normalized two-dimensional contours of the nine most energetic POD modes for the **Ideal 1** model: (top) v_x component in the A-A' plane; (bottom) v_y component in the B-B' transversal plane.

Finally, Modes 4 to 6 (Fig. 4.4d–f) capture the progressive disintegration of the primary vortex and the initial dissipation of secondary structures. These modes, although lower in energy, exhibit higher harmonic content and smaller-scale features. They provide important insight into the mechanisms driving vortex fragmentation and the energy cascade associated with flow unsteadiness.

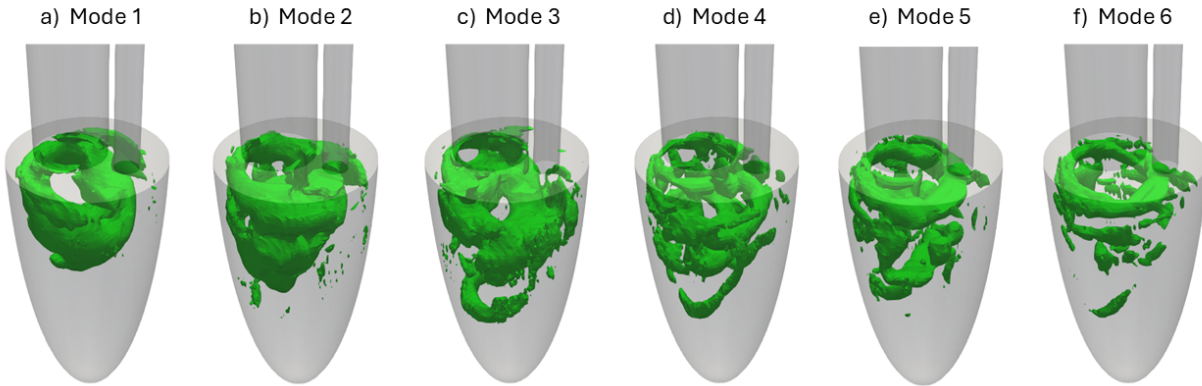


Figure 4.4: Three-dimensional isocontours of the normalized POD modes showing the Q-criterion for the first six most energetic modes of the **Ideal 1** model.

As discussed above, the dataset presents a rich spectral structure. While the POD and FFT analyses provide a first insight into its dominant frequencies, further refinement is achieved through the application of HODMD (see Sec. 2.3.3). This method decomposes the flow field into modes associated with specific temporal frequencies, offering improved spectral resolution.

Figure 4.5 shows the amplitude spectra of the HODMD modes as a function of frequency, computed under various algorithm configurations defined by the tolerance parameter ε and the window size d . The exploration of the d - ε parameter space follows the methodology

described in Le Clainche and Vega, 2017a.

Since HODMD aims to minimize reconstruction error, following the DMD expansion in Eq. 2.11, it may capture DMD modes related to either small scale or noise during the fitting process. To ensure the physical relevance of the extracted modes, a calibration procedure is conducted. This involves systematically testing multiple combinations of d and ε through a trial-and-error approach. Across all tested configurations, modes associated with the fundamental frequency and its harmonics consistently appear as high-amplitude groups, confirming their physical significance. In contrast, the remaining modes, associated with numerical noise or non-physical artifacts, are characterized by low amplitudes and exhibit inconsistent frequency or amplitude across different calibration cases, or may not appear at all.

Importantly, the amplitudes of the modes at 2π and 4π are found to be of similar magnitude. This observation reinforces the significance of the double-pulsed inflow behavior, linked to the E- and A-wave phases, and suggests it plays a role as important as the overall periodicity of the cardiac cycle. Higher harmonics, as expected, display a gradual decay in amplitude, consistent with their association to finer-scale, less energetic features in the flow.

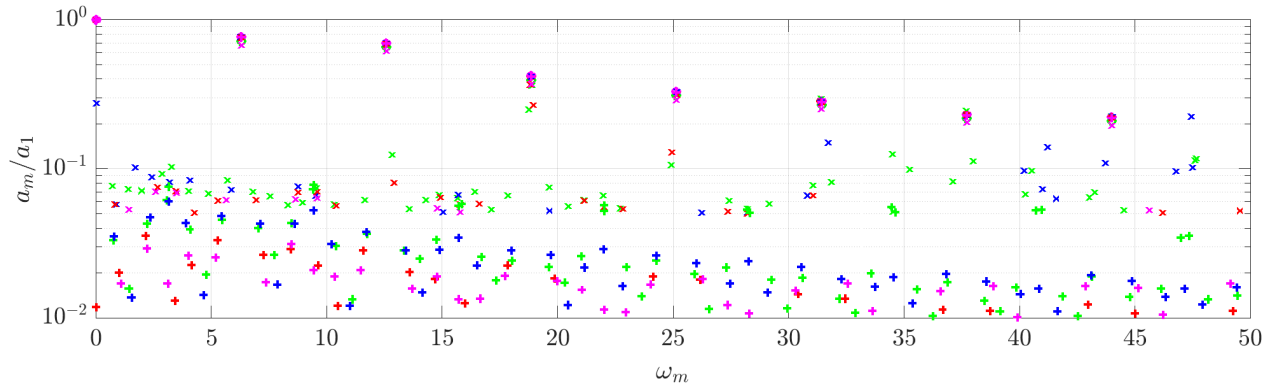


Figure 4.5: Amplitude against frequency spectrum of the DMD modes for the `Ideal 1` database and different calibrations of d and ε .

To examine the spatial structure of the DMD modes, we present two-dimensional visualizations of their real and imaginary parts. Figure 4.6 displays the real part of the mean flow, the dominant DMD mode, and its main harmonics for the `Ideal 1` dataset. The top row corresponds to the v_x component on the A-A' (X-Z symmetry) plane, while the bottom row shows the v_y component on the B-B' (Y-Z inlet) plane.

As DMD modes are intrinsically linked to specific frequencies, the dominant mode reveals the characteristic recirculating motion of the main vortex ring during early diastole. The 4π harmonic, associated with the double-pulsed inflow, captures the formation of a secondary ring. This structure becomes even more prominent at the 8π frequency, a higher harmonic of the same mechanism.

Higher-frequency modes expose finer-scale features, particularly concentrated near the vortex breakdown region. These structures are especially visible in the Y-Z plane, where the fragmentation of coherent flow and the onset of the energy cascade are most pronounced.

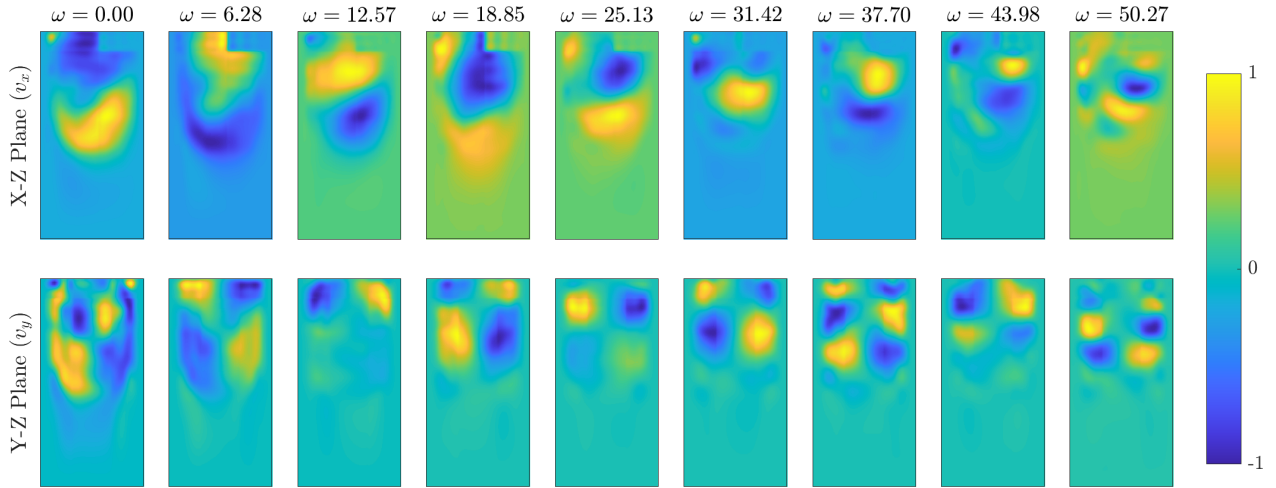


Figure 4.6: Real part of the DMD modes for the *Ideal 1* model: (top) v_x component in the X-Z symmetry plane; (bottom) v_y component in the Y-Z inlet plane. The figure includes the mean flow, the dominant mode, and its main harmonics.

Figure 4.7 shows the imaginary parts of the same DMD modes, providing additional insight into their phase dynamics. When examined alongside their real counterparts, these visualizations reveal the temporal evolution of the coherent structures.

In the dominant mode, for instance, the vortex ring located near the inlet in the real part is observed to shift downstream in the imaginary component, illustrating its progression. A similar behavior appears in the 8π mode: a vortex structure advances toward the apex while a new one begins to form near the inlet. This behavior further confirms the connection between this mode and the double-pulsed inflow pattern.

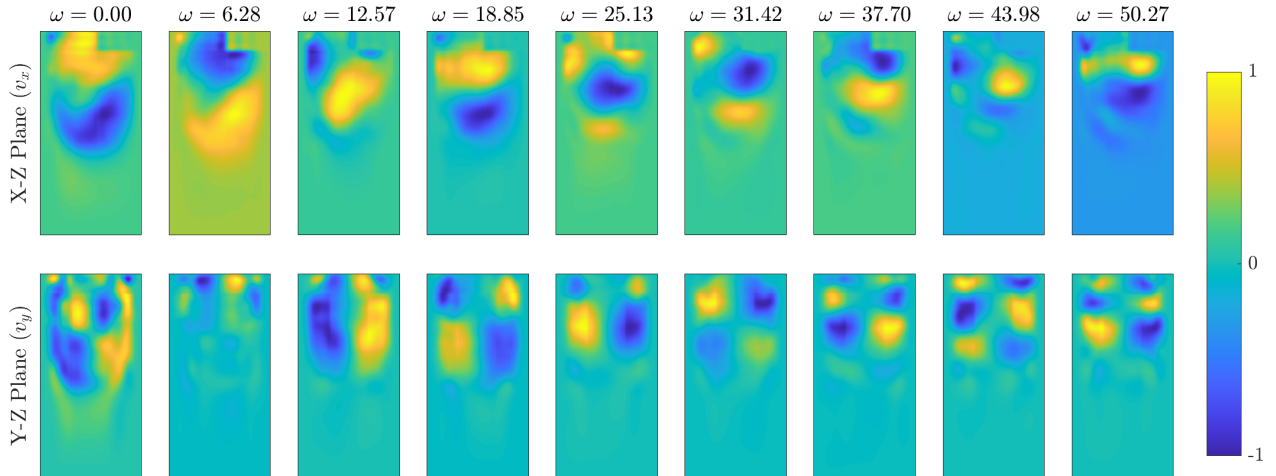


Figure 4.7: Counterpart of Fig. 4.6 for the imaginary part.

To complement the 2D analysis, Fig. 4.8 presents three-dimensional Q-criterion isocontours of the real and imaginary parts of the dominant DMD mode and its first three harmonics. The mode at $\omega = 2\pi$ captures the evolution of a single vortex ring throughout the cardiac

cycle. At $\omega = 4\pi$, a second ring appears, interacting with the primary one. This interaction is evident from the phase shift between the real and imaginary components, reinforcing the link between the 4π mode and the double-pulsing inflow.

At $\omega = 6\pi$, the structure is still dominated by a single ring, though faint traces of a secondary feature begin to emerge. In contrast, the mode at $\omega = 8\pi$ shows a clear formation of two distinct vortex rings, providing further evidence that higher harmonics of 4π are strongly tied to the double-pulse dynamics.

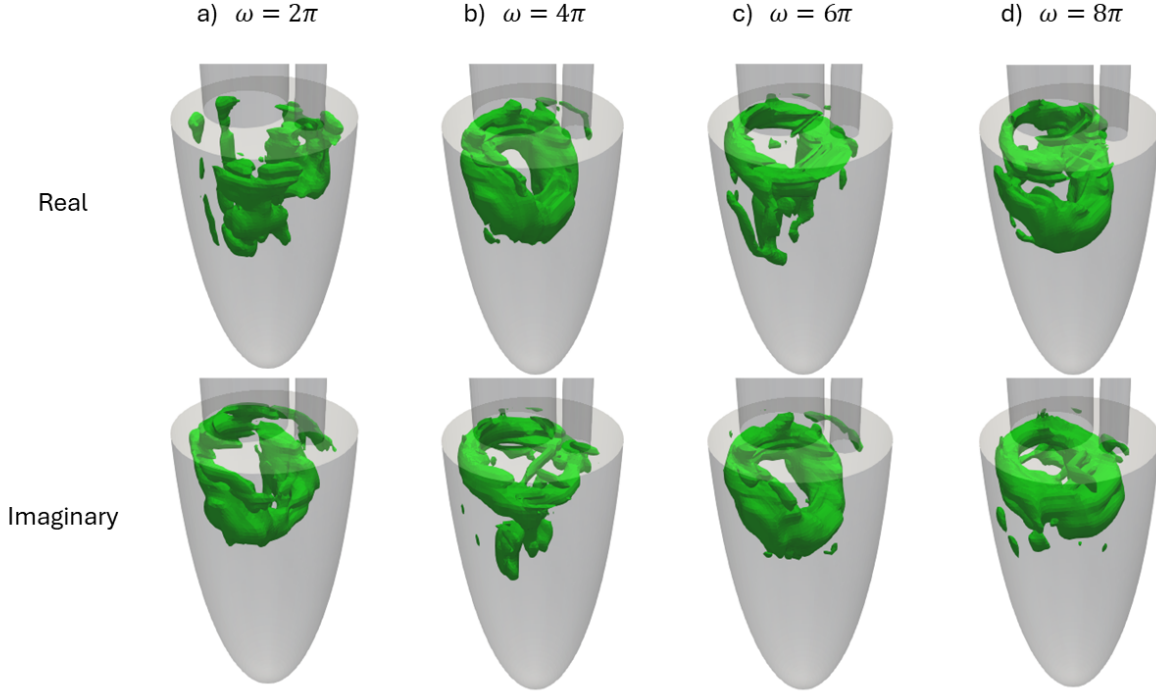


Figure 4.8: Three-dimensional Q-criterion isocontours at level 2000 for the real (top) and imaginary part (bottom) of the dominant DMD mode and its first three harmonics in the **Ideal 1** model: (a) 2π , (b) 4π , (c) 6π , and (d) 8π .

Figure 4.9 displays the three-dimensional Q-criterion isocontours for the next four higher-frequency DMD harmonics. These modes reveal increasingly fragmented and spatially complex structures, indicative of finer flow scales and more irregular, turbulent dynamics. Despite this, signatures of the double-pulsing behavior remain evident, likely arising from nonlinear interactions between the dominant mode and its first harmonic.

To complete the analysis, we compare the frequency content extracted from HODMD with that obtained from the FFT of the POD temporal coefficients. The dominant DMD modes, ranging from $\omega = 2\pi$ to $\omega = 8\pi$, are primarily associated with the first three POD modes. These correspond to the main vortex ring, its initial breakdown, and the emergence of the double-pulsing effect. In contrast, higher-frequency DMD modes, such as those at $\omega = 10\pi$ and above, are more closely aligned with POD modes 4 to 6, which represent smaller-scale features and later stages of the flow evolution.

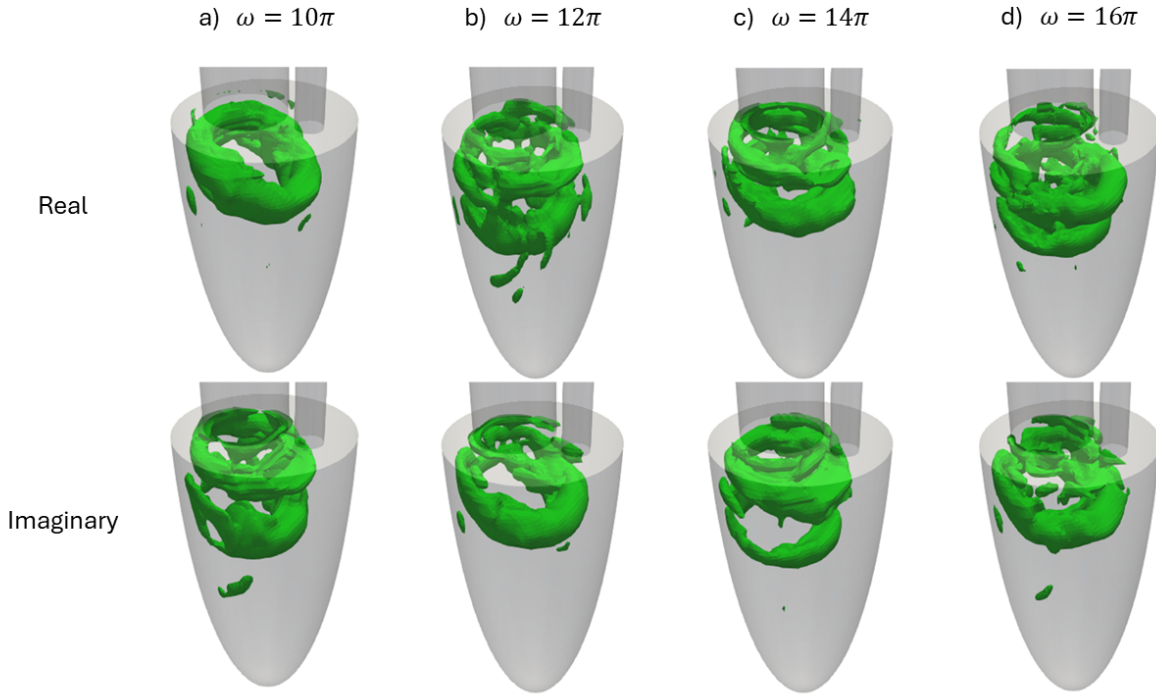


Figure 4.9: Same as Fig. 4.8 for the higher harmonics: (a) 10π , (b) 12π , (c) 14π , and (d) 16π .

This correspondence reinforces the conclusion that interactions between the secondary and primary vortices play a significant role in the disruption of the main vortex ring. The frequency-resolved structure provided by HODMD complements the energy-based analysis of POD, offering a more detailed picture of the spectral organization and dynamical mechanisms underlying vortex breakdown.

4.2 Ideal 2: Geometry based on experimental setup.

As noted in Sec. 4.2, the *Ideal 2* dataset offers a clearer depiction of intraventricular flow dynamics. This can be attributed to the slower progression of vortex breakdown, driven by a smaller volume change during the cardiac cycle. As a result, the primary vortex ring is able to travel further and nearly reach the apex before dissipating. Compared to the previous case, this leads to a distinct breakdown mechanism and a more coherent flow evolution.

We begin the analysis by applying POD and evaluating the singular value decay, normalized by the first mode, as shown in Fig. 4.10. Similar to *Ideal 1*, the decay is steep, with the first 15 modes ($\sum_{n=1}^{15} e_n$) capturing approximately 99% of the total energy (Eq. 2.9). However, in contrast to simpler periodic flows where energy-balanced mode pairs often appear, the POD modes in this case do not exhibit such pairing. This points to a more complex and nonlinear dynamic behavior, even though the simulation remains globally periodic.

The analysis of the POD modes and the corresponding FFT of the chronos matrix reveals notable differences from the *Ideal 1* case. Figure 4.11 shows the FFT spectra for the six

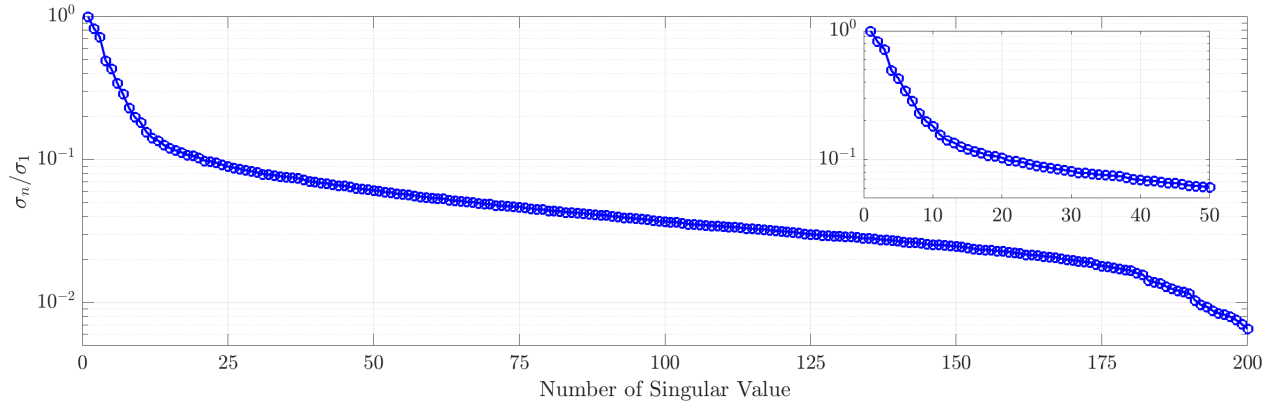


Figure 4.10: Counterpart of Fig. 4.1 for the Ideal 2 database.

most energetic modes. As expected, the dominant frequency at 2π , associated with the heart rate, is clearly captured, along with the secondary peak at 4π , reflecting the double-pulsed inflow. Higher harmonics are also present but less pronounced.

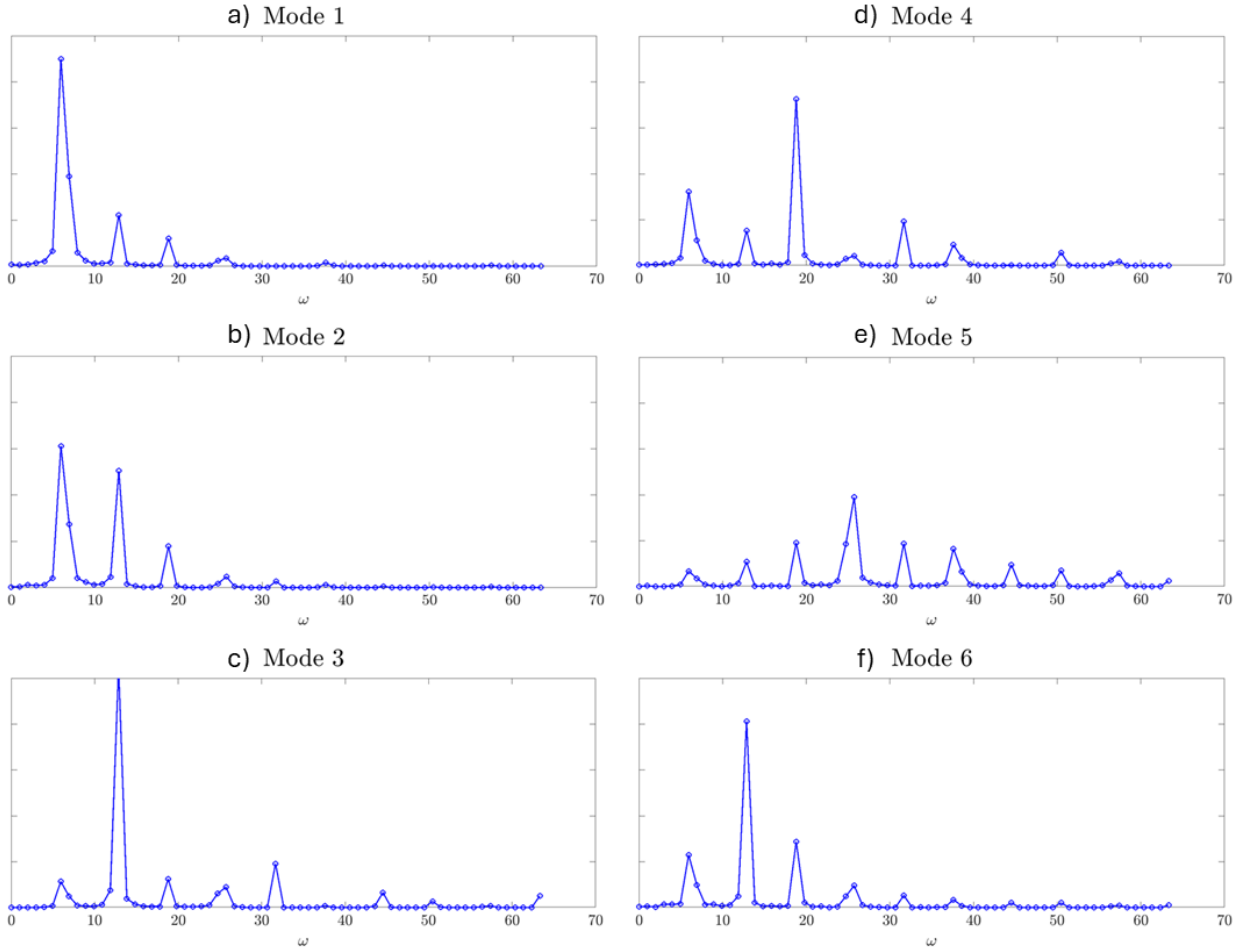


Figure 4.11: Counterpart of Fig. 4.2 for the Ideal 2 database.

Unlike the more entangled dynamics of **Ideal 1**, the modal structure here is more clearly separated. Mode 1 is dominated by the fundamental 2π frequency. Mode 3 is primarily governed by the 4π component. Mode 2 exhibits a balanced contribution from both, suggesting an interaction between the main and secondary inflow events.

Lower-energy modes show evidence of nonlinear coupling between frequencies, although these interactions remain limited to the lower harmonics. In contrast to the richer high-frequency content observed in Fig. 4.4(d–f), the spectral range in this case is narrower. Capturing more complex interactions at higher frequencies would require analyzing POD modes beyond those currently presented.

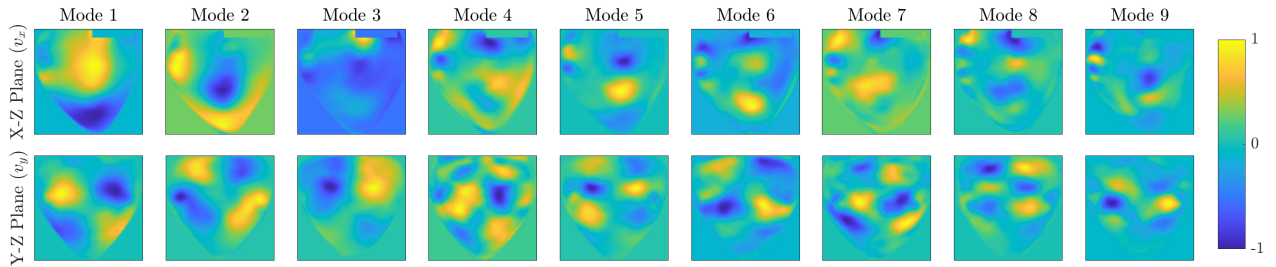


Figure 4.12: Counterpart of Fig. 4.3 for the **Ideal 2** database.

Figure 4.12 presents the two-dimensional projections of the most energetic POD modes for the **Ideal 2** case, following the same format as in Sec. 4.1. Mode 1 captures the main vortex ring with a pronounced tilt, characteristic of the early filling phase. Mode 3 highlights the formation of a secondary vortex near the inlet, while Mode 2 reflects a combination of both behaviors, showing a tilted primary ring accompanied by downstream flow features.

The lower-energy modes emphasize finer-scale structures and provide a clearer view of the energy cascade occurring during vortex evolution and dissipation. As shown in the figure, the spatial extent of the dominant structures decreases with increasing frequency content, indicating that higher-frequency harmonics are associated with smaller and more localized flow features.

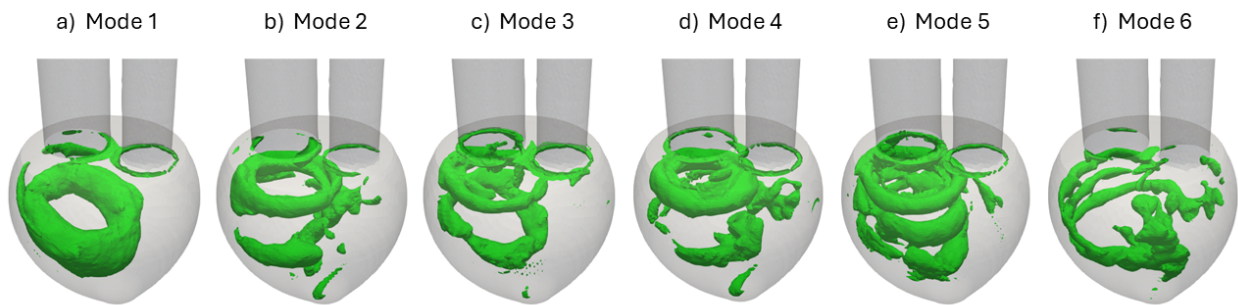


Figure 4.13: Counterpart of Fig. 4.4 for the **Ideal 2** database.

These results are reinforced by the three-dimensional Q-criterion isocontours of the POD

modes shown in Fig. 4.13. Mode 1, associated with the fundamental frequency 2π , captures the primary recirculating structure around the main vortex ring. This ring extends longitudinally through the ventricle, in agreement with the behavior observed in Fig. 3.7, where the vortex progresses toward the apex before undergoing breakdown.

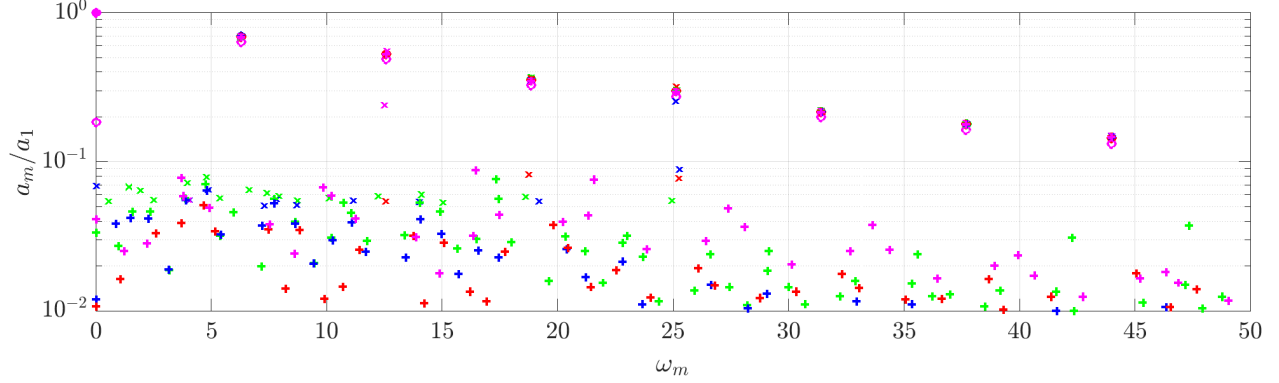


Figure 4.14: Counterpart of Fig. 4.5 for the *Ideal 2* database.

The second POD mode reflects an interaction between the 2π and 4π frequency components. Its Q-criterion isosurface captures the formation of a vortex near the inlet and the gradual dissipation of the main structure as it moves toward the apex. Mode 3, more clearly associated with the 4π frequency, likely represents the double-pulsing mechanism observed in the simulation. The isosurface reveals a vortex near the apex and another developing close to the inflow region, consistent with the secondary filling phase.

In contrast to the *Ideal 1* case, where most modal activity was localized near the inlet (see Fig. 4.4), the modes here span the entire ventricular domain. This suggests a more complete evolution of the vortex ring, which travels farther before breakdown occurs. Modes 1-3 primarily capture the formation, progression, and interaction of the main and secondary vortices.

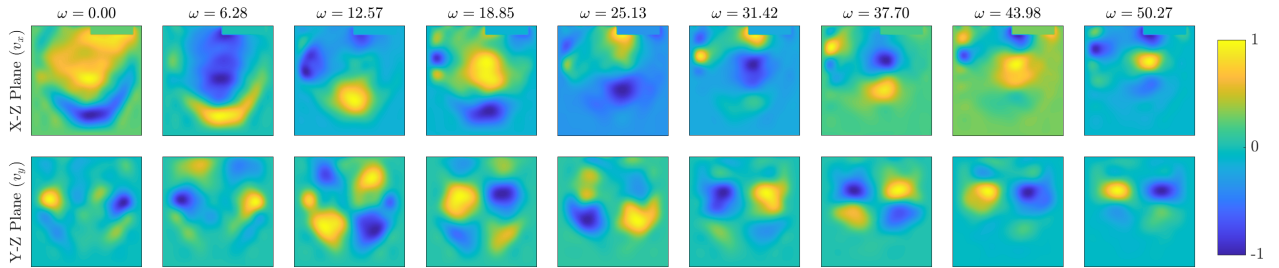


Figure 4.15: Same as Fig. 4.6 for the *Ideal 2* database.

Modes 4 and 5 (Fig. 4.13d–e), associated with higher harmonic content, reveal finer flow structures and increased spatial complexity. These features are indicative of nonlinear interactions that contribute to the eventual destabilization of the vortex ring. Mode 6 again emphasizes the secondary vortex, with a weaker imprint of the primary structure. Notably, its spatial pattern resembles that of Mode 3, but with reduced energy content, suggesting a redistribution of energy across similar flow features at different frequencies.

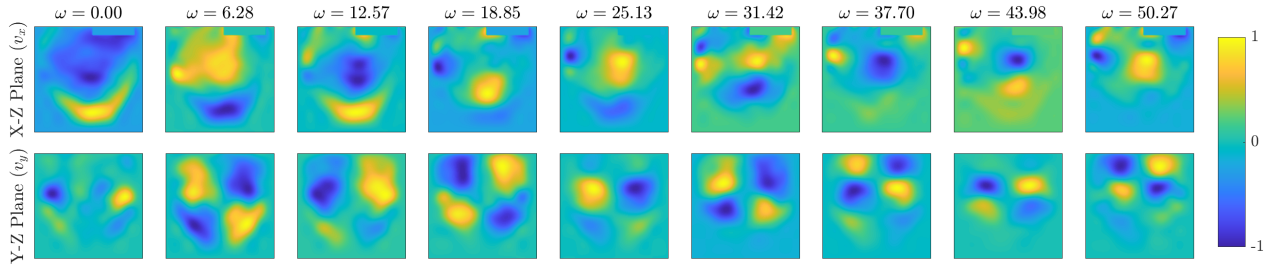


Figure 4.16: Same as Fig. 4.7 for the *Ideal 2* database.

To gain further insight into the temporal dynamics, we apply HODMD to this dataset as in the previous case (Sec. 4.1). The resulting amplitude spectra, shown in Fig. 4.14, highlight clusters of dominant modes at 2π and its harmonics. These peaks stand out clearly above the background, which consists mostly of spurious modes with negligible amplitude. In this case, however, the decay of amplitudes across harmonics is more gradual and uniform, while the 2π component remains the most dominant.

A similar modal structure is observed in the *Ideal 2* dataset. Figures 4.15 and 4.16 display the real and imaginary parts, respectively, of the mean flow and selected DMD modes. The dominant mode again captures the large-scale recirculating motion of the primary vortex ring. The first harmonic highlights flow disturbances near the inlet, corresponding to the double-pulsed inflow pattern.

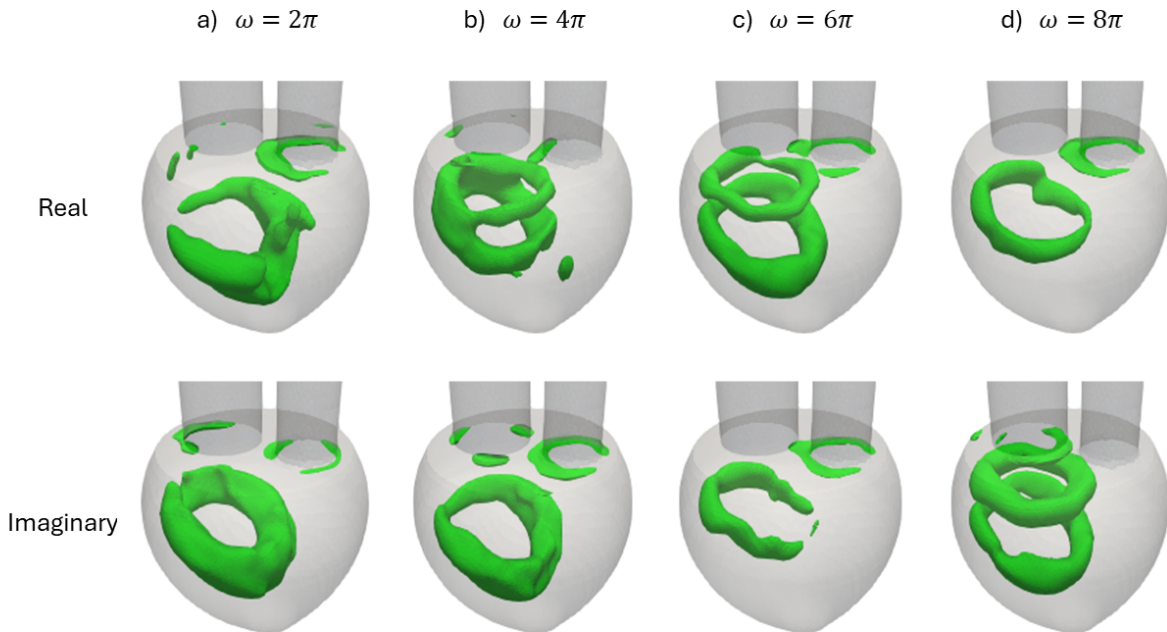


Figure 4.17: Same as Fig. 4.8 for the *Ideal 2* database.

Higher-frequency modes reveal more intricate structures and complex flow interactions. This

is particularly evident in the 8π mode, which exhibits features resulting from nonlinear interactions between the primary and secondary inflow pulses. The phase shift between the real and imaginary components provides additional insight into the temporal progression of these coherent structures throughout the cardiac cycle.

As in the **Ideal 1** case, the DMD analysis of the **Ideal 2** model is further enriched by examining the three-dimensional Q-criterion isocontours of the real and imaginary parts of each mode, shown in Fig. 4.17. At first glance, the flow structures appear cleaner and more coherent than in the previous case, which can be attributed to the slower and more regular dynamics of this simulation.

The dominant mode again captures the primary vortex ring, aligned with the fundamental periodicity of the flow. At $\omega = 4\pi$, two separate vortex rings are already visible in the real part, providing a clearer manifestation of the double-pulsing behavior. The nonlinear interaction between the fundamental and its first harmonic is more evident here than in **Ideal 1**, particularly in the $\omega = 6\pi$ mode, which reveals one ring near the inlet and another closer to the ventricle's center.

This pattern becomes even more pronounced at $\omega = 8\pi$. As the phase evolves, the initial vortex ring moves toward the apex while a second ring begins to form at the inlet. Once the latter is fully developed, the former starts to dissipate, clearly illustrating a cyclic generation and dissipation sequence consistent with double-pulsed inflow dynamics.

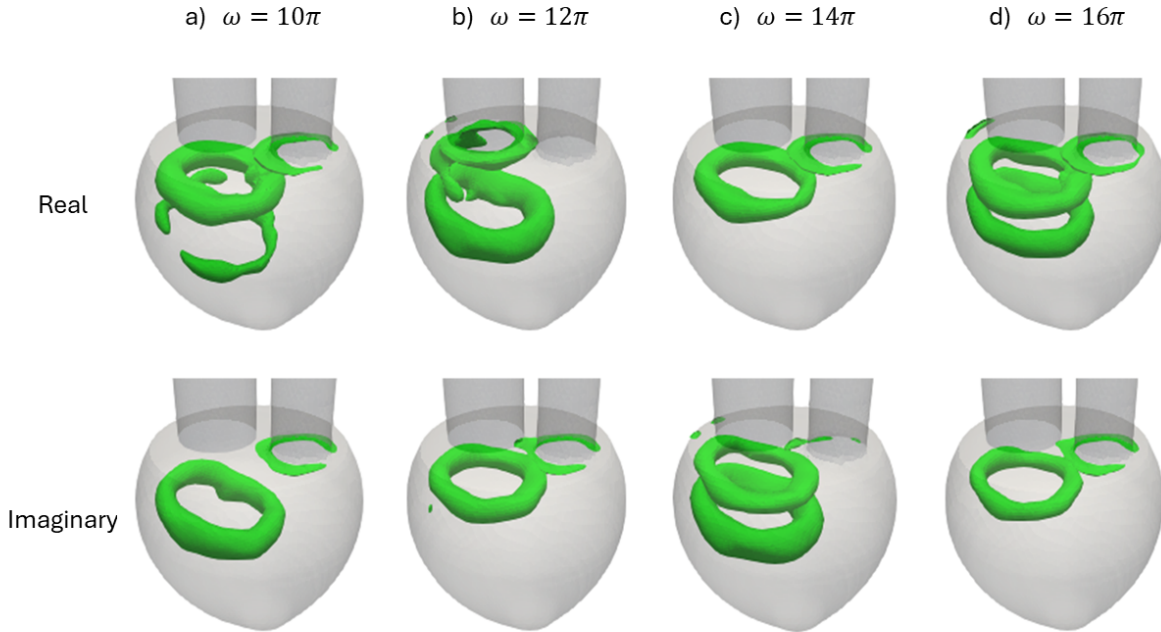


Figure 4.18: Same as Fig. 4.9 for the **Ideal 2** database.

Figure 4.18 displays the Q-criterion isocontours corresponding to the higher-order DMD harmonics. As previously discussed, the strong coupling between the fundamental periodic

motion and the double-pulsed inflow gives rise to flow structures that reflect characteristics of both phenomena. The visualizations often reveal two simultaneous vortex rings within the left ventricular chamber, along with clear signatures of vortex formation, dissipation, and interaction near the outlet region. These features emphasize the complexity of the dynamics captured at higher frequencies.

To complete the analysis, we compare the POD and DMD results to better characterize the spectral organization of the flow structures. The first POD mode captures the primary vortex ring, including its characteristic tilt and recirculation pattern, and corresponds well with the dominant DMD mode at the fundamental frequency 2π . The third POD mode, which features two spatially separated vortical structures, aligns with the double-pulsing behavior observed in the simulation. The second mode appears to represent a nonlinear combination of the primary and secondary vortices. Lower-energy POD modes reveal finer structures, indicative of higher-frequency content and nonlinear interactions.

While POD hints at the presence of these phenomena, HODMD offers more accurate temporal resolution. The main vortex ring is clearly isolated in the 2π mode, while the emergence of the secondary vortex begins at 4π and becomes dominant at 8π . From that point onward, both structures are consistently captured across all higher-frequency DMD modes, confirming their coexistence and dynamic interaction throughout the cardiac cycle.

Chapter 5

Reduced order model for intraventricular flows

To evaluate the performance of the ROM described in Sec. 2.3.4, we apply it to the two idealized left ventricle (LV) databases introduced in Chapter 4. As previously shown, the vortex ring dynamics differ significantly between geometries. In the **Ideal 1** configuration, the narrower chamber leads to early vortex-wall interaction, triggering breakdown before the ring reaches the apex. Conversely, in **Ideal 2**, the wider chamber allows the ring to develop fully, propagate toward the apex, and break down due to combined wall effects and velocity decay.

These contrasting behaviors arise from two primary factors:

1. The narrow geometry of **Ideal 1** intensifies vortex-wall interactions, limiting ring propagation.
2. **Ideal 2** exhibits lower ejection fraction and volume change, reducing pressure gradients and flow velocities.

Such differences are critical for assessing the ROM’s robustness under varying hemodynamic regimes.

Each simulation spans 20 cardiac cycles, with fields sampled every $\Delta t^* = 0.05$, yielding 20 snapshots per cycle and $K = 400$ snapshots in total. The ROM is trained on the first 10 cycles, including the transient regime, while the remaining 10 are reserved for validation, reflecting the converged dynamics. DMD analysis confirms that growth rates stabilize only during the final cycles, justifying this partition.

While typical studies limit simulations to 6 cycles (Canè et al., 2022; Grünwald et al., 2022; Korte et al., 2023), our results indicate that transient behavior persists beyond this window. Extended simulations are therefore essential to ensure modal convergence and the reliability of ROM predictions.

Table 5.1 summarizes the cases used for both geometries. Naming conventions are preserved for consistency. Each case defines a training or validation interval and the associated tuning

threshold δ_{tune} , which filters out unstable or spurious modes in the HODMD analysis.

Case	No. of Cycles	Time Interval t^*	Snapshots K	Purpose	δ_{tune}
T-1.5	1.5	[0, 1.5]	30	Training (transient)	1.0
T-3	3	[0, 3]	60	Training (transient)	0.5
T-5	5	[0, 5]	100	Training (transient)	0.1
T-10	10	[0, 10]	200	Training (transient)	0.01
V-10	10	[10, 20]	200	Validation (converged)	0.01

Table 5.1: Simulation cases used for ROM training and validation, indicating time intervals, number of cycles, and selected growth rate threshold δ_{tune} .

Despite the periodic boundary conditions, moving-wall CFD introduces unavoidable variability across cycles (Chnafa et al., 2014). While large-scale features, such as vortex rings and outflow jets, are consistently reproduced, smaller-scale structures may vary.

To quantify this variability, we integrate the TKE over each cardiac cycle:

$$\text{TKE}_i = \int_{i-1}^i \text{TKE}(t^*) dt^*, \quad i = 1, \dots, 20. \quad (5.1)$$

We then define the RRMSE with respect to the final cycle as:

$$\text{RRMSE}_{\text{TKE}}(\%) = \frac{|\text{TKE}_{20} - \text{TKE}_i|}{|\text{TKE}_{20}|} \cdot 100. \quad (5.2)$$

As shown in Fig. 5.1, the RRMSE falls below 4% in both models, confirming convergence of global dynamics. However, localized flow quantities may exhibit greater variability. Accordingly, ROM accuracy should be interpreted within an intrinsic uncertainty margin of 5–10%.

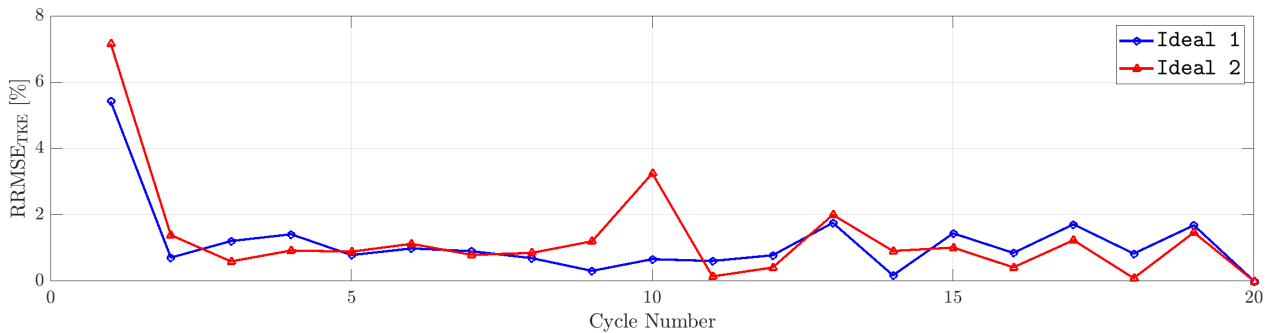


Figure 5.1: Cycle-to-cycle variability in total kinetic energy for **Ideal 1** and **Ideal 2** geometries.

We begin the analysis by applying HODMD to case V-10 of the **Ideal 1** model. The resulting spectrum is shown in Fig. 5.2, with normalized mode amplitudes (left) and growth rates (right) plotted against frequency. Different window lengths d and tolerances ε are included, illustrating the consistency of extracted modes across parameter choices (A. Hetherington et al., 2024).

The dominant frequencies (e.g., 2π , 4π , 6π , ...) consistently exhibit large amplitudes, indicating robust physical relevance. In contrast, low-amplitude modes correspond to numerical artifacts. Growth rate analysis confirms this: physical modes remain near-neutral (below 10^{-2}), while spurious modes decay rapidly.

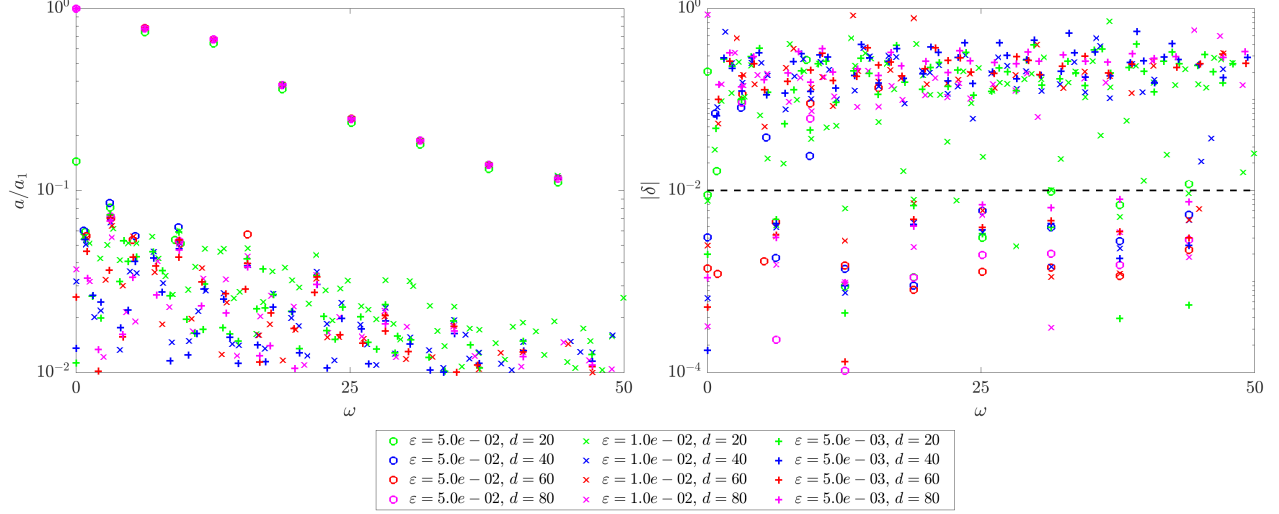


Figure 5.2: Spectrum of DMD modes for the **Ideal 1** model. Left: normalized amplitude vs. frequency. Right: growth rate vs. frequency. Dashed line at $< 10^{-2}$ separates persistent from transient modes.

The selected threshold $\delta_{tune} = 10^{-2}$ distinguishes stable, recurring dynamics from transient components. Below this value, modes are consistent across calibrations and align with dominant frequencies. Above it, they become scattered and non-physical. The same behavior is observed for the **Ideal 2** model and is omitted here for brevity.

5.1 Ideal 1: Geometry based on a semi-ellipsoid.

For the **Ideal 1** model, HODMD is applied to multiple training subsets, each containing a different number of cardiac cycles as specified in Table 5.1. The goal is to assess how many cycles are required to reliably capture the system's temporal dynamics. To this end, we reconstruct the temporal evolution using the frequencies and growth rates obtained from HODMD. Two reconstruction scenarios are considered: (i) using the original growth rates, and (ii) assuming purely periodic behavior by setting all growth rates to zero.

Figure 5.3 compares the reconstructed temporal coefficients $\hat{T}$ across different training cases. The left column shows reconstructions using the original growth rates from HODMD, while the right column displays the same reconstructions with growth rates set to zero, enforcing purely oscillatory behavior.

With only 1.5 cycles (case a), the dominant frequency is roughly captured, but the temporal evolution is inaccurate due to a strongly negative growth rate and poor resolution of higher harmonics. Setting the growth rate to zero slightly improves the result, though the reconstruction remains unsatisfactory. At 3 cycles (b), the dominant frequency is well identified,

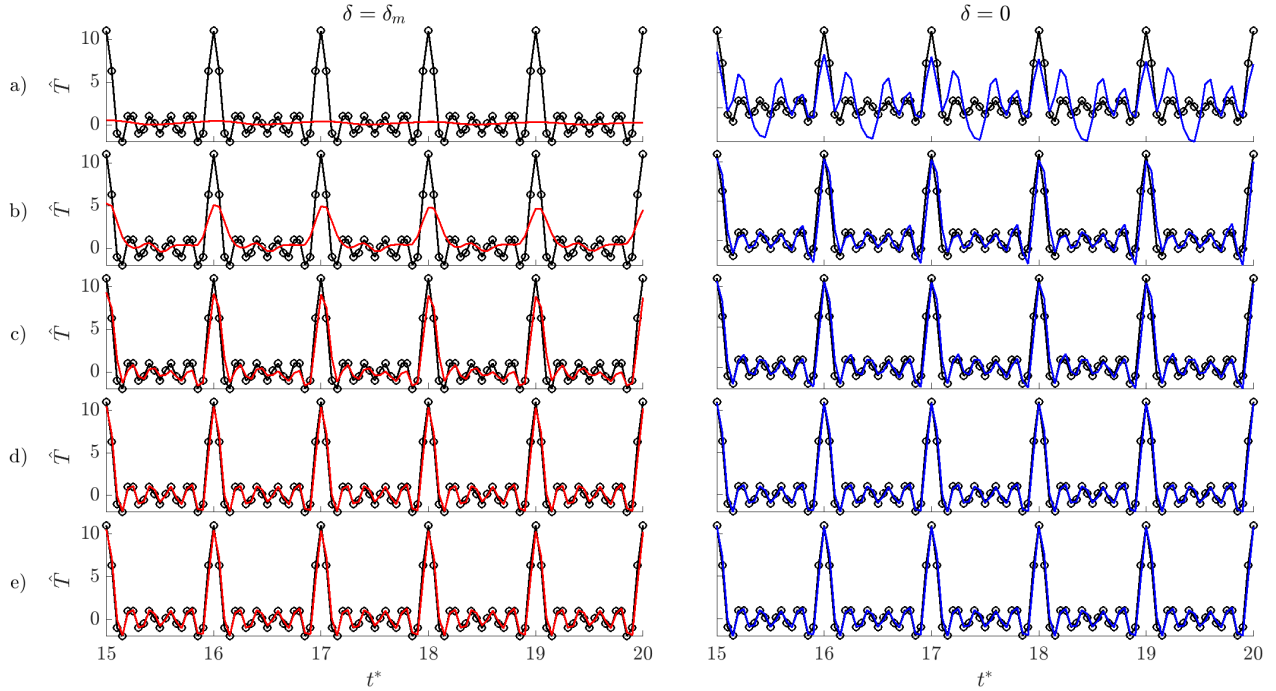


Figure 5.3: Comparison of the temporal evolution calculated with HODMD against the true system (black) for the *Ideal 1* model: (left, red) computed growth-rate and (right, blue) growth-rate set to zero. The cases are listed in rows as: (a) T-1.5, (b) T-3, (c) T-5, (d) T-10, and (e) V-10 cases.

but the dynamics are still distorted by a high negative growth rate. When zero growth is imposed, the reconstruction aligns closely with the expected evolution. For larger datasets (T-5 and T-10), both frequency and growth rate estimates improve significantly, yielding accurate reconstructions even without imposing the zero-growth constraint. The V-10 case (e), which includes only converged cycles, shows nearly identical frequencies to the ground truth and negligible growth rates, confirming the robustness of the extracted modes.

Having established that the spectral features of the simulations can be accurately captured using only three cardiac cycles—provided that the growth rates are set to zero—we now extend the analysis to the spatial domain. Specifically, we perform flow reconstructions using DMD modes extracted from training datasets of varying lengths (excluding the 5-cycle case for brevity, as its results closely resemble those of the 10-cycle case). For each dataset, two reconstruction scenarios are considered: (i) using the original growth rates and (ii) imposing zero growth. Furthermore, we evaluate two modal selections: one using all extracted modes, and another using only the dominant mode and its harmonics.

Figure 5.4 shows the temporal evolution of the vertical velocity component v_z at probe point P1. This component is selected because the flow is primarily oriented along the vertical axis, making v_z the most representative measure. Predictions using the full set of modes (blue) and the reduced subset of representative modes (red) are compared against the reference data from case V-10 (black). From top to bottom, each row corresponds to a different training case: T-1.5, T-3, and T-10. The left column presents reconstructions using the original HODMD

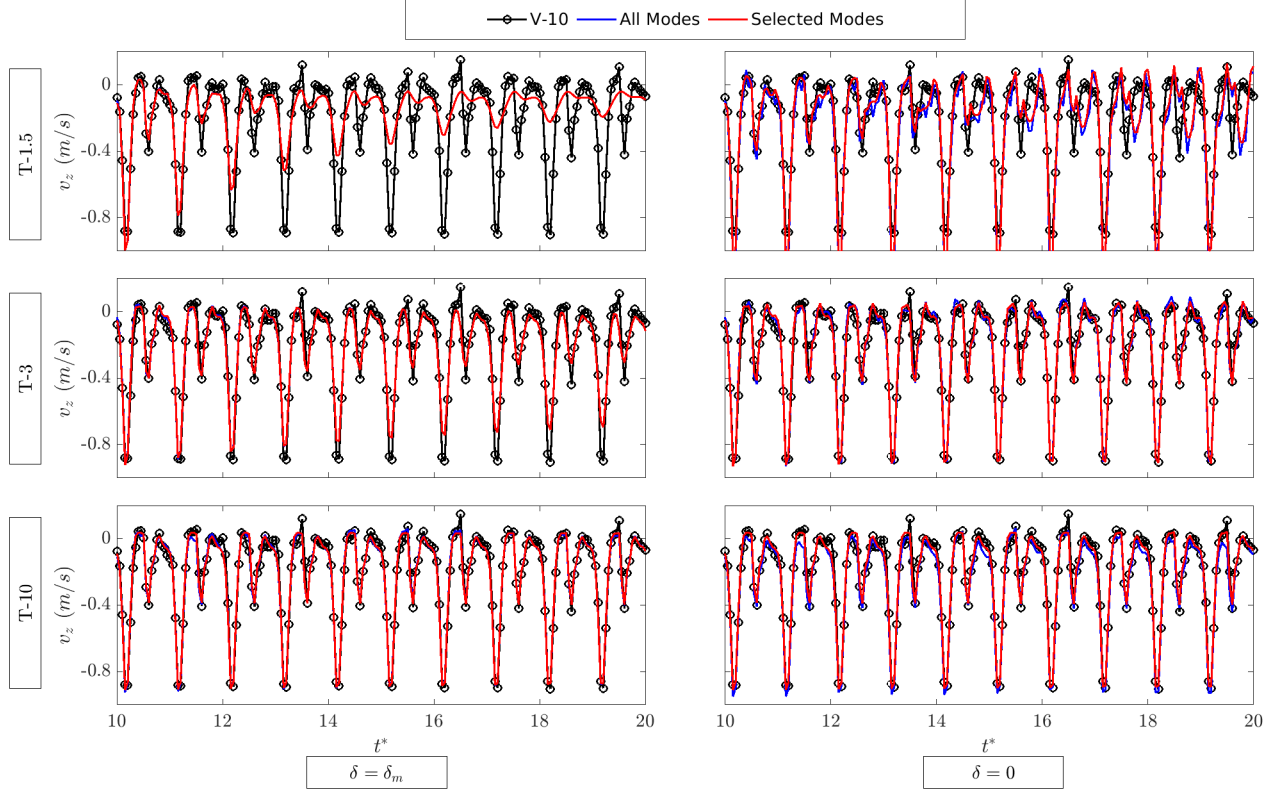


Figure 5.4: Comparison of the temporal evolution of the v_z velocity component in P1 (see Fig.2.2), between the predictions using all modes (blue) and a selected subset of modes (red) against the ground truth (black) for the *Ideal 1* model. The first column displays the results when maintaining the original growth rate ($\delta = \delta_m$), whereas the second column enforce a zero growth rate ($\delta = 0$). Each row corresponds to a different training case: (top) T-1.5, (middle) T-3, and (bottom) T-10.

growth rates, while the right column shows results with zero growth imposed.

The temporal evolution of the flow at this location is primarily influenced by the conditions imposed at the nearby inflow region. In all cases, the most accurate predictions are achieved when retaining only the dominant mode and its harmonics, as this selection filters out spurious components that would otherwise introduce noise. This effect is further enhanced when setting the growth rates to zero, ensuring that all modes contribute uniformly over time.

When using only 1.5 cycles for model construction, the predictions are notably inaccurate, with limited potential for improvement. Extending the training set to 3 cycles leads to a marked increase in accuracy, particularly when the zero-growth condition is applied, which prevents artificial amplitude decay throughout the prediction window.

A similar comparison is shown in Fig. 5.5 for probe point P2, located at the center of the LV chamber. Unlike the inlet region, this location is characterized by more complex flow features, including vortex tilting, dissipation, and recirculation. Consequently, accurately capturing the temporal evolution at this point is more challenging.

As before, retaining only the dominant modes yields the best performance. The T-1.5 case

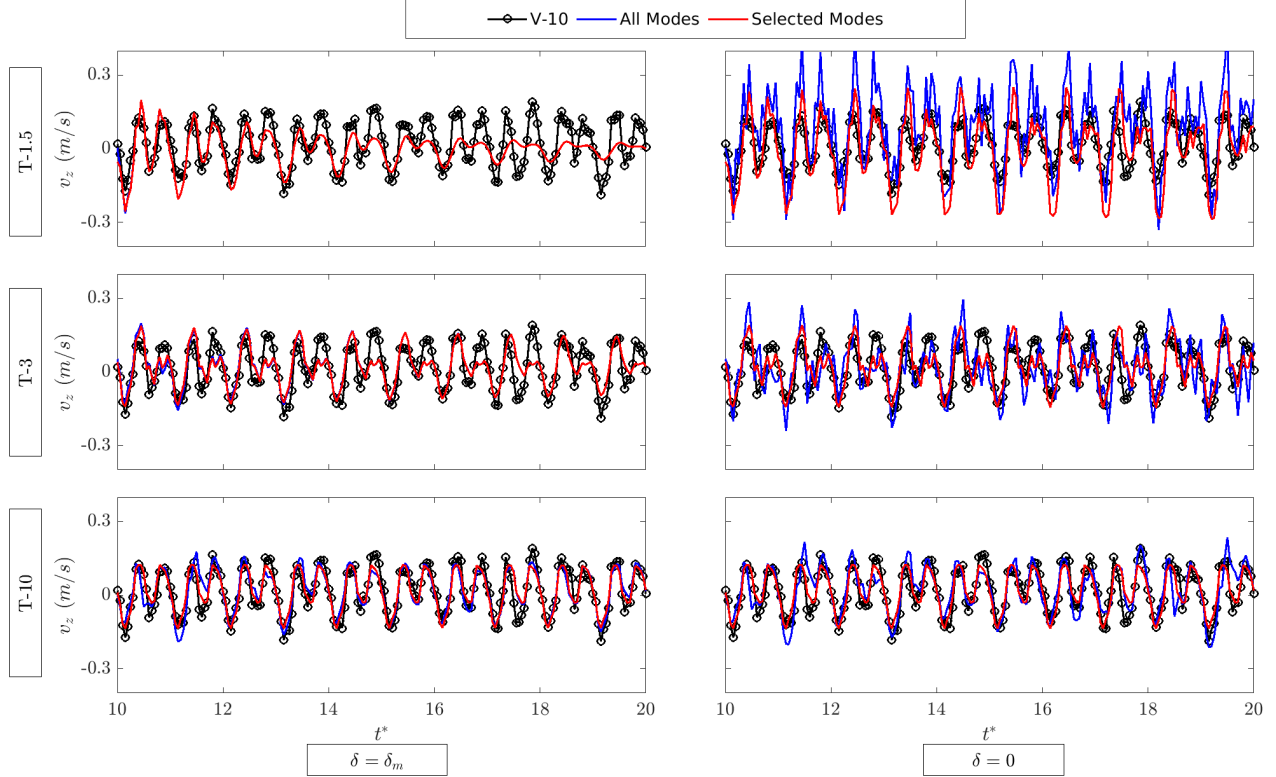


Figure 5.5: Counterpart of Fig. 5.4 for the spatial point P2 (see Fig.2.2).

fails to reproduce the flow dynamics at this location, and its predictions are significantly inaccurate. With 3 cycles, the reconstruction improves, though some discrepancies persist due to the complexity of the flow. Even in the T-10 case, minor deviations remain, reflecting the inherent difficulty in reconstructing highly nonlinear behavior. Nevertheless, considering the simulation’s intrinsic uncertainties, the predictions are considered reliable.

To better interpret the model’s predictive capabilities, we focus on the most accurate configurations, those obtained by selecting modes with growth rates below the threshold and imposing zero growth. Figure 5.6 presents 2D contours of the v_x velocity component on the A–A’ plane at $t^* = 19.25$ for the *Ideal 1* case, comparing configurations T-1.5, T-3, and T-10 (top row). All cases qualitatively reproduce the key features observed in the reference solution V-10, such as the inflow and recirculation zones. However, the T-1.5 case shows significant errors, particularly a spurious influence of the outflow, which is unphysical at this phase of the cardiac cycle.

These findings are corroborated by the absolute error maps shown in the bottom row of Fig. 5.6, computed as the pointwise difference with respect to the V-10 reference. The T-1.5 case exhibits the largest discrepancies, especially near the outlet. In contrast, the T-3 configuration reduces the error substantially, achieving accuracy comparable to that of the T-10 case.

It is important to recognize the intrinsic uncertainty associated with moving-wall CFD simulations. Even among different cycles of the reference simulation, minor variations are

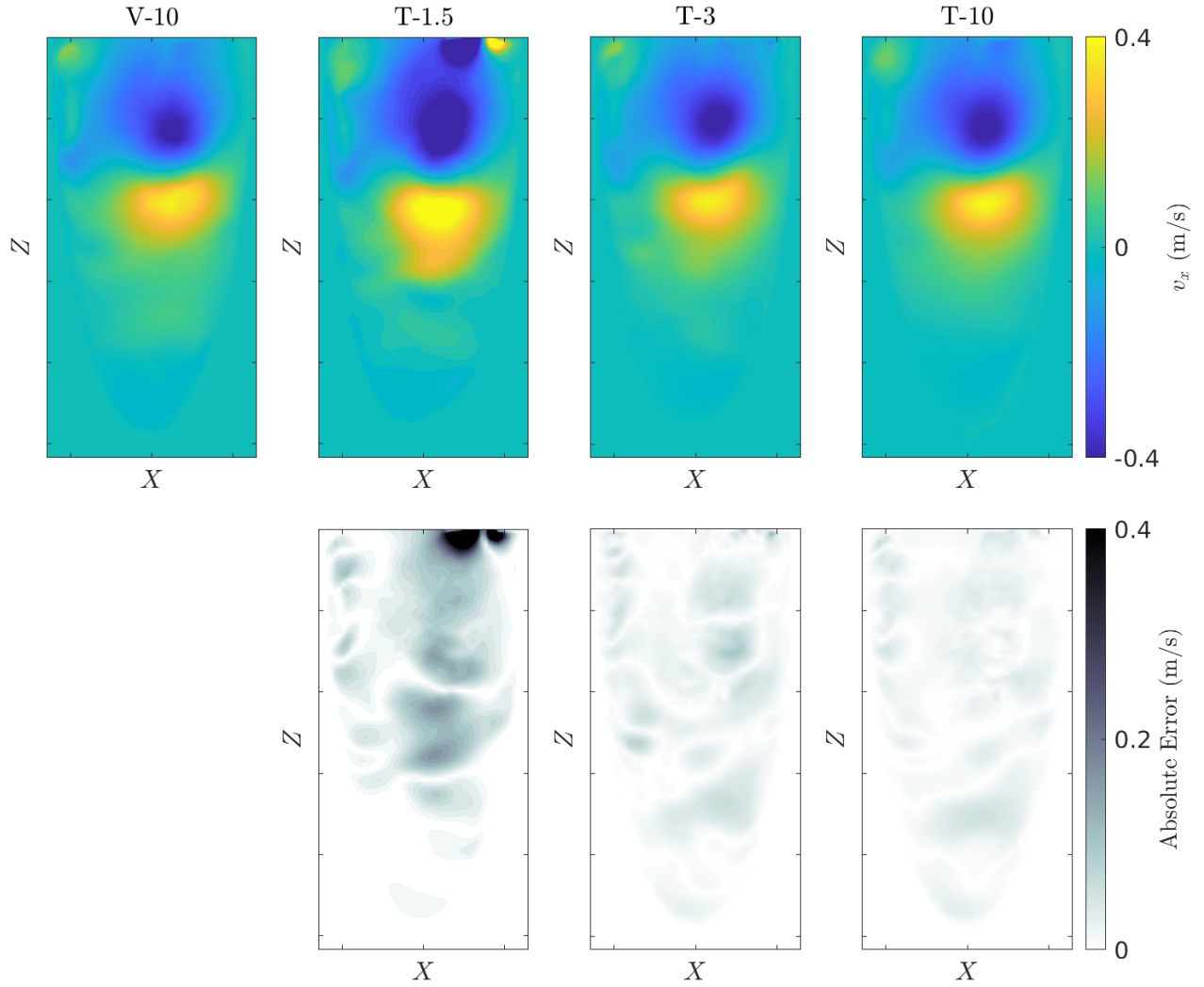


Figure 5.6: Comparison of the v_x velocity component in the A-A' plane at $t^* = 19.25$ for the *Ideal 1* case using ROMs constructed from training sets T-1.5, T-3, and T-10 (top row), along with the corresponding absolute error with respect to the reference case V-10 (bottom row).

observed. In light of this variability, the accuracy achieved by the ROM is particularly noteworthy given its drastically reduced computational cost.

The main advantage of the ROM lies in this cost reduction. For example, the full-order CFD simulation, run on 40 CPUs, required approximately 38 hours to compute 10 cardiac cycles using a high-resolution mesh. In contrast, the ROM prediction over the same interval was completed in just 36 seconds, resulting in a speed-up factor (SUF) of 1.5×10^5 .

However, this efficiency comes with a trade-off between computational savings and reconstruction fidelity. Shorter training sets, such as case T-1.5, lower the offline cost but fail to capture essential flow features, leading to poor performance. Our results indicate that case T-3 provides a balanced compromise: it captures the dominant flow dynamics with acceptable accuracy while offering significant savings in computational time compared to longer training

sets like T-10.

5.2 Ideal 2: Geometry based on experimental setup.

Having analyzed the tuning and performance of the ROM using the *Ideal 1* geometry, we now extend the study to the *Ideal 2* model. This configuration serves as a benchmark to assess the method's robustness under different intraventricular flow conditions, which in this case evolve more slowly and exhibit distinct dynamics. Further details on the flow patterns and instability development for this geometry are discussed in Sec. 4.1.

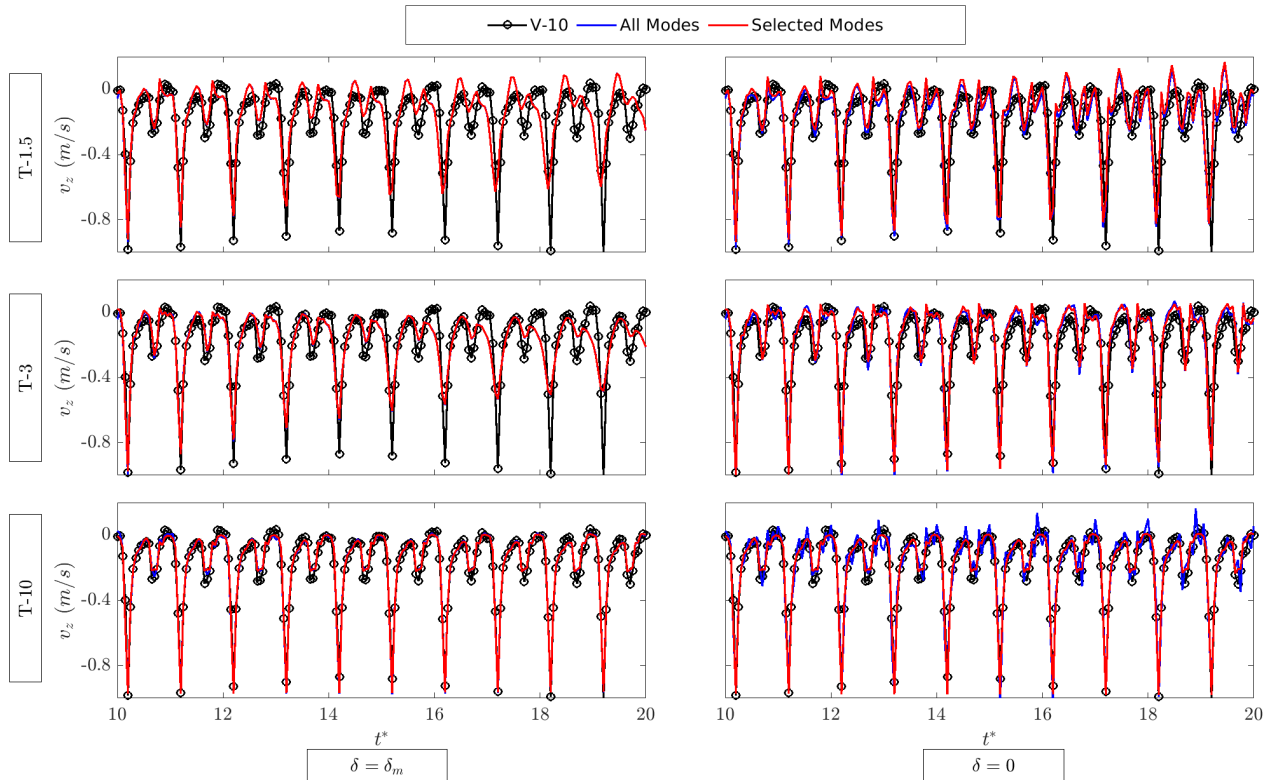


Figure 5.7: Counterpart of Fig. 5.4 for the *Ideal 2* model (see Fig.2.3).

Since the frequency estimation with HODMD yields results comparable to those in Fig. 5.3, a detailed spectral analysis is omitted for brevity. As previously noted, while the dominant frequency is well captured even with only 1.5 cycles, the growth rate remains poorly estimated. Thus, accurate temporal predictions require either extending the training dataset or enforcing zero growth.

A central element of this analysis is the evolution of the vertical velocity component v_z at selected probe locations within the chamber, comparing ROM predictions to the original CFD results. Figure 5.7 shows the temporal evolution of v_z at a point near the inlet tube (P1), evaluated under two conditions: with the original growth rates (left column) and with growth rates set to zero (right column). In both cases, predictions using the full mode set and a reduced set (dominant mode at 2π and its harmonics) are compared against the reference

data.

The results reveal that some extracted modes exhibit strongly negative growth rates (e.g., $\delta \approx -0.3$), which introduces artificial damping over time. This behavior, consistent with the DMD expansion in Eq. 2.11, leads to exponential amplitude decay and degrades prediction accuracy. Enforcing a zero growth rate effectively mitigates this issue, stabilizing the reconstruction and better preserving the periodic behavior of the flow.

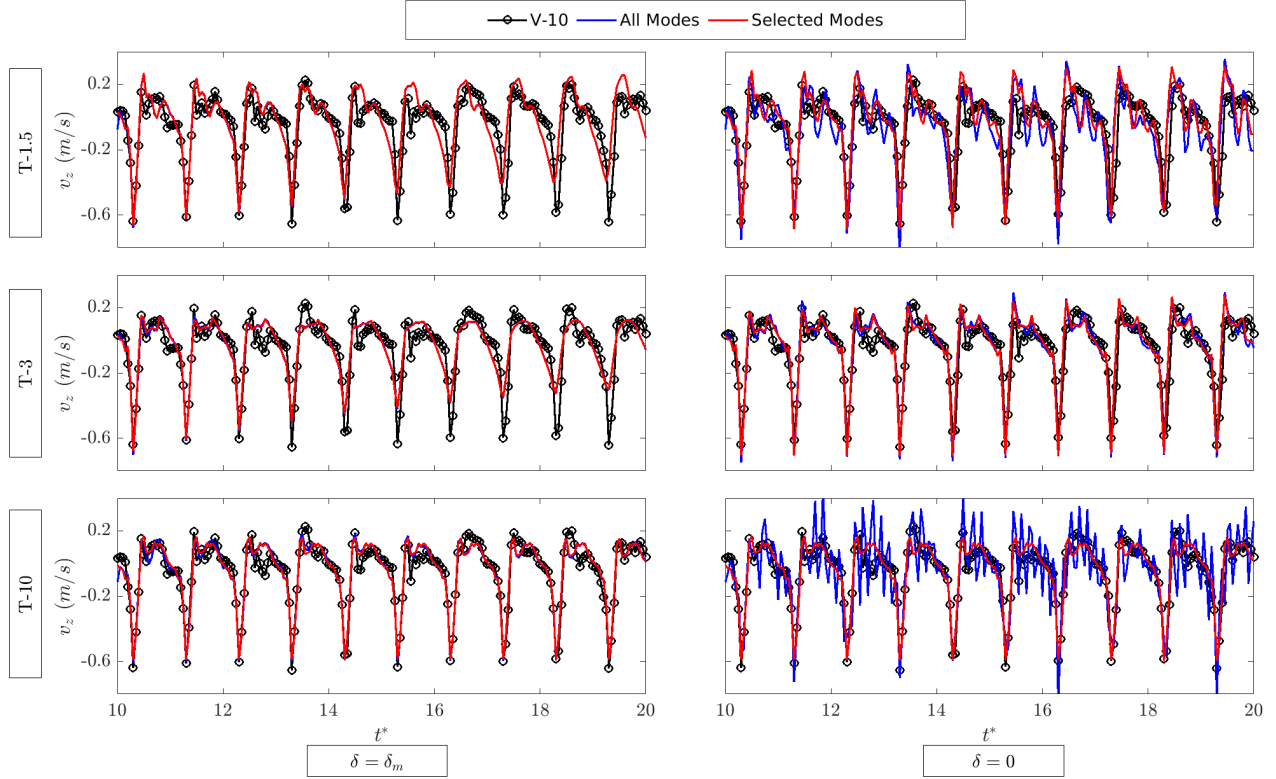


Figure 5.8: Counterpart of Fig. 5.5 for the *Ideal 2* model (see Fig.2.3).

Including all modes introduces spurious contributions and numerical noise, reducing reconstruction accuracy. In contrast, retaining only the principal modes—namely the dominant frequency and its harmonics—proves sufficient to recover the main dynamics. Although 1.5 cycles are adequate to reproduce the general trend, at least 3 cycles are needed to achieve more detailed and reliable predictions.

A similar trend is observed at probe point P2, located near the center of the LV chamber, as shown in Fig. 5.8. The flow at this location is more complex due to weaker geometric constraints compared to the inlet region, making prediction accuracy more challenging. Retaining the original growth rates leads to excessive amplitude decay, while including all modes amplifies noise. The best results appear in the second column of the figure, where only persistent modes are used and the growth rates are set to zero. Nevertheless, even with 3 cycles, the reconstruction remains limited in accuracy, and 10 cycles are required to resolve finer-scale features—though the results still fall short of those obtained at the inlet.

Figure 5.9 presents contours of the v_x velocity component in the A–A' plane at $t^* = 19.25$,

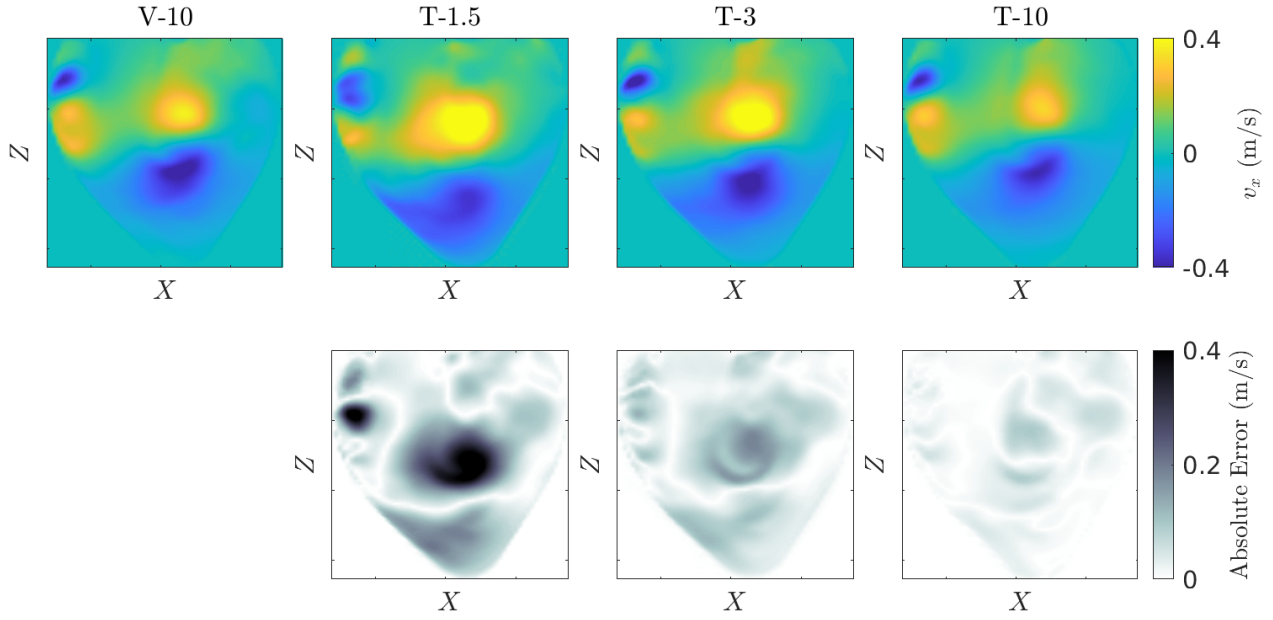


Figure 5.9: Counterpart of Fig. 5.6 for the `Ideal 2` model.

comparing configurations T-1.5, T-3, and T-10. The lower row shows the corresponding absolute error fields with respect to the reference solution V-10. For the T-1.5 case, the reconstruction error remains high; however, unlike in the `Ideal 1` model (see Fig. 5.6), the spurious outflow is absent. This may be attributed to the simpler vortex evolution observed in `Ideal 2`, where late-stage breakdown results in more coherent dynamics, as discussed in Chapter 4. Despite the limitations, the main flow structures are correctly captured.

Accuracy improves significantly with the T-3 configuration and is further enhanced with T-10, where the training data is more converged. Still, the results obtained with T-3—and even T-1.5—remain attractive considering the substantial computational savings compared to using 10 or more cycles.

These results become even more compelling when accounting for the computational cost reduction, as reflected in the speed-up factor (SUF). For this idealized case, the high-fidelity CFD simulation required approximately 48 hours on 40 CPUs to compute the interval between $t = 10$ and $t = 20$. In contrast, the ROM completed the same prediction in just 41 seconds, yielding an SUF of 1.7×10^5 .

As discussed in Sec. 5.1, a trade-off exists between ROM accuracy and computational efficiency. In the `Ideal 2` model, training with only 1.5 or 3 cycles drastically reduces both data volume and offline computational cost compared to using the full 10-cycle dataset. While the T-1.5 case already achieves reasonable accuracy, the T-3 configuration is preferred as it provides improved reconstruction performance with minimal additional cost.

Chapter 6

Discussion

6.1 General Discussion

The main focus of this Doctoral Thesis has been the modeling, analysis, and acceleration of intraventricular blood flow simulations using computational fluid dynamics (CFD) and data-driven methods. The different studies carried out across the manuscript address three major areas: (i) the impact of simulation setup on flow fidelity and computational performance, (ii) the extraction and interpretation of key flow patterns using machine learning tools, and (iii) the development of a predictive reduced-order model (ROM) based on higher order dynamic mode decomposition (HODMD). The discussion below synthesizes the key insights from each study and places them within the context of existing literature.

6.1.1 Simulation methodology and physiological fidelity

This work has shown that the accuracy of LV flow simulations is highly sensitive to choices made in the simulation setup. In particular, the use of idealized geometries enables a reduced computational cost while still reproducing essential flow features, such as the formation and evolution of the diastolic vortex ring. This trade-off between complexity and physiological realism is well known in the literature (Chnafa et al., 2014; Sotiropoulos et al., 2016), and our findings further support the use of idealized models as a first step toward understanding the core mechanisms of LV hemodynamics.

Among the two geometries investigated, **Ideal 1** and **Ideal 2**, the former is a semi-ellipsoid with two tubes attached at its base (modeling mitral and aortic valves as inlet and outlet respectively), representing more closely a healthy left ventricle due to its narrower chamber. Wall motion is prescribed to produce uniform volumetric changes extracted from flow-rate curves. In contrast, **Ideal 2**, derived from an *in silico* marker-based experiment (Vedula et al., 2014). The chamber is wider in comparison to its counterpart and has analogous inlet and outlet tubes.

The choice of laminar flow modeling and the incorporation of moving-wall boundaries allowed us to achieve realistic flow dynamics without relying on turbulence models, echoing prior

studies that report laminar-like behavior in the physiological Reynolds number range of the LV (He et al., 2022; Tagliabue et al., 2017). Furthermore, mesh refinement near the endocardial surface proved critical in resolving the small-scale flow features induced by wall motion.

Validation against commercial solvers (Ansys Fluent and STAR-CCM+) and literature (Kjeldsberg et al., 2023; Vedula et al., 2014; Zheng et al., 2012) confirmed the reliability of the proposed framework, with kinetic energy levels and vortex topologies in close agreement. This cross-verification strengthens the trust in our simulation choices and supports the reproducibility of the results.

6.1.2 Flow pattern analysis and modal decomposition

To better understand the internal flow dynamics and vortex evolution, we employed two modal decomposition techniques, proper orthogonal decomposition (POD) and HODMD, on both geometries under physiological inflow conditions. This analysis revealed that the fundamental frequencies driving the flow are consistent across geometries, but the modal content and coherence are highly geometry-dependent.

In **Ideal 1**, the strong inflow conditions generated an intense vortex ring that rapidly interacted with the chamber wall, resulting in an early and chaotic breakdown. This is reflected in the modal analysis, where POD modes are fragmented and affected by high-frequency interactions. In contrast, **Ideal 2** displayed a more ordered structure, with clearer modal separation and more interpretable dynamics. These results align with prior literature that associates smoother geometries with more stable vortex propagation (Le et al., 2012).

In terms of data-driven pattern extraction, our findings align conceptually with the recent study by Wu et al., 2023, which applied POD to left ventricular flow measured via 4D Shake-the-Box particle tracking. Both works reveal similar structures in the two-dimensional POD modes: a dominant recirculating pattern associated with the vortex ring in the most energetic mode, followed by increasingly fragmented structures indicative of an energy cascade. However, the present study builds upon this approach by incorporating spectral analysis through the fast Fourier transform (FFT) and systematically comparing the results with those obtained via HODMD. This combined spatial-spectral framework offers a more detailed interpretation of the underlying flow dynamics, particularly regarding vortex breakdown and transitions in flow regimes.

HODMD, by isolating specific frequencies, provided further clarity on the temporal evolution of vortex structures. It was particularly effective in identifying and separating the dynamics associated with the primary and secondary vortex rings. The cleaner separation observed in **Ideal 2** suggests that smoother flow conditions favor better decomposition in modes, which is crucial for future efforts in flow classification and patient-specific diagnosis based on modal features.

6.1.3 ROM development and acceleration

The final contribution of this thesis is the implementation of a predictive ROM based on HODMD (Le Clainche and Vega, 2017b). Unlike traditional uses of modal decomposition

focused on reconstruction or analysis (Corrochano et al., 2024; Lazpita et al., 2022), the ROM developed here forecasts future flow states using limited training data.

The approach demonstrated low error rates and strong spatial and temporal agreement with full-order simulations in both *Ideal 1* and *Ideal 2* cases. Its ability to provide accurate predictions using as little as 1.5–3 cardiac cycles as training data is especially promising for clinical translation, where data availability may be limited. The achieved speed-up factors ($\text{SUF} > 10^5$) represent a significant step toward real-time simulation capabilities, an area of increasing interest in cardiovascular modeling (Lopez-Perez et al., 2019; Müller et al., 2018; Pekkan et al., 2008).

Notably, the performance of the ROM is enhanced when the underlying flow is more structured, as seen in *Ideal 2*. This observation supports the notion that flow regimes with coherent modal content are more suitable for ROM applications (Rowley et al., 2004; Taira et al., 2017), which may inform future geometry design for modeling and data acquisition.

6.2 Novelty of the Thesis

This thesis delivers five main interrelated innovations, detailed across Chapters 2–6:

1. **Open-source automated CFD pipeline (Chapter 2).** A fully scripted workflow, from geometry import and cleanup to mesh generation, boundary-condition setup, solver execution and post-processing. Discussion of how geometry choices, boundary conditions and modeling assumptions affect results.
2. **Synthetic cardiac-motion generator (Chapter 2).** A parametric module prescribing wall displacement via volumetric curves for both idealized and patient-specific models. Outputs STL files and includes example scripts.
3. **Extended validation and feature visualization (Chapter 3).** Using *Ideal 1* and *Ideal 2* geometries, we compare velocity and vorticity fields against benchmark data. Vortex-core detection and vorticity contours highlight key flow structures.
4. **Data-driven pattern analysis of intracardiac flows (Chapter 4).** POD and HODMD on intraventricular flow databases to extract dominant modes and classify ventricular regimes. This framework reveals vortex-breakdown physics and, in the near future, may support discrimination of healthy versus pathological patterns.
5. **Reduced-order model for rapid cycle prediction (Chapter 5).** A ROM based on HODMD that predicts subsequent cardiac cycles with high accuracy from as few as three initial cycles, achieving substantial computational speed-up.

Chapter 7

Conclusions

This doctoral thesis has undertaken a comprehensive study of intraventricular flow using advanced computational tools and modal analysis techniques, with the ultimate goal of contributing to a deeper understanding of cardiac dynamics and their potential clinical implications. The main focus has been on the generation and evolution of the diastolic vortex ring, one of the most representative structures of left ventricular (LV) flow and a potential functional indicator of cardiac health.

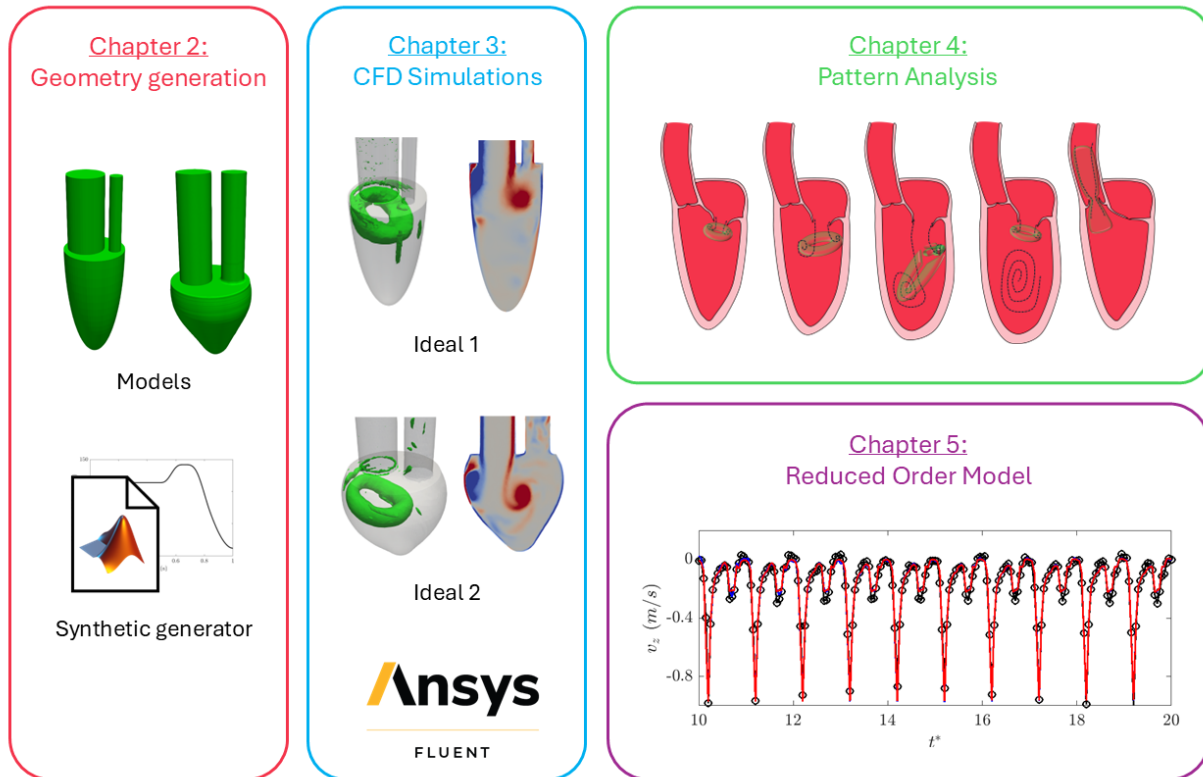


Figure 7.1: Summarizing scheme of the main developments of the present Doctoral Thesis.

First, a robust numerical methodology was developed to simulate intraventricular flow, incorporating physiologically relevant features such as dynamic wall motion, pulsatile boundary conditions, and suitable numerical schemes to resolve the transient and complex nature of cardiac flow. This computational framework (described in Chapter 2) allowed for the accurate capture of key diastolic flow features, including the formation, propagation, and eventual breakdown of the vortex ring, in agreement with previous benchmark studies.

To investigate the influence of anatomy on flow dynamics, two idealized LV geometries were employed. These geometries served as test cases to explore how morphological variations affect flow organization and vortex ring behavior. The results analyzed in Chapter 3, show that geometric differences lead to noticeable changes in the location, intensity, and stability of the main vortex ring. This confirms that even simplified models can capture essential aspects of flow mechanics inside hearts with distinct morphologies.

From a data analysis perspective, a dedicated postprocessing pipeline was developed to extract meaningful information from the simulation data in Chapter 4. Using modal decomposition techniques such as proper orthogonal decomposition (POD) and higher order dynamic mode decomposition (HODMD), dominant flow structures were identified, their temporal evolution characterized, and coherent modes associated with specific system frequencies estimated. The POD modes, combined with a fast fourier transform (FFT) analysis, revealed the main flow scales and their frequency content but often produced mixed-frequency modes, limiting interpretability. In contrast, HODMD provided a cleaner spectral separation and more coherent spatiotemporal patterns, allowing a clearer distinction between primary and secondary vortex dynamics. This approach offered a more structured and interpretable view of intraventricular flow, surpassing the limitations of purely qualitative visualization and enabling more precise analysis of flow regime transitions.

Finally, the potential of reduced-order models (ROMs) for efficient flow prediction was explored. In particular, the HODMD technique was employed to construct predictive models based on a limited set of snapshots. In Chapter 5, we demonstrate that future flow evolution can be predicted with high accuracy and significantly reduced computational cost compared to full-order simulations. A key finding is the trade-off between accuracy and computational efficiency: while models trained with only 1.5 cardiac cycles achieve substantial speed-ups (with speed-up factors exceeding 10^5), increasing the training set to 3 or more cycles yields noticeably better temporal and spatial fidelity. This balance allows the ROM to be adapted depending on the precision and real-time constraints of the intended application, paving the way for future deployment in clinical scenarios where both reliability and speed are essential.

Overall, the thesis addresses the key challenges originally posed; from building a CFD methodology that integrates wall motion and physiological conditions, to developing tools for modal analysis and reduced-order prediction. The contributions made represent a step toward more accessible, interpretable, and clinically applicable models, with the potential to be integrated into broader frameworks for personalized simulation and diagnostic support.

7.1 Outlook and Future Directions

This thesis opens multiple avenues for research in three broad areas: clinical translation, model extensions, and data-driven methods.

7.1.1 Clinical translation

- **Personalized geometries:** Incorporate patient-specific anatomies from MRI, CT or 3D echo to capture inter-individual variability and tailor simulations to patient physiology.
- **Clinical integration pathways:** Develop automated segmentation, boundary-condition extraction, uncertainty propagation and compliance protocols to enable point-of-care CFD workflows.
- **Pathological heart simulations:** Apply the framework to dilated or hypertrophic cardiomyopathy, valve regurgitation and other pathologies to identify hemodynamic biomarkers of dysfunction.

7.1.2 Model extensions

- **Complex flow regimes:** Extend to transitional and turbulent models (LES, RANS) to resolve multiscale phenomena in pathological conditions.
- **Fluid–structure interaction:** Implement fully coupled FSI with finite-element myocardium models to capture bidirectional blood–wall interactions.
- **Comparative studies:** Systematically compare idealized, healthy patient-specific and pathological geometries to define normative flow metrics and identify disease thresholds.

7.1.3 Data-driven methods

- **Expanded ROM validation:** Test the sparse-trained HODMD ROM across varied shapes, heart rates and loading conditions to assess uncertainty and generalizability.
- **Advanced pattern recognition:** Combine POD/HODMD modes with clustering or manifold learning to classify flow signatures and support patient stratification.
- **Hybrid machine-learning frameworks:** Integrate modal decomposition with autoencoders, LSTMs or physics-informed neural nets to capture nonlinear dynamics and improve predictive accuracy.
- **Real-time simulation platforms:** Develop interactive tools that couple fast ROM solvers with visualization interfaces for live assessment during interventions.

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