UNIVERSIDAD POLITÉCNICA DE MADRID

ESCUELA TÉCNICA SUPERIOR DE INGENIERÍA AERONÁUTICA Y DEL ESPACIO

Post-processing enhancement: feature detection and evaluation of unsteady/steady flows

Doctoral Thesis for
Ph.D. in Aerospace Engineering

Nuno Filipe da Costa Vinha
Aeronautical Engineer

MADRID, JUNE 2017

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Abstract

The exponential growth in computational capabilities, and the increasing reliability and precision of current simulation solvers, has fostered the use of Computational Fluid Dynamics (CFD) in the analysis of highly non-linear and complex flow problems. The nature of these flows usually involves a large number of scales and flow features, which makes it very challenging to achieve a clear understanding of the inherent problem. Additionally, current numerical simulations produce large amounts of raw data that needs to be evaluated. However existing post-processing tools are unable to extract with accuracy and efficiency all the valuable information contained in it.

Searching for meaningful structures through the entire dataset, by means of classical visualization techniques, might result in a fruitless, or at least inefficient, effort. Alternatively, with the use of flow feature detection and data decomposition techniques, the identification of the relevant features becomes much more straightforward, allowing more accurate visualizations and faster analysis, with lower uncertainties. In this thesis, these two promising post-processing approaches are studied, and applied to problems of physical and industrial relevance: a three-dimensional open cavity flow, and a Counter-Rotating Open Rotor (CROR) engine. On the one hand, amongst current feature detection techniques, Region-based (RB) vortex detection methods can delimit rotating regions in the flow, while Line-based (LB) ones are capable of reconstructing the imaginary center lines of the vortices. On the other hand, the Dynamic Mode Decomposition (DMD) is a recent tool used to decompose oscillatory dominated flows into spatial modes, with the advantage of associating each extracted dynamic mode to a single frequency.

At first, the DMD technique is employed to investigate the dynamics of saturation inside a rectangular open cavity. Previous experiments and linear stability analysis of the problem completely described the flow in its onset, as well as in a saturated regime, characterized by coherent three-dimensional centrifugal modes. The morphology of the modes observed in the experiments matched the ones predicted by linear analysis, but with a shift in frequencies for the dominant oscillating modes. This work presents a detailed numerical simulation of the entire saturation process, from 2D to 3D flow, shedding

some light on the main mechanism that produces the discrepancies encountered between both approaches. The capability of the DMD to analyze the underlying dynamics inside the cavity is demonstrated in this thesis, enabling to explain the main reason for the aforementioned differences in frequency.

Finally, some vortex detection algorithms are applied to the particular case of CROR, aiming the monitoring and visualization of the trajectory of the vortices generated at the tip of the front rotating blades. This is of critical importance to understand and prevent vortex-blade interaction with subsequent stages, as this non-linear flow topology strongly influences the aerodynamic performance and acoustic footprints of the engine. The suitability and performance of four typical Region-based (RB) vortex detection criteria, and one Line-based (LB) method, are firstly evaluated. Then, two new methodologies are introduced that improve the original assortment of seeds required by the tested LB method, as they increase the probability of the selected seeds to grow into a tip vortex line, providing faster and more accurate answers during the design-to-noise iterative process.

Resumen

El crecimiento exponencial de la capacidad de cálculo de los ordenadores, así como la elevada fiabilidad y precisión de códigos de simulación actuales, han motivado un uso cada vez mayor de la Mecánica de Fluidos Computacional (conocida por sus siglas en inglés, CFD) en el análisis de problemas de fluidos complejos y altamente no lineales. Estos flujos normalmente abarcan un gran número de escalas y estructuras fluidas, y su elevada complejidad hace que sea un desafío alcanzar una clara comprensión del problema inherente. Además, las simulaciones numéricas actuales generan grandes cantidades de datos que tienen que ser evaluados. No obstante, las herramientas de post-proceso existentes en la actualidad no permiten extraer con precisión, y de forma eficiente, toda la información relevante contenida en los datos.

La búsqueda de estructuras fluidas de relevancia a través de técnicas de visualización clásicas, podría resultar en un esfuerzo ineficaz o, al menos, ineficiente. Alternativamente, con el uso de técnicas de detección de estructuras fluidas y de descomposición modal, la identificación de las estructuras fluidas relevantes se hace de una manera mucho más directa, posibilitando visualizaciones más precisas y análisis más rápidos. En esta tesis, se estudian estas dos metodologías punteras de post-proceso, y se aplican a problemas con fuerte componente físico e industrial: el flujo sobre una cavidad abierta tridimensional, y el motor de rotor abierto (siglas en inglés CROR). Por un lado, y entre las técnicas existentes para la detección de estructuras fluidas, están los métodos de detección de torbellinos que delimitan zonas de flujo rotatorias (conocidos en inglés por métodos *Region-based*, RB), y los métodos que permiten la reconstrucción de las líneas imaginarias que siguen el centro de los torbellinos (conocidos en inglés por métodos *Line-based*, LB). Por otro lado, el método de descomposición dinámica de modos (siglas en inglés DMD) es una herramienta reciente utilizada para descomponer flujos con comportamiento oscilante en modos espaciales, con la ventaja de asociar cada modo dinámico a una sola frecuencia.

En primer lugar, la técnica de DMD se utiliza para investigar el proceso de saturación producido dentro de una cavidad abierta rectangular. Estudios anteriores, basados en experimentos y en análisis de estabilidad lineal del problema, permitieron una descripción

completa del flujo en un estado inicial, así como en un régimen saturado, caracterizado por la existencia de modos centrífugos tridimensionales. La morfología de los modos observados en la campaña experimental coincide con la obtenida a través de análisis de estabilidad, pero con diferencias considerables en frecuencia entre los modos oscilatorios dominantes. Este trabajo presenta una simulación numérica detallada de todo el proceso de saturación, desde el flujo 2D a 3D, centrándose en el mecanismo primordial que produce dichas discrepancias. La capacidad del DMD para analizar la dinámica relacionada con este problema se demuestra en esta tesis, permitiendo explicar la naturaleza principal de dichas diferencias.

En segundo lugar, se aplican algunos algoritmos de detección de torbellinos al caso específico de CROR, con el objetivo de rastrear y visualizar la trayectoria de los torbellinos generados en la punta de las palas. Esta información es indispensable para percibir y prevenir posibles situaciones de impacto entre torbellinos y las palas de los rotores subsiguientes, ya que esta situación influye negativamente en el comportamiento aerodinámico y acústico del motor. Primero, se evalúa la idoneidad y el desempeño de cuatro criterios fundamentales de detección de torbellinos RB, y de un método de detección LB. Posteriormente, se introducen dos nuevas metodologías que mejoran el proceso de inicialización requerida por el método LB implementado, facilitando resultados más rápidos y precisos durante el proceso iterativo de desarrollo.

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1

Introduction

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1.1 Preface

A thorough understanding of the physics involved in a fluid flow problem is of critical importance during the design and optimization process of any aircraft component, in the endeavour of achieving enhanced aerodynamic performance and minimized fuel consumption and emissions. This plays a vital role from the moment industry is committed to high aerodynamic efficiencies and low operational costs. Besides that, noise regulations within

the airspaces are becoming more and more strict, obliging the designers to be aware of any possible source of aeroacoustic noise being generated or interacting with the airframe. The design process is led by tight noise and performance requirements from a very early stage, thus requiring a deep and accurate investigation of the acoustic and aerodynamic behaviour of the flow.

The extraordinary growth in computational capabilities over the last few decades has enabled the numerical simulation of massive and complex flow problems with high accuracy. In the aerospace industry for example, the direct consequence of such exponential evolution has been the increasing reliance on Computational Fluid Dynamics (CFD) in the aircraft design process [47, 1], as it is illustrated in Figure 1.1. Around 1965 only potential models were used to design airfoils and wings, while in the present moment fully three-dimensional, time-dependent Navier-Stokes simulations are performed to model highly non-linear flow topologies in complex aircraft configurations, providing high-quality and high-fidelity solutions. Not surprisingly, CFD has become nowadays a crucial tool in the design of pioneering aircraft structures and engine architectures.

Figure 1.1: Evolution of the CFD models used inside Airbus over the last 50 years (adapted from [40, 10]).

One of the biggest drawbacks characterizing current numerical simulations is related

to the significant amount of raw data that these simulations often generate. In certain industrial problems, the size of a single solution snapshot can easily reach the order of Terabytes, demanding massive storing capabilities if saving several snapshots from an unsteady CFD simulation. Moreover, with a huge amount of CFD raw data, the complexity of the subsequent post-processing step is directly affected, and the time required to perform a detailed and accurate analysis of the flow is also increased. Depending on the level of complexity of the investigated flow problem, the time necessary to correctly post-process the entire CFD data might be of the same order of magnitude of the time already spent to converge the numerical solutions.

Because CFD simulations will undoubtedly continue to increase in size and complexity, one of the challenges that arises nowadays is the development of post-processing tools that allow an efficient, (i.e. without consuming excessive user's time and computational resources) and, at the same time, an accurate flow data processing and analysis, characterized by low uncertainties and minimum user input. State-of-the-art flow feature detection and data decomposition techniques should definitely play a more decisive role in current post-processing tools, with particular relevance to industrial flow problems. The general idea behind both techniques is to detect and extract parts of the original numerical domains, that contain structures or features of relevance for a certain academic or engineering problem.

1.2 Flow Feature Detection

When we have to analyse a huge amount of CFD data, possibly obtained from three-dimensional, large scale, unsteady simulations, the interpretation of the flow physics involved becomes naturally more straightforward by concentrating the analysis on certain regions of the whole flow field that contain information with physical meaning. Searching for those regions through the entire dataset, by means of classical direct visualization techniques, might result in a fruitless and inefficient effort. Alternatively, flow feature detection techniques aim to extract directly from the raw data regions containing a phenomena, structure, or object that is of interest for a certain engineering problem [70]. With

such an approach, the access to the original dataset is only required for the geometrical reconstruction of those features. Examples of flow features that can be found in nature are vortices or rotating flow structures, shock waves, boundary layers, and separation and attachment lines.

Conventional feature detection methodologies apply a set of numerical algorithms or schemes directly to a fluid data model, which can comprise CFD datasets, experimental measurements, or even analytical solutions. The purpose is to extract a certain physical or mathematical property of relevance, characterizing the flow field. The resulting output consists of a set of points, lines, surfaces, or regions that geometrically describe the identified feature, as Figure 1.2 exemplifies.

Figure 1.2: Examples of extracted flow features from the literature (top-left from [37]; bottom-left and top-right from [70]; bottom-right from [104]).

The advantages introduced by this feature-based post-processing approach are, as follows:

- *Higher level of abstraction:* the information content of the original dataset can be increased by simply extracting and preserving the important features contained on it [70]. This methodology favours also the identification of the relevant features of the flow in comparison with other visualization techniques, as the complexity of the visualization is reduced beforehand [68].

- *Large data-size reduction:* according to the work of Sahner [85], the original raw data content can be reduced to a very small fraction of it, which can reach the order of 1000 times [70, 57]. Moreover the data reduction is content-based only, ensuring that relevant information is not erased or lost throughout the entire extraction phase [70].
- *Batch processing:* the detection and extraction of the flow features can be computed concurrently, along with the CFD simulations [85], allowing important storage savings. For the particular case of an unsteady computation, we are able to extract features from the available snapshots without suspending or stopping the ongoing simulation. As soon as the detection algorithm completes its tasks for a certain snapshot, the unimportant data contained on that snapshot can be immediately erased, and the algorithm can then be instructed to execute the detection for the subsequent snapshot.
- *Faster and more efficient analysis:* this advantage is a direct consequence of the three previous points. As we are now focused on a much smaller amount of raw data with higher level of abstraction, the following post-processing step can naturally be shortened and performed more efficiently. Furthermore, the extracted features can still be described on both a qualitative and quantitative way, providing more realistic representations of the flow field. Ideally the feature extraction process should be done in an automated way, with minimum user interference, and targeting a variety of flow conditions and scenarios.

A standard feature extraction pipeline is shown in Figure 1.3. For more complex and demanding CFD simulations, the application of a feature detection algorithm directly to the original flow dataset may result in unclear and unfocused visualizations. This situation can be exemplified with the burner application of Guedot et al. [33], displayed on the right side of this figure. By increasing the grid resolution from 41 to 110 million points, and after applying the Q-criterion (more details about this vortex detection method will be given in Chapter 4), the authors were able to capture smaller vortical scales. Nonetheless, the visualization of the results obtained with the most refined mesh became even more blurred and unfocused, preventing, from the side of the user, an accurate interpre-

tation of the results. With the introduction of a condensation step right after applying the aforementioned feature detection algorithm to the original dataset, the authors were finally able to achieve a focused output with meaningful information content. This condensation step generally consists of thresholds, high-order filters, smoothing, reduction, simplification or mapping techniques, or even a combination of several methods, allowing a more effective representation of the most relevant structures.

Figure 1.3: Conventional feature extraction pipeline (adapted from [68]), exemplified on the right with the extraction of coherent vortices in a burner application, for two distinct grid resolutions (adapted from [33]).

Despite all the advantages introduced by feature detection techniques to the flow visualization field, there are still some important limitations that should always be taken into account, as pertinently discussed by Lively [57] in his thesis. The first problem is related with the computational burden required to execute a certain feature detection algorithm. If the extraction process takes too long, we are actually losing some of the aforementioned advantages. Nevertheless, this limitation can always be minimized by performing a concurrent feature detection, together with the CFD simulation.

The second drawback comes directly from the definition given to the feature that we are searching in the flow field. Different mathematical definitions describing the exact

same physical flow feature may arise within the fluid dynamics community, leading to the appearance of a plurality of feature extraction algorithms. A direct consequence of this situation would be that, for each feature, there is not one markedly superior algorithm that accurately extracts all features within the spacial and temporal flow domain, as stressed by Lively [57]. This is a very sensitive point for the case of vortex detection, as a precise and unique mathematical definition of a vortex has never existed in literature. After applying several vortex extraction methods to practical engineering test-cases, Roth [80] concluded that none of the methods is clearly superior in all the tested datasets. This suggests that each vortex detection technique aims to extract a certain type of vortex that appears in a particular flow problem. But in a completely different scenario, the same methodology might fail in capturing the existing vortices, or even return false positive results. This issue will be addressed with more detail in Chapter 4.

Similar problems can equally be observed for the case of shock-wave detection. In Ma et al. [59], the authors subscribe that no single best shock detection algorithm exists for locating and visualizing with accuracy all the three-dimensional shock waves. Obviously this situation is not desirable if we seek for an accurate and efficient iterative design or optimization loop, relying exclusively on feature detection methods. Moreover, any new flow solutions tested with multiple detection algorithms would have to be carefully validated first and, most of the times, experimental confrontation is not affordable.

More recently, computer vision and artificial intelligence concepts have been introduced in the field of flow feature detection. In his Ph.D. thesis, Roth [80] writes that future research directions should rely on systems that detect a certain feature according to a set of definitions, and then try to use knowledge about the strengths and weaknesses of each method to determine a single set. In the work of Gosnell et al. [31], an overview of the CAFÉ (Concurrent Agent-Enabled Feature Extraction) concept has been presented. Their idea uses subjective logic to determine in an autonomous way whether a detected feature exists effectively in the flow field, or it is a result of a false positive detection or a not converged CFD solution. The results obtained by the authors were quite promising about the capabilities of this new concept. However, its suitability for current industrial problems still needs to be demonstrated.

1.3 Flow Data Decomposition

Conventional flow feature extraction techniques usually apply a detection algorithm directly to the original raw dataset, as previously shown in Figure 1.3. In complex, time-dependent industrial flow problems, we can easily end up with several solution snapshots, and a huge amount of raw data to post-process. The time required to perform the detection of features might easily become too large in these cases, making it difficult to take full advantage of such a methodology. Furthermore, and citing Pobitzer et al. [68], a proper assessment on what can be removed and what can actually be retained in the data is very difficult to perform. This statement is even more evident when dealing with a complex, non-linear, and turbulent flow, whose spectrum is characterized by a plurality of coherent structures with different sizes, energies, and oscillation frequencies, that can also interact with each other.

One solution to overcome this drawback would be to perform a preliminary decomposition of the original data guided by the underlying dynamics of the flow field, by means of purely algebraic manipulations. The idea is to achieve a data size reduction taking into account the dynamic relevance of the different coherent structures contained in the whole flow field, ensuring at the same time that only the important dynamic features are selected [68]. This data decomposition based procedure is illustrated in Figure 1.4.

Data-sequences of snapshots collected from numerical simulations (or derived from experimental measurements as well) can be used to approximate the inherent fluid flow into dynamic modes, allowing thus the identification of the relevant coherent features of the flow. This process is achieved by means of a data matrix decomposition, as illustrated in Figure 1.5. The original input data matrix $\mathbf{S}$ contains several snapshots collected from CFD, that are sorted in here by space and time. This matrix can be constructed with one or several variables of the flow field, such as velocity, pressure, or vorticity fields, or with any other parameter that can track the dynamics of the system. The main aim is to decompose this data/snapshot matrix $\mathbf{S}$ into spatial structures/modes, contained in the columns of matrix $\mathbf{A}$, their respective amplitude or dynamical relevance, contained in the diagonal of $\mathbf{B}$, and their temporal evolution, contained in the rows of matrix $\mathbf{C}$ [91].

Figure 1.4: Feature extraction pipeline with a preliminary decomposition of the input data (adapted from [68]).

The most commonly used data-based decomposition techniques so far are the Fourier Transform analysis, the Singular Value Decomposition (SVD), the Proper Orthogonal Decomposition (POD) and, more recently, the Dynamic Mode Decomposition (DMD). The first approach is particularly efficient when dealing with periodic sampled solutions. However, it may lose accuracy when dealing with more complex, non-linear, and transient flow fields. With the SVD and POD, we are able to extract the relevant spatial structures in the flow, ranked by their energy content. By performing the SVD/POD to the velocity field for example, the information is sorted according to its kinetic energy. Nonetheless, the temporal behaviour of the extracted modes is characterized by the presence of multiple frequencies, as a result of the orthogonalization in space of the two decompositions. For a detailed and complete discussion about the POD and its relation to SVD, the reader is directed to the paper of Berkooz et al. [12] and to the book of Holmes et al. [41].

The SVD and POD are currently very attractive decomposition techniques in the

Figure 1.5: Decomposition of a flow data matrix.

post-processing of numerical and experimental data, mainly due to their ease of implementation, efficient energy-based analysis, inherent low computational cost, and possibility of application to large datasets or to sub-domains of a flow region. For these reasons, they are also widely used in the development of Reduced-Order Models (ROMs) for non-linear, time-dependent fluid flow problems. According to Rempfer [73] and Terragni et al. [102], these models are normally constructed by Galerkin projection of the governing equations onto bases of SVD/POD eigenfunctions, obtained from SVD/POD of the original sequence of snapshots. Nowadays ROMs can provide very accurate approximations of complex fluid flow problems, with reduced computational effort.

The DMD allows the extraction of spatial modal structures from a flow field, where each identified dynamic mode is associated to a single and unique frequency, consequence of the orthogonalization in time enforced to the temporal matrix $\mathbf{C}$ (see Figure 1.5). This decomposition technique is based on the Koopman analysis of a non-linear dynamical system [82], aiming to approximate the Koopman modes and eigenvalues of a linear infinite dimensional operator that describes the system. For a system with linear behaviour, the extracted DMD modes are expected to match the global stability modes. If the dynamic behaviour of the system is non-linear, the structures result from a linear tangent approximation of the underlying dynamics [90]. Rowley et al. [82] analytically demonstrated that the DMD is identical to a discrete temporal Fourier Transform, in case the dynamic decomposition is performed over periodic solutions. Contrary to the POD, the DMD does

not rank the extracted coherent structures in terms of energy content. However, their amplitudes can be recovered, providing a feedback about the individual contribution of a specific mode to the original system [92], and granting also to the DMD the possibility of obtaining models of lower complexity [48], as it already happens with the POD.

The DMD has demonstrated superior performance, over other traditional data-based decomposition techniques, for oscillatory dominated flow problems [92], and for fluid flows presenting strong peaks in the spectrum [64]. Its algorithm is relatively simple and of easy implementation, and with the DMD a sub-domain analysis is also possible [91]. Furthermore, Schmid [90] proved that this technique can alternatively be used in a spatial framework. Nonetheless, the DMD has still some relevant limitations, as recognized by Schmid [91] and Bagheri [5]. According to this last reference, there is yet no validation between Koopman and DMD modes for chaotic and noisy high-Reynolds number flows. Based on the work of Duke et al. [24], the decomposition can also be sensitive to the presence of noise in the flow field, and to aliasing. Besides that, in a flow characterized by a broad frequency spectrum without dominant spectral peaks, Muld et al. [65] observed no particular differences between the POD and the DMD modes. Finally, the standard DMD technique may not guarantee the best possible approximation of the flow field, allowing improved variants of its original algorithm to emerge. In the works of Jovanovic et al. [48] and Chen et al. [17] for example, optimization techniques are combined with the DMD to direct the selection of modes, and to improve the accuracy of the approximation.

1.4 Objectives and Motivations

The present thesis concentrates efforts on the development of post-processing tools that enable CFD users or experimentalists the detection and extraction of the relevant flow features existing in fluid flow problems. The identification of these features is performed according to different criteria and algorithms, and taking into account both academic and industrial needs. For this purpose, research and industrial activities were performed at UPM (Madrid), Airbus-SP (Getafe), and Airbus-GE (Bremen). It is expected that the developed numerical tools can provide valuable feedback to industrial designers that look for

improved aerodynamic configurations, and precious guidelines about possible mesh refinement areas, with the strong possibility to be combined with mesh adaptation strategies. These tools can also be utilized in a more academic framework to investigate the dynamics of fluid flows with high level of complexity, and to support the validation/evaluation of new CFD solvers or post-processing methods.

The first objective of this Ph.D. was to carry out an intense literature survey in order to collect state-of-the-art information on existing flow feature detection and data decomposition techniques, within CFD solutions. Amongst the several approaches found in literature, some vortex detection methodologies were chosen to analyse a particular aeroacoustic interest to Airbus-SP. On the other hand, the Dynamic Mode Decomposition (DMD) technique was selected, with the objective to investigate the spanwise dynamics of a typical academic time-dependent flow problem, such as the open cavity flow.

Regarding the first industrial campaign performed at Airbus-SP, the objectives to achieve were, as follows:

- Get familiar with the current software and numerical tools from Airbus, and with its working environment.
- Identify methodologies aiming at an efficient detection and tracking of vortical structures.
- Implement the selected algorithms in a completely industrial environment, using current Airbus post-processing tools.
- Validate and assess the implemented methods using typical large-scale test-cases from Airbus. The evaluation step should comprise: (1) strengths/weaknesses of each individual algorithm; (2) its computational efficiency; (3) prediction of possible spurious structures.

On the other hand, the following research objectives were proposed for the academic work carried out at UPM:

- Develop a generic numerical tool containing the DMD technique.

- From DNS solutions of a particular open cavity flow problem, use the aforementioned tool to completely describe the underlying spanwise dynamics, motivated by saturation of three-dimensional perturbations that linearly grow inside the cavity.
- Compare the DMD results with experimental and linear stability analysis data, previously obtained by our research group, and assess the suitability of this dynamic decomposition to the investigated flow problem.

In a last phase, a numerical tool containing a parallel version of the DMD was developed in Airbus-GE, in a completely industrial environment. The objective of this work was to extend the use of the DMD technique to a thoroughly industrial framework, particularly targeting complex, unsteady, and large-scale aeroacoustic problems that currently exist in Airbus.

1.5 Structure of the Thesis

The present thesis has been structured as follows:

- Chapter 1 provides an overall background of the project. It starts with a discussion of the advantages and benefits of including flow feature detection and data-based decomposition techniques in current post-processing tools. The objectives and motivations driving the present thesis are also depicted in this chapter. At the end, the relevant dissemination actions accomplished during the ongoing of the thesis are listed.
- Chapter 2 presents a complete numerical investigation of the saturation process in the open cavity flow, using the Dynamic Mode Decomposition (DMD) technique. After introducing the physical problem behind open cavity flows, and describing the numerical methodology used for this work, a preliminary study of the saturation process with simplified computational domain is shown. A detailed analysis of the dynamics of saturation inside the open cavity is then presented, reproducing the full dynamics of the experiments. At the end of this chapter, the main findings of this research are summarized.

- Chapter 3 extends the DMD technique towards industrial applications, by means of a parallel implementation of this method. A numerical tool containing the parallel DMD algorithm was implemented in Airbus, aiming large-scale unsteady industrial test-cases. Numerical details regarding its implementation and industrialization are provided in this chapter. Finally, in Section 3.3, the validation of this tool using an open cavity test-case is shown, and its computational performance evaluated.
- In Chapter 4, vortex-blade interactions occurring in a Counter Rotating Open Rotor (CROR) test-case are evaluated, utilizing flow feature detection techniques. After the introduction, a comprehensive review of the state-of-the-art in vortex detection is provided. Section 4.3 describes the numerical methodology, and briefly introduces the vortex detection library implemented in Airbus. The results obtained with this numerical tool applied to the CROR test-case are then discussed in Section 4.4. Two novel initialisation methods, that allow a more intelligent selection of candidate seeds in our line-based implementation, are suggested in Section 4.5. Finally, the most important conclusions reached with this industrial work are then summarized.
- Chapter 5 resumes the main conclusions and contributions of the present thesis, and discusses possibilities for future work.

1.6 The AIRUP Project and Industrial Placements

The present Ph.D. work was conducted within the European project AIRUP (*Airbus-UPM European Industrial Doctorate in mathematical methods applied to aircraft design*¹). AIRUP is an EC-funded academia-industry based project under the Marie Curie Initial Training Network (ITN) program, as part of the EU's Seventh Framework Program (FP7-PEOPLE), with grant agreement number PIAP-GA-2013-608087. Its main target is to foster R&D cooperation between academia and the aerospace industry sector, consolidating a joint Ph.D. training program between Universidad Politécnica de Madrid (UPM) and the following industrial partners: Airbus, Altran, and INTA.

¹<http://www.airup-itn.eu/home/about-airup>

Research and industrial activities were developed at UPM (Applied Mathematics Department in Madrid, Spain), Airbus-SP (EGDCS Flight Physics Capability Development in Getafe, Spain), and Airbus-GE (EGDCB Flight Physics Capability Development in Bremen, Germany). The chart in Figure 1.6 shows how these activities were distributed in time, and specifies the total number of months spent in the aforementioned organizations.

Figure 1.6: Distribution of the academic and industrial secondments.

1.7 Scientific Publications and Conferences

The publications resulted from the present Ph.D. work are listed in this section. This thesis combines most of the contents already presented in the publications listed below, together with some additional technical details.

- **Journal papers:**

- **N. Vinha**, F. Meseguer-Garrido, J. de Vicente, and E. Valero. Numerical investigation of the saturation process in an incompressible cavity flow. Submitted to *Journal of Fluid Mechanics*.
- **N. Vinha**, D. Vallespin, E. Valero, and V. de Pablo. Evaluation of vortex-blade interaction utilizing flow feature detection techniques. Submitted to *Aerospace Science and Technology*.
- **N. Vinha**, F. Meseguer-Garrido, J. de Vicente, and E. Valero. A dynamic mode decomposition of the saturation process in the open cavity flow. *Aerospace Science and Technology*, 52:198-206, 2016.

- **Patents:**

- **N. Vinha**, D. Vallespin, E. Valero, and V. de Pablo. Computer aided-method for a quick prediction of vortex trajectories on aircraft components. Patent Application No. 16382603.5 - 1954, filed on 15.12.2016.
- **N. Vinha**, D. Vallespin, E. Valero, and V. de Pablo. Computer aided-method for a quick prediction of vortex trajectories on aircraft components checking high pressure gradients and high drag friction components. Patent Application No. 16382604.3 - 1954, filed on 15.12.2016.

- **Conferences:**

- **N. Vinha**, F. Meseguer-Garrido, J. de Vicente, and E. Valero. A numerical study of the saturation process in an open cavity flow. In *Proceedings of the 46th AIAA Fluid Dynamics Conference*, Washington, D.C., June 2016. AIAA 2016-3316.
- **N. Vinha**, D. Vallespin, E. Valero, and V. de Pablo. Evaluation of vortex-blade interaction utilizing flow feature detection techniques. In *13th U.S. National Congress on Computational Mechanics*, San Diego, CA, July 2015. USNCCM13-589.

2

Numerical Investigation of the Saturation Process in the Open Cavity Flow

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2.1 Introduction

The open cavity flow problem has been extensively investigated in literature, aiming to predict and understand the relevant flow instabilities emanating inside cavities. This problem appears in numerous industrial applications, including open roofs on motor vehicles, landing gears in aeroplanes, or even weapon bays. Understanding the richness of the physics involved in this problem is therefore indispensable to the designers in their endeavour of reducing noise levels, vibrations, and drag in open cavity configurations.

The majority of the early work focused on the two-dimensional flow/acoustic resonance that produces self-sustained oscillations in the shear layer, commonly known as the Rossiter modes [79, 76, 78]. As the incoming flow goes through the leading facing step of the cavity, recirculation vortices are developed and travel with the flow, impinging the rear face of the cavity and generating acoustic pressure waves that propagate upstream. These waves will reach the leading edge of the cavity, creating an acoustic feedback mechanism that continually reinforces the shear layer oscillations, resulting in vortex-shedding at the leading edge [71]. This resonance process is illustrated in Figure 2.1.

Figure 2.1: Resonance mechanism in open cavity flows.

In compressible flow, Rossiter modelled an empirical formula to predict the discrete locked-on frequencies of the self-sustained modes, based on the parameters free-stream

velocity and cavity length [72, 79]. Subsequent studies demonstrated that the acoustic feedback phenomenon is instantaneous in the incompressible regime (Mach number = 0) [87, 8, 109].

Further research observed a modulation of the shear layer modes at smaller frequencies [77, 51, 111, 55, 66], as a result of the onset of centrifugal instabilities along the recirculating flow [96] that causes the growth of three-dimensional coherent structures, pulsating and coiling around the main recirculating vortex inside the cavity [9]. The distribution of such spanwise perturbations inside a rectangular open cavity is exemplified in Figure 2.2, for illustrative purposes only. The first linear computations of these three-dimensional instabilities were presented in Theofilis and Colonius [103], and they were proven to be dominant under certain flow conditions [13], as well as independent from the two-dimensional shear layer modes. More recently, experimental campaigns have focused in the characterization and visualization of these centrifugal modes, such as the work of Faure et al. [26] and Basley et al. [8].

Figure 2.2: Spanwise instabilities inside an open cavity.

For a deeper understanding of the physics involved, an extensive parametric study of the three-dimensional dynamics inside the cavity, using linear stability analysis, was presented in Meseguer-Garrido et al. [63] for the incompressible limit. By investigating the behaviour of the linear eigenmodes for the significant parameters of the problem (i.e. length-to-depth aspect ratio of the cavity L/D ; Reynolds number based on the cavity

depth Re_D ; incoming boundary layer momentum thickness θ_0/D ; and spanwise length of the perturbation L_z/D , which can also be considered through the spanwise wavenumber, β), the authors were able to extract the morphological structures and characteristic frequencies of the eigenmodes, and present neutral stability curves and dependence laws between the different parameters.

In de Vicente et al. [22], the results described by linear analysis were compared to experimental results for two different setups, in a $L/D = 2$ cavity: $\text{Re}_D = 1500$ (Case A), and $\text{Re}_D = 2400$ (Case B). The main coherent structures present in the saturated and wall-bounded regime were found to match the ones of linear stability analysis, given the difference in flow conditions. Nonetheless, one of the main results obtained from the aforementioned experimental campaign was the apparent reduction of the characteristic frequencies of the most energetic Fourier eigenmodes from the theoretical value predicted by the linear analysis. The authors postulated that this frequency reduction was a consequence of the presence of the spanwise walls, which had the effect of slowing down the main centrifugal recirculation vortex, thus reducing the characteristic Strouhal number of these structures. Other possible sources for this phenomenon not considered in de Vicente et al. [22] could be the saturated regime of the flow, or the onset of non-linear interactions between several unstable eigenmodes.

In an attempt to separate these three effects, a preliminary numerical study on the saturation phenomena was presented in Meseguer-Garrido et al. [62]. Three-dimensional Direct Numerical Simulations (DNS) were performed for the same flow parameters of the above-mentioned cases A and B. The effect of the presence of end-walls was neglected by setting periodic boundary conditions on the simulations. Moreover, a restriction was done on the spanwise wavenumber β to limit the number of interacting eigenmodes, leaving the saturation as the main mechanism present in the study. This work relied only on the analysis of instantaneous snapshots, as well as on the evolution of several flow variables at one control point. The authors also detected similar reduction of characteristic Strouhal number in the DNS results, however no relevant conclusions could be drawn once the saturated state had been reached, due to the high complexity of the flow.

The present chapter endeavours to further investigate the physics that led to the

reduction of the characteristic Strouhal number of the most energetic mode, extending the previous research of our research group [22, 63, 62, 61] on the spanwise dynamics of saturation inside the open cavity. For this purpose, new three-dimensional unsteady DNS of the incompressible fluid flow over the rectangular open cavity of Meseguer-Garrido [61] were employed, and the results were analysed using the original formulation of the Dynamic Mode Decomposition (DMD) technique [90]. Using this methodology, we also seek to track the evolution of spanwise instabilities of the flow inside the cavity, and understand the possible interactions that may occur between different dynamic modes. Some implementations of this tool for cavity problems can be found in the literature [94, 30, 27, 107]. The case studied and presented in this thesis corresponds to the experimental case B of de Vicente et al. [22] ($Re_D = 2400$), as it is characterized by a greater variety of linearly unstable modes [61]. The numerical details of the different methods used in the present investigation are explained in Section 2.2.

In a preliminary study, the DMD technique was applied to the incompressible open cavity flow from the linear to the saturated regime, restricting the spanwise length of the computational domain L_z/D to $2\pi/6$ in order to simplify the analysis. By doing this, we were able to reduce the amount of interactions between the different modes, guaranteeing that only the modes of β multiple of 6, which are those corresponding to the β of maximum amplification of the linear modes ($\beta = 6$ and $\beta = 12$), appeared in the DNS solutions. As in Meseguer-Garrido et al. [62], spanwise periodic boundary conditions were imposed to avoid the effect of the presence of spanwise bounding walls. The results derived from this first analysis are presented in Section 2.3, and were already published in the paper of Vinha et al. [107].

In Section 2.4, a deeper analysis of the entire saturation process in the open cavity flow is presented. Additional DNS simulations of the full open cavity geometry were performed for the same inflow conditions of the experimental case B of de Vicente et al. [22], with a spanwise length of the computational domain L_z/D in agreement with the experimental one. Thus, the forced selection of spanwise wavenumber is diminished, allowing a greater variety of modes to interact. Two distinct spanwise boundary conditions were imposed in order to determine the true nature of the reported drop in the characteristic Strouhal

number: spanwise walls bounding the computational domain, in an attempt to capture the full dynamics of the experiments; but also spanwise periodic boundary conditions to cancel the effect of the presence of walls, allowing more comprehensive comparisons. The original DMD technique was again applied to both cases, allowing the identification of the relevant dynamic modes within the saturated flow. Both temporal and spatial modal analysis were performed to capture the frequency and spanwise wavenumber of the relevant perturbations. The validity of this research was also assessed considering the experimental results of de Vicente et al. [22] and Basley [7], and the ones obtained using linear stability analysis in Meseguer-Garrido et al. [63] and Meseguer-Garrido [61].

2.2 Numerical Methodology

2.2.1 Problem Description

A schematic representation of the flow configuration is depicted in Figure 2.3. The parameters that completely define the incoming flow are: (i) the Reynolds number based on cavity depth (Re_D), and (ii) the incoming boundary layer momentum thickness (θ_0/D). The geometrical parameters of the cavity are: (i) the length-to-depth aspect ratio (L/D), and (ii) the wavelength in the spanwise direction normalized by the cavity depth (L_z/D), related with the corresponding wavenumber $\beta = 2\pi/L_z$. The case studied in the present work corresponds with the experimental case B of de Vicente et al. [22], with $Re_D = 2400$ and $\theta_0/D = 0.036$, in a cavity with geometrical parameters $L/D = 2$. In Section 2.3, the spanwise length of the cavity was restricted to $L_z/D = 2\pi/6$, as explained in the introduction of the present chapter. In Section 2.4, this parameter was set to $L_z/D \sim 10$, to match the experimental setup of de Vicente et al. [22].

2.2.2 Linear Stability and Experimental Analysis

The linear stability theory is concerned with the evolution of disturbances of small amplitude superimposed over a basic state ($\bar{\mathbf{q}}$). In this case, BiGlobal instability analysis, in

Figure 2.3: Schematic description of the three-dimensional rectangular open cavity, and problem parameters.

which the three-dimensional space comprises an inhomogeneous two-dimensional domain which is extended periodically in z , was used to analyse the flow over an open cavity.

The linearisation of the incompressible Navier-Stokes (NS) equations around $\bar{\mathbf{q}}(x, y)$ results in:

$$\mathbf{q}(x, y, z, t) = \bar{\mathbf{q}}(x, y) + \epsilon \hat{\mathbf{q}}(x, y) e^{i(\beta z - \omega t)}, \quad (2.1)$$

giving rise to the following complex generalised eigenvalue problem:

$$\mathbf{A}(\bar{\mathbf{q}}) \hat{\mathbf{q}} = \omega \hat{\mathbf{q}}, \quad (2.2)$$

where $\mathbf{A}(\bar{\mathbf{q}})$ is a linear NS operator.

The associated eigenvalue problem is then solved, for the determination of the complex eigenvalue:

$$\omega = 2\pi \frac{\text{St}_D U_\infty}{D} + i\sigma, \quad (2.3)$$

where σ is the amplification/damping rate of the disturbance, and the Strouhal number (St_D) represents the dimensionless frequency, based on cavity depth.

In the range of parameters close to the limit of stability, a detailed linear stability

analysis was performed by Meseguer-Garrido et al. [63], showing the presence of three main branches of unstable eigenmodes. These branches can be seen in the neutral curves for $L/D = 2$, depicted in Figure 2.4-A. The mode that becomes unstable at lower Reynolds number, Mode I (represented in red in Figure 2.4-A), is a travelling disturbance that is more unstable in the proximity of $\beta \simeq 6$ and $\beta \simeq 12$. Mode II (represented in blue in Figure 2.4), the second to become unstable, is stationary at higher β , and undergoes a bifurcation at $\beta \simeq 9$, resulting in a pair of complex conjugate eigenvalues (so it is also a travelling mode) for values of β lower than that. The third mode to become unstable, Mode III (represented in grey in Figure 2.4), is also a travelling disturbance with negligible relevance for the Reynolds number of the study ($Re_D = 2400$). A more detailed description of the BiGlobal analysis, base flow calculations, and nature and behaviour of the aforementioned modes can be found in Meseguer-Garrido [61].

Figure 2.4: Neutral stability curves for the $L/D = 2$ cavity in the Re_D vs β plane (A) (adapted from Meseguer-Garrido [61]). St_D vs β map of unstable eigenmodes for both experimental and linear stability analysis at $Re_D = 2400$ (B).

For this flow configuration, the comparison between linear stability and experimental results can be seen in Figure 2.4-B, for both Mode I and II in the $St - \beta$ plane. The red and blue symbols refer to the Modes I and II of the linear stability analysis, while the grey areas show the natural frequencies of the spanwise structures of the real flow in the experiments. This Figure shows the discrepancy on the Strouhal numbers, already

discussed in Section 2.1, between the $\beta = 2\pi$ eigenmode of Mode I (represented by A) and low- β branch of Mode II (represented by B) and the corresponding Fourier modes extracted from the experiments. The present chapter intends then to delve in the possible causes for those discrepancies in Strouhal number.

2.2.3 Direct Numerical Simulation

The numerical solutions required to construct the data-sequences of snapshots for the DMD were obtained by means of a three-dimensional unsteady DNS solver. The compressible laminar Navier-Stokes (NS) equations constitute a system of partial differential equations which can be written in vector form as:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = 0, \quad (2.4)$$

where $\mathbf{U}$ represents the vector of conservative variables, and $\mathbf{F}(\mathbf{U})$ represent the convective and diffusive 3D fluxes.

The computationally-demanding nature of the NS solution, in the stability analysis context, leads to the selection of high-order numerical schemes for the numerical discretization of system (2.4). High order, spectral type methods have been extensively used in computational fluid dynamics due to their accuracy and efficiency in the simulation of fluid flows. In particular, these methods are suitable for problems where high accuracy is required and, hence, are well suited to track the evolution of small flow perturbations.

In this context, a spectral discontinuous Galerkin method is used in this work to solve Equation (2.4). The original domain, Ω , is divided into non-overlapping hexahedral sub-domains, E_k , such that $\Omega = \sum_k E_k$. Inside each sub-domain, a polynomial of degree N is used to approximate the unknowns and the fluxes, $\mathbf{U}, \mathbf{F}$, thus:

$$\mathbf{U}^N = \sum_{i,j,k=0}^N \mathbf{U}_{i,j,k} \Phi_{i,j,k}, \quad \mathbf{F}^N = \sum_{i,j,k=0}^N \mathbf{F}(\mathbf{U}_{i,j,k}) \Phi_{i,j,k}, \quad (2.5)$$

where

$$\Phi_{i,j,k} = L_i(x)L_j(y)L_k(z)$$

is the tensor product of the Lagrange interpolant in the nodes i, j, k and $\mathbf{U}_{i,j,k}$ is the value of the unknown in each computational node. In this work, the nodes in each direction follow a Gauss-Legendre distribution, and the basis functions $L_{(i,j,k)}$ are taken as the Lagrange interpolant at these nodes.

Reconsidering Equation (2.4), we obtain, at an element level, the following discretized equation:

$$\frac{\partial \mathbf{U}^N}{\partial t} + \nabla \cdot \mathbf{F}^N = 0. \quad (2.6)$$

The Discontinuous Galerkin-Spectral Element method (DG-SEM [54]) makes use of the Galerkin weak form of the equations and a discontinuous treatment of the interfaces and boundaries. Thus, Equation (2.6) is multiplied by a test function (the same function as the basis for the Galerkin method) and integrated in the computational space. The error is then forced to be orthogonal at each test function $\Phi_{i,j,k}$ in a mesh element E_k , yielding:

$$\left(\frac{\partial \mathbf{U}^N}{\partial t}, \Phi_{i,j,k} \right)_{E_k} + (\nabla \cdot \mathbf{F}^N, \Phi_{i,j,k})_{E_k} = 0, \quad (i, j, k) = 0 \dots N,$$

with $(a, b)_{E_k} = \int_{E_k} ab \, d\mu$ defining an inner product (typically the L_2 -inner product). After integrating by parts we obtain:

$$\left(\frac{\partial \mathbf{U}^N}{\partial t}, \Phi_{i,j,k} \right)_{E_k} - (\nabla \Phi_{i,j,k}, \cdot \mathbf{F}^N)_{E_k} + \int_{\partial E_k} \Phi_{i,j,k} \mathbf{F}^N \cdot \mathbf{n} \, dS = 0, \quad (2.7)$$

where the third term (the surface integral) extends over the boundary ∂E_k of the computational element E_k , with external pointing normal $\mathbf{n}$. This boundary may lie at the interface between two elements or at a physical boundary condition and, in both cases, the treatment is similar. Note that all integrals in Equation (2.7) can be numerically evaluated using Gauss quadrature.

To obtain a solution over the complete discretized computational domain ($\Omega =$

$\sum_k E_k$), it is necessary to sum all the element contributions, as follows:

$$\left(\frac{\partial \mathbf{U}^N}{\partial t}, \Phi_{i,j,k} \right)_{\Omega} - (\nabla \Phi_{i,j,k}, \cdot \mathbf{F}^N)_{\Omega} + \sum_{\gamma \in \Gamma} \int_{\gamma} \Phi_{i,j,k} \mathbf{F}^*(\mathbf{n}, \mathbf{U}^L, \mathbf{U}^R) d\vec{S} = 0, \quad (2.8)$$

where Γ denotes the set of internal edges in the mesh Ω . In addition, note that we have replaced $\mathbf{F}^N$ by $\mathbf{F}^*(\mathbf{n}, \mathbf{U}^L, \mathbf{U}^R)$ in the surface integral. $\mathbf{F}^*(\mathbf{n}, \mathbf{U}^L, \mathbf{U}^R)$ represents the numerical flux between two consecutive elements in the mesh (**Left** and **Right**). This numerical flux arises from the discontinuous Galerkin setting, where we consider that each element is disconnected from the next, and hence contains a complete set of degrees of freedom to represent a polynomial of order N .

Taking into account the decomposition of the unknown (Equation (2.5)) and the orthogonality of the Lagrange basis in the Gauss nodes, the following expression is finally obtained for the integrals of Equation (2.8).

$$\frac{\partial \mathbf{U}_{i,j,k}}{\partial t} + \mathcal{D}_x \mathbf{F}_{i,j,k}^1 + \mathcal{D}_y \mathbf{F}_{i,j,k}^2 + \mathcal{D}_z \mathbf{F}_{i,j,k}^3 = 0, \quad \text{with } (i, j, k) = 0, \dots, N. \quad (2.9)$$

The discrete divergence (second term of the previous equation) is obtained after the numerical integration of the second and third terms of Equation (2.8). Gauss quadrature is used to evaluate these integrals, giving:

$$\begin{aligned} \mathcal{D}_x \mathbf{F}_{i,j,k}^1 &= \mathbf{F}^{1*}(x, y_j, z_k) \frac{L_i(x)}{w_i} \Big|_{x=0}^{x=1} - \sum_{m=0}^N \mathbf{F}_{m,j,k}^1 d_{i,m}, \\ \mathcal{D}_y \mathbf{F}_{i,j,k}^2 &= \mathbf{F}^{2*}(x_i, y, z_k) \frac{L_j(y)}{w_j} \Big|_{y=0}^{y=1} - \sum_{m=0}^N \mathbf{F}_{i,m,k}^2 d_{j,m}, \\ \mathcal{D}_z \mathbf{F}_{i,j,k}^3 &= \mathbf{F}^{3*}(x_i, y_j, z) \frac{L_k(z)}{w_k} \Big|_{z=0}^{z=1} - \sum_{m=0}^N \mathbf{F}_{i,j,m}^3 d_{k,m}, \end{aligned} \quad (2.10)$$

with

$$d_{m,n} = \frac{L'_m(s_n) w_n}{w_m}. \quad (2.11)$$

In the previous expression, w_n are the Gauss integration weights in x, y , or z dimension, $L'_m(s_n)$ is the derivative of the Lagrange interpolant evaluate in the node s_n , and $\mathbf{F}^*$ are the interface fluxes. These fluxes can be differentiated into viscous or inviscid.

Computation of inviscid fluxes requires taking into account the left and right values

of the unknowns at each interface. Let us note that by taking the average value of the unknowns $\mathbf{U}$ at the interface (equivalent to a central scheme), it provides a numerically unstable scheme when the convective terms dominate, and is only recommended at very low Reynolds numbers. For larger Re , an upwinding scheme should be used instead. The most common way to introduce upwinding in the scheme is by solving the equivalent Riemann problem at the interface. For the particular case of Euler equations (or inviscid NS), a different Riemann solver has already been developed. In this work, a standard Roe Riemann solver has been used in the computations [105].

The viscous fluxes require discretization for elliptic type equations. A simple approach consists of averaging the right and left viscous fluxes at the interface, but this solution has been proved numerically unstable for implicit schemes. A more general framework for derivation and analysis of discontinuous Galerkin methods for elliptic equations (e.g. Interior Penalty, Local Discontinuous Galerkin, Bassi-Rebay) was derived in Arnold et al. [4]. For additional details on implementation, methodology, and numerical validation of the employed spectral discontinuous tool, the reader is directed to Kopriva [54], Kopriva [53], Jacobs et al. [43], and Vinha et al. [107].

The DNS code used for the present work was compiled and executed using 64 nodes in the HPC cluster *Magerit*, installed in the Supercomputing and Visualization Center of Madrid (CeSViMa¹, Universidad Politécnica de Madrid).

2.2.4 Dynamic Mode Decomposition

The Dynamic Mode Decomposition (DMD) is a recent data-based technique, introduced by Schmid [90], that follows the Koopman analysis of a dynamical system [82, 64] to find the relevant spatial modes that evolve in a flow field, as previously introduced in Section 1.3.

Let's consider one has a dynamical system evolving on a manifold $\mathcal{M}$ such that, for all $x_i \in \mathcal{M}$:

$$x_{i+1} = f(x_i). \quad (2.12)$$

¹<http://www.cesvima.upm.es/infrastructure/hpc>

The Koopman operator is a linear operator $\mathbf{U}$ that maps g into a new function $\mathbf{U}g$, for any scalar-valued function $g : \mathcal{M} \rightarrow \mathbb{R}$, i.e.:

$$\mathbf{U}g(x) = g(f(x)). \quad (2.13)$$

Note that $\mathbf{U}$ is a linear infinite dimensional operator, although the dynamical system is non-linear and finite dimensional.

With the eigendecomposition of $\mathbf{U}$,

$$\mathbf{U}\phi_j(x) = \mu_j\phi_j(x), \quad (2.14)$$

we can expand the vector-valued observable g in terms of:

$$g(x) = \sum_{j=1}^{\infty} \phi_j(x)v_j, \quad (2.15)$$

where $\{v_j\}_{j=1}^{\infty}$ represents a set of vector coefficients called Koopman modes, corresponding to the observable g .

Using (2.14) and (2.13), iterates of x_0 are given by:

$$g(x_i) = \sum_{j=1}^{\infty} \mu_j^i \phi_j(x_0)v_j. \quad (2.16)$$

The Koopman eigenvalues $\{\mu_j\}_{j=1}^{\infty}$ completely characterize the temporal behaviour of the corresponding mode v_j :

- its phase determines the frequency of v_j ;
- its magnitude determines the growth rate of v_j .

The DMD aims to approximate the Koopman modes and eigenvalues from a finite set of snapshots. It is thus classified as a data-based technique because the only input required by this post-processing method is a set of data snapshots, coming from numerical simulations or experimental measurements. These flow field snapshots have to be collected with a constant sampling frequency, dictated by the Nyquist criterion. Therefore, in order

to avoid aliasing and a diverged decomposition, the data must be sampled at least at twice the highest frequency of the dynamic modes to be captured from the analysed flow field [3]. A snapshot matrix can then be constructed containing the selected N snapshots, temporally ordered and equally spaced by the aforementioned constant sampling time Δt :

$$\mathbf{V}_1^N = (v_1, v_2, v_3, \dots, v_N). \quad (2.17)$$

The matrix $\mathbf{V}_1^N$ may be composed of one or all available variables of the flow field. Figure 2.5 shows the shape of this matrix, and how the flow variables' array $\mathbf{v} = [u_1, u_2, \dots, u_i]$ is organized inside of it. Note that, in this figure, n_x , n_y , and n_z represent the total number of elements in the x , y , and z -direction, respectively. If we consider only one flow variable, the computational burden of the DMD is substantially reduced. Nevertheless, to describe more accurately the whole dynamics of the system, as much flow field variables as possible should be included, given that the basis of the dynamic modes are common to all of them [74].

Let's assume one has a linear dynamical system:

$$v_{i+1} = \mathbf{A}v_i. \quad (2.18)$$

The eigenvalues and eigenvectors of matrix $\mathbf{A}$ completely characterize the behaviour of the dynamical system.

The snapshot sequence of Equation (2.17) can be formulated as a Krylov sequence, as follows:

$$\mathbf{V}_1^N = (v_1, \mathbf{A}v_1, \mathbf{A}^2v_1, \dots, \mathbf{A}^{N-1}v_1). \quad (2.19)$$

The fundamental idea of the DMD is to extract the dynamic characteristics of the linear operator $\mathbf{A}$, which approximates the dynamical process between two consecutive snapshots in the sequence $\mathbf{V}_1^N$.

Suppose that we can express v_N as a linear combination of the previous $N - 1$ vectors,

$$\begin{array}{c}
\text{time} \xrightarrow{\hspace{10em}} \\
\begin{array}{c}
\downarrow \text{space} \\
\left[\begin{array}{cccc}
u_{1,1}(x_1, y_1, z_1) & u_{1,2}(x_1, y_1, z_1) & \dots & u_{1,N}(x_1, y_1, z_1) \\
\vdots & \vdots & \vdots & \vdots \\
u_{1,1}(x_{n_x}, y_1, z_1) & u_{1,2}(x_{n_x}, y_1, z_1) & \dots & u_{1,N}(x_{n_x}, y_1, z_1) \\
u_{1,1}(x_1, y_2, z_1) & u_{1,2}(x_1, y_2, z_1) & \dots & u_{1,N}(x_1, y_2, z_1) \\
\vdots & \vdots & \vdots & \vdots \\
u_{1,1}(x_{n_x}, y_2, z_1) & u_{1,2}(x_{n_x}, y_2, z_1) & \dots & u_{1,N}(x_{n_x}, y_2, z_1) \\
\vdots & \vdots & \vdots & \vdots \\
u_{1,1}(x_1, y_{n_y}, z_1) & u_{1,2}(x_2, y_{n_y}, z_1) & \dots & u_{1,N}(x_1, y_{n_y}, z_1) \\
\vdots & \vdots & \vdots & \vdots \\
u_{1,1}(x_{n_x}, y_{n_y}, z_1) & u_{1,2}(x_{n_x}, y_{n_y}, z_1) & \dots & u_{1,N}(x_{n_x}, y_{n_y}, z_1) \\
u_{1,1}(x_1, y_1, z_2) & u_{1,2}(x_1, y_1, z_2) & \dots & u_{1,N}(x_1, y_1, z_2) \\
\vdots & \vdots & \vdots & \vdots \\
u_{1,1}(x_{n_x}, y_{n_y}, z_{n_z}) & u_{1,2}(x_{n_x}, y_{n_y}, z_{n_z}) & \dots & u_{1,N}(x_{n_x}, y_{n_y}, z_{n_z}) \\
u_{2,1}(x_1, y_1, z_1) & u_{2,2}(x_1, y_1, z_1) & \dots & u_{2,N}(x_1, y_1, z_1) \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
u_{i,1}(x_{n_x}, y_{n_y}, z_{n_z}) & u_{i,2}(x_{n_x}, y_{n_y}, z_{n_z}) & \dots & u_{i,N}(x_{n_x}, y_{n_y}, z_{n_z})
\end{array} \right] = \mathbf{V}_1^N
\end{array}
\end{array}$$

Figure 2.5: Shape and composition of the DMD input matrix $\mathbf{V}_1^N$.

for a sufficiently long sequence of snapshots:

$$v_N = a_1 v_1 + a_2 v_2 + \dots + a_{N-1} v_{N-1} + r = V_1^{N-1} a + r. \quad (2.20)$$

We can also write Equation (2.20) in the form:

$$\mathbf{A}\{v_1, v_2, \dots, v_{N-1}\} = \{v_2, v_3, \dots, v_N\} = \{v_2, v_3, \dots, \mathbf{V}_1^{N-1} a\} + r e_{N-1}^T, \quad (2.21)$$

or in the following matrix form:

$$\mathbf{A} \mathbf{V}_1^{N-1} = \mathbf{V}_2^N = \mathbf{V}_1^{N-1} \mathbf{S} + r e_{N-1}^T, \quad (2.22)$$

where $\mathbf{S}$ is a companion matrix, defined as:

$$\mathbf{S} = \begin{bmatrix} 0 & & & a_1 \\ 1 & 0 & & a_2 \\ & \ddots & \ddots & \vdots \\ & & 1 & 0 & a_{N-2} \\ & & & 1 & a_{N-1} \end{bmatrix}.$$

By decreasing the residual term in Equations (2.20)-(2.22), the eigenvalues and eigenvectors of $\mathbf{S}$, given by $\mathbf{S}\mathbf{y} = \mu\mathbf{y}$, will converge towards some eigenvalues and eigenvectors of $\mathbf{A}$, since [34]:

$$\mathbf{A}(\mathbf{V}_1^{N-1}\mathbf{y}) = \mathbf{V}_1^{N-1}\mathbf{S}\mathbf{y} = \mu(\mathbf{V}_1^{N-1}\mathbf{y}). \quad (2.23)$$

As the present equation suggests, an explicit knowledge of matrix $\mathbf{A}$ is not required. The only unknowns are thus the coefficients $a_1, a_2, \dots, a_{N-1}$ of the companion matrix $\mathbf{S}$. The eigenvalues of $\mathbf{S}$ are usually named Ritz values, while the corresponding approximate eigenvectors are called Ritz vectors, being given by $\mathbf{V}_1^{N-1}\mathbf{y}$.

For a sufficiently long sequence of snapshots, the original DMD [90] performs initially a Singular Value Decomposition (SVD) on the snapshot matrix $\mathbf{V}_1^{N-1} = \mathbf{U}\mathbf{\Sigma}\mathbf{W}^H$, in order to compute the companion matrix $\mathbf{S}$. This guarantees higher robustness in the presence

of noise and other uncertainties, or in case of rank-deficiency data [92]. Substituting the SVD into $\mathbf{A}\mathbf{V}_1^{N-1} = \mathbf{V}_2^N$, and manipulating the resulting expression, one gets [92]:

$$\mathbf{U}^H \mathbf{A} \mathbf{V}_1^{N-1} \approx \mathbf{U}^H \mathbf{V}_2^N \quad (2.24a)$$

$$\mathbf{U}^H \mathbf{A} \mathbf{U} \mathbf{U}^H \mathbf{V}_1^{N-1} \approx \mathbf{U}^H \mathbf{V}_2^N \quad (2.24b)$$

$$\mathbf{U}^H \mathbf{A} \mathbf{U} \Sigma \mathbf{W}^H \approx \mathbf{U}^H \mathbf{V}_2^N \quad (2.24c)$$

$$\mathbf{U}^H \mathbf{A} \mathbf{U} \approx \mathbf{U}^H \mathbf{V}_2^N \mathbf{W} \Sigma^{-1} \quad (2.24d)$$

$$\tilde{\mathbf{S}} \approx \mathbf{U}^H \mathbf{V}_2^N \mathbf{W} \Sigma^{-1} \quad (2.24e)$$

Following this approach, we have reached a matrix $\tilde{\mathbf{S}}$ that can describe the dynamics of the unknown matrix $\mathbf{A}$, projected onto a POD basis. Note that the matrix $\mathbf{U}$ contains the POD spatial modes.

The following step consists on solving the eigenvalue problem $\tilde{\mathbf{S}}y_i = \mu_i y_i$. The dynamic modes can finally be recovered using the expression:

$$\phi_i = \mathbf{U} y_i, \quad (2.25)$$

where y_i represents the eigenvectors of $\tilde{\mathbf{S}}$, and $\mathbf{U}$ the left singular vectors of the snapshot sequence $\mathbf{V}_1^{N-1}$. The dynamic modes ϕ_i are then expressed in the POD-basis of $\mathbf{V}_1^{N-1}$. From the imaginary part (ω_i) and real part (σ_i) of the eigenvalues of $\tilde{\mathbf{S}}$, we retrieve the frequency information and growth rates of the dynamic modes, respectively.

Once the DMD assumes that each snapshot in the sequence $\mathbf{V}_1^{N-1}$ evolves in time by $e^{\lambda_i \Delta t}$, the eigenvalues of $\tilde{\mathbf{S}}$ can be expressed in terms of physical or dynamic information by:

$$\lambda_i = \frac{1}{\Delta t} \log \mu_i. \quad (2.26)$$

In order to recover the amplitude information of the DMD modes, and taking advantage that the dynamic modes ϕ_i are expressed in the POD-basis of $\mathbf{V}_1^{N-1}$, we can decompose matrix $\mathbf{V}_1^{N-1}$ into [92]:

$$\mathbf{V}_1^{N-1} = \mathbf{U} \Sigma \mathbf{W}^H = \mathbf{U} y_i \mathbf{D} \mathbf{C}, \quad (2.27)$$

or,

$$\mathbf{V}_1^{N-1} = \mathbf{\Phi} \mathbf{D} \mathbf{C}, \quad (2.28)$$

with $\mathbf{\Phi} = [\phi_1, \phi_2, \dots, \phi_{N-1}]$. Matrix $\mathbf{C}$ is a Vandermonde matrix that contains the identified discrete frequencies μ_i , being expressed by:

$$\mathbf{C} = \begin{bmatrix} 1 & \mu_1 & \mu_1^2 & \dots & \mu_1^{N-2} \\ 1 & \mu_2 & \mu_2^2 & \dots & \mu_2^{N-2} \\ \vdots & & & \ddots & \vdots \\ 1 & \mu_{N-1} & \mu_{N-1}^2 & \dots & \mu_{N-1}^{N-2} \end{bmatrix}.$$

$\mathbf{D}$ is the diagonal matrix containing the amplitude of the respective modes. To avoid an inversion of matrix $\mathbf{C}$ and an ill-conditioned operation, one has to look for the inverse of the amplitude matrix $\mathbf{D}$, following the expression [92]:

$$\mathbf{D}^{-1} = \mathbf{C} \mathbf{W} \mathbf{\Sigma}^{-1} \mathbf{y}_i. \quad (2.29)$$

Note that $\mathbf{D}$ is much easier to invert than matrix $\mathbf{C}$. With this approach, it is possible to recover all the amplitudes of the dynamic modes. Algorithm 2.1 resumes all the steps of the DMD technique.

Our DMD implementation was written in the Fortran programming language. For the computation of the SVD and eigenvalue problem, the subroutines *dgesvd* and *dgeev* of LAPACK (*Linear Algebra PACKage*²) were used, respectively.

2.3 Preliminary Study with Reduced Domain

2.3.1 Computational Setup and Numerical Details

The chosen flow conditions were the same as in the linear analysis, with the exception of the Mach number ($M = 0.2$). A good agreement between incompressible results from linear

²<http://www.netlib.org/lapack>

Algorithm 2.1 DMD (edited from [92]).

- 1: Split the snapshot sequence $\mathbf{V}_1^N$ into $\mathbf{V}_1^{N-1} = [v_1, v_2, \dots, v_{N-1}]$ and $\mathbf{V}_2^N = [v_2, v_3, \dots, v_N]$
- 2: Orthogonalize the left data matrix: $[\mathbf{U}, \mathbf{\Sigma}, \mathbf{W}] = \text{svd}(\mathbf{V}_1^{N-1})$
- 3: Pseudo-inverse onto the right data matrix: $\tilde{\mathbf{S}} = \mathbf{U}^H \mathbf{V}_2^N \mathbf{W} \mathbf{\Sigma}^{-1}$
- 4: Determine eigenvalues and eigenvectors: $[\mu, \mathbf{X}] = \text{eig}(\tilde{\mathbf{S}})$
- 5: Map eigenvalues into frequencies: $\lambda_j = \log \mu_j / \Delta t$
- 6: Reconstruct dynamic modes: $\phi_j = \mathbf{U} \mathbf{X}_{(:,j)}$
- 7: Form the Vandermonde matrix from the frequencies:

$$\mathbf{C} = \begin{bmatrix} 1 & \mu_1 & \mu_1^2 & \dots & \mu_1^{N-2} \\ 1 & \mu_2 & \mu_2^2 & \dots & \mu_2^{N-2} \\ \vdots & & & \ddots & \vdots \\ 1 & \mu_{N-1} & \mu_{N-1}^2 & \dots & \mu_{N-1}^{N-2} \end{bmatrix}$$

- 8: Compute the inverse amplitude matrix $\mathbf{D}^{-1} = \mathbf{C} \mathbf{W} \mathbf{\Sigma}^{-1} \mathbf{X}$
 - 9: Extract the amplitudes from the diagonal $d_j = \frac{1}{D_{j,j}^{-1}}$
-

analysis and the low Mach case of Brès and Colonius [13] is shown in Meseguer-Garrido et al. [63], once compressibility effects are still negligible at this low Mach number.

A multi-block structured mesh with a total of 104 hexahedral sub-domains was used for the DNS computations, with 9 sub-domains in the streamwise direction, 2 in the spanwise direction, and 8 in the normal direction. Inside each sub-domain, a polynomial of degree $(N_x, N_y, N_z) = (12, 12, 12)$ was defined. The streamwise length of the computational domain upstream of the cavity was set to half of the cavity's length ($L/2$), while the one downstream was set to two times the length of the cavity ($2 \times L$). The length of the domain above the cavity, in the y-direction, was defined to match the length of the cavity (L). As it was previously mentioned, the spanwise length of the computational domain was selected in order to reduce the amount of interaction between the different modes. By using a $L_z/D = 2\pi/6$ only the modes of β multiple of 6 can appear, and those correspond with the β maximum amplification of the linear modes ($\beta = 6$ and $\beta = 12$), as it could be seen in Figure 2.4 (right). The resulting three-dimensional grid is shown

in Figure 2.6 (top). The mesh generated near the walls was refined enough to compute accurately the boundary layer. This can be observed in Figure 2.6 (bottom), that depicts the mesh resolution in the near-wall leading edge region of the cavity.

Figure 2.6: Multi-domain structured mesh of the cavity at the: streamwise/normal plane (A); spanwise/normal plane (B), showing the location of the probe point P_1 (top). Boundary layer profile (black line) at the leading edge of the cavity, and grid lines in the y -direction (in red) near the wall (bottom).

Boundary conditions were always imposed in a weak form through the fluxes, normally solving a Riemann problem at the boundary. At the inlet of the computational domain, a Blasius compressible flow profile with boundary layer momentum thickness of $\theta_{inlet}/D = 0.034$ was imposed. Together with a $Re_D = 2400$, the latter guarantees an incoming boundary layer momentum thickness of $\theta_0/D = 0.036$ at the leading edge of the cavity, matching the one from the experimental Case B of Meseguer-Garrido et al. [63]. Spanwise periodic boundary conditions were used to avoid the effect of the spanwise walls,

as previously explained. At the solid wall boundaries, Dirichlet boundary conditions were applied for an adiabatic wall by prescribing a zero value of velocity at these boundaries. In the farfield region, constant free stream boundary conditions for the u -velocity, pressure, and temperature were imposed. The v -velocity was assumed to change according to a boundary layer flow at the same Reynolds number. Finally at the outlet region, the flow was supposed to recover the boundary layer profile of the unperturbed Blasius flow. Additionally, Neumann boundary condition for the viscous flux was also imposed.

For the chosen flow conditions the two-dimensional stationary solution was extended periodically in the whole domain, and then a random noise of 10^{-8} was introduced to kick-start the growth of the linearly unstable modes. The flow variables in a point P_1 located in the middle of the cavity, with coordinates $(x, y, z) = (L/2, -D/2, L_z/2)$ relative to the leading edge of the cavity, were recorded and snapshots of the whole flow field were saved each 10 non-dimensional time units.

2.3.2 Results

In the investigated fluid flow over a rectangular open cavity, five instability regions of spanwise velocity component are identified from the linear to the saturated regime, as reported in Meseguer-Garrido et al. [62]. Those five regimes can be seen in Figure 2.7, that shows the temporal evolution of the spanwise velocity component in the control point set in the middle of the cavity. A DMD was thus applied to regions II to V. Convergence for each regime was accepted when the residual norm of the DMD became sufficiently low, and when the eigenvalues corresponding to the most relevant dynamic modes became independent of the total number of snapshots comprising matrix $\mathbf{V}_1^N$.

Once the present research was only focused on the spanwise perturbations evolving inside the open cavity, and not on the whole dynamics of the system, the results presented and discussed in the following subsections are therefore those obtained from the DMD using only a single variable (the spanwise velocity component). With this approach, we avoid the introduction of the dynamics related to the two-dimensional shear layer modes into the decomposition, favouring the subsequent selection of the relevant 3D modes, while

reducing at the same time the computational costs of the DMD.

Figure 2.7: Temporal evolution of the absolute value of the spanwise velocity component in the control point P_1 , located in the middle of the cavity.

2.3.2.1 Regime I

The preliminary study conducted in Meseguer-Garrido et al. [62] shows that the behaviour of the DNS in the linear growth phase (region I of Figure 2.7) matches perfectly with the results predicted by linear analysis, with the most unstable eigenmode appearing and growing exponentially with the predicted σ . Those results will not be repeated here. The aforementioned study has also served as a validation for the DNS code.

2.3.2.2 Regime II

In regime II, after the linear growth phase, saturation of the leading mode occurs ($t = 500$) and the stationary disturbance starts to pulsate with a St_D of 0.0098. The physical morphology of the mode does not change, and the oscillation gets dampened with time. The St_D number of these oscillations matches the $St_D = 0.0099$ of the $\beta = 6$ branch of Mode II. The behaviour seems to be that after saturation the amplitude of the stationary

mode is too high, so it starts vibrating, and that vibration is progressively dampened. In this case, the mode is stationary, so it has no natural frequency, but the strong selection of L_z/D makes then the structure resonate at the characteristic frequency of the same branch of said mode at $\beta = 6$, even though the structures do not change their characteristic $\beta = 12$. This is a very interesting behaviour, as the mode tends to vibrate with a frequency which is somehow natural to it (although for a different β), even though for this β it is inherently stationary. The DMD analysis of regime II can be seen in Figure 2.8. The DMD results show a strong presence of a stationary mode (A), with a pulsation of the same structure (B). The morphology of these structures is identical to those of the stationary branch of the BiGlobal analysis (Figure 2.8 center and right, respectively).

Figure 2.8: DMD modes on regime II, obtained using 35 snapshots and starting the decomposition at $t = 650$. On the left, situation in the St_D vs β plane of DMD modes A and B (center). On the right, BiGlobal mode corresponding with point A (Mode II for $\beta = 12$).

2.3.2.3 Regime III

Once the oscillations characterizing regime II have almost vanished, a new mode starts to grow in regime III ($t = 1500$ to $t = 2100$). Figure 2.9 (top) shows two instantaneous flow fields belonging to that period of time, compared with the linear composition of the low β branch of Mode I and the high β branch of Mode II of linear analysis (bottom). The

oscillating mode has $\beta = 6$ and $St_D = 0.0194$, according to DNS results. That frequency is smaller than the one predicted from linear analysis ($St_D = 0.025$), but the identified mode is the same Mode I (Figure 2.9). As it was previously discussed, the reduction of the characteristic frequency of this dominant mode with $\beta = 6$ was already observed in the experimental work of de Vicente et al. [22]. These observations point to the fact that both the saturation process and the non-linear interaction of the modes are enough to produce the St_D reduction, without the presence of spanwise walls.

Figure 2.10 shows the results obtained with DMD for the same regime III. The short period of time and limited sampling frequency available, coupled with the nature of the growth of the second mode, constitutes a limitation for the DMD methodology. The two main structures that can be appreciated in this regime are the aforementioned mode A, still stationary and strongly resembling the stationary branch of BiGlobal Mode II, and a structure pulsating with $St_D = 0.019$ (mode C in Figure 2.10) that bears some similarity with the linear structure of $\beta = 6$ of Mode I (shown in the left part of Figure 2.9 bottom). In this case the mere composition of linear modes recover the instantaneous flow field.

2.3.2.4 Regime IV

The next step in the DNS evolution, regime IV ($t = 2100$ to $t = 2900$), features the apparition of a secondary oscillation in counter-phase with the main one, producing a shifting of the frequency to $St_D = 0.015$. This regime is at first stable in amplification, until $t \simeq 2700$. At this stage the iso-contour structures of spanwise velocity component exhibit such a complexity not easy to recreate by combinations of linear modes. The latter frequency is once more in the range of frequencies of high energy in the experiments of de Vicente et al. [22].

The results of the DMD analysis for this regime can be seen in Figure 2.11, and allow the separation of the flow features into identifiable structures. Mode A is still the stationary branch of the linear mode, although the mode has varied morphologically. Since the structures coiling around the main recirculating vortex have started breaking it, the modes are no longer restricted to coil around the exterior part of the vortex, filling

Figure 2.9: Two instantaneous flow fields in region III (top). Composition of the two linear β_6 and β_{12} branches of Mode II, which yields a similar flow field (bottom).

Figure 2.10: DMD modes on regime III, obtained using 25 snapshots and starting the decomposition at $t = 1600$. Situation in the St_D vs β plane of DMD modes A and C.

now a greater fraction of the cavity space. A similar phenomenon occurs to mode C which still corresponds, as before, with the linear mode in Figure 2.9, but with a frequency of $St_D = 0.015$ (also within the range of St_D of the dominant mode in de Vicente et al. [22]). Other structures appear here: one of $St_D = 0.030$ and $\beta = 12$, which corresponds with the aforementioned counter-phase oscillation (mode E); and another one in which two different β can be seen (mode D), with a frequency in line with the linear mode, $St_D = 0.025$. Since DMD does a separation by frequency, the two structures that oscillate with $St_D = 0.025$, one with $\beta = 6$ and the other with $\beta = 12$, get combined into a single DMD mode. It is reasonable to assume that the linear composition of different structures of the linear Mode I of different β could produce structures similar to mode D. On the other hand those two modes could correspond with flow features related with non-linear interaction between the different structures in the saturated regime. It seems relevant that the appearance of a mode with $St_D = 0.030$, which does not appear in the linear analysis nor was present in the experiments conducted in de Vicente et al. [22], coincides with the reduction of the characteristic frequency of mode C from $St_D = 0.019$

to $St_D = 0.015$, which is exactly half of the one of mode E. There seems to be some sort of coupling between those modes in frequency, with stable amplitude. That constant amplitude changes after $t \simeq 2700$, leading to regime V.

Figure 2.11: DMD modes on regime IV, obtained using 35 snapshots and starting the decomposition at $t = 2100$. Situation in the St_D vs β plane of DMD and modes A, C, E and D.

2.3.2.5 Regime V

After the breaking of the amplitude-stable counter-phase oscillation at $t \simeq 2700$ another change occurs, as the structures trespass the $x-y$ plane in the middle of the computational domain. This produces a drastic increase in the complexity of the structures present in the flow, as different packs of waves start travelling left or right, instead of just staying stationary, or pulsating without changing position. These complex structures characterize the behaviour of regime V ($t = 2900$ onwards). The possibility of having travelling structures appears in the linear analysis, as the non-travelling ones are just a single combination of complex conjugate eigenvectors; but once the flow starts developing this kind of structures, those shift in short periods of time. This might explain the poor convergence of the DMD technique for the present regime. The physics of the problem

still selects some natural frequencies, so the DMD modes are extracted with constant Strouhal numbers, but the shape of the modes varies greatly. Nevertheless, the results of the DMD of regime V can be seen in Figure 2.12, and some of the familiar structures are still present: the stationary mode A, the dominant mode C, or mode E. The nature of the mode on the $St_D = 0.021 - 0.025$ band experiences the most salient changes, as structures of all possible β (0, 6 and 12) merge in a single mode. An example of such is mode F in Figure 2.12.

Figure 2.12: DMD modes on regime V, obtained using 35 snapshots and starting the decomposition at $t = 2900$. Situation in the St_D vs β plane of DMD and modes A, C, E and F.

2.3.3 Overview

In this preliminary study using a cavity with limited spanwise length, we were able to identify with the DMD the two most relevant linear modes well outside the linear regime of the DNS computation. The description of the dominant structures in the five different flow regimes allowed us to better understand how the process of saturation affects the morphology of the modes, as well as their characteristic frequencies, without having to deal with the effects of spanwise walls, unavoidable in an experimental setup. The reduction of

the characteristic Strouhal number of the dominant mode was found again after applying the DMD to snapshots within the saturated regime, contradicting the hypothesis deduced in de Vicente et al. [22]. Nonetheless, the nature of this study and its simplifications have not proved sufficient to determine whether this effect is due to secondary instabilities on saturated flow, or to non-linear interactions occurring between the different dynamic modes. These issues are addressed with greater depth in the following Section 2.4.

2.4 Detailed Analysis of the Saturation Process

2.4.1 Computational Setup and Numerical Details

In a cavity with length-to-depth aspect ratio L/D to 2, two types of spanwise boundary conditions were investigated: spanwise bounding walls and spanwise periodicity. For the periodic case, the spanwise length was set to 10 times the one chosen in Section 2.3 (i.e. $L_z/D = 10 \times 2\pi/6$), while for the second configuration this parameter was fixed to $L_z/D = 10$, reproducing the same cavity domain as in the experiments of de Vicente et al. [22]).

A multi-block structured mesh with a total of 416 hexahedral sub-domains was used for the DNS computations, with 9 sub-domains in the streamwise direction, 8 in the spanwise direction, and 8 in the normal direction. Inside each sub-domain, a polynomial of degree $(N_x, N_y, N_z) = (12, 12, 12)$ was defined. The resulting three-dimensional grid generated for the DNS can be shown in Figure 2.13. Note that the grid generated near the boundaries was refined enough to compute the boundary layer with accuracy.

The numerical simulations were computed under the same flow conditions as the ones applied in the previous preliminary study. For additional details regarding the boundary conditions at the inlet of the computational domain, farfield region, and outlet region, the reader is thus directed to Section 2.3.1.

The two-dimensional stationary solution was again extruded periodically in the whole computational domain, and then a random noise of 10^{-8} was introduced to kick-start the

Figure 2.13: Multi-block structured mesh of the cavity at the: streamwise/normal plane (A) and spanwise/normal plane (B).

linear growth of the unstable modes. Solution snapshots of the whole flow field were saved within a period between 1 to 5 non-dimensional time units. The L_∞ -norm of the spanwise velocity component of the perturbed flow was also monitored as a function of non-dimensional time ($t = \tau U_\infty / D$) at several control points located inside the cavity, in order to determine the different flow regimes inside the cavity. This information is indispensable to perform the DMD, as it is discussed in the following subsection. Moreover, since the value of this velocity component is zero in the two-dimensional base flow, the whole effect corresponds to perturbation, giving greater detail about the underlying spanwise dynamics.

All the following DMD results were obtained considering only the spanwise velocity component into the decomposition. This choice was based on the reasons explained in

the previous Section 2.3.2, and permits modal analysis only focused on the spanwise perturbations developed inside the cavity. For bigger computational domains, such as the ones utilized in the present section, it also reduces significantly the computational cost associated with the DMD.

2.4.2 Cavity with Periodic Boundary Conditions

When periodic boundary conditions are imposed to the investigated open cavity flow, two instability regions for the spanwise velocity component are identified. These regimes can be seen in Figure 2.14-left, which shows the temporal evolution of spanwise velocity component for three control points placed inside the cavity, with different spanwise locations. The coordinates of those points are indicated above each curve in Figure 2.14-left. As expected, the aforementioned velocity component exhibits at these control points a linear growth phase followed by a saturated regime. As it is shown in Figure 2.14-right, the exponential growth slopes at the three DNS control points match the one predicted by the linear stability analysis. In the center of the computational domain differences between DNS and linear growth rates are within 1%, while in regions closer to the periodic boundaries discrepancies can reach 7%.

Figure 2.14: Temporal evolution of the absolute value of spanwise velocity component at three control points located inside the cavity, from the linear to the saturated regime (on the left). Detail of the linear zone in logarithmic scale, and comparison to linear analysis (on the right).

From Figure 2.14 it can also be inferred that saturation does not occur at the same

moment for the three investigated control points, due to the fact that a random numerical noise was imposed for the onset of spanwise perturbations. At P_1 and P_3 saturation of the leading mode happens around 700 time units, while at P_2 saturation seems to occur earlier. After the occurrence of saturation, the spanwise velocity component experiences an oscillatory behaviour with unstable amplitude at the three control points, with $St \approx 0.020$.

The DMD technique was applied to each of the identified regimes, in order to investigate the morphology and characteristic frequencies of the relevant modes appearing in each regime. Convergence of the DMD was assumed when the residual norm of the decomposition and the eigenvalues corresponding to the most relevant dynamic modes became independent of the number of snapshots comprising the initial matrix $\mathbf{V}_1^N$. The solution snapshots were also collected with a constant sampling frequency, which was selected taking into account the temporal evolution of the spanwise instabilities. The following subsections describe the most relevant results obtained with the DMD.

2.4.2.1 Linear Regime

A modal analysis was conducted by applying the DMD to the linear growth regime. Recovering the first solution snapshot at $t = 250$, this technique took 40 DNS snapshots temporally spaced by a constant $\Delta t = 5$. Note that only the spanwise velocity component was added to the snapshot matrix for the decomposition, as previously explained in Section 2.2.4.

The obtained DMD spectrum is compared to the BiGlobal stability analysis performed by Meseguer-Garrido et al. [63]. In Figure 2.15, the real and imaginary parts of the eigenmodes are plotted. The eigenvalues from linear stability analysis are coloured with respect to the wavenumber of the perturbations. We can observe that both frequency and growth rate of all unstable DMD modes are in agreement with linear stability analysis results. The dominant DMD modes in the decomposition, matching each branch of the most unstable BiGlobal modes (Modes I and II in Figure 2.4), were selected to evaluate the spatial wavenumbers of those modes. DMD modes A, B, and C correspond to the

stationary branch of linear Mode II, DMD mode D to the low- β branch of linear Mode II, and DMD modes E and F to the linear Mode I.

Figure 2.15: Comparison between the obtained DMD spectrum (in empty rhombus), and the linear stability analysis (in filled dots), coloured as a function of the spanwise wavelength of the linear eigenspectrum.

The morphology of the selected unstable DMD modes is represented on the left half of Figure 2.16 by iso-surfaces of spanwise velocity. On the right, the averaged results obtained from a space Fourier analysis of each DMD mode are shown. The spatial Fast Fourier Transforms (FFTs) were performed on the spanwise velocity component over several x positions in the $y/D = -0.1$ plane. The shape of the growing DMD mode A resembles the leading disturbance from linear stability analysis, displayed in the work of de Vicente et al. [22]. The FFT demonstrates an amplitude peak for $\beta = 11.6$, being this wavenumber in accordance with the BiGlobal analysis for the leading unstable mode. DMD mode A did not grow uniformly over the spanwise direction, as instabilities start growing first at the center of the cavity and later towards the periodic boundaries. This lack of isotropy over the spanwise direction can also be observed in DMD modes B and E, and it was already observed in the experimental work of de Vicente et al. [22]. The

random nature of the initial seeding makes that the base upon which the exponential growth starts, can be different in each part of the computational domain. In the same way, slight inequalities in the incoming flow on the experimental setup can affect the local morphology of the flow inside the cavity. Figure 2.16 shows also that the shape of all the unstable DMD modes is in agreement with linear stability results, as the wavenumbers retrieved by the FFTs match the β values of the corresponding linear eigenmodes (shown in Figure 2.15).

2.4.2.2 Transition to the Non-Linear Regime

In an attempt to characterize how transition from the linear to the non-linear regime is produced, a spatial Fourier analysis was conducted. From the beginning of the periodic DNS until $t = 1200$, spatial FFTs were performed on the spanwise velocity component, over several streamwise positions in the $y/D = -0.1$ plane. The results obtained are combined in Figure 2.17.

The linear growth phase can clearly be observed in Figure 2.17a. Modes with wavenumbers in the β range $11.5 - 12$ are the most unstable growing ones and dominate the spectrum until saturation of these modes occurs. These observations are consistent with the DMD analysis presented in Section 2.4.2.1 for the linear regime. Just before the leading modes saturate, at approximately $t \simeq 650$, we can observe that the slopes of the low- β growing modes suddenly increase, suggesting that saturation of the first modes triggers a faster growth of the latter. After this moment, $t \simeq 850$, the flow enters in a completely non-linear regime, with no apparent predominance of a certain spanwise perturbation over the others.

Figure 2.17b concentrates the FFT data for the saturated regime, allowing us to track in time the evolution of power spectral density (PSD) of a certain mode. In the first periods right after saturation, modes with wavenumbers around $\beta \simeq 9$ are clearly dominating the spectrum. Nonetheless the figure displays also an increase of the energy of space scales with wavenumbers in the proximity of $\beta \simeq 2\pi$, suggesting that these structures turn dominant after a short amount of time. The strong PSD oscillations in

Figure 2.16: Iso-surfaces of spanwise velocity (on the left) and spatial FFTs (on the right) of the selected unstable DMD modes in the linear regime. Coordinate axes shown in (a).

Figure 2.17b are related with the highly complex spanwise behaviour of the flow, and with non-linear interactions occurring between the different modes.

(a) Linear regime towards transition to the saturated regime.

(b) Saturated regime.

Figure 2.17: Spatial FFT power spectral density performed on the spanwise velocity component for each DNS snapshot. PSD is averaged for several streamwise locations in the $y/D = -0.1$ plane.

A spatial DMD analysis was additionally conducted in an attempt to track the evolution in time of structures with characteristic wavenumber in the order of $\beta \simeq 2\pi$. In the spatial framework, the DMD is able to split the spectrum into spanwise wavenumbers, retrieving modes evolving in the time dimension. For this purpose, solution snapshots with spanwise velocity $w(x, y, t)$ were taken at several spanwise positions, equally spaced by a Δz in accordance with the Nyquist sampling criterion. Once the computational grid

was not equidistant in the spanwise direction, Tecplot was used to extract the spanwise cuts inside the cavity, allowing afterwards to build the spatial DMD input matrix $\mathbf{V}_1^N$, as follows:

$$\mathbf{V}_1^N = [w(z_1), w(z_2), \dots, w(z_n)]. \quad (2.30)$$

For the DNS time interval $t = 250 - 1750$, Figure 2.18 shows the two dominant DMD modes obtained with the present spatial analysis, at the $y/D = -0.1$ plane. The spanwise velocity contours suggest that these modes are originated after the occurrence of saturation of the linearly growing modes. From $t \simeq 1100$, and according to the FFT results on the right, these spanwise perturbations pulsate with a dominant frequency $St \simeq 0.187$. These values express once again a strong agreement with the correspondent experimental results of de Vicente et al. [22].

Figure 2.18: Spatial DMD modes. On the left, spanwise velocity contours of the mode at the plane $y/D = -0.1$. On the right, averaged FFT spectrum of the spanwise velocity.

A three-dimensional representation of the morphology of these two spatial DMD modes is displayed in Figure 2.19, allowing to visualize in greater detail the evolution over time of these two prevailing spatial modes. From this figure, showing iso-surfaces of

the spanwise velocity component, it can be observed that structures composing these two modes begin their growth around $t \approx 750$. When transition to the non-linear regime is completely produced, these three-dimensional structures exhibit a coherent pattern over time, which represents no more than their dominant oscillation frequency (previously shown in Figure 2.17-right).

Figure 2.19: Three-dimensional representation of two dominant modes extracted from the spatial DMD analysis.

2.4.2.3 Saturated Regime

After an initial linear growth phase, saturation of the leading mode occurs, and perturbations start to fluctuate with a characteristic Strouhal number, as previously shown in Figure 2.14. This can also be seen in Figure 2.20, showing for a longer DNS time the evolution of spanwise velocity component at eight probes. These new control points are distributed over the two central sub-domains of the cavity, sharing the same axial and normal coordinates, but having different spanwise positions. Their coordinates are shown on the top of each graph in Figure 2.20. The close spanwise proximity between those points allows us to capture with higher confidence the nature and characteristics of the dominant perturbations occurring in a central region of the cavity. This also influences the sampling rate at which flowfield snapshots are taken from the DNS to perform the dynamic decomposition. All the aforementioned control points track a pulsating behaviour for the entire recorded time just after saturation, with a dominant frequency in the range $St \in (0.017, 0.020)$. These values are within the Strouhal number range of the most predominant dynamics revealed by the experiments of de Vicente et al. [22], and represented in Figure 2.4 by the grey area intersected by the blue horizontal dashed line C. This behaviour was not recovered by linear stability analysis.

Figure 2.20: Saturated regime inside the open cavity. Temporal evolution of the absolute value of spanwise velocity component at eight probes in the middle of the cavity $(0.5L, -0.5D, z)$, with different spanwise locations.

In a first attempt to clarify the space-time dynamics of the saturated flow, Figure 2.21 shows space-time diagrams over the spanwise direction, at the planes $y/D = -0.1$

and $x/D = 0.5$, for two different DNS segments: $1200 \leq t \leq 1700$ on the left, and $3000 \leq t \leq 3500$ on the right, being t the DNS dimensionless time. Contours of spanwise velocity component are shown in this figure. In the saturated regime, the flow is characterized by the presence of highly coherent left and right travelling waves. The phase velocity of these structures over the spanwise direction can be estimated from slopes in the space-time diagram (Δm), as depicted in Figure 2.21 by the lines (1), (2), (3), and (4), and it can provide a rough indication about the Strouhal number of these perturbations through the expression [7]:

$$\text{St} = \frac{w}{U_\infty} \frac{\beta}{2\pi} = \Delta m \frac{\beta}{2\pi}. \quad (2.31)$$

For the dominant wavenumber of the experiments, $\beta \simeq 6$, and $\text{St} \approx |\Delta m|$. The absolute values of the slopes drawn in Figure 2.21 are, as follows: $\Delta m_1 = 0.019$, $\Delta m_2 = 0.022$, $\Delta m_3 = 0.018$, and $\Delta m_4 = 0.017$. These values are in agreement with the experimental results described in the Part II of Basley [7], and suggest that the leading spanwise dynamics inside the cavity remain practically unchanged after the occurrence of saturation.

Figure 2.21: Space-time diagrams of spanwise velocity component, extracted at $y/D = -0.1$ and $x/D = 0.5$, for the DNS time intervals 1200 – 1700 on the left, and 3000 – 3500 on the right, with periodic boundary conditions. Lines (1) and (3) indicate left-travelling waves, while lines (2) and (4) right-travelling waves.

The aforementioned behaviour was also found after performing a spatial DMD analysis within the fully saturated regime, similar to the one presented in the previous Section

2.4.2.2. Figure 2.22 shows the reconstruction in (x, y, t) of a high-energy spatial DMD mode, with wavenumber $\beta = 6$, in the form of iso-surfaces of spanwise velocity component. Note that this decomposition was performed for the DNS time interval 2000 – 3000, after splitting the spanwise domain in 100 equally spaced cut sections. The shape of this mode does not suffer important changes within this time interval, indicating that it is pulsating around the recirculation vortex with a dominant frequency $St = 0.018$. This value was recovered by means of a FFT analysis at the plane $y/D = -0.1$. The results obtained from this preliminary spatial analysis are once again consistent with experimental data.

Figure 2.22: Spatial DMD mode with $\beta = 6$, and its FFT spectrum of the spanwise velocity averaged at the plane $y/D = -0.1$.

2.4.2.3.1 DMD Analysis The DMD was applied to the saturated regime, starting the decomposition at $t = 1222$. The results discussed in the present subsection were obtained using 272 DNS snapshots, temporally spaced one from each other 1 non-dimensional time units, (i.e. approximately five oscillation periods were covered), that demonstrated to be enough for a converged decomposition. Inside the $St \in (0, 0.030)$ range, the DMD technique captured nine modes, associated with nine eigenvalues of $\mathbf{S}$ with negative real part. These modes are plotted in the $\beta - St$ plane of Figure 2.23a, where to each DMD mode corresponds only a single frequency, represented in this graph by a set of horizontal

blue diamonds. In the $y/D = -0.1$ plane of each mode, spatial FFTs were performed on the spanwise velocity component over various x positions. In Figure 2.23a, the size of the blue diamonds is proportional to the amplitude of the averaged power spectral density in the above-mentioned plane. The DMD spectrum is also compared in this figure with linear stability analysis (BiGlobal) and experimental results, both derived from the work of de Vicente et al. [22].

The DMD performed for the present regime was able to capture the experimental modes, represented in Figure 2.23a by the grey regions. For each DMD mode, spanwise FFTs do not exhibit a dominant wavenumber, but instead a range of prevailing wavenumbers, as shown in the experiments. For a comprehensive comparison, four DMD modes with closer frequency to the experimental modes described in de Vicente et al. [22] were selected, in order of increasing St : stationary DMD mode A; DMD mode B with $St = 0.0059$; DMD mode C with $St = 0.018$; and DMD mode D with $St = 0.025$. Figure 2.23b displays the iso-surfaces of spanwise velocity for these modes, in the zy and zx planes.

DMD mode A contains several coherent structures with similar morphological shape along the entire spanwise direction, however with different wavenumbers. The spanwise FFTs in the $y/D = -0.1$ plane returned amplitude peaks within the range of $\beta \in (9, 12)$, resembling these structures the stationary branch of linear bifurcated Mode II. This mode comprises also low- β structures, as indicated by the FFTs and iso-surfaces of spanwise velocity, fitting the corresponding experimental shade. Note that the distribution of all these stationary structures inside the cavity is anisotropic.

Low- β perturbations can also be found in DMD mode B, with higher energy structures inside the range $\beta \in (4.8, 7)$. Along the spanwise direction, these structures can mainly be found in two portions of the cavity: $2.5 \leq z/D \leq 4.5$, and $7.5 \leq z/D \leq 10$. Even if these characteristic wavenumbers are slightly lower than the ones predicted by linear stability analysis, but within the range of the experiments, the associated structures seem to correspond to the oscillatory branch of linear Mode II. Moreover, the increase of Strouhal number with the decrease of associated spatial wavenumber can also be observed with the DMD.

(a) Extracted DMD modes in the $\beta - St$ plane. Each mode is associated with a single frequency, represented by a set of horizontal blue diamonds. The size of the diamonds is proportional to the amplitude of the power spectral density performed on the spanwise velocity component of each DMD mode. DMD results are compared with data from BiGlobal (red dots) and experiments (grey areas) of de Vicente et al. [22].

(b) Iso-surfaces of spanwise velocity of the aforementioned DMD modes, in the zy and zx planes.

Figure 2.23: Extracted DMD modes for the saturated regime, starting the decomposition at $t = 1222$ and using 272 DNS snapshots.

DMD mode C is inside the Strouhal range of the most energetic mode of the experiments, oscillating with $St = 0.018$. Coherent low- β structures can be recognized in Figure 2.23b for this mode, being in agreement with the PSD peaks shown above between the range $\beta \in (4.8, 6.6)$. They can be favourably compared to the low- β structures of travelling linear Mode I, however with lower frequency but in accordance with the experiments. Similarly to what happens with the other discussed DMD modes within the saturated regime, and also in agreement with the experiments, these structures lose periodicity inside the cavity over the spanwise direction, and become anisotropic.

Finally, DMD mode D is characterized by the presence of some coherent high- β structures, confined to small spanwise subregions of the cavity (see $1.5 \leq z/D \leq 5$ and $7.5 \leq z/D \leq 10$). The highest FFT peak occurs for $\beta = 10.3$, nonetheless other relevant structures involving wavenumbers in the range $\beta \in (3, 12)$ are also obtained for this mode. Despite its highly dynamic complexity, this highly anisotropic mode exhibits properties that bear strong similarity to various eigenmodes of linear Mode I.

Similar DMD analyses were also carried out utilizing later time windows within the saturated regime into the decomposition, and their results resembled the dynamics already described in the present subsection and did not add new relevant information. Despite the highly non-linear and complex nature of the saturated flow inside the cavity, the DMD technique was able to identify the most relevant modes of the linear stability analysis and of the experiments. The reported drop in St was also revealed in the absence of spanwise walls, strongly suggesting that this effect is directly associated with the saturation process.

2.4.3 Cavity with Spanwise Wall Boundary Conditions

Similar investigation considering the effect of spanwise walls was also carried out. New computations were performed imposing solid wall boundary conditions at the spanwise limits of the computational domain, for the same inlet flow conditions of the periodic case. The evolution of the spanwise velocity component was tracked at eight control points, distributed over the two central sub-domains of the cavity. Figure 2.24 shows the temporal evolution of spanwise velocity at these probes, from the beginning of the DNS.

The coordinates of those control points are shown on the top of their corresponding plot. Contrary to what happened in the periodic study, a linear growth regime could not be recognized for the present case. The numerical noise introduced by the growth of the boundary layer due to the presence of the walls overcomes the artificial noise introduced to kick-start the DNS, triggering a faster growth of the linearly unstable modes.

Figure 2.24: Temporal evolution of the absolute value of spanwise velocity component at eight probes, in the middle of the cavity with spanwise walls.

From the beginning of the DNS all control points show a wavering growth phase, before spanwise velocity perturbations reach a saturated state at about $t = 420$. From this moment, the spanwise velocity component fluctuates with a dominant frequency within the range $St \in (0.017, 0.018)$, inside the St range of the most predominant dynamics revealed by the experiments (middle grey zone in Figure 2.4-B), and it is related with low- β travelling modes. These oscillations seems to reach a more stable regime around $t = 2000$ for the majority of the control points. Nonetheless its dominant frequency remains unchanged from saturation point till the end of the computation.

As in Section 2.4.2.3, space-time diagrams were constructed to track the temporal evolution of spanwise velocity perturbations in the saturated regime, with the presence of walls in the spanwise confinements of the cavity. Once again this variable was extracted at the $y/D = -0.1$ and $x/D = 0.5$ planes, for two distinct DNS windows: $500 \leq t \leq 1000$, on the left; $2000 \leq t \leq 2500$, on the right. These values were selected in order to allow a comprehensive coverage of the two main regions of velocity fluctuation previously displayed in Figure 2.24. The aforementioned diagrams are shown in Figure 2.25 in the

form of spanwise velocity contours.

Due to the presence of solid walls at $z/D = 0$ and $z/D = 10$, a thick vertical band appears in both diagrams next to these two boundaries, delimiting a region where no periodic or stationary structures stand out. The main differences between the left and right plots occur in the central region of the cavity, for $3.5 \leq z/D \leq 6.5$. In Figure 2.25-left, we can observe some vertical stripes within this central region, revealing the existence of stationary perturbations. Furthermore, left and right travelling waves coexist as well in the center of the cavity, as it is suggested by the slopes (5) and (6) drawn in this left diagram, with absolute value $\Delta m_5 = 0.021$ and $\Delta m_6 = 0.017$, respectively. As explained in the previous section, the phase velocity of the travelling waves can be deduced from these values.

Figure 2.25: Space-time diagrams of spanwise velocity component, extracted at $y/D = -0.1$ and $x/D = 0.5$, for the DNS time intervals 500 – 1000 on the left, and 2000 – 2500 on the right, with spanwise bounding walls. Lines (5) and (7) indicate left-travelling waves, while lines (6) and (8) right-travelling waves.

The central stationary oscillations tend to vanish with the increase of DNS time, as a result of saturation and non-linear interactions between the coexisting structures. In the space-time diagram of Figure 2.25-right, left and right travelling waves clearly dominate the spectrum inside the cavity. The absolute values of the slopes drawn in this right plot are: $\Delta m_7 = 0.018$, and $\Delta m_8 = 0.019$. For the dominant wavenumber of the experiments

($\beta \simeq 6$), these two slopes approximate the characteristic Strouhal number of the left and right waves (as previously shown by Equation (2.31)).

2.4.3.1 DMD Analysis

Two different DNS time frames were selected to perform the DMD analysis. The first one started at $t = 417$ and comprised 228 snapshots, while the second time interval started at $t = 1985$ and contained 291 snapshots. In both cases, the snapshots were equally spaced by a constant $\Delta t = 1$. These values were chosen after performing a DMD convergence study for the two cases. Furthermore, the spatial domain of the decompositions was reduced to the six central sub-domains of the mesh ($1.25 \leq z/D \leq 8.75$), in order to avoid the perturbations introduced by the presence of walls into the DMD, with the added benefit of reducing the computational cost of the decomposition.

Figures 2.26-2.27 resume the most important results obtained by means of the two DMDs. The plots of Figure 2.26 were constructed for the DMD started at $t = 417$, while the ones of Figure 2.27 for the DMD initiated at $t = 1985$. The modes extracted inside the $St = 0 - 0.030$ range are plotted in the $\beta - St$ planes of Figures 2.26a-2.27a, where the frequency of each mode is represented by a set of horizontal diamonds. Note that the corresponding eigenvalues of all these modes have a stable behaviour. The size of the plotted diamonds is once again proportional to the amplitude of the spatial Fourier averaged power spectral density, performed for both cases on the spanwise velocity component over various streamwise positions in the plane $y/D = -0.1$. The DMD spectrum is again confronted with data from linear stability analysis and experimental measurements, both obtained from the work of de Vicente et al. [22].

For the investigated wall-bounded cavity, both DMDs were capable to capture modes inside the three grey areas of the experiments, with a sharp abundance of wavenumbers inside them. For a deeper comparison between the experimental Fourier and BiGlobal modes, and the extracted DMD modes, four DMD modes with closer frequency to the experimental ones were chosen. These modes are labelled by circled letters A to D in Figures 2.26a-2.27a, in the order of increasing St . In the bottom, Figures 2.26b-2.27b

show the morphology of the DMD modes associated with those four letters, by means of iso-surfaces of the spanwise velocity component (blue A to D on the first figure for DMD started at $t = 417$; black A to D on the second figure for DMD started at $t = 1985$).

In Figure 2.26b, blue DMD mode A exhibits the most coherent structures in the center of the cavity, with wavenumbers in the order of $\beta \simeq 11$. Note that this value is close to the wavenumber for maximum amplification according to linear stability analysis ($\beta \simeq 12$), and in agreement with the experiments. We can also notice that structures of this same mode lose some coherence in the vicinity of the walls, due to the numerical establishment of the boundary layer. The existence of stationary structures mainly in the center of the cavity was also observed in the space-time diagram of previous Figure 2.25-left.

Black DMD mode A, belonging to the second DMD time interval considered for the present analysis and illustrated in Figure 2.27b, shows a different morphology compared to the blue DMD mode A. We can visualize now some well-defined structures within the spanwise range $3 \leq z/D \leq 5$, with wavenumbers around $\beta \simeq 9$, which is the bifurcation point from the stationary to the oscillatory branch of linear Mode II. Some other structures can be seen more to the right side of the cavity ($6 \leq z/D \leq 8$), indicating that the distribution of structures of this stationary mode is not any more uniform inside the cavity, but anisotropic as in the experiments.

Blue and black DMD mode B exhibit low- β structures with wavenumbers that match the experimental grey area of Figures 2.26a-2.27a, and they are confined to several portions of the cavity, as suggested by the iso-surfaces of spanwise velocity. Other structures with smaller wavenumbers emerge as well inside the cavity, possibly as a result of the growth of the boundary layer in the spanwise boundaries. Nonetheless, for the corresponding perturbation frequencies (blue DMD Mode B: $St = 0.0055$, black DMD Mode B: $St = 0.0048$), experimental measurements also detected highly anisotropic structures with a pronounced range of wavelengths in the spanwise direction.

Similar situation occurs with the two DMD modes D displayed in Figures 2.26b-2.27b, that are also characterized by a strong plurality of wavenumbers. Blue DMD

mode D is pulsating with a $St = 0.0248$, while black DMD mode with a $St = 0.0224$. The iso-surfaces of spanwise velocity display several highly anisotropic structures with certain coherence near the region of the walls, resembling some of the dynamics of the matching experimental mode. However these features are not relevant in terms of energy, in comparison to the ones composing the other DMD modes distinguished in Figures 2.26-2.27, and likely evolve from non-linear interactions between the different structures.

The most relevant mode revealed by both decompositions is DMD mode C. The blue DMD mode C oscillates with a characteristic $St = 0.0185$, while the black mode C with a $St = 0.0174$. Both DMD modes contain clearly-defined features uniformly distributed along the majority of the spanwise length of the cavity, with wavenumbers in the order of $\beta \approx 2\pi$. On the left figure, its FFT amplitude peak occurs for $\beta \simeq 5$, while structures on the right figure present a dominant wavenumber of $\beta \simeq 6$ for this mode C. In both cases, these dominant structures consist of highly coherent right or left-travelling waves, previously observed in the space-time diagram of Figure 2.25. The morphological shape of the present DMD modes bear thus strong similarity with the most energetic one described by the experiments, with identical shift in frequency in comparison with the linear Mode I. Note that similar mode was also recovered in Section 2.4.2.3 considering periodic boundary conditions, disclosing that the above-mentioned discrepancy in frequency is not an exclusive effect of the presence of spanwise walls.

The two DMD analysis of Figures 2.26-2.27 recovered the dominant mode of the experiments, however a small discrepancy in frequency can be observed between the blue DMD mode C (in Figure 2.26) and the black DMD mode C (in Figure 2.27). Figure 2.28 compares the streamwise velocity profiles in the $y/D = -0.1$ plane, averaged for the two following temporal scenarios: solid blue line uses the same DNS snapshots as in Figure 2.26, while dashed black line takes the same DNS solutions as in Figure 2.27. It can be seen that the streamwise velocity in the region of the main recirculation is lower for the second case, suggesting that the saturation process has the effect of slowing down the main centrifugal vortex inside the cavity, causing the aforementioned drop in St .

(a) Extracted DMD modes in the $\beta - St$ plane. Each mode is associated with a single frequency, represented by a set of horizontal blue diamonds. The size of the diamonds is proportional to the amplitude of the power spectral density performed on the spanwise velocity component of each DMD mode. DMD spectrum is compared with data from BiGlobal analysis (red dots) and experimental measurements (grey areas) of [22].

(b) Iso-surfaces of spanwise velocity of the aforementioned DMD modes, in the zy and zx planes.

Figure 2.26: Extracted DMD modes for DNS solutions with spanwise walls boundary conditions, starting the decomposition at $t = 417$ and using 228 snapshots. The spatial domain of the DMD was reduced to the six central sub-domains of the mesh.

(a) Extracted DMD modes in the $\beta - St$ plane. Each mode is associated with a single frequency, represented by a set of horizontal blue diamonds. The size of the diamonds is proportional to the amplitude of the power spectral density performed on the spanwise velocity component of each DMD mode. DMD spectrum is compared with data from BiGlobal analysis (red dots) and experimental measurements (grey areas) of [22].

(b) Iso-surfaces of spanwise velocity of the aforementioned DMD modes, in the zy and zx planes.

Figure 2.27: Extracted DMD modes for DNS solutions with spanwise walls boundary conditions, starting the decomposition at $t = 1985$ and using 291 snapshots. The spatial domain of the DMD was reduced to the six central sub-domains of the mesh.

Figure 2.28: Averaged dimensionless streamwise velocity profiles in the $y/D = -0.1$ plane, considering the same DNS snapshots as in the DMDs of previous Figures 2.26-2.27.

2.4.4 Discussion of Results

With and without the presence of solid bounding walls inside the open cavity, the DMD technique was able to recover, from a highly non-linear and saturated flow regime, high energy modes containing features that resemble the dominant structures obtained in the experimental campaign of de Vicente et al. [22]. The frequency of those DMD modes was also matching the St range of the experiments, and confirmed the shift in frequency from the corresponding oscillatory BiGlobal Mode I.

Figure 2.29 shows averaged dimensionless streamwise velocity profiles for the two DNS cases studied in the present paper. Both profiles were taken in the $y/D = -0.1$ plane, and are compared with the 2D base flow from linear stability analysis, and with the experimental mean flow, both from the work of de Vicente et al. [22]. Within the saturated regime, we observe for both DNS cases a strong reduction of the velocity of the main recirculation, which explains the said drop in Strouhal number.

A secondary effect arises from the presence of spanwise walls, leading to an additional decrease in the velocity of the main centrifugal recirculation. The presence of end-wall vortices slowing down the main centrifugal recirculation vortex inside the cavity, was firstly

Figure 2.29: Averaged dimensionless streamwise velocity profiles within the saturated regime, in the $y/D = -0.1$ plane. DNS profiles are compared with the BiGlobal and experimental ones, published in the work of de Vicente et al. [22].

described in the literature by Shankar and Deshpande [95]. This braking phenomenon was also observed in the experiments. Nonetheless this effect is not as strong as the one measured inside the experimental cavity. Such discrepancies can be explained by the development of end-wall effects from the inlet of the experimental test-section, yielding to more developed lateral boundary layers at the leading edge of the experimental cavity. Nevertheless new evidences point out that the main mechanism for the reduction of frequency is the reduction of the velocity of the main vortex, and that such reduction occurs mainly due to the saturation process, not to the presence of walls.

In order to attest that relationship between recirculation velocity and associated Strouhal number of the leading perturbation, the behaviour of the peak velocity of the main vortex with time, and of the frequency of the dominant DMD mode, is plotted in Figure 2.30 for both investigated DNS cases. The three velocity points depicted in the figure were averaged in three DNS time intervals, and the DMDs were performed for the corresponding interval. For the periodic case on the top (Figure 2.30a), the clear trend is that the saturation process reduces the recirculation velocity inside the cavity, and the

frequency of the modes is reduced in the same fashion. For later simulation times, we can observe a slight increase of the streamwise velocity, possibly induced by non-linear interactions occurring inside the cavity, resulting in a small increment of the Strouhal number.

(a) DNS with spanwise periodic boundary conditions.

(b) DNS with spanwise wall boundary conditions.

Figure 2.30: Trend of the maximum value of averaged dimensionless streamwise velocity (squared blue markers) in three DNS time intervals, compared with the dominant Strouhal number (circled red markers) retrieved by the DMD for the same time intervals.

For the case where lateral wall boundary conditions were imposed, Figure 2.30b shows an initial trend in line with the periodic case, confirming that the reduction of Strouhal number of the leading mode is a consequence mainly of the saturation mechanism. Nonetheless the effect of the presence of end-walls also contribute to a further decrease in the velocity of the main centrifugal vortex, resulting in a stronger drop of the Strouhal number.

2.5 Summary

This study demonstrated the capability of the DMD to analyse the spanwise perturbations occurring in an open cavity flow problem, within the completely saturated regime. This technique was applied to a set of snapshots obtained from DNS, imposing lateral periodic and solid wall boundary conditions, in order to investigate the possible cause for the drop of characteristic Strouhal number of the most energetic mode of the experiments of de Vicente et al. [22]. Despite the highly non-linear regime inside the cavity triggered by saturation of linearly unstable modes, the DMD was able to retrieve the morphological shape and oscillation frequency of the most relevant modes of the linear stability analysis and of the experiments.

The reported reduction of Strouhal number of the dominant mode from the value predicted by linear analysis was again found in the present analysis, with or without the presence of spanwise bounding end-walls. We have found that this behaviour is mainly due to the saturated regime of the flow, which has the effect of slowing down the main centrifugal recirculation vortex, thus reducing the characteristic Strouhal number of the modes. The presence of end-wall vortices near the spanwise confinements of the cavity only strengthens this effect, and its overall weight is always lower in comparison to saturation.

The DMD technique revealed to be a powerful instrument in the analysis of this particular open cavity flow problem. Using this post-processing tool, we were able to establish the link that was missing between the experimental results, linear stability analysis, and DNS data, and find the true nature of the decrease in Strouhal number. Moreover, with the reconstruction of the dynamic modes, the DMD technique demonstrated also to be a very useful tool for the visualization of the characteristics of complex flows, in both space and time domain. In this particular numerical investigation, we were able to visualize the morphology of the relevant spanwise modes developed inside the open cavity. The spatial DMD formulation allowed also to visualize how these modes were evolving in time.

3

DMD Towards Industrial Applications

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3.1 Introduction

In the previous Chapter 2, the DMD technique demonstrated to be a very useful tool for the analysis of a complex problem, such as the open cavity flow. Based on the high number of publications using the DMD to study wake, jet, turbulent, or separated flows (e.g. [90, 39, 32, 17, 110]), this recent technique is becoming one of the preferred data-based decomposition methods for the analysis of oscillatory flow problems, characterized by coherent structures. Simplified computational geometries or experimental setups (comprising rectangular cavities, flat plates, cylinders, airfoils, etc.) are widely used to perform fundamental research within a more academic framework, and the concurrent

data sampling process normally do not produce datasets with very high dimensions. In this context, the original DMD formulation [90] has a relatively low computational cost in terms of CPU and memory.

Within an industrial framework, where the level of complexity is much higher, very small time-steps and a huge amount of grid cells are generally required to perform very accurate CFD simulations. To give the reader an idea about the order of magnitude of an industrial engineering problem, a single solution snapshot of the CROR test-case used in Chapter 4 for vortex detection consists of 95 million grid points. The combination of several snapshots with large number of points and uniformly sampled in time, into a snapshot matrix $\mathbf{V}_1^N$ in the way shown in Figure 2.5, will certainly originate a matrix $\mathbf{V}_1^N$ where the number of rows is far larger than its column size. This particular matrix is commonly dubbed in literature as “tall-and-skinny” (TS) matrix [11]. In the DMD analysis of three-dimensional, large-scale problems, the greatest challenge is performing the Singular Value Decomposition (SVD) of such snapshot matrix. In a serial computation environment, the memory required for this factorization will certainly exceed the memory available in the system. Alternatively, we could consider reducing the complexity of the problem, by selecting a smaller sub-domain of the original dataset where dynamically interesting phenomena are expected to occur [90]. Nonetheless, on the one hand, this approach does not guarantee that memory problems are completely suppressed. On the other hand, a proper preliminary sub-domain selection is not always easy to achieve without a priori knowledge of the flow. Hemati et al. [38] and Guéniat et al. [35] recently proposed two methodologies aiming to reduce the computational cost of the DMD for large datasets, but the applicability of their algorithms to industrial flow problems was not properly assessed.

A truly parallel implementation of the original DMD algorithm, which addresses a solution to the aforementioned memory constraints on a single processor, was firstly introduced by Sayadi and Schmid [88]. Their approach takes advantage of the TSQR method, a parallel QR factorization algorithm suitable for TS matrices, developed by Demmel et al. [23]. By using a Message Passing Interface (MPI) implementation of the TSQR method as a basis for the SVD [88], their parallel DMD algorithm can be easily

compiled and executed in a High-Performance Computing (HPC) environment, keeping the simplicity and robustness of the original DMD and requiring very low number of communications between processors [88].

During the secondment in Airbus-GE, the parallel DMD algorithm of Sayadi and Schmid [88] was entirely implemented in Airbus tools, with the objective to analyse a particular Nose Landing Gear (NLG) problem. Numerical implementation and industrialization details are provided in Section 3.2. The main target was to track a large noise response experienced in a NLG cavity bay, causing nuisance to the crew and passengers, and structural vibrations. The DLR-TAU solver was used to perform an unsteady Detached Eddy Simulation (DES), with unsteady physical time step size in the order of the milliseconds, allowing to resolve all time-scales of interest for the dynamics of the problem. The tested computational domain comprised around 40 million cells. Due to strict confidentiality policies from Airbus, the provided test-case and results obtained with the parallel DMD analysis cannot be published in this thesis. Nonetheless, a preliminary validation of the implemented parallel DMD tool is presented in Section 3.3, using the open cavity test-case of Chapter 2. Some figures regarding its computational performance are also given in the same section.

3.2 Numerical Implementation and Industrialization

The parallel DMD algorithm suggested by Sayadi and Schmid [88] encompasses three essential steps: (1) Parallel QR-factorization, based on the TSQR method of Demmel et al. [23], (2) Parallel SVD, and (3) DMD and extraction of the dynamic modes and corresponding spectrum.

Figure 3.1 shows a schematic diagram of its first step, using four processors for illustration purposes only. The objective of this step is the computation of $\mathbf{Q}$ and $\mathbf{R}$ matrices of the input snapshot matrix $\mathbf{V}_1^N$, represented in the figure by letter $\mathbf{A}$. The shape and composition of this matrix was previously discussed in Chapter 2, and schematically shown in Figure 2.5. Matrix $\mathbf{A}$ needs first to be distributed among the processors and,

according to the authors [88], there is no special restriction on how this matrix can be split. After that, a first QR-factorization is applied to each of the sub-matrices $\mathbf{A}_i$, previously distributed among the i processors. The resulting upper-triangular matrices $\mathbf{R}_i$ are then gathered on each processor into a single matrix ($\mathbf{R}'$), as Figure 3.1 depicts, while $\mathbf{Q}_{1i}$ are stored for a later operation. Afterwards, a second QR-factorization is performed by each processor on the gathered matrix $\mathbf{R}'$. The outcoming upper-triangular matrix $\mathbf{R}$ is the final $\mathbf{R}$ matrix of the initial snapshot matrix $\mathbf{A}$. In order to obtain the final orthonormal $\mathbf{Q}_i$ matrices of the system, we need to multiply the two $\mathbf{Q}$ matrices resulting from the two previous QR-factorizations, $\mathbf{Q}_{1i}$ and $\mathbf{Q}_{2i}$ respectively, that are already distributed among the processors.

Figure 3.1: Step 1 of the parallel DMD algorithm: computation of $\mathbf{Q}_i$ and $\mathbf{R}$ of the input snapshot matrix $\mathbf{A}$, using four processors (adapted from [11, 88]).

The second step of the parallel DMD algorithm starts with the SVD of the upper-triangular matrix $\mathbf{R}$, performed on each processor. Note that the dimension of this square matrix is only equal to the number of snapshots (i.e. number of columns) composing the initial snapshot matrix $\mathbf{V}_1^N$, which has far more rows than columns. Therefore, the computational burden associated with this operation is much lower than performing the SVD of the original $\mathbf{V}_1^N$ matrix, as in the original DMD algorithm of Schmid [90]. At each processor, the resulting left singular vectors are then multiplied by the $\mathbf{Q}_i$ matrices previously obtained at the end of Step 1. With this last operation we retrieve the left

singular vectors of the snapshot matrix $\mathbf{V}_1^N$, required to compute the DMD companion matrix $\tilde{\mathbf{S}}$ (previously defined in Equation (2.24)).

The third and final step of the parallel DMD is no more than the replication of its original algorithm after the SVD, within a parallel framework. All the steps comprising the original DMD were previously enumerated in Algorithm 2.1.

All the fundamental steps of the parallel DMD technique of Sayadi and Schmid [88] are resumed in Algorithm 3.1. Note that MPI communications among the i processors are only required at executions 1, 3, and 11.

Algorithm 3.1 Parallel DMD.

Input: Snapshot matrix $\mathbf{V}_1^N = [v_1, v_2, \dots, v_n]$

1: Distribute $\mathbf{V}_1^N$ among i processors: $\mathbf{V}_1^N \xrightarrow{\text{scatter}} \mathbf{V}_{1,i}^N$

Step 1: Parallel QR-factorization

Input: $\mathbf{A}_i = \mathbf{V}_{1,i}^{N-1}$, distributed among the processors

2: QR-factorization on $\mathbf{A}_i$: $\mathbf{Q}_{1i}, \mathbf{R}_i = \text{qr}(\mathbf{A}_i)$

3: Gather $\mathbf{R}_i$ in $\mathbf{R}'$ in all processors: $\mathbf{R}_i \xrightarrow{\text{allgather}} \mathbf{R}'$

4: QR-factorization on $\mathbf{R}'$: $\mathbf{Q}_{2i}, \mathbf{R} = \text{qr}(\mathbf{R}')$

5: Compute $\mathbf{Q}_i = \text{matmul}(\mathbf{Q}_{1i}, \mathbf{Q}_{2i})$

6: **return** $\mathbf{Q}_i, \mathbf{R}$

Step 2: Parallel SVD

Input: $\mathbf{Q}_i$ and $\mathbf{R}$

7: Compute SVD of matrix $\mathbf{R}$: $\mathbf{U}_R, \mathbf{\Sigma}, \mathbf{W}^T = \text{svd}(\mathbf{R})$

8: Compute $\mathbf{U}_i = \text{matmul}(\mathbf{Q}_i, \mathbf{U}_R)$

9: **return** $\mathbf{U}_i, \mathbf{\Sigma}, \mathbf{W}^T$

Step 3: DMD

Input: $\mathbf{U}_i$ and $\mathbf{A}_i = \mathbf{V}_{2,i}^N$, distributed among the processors, $\mathbf{\Sigma}, \mathbf{W}^T$

10: Compute matrix $\mathbf{B}_i$: $\mathbf{B}_i = \mathbf{U}_i^T \times \mathbf{A}_i$

11: Sum $\mathbf{B}_i$ across all processors and store the result in $\mathbf{C}$: $\mathbf{B}_i \xrightarrow{\text{allreduce}} \mathbf{C}$

12: Compute matrix $\tilde{\mathbf{S}}$: $\tilde{\mathbf{S}} = \mathbf{C} \times \mathbf{W} \times \mathbf{\Sigma}^{-1}$

13: Determine eigenvalues and eigenvectors: $[\mu, \mathbf{X}] = \text{eig}(\tilde{\mathbf{S}})$

14: Reconstruct dynamic modes: $\Phi_i = \text{matmul}(\mathbf{U}_i, \mathbf{X})$

15: **return** Φ_i, μ

A library containing the aforescribed parallel DMD algorithm was written in Python and completely integrated with the Airbus Flow Simulator, allowing parallel DMD jobs to be executed on the Airbus HPC cluster. For the computation of the QR-factorization, SVD, and eigenvalue problem, linear algebra routines from Numpy are called. The developed library makes also use of other scientific and software libraries, such as SciPy, mpi4py (MPI for Python package), and NetCDF. This last library is particularly used to read TAU solution files in the NetCDF format, and to write the reconstructed DMD modes in the same format.

3.3 Validation and Computational Performance

A preliminary validation of the parallel DMD tool implemented in Airbus was carried out, using the open cavity test-case shown in Figure 2.27 comprising 291 DNS snapshots. Figure 3.2 compares the eigenvalues and spectrum of the DMD modes obtained with the parallel code using 4 and 8 processors, with results from the original DMD version executed on a single processor. We can observe that on both graphs all the points are overlapping, disclosing a strong agreement between the original and the parallel DMD implementations. Eigenvalues and DMD spectrum are also independent of the number of processors used.

Table 3.1 shows the computational times required by the parallel DMD implementation to complete its three fundamental steps, using the aforementioned open cavity test-case. These values are also confronted with the ones required by the original DMD version of Schmid [90], employing just one processor. With 8 processors, we are able to achieve a reduction of about 50% on the total DMD time, in comparison with a single processor computation. As expected, the computational load associated with the SVD in the second step is strongly reduced with the parallel algorithm. For this particular open cavity test-case, we can also observe from the table that it is not profitable to execute the parallel DMD using more than 4 processors, because the gain in computational time is negligible with the inclusion of additional processors.

(a) Eigenvalues

(b) Spectrum

Figure 3.2: Comparison between the eigenvalues and spectrum of the DMD modes obtained with the parallel algorithm, with the ones obtained with the original DMD formulation using a single processor. Open cavity test-case shown in Figure 2.27 used for the present validation.

Table 3.1: Computational performance of the developed parallel DMD library, using the open cavity test-case shown in Figure 2.27, and compared to the performance of the original DMD of Schmid [90], indicated in the table by the symbol *.

No of Processors	Step 1 (s)	Step 2 (s)	Step 3 (s)	Total (s)
1*	n.a.	17.93	18.01	35.94
1	27.95	2.88	17.83	48.66
2	13.67	1.44	8.94	24.04
4	11.34	1.22	8.16	20.72
8	10.44	1.31	8.45	20.20
16	10.42	1.38	9.75	21.55
32	9.27	1.28	9.05	19.59

4

Evaluation of Vortex-Blade Interaction on CROR Engines

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4.1 Introduction

In recent years Counter Rotating Open Rotor (CROR) engines have become of prime interest in the aeronautical industry, in search for more efficient aircraft configurations. Amongst all potential future propulsion systems, the open rotor concept offers the most significant fuel consumption and CO₂ emissions improvement [101], as shown in Figure 4.1. The biggest drawbacks in these particular engine types are the high levels of noise generated, both broadband and tonal, due to the absence of a cold stream duct, thus design focus is placed on trying to reduce it in order to meet tighter noise regulations within the airspaces. As it is well known a major contribution to tonal noise is caused by the first stage rotor blade tip vortices interacting with the second stage rotor [98]. This impact condition is also undesirable from the aerodynamic and structural point of view, as it penalizes drag, and increases significantly vibrations and fatigue loads nearby the impact regions. On the other hand, broadband noise is directly associated with the breakdown of trailing vortices. Figure 4.2 schematically illustrates the origin of such CROR noise sources. An effective and efficient tracking of these two vortex topologies is therefore indispensable to the designers that look for advantageous configurations.

Figure 4.1: Efficiency in terms of fuel burn versus improved noise in future aircraft engine architectures (from [60]).

Thanks to the development in Computational Fluid Dynamics (CFD) techniques and

Figure 4.2: Acoustic sources on CROR.

the exponential growth in computational power, today it is possible to obtain with high accuracy detailed flow behaviour predictions under normal operating conditions. Not surprisingly, over the last few decades the reliance on CFD in the design process of pioneering aircraft engine architectures has increased significantly. Noise and performance requirements lead this design process from a very early stage, thus requiring deep investigation and complete understanding of the acoustic and aerodynamic behaviour within numerical solutions.

A new problem arises from current industrial simulations, which is the large amount of CFD data that needs to be processed to be able to derive valuable conclusions. In particular, the simulations focusing on noise prediction require very small time steps and very large meshes which increases the burden on data reduction prior to analysis on the part of the designer. Most methodologies in noise prediction move from the CFD analysis directly to noise propagation models based on pressure data around known noise sources, which gives quantitative noise information in the form of sources and footprints at high computational costs [108].

Alternatively, flow feature detection techniques focus the analysis on regions of relevance within large CFD data domains. These techniques aim to extract flow features that are of interest for a certain engineering problem in a numerically efficient manner. Tip vortices and vortex breakdown are the features of interest for the particular case of CROR

engines in the current design-to-noise mindset, where ideally original data would only be accessed for the reconstruction of such structures. Without adding excessive computational burdens to the CFD, this methodology offers an important size and complexity reduction to the original data and a higher level of abstraction [70, 68, 85], providing faster and more accurate answers to the designers.

In the present chapter, one first evaluates the suitability of traditional region and line-based vortex detection techniques, available in the literature, for the particular case of CROR. Four region-based methods based on the velocity gradient tensor and one line-based algorithm were selected for the visualization and tracking of the tip vortices produced at the first engine stage and interacting with the second. The strengths and weaknesses of each individual algorithm and its computational performance are also discussed in this chapter. Following this comparative analysis, two new initialization methods are presented to improve the original selection of seeds required by the tested line-based method. The first methodology uses the information given by the four region-based detection methods previously tested as an input for the aforementioned line-based method. For the second method, the selection of seeds is driven by high friction drag and pressure gradient criteria.

4.2 Detection of Vortices

It is surprising that a precise and unique mathematical definition of a vortex does not exist in literature. Lugt defined in 1979 a vortex as “the rotating motion of a multitude of material particles around a common center” [58]. Later on, Robinson provided the following definition for a vortex: “a vortex exists when instantaneous streamlines mapped onto a plane normal to the vortex core exhibit a roughly circular or spiral pattern, when viewed from a reference frame moving with the center of the vortex core” [75]. More recently Portela introduced his own definition of a vortex, considering that “a vortex is comprised of a central core region surrounded by swirling streamlines” [69].

The lack of consensus for a rigorous and unique definition of a vortex gave rise to the

development of several vortex detection algorithms. Epps provided in [25] an updated comprehensive review of the state-of-the-art in vortex identification, enumerating more than thirty vortex detection methods developed in the last three decades. The majority of these methods take the assumption that a coherent vortical structure can be described as a vortex core line, also designated in literature as skeleton line, with a swirling fluid motion around it. Hence, two main categories of vortex extraction methodologies can be found currently in literature:

- Methods that look for vortex core lines, or the imaginary centres of rotational motion, are usually called Line-Based (LB) methods (exemplified in Figure 4.3a).
- Methods that search for vortex core regions or “regions of influence” of a vortex core line [28] (exemplified in Figure 4.3b). These schemes are commonly known as Region-Based (RB) methods, mainly allowing the visualization of iso-surfaces of a certain scalar field that represent the vortex core boundary. A very complete and recent review of the available RB methods so far can be found in [25].

Figure 4.3: Vortex detection on a generic fighter aircraft.

As described in [46], RB methods are easier to implement and require less computational burden in comparison to LB schemes. However, the latter can provide a more accurate representation of the vortex, especially when the distance between two individual structures is considerably small. In LB methods, the region of rotational influence of a vortex can additionally be estimated, using surface-based techniques. Several surface methods developed particularly for this purpose can be found in [29].

Vortex detection methods can also be classified as Galilean invariant (GI) or not invariant (GNI). Jiang et al. explain in [46] the importance of such property for the extraction of vortices in unsteady flow problems. Relying on [58] and [75], they state that in a time-dependent flow problem a vortex can only exhibit swirling motion if viewed from a reference frame moving with that vortex. For an objective vortex identification in such kind of flow problems, the algorithm must satisfy the Galilean invariance condition, i.e. when a vortex detection method produces exactly the same results using different moving reference frames. This is the case for methods relying on the static pressure or vorticity as a detection criterion, as they do not depend directly on the velocity [46]. Nonetheless, schemes relying on the velocity field normally are Galilean not invariant methods.

A third property can also be used to classify vortex extraction algorithms, depending on which part of the computational domain the method is applied. On the one hand, a method is considered to have local nature (L) if it is applied individually to each grid cell, as it normally happens with methods relying on the velocity gradients. On the other hand, if the algorithm needs to evaluate more than one grid cell in a single computation step, it is known to be a global method (G). From the computational point of view, global methods are usually more expensive than local ones. Nonetheless they are more suitable to trace vortex core lines that define the skeleton of a vortex.

There is no generic vortex detection method valid for the wide range of conditions under which a vortex may occur. This means that each approach has a preferred vortex type based on strength, rotation rate, shear rate, curvature, or on relative distance to the solid surface and its boundary layer. Roth in [80] evaluated the performance of six LB methods, representative of the state-of-the-art, using several turbomachinery data sets. Even if the Eigenvector method (Sujudi & Haimes [100]), the Parallel Vectors method (Roth & Peikert [81]), and the Normalized Helicity method (Levy et al. [56]) performed globally better for the tested flows, the author concluded that, among all the tested methods, there is not one clearly superior method that extracts coherently all the vortices. The works of Post [70], Jiang [46], and Rutten [84] compare typical RB and LB vortex detection methods available in literature, that offer good results in most CFD applications. Nonetheless, as each individual algorithm has its own advantages and

limitations depending on the flow conditions and on the quality of the CFD, it is impossible to select one superior method over the others for all applications. These studies stress the importance of evaluating in a preliminary step the suitability of a vortex detection technique for a particular engineering problem. Table 4.1 compiles the most typical LB methods used in the literature and briefly describes them according to their preferred applicability and reported limitations, in an attempt to assist the reader in the endeavour of extracting vortex core lines from their own CFD solutions.

The evaluation of the strengths and weaknesses of an individual algorithm might reveal insights into the development of variances from the original method, or alternatively into the exploitation of coupling methodologies. Chakraborty et al. introduced in [16] an enhanced RB vortex identification scheme, after performing a study about the relationship between the most common gradient-based methods. Haller in [36] presented an objective frame-independent RB vortex definition, while Kolar formulated in [52] a triple decomposition method that separates pure shearing from actual swirling motion of a vortex. For large CFD data sets the quality of the detection using LB techniques can be greatly increased by performing a preliminary identification using RB gradient-based methodologies, as demonstrated in [44, 97, 83, 89].

4.3 Numerical Methodology

4.3.1 Computational Domain and Mesh

The CROR test case used for this work comes from a Z08 open rotor configuration, based on the geometry of the generic 14ft diameter open rotor AI-PX7 from Airbus Operations at scale 1/7. It features 11 blades in the first rotating row, and 9 blades in the following counter-rotating part. A multi-block structured grid was generated, comprising 825 blocks and 95 million grid points, and modelling the entire annular section. The first rotating row was connected to the second counter-rotating row through a sliding plane. Figure 4.4 shows the geometry, the computational domain, and the structured mesh of the CROR test case used in the present work. For additional details, the reader is directed to [19, 20].

Table 4.1: Line-based vortex detection methods.

Method	Preferred applicability	Known limitations
Helicity (Levy et al. [56]) Maxima points of normalized helicity. Type: LB, GNI, L	Primary and secondary vortices distinction (such as in hemisphere and ogive cylinder data sets [56]).	False detections for curved vortices. Rarely used.
Predictor-Corrector (Banks & Singer [6]) Vorticity predictor step, followed by pressure corrector step. Type: LB, GI, G	Elongated, hairpin, and spiral vortices, vortices in a shear layer near a wall. General engineering flows (e.g. serrated wings, and canted tail fins and canards of a missile [44]).	Broad vortex sheets. Limited performance detecting highly curved vortices (typical of turbomachinery flows). Large initialization based on arbitrary thresholds. Global method, more demanding parallelization.
Eigenvector (Sujudi & Haimes [100]) Eigenvectors of the velocity gradient tensor. Type: LB, GNI, L	Straight and high strength vortex lines. Numerous CFD applications (e.g. wing tips, helicopter rotor hover, vortex breakdown in high AoA rolling delta wings, and vortex burst on a F/A-18 fighter [49]).	Requires tetrahedral cells. Limited performance if grid cells are large or very irregular. Non-contiguous lines. Negative detections under boundary layer formation. Sensible to other non-local vector features and to the strength of the vortex. Expensive computation.
Parallel Vectors (Roth & Peikert [81]) High-order method based on parallel vectors. Type: LB, GNI, L	Bent vortices. Low strength vortex lines. Typical turbomachinery applications with strongly curved vortices (e.g. Francis turbine runner, and stator of pump-turbine [80]).	Can extract less coherent lines than others. Not always produce the best results on typical turbomachinery flows. Vortex lines with gaps. Requires the calculation of accurate higher-order derivatives.
Kida and Miura [50] Sectional-swirl and pressure-minimum. Type: LB, GI, G	Swirling slender vortices. Demonstrated in isotropic turbulence and inhomogeneous shear flows [50], and in a draft tube with swirling flows [80].	Limited performance detecting highly curved vortices (typical of turbomachinery flows). Rarely used.
Maximum Vorticity (Strawn et al. [99]) Local maxima of vorticity magnitude in a plane normal to the vorticity. Type: LB, GI, L	Free-shear vortices. Demonstrated for rotorcraft problems (e.g. V-22 tiltrotor blades [1]). Individual vortices distinction (e.g. delta wing [99]).	Not applicable to shear layers. Requires structured-grid data sets. Limited performance detecting highly curved vortices (typical of turbomachinery flows). Rarely used.

Figure 4.4: Computational domain and structured mesh of the CROR engine.

4.3.2 Solver Settings

The elsA solver [14, 15], developed by ONERA, was used to perform time-dependent, compressible Reynolds-Averaged Navier-Stokes (URANS) simulations, adopting the one-equation Spalart-Allmaras turbulence model. The computations allow the simulation of the actual CROR engine conditions in terms of Reynolds and Mach numbers ($Re = 4.5 \times 10^6$ and $M = 0.2$). The working fluid was assumed to be a thermally and calorically perfect gas. Spatial discretization was carried out using the cell-centred finite volume method with second order upwind. The Roe scheme was used to compute the viscous fluxes. For the temporal discretization, the implicit dual time stepping method was used with backward Euler integration with implicit LU schemes. The CFL number was adjusted to 1.

4.3.3 Vortex Detection Library

Four RB vortex detection methods relying on the velocity gradients (Q -criterion, Kinematic vorticity number, Δ -criterion, and λ_2 -criterion), and one LB method (Predictor-

Corrector method) were selected and implemented within an internal Airbus object-oriented post-processing library. This tool follows a pipeline programming philosophy written in Python and making use of scientific and visualization libraries, such as NumPy, SciPy, and VTK. Each of the selected vortex detection methods is described in this section.

4.3.3.1 Q -Criterion

The Q -criterion was proposed by Hunt et al. [42] and searches for coherent vortex structures based on the properties of the local velocity gradient tensor $\nabla \mathbf{v}$, that can be written in the following form:

$$\nabla \mathbf{v} = \begin{pmatrix} \frac{dv_x}{dx} & \frac{dv_x}{dy} & \frac{dv_x}{dz} \\ \frac{dv_y}{dx} & \frac{dv_y}{dy} & \frac{dv_y}{dz} \\ \frac{dv_z}{dx} & \frac{dv_z}{dy} & \frac{dv_z}{dz} \end{pmatrix}. \quad (4.1)$$

where (v_x, v_y, v_z) correspond to the velocity components in the Cartesian coordinates (x, y, z) , respectively. The velocity gradient tensor $\nabla \mathbf{v}$ can then be decomposed into its symmetric part $\mathbf{S}$ and antisymmetric part $\mathbf{\Omega}$, as follows:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T); \quad (4.2)$$

$$\Omega_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right) = \frac{1}{2} (\nabla \mathbf{v} - \nabla \mathbf{v}^T). \quad (4.3)$$

The component $\mathbf{S}$ represents the shear contribution of the velocity gradient tensor, whereas the part $\mathbf{\Omega}$ is associated with the rotational contribution of $\nabla \mathbf{v}$.

The Q -criterion is then defined as the second invariant of $\nabla \mathbf{v}$, allowing to compare the influence of local fluid shear to rotation, as follows:

$$Q = \frac{1}{2} \left(|\mathbf{\Omega}|_F^2 - |\mathbf{S}|_F^2 \right), \quad (4.4)$$

where $|\cdot|_F$ represents the Froebenius norm of the tensors. The general idea behind this criterion is to look for areas of the flow where $Q > 0$, meaning that the local rotation rate is dominating the local shear rate, and thus suggesting the existence of a vortical

structure.

The present criterion is quite well accepted among the post-processing community because it can provide reliable visualizations, with a simple implementation and relatively cheap and fast computations. Nonetheless, it requires the selection of a fully arbitrary threshold that may vary from one flow problem to another, and so the value of the threshold must be chosen carefully in order to properly visualize the structures of interest. Moreover, and due to its nature, the method is sensitive to the quality of the velocity derivatives, which in some cases can be difficult to be computed [28].

4.3.3.2 Kinematic Vorticity Number

The kinematic vorticity number is a parameter introduced by Truesdell [106], which measures the “quality of rotation” regardless of the local magnitude of vorticity. Following the Einstein summation convention, it is defined as:

$$N_k = \frac{|\mathbf{\Omega}|_F}{|\mathbf{S}|_F} = \sqrt{1 + \frac{2Q}{S_{ij}S_{ij}}}. \quad (4.5)$$

Basically this criterion highlights a vortex core region in zones where $N_k \geq 1$, i.e. when the rotational part of the local $\nabla \mathbf{v}$ out-balances its shear part.

The parameter N_k is low inside boundary layers, where vorticity magnitude usually is high, and is appropriate to be used for the detection of a vortex in a boundary layer flow [93]. Similarly to the Q-criterion, this method is of easy implementation and computationally cheap. Nonetheless it might extract vortical structures that are not dynamically relevant for the problem under investigation, especially in regions where both $|\mathbf{S}|_F$ and $|\mathbf{\Omega}|_F$ are negligible [93].

4.3.3.3 Δ -Criterion

Dallmann [21] and Chong et al. [18] proposed a different criterion derived from the characteristic polynomial of the local velocity gradient tensor, taking advantage of the

existence of complex eigenvalues of this tensor when the fluid experiences rotation in a cell or point. The characteristic equation for $\nabla \mathbf{v}$ is given by:

$$\lambda^3 + P\lambda^2 + Q\lambda + R = 0, \quad (4.6)$$

where the three invariants of the velocity gradient tensor $\nabla \mathbf{v}$ are given by:

$$P = -\text{trace}(\nabla \mathbf{v}); \quad (4.7)$$

$$Q = \frac{1}{2} \left(P^2 - \text{trace}(\nabla \mathbf{v})^2 \right); \quad (4.8)$$

$$R = -\det(\nabla \mathbf{v}). \quad (4.9)$$

The discriminant of the characteristic Equation (4.6) is given by:

$$\Delta = 27R^2 + (4P^3 - 18PQ)R + (4Q^3 - P^2Q^2). \quad (4.10)$$

The Δ -criterion defines then a vortex region in cells or points of the fluid domain where Δ has a positive value (i.e. $\Delta > 0$). In those points, the characteristic Equation (4.6) has one real root and two complex roots, conjugated to each other.

From the practical point of view, the Δ -criterion does not offer significant vortex detection performance improvements in comparison to the Q -criterion, that provides a more restrictive selection [16], even though the latter has a simpler definition. Furthermore, and similarly to previous vortex identification methods, the Δ -criterion always requires a certain threshold value, that needs to be selected carefully.

4.3.3.4 λ_2 -Criterion

Jeong and Hussain [45] developed the λ_2 -criterion, that aims to detect cells or points of the flow where the pressure is minimum. Vortices are commonly associated with low pressure regions, once a vortex normally rotates around areas of low static pressure. These low pressure regions are a consequence of the centrifugal force that induces a pressure gradient

in the fluid, oriented perpendicular to the axis of rotational motion. However, the authors pointed out that the condition of minimum pressure is not always sufficient to guarantee the presence of a vortex in the flow. On the one hand, strong unsteady irrotational straining can also originate a pressure minimum in the flow. On the other hand, pressure minima regions within a vortex can disappear due to viscous effects [46]. In order to take into account those effects, the authors formulated the following condition (obtained from the incompressible Navier-Stokes equations, as demonstrated in [67]):

$$\mathbf{\Lambda} = \mathbf{S}^2 + \mathbf{\Omega}^2 = S_{ik}S_{kj} + \Omega_{ik}\Omega_{kj} = -\frac{1}{\rho} \frac{\partial^2 p}{\partial x_i \partial x_j}. \quad (4.11)$$

The sum on the left-hand side of Equation (4.11) is real and symmetric, therefore has three real eigenvalues ranked as $\lambda_1 \geq \lambda_2 \geq \lambda_3$. A pressure minimum exists in a cell or point where two of the three eigenvalues are negative. A vortical structure can thus be identified through manual inspection of the iso-surfaces of negative λ_2 .

Nowadays the λ_2 -criterion is widely used in several post-processing tools due to its improved accuracy over other RB methods derived from the velocity gradient tensor, especially under strong external strains [86]. Another advantage offered by this criterion is related with its precise and nearly automatic threshold [28]. However, [86] warns about the possibility that in some turbomachinery problems, λ_2 can be negative almost everywhere in the fluid domain. For these cases, a stronger and more selective threshold is therefore required in order to extract regions with strong vortical behaviour.

In terms of computational performance, the λ_2 -criterion is more demanding and takes more time to compute, as it involves the calculation of the eigenvalues of a real and symmetric tensor at every cell or point of the fluid domain. Another limitation of the method is based on its difficulty to make a precise distinction of an individual vortex, in regions where several vortices coexist [46]. Finally, as [67] stresses, boundary layers can also fulfil the λ_2 -criterion, originating false vortex detections.

4.3.3.5 Predictor-Corrector Method

The vorticity-Predictor pressure-Corrector method is a well-known LB method, introduced by Banks and Singer in 1995 [6]. The algorithm extracts streamlines of the vorticity field during a predictor step, correcting these predictions based on the local minimum pressure in a corrector step, and providing a more precise approximation of a vortex core skeleton. The method relies on both a low static pressure and a high vorticity magnitude criterion to investigate if a certain point belongs to a vortex skeleton. Nonetheless, and according to [6], it is possible to have regions with low pressure or with high vorticity magnitude without being associated with a vortex. Examples of such cases are the flow downstream of an obstacle and a shear flow, respectively. Nevertheless, the authors believe that the combination of these two criteria is a powerful indication of the presence of a vortex.

The original Banks & Singer algorithm starts by an initialization step, which looks for possible candidate seeds at every grid point of the fluid domain. It is based on arbitrary user inputs which may be inferred from thresholds of low static pressure and high vorticity magnitude. A good candidate point is thus a grid point that satisfies the two thresholds which must be found and selected manually. The method also foresees corrections to the position of these candidate points, so that they are not constrained to the grid.

From the candidate points extracted during the pre-processing step, the algorithm starts developing the vortex core lines. At each iteration point, a predictor step is firstly applied, followed by a correction treatment, as one can observe in the pseudo-code of Algorithm 4.1. The steps comprising the original predictor-corrector method are schematically sketched in Figure 4.5. Note that for the predictor and corrector steps the method uses only vectorial quantities.

In our implementation of the Predictor-Corrector method, the vorticity integration is achieved by means of a fourth-order Runge-Kutta approach. For the corrector step, the method of steepest gradient descent is used to locate the local minimum of static pressure in the plane perpendicular to the vorticity vector. Finally VTK interpolation functions are used to perform the required interpolations.

Algorithm 4.1 Predictor-Corrector method (adapted from [46]).

- 1: **initialization:** locate seeds with low pressure P and high vorticity magnitude $|\omega|$
 - 2: **for** all seeds **do**
 - 3: **repeat**
 - 4: compute ω_i at current seed point p_i (Fig. 4.5 - 1)
 - 5: step in ω_i to predict next point p_{i+1} (Fig. 4.5 - 2)
 - 6: compute ω_{i+1} at predicted point p_{i+1} (Fig. 4.5 - 3)
 - 7: **procedure** (find P_{min} on plane $\perp \omega_{i+1}$ (Fig. 4.5 - 4))
 - 8: **if** $\angle(\omega_{i+1}, \omega_{P_{min}}) < \text{limit}$ **then**
 - 9: correct predicted point p_{i+1} to $p_{P_{min}}$
 - 10: **else**
 - 11: quit corrector phase
 - 12: **until** skeleton exits domain **or** is too long
-

Figure 4.5: The four steps of the Predictor-Corrector method (from [6]).

The original algorithm expects that any vortex core line stops growing when it starts leaving the computational domain, and when the total arclength along a skeleton line is at least two times bigger than the longest grid dimension [6]. The method is also capable of eliminating redundant seeds, skeletons, and any spurious feeders that may appear during its computation. The Banks & Singer method can additionally be combined with techniques that provide a geometrical approximation of the vortex shape, from cross-sections of vortex tubes in planes perpendicular to the imaginary core. For additional implementation details the reader is forwarded to Banks and Singer [6].

4.4 Vortex Detection on CROR

4.4.1 Search of Vortex Core Regions

Figures 4.6, 4.7, 4.8, and 4.9 show the iso-surfaces of different threshold values for the parameters Q , N_k , Δ , and λ_2 , respectively, applied to one snapshot of the CROR solution. For the lower absolute threshold values selected, all these four methods successfully predict the trajectory and the shape of the vortices developed at the tip of the blades comprising the front rotating rotor, and a tip-vortex impact condition with the subsequent rotor stage can be observed. Downstream of the second rotor stage significant vortex interactions occur, and none of the four RB methods is capable to provide a clear representation of all the individual coherent vortex regions.

As one increases the absolute value of these four parameters the low energy structures can be filtered, allowing a clearer representation of the tip vortices. However, if the selected thresholds are too high, the trajectory of the tip vortices cannot be visualized correctly. For the highest threshold values of Q and Δ shown in Figures 4.6 and 4.8, respectively, tip vortices are not extracted. However, these two RB methods extract always regions representing boundary layers. This is not the case for the other two RB methods. Applying the kinematic vorticity method, boundary layer regions are removed almost automatically. Using the λ_2 -criterion, one is able to vanish the boundary layer in the shaft imposing strong negative values.

Figure 4.6: Representation of iso-surfaces of Q . Figure 4.7: Representation of iso-surfaces of kinematic vorticity number N_k . Figure 4.8: Representation of iso-surfaces of Δ .

Figure 4.9: Representation of iso-surfaces of λ_2 .

All the four RB methods are applied locally to each grid cell, making them relatively easy to parallelize across multiple processors. Figure 4.10 shows the processing time required by the four methods, using 2, 4, and 12 processors. When passing from 2 to 12 processors the running time decreases about 85%. The most time consuming method, the λ_2 -criterion, requires about 10 minutes of computation time using 12 processors. These figures would drop significantly if one takes the same number of processors used for the CFD simulations, making the post-processing time required by these RB methods irrelevant in comparison to the simulation.

Figure 4.10: Computation time required by the selected RB methods.

4.4.2 Search of Vortex Lines

In order to investigate the suitability of the Predictor-Corrector method for the particular case of CROR engines, five representative candidate seeds were selected relying on both low static pressure and high vorticity magnitude thresholds. The spatial location of these points in the computational domain is depicted in Figure 4.11. The original Predictor-Corrector method was then initiated individually on each of these candidate seeds.

Figure 4.11: Location of the selected candidate seeds for the Predictor-Corrector method.

Figure 4.12 shows (in blue) the vortex axis developed from seed P_1 using the Predictor-Corrector method, together with iso-surfaces of $\lambda_2 = -5$ (in red). This line clearly defines the skeleton of the corresponding vortex core region extracted with the λ_2 -criterion, both in upstream and downstream directions. In the backwards direction to the flow, the line grows from its starting point P_1 , to the onset location of the matching tip vortex TV1. Initially, in the forward direction to the flow, the skeleton line follows correctly this tip vortex, until there is an impact with a second stage blade. At this intersection point the line extracted for TV1 stops its growth, and then a different skeleton line belonging now to the tip vortex TV2 starts to develop in the backwards direction, stopping at the exact location where TV2 is originated. From Figure 4.12 one can also observe some vortex line oscillations near the sliding plane region, that the Predictor-Corrector method cannot avoid.

Figure 4.12: Vortex line developed from P_1 . Results are compared with $\lambda_2 = -5$ regions.

Similar results can be obtained starting the Predictor-Corrector algorithm from seed points P_2 and P_3 , as shown in Figure 4.13. Note that P_2 is located near the mid-region between CROR stage 1 and stage 2, while P_3 is close to the tip of a front rotating blade of Stage 1. The vortex lines obtained from these two candidate seeds have a very similar shape and are almost superimposed in space, as they belong to the same tip vortex (TV1 in Figure 4.13). These results are shown here only as an illustrative example about the suitability of the Banks & Singer method to the present CROR test case, once the original algorithm already expects that a pre-selected candidate point belonging to an already extracted vortex is eliminated from the list of possible candidate seeds, avoiding the growth of the same vortex (as seen in Figure 4.13) and any possible redundancies, and thus less examinations.

Figure 4.14 shows the results obtained from two candidate seeds located downstream of the counter-rotating Stage 2, in the vortex breakdown region. On the left side, the extracted vortex line inherent to the tip vortex TV2, represented in the figure by a blue tube, grows correctly in the backwards direction from the seed P_4 to the tip of the blade

Figure 4.13: Vortex lines developed from P_2 (on the left) and from P_3 (on the right), belonging to the same tip vortex TV1. Results are compared with regions of $\lambda_2 = -5$.

where this vortex is originated. Note that the intersection of tip vortices TV2 and TV1' does not interfere with this last growth. Nonetheless, in the other direction from P_4 , the intersection between TV2 and TV1 causes this vortex line to deviate into the tip vortex TV1, coming from the first stage rotor. This vortex line continues then its growth towards upstream, until the moment it intersects a Stage 2 blade, breaking its growth. This is another indication suggesting the first stage vortices are impacting the second stage rotor. On the right side of Figure 4.14, the vortex line developed from P_5 does not divert significantly from the center of the tip vortex core region TV2, represented in the figure by iso-surfaces of $\lambda_2 = -5$ (in red). However, the extracted vortex line suffers from severe “zig-zags” in the trailing breakdown region. This effect results from the inevitable tip vortex interactions that occur in the area.

The biggest problem encountered with the original Predictor-Corrector method [6] is related with its high computational demands. At each pressure correction step, the method needs to interpolate over the computational domain in order to reach the local pressure minimum, and for a big test case such as the full annulus CROR this process can

take long computation times. Table 4.2 shows the computation times required to build the vortex core lines shown in Figures 4.12, 4.13, and 4.14, using one single processor. Besides that, the method is extremely sensitive to the quality of the prior initialization. For the CROR test case, the original selection of candidate seeds relying on pressure and vorticity thresholds provides a significant amount of points that do not evolve in a vortex line, increasing the already high computation costs of the method.

Figure 4.14: Vortex lines developed from P_4 (on the left) and from P_5 (on the right), both situated downstream of the second rotating row. Results are compared with regions of $\lambda_2 = -5$.

Table 4.2: Computation time required by the Predictor-Corrector method to build vortex core lines from points P_1 to P_5 , using one processor.

Vortex line from point	Computation time
P_1	15 min 11 sec
P_2	26 min 56 sec
P_3	22 min 43 sec
P_4	11 min 20 sec
P_5	55 min 35 sec

4.5 Improving the Initialization of the Banks & Singer Method

As explained in Section 4.3.3.5, the original Predictor-Corrector method makes the selection of candidate seeds according to high vorticity and low static pressure threshold criteria. Normally this methodology is enough for simple academic test cases, with a low number of grid points. However, when dealing with a large scale industrial case with high flow complexity, such as the present CROR test case with 95 million points, the original initialization may return a huge amount of candidate points. This will directly penalize the subsequent predictor-corrector step, once it has to be started from each one of those candidate points, resulting in excessive and prohibitive computational costs. Furthermore, by relying exclusively on those two threshold criteria, there is not a physical guarantee that the selected thresholds contain the most relevant features. For the present CROR test case, by setting a threshold for cells whose vorticity magnitude is higher or equal to only 0.15% of the maximum vorticity of the computational domain, this criterion fails to extract cells related to the tip vortex emerging from the first rotating row. The output of the aforementioned vorticity threshold is only associated with the boundary layer of the rotating surfaces, where vorticity can also be high. Alternatively, for the lowest static pressure values of the domain, the corresponding threshold filter retrieves no more than points or cells located in low pressure zones of the blades. Furthermore, significant trial and error tests were required to correctly tune a static pressure threshold that allowed the extraction of cells or points related to tip vortices.

The original initialization process relies only on thresholds, and so there is always a user interference that cannot be avoided in the Predictor-Corrector method. Moreover, as the present CROR test case demonstrated, it is not a straightforward task for the designer to correctly adjust thresholds relying on static pressure and vorticity magnitude. There are several flow regions apart from the tip vortices where the static pressure is low and the vorticity is high, reducing the probability of those two criteria to extract cells or points associated to tip vortices. Furthermore, the pressure and vorticity thresholds set for one case probably have to be changed for different flow problems.

Two initialization methodologies are presented to address this problem.

4.5.1 Initialization Based on RB Vortex Detection Criteria

This initialization uses the RB vortex detection methods described in Section 4.3.3 to build a set of candidate points for the Predictor-Corrector method, increasing its probability to find candidate seeds that will develop into a tip vortex core line. With the inclusion of these four gradient-based methodologies, the extraction of candidate seeds being related with a tip vortex becomes also less sensitive to the selection of thresholds, contrary to what happens with the thresholds of vorticity magnitude and static pressure. The steps comprising the method are presented in the pseudo-code of Algorithm 4.2.

Algorithm 4.2 Initialization based on gradient-based vortex detection methods.

- 1: select only one of the four RB vortex detection methods described in Section 4.3.3
 - 2: calculate the parameter related with the chosen method over the fluid domain
 - 3: **if** *Q-criterion is selected* **then**
 - 4: set a positive $Q_{threshold}$ and extract cells or points where $Q > Q_{threshold}$
 - 5: **else if** *Kinematic vorticity number is selected* **then**
 - 6: set a positive $N_{k,threshold}$ always higher than 1 and extract cells or points where $N_k > N_{k,threshold}$
 - 7: **else if** Δ -*criterion is selected* **then**
 - 8: set a positive $\Delta_{threshold}$ and extract cells or points where $\Delta > \Delta_{threshold}$
 - 9: **else if** λ_2 -*criterion is selected* **then**
 - 10: set a negative $\lambda_{2,threshold}$ and extract cells or points where $\lambda_2 < \lambda_{2,threshold}$
 - 11: update fluid domain: it contains now only the extracted cells or points
 - 12: refine the previous extraction by selecting an alternative RB method
 - 13: **repeat**
 - 14: **go to** 2
 - 15: **until** the four RB methods are used
-

The advantages introduced by such initialization are presented in Table 4.3, for the example being considered, with respect to one snapshot of the CROR simulation. This table shows, for three threshold values of static pressure (p), vorticity magnitude ($|\omega|$), Q , Δ , λ_2 , and N_k , the ratio of volumes extracted over the total volume of the computational domain, and information about whether the extracted volumes contain cells that are

related with the tip vortex generated from the first blade row. Note that the thresholds exhibited for Q , N_k , Δ , and λ_2 were previously shown in Figures 4.6 to 4.9, respectively, in the form of iso-surfaces of that threshold value.

Table 4.3: Thresholds applied to the CROR test case regarding initialization 1.

	Threshold on					
	p	$ \omega $	Q	Δ	λ_2	N_k
Threshold 1	$3.5p_{min}$	$0.8 \omega _{max}$	1.1	50	-1	1.1
Vol_1/Vol_{domain} [%]	0.0000	0.0000	0.0381	0.0258	0.0057	1.3949
Cells within tip vortex from 1 st row	NO	NO	YES	YES	YES	YES
Threshold 2	$5.0p_{min}$	$0.1 \omega _{max}$	50	2000	-5	2.5
Vol_2/Vol_{domain} [%]	0.0002	0.0000	0.0044	0.0126	0.0019	0.0035
Cells within tip vortex from 1 st row	NO	NO	YES	YES	YES	YES
Threshold 3	$6.0p_{min}$	$0.01 \omega _{max}$	2500	1.00E+08	-50	5
Vol_3/Vol_{domain} [%]	0.0025	0.0001	0.0007	0.0017	0.0002	0.0001
Cells within tip vortex from 1 st row	YES	NO	NO	NO	YES	YES

For the highest threshold values of Q and Δ exemplified in Table 4.3, tip vortices are not extracted. However, for all the selected thresholds of λ_2 and N_k shown in this table, cells belonging to tip vortices are always extracted, demonstrating that the suggested initialization is much less sensitive to the selection of those values, when confronted to pressure and vorticity magnitude thresholds. For the latter, even with a threshold of 1% the maximum vorticity magnitude of the computational domain, no cell associated with the tip vortex is extracted. And for the static pressure, only with a threshold from 6 times its minimum value inside the computational domain, the extraction of cells related with the tip vortex is possible.

Table 4.3 shows also that for higher thresholds of Q , Δ , and N_k , and lower values of λ_2 , the ratio of volumes extracted over the total volume of the computational domain (Vol/Vol_{domain}) decreases, lowering the number of candidate seeds extracted and thus reducing the computational burden of the Predictor-Corrector method, once less evaluations are required. Moreover any threshold value of the aforementioned gradient-based parameters combined is able to extract cells belonging to tip vortices, enhancing the probability

of the proposed initialization to extract candidate cells or points that have the potential to grow into a tip vortex core line.

4.5.2 Initialization Based on High Pressure Gradients & Friction Drag

Similarly to the previous method, an initialization relying on high pressure gradients and high friction drag allows to improve the quality and to reduce the uncertainty of the original initialization of the Predictor-Corrector method, as it increases as well the probability of the aforementioned LB method to find candidate cells or points that will develop into a tip vortex core line. On the one hand, adverse pressure gradients in the direction of the flow induce the formation of the “separated” tip vortex from the first blade row. The extraction of cells or points where this parameter is higher than zero enhances thus the probability to find good candidate seeds. On the other hand, the proposed methodology searches also for surface cells or points where the drag friction coefficient is high, suggesting high local aerodynamic losses. In CROR engines, the formation of tip-vortices and possible tip-vortex-blade impact conditions have a significant contribution to the overall aerodynamic losses of the system. With the combination of these two superficial aerodynamic parameters, a more intelligent selection of candidate seeds is granted, but also the quality of the initialization process becomes less dependent upon arbitrary threshold selection, in comparison to the thresholds of vorticity magnitude and static pressure from the original initialization. Algorithm 4.3 shows the pseudo-code used for the presented methodology.

The advantages given by the present initialization based on high pressure gradients and high drag friction coefficient are resumed in Table 4.4, for the example being considered with respect to one snapshot of the CROR simulation. This table compares the number of points extracted with the original static pressure (p) and vorticity magnitude ($|\omega|$) threshold method, with those obtained after applying thresholds of dp/dX and C_{df} to the same data set, and provides information about whether the extracted points are related with the tip vortex generated from the first blade row. The graphical informa-

Algorithm 4.3 Initialization based on high pressure gradients and high drag friction.

- 1: calculate $\nabla \mathbf{v}$ and ∇p at each cell or point of the computational domain
- 2: compute the pressure gradient in the direction of the flow, as the scalar projection of ∇p onto $\mathbf{v}$:

$$\frac{dp}{dX} = \frac{\nabla p \cdot \mathbf{v}}{|\mathbf{v}|} = \frac{(dp/dx)v_x + (dp/dy)v_y + (dp/dz)v_z}{\sqrt{v_x^2 + v_y^2 + v_z^2}} \quad (4.12)$$

- 3: project the volume information into the matching superficial nodes, and obtain a superficial dataset
- 4: at each cell or point of the superficial dataset, approximate the nine single components of the stress tensor by:

$$\tau_{ij} = -p\delta_{ij} + \mu \left(\frac{dv_i}{dx_j} + \frac{dv_j}{dx_i} \right) \quad (4.13)$$

where

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (4.14)$$

- 5: calculate the drag friction coefficient, as follows:

$$C_{df} = C_{df,x} + C_{df,y} + C_{df,z} \quad (4.15)$$

with

$$C_{df,x} = \frac{(\tau_{xx} \cos \alpha \cos \beta + \tau_{yx} \cos \alpha \sin \beta + \tau_{zx} \sin \alpha) \times Normal_s_x}{S_{ref}} \quad (4.16a)$$

$$C_{df,y} = \frac{(\tau_{xy} \cos \alpha \cos \beta + \tau_{yy} \cos \alpha \sin \beta + \tau_{zy} \sin \alpha) \times Normal_s_y}{S_{ref}} \quad (4.16b)$$

$$C_{df,z} = \frac{(\tau_{xz} \cos \alpha \cos \beta + \tau_{yz} \cos \alpha \sin \beta + \tau_{zz} \sin \alpha) \times Normal_s_z}{S_{ref}} \quad (4.16c)$$

where α represents the angle of attack, β the angle of sideslip, S_{ref} the reference area, and $Normal_s_i$ the surface normals in the i -direction.

- 6: **for** dp/dX : set a positive $dp/dX_{threshold}$ and extract cells or points where $dp/dX > dp/dX_{threshold}$ from the superficial dataset previously created in 5
 - 7: create a new superficial dataset, containing only the extracted candidate seeds from 6
 - 8: **for** C_{df} : set a positive $C_{df,threshold}$ and extract cells or points where $C_{df} > C_{df,threshold}$ from the superficial dataset created in 5
 - 9: update the superficial dataset of step 7 with the information derived from 8. This final dataset contains the candidate seeds for the Predictor-Corrector method
-

tion for the threshold 1 and 3 of dp/dX and C_{df} is displayed in Figures 4.15 and 4.16, respectively.

Table 4.4 confirms that the proposed initialization is much less sensitive to the selection of thresholds, when confronted to pressure and vorticity magnitude thresholds. For the latter, seeds associated with the tip vortex can only be extracted with a threshold in the order of 0.0003 the maximum vorticity magnitude present in the computational domain. And for the static pressure, as discussed in Section 4.5.1, only by setting a threshold from 6 times its minimum value inside the computational domain, the extraction of cells related with the tip vortex is possible. This new initialization also enables a significant drop of the number of candidate seeds extracted, allowing thus an important reduction of the computational burden of the original Pressure-Correction method for the particular case of CROR.

Table 4.4: Thresholds applied to the CROR test case regarding initialization 2.

	Threshold on			
	p	$ \omega $	dp/dX	C_{df}
Threshold 1	$6.0p_{min}$	$0.0003 \omega _{max}$	$0.04dp/dX_{max}$	$0.70C_{df,max}$
# Pts_1	10619111	19806357	6319	701
Pts within tip vortex from 1 st row	YES	YES	YES	YES
Threshold 2	$5.0p_{min}$	$0.1 \omega _{max}$	$0.17dp/dX_{max}$	$0.82C_{df,max}$
# Pts_2	2357355	387408	2042	60
Pts within tip vortex from 1 st row	NO	NO	YES	YES
Threshold 3	$3.5p_{min}$	$0.8 \omega _{max}$	$0.35dp/dX_{max}$	$0.94C_{df,max}$
# Pts_3	456848	84	702	60
Pts within tip vortex from 1 st row	NO	NO	NO	YES

The vortex core lines obtained with the Banks & Singer method, from the seeds illustrated in Figure 4.16-right, are shown in Figure 4.17. Prior to the beginning of the growth of each vortex line, the original position of each seed was refined in order to match the local point of maximum kinematic vorticity number (N_k). As it can be observed

from the figure, all candidate seeds correctly end up in lines that accurately describe the trajectory of the corresponding tip vortices. From Figure 4.17 we can also visualize that all the extracted vortex lines are impacting the second stage counter rotating blades of the tested CROR configuration, as expected. The computation time required for the growth of one of these lines was, in average and using one processor, 8 minutes and 35 seconds.

Figure 4.15: Points extracted after performing step 6 of Algorithm 4.3, for two thresholds of dp/dX .

Figure 4.16: Points extracted after performing step 8 of Algorithm 4.3, for two thresholds of C_{df} .

(a) Side view

(b) Front view

Figure 4.17: Vortex core lines obtained with the Predictor-Corrector method, after applying the threshold $C_{df} = 0.94C_{df,max}$ to the initialization step.

4.6 Summary

For large and complex industrial simulations, flow feature detection techniques can provide fast and very accurate information about existing non-linear flow features. Using a typical industrial CROR test case, this work shows that both Region and Line-based vortex detection methods are very convenient tools to visualize and to track the vortices generated at the tip of the blades, providing feedback about possible vortex-blade impacts.

All the four implemented RB methods (Q , N_k , Δ , and λ_2 criteria) successfully depict the trajectory of the tip vortices, nonetheless they strongly depend on fully arbitrary thresholds. Boundary layer removal is almost automatic using the N_k method, a valuable feature considering the boundary layer is of no interest to the current study. For the particular case of CROR, the tested Predictor-Corrector method, by Banks and Singer, provides a precise tip vortex tracking and a near automatic impact evaluation, once its algorithm breaks when a vortex core line intersects a blade. However, the method cannot guarantee the correct development of a tip vortex line when it interacts with other rotating structures. Furthermore its original seeding selection (or initialization) is somehow limited.

Two initialization methodologies are proposed to address the solution of this last problem, by increasing the probability of finding good candidate points that develop into a tip vortex core line. The first initialization scheme relies on the aforementioned RB methods, and can be applied to any generic dataset containing rotating structures. The second initialization method is geared towards particular flow problems where fluid-structure interaction exist, and where the formation of vortices is linked to high pressure gradients and high friction drag on the structures, as in this concrete CROR test case.

5

Concluding Remarks

Flow feature detection and data-based decomposition techniques are valuable post processing tools when it comes to identifying relevant features existing in a certain fluid flow problem. Relying only on flow snapshots, directly obtained from numerical simulations or derived from experimental measurements, these techniques provide fast and accurate representations of the main structures, at a relatively low computational cost.

In the present thesis, a flow feature detection approach was followed to identify vortices in a large-scale CROR test-case, provided by Airbus. For this purpose, a vortex detection library was developed and completely integrated with current Airbus post-processing tools. This library is nowadays accessible to everybody within Airbus, for steady solutions. At the moment it comprises the Q , N_k , Δ , and λ_2 criteria, and the Pressure-Corrector method, but other vortex detection methodologies can easily be added to broaden this tool. With all the above-mentioned methods, we were able to predict the trajectory of the tip vortices generated from the first rotating row, and identify an impact situation with the following counter-rotating blades.

In their original formulation, all the five methods require strong external dependencies, as arbitrary thresholds have to be tuned. To reduce the user's dependence upon

the selection of candidate seeds for the Predictor-Corrector method, two initialization methodologies were presented. The first one relies on Region-based methods, and it is basically a combination of several vortex detection criteria. The second method is based on high local pressure gradients and high drag friction, being particularly suitable for this CROR test-case. Future work to improve the present vortex detection library should include the following directions: parallelization of the Pressure-Corrector method; development of a more intelligent and user's free methodology for the selection of thresholds; tracking and visualization in time of the evolution of a vortex; and combination with mesh refinement and design/optimization tools.

The dynamics of saturation inside an open cavity was also investigated in this thesis, using three-dimensional DNS simulations together with the DMD. Despite the highly non-linear complexity of the flow, this data-based decomposition technique was demonstrated capable of extracting the frequency and the shape of the most relevant modes emanating inside the cavity, and both in agreement with previous linear stability analysis and experimental results. With this modal analysis, we were able to find the true nature of the decrease in the characteristic Strouhal number observed for the dominant mode of the experiments. This behaviour is mainly due to the saturated regime of the flow, producing a reduction of the velocity of the main centrifugal vortex, responsible for the said discrepancy in frequency. The presence of end-wall vortices near the spanwise confinements of the cavity strengthens this effect, however always with a lower contribution.

A parallel version of the DMD was also implemented in current Airbus simulation tools, allowing its use in typical large scale industrial problems of Airbus. This numerical tool was properly validated, and its computational performance evaluated. Besides all the advantages offered by the DMD, this technique still requires a manual selection of modes, a study about the convergence of the decomposition, and a priori knowledge of the physical problem under investigation. Future versions of our DMD tool should include algorithms that allow an intelligent selection of modes, and a nearly-automatic convergence of the DMD. After this sensitive step, we would be able to perform concurrent DMD analysis along with the numerical simulations. The inclusion of statistical components into the decomposition is also a potential future topic of investigation.

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