General Proper Orthogonal Decomposition, Modal Correction, Inter-Modal Interactions, and Sequencing

by

Mahdi Hosseinali

Master of Science, Amirkabir University of Technology, 2013
Bachelor of Science, University of Tabriz, 2009

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

Doctorate of Philosophy

In the Graduate Academic Unit of Mechanical Engineering

Supervisor(s): Joseph W. Hall, PhD, Mechanical Engineering
Examining Board: Tiger Jeans, PhD, Mechanical Engineering, Chair
Andrew Gerber, PhD, Mechanical Engineering,
Gordon Halloway, PhD, Mechanical Engineering
External Examiner: Arash Habibi Lashkari, PhD, Computer Science
Lawrence S. Ukeiley, PhD, Mechanical Engineering,
University of Florida

This dissertation is accepted by
The Dean of Graduate Studies

THE UNIVERSITY OF NEW BRUNSWICK
July, 2019
©Mahdi Hosseinali, 2019
Abstract

This study revisits key points, and develops new tools for a better understanding of
the Proper Orthogonal Decomposition method (POD), a popular approach to edu-
cate researchers about the underlying mechanisms in fluid flow. First, the implement-
tation of a Jacobian matrix is revised to develop a general form that is implementable
on arbitrary grids, coordinate systems, and variations of POD with ease. Using the
general approach developed herein, the scalar and vectorial kernel are analytically
compared to show the superiority of the latter. The commonly accepted concept of
POD equivalency with the Fourier transform in homogeneous directions is challenged
using an analytical test function to show it does not always hold true. Moreover,
a summary of the practical difficulties of the Fourier transform are presented and
a discussion of how POD overcomes these difficulties is presented. Next, tools for
selecting the number of modes for low-dimensional reconstruction and choosing the
best instances to represent such reconstructions are developed. Then, the eigenvalue
degeneracy and its effect on the globality of POD modes are investigated for the
first time. A correction method has been developed to increase the locality of the
modes through the use of a blind source separation algorithm and eigenvalue uncer-
tainty. Furthermore, two new criteria are developed to discover the modes associated
with traveling waves with the least possible assumptions. Finally, a novel method is
developed to provide sequences of instances from a non-time-resolved dataset.
Acknowledgements

I wish to acknowledge my mentor, Dr. J. W. Hall for all the support, guidance, and most importantly patience that he displayed during the course of this ever-evolving thesis. I would like to extend a sincere thanks to Atlantic Computational Excellence Network for the two year research fellowship, Compute Canada for invaluable resources, Mitacs Accelerate for the opportunity of extending my capabilities, NSERC and NBIF for financial support, all of which played important roles in this thesis. Also, a special note of thanks to students, faculty, and support staff of Department of Mechanical Engineering at University of New Brunswick who’s name will not be written here for risk of leaving somebody out. Finally and most importantly, I wish to express sincerest gratitudes to my parents for a life-long support.
Table of Contents

Abstract ii

Acknowledgments iii

Table of Contents vi

List of Tables vii

List of Figures xiv

1 Introduction 1

2 General Proper Orthogonal Decomposition and Kernel Choice 7

2.1 Introduction .......................................................... 7

2.2 Classical POD ........................................................ 11

2.3 The Method of Snapshots ........................................... 14

2.4 Singular Value Decomposition and General POD ................. 16

2.5 POD Kernels ......................................................... 25

2.6 Free Jet Experimental Setup ...................................... 28

2.6.1 Facility ............................................................ 28

2.6.2 Instrumentation .................................................. 28

2.6.3 Validation ........................................................ 30

2.6.4 Grid Transformation ............................................ 34

2.7 Implementation ..................................................... 36
# List of Tables

2.1 Energy content of kernels. .............................................. 42

4.1 Asymptotic eigenvalues of random covariance matrix at 100%, 95%, and 50% confidence. ............................................. 69

5.1 Theoretical and numerical energy contents of numerical test function. 96
5.2 Association matrix of original POD coefficients by Frequency Criteria 110
5.3 Association matrix of original POD coefficients by Derivative Criteria 110
5.4 Association matrix of corrected POD coefficients by Frequency Criteria 111
5.5 Association matrix of corrected POD coefficients by Derivative Criteria 111
5.6 Energy content of POD and Fourier modes for numerical test function
    (u5). ................................................................. 112
5.7 Compared references and corresponding symbols ..................... 117

6.1 Distance of instances in POD coefficient space with different number
    of modes. ............................................................ 170
6.2 Cosine of angle between three consecutive instances in POD coefficient
    space with different number of modes. ............................. 173
6.3 Cosine of angle between three consecutive instances in POD coefficient
    space with all modes and different temporal resolution. The last row
    has 12 modes with the sampling of the row above it. .............. 173
List of Figures

2.1 Samples in a space with higher dimension. (a) Two sampled vectors in a two-dimensional space. (b) Two sampled vectors in a three-dimensional space. 19

2.2 Over-sampled data in column and row space. (a) Three sampled vectors in a the column space. (b) Three sampled vectors in the row space. 20

2.3 Experimental setup and coordinate system. 29

2.4 Contours of mean velocity components. 31

2.5 Turbulent kinetic energy and Reynolds stresses. 32

2.5 (continued) Turbulent kinetic energy and Reynolds stresses. 33

2.6 Mean streamwise velocity component and its fluctuation. 35

2.7 Selected streamwise modes of the scalar kernel. Solid and dash contour lines are positive and negative, respectively. 38

2.8 Selected cross-stream modes of the scalar kernel. Solid and dash contour lines are positive and negative, respectively. 39

2.9 Selected streamwise modes of the vectorial kernel. Solid and dash contour lines are positive and negative, respectively. 40

2.10 Selected cross-stream modes of the vectorial kernel. Solid and dash contour lines are positive and negative, respectively. 41

2.11 Low-dimensional reconstruction of the streamwise velocity components with scalar kernel. 43
2.12 Low-dimensional reconstruction of the cross-stream velocity components with scalar kernel. ........................................ 44
2.13 Low-dimensional reconstruction of the streamwise velocity components with vectorial kernel. ........................................ 46
2.14 Low-dimensional reconstruction of the cross-stream velocity components with vectorial kernel. ........................................ 47
3.1 Temporal evolution of the parametric test functions. ............... 52
3.2 Windowing effect on decompositions methods. Top: input signal and window size, middle: Fourier modes of full domain (horizontal hatch) and windowed domain (oblique hatch), bottom: energy of POD modes of full (horizontal) and windowed (oblique) signal. ...................... 59
4.1 Temporal evolution of clean $u_5$, correlated normal noise, and the summation. Temporal evolution is depicted by faded color lines. ...... 65
4.2 First 8 original modes of test function $u_5$. .......................... 67
4.3 Modal energy of the test function $u_5$. ................................. 68
4.4 First and 7th POD coefficients of test function $u_5$ before (left) and after (right) added noise. .............................................. 71
4.5 Effect of noise on POD coefficients of modes 1 to 6, excluding mode
3. Solid line is without noise, color of dots is based on noise. ......... 72
4.6 Different ratios of noise-to-signal-ratio between instances. ........ 74
4.7 Effect of noise on POD coefficients of modes 1 to 6, excluding mode
3. Solid line is without noise, color of dots is based on noise. ......... 75
4.8 Third-order velocity fluctuation moments with low-dimensional reconstructions. ................................................................. 79
4.9 Streamwise component of first twelve POD modes of the jet flow. Solid and dash contour lines are positive and negative, respectively. .... 83
4.10 Similar instance with different noise-to-signal-ratio thresholds computed by 7 modes. ................................. 84
4.11 Similar instance with different noise-to-signal-ratio thresholds computed by 9 modes. ................................. 85

5.1 POD reconstruction of uncorrelated independent signals. Top: original signals, bottom: reconstructed signals, left: joint PDF, right: univariate PDF ................................................................. 94
5.2 Uncertainty of $u_5$ eigenvalues with different confidence levels ... 100
5.3 First 8 corrected modes of test function $u_5$ ............... 102
5.4 Geometry of numerical simulations. .............................. 114
5.5 Simulation grid at the inlet boundary condition. .............. 116
5.6 Mean velocity and normal Reynolds stresses of pipe flow simulation. For symbols see Table 5.7. ......................... 119
5.7 Mean velocity and normal Reynolds stresses of channel flow simulation. For symbols see Table 5.7. ......................... 120
5.8 Streamwise velocity component of the pipe flow original POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively. ................................. 124
5.9 Streamwise velocity component of the channel flow original POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively. ................................. 125
5.10 Rotation of first two POD modes of pipe flow in streamwise plane (streamwise components). Blue crosses are POD coefficient, arrows are rotated axes with corresponding POD mode at the end of each arrow. Black contour lines are fitted multivariate Gaussian. Subplot captions are corresponding kurtosis. ................................. 126
5.11 Streamwise velocity component of the pipe flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively. .................................................. 128

5.12 Streamwise velocity component of the channel flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively. .................................................. 129

5.13 Relative energy contents of the first original and corrected 40 modes in streamwise plane. Top: pipe, bottom: channel. .......................... 130

5.14 Association map of pipe flow original and corrected POD modes in the streamwise plane. Pure black and white are perfect and no associations, respectively. .................................................. 131

5.15 Association map of channel flow original and corrected POD modes in the streamwise plane. Pure black and white are perfect and no associations, respectively. .................................................. 133

5.16 Streamwise velocity component of the pipe flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively. .................................................. 134

5.17 Corrected POD coefficients of modes 7, 10, and 12 of pipe flow in streamwise plane. .................................................. 136

5.18 Rotated POD modes to increase modal interaction. CM: Corrected Mode, RM: Rotated Mode after correction, k: kurtosis. Solid and dash contour lines are positive and negative, respectively. ........... 137

5.19 Corrected POD coefficients of modes 24, 25, 28, and 30 of pipe flow in streamwise plane. .................................................. 138

5.20 Original and corrected coefficients and POD modes of pipe flow. . . . 141

5.21 Time history of POD original and corrected coefficients and their Energy-Ratios. .................................................. 142
5.22 Streamwise velocity component of the pipe flow original POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively. 144

5.23 Streamwise velocity component of the channel flow original POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively. 145

5.24 Streamwise velocity component of the pipe flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively. 146

5.25 Streamwise velocity component of the channel flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively. 148

5.26 Relative energy contents of the first original and corrected 40 modes in cross-stream plane. Top: pipe, bottom: channel. 150

5.27 Association map of original and corrected POD modes of pipe and channel flow in the cross-stream plane by DC. Pure black and white are perfect and no associations, respectively. 151

5.28 Velocity components of pipe flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively. 153

5.29 Cross-stream velocity components of pipe flow corrected POD modes in cross-stream plane. 154

5.30 Combined Energy-Ratio of modes 17, 18, 40, and 43 of pipe flow in cross-stream plane. 155

6.1 Example of extracting low-dimensional dynamics from an under-sampled high-dimensional space. 161

6.2 Rate of velocity change by the angle between data points. 164
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3</td>
<td>Sequencing of low-dimensional reconstruction of test function u5.</td>
</tr>
<tr>
<td>6.4</td>
<td>Distance between instances in original POD coefficient space of pipe flow in streamwise plane with different mode numbers.</td>
</tr>
<tr>
<td>6.5</td>
<td>Angle change in POD coefficient space with fine (top) and coarse (bottom) time steps.</td>
</tr>
<tr>
<td>6.6</td>
<td>Interpolated POD coefficients of streamwise plane of pipe flow with spline method for different sampling rates ($tU/D$ is Eddy-turn-over time).</td>
</tr>
<tr>
<td>6.7</td>
<td>Interpolated time-resolved POD coefficients of mode 19 ($\Delta tU/D = 1.93$) by time, distance in 19 modes, and distance in P50 modes.</td>
</tr>
<tr>
<td>6.8</td>
<td>Sequencing time-resolved pipe flow data with 3 Modes and different sampling rates.</td>
</tr>
<tr>
<td>6.9</td>
<td>Sequencing time-resolved pipe flow data with 6 Modes and different sampling rates.</td>
</tr>
<tr>
<td>6.10</td>
<td>Sequencing time-resolved pipe flow data with 12 Modes and different sampling rates.</td>
</tr>
<tr>
<td>6.11</td>
<td>Sequencing time-resolved pipe flow data with 19 Modes and different sampling rates.</td>
</tr>
<tr>
<td>6.13</td>
<td>Sequenced and time-resolved POD coefficients of first 6 modes of pipe flow. The reference instance is at $tU/D = 66$.</td>
</tr>
<tr>
<td>6.14</td>
<td>Time-resolved and sequenced instances (with first 6 modes) from pipe flow. The reference instance is at $tU/D = 66$.</td>
</tr>
<tr>
<td>6.15</td>
<td>Sample sequence of streamwise velocity component of jet flow in cross-stream plane. The sequence has been down-sampled by showing one out of every 5 instances.</td>
</tr>
</tbody>
</table>
D.1 Annotation of triangle to calculate area contributed to each node. . . 228
Chapter 1

Introduction

It has long been believed that coherent structures are responsible for the governing dynamics in turbulent flow. The first to note the presence of these structures was likely Da Vinci in his sketches of vortices, but the first systematic investigations of them may have been by Brown [18] who used flow-visualization of these structures to infer the behaviour of instability mechanisms in the free jet. Many techniques for analyzing coherent structures have been used over the years such as flow visualization [18, 66], Conditional Sampling [150], Linear Stochastic Estimation [2], Wavelets [35], Spatial Filtering [3], and Dynamic Mode Decomposition [129] but the current work focuses on one of the most widely used, the Proper Orthogonal Decomposition (POD) [90].

The POD method developed by Pearson [111], and first introduced to the turbulence community by Lumley [90], attempts to capture the coherent structures in an unbiased way by maximizing their projection onto the turbulent velocity field in a mean square sense. As a result, the eigenfunctions are the most likely occurrences of velocity fluctuations [48]. In simpler terms, the eigenfunctions are the best orthogonal representation of correlations in a dataset. The method has gained popularity over the decades and has caused numerous variations such as Extended POD [94, 16]
or Spectral POD [149]. Chapter 2 examines the derivation of the most common variation; the Method of Snapshots [138]. Using the insight of previous researches and Glauser’s generalization [48] of Lumley’s classical formulation [90], the base matrix is redefined so both classical POD and the Method of Snapshots could be used, conveniently, in conjunction with any POD variation on an arbitrary coordinate system and grid. Then the coordinate system dependence of two widely used kernel definitions, scalar and vectorial, are analytically investigated to show that the modes of the scalar kernel could be misleading.

Chapter 3 covers another basic concept in the POD implementation. POD is often employed in flows where one or more dimensions can be considered homogeneous. Lumley [90] addresses POD behavior in a homogeneous direction in his original paper by stating, ”In any homogeneous direction, the harmonic functions are suitable solutions of POD”. The generally accepted implication of POD modes degenerating into harmonic functions has also been mentioned by others [61, 43]. The logic of the implication is that the reconstruction of the kernel by eigenfunctions and eigenvalues in discrete [61] (equation 2.7) or continuous form [90] is analogous to discrete or continuous Fourier transform respectively; therefore, the modes of both decomposition methods can be equivalent. Bakewell and Lumley [9] were the first to perform dimensionally decoupled POD analysis on experimental data of a pipe flow where the azimuthal and axial directions were represented by Fourier modes, and many other researchers [47, 96, 13, 11, 128, 26, 15, 27, 22, 76, 42, 73, 151, 147, 122] have followed the same procedure. Although previous studies have presented formulations to support the implication, neither have explored the possibility that the POD modes could be a combination of Fourier modes. For example, Pinier [113] discussed this possibility qualitatively in velocity measurements of free jet. In the current study, analytical test functions and POD solution are used to prove by contradiction that the equivalency of the two methods is not always true. With fundamental concepts
regarding the implementation of POD being covered, the next chapters focus on the proper application of results.

Although low-dimensional reconstruction is the main purpose of POD, similar to any other decomposition method, the fluid mechanics community suffers from the lack of any systematic method to choose the cut-off mode number and the reconstructed instances. Current approaches to select the cut-off mode number are either vague, or intuitive, such as: arbitrary selection of modes [5], maintaining a high energy percentage, which no threshold is generally accepted, [38, 72, 115, 143], to reconstruct a specific structure [147, 121], or an abrupt drop in the energy [107, 57, 122]. Also, the low-dimensionally reconstructed instances for inspection are often selected randomly which raises questions toward the application and interpretations of POD analysis. Chapter 4 introduces the methods used in other fields for selection of the cut-off mode number and adapts them to fluid mechanics context. Moreover, new methods will be developed to efficiently under-sample the instances and select the ones that are most representative of the desired subspace.

As stated, the main purpose of POD is to understand the physics of coherent structures which are known to be advective [145], so POD is expected to reflect this. In fact, one of the known weaknesses of POD is that the modal interactions are unclear using the standard analysis. Due to experimental limitations, the domain of POD analysis is usually space-only so a single mode, which is time independent, cannot represent a traveling structure. Shlens [136] uses the example of a person on a Ferris wheel to show that the appearance of multiple modes for a single transitional wave is a result of improper frame of reference. Although the movement of the Ferris wheel can be explained by only one bases (angle of rotation), a Cartesian frame of reference needs two bases to capture the movement. Feeny [36] explains that a traveling wave is represented by a continuous transition of energy between two modes with similar energy content. Feeny’s finding is inline with many other
studies such as analytical POD modeling of Kuramoto-Siavshinsky equation [124], numerical simulations of cylinder wakes [105], experimental velocity measurements of rectangular jet [54, 56], axisymmetric wall jet [63], axisymmetric free jets [148], and numerical and experimental investigation of swirling jets [107]. Chapter 5 reviews previous methods of capturing traveling waves in more detail. A known obstacle in understanding the traveling waves is the global shape of modes (i.e., the modes are non-zero in full field). However, contrary to the common belief, the globality is not an inherent property of POD. A method is developed to enhance the locality of the mode shapes which in turn reduces the complexities of discovering traveling waves. The correction method can also be used in time-resolved data or when the domain is not limited to space, such as spectral POD [149]. Finally, two new criteria are defined based on POD coefficients to quantify the level of modal interactions.

The methods developed in Chapter 4 provide a guideline to narrow down the number of realizations used in the interpretation of the flow, but in non-time-resolved datasets the interpretation of the low-dimensionally reconstructed field needs further attention. The underlying mechanisms are frequently examined by presenting a series of low-dimensional reconstructions but there is no guideline to reliably find such a sequence of instances from non-time-resolved data (like PIV), or measure their validity. Chapter 6 tackles this problem, for the very first time, by deriving relations between distances and angles in the POD coefficient space and time differences and rates of momentum change.

In summary, the objectives of this thesis aim to improve our understanding of POD analysis including addressing the direct formulation of POD and the subsequent interpretation and understanding of the POD solutions. To undertake the first objective, understanding the formulation of the POD problem, prior to solving, is crucial. Chapter 2 and 3 focus primarily on improving the formulation of the POD problem. In particular, Chapter 2 builds upon the current formulation and implementation of
POD and combines them into a unified Generalized POD approach that can be used with arbitrary coordinate system, non-uniform grids, and other extensions of POD. The same chapter also formally examines how the choice of POD kernel impacts the resulting POD modes and low-dimensional reconstructions. Often, researchers make the choice to replace POD analysis in homogeneous directions with the Fourier transform, and this choice on the POD solution is critically analyzed in Chapter 3.

Chapters 4, 5 and 6 are directed at improving our understanding of the resulting POD solutions. Although many methods are developed throughout these chapters, the major contributions are Energy-Ratio, Modal Correction, Traveling Wave Criteria, and the Sequencing Method. The Modal Correction method developed in Chapter 5 resolves the previously unknown cause of global mode shapes which leads to better understanding of the underlying dynamics of the turbulence. Two methods, namely Derivative and Frequency Criteria, are developed in the same chapter as measures of the inter-modal interactions which might be representative of the advection of turbulent structures. The methods of Chapter 5 along with cut-off mode criteria developed in Chapter 4 provides insight into choosing the most important modes for a low-dimensional reconstruction. Then the Energy-Ratio method, which is developed in Chapter 4, can be used to find the best instances where the desired modes have significant dynamical importance in a low-dimensional reconstruction. Lastly, Chapter 6 develops an algorithm to find the most probable sequence of events in non-time-resolved datasets which are common in experimental measurements of complex flows.

In the entirety of this thesis, the developed methods and concepts are examined or illustrated using multiple datasets. Analytical test functions are used when validity of existing concepts are addressed. A numerical test function is used for illustration of concepts as the new methods are developed. Experimental measurement of the velocity field of an axisymmetric free jet and numerical simulations of pipe and
channel flow are used in different chapters to demonstrate the usefulness of the methods in practical cases.
Chapter 2

General Proper Orthogonal Decomposition and Kernel Choice

2.1 Introduction

This chapter will take a closer look and extend the usefulness of likely the biggest contribution known by the community, the Method of Snapshots [138]. This method is particularly important for newer, information dense methods such as Particle Image Velocimetry (PIV) and Computational Fluid Dynamics (CFD). The main assumption in the development of this method is that POD modes are expressible as a linear combination of the velocity field. The equivalency of the classical POD and the Method of Snapshots have been numerously studied [140, 61, 119, 144]. Raiola et al. [119] used SVD to show the equivalence of the methods and that the extra eigenvalues produced by the classical POD are zero. Taira et al. [144] later provided a comprehensive overview of POD and its relation to Singular Value Decomposition (SVD) and other modal analysis methods.

The Method of Snapshots was originally developed on a uniform and Cartesian grid as quadrature and Jacobian matrices were not considered in the algorithm. This
can be verified as equation 3.3 of the original paper [138] only integrates over time and not space. This prohibits its use in cases where other coordinate systems are of interest. An example of such cases is Wanstrom et al. [153] where they had to adopt their variation of the Method of Snapshots to calculate the modes in a polar coordinate system. Another example of using classical POD on PIV data where the Method of Snapshots would be computationally more desirable is Tinney et al. [147] who interpolated their data on a polar grid and used Fourier-POD analysis. Although this obstacle has been properly resolved as pointed by Taira et al. [144], the generated eigenfunctions are no longer orthonormal which is needed in other chapters of this thesis. Moreover, the POD method has also been developed tremendously in other fields without consideration for Jacobian matrices. Examples of these developments are Functional, Simplified, Robust Principle Component Analysis (PCA) [77], randomized Singular Value Decomposition (SVD) [53], and kernel PCA [130] for non-linear projection. A special extension of POD which is useful for calculating the most energetic modes of very large datasets (such as in Computational Fluid Dynamics (CFD)) is Incremental Principal Component Analysis (IPCA) [123]. All such methods would be readily available to the fluid mechanic community by embedding the Jacobian and quadrature matrix inside the base matrix. A technique will be developed herein to maintain the orthonormality of the eigenfunctions by including the Jacobian, quadrature, and other coefficients on the base matrix. Also arbitrary coordinate systems can be used conveniently for datasets with arbitrary grids. Perhaps most importantly, this will allow us to better understand the effect of coordinate system choice and the number of velocity components on POD solutions.

POD is an analytical tool that yields insight to the data, so the choice of the kernel (or base matrix \( U \) as will be accurately defined later) has important effects on the output of the method and subsequently the researcher’s understanding of the physics. Normally the kernel choices are either scalar, 2, or 3 component vectorial.
The earliest study known to authors that addresses kernel formation is by Glauser [46]. His investigation of the vectorial POD included both axial and radial velocity components and compared the reconstruction of the velocity signal to conclude that even though the vectorial kernel has higher energy than the scalar, it did not reveal any extra physical phenomenon. Further investigations of the energy convergence and mode shapes in planar mixing layer [27], planar jet [49], and far-field wake [76] agreed with Glauser. However, later studies [153, 73] compared two-component and three-component vectorial POD and observed that the azimuthal Fourier mode with the maximum energy shifts by including the third velocity component. Tutkun et al. [151] and Tinney et al. [147] used the same approach and reported the most energetic mode occurs at lower Fourier modes when all the components are included. Appealing to the optimality of POD, they stated the kernel which captures the most energy in the fewest modes is presumed to be better. Another study that is not consistent with any of the aforementioned groups above is Delville [26]. Delville’s work shows that the scalar and two-component vectorial kernels have the same amount of relative energy in his mixing layer, axisymmetric jet of Glauser [46], and far wake of a flat plate but the vectorial kernel results in a better spatio-temporal reconstruction. Although the aforementioned criteria are reasonable, they have not provided any definite conclusions about the kernel choice. The conclusions based on previous criteria are not clear due to lack of guidelines for the cut-off mode number or meaning of the POD modes. Such unclear concepts cannot be used as a criteria to make a decision on the choice of kernel.

The present work aims to rigorously investigate the effect of the kernel choice on the POD modes and the resulting low-dimensional reconstruction using a more proper criteria with a priori known expectation of the results. If the POD modes or low-dimensional reconstructions are truly indicative of physical phenomenon, they should be invariant to the coordinate system. To the best knowledge of the author,
no previous study has isolated the effect of the coordinate system transformation on kernels. Studies that have used the polar coordinate system are either captured on a polar grid \([45, 21]\) and solved on polar coordinates but never examined on a Cartesian coordinate system, or have compared the modes from a Cartesian coordinate system with Cartesian grid to polar coordinates system with polar grid after interpolation \([153, 146]\). The caveat of interpolating on a polar grid is that the effect of the coordinate system is not isolated from the interpolation error or grid clustering. Also no study has conducted a two dimensional vectorial POD on polar coordinate system (as Fourier-POD is commonly implemented, and as will be shown in Chapter 3, it is not the same as a two-dimensional POD).

The chapter is organised as follows. First, the classical POD will be briefly reviewed as the equations will be used both in this chapter and later. Then a linear algebraic derivation of the Method of Snapshots will be presented (Section 2.3) to show the inherent assumption in the original derivation which has been overlooked formerly. The next section (2.4) uses the more advanced SVD method in linear algebra to show the link between the classical POD and the Method of Snapshots without any assumption, and the meaning of the extra eigenvectors. A new definition of the base matrix is introduced by comparing Glauser’s generalization of the classical POD and SVD formulation. Section 2.5 uses the kernel definitions to analytically prove that only the vectorial POD has coordinate system invariant modes and reconstructions. Section 2.7 illustrates the implementation of the modified base matrix using three-component velocity measurements in a turbulent free jet as well as examining the coordinate system dependence of scalar and vectorial POD.
### 2.2 Classical POD

A basic knowledge of POD is necessary for the reader to better understand the history and evolution of POD, so the very basic theory and derivation of POD is presented here. The POD method [90] is derived by projecting the velocity field \( (u) \) onto a set of unknown basis functions \( (\psi) \), and normalizing it:

\[
\frac{< u, \psi >}{|\psi|^{1/2}}
\]  

(2.1)

Maximizing this projection produces the most uncorrelated bases. The maximization is done by calculus of variations and leads to a Fredholm integral of the second type:

\[
\int K_{ij}(x, x') \psi_j(x') dx' = \lambda \psi_i(x) + f(x) \]  

(2.2)

The \( f(x) \) here is the forcing function which is zero in a homogeneous integral equation (not to be confused with statistically homogeneous function). Here, \( \lambda \) is the eigenvalue(s) of the equation and the kernel of the integral is the two-point correlation matrix formed by:

\[
K_{ij}(x, x') = < u_i(x) u_j(x') > \]  

(2.3)

In the above equation, the angled brackets denote ensemble averaging. Since the kernel \( K_{ij}(x, x') \) is symmetric, the Hilbert-Schmidt theory can be used to solve the Fredholm integral (equation 2.2). Lumley considered the domain of the correlation \((x)\) to be physical space and time, but it can be space or a subset of spatial dimensions (for example two-dimensional). Then, every realization of the velocity space can be described as a linear summation of the eigenfunctions:

\[
u_i = \sum_{n=1}^{\min(S,N)} a_n \psi_i^{(n)} \]  

(2.4)
where \( S \) is the number of realizations and \( a_n \) represents the POD coefficients which can be calculated using the orthogonality of the eigenfunctions as:

\[
a_n = \int u_i \psi_i^n \, dx
\]  

(2.5)

The eigenfunctions of 2.2 are the so-called POD modes and the eigenvalues are intended to represent the kinetic energy contained in every mode (the square of the eigenfunction’s scale in the velocity space).

POD modes and their coefficients have useful properties. All the POD modes inherit the properties of the original set, such as boundary conditions and continuity. Also, the POD coefficients are uncorrelated and their variance is equal to the corresponding eigenvalues:

\[
< a_n a_m > = \delta_{mn} \lambda_m
\]  

(2.6)

The two-point correlation can be generated by eigenfunctions:

\[
K = \psi \lambda \psi^T
\]  

(2.7)

Numerical integration of 2.2 on an arbitrary grid and coordinate system results in:

\[
KQ \Psi = \Lambda \Psi
\]  

(2.8)

Here \( Q \) is multiplication of the Jacobian and quadrature coefficients of the integration. Ensemble averaging of the correlation kernel yields:

\[
K = \frac{1}{S} U U^T
\]  

(2.9)

where \( U \) is called the base matrix and might have different definitions based on the intent of the kernel (as will be discussed later). The \( 1/S \) coefficient is commonly
dropped for simplicity as it does not affect the results; it only leads to a constant
factor on the absolute value of all the eigenvalues but the relative energy in the
modes, which is of interest here, does not change. The eigenvalue problem then can
be written as:

\[ \mathbf{U} \mathbf{U}^T \mathbf{Q} \boldsymbol{\Psi} = \Lambda \boldsymbol{\Psi} \]  \hspace{1cm} (2.10)

However, this is no longer a symmetric eigenvalue problem. To overcome this,
Glauser [47] suggested to left multiply above equation by \( \mathbf{Q}^{1/2} \) and rewrite it as:

\[ \mathbf{Q}^{1/2} \mathbf{U} \mathbf{U}^T \mathbf{Q}^{1/2} \mathbf{Q}^{1/2} \boldsymbol{\Psi} = \Lambda \mathbf{Q}^{1/2} \boldsymbol{\Psi} \]  \hspace{1cm} (2.11)

Considering the Hermitian kernel as \( \mathbf{K}_q = \mathbf{Q}^{1/2} \mathbf{U} \mathbf{U}^T \mathbf{Q}^{1/2} \) and new eigenvectors as
\( \Phi = \mathbf{Q}^{1/2} \boldsymbol{\Psi} \) results in a well posed eigenvalue problem with real eigenvalues and
eigenvectors. The original eigenvectors can be recovered by left multiplying new
eigenvectors by \( \mathbf{Q}^{-1/2} \). Notice that in linear algebra, multiplication of two matrices
(\( \Lambda \) and \( \mathbf{Q}^{1/2} \)) is generally not commutative unless one of them is zero or identity, or
both are diagonal matrices. In other words, the above equation is only valid when
the coefficient matrix (\( \mathbf{Q}^{1/2} \)) is diagonal which can be obtained when the quadrature
method is zeroth order.

The POD coefficients in matrix form can be calculated using:

\[ \mathbf{A} = \Psi^T \mathbf{Q} \mathbf{U} \]  \hspace{1cm} (2.12)

and a low-dimensional reconstruction based on an arbitrary number of modes is
obtained by:

\[ \mathbf{U}_n = \Psi_{N,n} \mathbf{A}_{n,S} \]  \hspace{1cm} (2.13)

The subscripts in equation 2.13 represent the matrix dimensions, \( n \) is the desired
number of modes in the reconstruction, \( N \) is the number of grid points (or grid points
times velocity components for a vectorial implementation), and \( S \) is the number of realizations. The next section reviews the most popular extension of POD as well as providing a deeper insight of the method itself.

### 2.3 The Method of Snapshots

The original formulation of POD as presented in the previous section can be computationally inefficient when the spatial resolution of the data is high. For example, solving vectorial POD on the velocity data measured by Stereo Particle Image Velocimetry (PIV) with moderate spatial resolution of 20,000 grid points leads to an eigenvalue problem of \( 60,000 \times 60,000 \). The size of the problem increases by the use of Tomographic PIV that measures velocity in a volume rather than a plane. With existing computational power, grid sizes of a million points are very common in mid-size numerical simulations. The size of the kernel for a three-dimensional classical POD solution of such simulation will be \( 10^6 \times 10^6 \). A double precision storage, without any addressing overhead, needs 7.3 Terabytes of memory, which is essentially impossible to store on most of the powerful clusters of today, let alone to solve the eigenvalue problem. Hence, the early implementation of POD in CFD studies is limited to cases with homogeneous directions.

The Method of Snapshots, developed by Sirovich [138], provides a tool to use POD when the spatial resolution is higher than the number of ensembles and most likely to this day remains by far the biggest contribution of the method since Lumley’s original development. The main assumption in the development of this method is that POD modes are expressible as a linear combination of the velocity field. The equivalency of the classical POD and the Method of Snapshots has been a subject of some research. Smith et al. [140] used an analytical proof and noted different numbers of eigenvalues and modes were obtained from each method, but did not address
the meaning or reason of the extra modes. Wanstrom et al. [153] mentioned that the kernels of classical POD and the Method of Snapshots have different ranks which produces a different number of modes for each method. Holmes et al. [61] derived an analytical comparison for a single mode (shorter than the original derivation by Sirovich) and concluded that given the realizations are independent, both methods produce the same modes but did not comment on the known different number of modes produced by each method. Frederich and Luchtenburg [38] noticed that both methods are the same in a linear algebraic sense but did not mention different number of modes. Later, Raiola et al. [119] and Taira et al. [144] used SVD to show the equivalence of both methods and that extra eigenvalues are zeros.

In the following, first linear algebra is used to show the shortcoming of the original derivation of the method, then SVD will be used in next section to prepare the bases for further developments. Studying the Method of Snapshots with linear algebra reveals the ambiguity of its equivalence to the classical POD in Sirovich’s derivation [138]. The key idea is to assume a degenerate form of the eigenvectors based on the velocity field:

\[
\psi = \sum_{m=1}^{M} p_m u^{(m)}
\]

which in matrix form is:

\[
\Psi = UP
\]  \hspace{1cm} (2.14)

where constants \(p_m\) in the \(P\) matrix, remain to be determined. To solve, the above equation needs to be substituted in 2.8:

\[
UU^TUP = \Lambda UP
\]  \hspace{1cm} (2.15)

This is no longer an eigenvalue problem and needs modification. The next step to derive the Method of Snapshots from classical POD is not mentioned in the original paper [138] or others [61, 140]. To form a proper eigenvalue problem, a Moore-
Penrose pseudo-inverse [112] must be left multiplied on each side:

\[ U^+ UU^T U P = U^+ \Lambda U P \]  \hspace{1cm} (2.16)

A basic property of the pseudo-inverse matrix is:

\[ U^+ UU^T = U^T \]

when substituted in equation 2.16, it simplifies to the Method of Snapshots:

\[ U^T U P = \Sigma P \]  \hspace{1cm} (2.17)

the new set of eigenvalues are defined as:

\[ \Sigma_{SS} = U^+_{S,N} \Lambda_{N,N} U_{N,S} \]  \hspace{1cm} (2.18)

Equation 2.17 is now a well posed eigenvalue problem and can be solved for \( P \). Then using 2.14, the original eigenvectors can be regenerated whereas their number is smaller than those calculated via classical POD. Additionally, considering that this equation is not a similarity transform [142] \((UU^+ \neq I)\), the eigenvalue matrices in equation 2.18 have different sizes, so one cannot generally conclude that they are the same. Together, the eigenspace is not necessarily preserved between the classic POD and the Method of Snapshots according to this derivation.

### 2.4 Singular Value Decomposition and General POD

A simpler, yet more robust way to show the equality of the Method of Snapshots and the classical POD is to apply SVD [142] on the base matrix \( U \). SVD breaks every rectangular matrix into an eigenvalue matrix \( \Gamma \) and two sets of orthonormal
eigenvectors, namely left ($L$) and right ($R$):

\[ U = L \Gamma R^T \]  \hspace{1cm} (2.19)

To calculate the left eigenvector, both sides of equation 2.19 would be right multiplied by its conjugate transpose (velocity field is real variable, so the transpose is equivalent to the conjugate transpose):

\[ UU^T = L \Gamma R^T R \Gamma L^T \Rightarrow UU^T = L \Gamma^2 L^T \Rightarrow UU^T L = \Gamma^2 L \]  \hspace{1cm} (2.20)

This equation is the matrix form of the classical POD (2.10) when quadrature matrix ($Q$) is identity and the left eigenvectors are classical POD modes. To calculate the right eigenvectors, each side of equation 2.19 would be left multiplied by its conjugate transpose:

\[ U^T U = R \Gamma L^T L \Gamma R^T \Rightarrow U^T U = R \Gamma^2 R^T \Rightarrow U^T U R = \Gamma^2 R \]  \hspace{1cm} (2.21)

The last equation is equivalent to equation 2.17 which shows the Method of Snapshots solves for the right eigenvectors of the base matrix in SVD notation.

The left eigenvectors can be partially calculated from the right eigenvectors by right multiplying 2.19 by $R \Gamma^+$ and noting that the pseudo-inverse of a diagonal matrix is the inverse of every diagonal element. In practice, due to the round-off errors of the smallest eigenvalues, eigenvectors are directly normalized instead of dividing by the eigenvalues. This formulation also shows that if the modes are not used to project other fields, the Method of Snapshots can be conducted as a Compact
Formulation:

\[ K = U^T U \]

\[ KP = \Lambda P \]

\[ \Psi = UP \]

\[ U^{(n)} = \Psi^{(n)} (P^T)^{(n)} \]

For future reference, the kernels formed by equations 2.20 and 2.21 will be called left and right kernel respectively.

Before proceeding further on the possible formulations to obtain POD modes and lower-dimensional reconstructions, it is constructive to understand results of using SVD and the meaning of extra eigenvectors. One of the major advantages of this simple change of perspective lies in the fact that, without any assumptions, it shows the Method of Snapshots and classical POD are the same. The dimension of the SVD eigenvalue matrix is \( N, S \) in equation 2.19 (rectangular rather than square as in classical POD or the Method of Snapshots). So the differences in the number of eigenvalues obtained from the classical POD and the Method of Snapshots can be explained; the extra eigenvalues in the classical POD are always zeros, and the corresponding eigenvectors (extra eigenvectors of the classical POD) are the bases of the row null space.

To better understand these null spaces, one can consider the simpler example of vectors in a plane as shown in Figures 2.1 and 2.2. Dotted and solid arrows are principal axes and sampled vectors, respectively. In order to have a well posed system with no null space, the number of sampled vectors should be equal to the dimensions of the space they are introduced at (Figure 2.1a), which would be two vectors in a two-dimensional plane. Having a higher number of grid points than the number of snapshots (such as occurs with PIV or CFD which are dense in space by normally less
ensambles than grid-points) is equivalent to presenting our two vectors in a three-dimensional space rather than a plane; therefore a row null space is included (Figure 2.1b). The extra dimension does not provide any extra information but produces an extra base which is orthogonal to the plane of our vectors.

Neither of the two sampled vectors nor any linear combination of them (i.e. a low-dimensional reconstruction of them) would have any component in the third dimension because of its zero energy content. Solving for the extra bases is what a left solution spends a tremendous computational effort on, when applied to CFD or PIV data, whereas a right solution ignores them.

On the other hand, the column null-space happens when the number of sampled instances is higher than the number of grid points (such as measurements taken using hot-wire rakes or microphones) similar to more than two vectors in a two-dimensional plane; illustrated in Figure 2.2. To explain further, assume three sampled velocity measurements from a cross hot wire are vectors in Figure 2.2a. As the data are only two components of the velocity, the space they generate for every point can only be two-dimensional and hence only a plane is needed to present them. The classical POD (the left solution) thus solves the vector space without any null information.
Figure 2.2: Over-sampled data in column and row space. (a) Three sampled vectors in the column space. (b) Three sampled vectors in the row space.

However, the Method of Snapshots (the right solution) works in row space which means the u-component and v-component of each sample represents a single vector in the row space. Consequently, the samples are two vectors in a three-dimensional space (or a higher dimension if more samples were taken). Oversampling increases the dimensions of the row space while the spatial resolution (number of vectors in row space) remains constant. As shown in Figure 2.2b, high sampling also leads to null dimensions.

The second example shows that over sampled data is in fact linearly dependent which violates the necessary condition of linearly independent data posed by Holmes et al. [61]. However, in practice having linearly independent data (not instances) is never feasible; for example, to reduce the uncertainty in an experiment, naturally large number of samples are required to ensure the convergence of turbulence statistics. On the other hand, high spatial resolution is vital in CFD to resolve the smallest scales but the number of temporal samples is normally much less than the number of spatial grid points. In each case, the extra grid points or additional temporal samples that cause the null-spaces are necessary. Solving for these large null-spaces can be avoided by appropriately choosing the left or right solution. Of course, the
fluid mechanics community has been making the choice of solution type correctly for years, where possible, by using the classical POD for spatially sparse but time-resolved hot wire or microphone data [54, 122] and the Method of Snapshots for PIV data that are spatially dense but have fewer instants in time [101, 135].

In essence, the extra eigenvectors are null bases of a necessarily ill posed problem. For a rectangular matrix (or any matrix produced by it, such as the correlation kernel), with linearly independent rows or columns, the rank of the matrix is equal to the size of the smaller dimension. For example, by applying both classical POD and the Method of Snapshots to PIV data, the former produces a bigger kernel yet the ranks of both kernels are still the same, as multiplying the base matrix by its transpose (be it from right or left) does not generate any new information about the system. This is in contrast with [153], which states that the rank of each kernel is its size. This approach also shows that almost always, either row or column null space exists in the data as experimental or simulation dataset matrices are rarely ever square..

A general form of the POD method can be derived by comparing the left eigenvectors from SVD (equation 2.20) and Glauser’s [47] extension of the classical POD for a polar coordinates (equation 2.11). Assuming the quadrature matrix is symmetric, equation 2.11 can be modified to the following form:

\[
Q_2^T U U^T Q_1^T Q_2 \Psi = \Lambda \left[ Q_2^T U \right] \left[ Q_2^T U \right]^T \left[ Q_2^T \Psi \right]
\]

This shows that the classical POD applied in a general form can be considered as a left solution of a modified base matrix:

\[
U_q = Q_2^T U
\]

New formulations to solve the POD modes and low-dimensional reconstructions
can be devised by left multiplying the SVD equation (2.19) by the coefficient matrix and rewriting it:

\[
Q^\frac{1}{2}U = Q^\frac{1}{2}LR^T
\]

\[
U_q = L_qR^T
\]  
(2.24)

Including the coefficients matrix into The Method of Snapshots as mentioned in many other studies would follow readily (along with the SVD notation):

\[
U^TQU = \Lambda P = \Gamma^2R
\]

\[
\Psi = UPA^{-\frac{1}{2}} = L
\]

\[
A = \Psi^TQU = \Gamma R^T
\]

\[
U^{(n)} = \Psi^{(n)}A^{(n)} = L^{(n)}\Gamma^{(n)}R^{(n)T}
\]  
(2.25)

However if higher modes are needed (for example for filtering), the round-off error of directly inversing the eigenvalues can be problematic due to the fast convergence of POD energy. Also the modes are not orthonormal anymore, instead the orthonormality condition is satisfied through \(\Psi Q\Psi = I\). To maintain the orthonormality of the modes it is suggested to use the modified base matrix through the calculation as:

\[
U_q^TU_q = \Lambda R
\]  
step-1

\[
L_q = \frac{U_qR}{\|U_qR\|}
\]  
step-2

\[
A_q = \Lambda^\frac{1}{2}R^T
\]  
step-3

\[
U_q^{(n)} = L_q^{(n)}A^{(n)}
\]  
step-4

\[
U^{(n)} = Q^{-\frac{1}{2}}U_q^{(n)}
\]  
step-5  
(2.26)
Note that if step 3 in the above equation is replaced with $A_q = L_q^T U_q$ then steps 1 to 4 are the conventional steps for the Method of Snapshots seen in many references such as [95] but applied to the modified base matrix.

Although the method in equation 2.26 seems more elaborate than the one in equation 2.25, the numerical implementation will never be used as such. In practice, the SVD functions of numerical packages would be directly used on the modified base matrix to yield the modified left ($L_q$) and right eigenvector ($R$) as well as the square root of the modal energy ($\Gamma$). Then, the low-dimensional reconstruction can be obtained by:

$$U_q(n) = L_q(n)\Gamma(n)R(n)^T$$

$$U(n) = Q^{-\frac{1}{2}}U_q(n)$$

The SVD packages are impractical for datasets with very large spatial dimension (such as those in CFD) as loading all the data in memory is not feasible. Instead, the incremental methods such as IPCA which have efficient implementations (for example in scikit-learn\(^1\)) can be used to calculate the first few hundred modified left eigenvectors. The corresponding coefficients and low-dimensional reconstructions can be calculated using steps 3 to 5 of 2.26.

Neither the coefficient nor the Jacobian or quadrature matrix are limited to the fluid mechanic community. Chatterjee [20] explains that the energy of POD modes does not always correspond to a meaningful definition of the energy in the system. He presents an example of two vibrating masses connected by a spring, a heavy mass with a small amplitude and a small mass which vibrates with large amplitude. As he noted the first POD mode would represent the smaller mass despite its lower kinetic energy. However, this is a matter of wrongful kernel definition; the square root of the masses as coefficient matrix would preserve the proper order in this

\(^1\text{sklearn.decomposition.IncrementalPCA()}\)
example. Similar problems appear in the POD analysis of compressible flow where
the natural choice is to consider the square root of the density in the coefficient
matrix as done by Rowly et al. [125]. Although it is not possible for any individual
to review POD studies in all fields, the author did not find any study that expresses
the importance of the spatial weighting (Jacobian matrix) in the POD calculations
outside the fluid mechanic literature. Any dataset with a spatial distribution (such as
Electroencephalography (EEG) [109] to real estate [83]) should use the modified base
matrix to avoid a bias in mode shapes toward locations with dense measurements.

The prominence of modifying the base matrix by the square root of coefficients in-
stead of its implementation in the kernel is that previously developed POD variations
and related methods in image processing or other fields are readily implementable
on arbitrary grid and coordinate systems. Since the coefficient matrix accounts for
the inner product (integration of the Fredholm equation), the elements of the base
matrix can be described in any coordinate system. So extended [16] or spectral
POD [149] can be applied to CFD data in arbitrary coordinate system without any
extra effort. Other than IPCA which is already mentioned, affinity transformation
can be used dynamically to center a desired target for more consistent modes [123].
Such methods could be valuable to study the dynamics of the flow in the vicinity
of a moving object without obscuring the modes by the movement of the object.
Moreover, since the modified base matrix is formed by element-wise multiplication
of the coefficients and measurements, the domain can be both spatial and temporal
as originally defined by Lumley [90]. Hence, implementation of any POD variation
(extended POD for example) with time in the domain of the measurement is trivial.
2.5 POD Kernels

This section introduces scalar and vectorial kernels and analytically examines their invariance under coordinate system transformation. Each kernel can have the left or right form (base matrix multiplied by its transpose from right or left, respectively) but the kernel type is determined by the definition of the base matrix. Each column of the base matrix contains all the domain (either spatial only, or spatial and temporal) of each realization (temporal samples or blocks of measurement). In case of space only POD, the base matrix of the scalar kernel has the following form:

\[ U = \begin{bmatrix}
  u_1^{(1)} & u_1^{(2)} & \ldots & u_1^{(S)} \\
  u_2^{(1)} & u_2^{(2)} & \downarrow & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  u_N^{(1)} & u_N^{(2)} & \ldots & u_1^{(S)}
\end{bmatrix} \]  \hspace{1cm} (2.27)

Similarly, the base matrix for the vectorial kernel:

\[ U = \begin{bmatrix}
  u_1^{(1)} & u_1^{(2)} & \ldots & u_1^{(S)} \\
  u_2^{(1)} & u_2^{(2)} & \downarrow & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  u_N^{(1)} & u_N^{(2)} & \ldots & u_1^{(S)} \\
  v_1^{(1)} & v_1^{(2)} & \ldots & v_1^{(S)} \\
  v_2^{(1)} & v_2^{(2)} & \downarrow & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  v_N^{(1)} & v_N^{(2)} & \ldots & v_1^{(S)}
\end{bmatrix} \]  \hspace{1cm} (2.28)

The general proof of transformation invariance is presented for any isometric linear transformation in Hilbert space. This means the invariance of modes and reconstructions are studied under any coordinate system transformation that does
not change the distances in the space (length of the velocity vectors). Each element of the right solution kernel for vectorial base matrix 2.28 in space \( \mathbf{X} \), are calculated by multiplying columns \( m \) and \( n \) from equation 2.28:

\[
K^{(mn)}(X) = \sum_{i=0}^{N} [u_m^i u_n^i + v_m^i v_n^i + w_m^i w_n^i]
\] (2.29)

The matrix form of which, is:

\[
K^{(mn)}(X) = \sum_{i=0}^{N} V_i^{(m)} \mathbf{T} V_i^{(n)}
\] (2.30)

where

\[
V_i^{(m)}(X) = \begin{bmatrix}
  u_m^i \\
  v_m^i \\
  w_m^i
\end{bmatrix}
\] (2.31)

If transformation matrix \( \mathbf{M} \) transforms space \( \mathbf{X} \) to \( \mathbf{Y} \) by \( \mathbf{Y} = \mathbf{MX} \), then the velocity at point \( i \) and realization \( m \) in the new coordinate system is:

\[
V_i^{(m)}(Y) = \mathbf{MV}_i^{(m)}(X)
\] (2.32)

replacing the transformed velocity into 2.30:

\[
K^{(mn)}(Y) = \sum_{i=0}^{N} \left( \mathbf{MV}_i^{(m)} \right)^T \left( \mathbf{MV}_i^{(n)} \right)
\]

\[
= \sum_{i=0}^{N} V_i^{(m)} \mathbf{T} \mathbf{M}^T \mathbf{MV}_i^{(n)}
\]

\[
= \sum_{i=0}^{N} V_i^{(m)} \mathbf{T} V_i^{(n)}
\]

\[
= K^{(mn)}(X)
\]

if the transformation matrix is unitary (\( \mathbf{M}^T \mathbf{M} = \mathbf{I} \)) such as an isometric transformation. This shows the vectorial base matrix has invariant right kernel and right
eigenvectors under any isometric coordinate system transformation (for example polar and spherical).

The invariance of the POD modes, which are left eigenvectors, can be deduced by linear algebra. The mode \( n \) at point \( m \) in space \( \mathbf{X} \) is calculated by:

\[
L_n(\mathbf{X}_i) = \sum_{j=1}^{S} U_j(\mathbf{X}_i) R_{j,n}
\]

Similarly, modes in space \( \mathbf{Y} \) are calculated by left multiplying the transformed base matrix by the right eigenvectors:

\[
L_n(\mathbf{Y}_i) = \sum_{j=1}^{S} M U_j(\mathbf{X}_i) R_{j,n}
\]

It is clear that the POD modes in the transformed space are just the transformation of the POD modes in the original space \( L(\mathbf{Y}_i) = M \Psi(\mathbf{X}_i) \). The invariance of low-dimensional reconstructions is trivial using the last equation in 2.25 as the kernel and both eigenvectors are coordinate system invariant, so is their multiplication. In comparison, the scalar kernel only has isolated elements of the transformation matrix so the single element in the transformatin matrix does not reduce to one. Hence the scalar kernel has coordinate system dependence. Appendix A is a specific case of the general solution for transformation from Cartesian to polar coordinate systems.

Experimental results will be used to test and implement these concepts. It is noteworthy that a full dimensional POD on polar coordinate system has never been conducted in free jet literature.
2.6 Free Jet Experimental Setup

2.6.1 Facility

Air is supplied by a 6.5HP, single stage centrifugal blower in a settling chamber (0.9m × 0.9m × 0.9m) and conditioned through three sets of grids with mesh size of 10mm. Next, a flow straightener placed inside a pipe with diameter of 0.2m delivers the uniform flow to a screen that breaks down any wake generated by a honeycomb [88]. A contoured nozzle with exit diameter of 38.1mm and area contraction ratio of 28:1 is used to generate a top hat velocity profile. Air then flows into quiescent surroundings to form an axisymmetric free jet. The jet velocity is calculated using the stagnation pressure of the settling chamber and quiescent surroundings (jet pressure) by a linear pressure transducer. The Reynolds number based upon jet diameter and jet exit velocity was $Re = 28000$. As discussed by [102] the turbulent intensity at nozzle outlet is less than 0.25%.

2.6.2 Instrumentation

A LaVision stereo (three-component) Particle Image Velocimetry (PIV) system has been used to measure the velocity in the cross-flow plane at $x/D = 10$ and is set up as shown in Figure 2.3. The system includes two 12 bit resolution CCD cameras (LaVision Image intense). Both cameras were equipped with AF Nikkor lenses and yield $1376 \times 1040$ square pixels with pixel sizes of 6.45$\mu m$ on both sides of the jet. The laser sheet is generated by a Solo 120XT Nd:YAG with pulse energy of 120$mJ$ and illuminates the flow from below, as shown. The pulse separation was set to 80$\mu s$ and the laser sheet width was adjusted to ensure all seeding particles remain in the laser sheet between two pulses. Inspection of the velocity PDF ensured that peak locking effect does not occur at any time [85].

A Laskin-type atomizer was used to seed the flow with olive oil droplets with a
mean diameter of 3µm. The room was first seeded to an appropriate level before the measurements start to avoid entrainment of unseeded air and biased results on the edges of the measuring window. The captured images were processed using LaVision flow manager (DaVis 8.0). Multi-pass decreasing interrogation windows have been used starting at 64 × 64 pixels, decreasing to a final window size of 32 × 32 with 50% overlap. The normalized correlation function was used for three passes on the smaller window size. The velocity field is reconstructed using Whittaker algorithm [154]. Self calibration of the data puts the root mean square (RMS) fit of pixels at 0.08 < 0.3 which is in the "excellent" range.

A total of 1950 pairs of statistically independent images are taken to ensure statistical convergence. The uncertainty of the streamwise component at the jet centerline at the 95% confidence interval is 0.728% and the uncertainty of streamwise RMS velocity is 3.98% as calculated based on [44, 155].
2.6.3 Validation

It should be noted that the importance of the current dataset is its azimuthal symmetry with reasonable uncertainty, so the extent of the measurement error on the kernel could be assessed. Figure 2.4 shows the mean velocity contours in Cartesian coordinate system. As expected, the streamwise component is almost perfectly circular. Cross components are orders of magnitude smaller than the streamwise direction and display entrainment of the flow into the jet.

The turbulent kinetic energy and shear stresses measured in the jet are shown in Figure 2.5. As expected, the turbulent kinetic energy distribution is circular and is largest in the centre of the jet (Figure 2.5a) at this location downstream of the jet, similar to [10, 37]. The Reynolds shear stresses, $\overline{u\varepsilon}$ and $\overline{uw}$, shown in figures 2.5c and 2.5d, respectively, are symmetric toward the axis of the cross-stream components as expected from a flow with azimuthal symmetry.

The mean streamwise velocity component and its fluctuation are demonstrated in Figure 2.6 and compared to others. Reynolds number of the other sources in the plot are 30000, 26400, 40000, 100000 for Fellouah [37], Abdel-Rahman [1], Gammard, and Hussein [67], respectively. The profiles of Hussein [67] are modeled based on measurements well downstream ($x/D > 70$) and for a much higher Reynolds number but are included because according to Hinze [60], profiles show qualitative similarity at $x/D > 8$. The horizontal axis is normalized with the half-width of the jet which is determined by the radius where the jet velocity is half the maximum at the centerline. The vertical axis of both figures are normalized by the maximum local velocity. The mean velocity profile agrees well with other data in the literature. The RMS of the velocity fluctuation agrees reasonably with Fellouah [37] at $x/D = 10$. Although the potential core decays by $x/D = 6$, but the normalized velocity RMS continuously increases until $x/D = 20$ where its dependence on the streamwise location decreases [37]. This explains the deviation of the current measurement from the literature.
Figure 2.4: Contours of mean velocity components.
Figure 2.5: Turbulent kinetic energy and Reynolds stresses.
Figure 2.5: (continued) Turbulent kinetic energy and Reynolds stresses.
measured further downstream of the jet. Unfortunately RMS data at $x/D = 10$ are scarce.

### 2.6.4 Grid Transformation

To investigate the effect of the interpolation and coordinate system transformation in the next chapter, the velocity measurements need to be interpolated on a polar grid. Interpolation affects the TKE depending on the flow structures and/or the interpolation method. The change in TKE will affect the trace and determinant of the POD kernel and subsequently affects the eigenvalues and eigenvectors. Even though interpolation on a polar grid is not necessary for implementing a right solution in a polar coordinate system, it is conducted to investigate the effect and to keep the steps consistent with other studies [44, 22, 146]. The origin of the polar coordinates is the nozzle centre (which is also the location of the maximum mean streamwise velocity) and the grid increment has been determined based on the study by Hosseinali \textit{et al.} [63]. The Cartesian grid is consisted of $68 \times 59$ grid horizontally and vertically, respectively, while the polar grid is $120 \times 40$ in azimuthal and radial direction, respectively. Use of linear and spline interpolation methods were determined not make a difference on POD modes so the former has been used. To compare the validity of the grid transformation, the turbulent kinetic energy (TKE) integrated over the whole field was calculated to be $0.279 m^3/s^2$ and $0.259 m^3/s^2$ on the Cartesian and polar grid, respectively, which is 7.2% lower for the polar grid. The effect of interpolation on contour plots of instantaneous velocity or TKE are indiscernible, so are not shown here for the sake of brevity.
Figure 2.6: Mean streamwise velocity component and its fluctuation.

(a) Mean streamwise velocity $U$

(b) $u'$ Reynolds stress
2.7 Implementation

This section confirms the effect of coordinate system transformation and interpolation on modes and low-dimensional reconstructions of scalar and vectorial kernels. As mentioned previously (Section 2.5), modes and reconstructions of the vectorial kernel are invariant to coordinate system but their sensitivity to interpolation needs further investigation. Thanks to the new approach outlaid in Section 2.4, scalar and vectorial POD are applied on the free jet velocity measurements in three different ways. First, the conventional Method of Snapshots is used on a Cartesian coordinate system with the original Cartesian grid (case 1). Next, the coordinate system is transformed to polar coordinates while keeping the original grid (case 2); the area contributed to every grid point is constant, as in case 1, so the Jacobian matrix is a constant scalar and can be ignored. Then, the polar velocity components of case 2 are interpolated to a polar grid (case 3). Lastly, scalar and vectorial POD solution are conducted for all cases. Since the mode shapes are not to be interpreted, only selected modes of each kernel are shown in figures 2.7 to 2.10. The columns of each figure represent modes of three cases and the labels are their relative energy content.

Selected modes of the streamwise component of scalar POD are shown in Figure 2.7. The first and second column have identical values in this case since the out of plane component does not change with coordinate system transformation, thus all the modes look exactly the same. Comparing the last column with the other two reveals the effect of interpolation is negligible. The shape of the modes are retained for a very high number of modes before the first diversion appears at mode 74. Despite the mode shape difference at mode 74, most of the modes with higher number have the exact same shape. So the change of the mode shapes is not a function of the energy content of the mode and is in fact irregular.

In contrast, the cross-stream components of the scalar kernel are dramatically affected by both the coordinate system transformation and interpolations (Figure
None of the modes show any resemblance between the first and second column. A thorough study of the modes showed that there is no similarity of the modes between two coordinate systems. Although the first mode of the second and last column are the same, the similarity of the modes decreases in higher modes until they show fundamentally different shapes. Interpolation causes modes 11 and 12 of the polar coordinate system to be different despite their relatively high energy content. Furthermore, it is notable that the energy of modes are reduced due to the coordinate system transformation (without interpolation) but are in the range of uncertainty (discussed later in equation 5.2) except for the first few modes.

The modes of the vectorial kernel (figures 2.9 and 2.10) confirm the coordinate system invariance as expected. This kernel also shows a very high consistency through interpolation for all components. The effect of interpolation on the modes is occasional (mode 56, for example) and does not carry into the higher modes. Based on the effect of coordinate system and interpolation, the vectorial kernel is performing considerably better than the scalar kernel.

Although the study of the mode shapes are constructive, the impact of the kernel type on the low-dimensional reconstruction is required as it is the most commonly used tool for POD interpretation. Low-dimensional reconstruction of three instances will be used for each kernel, one random instance (consistent through all cases) to compare the reconstruction of two kernels, and two instances with low and high Energy-Ratio (defined later in Chapter 4) within each kernel. The Energy-Ratio is a measure of instance importance in the selected low-dimensional space. In figures 2.11 to 2.14, the first column is the randomly chosen snapshot, the second column is a snapshot with low Energy-Ratio, and the third column is a snapshot with high Energy-Ratio. The first row is the original snapshot and the next three rows correspond to the three cases. Here, 13 modes have been used for the low-dimensional reconstruction and the corresponding energy content for each kernel and case is
Figure 2.7: Selected streamwise modes of the scalar kernel. Solid and dash contour lines are positive and negative, respectively.
Figure 2.8: Selected cross-stream modes of the scalar kernel. Solid and dash contour lines are positive and negative, respectively.
Figure 2.9: Selected streamwise modes of the vectorial kernel. Solid and dash contour lines are positive and negative, respectively.
Figure 2.10: Selected cross-stream modes of the vectorial kernel. Solid and dash contour lines are positive and negative, respectively.
The scalar kernel solves each component separately, so the low-dimensional reconstruction is expected to exhibit similar behaviour to that of mode shapes when subjected to coordinate system transformation and interpolation. The streamwise component mode shapes are not changed by the coordinate system transformation and are barely affected by the interpolation, thus consistently the low-dimensional reconstruction does not change, as shown in Figure 2.11. Figure 2.12 shows that the effect of coordinate system transformation is tightly related to the Energy-Ratio of the instances. The effect of the interpolation is not as dramatic as the coordinate system transformation, nonetheless is visible in the instance with high Energy-Ratio.

On the other hand, the vectorial kernel shows excellent consistency in the low-dimensional reconstruction, as expected. The reconstructions are invariant under the coordinates transformation and have barely changed due to interpolation for both the streamwise and cross-stream component of the velocity. Comparing the streamwise (figures 2.11 and 2.13) and cross-stream (figures 2.12 and 2.14) velocity component of the random snapshot shows that kernel choice could lead to different interpretations of the flow. Invariance of the modes and reconstructions of the vectorial kernel proves its superiority over the scalar kernel. In contrast, not only are the modes and reconstructions of the scalar kernel coordinate system dependent, but also dramatically affected by interpolation. This indicates that the scalar kernel is a less reliable choice to interpret any physical phenomena of a flow. The only advantage of using the scalar kernel is the rapid energy convergence, so it could still be used for filtering purposes as most of the energy is contained in only a few modes.
Figure 2.11: Low-dimensional reconstruction of the streamwise velocity components with scalar kernel.
Figure 2.12: Low-dimensional reconstruction of the cross-stream velocity components with scalar kernel.
For the rest of the thesis, only the vectorial kernel will be used.

2.8 Conclusion

This chapter used the Singular Value Decomposition theorem in linear algebra to show the equivalency of the Method of Snapshots and the classical POD. The different number of the eigenvalues and eigenfunctions between the classical and Snapshot POD are attributed to row or column null space which only produces zero eigenvalues and eigenfunctions that are orthogonal to the velocity field at hand.

The classical POD and the Method of Snapshots are, in fact, the left and right solution of an SVD problem, respectively. Using this new perspective on the POD methodology, a modified base matrix has been introduced by the aid of the coefficient matrix which can contain the Jacobian of integral, quadrature weights, and any physical properties. The simple modification on the base matrix makes all the POD variations available in general coordinate systems and unstructured grids with ease. This is of paramount importance as now PIV data with high spatial resolution can be used in a polar coordinate system for POD analysis in a computationally efficient manner. This also allows all variations of POD to be properly applied to CFD simulations with non uniform grid spacing in as efficient a manner as possible using available numerical packages.

Solving the POD for various kernels in both Cartesian and polar coordinate systems has yielded insight into POD modes and subsequently low-dimensional reconstructions. The POD modes and low-dimensional reconstructions of the vectorial kernel are proved to be invariant under coordinate systems transformation and only barely affected by grid interpolation. This means reconstruction using this kernel provides the best tool to study the cumulative effect of modes and for low-dimensionally filtering the domain. Both modes and reconstructions of the scalar
Figure 2.13: Low-dimensional reconstruction of the streamwise velocity components with vectorial kernel.
Figure 2.14: Low-dimensional reconstruction of the cross-stream velocity components with vectorial kernel.
kernel are coordinate system dependent which means this kernel should be avoided wherever possible
Chapter 3

Proper Orthogonal Decomposition, Fourier Transform, and Homogeneity

3.1 Introduction

Since using the Fourier Transform in the homogeneous direction before performing POD analysis is very common and the test cases of this thesis, like most flows, have homogeneous directions, it is useful to address the reasons for avoiding the use of Fourier Transform. The two step Fourier transform and POD analysis will be denoted as Fourier-POD decomposition herein to distinguish it from POD solutions on all dimensions simultaneously. Although harmonic functions are shown to be suitable bases of POD analysis, the possibility that bases of one method are combinations of the other, rather than direct equivalence, has never been examined. Thus, an analytical investigation of the relationship between the Fourier transform and POD in a homogeneous direction is the subject of this chapter. First, analytical test functions are defined to mimic homogeneous turbulence behavior in one dimension.
Next, the linear algebraic groundwork will be laid to rigorously show the bases of a homogeneous kernel are harmonic functions is presented. Then, the equivalency of two methods in a finite domain is analytically investigated. Finally, the shortcomings of Fourier-POD decomposition and practical superiority of full dimensional POD analysis are presented.

3.2 Analytical Test Function

In order to illustrate some of the problems that arise by specific assumptions in the literature, a priori tests are needed. One of the very few a priori tests has been done by Kevlahan et al. [80] who used an asymmetrical function in an analytical POD analysis and showed that the individual POD modes may not be the coherent structures. He used independent, normally distributed, random coefficients to generate samples of the structures, but this means his structures have no coherent temporal evolution. The current study will improve upon this by using a one-dimensional form of the series representation of stationary homogeneous turbulence introduced by Fung et al. [40] as test functions. Fung et al. [39] explain that their representation is capable of generating local structures of high vorticity or strain that manifest themselves in the flow as "beats" of high local energy or vortical structures. Even though vortical structures do not exist in one-dimension, beats of high energy could be constructed. The general one-dimensional form then could be written as:

\[ u(x, t) = \sum_{n=-N}^{N} \sum_{p=-P}^{P} A_{n,p} \cos(k_n x + w_p t) + B_{n,p} \sin(k_n x + w_p t) \]  \hspace{1cm} (3.1)

where \( A \) and \( B \) are random coefficients, \( k \) and \( w \) are spatial and temporal frequencies, respectively. As the purpose of test functions is used to illustrate specific problems in POD application, only a few of the terms in equation 3.1 will be used with accurately chosen coefficients. The legitimacy of the selected test function will be discussed
later. Also, only test functions $u_1$ and $u_3$ will be used in this chapter and the other two will be used later. The four analytical test functions in order of complexity are:

\[ u_1(x, t) = \sin(ax + mt) \] (3.2)
\[ u_2(x, t) = \sin(ax + mt) + d\cos(ax - mt) \] (3.3)
\[ u_3(x, t) = \sin(ax + mt) + d\cos(ax - mt) \]
\[ + \sin(bx + mt) + e\cos(bx - mt) \] (3.4)
\[ u_4(x, t) = \sin(ax + mt) + d\cos(ax - mt) \]
\[ + \sin(bx + nt) + e\cos(bx - nt) \] (3.5)

Here, the arbitrary constant parameters $a, b, m$ are real integers and $d, e$ are real numbers. The test function parameters are assumed to be integers because the limits of the kernel integration are not infinite. This choice is deliberate as infinite domain never happens in practice and the purpose of this document is to examine applicability of the method. Note that $u_3$ is a special case of $u_4$ where two waves propagate with different speeds but have the same temporal evolution. Figure 3.1 illustrates an instance of the parametric test functions with the solid line and their temporal evolution with faded lines.

The analytical solution of the Fredholm integral equation and its solution for test functions 3.2 to 3.5 are available in Appendix B\(^1\).

### 3.3 Eigenfunctions of Homogeneous Directions

A rigorous proof of discrete POD modes degenerating to Fourier modes has never been presented by the fluid mechanic community. Nevertheless, the idea has probably derived from circulant matrices in linear algebra. In a circulant matrix, every column

\(^1\)The python code is available at https://github.com/Mahdi-Hosseinali/FourierPOD
Figure 3.1: Temporal evolution of the parametric test functions.
is a permutation of the previous column by one, hence these class of matrices can be characterized by a single vector. The two point correlation matrix of a homogeneous turbulent flow should be a circulant kernel [51] due to transitional symmetry.

Multiplying a circulant matrix by vector $x$ creates a single polynomial equation called associated polynomial [51]:

$$f(x) = \sum_{j=0}^{N-1} c_j x^j$$

where $N$ is the dimension of the kernel which depends on the kernel type. Then the normalized $j^{th}$ component of the $k^{th}$ eigenvector is $w_j = \exp(\frac{2\pi I j k}{N})$ where $I = \sqrt{-1}$. So the eigenvector matrix is the discrete Fourier transform operator. Using this simplification, it is possible to perform a Fourier analysis in homogeneous direction(s) and then POD in inhomogeneous direction(s) for every Fourier mode.

The caveat of the Fourier-POD transform is that, unlike a linear system, waves in a turbulent flow propagate at different speeds as can be seen in Fung’s approximation of homogeneous turbulence (equation 3.1). Multi-speed waves can be problematic in a finite and discretized domain, especially since the two-point kernels are rarely ever circulant in practice. Attempt by Sieber et al. [137] of filtering the POD kernel in the cross-diagonal direction to achieve a form closer to a circulant matrix and harmonic bases is a witness to this impracticality of the assumptions.

**Proposition:** POD and Fourier transform in space are equivalent in a homogeneous direction.

**Proof.** Suppose the proposition is true. So equation 3.1 is already in the POD space. Because of the linearity and orthogonality of the eigenvectors, changing $A_{n,p}$ or $B_{n,p}$ in equation 3.1 only changes the eigenvalue and coefficients of the corresponding bases but not the eigenvector. Thus if a subset of the terms are retained (test functions) then only the corresponding eigenvectors which are harmonic modes, will
be extracted. If POD modes of the test functions are not harmonic, then it is proved by contradiction that the proposition is false.

In other words, since the coefficients of equation 3.1 are random then the test functions are probable, so POD modes should be harmonic. Use of only $u_3$ will suffice for the purpose of this proof. Two cases could be considered; averaging the kernel over time (similar to non-time-resolved analysis [148, 153]), using Fourier transform in time and POD on the Fourier coefficients (similar to time-resolved analysis [9, 47]).

In the time-averaged case, the test function has four independent terms so a Fourier transform produces 2 complex coefficients (four degree of freedom). However, the analytical POD solution, shown in appendix B, yields only two real modes:

$$\Lambda = \begin{bmatrix} f_0 \\ f_1 \end{bmatrix}, \quad \Psi = \begin{bmatrix} F_0[\sin(ax) - \cos(ax)] - \sin(bx) + \cos(bx) \\ F_1[\sin(ax) + \cos(ax)] + \sin(bx) + \cos(bx) \end{bmatrix}$$

where $f_i$, and $F_i$ are functions of the test function constants $c, d$. Also, both wavelengths ($a$ and $b$) appear in both modes. It is easy to see that POD combines all the terms of equation 3.1 with similar temporal frequencies. Moreover, adding extra waves to the test function with the same temporal evolution does not change the number of POD modes, but generates additional Fourier coefficients. Thus POD and Fourier modes are not equivalent and the proof is concluded for this case.

The case of time-resolved data is much easier using the Fourier transform but becomes much more complicated for POD. Since the test function is a combination of the harmonic functions, the Fourier coefficients in time and space are the complex form of the same equation; complex Fourier coefficients are $A + IB$ of equation 3.1 where $I = \sqrt{-1}$. So the Fourier transform has two complex coefficients for every temporal frequency which is eight degrees of freedom. For Fourier-POD in space and time, the Fourier transform will be applied to $t$ and POD will be conducted on every Fourier mode. The eigenvalues of positive and negative temporal frequency and the
corresponding eigenvectors are:

\[ \lambda_{-\omega,\omega} = f_2 \]

\[ \Psi_{\omega} = F_2 \cos(ax) + iF_3 \sin(ax) + 2 \cos(bx) + iF_4 \sin(bx) \]

\[ \Psi_{-\omega} = F_5 \cos(ax) + iF_6 \sin(ax) + 2 \cos(bx) + iF_7 \sin(bx) \]

Again \( f_2 \) and \( F_2 \) to \( F_7 \) are functions of the test function constants. Clearly the two complex eigenfunctions have four degree of freedom which is half of the Fourier transform, similar to the time-averaged kernel. Since frequencies are not linearly separable, eigenfunctions are not harmonic modes. This concludes our proof that POD and Fourier transform are not equivalent in a homogeneous direction when the limits of Lumley’s integral (equation 2.3) are finite. Frederich and Luchtenburg [38] had noticed that POD mixes scales in complex flows but did not examine the equivalence of POD and Fourier modes in a homogeneous direction.

A better understanding of the difference between POD and Fourier-POD can be achieved by considering the finite domain of practical cases and infinite dimensions of theoretical homogeneous directions. A circulant kernel is achievable on a finite domain only when a single wave travels at a single speed such as test function \( u_1 \). The wave may have any other shape (such as square root or saw-tooth), but as long as it is the only present wave and travels at a constant speed, the correlation kernel will be circulant. Adding another wave with a different temporal evolution compromises the statistical invariance under translation. If infinitely more waves with unique temporal evolutions are added and measured over infinite time, then the statistical translational invariance is obtained again. The reason is that each wave can be expressed by a summation of harmonic functions and when all wavelengths and frequencies are present, then the harmonic functions are the proper bases. This the-
oretical case is the fundamental premise of Lumley’s derivation which is not feasible to capture in a finite spatial or temporal domain. In practice, the presence of coherent structures means only limited wavelengths or frequencies are present. So POD properly combines the harmonic functions to capture these coherences while using Fourier transform obscures them by distributing the projection into dimensions that are not present (hence the extra degrees of freedom in our case).

Nonetheless, the above findings do not nullify the previous researches nor question their merits. Lumley’s proof [90] shows that decomposition of homogeneous and inhomogeneous directions can be decoupled. Therefore use of the Fourier transform in homogeneous directions is still mathematically correct, but it is not any more proper than other orthogonal decompositions and as shown above is not equivalent to POD. Thus the POD modes in the inhomogeneous direction would be different than a full dimensional POD. That being said, using the Fourier-POD transform raises numerous problems in application and interpretation of the modes. As George [43] mentioned, the Fourier-POD modes are complex and inverting them back to real space does not look like the original modes. Moreover, the Fourier transform can be used efficiently only when the grid is uniform in the homogeneous direction. For example, the data captured by PIV on an axisymmetric free jet are on a Cartesian grid while the homogeneous direction is azimuthal. For the Fourier-POD transform one has to interpolate the data on a polar grid first [148] or both Fourier transform and POD solution should be performed on a scattered grid which increases the complexity of the problem tremendously. Furthermore, interpolation to a polar grid either causes inaccuracy in a coarse grid (specifically the far-field) or is computationally demanding on a dense grid such as those in CFD.

Also the Fourier-POD approach breaks down a single two-dimensional POD mode to multiple one-dimensional Fourier and POD modes. As a result, low-dimensional reconstruction of the flow to understand the coherent structures either
needs the added choice of a cut-off Fourier mode, which currently does not have any sound guidelines in the community, and requires some intuition of the flow [148] to perform a selective mode reconstruction. Additionally, the POD modes could be ordered differently in each Fourier mode [24] which makes the selection of the modes difficult. Either approach is inconsistent with the spirit of the POD method to provide an unbiased understanding of the flow with the least manipulation.

Both Lumley [90] and George [43] pointed out that the theoretical energy of a homogeneous direction can be infinite and integration of the kernel (equation 2.2) does not converge. In practice, this infinite energy is not representable. For example, a homogeneous direction in experimental measurements is achieved by a sufficiently large dimension to ensure the three-dimensional effect does not affect the measurement window. So sampling of the data happens on a window of the homogeneous direction which means most frequencies of periodic signals are not captured at a full period. This experimental limitation is known as the windowing effect and leads to a problem known as spectral leakage [58]. Figure 3.2 compares the impact of the windowing effect on the energy of Fourier and POD modes of test function \( u_1 \). The windowed Fourier transform shows clear leakage of energy to neighbor modes since all the bases functions have to be periodic in the sampled domain. Reconstruction with poorly chosen number of modes can lead to misinterpretation in case of windowed samples. This leakage can be trivial or considerable depending on the clipped portion of a wave but in a continuous spectrum of turbulent flow, it is guaranteed that some structures are affected dramatically. Although numerical simulations do not have the windowing problem when periodic boundary conditions are used in a spatial homogeneous direction (symmetric boundary condition are prone to a specific case of windowing), but they only represent finite energy of the homogeneous direction [43] captured in the simulation domain. Also both numerical and experimental studies are affected by spectral leakage when Fourier transform is applied to
temporal direction.

On the other hand, POD is not affected by the windowing effect as much as the Fourier transform, as shown in Figure 3.2. The energy shifts from one mode to the other but the mode shapes (not shown here) are unaffected. For a more complex signal, the shape of the POD modes start to deform which in turn causes the energy content of the modes to be less sensitive to the windowing effect in contrast to the Fourier transform.

Fourier-POD can be intricate even in an azimuthal direction where the spectral leakage does not exist. For example, Fourier analysis of the free jet velocity is applied with regard to the jet center in the mean sense, as an instantaneous center is hard to define. This simple center selection can be challenging in experiments [113] and lead to misinterpretation. Two of proposed mechanisms in this flow (meandering [4] and vortex ring tilting [14, 52, 55]) move the instantaneous center of the azimuthal symmetry. Thus using the Fourier transform with respect to a constant center for all the instances can exacerbate misinterpretation. The importance of meandering on the analysis can be seen in more structured flows such as wing-tip vortices [28, 59, 6] where the meandering is removed from instantaneous measurements as the very first step. Pinier [113] has shown that non-azimuthal structures, which play an important role in the free jet dynamics, can be difficult to capture with Fourier-POD analysis. In contrast, a two dimensional POD analysis does not assume any center of symmetry, hence it is not subjected to such misinterpretations.

Lastly, the Fourier-POD method can be problematic when the vectorial POD is implemented. The conventional Fourier transform works only on a scalar variable, but to extend it to the vector form, Clifford algebra is needed [31]. None of the POD studies that have used the Fourier transform in the homogeneous direction has implemented Clifford algebra so far. As a result, vectorial POD with Fourier transform has the inherent inconsistency of using scalar decomposition in one direc-
Figure 3.2: Windowing effect on decompositions methods. Top: input signal and window size, middle: Fourier modes of full domain (horizontal hatch) and windowed domain (oblique hatch), bottom: energy of POD modes of full (horizontal) and windowed (oblique) signal.
tion and vectorial in the others. Albeit, the scalar kernel, as shown in Section 2.5, is coordinate dependent which raises more questions on the rigor of the combined scalar-vectorial Fourier-POD decomposition.

3.4 Conclusion

The equivalence of Fourier-POD and POD was reviewed and a counter example showed, for the first time, that they are not equivalent in finite domain. Also Fourier-POD modes are harder to interpret because of higher number of generated modes and the complex form of the Fourier-POD modes. Furthermore, susceptibility of the Fourier-POD transform to windowing effect was illustrated in contrast to the ability of POD to retain the same mode shapes in a similar case. Other practical difficulties of the Fourier-POD transform were reviewed to show the motive for using POD analysis in all dimensions. All the reasons add to the rationale of using the General POD introduced in the previous chapter over the Fourier-POD.
Chapter 4

Low-Dimensional Reconstructions and Selection of Best Instances

4.1 Introduction

Once the POD modes are available, the first step in the analysis is usually to choose a low-dimensional space for projection. The most common choice of cut-off number, intuitively, is to find an abrupt drop in the energy level, but this can be ambiguous in practice. This method, unbeknownst to most of the fluid mechanic community, called Scree [19], is applicable only when the flow has dominant structures such as vortex shedding behind cylinders [105, 104, 12] or a well defined wing-tip vortex [64]. However, fully turbulent flows have a continuous spectrum of structures which renders the Scree method inapplicable. Another problem of this approach is the dilemma of the proper choice when the energy content has multiple abrupt drops.

A computationally expensive method called Monte-Carlo [117] can be used to compare the solved modes with randomly generated data. The procedure is to generate $L$ Gaussian random datasets with the same variance of the original dataset and calculate the eigenvalues of their correlation matrices. The $j^{th}$ eigenvalue of
all sets is distributed over a certain range. The $j^{th}$ POD modes are kept if the corresponding eigenvalue is higher than 95% of the $j^{th}$ eigenvalues in $L$ (two standard deviation of a normally distributed random variable). The logic of the method is that modes which represent an orderly structure should have more energy than modes of randomly generated sets. Experimental methods with low spatial resolutions, such as hot-wire anemometry or microphone pressure recordings, can use this cut-off method. Since the randomly sampled data are independent, only the effective sample size of the measurements should be used to generate $L$, as will be explained in Section 4.3. Thus, increasing sampling frequency does not increases the size of the problem. This method is at a disadvantage for spatially dense datasets such as PIV measurements or CFD simulation. Although only the eigenvalues of the randomly generated datasets are solved, the size of the base matrix and the eigenvalue problems are considerably larger than spatially sparse datasets. So generating a high number of random sets to provide the 95% probability range is computationally demanding.

Mardia [93] and Preisendorfer [117] have noticed that for large number of samples, the eigenvalues of the randomly generated data converge to asymptotic values. Preisendorfer et. al. developed an equation to estimate the probability distribution of corresponding eigenvalues. The equation, called rule-N, can be used safely when the dimensions of the sampled signal (base matrix) are larger than 100.

Many other approaches exist for the choice of the cut-off mode number but most of them have been developed in non-engineering fields and are not based on the basic concepts of interest to fluid mechanics. For example, another method that is originated from factor analysis in psychology is Eigenvalue-one or Kaiser Criteria [79]. The original study normalizes the variance of input signals, then keeps the modes with energy content more than one. It will be shown that the Kaiser criteria is a specific case of rule-N when the number of samples is two orders of magnitude larger than the spatial resolutions. Also, in fluid mechanics, normalizing the variance
of every spatial node results in the enhancement of noise in the quiescent parts of the flow (for example the outer edge of a jet) which obscures the important structures, hence Kaiser criteria cannot be implemented directly.

An effective way to represent the cumulative effect of the modes is to reconstruct snapshots with only high energy modes and then randomly choose a few to investigate the underlying mechanisms. However these “randomly chosen” snapshots are not always the most representatives of the reconstructed field, or could be biased by the investigator. Randomly chosen instances might be helpful in small datasets but with the advancements in modern instrumentations, capable of capturing large number of samples, renders this approach inefficient as most of the available information (and probably better candidates) might be ignored. The author did not find any document related to the selection of instances in other fields, probably because most commonly the statistics and correlations of the low-dimensionally reconstructions are of interest rather than individual samples. This chapter develops two methods to overcome this: an effective under-sampling method and a criteria to rank instances based on the ratio of dynamics maintained in the low-dimensional space.

4.2 Numerical Test Function

A test function will be used similar to the previous chapter to better illustrate the rational and behavior of the methods in this chapter as they are presented. The test function is again based on Fung’s equation for the synthetic homogeneous turbulence
with added Gaussian noise (\(\mathcal{N}\)) to mimic error in experimental measurements:

\[
u_5(x, t) = \sin(3x + t) + 2\cos(3x - t) \\
+ \sin(5x + 2t) + 4\cos(5x - 2t) \\
+ 2.5\sin(7x + 3t) + 3.5\cos(7x - 3t) \\
+ 2\sin(11x + 6t) + 2\cos(11x - 6t) \\
+ \mathcal{N}(0, 1)
\] (4.1)

The noise term is drawn from a normal distribution with zero mean and unit standard deviation which produces noise-to-signal-ratio of 4\% (signal-to-noise-ratio of 13.97dB). A temporal correlation is embedded in the noise by a moving-average filter over a \(2\pi\) period as the experimental noise is not always independent between the instances (for example electrical noise). The numerical sampling is 256 spatial points over \(2\pi\) and 512 temporal samples over \(9.5\pi\) to demonstrate the windowing effect in time which was introduced in the previous chapter. The instances of the numerical test function are then shuffled to represent non-time-resolved measurements. Shuffling the instances has the same effect as non-time-resolved sampling (such as conventional PIV) or non-uniform times steps (such as LDA) on our test function because it is perfectly periodic. Figure 4.1 shows the advancement of uncontaminated \(u_5\) and noise in time as well as their superposition and shuffling.

The test function is designed to have 7 modes representing 3 traveling and one standing waves with wave-numbers 3, 5, 7, and 11. The original POD solution (Figure 4.2) does not show the intended waves (as will be explained in next chapter, Figure 5.3 shows the corrected POD modes represent the waves properly). As expected, the effect of noise becomes more dominant for higher modes. The noise energy is distributed between the rest of the modes because of its low correlation, so modes higher than 7 are a combination of noise and null spaces. The energy content of the
Figure 4.1: Temporal evolution of clean $u_5$, correlated normal noise, and the summation. Temporal evolution is depicted by faded color lines.
modes is presented in Figure 4.3. By design the energy content of modes 4 and 5 should be exactly equal, but the imperfect temporal truncation has caused a shift of energy from mode 5 to 4.

4.3 Cut-off Mode Number

As mentioned earlier, the Monte-Carlo method is impractical for large datasets so this section presents the formulation of rule-N. First, the equation to calculate the asymptotic limits is presented along with tabulated values for convenience. Next three important thresholds are introduced and their physical meaning is discussed. Finally, the effect of temporal correlation on rule-N is presented.

Preisendorfer [117] has estimated the probability that the eigenvalues of randomly generated data are at or below a threshold using asymptotic theory of eigenvalues of large symmetric random covariance matrix. Equation 4.2 calculates the probability of eigenvalues of normal random data that are higher than $x$.

$$P(x, \beta) = \frac{1}{2} + \frac{\beta}{2\pi} \left[ ((x-a)(b-x))^{1/2} + (ab)^{1/2} \arcsin \frac{(a+b)x - 2ab}{x(a-b)} \right]$$

Where $0 < P < 1$ is the confidence level, $a = (1 - \beta^{-1/2})^2$, $b = (1 + \beta^{-1/2})^2$, $\beta = S/N \geq 1$, $S$ is the number of samples, $N$ is the number of grid points (the POD domain), and the function domain is $a \leq x \leq b$. By choosing $P$, $x$ can be calculated using bisection algorithm as the function is monotonically increasing. Table 4.1 has a summary of the calculated $x$ for three different $P$ values.

Although the $\beta \geq 1$ condition of rule-N does not apply to spatially dense measurements or simulations, it does not cause any problem. Such datasets always
Figure 4.2: First 8 original modes of test function \( u_5 \).
have order of magnitude(s) larger spatial resolution than the number of samples. Since this class of data have adequately large number of samples to ensure statistical convergence, sampling further data to obtain $\beta = 1$ is redundant. Hence, the recommendation is to use $\beta = 1$ for spatially dense datasets when $\beta < 1$ so long as the number of independent samples is at least one order of magnitude larger than 100. For example a PIV measurement with 20,000 grid points and 1,500 snapshots that is statistically converged can use $\beta = 1$ in equation 4.2 although in reality $\beta = 0.075$.

The selection of the cut-off method is simple. Normalise the eigenvalues of POD problem by their average, then modes with eigenvalues larger than 4.0, 3.09, and 0.65 are more structured than random noise with 100%, 95%, and 50% confidence, respectively. Three p-values mentioned (either from the rule-N or Monte-Carlo) respectively indicate the modes that are ensured to be more structure than any noise (p100), modes that are mostly structures rather than noise (p95), and the limit that separates modes that are mostly dominated by noise (p50).

The P thresholds of the numerical test function (previous section) are $p_{100} = 5$ and $p_{95} = p_{50} = 7$. The p50 and p95 clearly separate the last meaningful mode from
Table 4.1: Asymptotic eigenvalues of random covariance matrix at 100%, 95%, and 50% confidence.

<table>
<thead>
<tr>
<th>β</th>
<th>1.0</th>
<th>1.1</th>
<th>1.2</th>
<th>1.3</th>
<th>1.4</th>
<th>1.5</th>
<th>1.6</th>
<th>1.7</th>
<th>1.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>100%</td>
<td>4.00</td>
<td>3.82</td>
<td>3.66</td>
<td>3.52</td>
<td>3.40</td>
<td>3.30</td>
<td>3.21</td>
<td>3.12</td>
<td>3.05</td>
</tr>
<tr>
<td>95%</td>
<td>3.09</td>
<td>2.97</td>
<td>2.87</td>
<td>2.78</td>
<td>2.71</td>
<td>2.64</td>
<td>2.58</td>
<td>2.52</td>
<td>2.47</td>
</tr>
<tr>
<td>50%</td>
<td>0.65</td>
<td>0.67</td>
<td>0.71</td>
<td>0.74</td>
<td>0.76</td>
<td>0.77</td>
<td>0.79</td>
<td>0.80</td>
<td>0.81</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>β</th>
<th>1.9</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>3.5</th>
<th>4.0</th>
<th>4.5</th>
<th>5</th>
<th>5.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>100%</td>
<td>2.98</td>
<td>2.91</td>
<td>2.66</td>
<td>2.49</td>
<td>2.35</td>
<td>2.25</td>
<td>2.16</td>
<td>2.09</td>
<td>2.03</td>
</tr>
<tr>
<td>95%</td>
<td>2.43</td>
<td>2.38</td>
<td>2.22</td>
<td>2.10</td>
<td>2.00</td>
<td>1.93</td>
<td>1.87</td>
<td>1.82</td>
<td>1.78</td>
</tr>
<tr>
<td>50%</td>
<td>0.82</td>
<td>0.83</td>
<td>0.86</td>
<td>0.89</td>
<td>0.90</td>
<td>0.92</td>
<td>0.93</td>
<td>0.93</td>
<td>0.94</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>β</th>
<th>6.0</th>
<th>6.5</th>
<th>7.0</th>
<th>7.5</th>
<th>8.0</th>
<th>8.5</th>
<th>9.0</th>
<th>9.5</th>
<th>10.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>100%</td>
<td>1.98</td>
<td>1.94</td>
<td>1.90</td>
<td>1.86</td>
<td>1.83</td>
<td>1.80</td>
<td>1.78</td>
<td>1.75</td>
<td>1.73</td>
</tr>
<tr>
<td>95%</td>
<td>1.74</td>
<td>1.71</td>
<td>1.68</td>
<td>1.66</td>
<td>1.63</td>
<td>1.61</td>
<td>1.54</td>
<td>1.58</td>
<td>1.56</td>
</tr>
<tr>
<td>50%</td>
<td>0.94</td>
<td>0.95</td>
<td>0.95</td>
<td>0.96</td>
<td>0.96</td>
<td>0.96</td>
<td>0.96</td>
<td>0.96</td>
<td>0.97</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>β</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>80</th>
<th>90</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>100%</td>
<td>1.50</td>
<td>1.40</td>
<td>1.34</td>
<td>1.30</td>
<td>1.27</td>
<td>1.25</td>
<td>1.24</td>
<td>1.22</td>
<td>1.21</td>
</tr>
<tr>
<td>95%</td>
<td>1.39</td>
<td>1.31</td>
<td>1.27</td>
<td>1.24</td>
<td>1.22</td>
<td>1.20</td>
<td>1.19</td>
<td>1.18</td>
<td>1.17</td>
</tr>
<tr>
<td>50%</td>
<td>0.98</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

the noise despite the very low energy content compared to the other modes. But p100 chooses a cut-off value which is contaminated by noise while it is expected to delineate the modes that are 100% more structured than noise; the reason lies in the inter-modal interaction. As mentioned in Section 4.2, modes 6 and 7 interact with lower modes to represent traveling waves. So the noise is propagated to the well-structured modes through this interaction. The next section describes this mechanism in more detail and presents a way to reduce the noise effect on reconstructions.

The rule-N needs independent data, so time-resolved datasets need specific treatment. The correlation in such data reduces the effective number of samples [117] and in turn affects $\beta$. To determine the effective sample size, first estimate the ensemble correlation between $u(x, t_i)$ and $u(x, t_{i+1})$ for every point:

$$
\rho(x) = \frac{\Sigma_{i=2}^{S} u(x, t_i)u(x, t_{i-1})}{\Sigma_{i=2}^{S} u^2(x, t_{i-1})}
$$
Then calculate the effective sample size for every spatial point:

\[ S_{V^*} \approx S \left[ \frac{1 - \rho^2}{1 + \rho^2} \right] \]

Finally the effective number of samples is the smallest \( S^* \) and correspondingly \( \beta = S^*/N \).

### 4.4 Denoising Technique

As mentioned in the previous section, rule-N and the numerical test function reveal an important point in noise propagation through POD modes not known before. The low energy of modes 6 and 7 makes them prone to be contaminated by noise, but modes before p100 are not expected to be affected. The designed mode pairs are (1,7), (2,4), and (5,6) but theoretical modes 4 and 5 are combined due to eigenvalue degeneracy (the next chapter elaborates on this effect). So the modal groups (1,7), (2,4,5), and (4,5,6) interact. Contaminated mode 6 propagates noise to modes 4 and 5, in turn mode 2 is also affected by noise to a lesser degree (Figure 4.2). The energy difference of the modes decreases the propagation of the noise, but one can still observe small noises in the first mode (visible in peaks). The noise is propagated through modal interaction as the third mode, which does not interact with any contaminated modes, is not affected despite its lower energy than the first two modes. The propagation of noise through traveling waves can be stronger in POD solutions of turbulent flows because of numerous modal interactions and close energy contents.

The propagation of noise also affects the POD coefficients. The noise in the 7th mode propagates into the first mode, so the coefficients have to adjust to represent the instances properly which causes two main effects observed in Figure 4.4, a shift of the paths and a spread of the coefficients around them. Temporal evolution of the
uncontaminated POD coefficients for the test function follows a smooth path along the circles in the left part of the figure. The spread of the coefficients around the circles is obvious after the noise is added. The outer circle at the bottom of the plot has drifted outward while the inner circle at the bottom have shifted closer to the center.

Knowing the boundary between modes dominated with noise and coherent structures, a new noise reduction method can be developed using the distance of the instances in the coefficient space. Since the POD transform is a unitary rotation of space, the similarity of two instances can be measured by the distance between them in the coefficient space. This distance can be calculated in specific subspaces instead of the whole space. Since modes after p50 are dominated by noise, they will be labeled as "noise space". In contrast, a "coherent space" can be formed by the desired modes for reconstruction or modes 1 to p100. The behavior of the modes’ coefficients in these spaces are inherently different. Higher energy of the lower modes means the coefficients have larger time-scales, while in the noise space the coefficients are mostly independent or have small time-scales (excluding perfectly correlated noises such as
Figure 4.5: Effect of noise on POD coefficients of modes 1 to 6, excluding mode 3. Solid line is without noise, color of dots is based on noise.

electrical noise as they represent physical behavior). As a result, similar instances have close POD coefficients in the coherent space but are distant in the noise space.

Figure 4.5 illustrates the strength of this behavior for lower modes. Six POD coefficients (excluding mode 3) are plotted as solid blue lines (test function without noise) and scattered dots (with added noise). The color of dots indicates the value of POD coefficient from a mode in the noise space. The right plot depicts the extent of the path shift due to the added noise. The distance of the coefficients in the noise space is large for lower modes as their timescale is much smaller than the coherent modes (left figure) so the color of every point is different from its neighbors. For higher modes (right figure), the time-scale of the noise and coherent mode are similar so the color does not change as drastically along a line but across it. This indicates that while the distance of the coefficients is close in the coherent space, it is in fact large in the noise space. This property can be used for noise reduction.

A noise-to-signal-ratio between each pair of instances can be calculated by dividing their distance in the noise and coherent space. Then a threshold can be chosen to select the instances which are more distant in the noise space rather than repre-
senting substantial difference in the coherent space. POD coefficients of the selected instances can be averaged to reduce the noise while the coherence is largely maintained. A universal threshold cannot be determined as the selection of the coherent space is arbitrary. The researchers should compare instances with different noise-to-signal-ratios and select the threshold accordingly. Also each mode shape can be smoothed with strength proportional to energy of p50 divided by the mode energy to reduce the effect of the noise on the bases of the space. It should be mentioned that smoothing affects the basic properties of the modes such as continuity or boundary conditions and should be done with proper caution. Figure 4.6 shows three instances of the test function with high, close to 1, and low noise-to-signal-ratio.

Averaging the POD coefficients changes their property which needs further attention. The energy is tied to the coefficients through equation 2.6 which also expresses their orthogonality as the right eigenvectors. The Denoising Technique changes the distribution of the coefficients which can reduce the energy of the modes. Also the denoised coefficients are now not orthogonal, but this does not affect the reconstruction process as the bases of the space has not changed. The denoised POD coefficients are no longer uncorrelated but a weaker version of 2.6 is valid on account of POD orthonormality:

\[ <a_n a_n> = \lambda_n \]  (4.3)

The energy change (loss of orthogonality) of the mode coefficients is negligible if the number of denoised instances is small or the coherent space is limited to lower modes. In case of considerable reduction of the number of instances or when the orthogonality of coefficients is required, the field can be reconstructed using modes 1 to p50 for a second POD solution. The modes of the new POD solution will be a combination of the previous POD modes to maximize the variance of the coefficients and regain the orthogonality of the right eigenvectors.

Figure 4.7 depicts the reduction of the spread of POD coefficients by the De-
Figure 4.6: Different ratios of noise-to-signal-ratio between instances.
noising Technique. As expected, the coefficients of the lower modes are loyal to the underlying behavior but the shift of the POD coefficients in the higher modes is inevitable. Researchers should be aware that the experimental noise can affect the way one observes and interprets the turbulent mechanisms even with a low-dimensional reconstruction. Also note, that as the number of samples is reduced (as similar instances are averaged). This reduction of samples is favorable in a low-dimensional reconstruction as a space with lower dimensions requires fewer samples to be represented.
4.5 Energy-Ratio

In order to find a better way of choosing the most representative snapshots of the reconstructed field, we write the TKE of velocity fluctuation based on snapshots:

\[
    u'^2 = \frac{1}{N} \sum_n u_n^2 = \frac{1}{N} \sum_n \left( \sum_m \psi_m a_{mn} \right)^2
\]

\[
    = \frac{1}{N} \sum_n \sum_l \sum_m \psi_m a_{mn} \psi_l a_{ln} \quad (4.4)
\]

\[
    = \frac{1}{N} \sum_l \sum_m \psi_m \psi_l \sum_n a_{mn} a_{ln}
\]

The last sum is the orthonormality condition of POD coefficients (2.6) so it can be simplified as:

\[
    \sum_n a_{mn} a_{ln} = a_{ml}^2 \delta_{ml}
\]

As a result the variance can be simplified to:

\[
    u'^2 = \frac{1}{N} \sum_n \psi_n^2 a_{nn}^2
\]

Integrating spatially to get the total turbulent kinetic energy in the field would yield:

\[
    \int u'^2 = \int \frac{1}{N} \sum_n \psi_n^2 a_{nn}^2 dx = \frac{1}{N} \sum_n \left( \int \psi_n^2 dx \right) a_{nn}^2 = \frac{1}{N} \sum_n a_{nn}^2
\]

Here, integration of the eigenvector squared reduces to identity matrix since they are normalized.

The last equation means that the square of the length of a POD coefficient is equal to the kinetic energy of that instance. Thus in a low-dimensional reconstruction with \( m \) modes, the ratio of the kinetic energy that is contained in instance \( i \) can be measured as:

\[
    \frac{\sum_{i=1}^{m} a_{si}^2}{\sum_{i=1}^{N} a_{li}^2}
\]
which will be delineated as the "Energy-Ratio" (ER). The algebraic meaning of ER is the distance of the instance to the origin of the coefficient space in the low-dimensional space divided by the distance in the original space. As an example consider a stochastic process where the trajectory of instances in the coefficient space are contained by a sphere. If the low-dimensional reconstruction uses $x$ and $y$, then instances that have high $z$ value but small $x^2 + y^2$ loose their dominant dynamics by this projections. Energy-Ratio provides a criteria to avoid using such instance for interpretation of the low-dimensional dynamics.

It should be emphasized that the ER is not a measure of the turbulent kinetic energy (TKE), as it is defined in an instantaneous manner rather than statistically, yet this analogy provides a measure for a better choice of the representative snapshots than is currently done by random selection. This criteria does provide a preference factor for every snapshot, but as rule of thumb, it is suggested to use instances with higher ER than percent of TKE contained in the low-dimensional reconstruction.

### 4.6 Implementation on Jet Flow

This section briefly shows the result of methods introduced or developed in this chapter on the measure velocity fluctuations of the turbulent jet flow introduced in Section 2.6. First, the effect of different cut-off mode numbers is shown on turbulent statistics to compare the consistency with the original values and effect of the noise. Next, the Denoising Technique is applied to a low-dimensional reconstruction to find the instances which are similar in the low-dimensional space. Lastly, ER is used to study the interaction of the mode groups in a low-dimensional space.

Since the cut-off mode number in a highly turbulent flow is large, its best application is filtering to maintain the peaks and reduce the noise. The cut-off numbers also will be used in the next chapter to reduce the calculations of degeneracy and
traveling waves. The cut-off mode numbers for the jet flow are $p_{100} = 100$, $p_{95} = 124$, and $p_{50} = 333$ with total energy of 0.72%, 0.77%, and 0.92%, respectively. Probably the best application of using the cut-off mode number for filtering is in higher order turbulent velocity moments since the noise increases by every multiplication. For example, the third-order moments of the velocity fluctuations (like those that appear in the TKE budget), calculated with 1950 snapshots, are shown in Figure 4.8, every column of this figure is a triad of turbulent mixing with the same contour within each column. The first row represents the calculation without any filtering, while the other rows are from low-dimensional reconstructions with labeled cut-off values. It is clear that choosing low cut-off numbers reduces both noise and peaks. The $p_{50}$ criteria shows a good compromise that has similar peaks to the no filtering case with smoothness comparable to $p_{95}$. This is useful from a purely statistical sense which is useful in studies which do not intend to use POD analysis.

The first step to denoise the instances of the jet flow is to select the modes of the low-dimensional reconstruction (coherent space). The streamwise component of the first twelve modes are shown in Figure 4.9. The mode groups based on the number of lobes are (1), (2,3), (4,6,7), and (8,9). The Denoising Technique will be conducted for low-dimensional reconstruction with 7 and 9 modes respectively. Similar instances according to different NSRs are illustrated in figures 4.10 and 4.11 with the same contour level within every row. Expanding the coherent space increases its energy while the noise energy remains constant, thus the proper threshold of NSR decreases by including more modes. This can be seen in the figure, as NSR=2 points to two drastically different instances in Figure 4.10 but the same thresholds finds more similar instances in Figure 4.11. The same effect is observable for NSR=5 with lesser degree. De-noising the coefficients with 9 modes and NSR=4 as threshold results in 219 samples reduction (original dataset has 1950 samples). Similarly, de-noising with 7 modes and lower threshold of NSR=6 reduces 406 samples. Comparing the
Figure 4.8: Third-order velocity fluctuation moments with low-dimensional reconstructions.
Figure 4.8 (cont.): Third-order velocity fluctuation moments with low-dimensional reconstructions.
Figure 4.8 (cont.): Third-order velocity fluctuation moments with low-dimensional reconstructions.
number of reduced samples illustrates the need for fewer instances in a subspace with fewer dimensions.

4.7 Conclusion

The methods in this chapter are mainly developed or introduced to support other chapters but can be used independently in special cases. The Monte-Carlo and Rule-N methods use a mathematical grounding for selection of modes which are representative of structures. In a fully turbulent flow without any dominant actuation, the cut-off values mentioned are larger than commonly chosen for low-dimensional reconstructions. In such flows, the main usage is an upper bound for methods developed in the next chapter. Also as shown, the p50 can be used for filtering to produce better statistics or smoother derivatives.

De-noising the instances has two main purposes; under-sampling, and reducing the effect of noise on the modal behavior. A lower-dimensional space requires less number of samples to be effectively represented. While higher number of samples provide a better resolution, it also increases the number of instances the researchers need to study to understand the modal interaction and underlying structures. The Denoising Technique reduces the number of samples effectively by combining the instances that are close to each other in the coherence space but far in the noise space so it does not reduces the effective resolution of the low-dimensional space. The other advantage of the Denoising Technique is to reduce the spread of the coefficients caused by the noise. It was shown that the underlying noise can scatter the coefficients of the instances from their true trajectories in the coefficient space and the Denoising Technique mitigates such deviations.

Finally, a systematical method of choosing reconstructed snapshots has been developed. The introduced Energy-Ratio suggests that instants with higher contri-
Figure 4.9: Streamwise component of first twelve POD modes of the jet flow. Solid and dash contour lines are positive and negative, respectively.
Figure 4.10: Similar instance with different noise-to-signal-ratio thresholds computed by 7 modes.
Figure 4.11: Similar instance with different noise-to-signal-ratio thresholds computed by 9 modes.
bution of their kinetic energy in the low-dimensional space represent the dynamics of the subspace better. The ER provides a tool to reduce the number of candidates that represent the subspace. Combined with the Denoising Technique, the total number of instances that describe a low-dimensional space decreases substantially to be manageable for researchers as well as reducing the bias caused by randomly chosen snapshots.
Chapter 5

Traveling and Independent Modes

5.1 Introduction

Traveling waves (convective structures) are often thought to be captured in two modes with similar energy levels and shapes [36, 71, 137, 105]. However, the numerical test function in the previous chapter shows that a beating wave can have associated modes with different energy levels. It is crucial to maintain all associated modes in a low-dimensional reconstructions for a proper understanding of the dynamics and this has been one of the largest criticism of POD. For example, excluding mode 7 of the numerical test function shown in chapter 4 has negligible effect on the total energy of the system but the moving dynamics of mode 1 will be lost. The majority of the previous research on traveling waves can be divided in two categories: \textit{a posteriori} which is identifying the associated modes after conducting space-only POD (either visually [105, 71, 107, 143], or systematically [137]), and \textit{a priori} which is transforming the domain of the problem (either by a variation of POD method [124, 36], or by preprocessing the data [121]).

The most common \textit{a posteriori} methods use the POD coefficients to study the modal interactions. In a well-defined flow with dominant convective structures
(swirling jet, actuated flows, or wing-tip vortex), the phase-plot of the POD coefficients should have clear circular behavior based on Feeny’s idea of energy transfer between associated modes. Oberleithner et al. [107] stated that such phase-plots are a special case of Lissajous curves. Further, they showed that modal interaction can occur between more than two modes which appears as higher Lissajous curves in phase-plots but the transfer of energy is mainly contained in the first Lissajous curve (which is a circle). A rudimentary approach to find the associated modes is by visual inspection of the phase-averaged POD coefficient plot [105, 107, 143]. However, this manual procedure can be cumbersome as it requires $n(n+1)/2-1$ plots to compare $n$ modes. A heuristic is to limit the visual inspection to the modes with similar energy level [71, 107, 137] based on Feeny’s observation. Unfortunately, the visual inspection is often not useful in fully developed turbulent flows such as channel flows and can ignore pulsating waves as will be shown in Section 5.3.

Smith et al. [141, 140] have studied the Lissajous curves in Couette flow in more detail by comparing the projections of DNS on POD modes with POD based models and found the modal interaction of the associated modes have radial fluctuating components. So circular estimation of phase-averaged coefficients removes some dynamics of the system. In addition, intermittency or multi-frequency interactions of two modes renders their phase-plot hard to understand. Alternatively, Seiber et al. [137] used Dynamic Mode Decomposition (DMD) on the coefficients. Given that all the modes are included, the DMD analysis decomposes every POD coefficient into harmonic functions that describe the interaction of that mode with other modes. Then a similarity measure is used to examine the DMD coefficients and find the modes that are closely associated with a quarter period shift. However their method was only successful on their SPOD which is diagonally averaged and modes are not orthogonal, so low-dimensional reconstruction is not possible. They also mentioned the Fourier transform of the coefficients can be used to detect the
traveling modes but are not as reliable as the DMD. Although they did not explain their Fourier analysis search algorithm, a logical approach is to calculate the time-delayed cross-correlation of coefficients and consider the highest peaks as indication of modal association. Nicholas et al. [103] have used this approach to calculate the correlation coefficients of the POD coefficients and surface pressures at different locations in a wall jet. The advantage of this method is that it accumulates the association across all frequencies, so associated modes without a visually clear phase-plot can be found. The disadvantages are the heuristics of peak selection and spurious association between unrelated modes with similar frequencies. Finally, Aubry et al. [7] investigated modes with close energy content for similar shapes by using symmetry operators. Modern image processing methods can be used to find similarities of modes shapes without the drawbacks of symmetry groups (as will be explained later) but similar shapes does not always mean their association is to represent a traveling wave, as will be shown in Section 5.5.

Although transforming the frame of reference (domain of the problem) sounds more reasonable, it likely needs a priori knowledge of the system, can be computationally demanding, or limited to special cases. The main essence of this group of methods is to use the statistical symmetry properties (translation, rotation, ergodic) of the system at some point so the traveling waves are stationary in the new frame (domain). Rowley et al. [124] redefined the modes as functions of time and space $\Psi(x-ct)$. They used template fitting on raw data to update the independent variable and correct the frame of reference. But the presence of multiple traveling waves with different speeds, as is always the case in turbulent flow, decreases the confidence in their method. Reiss et al. [121] refined the idea (shifted POD) by separating every wave in raw data and performing POD analysis on them individually which leads to many other problems. The wave speed should be calculated through peak monitoring, intuition of the problem, or template fitting; unfortunately only the latter
is data-driven. Also, the method needs to solve a SVD problem for every wave. Moreover, waves are over-represented when they cross each other so interpolation is needed inside the kernel for an accurate shift operator. The basic idea for both methods needs template fitting of raw data which is computationally intensive and depends on the coordinate system. For example, transitional waves over a bump in a channel cannot be captured by template fitting without a sophisticated mapping of the domain.

Also other researchers have developed variations of POD to capture a mode pair as a complex mode or used other dynamical methods for finding traveling waves. Feeny [36] has transfered the input signal into a complex form by adding its Hilbert transformation as the imaginary part. The POD modes then become complex where the real and imaginary parts describe a traveling wave. The downside of this approach is the implied assumption that phase-plot of the original POD coefficients is a circle. Thus, more sophisticated modal interactions such as multi-frequencies or intermittent associations could break into multiple complex modes. A different approach called advection mode decomposition (ADM) [72] replaces the correlation kernel with Wasserstein distance matrix to look specifically for the advection modes. ADM captures the traveling waves better than POD but is limited only to coupled modes, so it needs POD analysis to include non-advective features of the flow.

Although many of the aforementioned methods are successful in specific cases, they have shortcomings due to (implied) assumptions made in their developing. The methods that use symmetry reduction (included template fitting) do not perform well in anisotropic directions because they do not consider structure deformations. For example, structures traveling through an expansion are expanded laterally while their speed is reduced. Other assumptions are that traveling waves need only two POD modes or the energy of the associated modes are similar; as Oberleithner et al. [107] pointed, the modal interaction may occur over many modes. Even though they
considered only the most energetic interactions, Ilak and Rowley [71] delineate that “the most energetic modes are not always the most dynamically significant ones”. All things considered, the benefit of the variations and manipulations of raw data may not overweigh the extra computational cost or subsequent complications.

The known global behavior of POD [96, 80, 27, 120, 124, 71, 38], where the mode shapes are non-constant over a large part of the domain, is an obstacle, often overlooked, in detecting and understanding traveling waves as the turbulent structures usually have limited span. This is counter intuitive as the POD solution is based on the two-point correlation of the measurement which vanishes for long separation distances unless a well-defined or forced structure is present. For example, the POD modes of the jet flow outlined in chapter 2 are global while the two-point correlations measured by Ukeiley et al. [152] in the shear layer of the free jet clearly indicate limited streamwise and azimuthal spans. Local structures are obtainable using global base functions when a high number of mode are used (such as a single square wave can be reconstructed with harmonic functions) but it is counterproductive as the endeavor is to seek a low-dimensional space. On the other hand, reconstruction with a lower number of modes can lead to the misinterpretation that the structures are either global, or interact globally. Moin and Moser [96] performed POD analysis on sub-domains of the flow to overcome the globality of the modes. Similar method has been used later in the control theory [126]. A more rigorous technique called Sparse PCA [92] regularizes (Ridge or Lasso) maximization of the bases (equation 2.1) to acquire local modes. The method performs well in image processing but is computationally more demanding than regular PCA. Furthermore, tuning the regularization parameter is a manual process which needs intuition about the problem at hand (reasonable in image processing).

This chapter develops methods to reduce the globality of the POD modes and examine inter-modal interactions \textit{a posteriori} to better understand the traveling
structures. Section 5.2 shows the globality of the modes is not an inherent characteristic of POD, but rather an outcome of the eigenvalue degeneracy. The POD modes are uncorrelated by definition but not independent, which can be deleterious to understanding of the dynamical system. A class of algorithms called blind source separation are used in a novel approach to reduce the dependency of the modes (increasing their locality) without bargaining their orthogonality. Next, Section 5.3 develops two new criteria to discover modal interactions using POD coefficients. Groups of interacting modes can be used in low-dimensional reconstruction for a better understanding of traveling structures. The numerical test function from Chapter 4 visualizes the logic of the developed methods in sections 5.2 and 5.3 until Section 5.5 validates their effectiveness on the numerical simulation of pipe and channel flow.

5.2 Eigenvalue Degeneracy and Modal Correction

A frequent phenomena in POD applications that has not received the attention it rightly deserves is eigenvalue degeneracy. For a repeated eigenvalue, any linear combination of the corresponding eigenvectors is also a valid eigenvector. Consider two eigenvectors of a repeated eigenvalue $\lambda$, multiplied by arbitrary scalars $\alpha$ and $\beta$:

\[ \alpha K \psi_1 = \alpha \lambda \psi_1 \]
\[ \beta K \psi_2 = \beta \lambda \psi_2 \]

Summing both equations yields:

\[ K(\alpha \psi_1 + \beta \psi_2) = \lambda (\alpha \psi_1 + \beta \psi_2) \]
\[ K \psi_3 = \lambda \psi_3, \quad \psi_3 = \alpha \psi_1 + \beta \psi_2 \]
The last equation shows that $\psi_3$ is also a valid eigenvector for $\lambda$. Numerically, the non-uniqueness of the eigenvectors of a repeated eigenvalues means the same problem can be solved on two computers and produce different POD modes. Degenerate eigenvalues always form a homogeneous bases in which, POD does not find any preferred direction. A bigger problem that can arise from eigenvalue degeneracy is increased dependency of the modes as POD essentially finds the bases where the Probability Distribution Function (PDF) of the signal is closest to Gaussian [93, 117]. According to Central Limit Theorem, any linear combination of independent processes is closer to a normal distribution than either of the original processes. Since POD maximizes the variance of the variables, it is natural that when possible (similar eigenvalues), it combines two signals to generate a more Gaussian process. In practice, the flow structures rarely have normal distribution [116]. As an example assume the underlying dynamics of a system are uncorrelated and independent signals $X_1 = \sin(a(t))$ and $X_2 = \cos(b(t))$, where $a(t)$ and $b(t)$ are stochastic processes and the joint distribution of the samples is as Figure 5.1 (top). The low-dimensional reconstructions $Y_1$ and $Y_2$ of POD analysis is plotted in Figure 5.1 (bottom). Clearly POD has not introduced any new insight into the problem, but has increased the dependency of the variables which is unfavorable.

The tendency of POD to increase Gaussianity of the modes obscures the traveling waves. Degeneracy is not deleterious when there is only one traveling wave (beating or not). The problem arises when modes of different traveling waves have similar eigenvalues. For illustration, test function $u_4$ (equation 3.5) is used which consists of two beating waves traveling at different constant speed. Eigenvalues and
Figure 5.1: POD reconstruction of uncorrelated independent signals. Top: original signals, bottom: reconstructed signals, left: joint PDF, right: univariate PDF
eigenfunctions of this test function (see Appendix B for solution) are:

\[
\Lambda = \begin{bmatrix}
(d + 1)^2 \\
(e + 1)^2 \\
(d - 1)^2 \\
(e - 1)^2
\end{bmatrix}, \quad \Psi = \begin{bmatrix}
sin(ax) + \cos(ax) \\
\sin(bx) + \cos(bx) \\
\sin(ax) - \cos(ax) \\
\sin(bx) - \cos(bx)
\end{bmatrix}
\]

Here, modes (1,3) and (2,4) are indicative of two traveling structures. In the special case where \( e + 1 = d - 1 \), eigenvalues of modes 2 and 3, which have different wavelength and temporal frequency, will be equal. As a result, the numerical calculation often yields combinations of them rather than the current form. Any method seeking traveling waves severely under-performs as the degenerated modes (2 and 3) interact with each other as well as modes 1 and 4.

In practice, the degeneracy might occur without exactly equal eigenvalues. As shown in Section 3.3, windowing of the domain can change the eigenvalues. Numerical errors such as uncertainty and sampling error are other causes that can shift eigenvalues of modes with similar energy contents. The numerical test function is designed to depict such effects. Mode groups (1,7), (2,4), (5,6) are intended to represent traveling waves with degeneracy affecting modes (4,5) and (6,7) as noted in table 5.1. In theory, lower modes are not contaminated by noise as they have higher energy compared with the 4% energy of noise which should be distributed in modes higher than p100. In practice, the energy of the lower modes has increased slightly due to the noise propagation mechanism discussed in Chapter 4. Additionally, temporal sampling and its uncertainty, which is not over a perfect period, have caused a shift in the energy of modes (4,5) and (6,7) similar to the windowing effect shown in Section 3.3. Figure 4.2 shows that despite the different energy content of modes (4,5) and (6,7) in a numerical solution, the degeneracy has taken place.

North [106] derived the effect of sampling error on the energy contents and
Table 5.1: Theoretical and numerical energy contents of numerical test function.

<table>
<thead>
<tr>
<th>Modes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>35.64</td>
<td>24.75</td>
<td>15.84</td>
<td>8.91</td>
<td>8.91</td>
<td>0.99</td>
<td>0.99</td>
<td>&lt;3.96</td>
</tr>
<tr>
<td>Numerical</td>
<td>35.69</td>
<td>24.94</td>
<td>15.98</td>
<td>9.40</td>
<td>8.41</td>
<td>1.15</td>
<td>1.06</td>
<td>0.19</td>
</tr>
<tr>
<td>Difference</td>
<td>0.05</td>
<td>0.19</td>
<td>0.14</td>
<td>0.49</td>
<td>-0.50</td>
<td>0.16</td>
<td>0.07</td>
<td>-</td>
</tr>
</tbody>
</table>

showed the eigenvalue shift is stronger when theoretical eigenvalues have close values. Thus the continuous spectrum of the turbulent flow is very susceptible to eigenvalue degeneracy. A blind source separation algorithm called FastICA will be used to selectively reduce the dependency of POD modes.

Blind Source Separation (BSS) are a group of algorithms developed to acquire independent source signals from a mixture of them. Mathematically speaking, this is equivalent to calculate $A$ and $S$ from $X$ in $X = AS$ which is an under-defined problem but can be solved with proper conditions or assumption. A classical example is the Cocktail Party problem where $N$ microphones ($X$) record the sound of $N$ attendees ($S$) in the hope of isolating each speaker’s sound. Due to different distance between each source and microphone ($A$), the sampled data are a linear combination of independent sources: $X = AS$.

Independent Component Analysis (ICA) is a BSS method developed by Juette and Herault [78] and Comon [23] in signal processing which has gained popularity in many other fields. The original method has been developed for temporal data, but currently has many other applications ranging from image processing [139] and cyber-security [86] to economics [8]. The method looks for the non-Gaussian signals by maximizing the kurtosis. The original definition (which will be used in this study) also assumes the sources are stationary (speakers are not moving, not the same as stationary processes) so the mixing matrix $A$ is not time dependent and number of microphones and speakers are equal (square mixing matrix). The idea is to iteratively increase the non-Gaussianity of each signal. A detailed description of the method
and its common implementations can be found in [69]. The following presents a short overview of FastICA algorithm (for a complete explanation see the same reference).

In practice, the kurtosis of noisy data can be very inaccurate and misleading so instead, another factor called negentropy [69] is used which is the complementary of Shannon’s entropy [133]. The term ”entropy” in communication theory has indeed been borrowed from thermodynamics; the more chaotic the process, the higher the entropy. More specifically, the entropy of a signal is a measure of the amount of information contained in it. By definition, Gaussian distribution has the maximum entropy in comparison to any possible random distribution with the same mean and variance. The ICA algorithm uses negentropy which is the measure of how ordered the signal is. If entropy of a signal is measured by function \( H \), then the definition of negentropy of a signal \( X \) is:

\[
J(X) = H(X_{\text{gauss}}) - H(X)
\]

where \( X_{\text{gauss}} \) is the synthetic Gaussian random variable with the same mean and variance as \( X \). The fastICA algorithm uses an approximation of negentropy [68] which is:

\[
J(X) \approx [E\{G(X)\} - E\{G(X_{\text{gauss}})\}]^2
\]

Here \( E \) is the expected value and \( G \) is a slow growing function to decrease the effect of outliers on the negentropy, defined as:

\[
G(x) = \frac{1}{a_1} \log \cosh(a_1 x)
\]

where \( 1 \leq a_1 \leq 2 \). The algorithm uses a stochastic gradient method to iteratively reduce the approximate negentropy as cost function.

To enhance the convergence of fastICA and its performance, often pre-processing
of data is needed. The two most important pre-processes are centering and whitening [69] which are removing the mean and normalizing data. The velocity fluctuations are already centered because of their zero mean. A popular whitening method is by eigenvalue decomposition:

\[ \tilde{X} = \Psi \Lambda^{-1/2} \Psi^T X \]  \hspace{1cm} (5.1)

where \( \Psi \) and \( \Lambda \) are the eigenvector and eigenvalue matrices as introduced in Chapter 2. The whitening is essentially the same as diagonalizing the covariance matrix \( \tilde{X} \tilde{X}^T = I \) which is not favorable in the analysis of turbulent flows. Using SVD it can be shown that the whitening of signal (equation 5.1) is multiplying left and right eigenvectors (or normalized POD coefficients):

\[ \tilde{X} = \Psi \Lambda^{-1/2} \Psi^T X \]

\[ = L \Gamma^{-1} L^T L \Gamma R^T \]

\[ = LR^T \]

Despite the promising outlook of ICA, it cannot directly be used on turbulent velocity fluctuations due to three reasons. The main reason is that coherent structures in a turbulent flow are not all mutually independent (or so we believe) and ICA does not perform properly when dependent sources are present. Other problems are the stationary condition and the number of sources. As mentioned, traveling structures or waves are a characteristic property of turbulent flows and the original ICA performs poorly in this cases. Although ICA with a time-dependent mixing matrix is an active field of research, the developed methods [110, 109, 99, 118] rely on temporal behavior of the data, which is not always accessible, or can be sophisticated with more hyper-parameters to tune [70]. The third reason is the high number of sources. The continuous spectrum of turbulent flow means an infinite dimensional problem [61], which cannot be fully captured via experimental measurements or even
most of numerical simulations. Despite the dense spatial resolution of the most advanced experimental methods, the number of observations are still too coarse to be comparable to the number of sources. Fine numerical simulations such as DNS and LES might have enough number of features (i.e. spatial large enough resolution) to capture the important sources but the application would be limited and computationally expensive. The problem of more sources than sensors leads to a group of algorithms called over-complete or under-determined ICA. Naturally, extra assumptions are necessary to compensate the missing information [17, 127, 100, 87].

Despite the mentioned limitations, ICA has the potential to be used on a subset of POD modes. Although the POD modes are not always centered, by definition their covariance is the identity matrix which satisfies the whitening condition. Also as mentioned in introduction, POD decomposes traveling waves into multiple stationary modes which is a necessity for ICA.

The process of reducing modes dependency starts by calculating the eigenvalue uncertainty. North et al. [106] added random noise of order $N^{-1/2}$ to the covariance matrix and used linear analysis to estimate the eigenvalue uncertainty due to sampling:

$$\delta \lambda = C_f \lambda \left( \frac{2}{S} \right)^{1/2}$$  \hspace{1cm} (5.2)

The original formulation uses the 68% confidence interval ($C_f = 1$) to calculate the standard error. But higher values can be used to increase the confidence of finding eigenvalues with similar energy level. The proper choice of the confidence interval depends on the number of realizations used, but $C_f$ of 2 or 3 for confidence intervals of respectively 95% and 99% are sufficient in most cases. This formulation assumes samples are independent, so for time-resolved data the effective number of samples from Section 4.3 should be used instead of the number of realizations. Figure 5.2 shows that using 95% confidence interval, modes (4,5) and (6,7) are in the same uncertainty range although the latter is not obvious from the mode shapes (Figure
Figure 5.2: Uncertainty of u5 eigenvalues with different confidence levels

4.2).

The next step is to isolate groups of modes as inputs for ICA. In practice, higher modes have similar energy levels so the isolation method can be complicated. Two methods are developed here but other approaches can be crafted. Both methods start by forming a group of eigenvalues for every mode that are in its range of uncertainty.

The first method called progressive (which is used throughout this document) starts from the lowest modes and moves forward. The first mode of the first group is called the left bound. The last mode of the same group (called right bound) is chosen, then other groups are searched to find the last group that contains the current right bound. The last mode of the new group is updated as the right bound. The isolated group contains all the modes in the range of the left and right bounds. Then the left bound is updated to be the next mode after the previous right bound and this procedure is repeated until all the modes (p50 suffices) are in isolated groups.

The other method called Eigenvalue Gradient Based (EGB) calculates the energy change in every initial group:

\[
\Delta \lambda_i = \frac{\lambda_m - \lambda_n}{m - n}
\]  

(5.3)
Here \( m \) and \( n \) are the first and last eigenvalues in the uncertainty range of \( i^{th} \) mode. To create isolated groups, a group is chosen then all the modes included in that group should be removed from the others. Repeating this process generates non-overlapping mode groups. The order of removing the overlapping modes is mostly heuristic, for example one can start from the groups with the highest average energy (forward EGB) or the lowest ones (backward EGB). A more reasonable approach is to normalize the gradient by the \( i^{th} \) eigenvalue and start with the group that has the smallest normalized energy gradient (least EGB). Once the modes are grouped in non-overlapping batches, ICA can be applied to every batch to correct the modes. Figure 5.3 shows the corrected modes of the numerical test function which has separated the mode shapes properly.

After the modes are corrected, their energy and coefficients should also be updated accordingly. To calculate the corrected coefficients of the updated modes, the linear property of ICA is used:

\[
\phi_k = \sum_{i=m}^{n} c_i \psi_i
\]

Here the location of \( k \) is between \( m \) and \( n \) but undetermined. \( c_i \) is the mixing coefficients calculated by ICA. Substituting the above equation into 2.5:

\[
a_{kj} = \int u_j \phi_k dx \\
= \int u_j \sum_{i=m}^{n} c_i \psi_i dx \\
= \sum_{i=m}^{n} c_i \int u_j \psi_i dx \\
= \sum_{i=m}^{n} c_i a_{ij}
\]

(5.4)

Where \( c_i \) is factored out of the integral in the third line because it is independent of
Figure 5.3: First 8 corrected modes of test function $u_5$. 
In linear algebra, the above equation can be written in two forms:

\[ A_{ica} = C^T A_{POD} = W A_{POD} \]  

(5.5)

Where \( W \) is the unmixing matrix from ICA and produces better results. The unmixing matrix is by definition inverse of the mixing matrix \((CW = I)\), so the second equation is derived from reconstruction \((U = A\Psi = ACW\Psi)\).

The new eigenvalues can be calculated using the updated coefficients as in equation 2.6. Rewriting the left hand side of equation 2.6 using 5.4:

\[ <a_k a_l> = \langle \Sigma_i c_i a_i \Sigma_j c_j a_j \rangle \]
\[ \quad = \langle \Sigma_i \Sigma_j c_j c_i a_i a_i \rangle \]
\[ \quad = \Sigma_i \Sigma_j c_j c_i <a_j a_i> \]
\[ \lambda_k = \Sigma_i c_i^2 \lambda_i \]  

(5.6)

Similarly, the matrix form is:

\[ \lambda_{ica} = W^2 \lambda_{POD} \]

Here, the squared is elementwise. If all the modes in a group are degenerate, then the corrected modes have equal energy so their order is immaterial. But the uncertainty criteria can group modes that are not degenerate in nature. Using the corrected eigenvalues, the corrected modes can be sorted to preserve the POD optimality. In practice the shift in the eigenvalues is usually minuscule and in the order of eigenvalue uncertainty, for example the energy of modes 4 to 7 of \( u5 \) has changed from \((8.11, 8.04, 0.9918, 0.9686)\)% to \((8.08, 8.07, 0.9912, 0.9692)\)%.

The corrected modes from ICA are orthonormal since the POD modes are orthonormal [84]. It should be noted that the General POD of Chapter 2 should be used so the modes are orthonormal.
5.3 Traveling Waves, Frequency and Derivative Criteria

This section is directed at developing two simple \textit{a posteriori} methods without restrictions mentioned in introduction. The fundamental idea is borrowed from Granger-Causality [50] in economics; time series X is Granger-causing time series Y if lagged values of X are predictive of current value of Y. In simple language, a peak in Y is preceded by a peak in X. Since X should decrease after its maxima while Y increases and both variables should be differentiable in time (proved in next chapter), they form a concave curve in the phase-plot for this period of interaction. The lag between the peaks determines the radius of the tangential circle of the curve. If the transition of energy between modes are continuous, then the concave curves are maintained through the trajectory but this is not necessarily required. Notice that the only restriction is one mode Granger-causing the other so concaved curves can have arbitrary radius or be randomly placed in the phase-plot. The concaved curve formed by the coefficients of two associated modes can be expressed by sine and cosine as functions of time in the neighborhood of a point. Then the series expansion of this model, can be written as:

\begin{align}
  a_i &= \sum_k A_k \sin n_k t + \mathcal{N} \left(0, \sigma_i^2\right) \\
  a_j &= \sum_k B_k \cos n_k t + \mathcal{N} \left(0, \sigma_j^2\right)
\end{align}

(5.7)

where \( n_k \) has the same value in both equations and \( \mathcal{N} \) is a normally distributed noise with zero mean and unknown variance \( \sigma^2 \). The selection of terms distinguishes this method from a general Fourier transform analysis [137] which has poor performance. The representation of the traveling waves using their POD coefficients is independent of the spatial domain since equation 5.7 is only a function of time. Thus, traveling
waves with arbitrary streamlines or beating waves should be captured which are untraceable for template fitting.

To simplify the analysis, without loss of generality, only one term of the summation and part of the noise will be analyzed. To normalize the coefficients, they can be divided by the amplitude of the harmonic function. Thus the equations can be rewritten as:

\[
\begin{align*}
\frac{a_i}{A} &= \sin nt + \mathcal{N} \left( 0, \left( \sigma_1/A \right)^2 \right) \\
\frac{a_j}{B} &= \cos nt + \mathcal{N} \left( 0, \left( \sigma_2/B \right)^2 \right)
\end{align*}
\]  
(5.8)

Here the noise is divided by the number of frequencies (which is unknown but finite) to distribute it equally, so \( K \sigma_i^2 = \sigma_i \) where \( K \) is the total number of non-zero frequencies. Also the variance of normal distribution function has changed by dividing the amplitudes. It should be noted that the normalization does not affect the generality of the method because of its linear behavior, so it can be assumed that each term has been dealt with individually, then the results are summed and normalized again.

The Discrete Fourier Transform (DFT) of equation 5.8 in time is:

\[
\begin{align*}
F \left[ \frac{a_i}{A} \right] &= \mathcal{G}_{\sigma A} + I \left[ -\delta_n + \mathcal{G}_{\sigma A} \right], \quad \mathcal{G}_{\sigma A} = \mathcal{N} \left( 0, \frac{\sigma_1^2}{A^2 S} \right) \\
F \left[ \frac{a_j}{B} \right] &= \delta_n + \mathcal{G}_{\sigma B} + I \mathcal{G}_{\sigma B}, \quad \mathcal{G}_{\sigma B} = \mathcal{N} \left( 0, \frac{\sigma_2^2}{B^2 S} \right)
\end{align*}
\]  
(5.9)

where \( I = \sqrt{-1} \), \( \delta \) is the Dirac delta, and \( S \) is the number of temporal points. For an explanation of the DFT of the normally distributed random variable (the noise) see appendix C. Note that the delta function \( (\delta_n) \) is the indicator of the underlying mechanism and everything else is made from noise. Multiplying the conjugate of one
equation in 5.9 by the other yields:

\[ F[a_i/A] F[a_j/B]^* = 2G_{\sigma A}G_{\sigma B} \mp \delta_n G_{\sigma B} \pm \delta_n G_{\sigma A} \pm I\delta_n [1 + G_{\sigma A} + G_{\sigma B}] \]  

(5.10)

The sign change depends on which equation is conjugated. Since the DFT of sine and cosine are imaginary and real, only the imaginary part of their multiplication is of interest. Additionally, the interacting frequency \( \delta_n \) is not known beforehand, so equation 5.10 needs to be integrated over all frequencies. Excluding the real part, which only consists of noise, enhances the performance dramatically compared to the cross-correlated based method. The noise terms in the imaginary part have minimal effect on the results because they are multiplied by the Dirac delta function, so their integration is a single draw from a random variable with very small variance. Distributing the noise to all frequencies means the random variables have small noise-to-signal-ratio \( (\sigma/A \ll 1) \), so a single draw is less than 1 with 95% confidence \( (2\sigma/(A\sqrt{S}) \ll 1) \) and can be neglected.

This analysis shows the reason for poor performance by a full Fourier analysis. Keeping the real part maintains the integration of the first term which contaminates the result. To normalize this value, it should be divided by the absolute value of each equation in 5.9:

\[
\| F[a_i/A] \| = \sqrt{\int \left[ \delta_n + 2\Re \left( 0, \frac{\sigma^2_1}{A^2S} \right) \right]^2 d\omega} = \sqrt{1 + \frac{\sigma^2_1}{A^2}}
\]

\[
\| F[a_j/B] \| = \sqrt{\int \left[ \delta_n + 2\Re \left( 0, \frac{\sigma^2_2}{B^2S} \right) \right]^2 d\omega} = \sqrt{1 + \frac{\sigma^2_2}{B^2}}
\]

Integrating the squared of random variable is equal to its variance multiplied by number of temporal points \( (S) \) which yields the last term in the square root. So, the
maximum Frequency Criteria (FC) in the presence of noise is:

\[
\frac{1}{\sqrt{1 + \sigma_1^2/A^2}} \frac{1}{\sqrt{1 + \sigma_2^2/B^2}}
\]  

The numerical approach to calculate the inter-modal association is simple. First the Fourier Transform of the POD coefficient is calculated in temporal dimension. Next, this matrix is left multiplied by its conjugate transpose. Then the square roots of the real part of the diagonal elements are used to normalize the imaginary part of the resulting matrix. The elements of the final matrix (which are real) indicate the interaction of the modes. Since all the frequencies of POD coefficient contribute to the elements of the association matrix, sophisticated modal behavior can be captured.

Although the Frequency Criteria produces a reasonable measure of the modal association, it is not trivial when the time difference of the measurements are not equal. Another approach can be devised by calculating the derivate of one of the equations in 5.7 and then normalizing them.

\[
a_i/A = \sin nt + \mathbb{N}(0, (\sigma_1/A)^2)
\]

\[
a_j/(Bn) = \sin nt + \mathbb{N}(0, (2\sigma_2/(Bn))^2)
\]  

Here, the effect of the temporal derivation on the second equation is estimated by assuming the noise has identical independent distribution in every sample [97]. Multiplying both equation and averaging over time yields:

\[
\frac{1}{T} \int_0^T \frac{a_i a_j}{ABn} dt = \frac{1}{T} \int_0^T \sin^2 ntdt + \frac{1}{T} \int_0^T \mathbb{N}(0, (\sigma_1/A)^2) \mathbb{N}(0, (2\sigma_2/(Bn))^2) dt
\]  

The missing terms are a Gaussian random variable multiplied by a deterministic
function which changes the Probability Distribution Function (PDF) but not the mean as \( \sin nt \) is a symmetric function. The value of the first term on the right hand side is asymptotically 0.5 regardless of the frequency \( n \). The second term on the right hand side is the expectation of the multiplication of two uncorrelated random variables. Although an accurate value cannot be found due to unknown nature of the noise, the limits can be calculated by using the Cauchy-Schwartz inequality [108]:

\[
-\frac{\sigma_1}{A} \frac{\sigma_2}{Bn} \leq \frac{1}{T} \int_0^T \Re \left( 0, (\sigma_1/A)^2 \right) \Re \left( 0, (\sigma_2/(Bn))^2 \right) dt \leq \frac{\sigma_1}{A} \frac{\sigma_2}{Bn}
\]

The mean square average of each equation in 5.12 should also be used for normalization of equation 5.13. The integral of either equations in 5.12 can be written as:

\[
\frac{1}{T} \int_0^T \left[ \sin(nt) + G_X \right]^2 dt = \frac{1}{T} \int_0^T \sin^2(nt) dt + \frac{1}{T} \int_0^T G_X^2 dt + \frac{1}{T} \int_0^T \sin(nt) G_X dt
\]

The first integral on the right hand side reduces to 0.5 as before. The second term is the expectation of random variable squared which is its variance and the last term is zero with the same logic as equation 5.13. The maximum of Derivative Criteria (DC) is then:

\[
1 \pm \frac{4 \sigma_1}{A} \frac{\sigma_2}{Bn} \sqrt{1 + 2\sigma_1^2/A^2} \sqrt{1 + 2\sigma_2^2/(B^2n^2)}
\]

(5.14)

Comparing 5.11 and 5.14 shows a counter intuitive property. Although the Derivative Criteria (equation 5.14) has higher uncertainty in the numerator and the noise terms in denominator have a higher coefficient, \( n \) in \( \sigma_2^2/(B^2n^2) \) reduces the effect of noise when the interaction of higher and lower modes are studied. Numerically, the derivative of POD coefficients in time should be calculated first. Next, both the derivative and the coefficient matrix should be normalized to have unit length for every mode. Then the transpose of the normalized coefficients is left multiplied
by the derivative matrix.

Association matrices of the numerical test function are used to show the strength of methods developed in this section to capture multi-modal interactions as well as importance of the correction method developed in the previous section. Tables 5.2 and 5.3 show the modal association of the first 8 original modes of the test functions (plotted in Figure 4.2). The values higher than 0.2 are underlined for better visual understanding. Two modes are associated if they mutually have highest value in their corresponding columns. For example, the highest value of the first column is in row 7 and the highest value of column 7 is in the first row. This means modes 1 and 7 are associated. Similarly, modes (2,4), and (5,6) are associated, but mode 3 is not related to any other mode as expected. The second highest values shows a weaker modal interaction which is due to the degeneracy. The expected effect of the eigenvalue degeneracy has been captured by both methods properly which shows they are capable of detecting multi-modal interactions.

Two important differences in the methods can be identified by comparing the tables. The association matrix is symmetric for the Frequency Criteria but not the Derivative Criteria. For example, the DC of mode 1 to 6 is 0.506 but is less than half (0.227) and vice versa. This asymmetric behavior of the DC can be related to the direction of energy transfer using Granger-causality (one mode Granger-causes the other stronger), but this needs further investigation and is beyond the scope of this study. The impact of the noise on both criteria will be studied further in Section 5.5 using practical examples.

Tables 5.4 and 5.5 show the association matrices of corrected modes. It is evident that mode groups ((1,7),(2,4),(5,6)) that are related by design have stronger association than before. Additionally, no more than two modes are interacting, so modes of a traveling wave are much easier to find. Both corrected association matrices show weak interaction between modes (1,4) and (2,7) due to the degeneracy of
Table 5.2: Association matrix of original POD coefficients by Frequency Criteria

<table>
<thead>
<tr>
<th>Modes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.049</td>
<td>0.015</td>
<td>0.109</td>
<td>0.088</td>
<td>0.227</td>
<td>0.951</td>
<td>0.02</td>
</tr>
<tr>
<td>2</td>
<td>0.049</td>
<td>0</td>
<td>0.002</td>
<td>0.84</td>
<td>0.477</td>
<td>0.093</td>
<td>0.098</td>
<td>0.019</td>
</tr>
<tr>
<td>3</td>
<td>0.015</td>
<td>0.002</td>
<td>0</td>
<td>0.022</td>
<td>0.01</td>
<td>0.029</td>
<td>0.023</td>
<td>0.022</td>
</tr>
<tr>
<td>4</td>
<td>0.109</td>
<td>0.84</td>
<td>0.022</td>
<td>0</td>
<td>0.034</td>
<td>0.486</td>
<td>0.147</td>
<td>0.003</td>
</tr>
<tr>
<td>5</td>
<td>0.088</td>
<td>0.477</td>
<td>0.01</td>
<td>0.034</td>
<td>0</td>
<td>0.806</td>
<td>0.175</td>
<td>0.071</td>
</tr>
<tr>
<td>6</td>
<td>0.227</td>
<td>0.093</td>
<td>0.029</td>
<td>0.486</td>
<td>0.806</td>
<td>0</td>
<td>0.009</td>
<td>0.007</td>
</tr>
<tr>
<td>7</td>
<td>0.951</td>
<td>0.098</td>
<td>0.023</td>
<td>0.147</td>
<td>0.175</td>
<td>0.009</td>
<td>0</td>
<td>0.063</td>
</tr>
<tr>
<td>8</td>
<td>0.02</td>
<td>0.019</td>
<td>0.022</td>
<td>0.003</td>
<td>0.071</td>
<td>0.007</td>
<td>0.063</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 5.3: Association matrix of original POD coefficients by Derivative Criteria

<table>
<thead>
<tr>
<th>Modes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.086</td>
<td>0.032</td>
<td>0.024</td>
<td>0.074</td>
<td>0.075</td>
<td>0.233</td>
<td>0.956</td>
<td>0.007</td>
</tr>
<tr>
<td>2</td>
<td>0.067</td>
<td>0.061</td>
<td>0.017</td>
<td>0.846</td>
<td>0.467</td>
<td>0.065</td>
<td>0.205</td>
<td>0.01</td>
</tr>
<tr>
<td>3</td>
<td>0.008</td>
<td>0.001</td>
<td>0.176</td>
<td>0.002</td>
<td>0.011</td>
<td>0.008</td>
<td>0.002</td>
<td>0.005</td>
</tr>
<tr>
<td>4</td>
<td>0.134</td>
<td>0.936</td>
<td>0.009</td>
<td>0.035</td>
<td>0.015</td>
<td>0.247</td>
<td>0.147</td>
<td>0.005</td>
</tr>
<tr>
<td>5</td>
<td>0.126</td>
<td>0.718</td>
<td>0.018</td>
<td>0.102</td>
<td>0.057</td>
<td>0.633</td>
<td>0.106</td>
<td>0.011</td>
</tr>
<tr>
<td>6</td>
<td>0.506</td>
<td>0.08</td>
<td>0.03</td>
<td>0.314</td>
<td>0.607</td>
<td>0.053</td>
<td>0.116</td>
<td>0.002</td>
</tr>
<tr>
<td>7</td>
<td>0.955</td>
<td>0.116</td>
<td>0.013</td>
<td>0.064</td>
<td>0.057</td>
<td>0.007</td>
<td>0.081</td>
<td>0.004</td>
</tr>
<tr>
<td>8</td>
<td>0.026</td>
<td>0.03</td>
<td>0.001</td>
<td>0.003</td>
<td>0.017</td>
<td>0.019</td>
<td>0.004</td>
<td>0.063</td>
</tr>
</tbody>
</table>
Table 5.4: Association matrix of corrected POD coefficients by Frequency Criteria

<table>
<thead>
<tr>
<th>Modes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.05</td>
<td>-0.02</td>
<td>-0.14</td>
<td>0.018</td>
<td>-0.01</td>
<td>0.977</td>
<td>-0.02</td>
</tr>
<tr>
<td>2</td>
<td>-0.05</td>
<td>0</td>
<td>0.002</td>
<td>-0.97</td>
<td>-0.03</td>
<td>0.068</td>
<td>-0.12</td>
<td>-0.01</td>
</tr>
<tr>
<td>3</td>
<td>0.016</td>
<td>0</td>
<td>0</td>
<td>0.023</td>
<td>0.003</td>
<td>0.033</td>
<td>0.015</td>
<td>-0.02</td>
</tr>
<tr>
<td>4</td>
<td>0.139</td>
<td>0.966</td>
<td>-0.02</td>
<td>0</td>
<td>0.033</td>
<td>-0.05</td>
<td>-0.03</td>
<td>0.027</td>
</tr>
<tr>
<td>5</td>
<td>-0.02</td>
<td>0.029</td>
<td>0</td>
<td>-0.03</td>
<td>0</td>
<td>-0.97</td>
<td>0.004</td>
<td>-0.06</td>
</tr>
<tr>
<td>6</td>
<td>0.01</td>
<td>-0.07</td>
<td>-0.03</td>
<td>0.051</td>
<td>0.969</td>
<td>0</td>
<td>0.01</td>
<td>0.022</td>
</tr>
<tr>
<td>7</td>
<td>-0.98</td>
<td>0.119</td>
<td>-0.02</td>
<td>0.034</td>
<td>0</td>
<td>-0.01</td>
<td>0</td>
<td>0.054</td>
</tr>
<tr>
<td>8</td>
<td>0.022</td>
<td>0.013</td>
<td>0.016</td>
<td>-0.03</td>
<td>0.064</td>
<td>-0.02</td>
<td>-0.05</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 5.5: Association matrix of corrected POD coefficients by Derivative Criteria

<table>
<thead>
<tr>
<th>Modes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.086</td>
<td>0.033</td>
<td>0.024</td>
<td>0.102</td>
<td>0.026</td>
<td>0.015</td>
<td>0.983</td>
<td>0.008</td>
</tr>
<tr>
<td>2</td>
<td>0.068</td>
<td>0.061</td>
<td>0.016</td>
<td>0.965</td>
<td>0.039</td>
<td>0.017</td>
<td>0.216</td>
<td>0.007</td>
</tr>
<tr>
<td>3</td>
<td>0.008</td>
<td>0.001</td>
<td>0.176</td>
<td>0.007</td>
<td>0.009</td>
<td>0.008</td>
<td>0.004</td>
<td>0.005</td>
</tr>
<tr>
<td>4</td>
<td>0.148</td>
<td>0.975</td>
<td>0.013</td>
<td>0.057</td>
<td>0.025</td>
<td>0.001</td>
<td>0.083</td>
<td>0.008</td>
</tr>
<tr>
<td>5</td>
<td>0.023</td>
<td>0.011</td>
<td>0.012</td>
<td>0.11</td>
<td>0.022</td>
<td>0.955</td>
<td>0.019</td>
<td>0.003</td>
</tr>
<tr>
<td>6</td>
<td>0.032</td>
<td>0.023</td>
<td>0.039</td>
<td>0.001</td>
<td>0.8</td>
<td>0.035</td>
<td>0.096</td>
<td>0.001</td>
</tr>
<tr>
<td>7</td>
<td>0.957</td>
<td>0.12</td>
<td>0.009</td>
<td>0.029</td>
<td>0.005</td>
<td>0.008</td>
<td>0.089</td>
<td>0.004</td>
</tr>
<tr>
<td>8</td>
<td>0.029</td>
<td>0.029</td>
<td>0.001</td>
<td>0.013</td>
<td>0.014</td>
<td>0.019</td>
<td>0.003</td>
<td>0.063</td>
</tr>
</tbody>
</table>

modes (4,5) and (5,6). These interactions could be reduced further by including the associated modes in the correction groups but that is limited to time-resolved data. Also, such associations are much weaker than those directly caused by degeneracy, so can be safely neglected.

Since the corrected modes of the numerical test function are harmonic, it is constructive to further investigate the equivalency of POD and Fourier analysis as a short continuation of chapter 3. Each mode group of the test function is either a standing or a traveling harmonic structure with individual wave speeds so unlike test function \( u3 \), the mode shapes are maintained as harmonic functions with a \( \pi/4 \) lag (Figure 5.3). The normalized POD energy and real and imaginary parts of RMS Fourier coefficients are summarized in table 5.6. Two differences are evident; the
difference in energy levels within each traveling wave and the representation of the standing wave (wave number 11). In traveling waves, the POD energy is linked to the amplitude of fluctuation (beating); the higher the amplitude changes in time, the higher the energy difference of associated modes. So POD modes 1 and 7 which are associated with wave number 7 have the widest energy gap. On the other hand, the difference between the real and imaginary part of the Fourier transfer does not reflect such dependency. The other difference is that harmonic mode 11 is described by a single POD mode, while the Fourier transform has both the real and imaginary part as the test function has both sine and cosine functions. It is interesting to note that the difference in the real and imaginary part of the 11th harmonic is more than any of the traveling waves. These two differences are additional evidence that POD and Fourier transform are not equal (even when applied to the harmonic base functions).

### 5.4 Numerical Setup

#### 5.4.1 Solution Method for Pipe and Channel Flows

To assess the developed methods in a practical case, numerical simulations of channel and pipe flow will be used. The simulations have been conducted with a finite volume based, open source package; OpenFOAM® v5.0 [74]. The pimpleFoam solver [62] with PISO algorithm and two inner corrector loops have been used. The pimple al-
algorithm has two inner loop and one non-orthogonal corrector for the pipe simulation because of the non-Cartesian grid in pipe flow. The convection discretization scheme for velocity is second-order central with no limiters to minimize the numerical dissipation, nevertheless this method has higher dissipation than spectral method used in Direct Numerical Simulation (DNS) [33, 98, 65]. Hence lower Reynolds stresses are expected. Gradients are estimated by Gaussian integration estimation and linear interpolation from cell centers. The pressure correction and momentum equations have been solved iteratively with the Gauss-Seidel [62] method. The geometric algebraic multigrid [75] preconditioning is used for the pressure solution. The pressure correction and velocity equations are converged to $10^{-6}$ and $10^{-5}$, respectively. Second-order backward implicit time discretization is used for both simulations. The time steps have been chosen to limit the maximum Courant number to be smaller than 0.5 while the mean value is 0.2 and 0.18 for channel and pipe simulations, respectively. The WALE LES model [114] has been used to model the subgrid scale fluctuations without any wall model. The width of the spatial filter is considered to be the cubic root of the cell volume.

The geometry of the simulations for both cases are depicted in Figure 5.4. Boundary conditions are zero pressure gradient and velocity for no-slip walls, and periodic for all other faces. An iteratively corrected pressure gradient acts as momentum source for the inlet and outlet to ensure constant flow inside the domain. A superposition of laminar mean profile and near wall instabilities, as explained by Schoppa [132], is used to initialize the velocity field and trigger turbulence. For all the future plots, the streamwise direction and the wall normal directions are $x$ and $y$, respectively. The $z$ direction is perpendicular to $x$ and $y$.

The simulation dimensions and grid resolutions have been chosen to ensure the structures are properly resolved. The domain dimensions for channel flow are $2\pi h \times 2h \times \pi h$ in the streamwise, normal, and spanwise directions which is larger than the
Figure 5.4: Geometry of numerical simulations.
minimal channel approach of Fureby [41] (4h × 2h × 2h). The length of the pipe simulation is five times the diameter which is consistent with Eggels [33] and Loulou [89]. The maximum y+ near the walls is limited to less than 1 while the mean value is 0.8 and 0.5 for the channel and pipe flow respectively.

According to De Villers [25], the LES grid should not be any larger than Δx+ = 35, and Δz+ = 20 in the streamwise and spanwise directions to capture the structures near the wall. The channel flow has 90 × 110 × 85 grids in x, y, and z directions respectively which leads to Δx+ = 26 and Δz+ = 14. To avoid the singularity of the grids in the center of the pipe simulation, a semi-Cartesian grid is used in the center with 20 × 20 grid points for 30% of the radius and smoothly transitioned to the pipe walls over 51 grids. This setup is similar to 61 × 80 grids in the radial and azimuthal directions respectively, with 60 grid points distributed uniformly in the streamwise direction. The respective grid sizes in wall units for the pipe flow are Δx+ = 30 and Δz+ = 14. All grid sizes are within the required grid resolution to resolve the physical structures. The cross-section of the simulations in a plane parallel to the inlet boundary is depicted in Figure 5.5.

The quadrature matrix is calculated by triangulating the cloud of points and then using the method described in Appendix D. Calculating the average value in the center of triangulated fields looses the information on boundaries and subsequently, POD does not conform to the no-slip wall or periodic inlet-outlet boundary conditions.

5.4.2 Validation

The simulations are reproduced after previous works so the results would be comparable. The bulk and wall shear Reynolds numbers based on channel half-width are 5700 and 376 which is close to the DNS performed by Moser et. al. [98] at Reτ = 392. For the pipe flow, the bulk and wall shear Reynolds numbers are 5200
Figure 5.5: Simulation grid at the inlet boundary condition.
and 340, respectively, to reproduce the results of Eggels [33] at $Re_\tau = 360$. Other studies with similar Reynolds numbers are also used for validation which are summarized in Table 5.7. For the sake of clarity the symbols are mentioned in the Table but not in the plot captions. Among the different constants of the log law in literature, $U^+ = 2.5 \ln y^+ + 5.5$ was used according to the main references [33, 98].

Table 5.7: Compared references and corresponding symbols

<table>
<thead>
<tr>
<th>paper</th>
<th>Geometry</th>
<th>$Re_{bulk}$</th>
<th>$Re_\tau$</th>
<th>Method</th>
<th>symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bakewell &amp; Lumley [9]</td>
<td>pipe</td>
<td>8700</td>
<td>512</td>
<td>HFA</td>
<td>□</td>
</tr>
<tr>
<td>Eggels et. al. [33]</td>
<td>pipe</td>
<td>5300</td>
<td>360</td>
<td>DNS</td>
<td>......</td>
</tr>
<tr>
<td>Eggels et. al. [33]</td>
<td>pipe</td>
<td>5450</td>
<td>371</td>
<td>LDA</td>
<td>◄</td>
</tr>
<tr>
<td>Eggels et. al. [33]</td>
<td>pipe</td>
<td>5450</td>
<td>379</td>
<td>PIV</td>
<td>▼</td>
</tr>
<tr>
<td>Durst et. al. [30]</td>
<td>pipe</td>
<td>7742</td>
<td>500</td>
<td>LDA</td>
<td>○</td>
</tr>
<tr>
<td>Loulou et. al. [89]</td>
<td>pipe</td>
<td>5600</td>
<td>380</td>
<td>DNS</td>
<td>......</td>
</tr>
<tr>
<td>El Khoury et. al. [34]</td>
<td>pipe</td>
<td>5300</td>
<td>360</td>
<td>DNS</td>
<td>......</td>
</tr>
<tr>
<td>Present</td>
<td>pipe</td>
<td>5177</td>
<td>351</td>
<td>LES</td>
<td>......</td>
</tr>
<tr>
<td>Eckelmann [32]</td>
<td>channel</td>
<td>5600</td>
<td>-</td>
<td>HFA</td>
<td>□</td>
</tr>
<tr>
<td>Moser et. al. [98]</td>
<td>channel</td>
<td>-</td>
<td>392</td>
<td>DNS</td>
<td>......</td>
</tr>
<tr>
<td>De Villers [25]</td>
<td>channel</td>
<td>5775</td>
<td>363</td>
<td>LES</td>
<td>......</td>
</tr>
<tr>
<td>Hoyas et. al. [65]</td>
<td>channel</td>
<td>-</td>
<td>547</td>
<td>DNS</td>
<td>......</td>
</tr>
<tr>
<td>Present</td>
<td>channel</td>
<td>5774</td>
<td>375</td>
<td>LES</td>
<td>......</td>
</tr>
<tr>
<td>Theory [81, 33]</td>
<td>Wall function</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>●</td>
</tr>
</tbody>
</table>

Since the results are used to illustrate the methods developed in this section, POD analysis has been conducted on independent and time-resolved data on streamwise and cross-stream planes for each flow. The pipe and channel flow have respectively 6000 and 2300 independent instances, sampled at one eddy-turn-over-time apart ($\Delta t D/U_b = 1$) where the characteristic length scale $D$ is the pipe diameter or channel half-width and $U_b$ is the bulk velocity. The time-resolved datasets have 1500 and 3000 instances taken at 0.05 and 0.057 eddy-turn-overs for pipe and channel flow, respectively. The time-resolved samples are taken from short simulation runs after sampling the independent datasets to ensure there is no overlap or dependency. The number of samples ensured the convergence of the statistics and subsequently
POD kernels. In channel flow, the mean profile velocity of the upper and lower wall collapse perfectly which shows an adequate number of samples have been used and the statistics are converged. Also for the pipe flow, the sampled lines at different azimuthal angles overlap within a reasonable range. Details of the POD implementation will be presented in Section 5.5.

The mean and normal Reynolds stress profiles of pipe simulations are plotted in Figure 5.6. In pipe units, the agreement with other references is excellent. The mean velocity profile shown in wall units follows the linear law of the wall perfectly for \( y^+ < 5 \). The current simulation is slightly (5%) higher in the log-law than Eggels et al. Log-law regions with higher constants are commonly observed in pipe simulations such as in El Khoury et al. [34] and Loulou [89], as shown in the figure. Also the Reynolds number of this simulation is slightly smaller than others which in turn shifts the log section of the profile away from the wall [34]. The streamwise RMS velocity is in agreement with DNS investigations but the normal and cross-stream components, despite the similar trend, are underestimated. This is partly due to the dissipation of the second order discretization used. Also the lower Reynolds number of the simulation causes smaller Reynolds stresses which are mostly observable in the normal and cross-stream components [34].

The channel flow shows even better agreement with the literature as shown in Figure 5.7. The mean flow agrees well with others both in channel and wall units. The simulation of De Villers [25] uses a similar method to this study but with a smaller domain and a coarser grid (first node is at \( y^+ = 2 \)). Similar to the pipe simulation, the streamwise Reynolds stress is accurately predicted while the other components are underestimated for the same reasons. It should be noted that present simulations did not show any better accuracy with finer grids.

In summary, both simulations are in good agreement with the literature. As mentioned before, the main purpose of simulations is to present a benchmark with
Figure 5.6: Mean velocity and normal Reynolds stresses of pipe flow simulation. For symbols see Table 5.7.
Figure 5.7: Mean velocity and normal Reynolds stresses of channel flow simulation. For symbols see Table 5.7.
symmetry in the level of round-off error to investigate the power and sensitivity of POD and the developed methods. The statistics of both simulations satisfies this by having correct trends and reasonable uncertainty, if any.

5.5 Channel and Pipe Flow

To properly assess the ICA performance on increasing modes locality, it is beneficial to know about the well-established mechanisms in the flow. A well-known structure in the developed turbulence near walls, such as channel, pipe, and boundary layer flow, are long streaks which have limited span [82, 9, 96, 33, 131, 134, 29]. Loulou et al. [89] measured the two-point correlations in pipe flow simulation and found that the streamwise components are correlated over large streamwise separations near the wall because of the streaks. Due to their limited pipe length, the streaks occupied the whole domain length in the sub-layer but diminish beyond the buffer layer ($y^+ ≈ 22$). Eggels et al. [33] found similar results with correlations over longer separation distances outside the buffer layer. Azimuthal two-point correlations of Loulou et al. showed that the streaks are rather narrow with a width of $\lambda^+ ≈ 55$ and spacing of $\lambda^+ ≈ 110$. The interaction of the nearby streaks are reasonable but decreases for long separations, hence the small two-point correlation length in the azimuthal direction. So in the streamwise plane, structures near opposite walls should behave independently and consequently the POD modes are expected to reflect this local behavior as well. In the cross-stream plane, at least a few modes with limited azimuthal spans are expected to be observed.

The other expectations is that the POD modes in the pipe and channel flow are symmetrical in shape and behavior with respect to the centerline because of the geometrical symmetry. The mode signs are not important as the coefficients compensate them, but either the mode shapes should show the symmetry or symmetric
modes with respect to the centerline should exist. The interaction of the modes are also expected to be symmetric. For example, if two modes of the streamwise plane describe a traveling wave near the upper wall, similar behavior is expected to be observed near the lower wall. Moreover, similar mode shapes are expected to be observed in the near wall region for the pipe and channel flow as the main structures are similar.

The POD analysis here is conducted on the independent samples, then the time-resolved instances are projected on the bases. First, the General POD approach of Chapter 2 is used on the independent datasets to generate the modes and their coefficients. Next, the eigenvalue uncertainty is calculated and the modes are corrected to decrease the dependency. Then, the time-resolved datasets have been projected on original and corrected modes to calculate the time-resolved coefficients from a converged bases. Finally, original and corrected time-resolved coefficients are used to calculate the inter-modal interactions.

5.5.1 Channel and Pipe Flow Streamwise Plane

The original POD modes of the streamwise plane for the pipe (Figure 5.8) and channel (Figure 5.9) flow show the modes are global, asymmetrical, and not similar between the two flows for modes 7 and higher. It should be noted that the similarity of the first 6 modes in the two flows with slightly different Reynolds number is remarkable. The first two modes are stronger near one wall with a diminished effect near the other wall. The close energy level and similar shape infers that they represent the same structure near opposite walls. But one mode (1 in pipe, 2 in channel) has the same sign in all domain (suggesting it is a global mode) while the other mode changes signs inconsistently. Also the diminished part of each mode indicates interaction of structures near opposite walls which is not expected as explained.

The global behavior becomes stronger in higher modes. In both flows, modes
(3,4) and (5,6) have similar shapes that could describe two traveling waves near the lower and upper walls respectively with acceptable symmetry. All four modes are non-zero near all walls which again suggests the structures near opposite walls are interacting and the modal behavior is global. Symmetrical forms can be found in modes 7 to 12 of the pipe flow but not in channel flow. Moreover, the similarity between the two flows is very obscured and the connection between opposite walls are more visible in these modes. As explained, the eigenvalue degeneracy is the reason for the global mode shapes. Since similar structures near each wall are equally as likely, their energy level will be similar and in the same uncertainty range.

The degeneracy can be illustrated best in the first two modes as they form a two-dimensional bases portrayed in Figure 5.10. A fitted Gaussian PDF is shown by black contour lines for the POD coefficients of the first two modes of the pipe flow. Perfect circles near the origin demonstrates the shortcoming of POD method with regards to eigenvalue degeneracy. Any unitary rotation in this sub-space yields the same energy content, so maximizing the Gaussianity is futile. As a result, numerical solutions from different platforms or numerical packages can yield non-unique mode shapes.

For a meaningful preferred axes in such sub-spaces, extra assumptions should be considered. The kurtosis of the POD bases (not coefficients as they are Gaussian) are a good candidate as they contribute to the locality of the mode shapes. As Figure 5.10 shows, maximum and minimum kurtosis result in symmetric forms with respectively most local and global shapes. This is intuitive as kurtosis is a measure of tailedness of the PDF. A local mode where most of the domain is zero (or constant) has a very long tail. In contrast, values of global modes are more centered and have lower kurtosis. Since global mode shapes increase the dependency of the modes, which is counter productive to the intention of low-dimensional reconstruction, local modes are preferred.
Figure 5.8: Streamwise velocity component of the pipe flow original POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.9: Streamwise velocity component of the channel flow original POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.10: Rotation of first two POD modes of pipe flow in streamwise plane (streamwise components). Blue crosses are POD coefficient, arrows are rotated axes with corresponding POD mode at the end of each arrow. Black contour lines are fitted multivariate Gaussian. Subplot captions are corresponding kurtosis.
Correction of the POD modes using ICA reduces the globality of the mode shapes and their interactions, as expected. The corrected modes near each wall are fairly constant near the opposite wall for both flows (figures 5.11 and 5.12). None of the corrected modes 7 to 12 connects the structures near opposite walls contrary to the original modes. Additionally, the similarity of these modes between the two flows has increased considerably.

Figure 5.13 shows removing the eigenvalue degeneracy results in more even energy distribution. This plot also reveals the reason modes 7 to 12 of the two flows are not as similar. In the pipe flow, the energy content of modes 7 to 12 are beyond the uncertainty range of other modes. On the other hand, modes 7 to 16 of the channel flow have similar energy content, so the degeneracy has occurred between more modes. This is an example where modes which are not truly degenerate fall in the same certainty range. Nonetheless, the correction is reasonably acceptable as shown.

The association maps of the streamwise plane of pipe flow (Figure 5.14) supports the enhanced interaction of POD modes, thanks to the increased locality of mode shape. The modes (2,3) and (4,5) from the original POD are clearly associated according to both Derivative and Frequency Criteria. The original modes 7 and 11 which are on the top wall are also strongly associated. However on the bottom wall, three modes (8,9,10) have association (both DC and FC) which is not a symmetric behavior. Although the original DC shows a one way association of modes 11 and 12 but DC does not find such interaction. The association of the corresponding corrected modes are pronounced and symmetric for both criteria. Mode groups (8,9,11) and (7,10,12) have clear associations near the top and bottom walls, respectively.

The association map of the channel flow (Figure 5.15) also shows that increased locality of the modes leads to better insight into inter-modal interactions. For clarity, the absolute value of FC is plotted and levels of all association maps are set between
Figure 5.11: Streamwise velocity component of the pipe flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.12: Streamwise velocity component of the channel flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.13: Relative energy contents of the first original and corrected 40 modes in streamwise plane. Top: pipe, bottom: channel.
Figure 5.14: Association map of pipe flow original and corrected POD modes in the streamwise plane. Pure black and white are perfect and no associations, respectively.
0 and 1 for no, and perfect associations, respectively. Although original modes 4 and 6 are fairly constant near one wall, DC and FC show that modes 2 to 6 cannot be divided into two independent groups due to globality of mode 5. For the next group of associated modes, the original association map shows close interaction levels between many modes. After correction, modes (3,4) and (5,6) are clearly distinguished because of increased locality. Also modes (8,9,10) are associated near the lower wall similar to modes (7,10,12) of the pipe flow. Unfortunately, the counterpart mode group is not as clear. Despite the interaction of modes (7,11,12), there is a close association level between this group and modes 13 to 17. As mentioned before, the reason of mixed association is due to the close energy level of other modes which may have been caused because of the lower number of samples compared to the pipe flow data.

The locality decreases at higher modes because a vast scale of modes fall into the same uncertainty range. But decreased performance at higher modes does not pose a substantial problem as researchers often favor the lower modes. Nonetheless, occasional mode groups that maintain their local and symmetric behavior can be observed in the very high modes. For example, figures 5.14c and 5.14d show clear association within mode groups (26,31) and (27,29). These mode groups are traveling waves near each wall similar to modes 2 to 6 but with smaller streamwise wave length (Figure 5.16).

The shortcoming of ICA is that it cannot reduce dependency locally. In the cocktail party example, two speakers can be distinguished well when they are far apart in the room, but not when standing close to each other. Mode groups with three modes in the pipe flow are a good example of this. Figure 5.17 shows the POD coefficients of modes 7, 10, and 12 in two different angles to demonstrate a more proper rotation exists. The corrected POD modes after rotation with such angle (Figure 5.18) illustrates that this group consists of a traveling and a standing wave.
Figure 5.15: Association map of channel flow original and corrected POD modes in the streamwise plane. Pure black and white are perfect and no associations, respectively.
Figure 5.16: Streamwise velocity component of the pipe flow corrected POD modes in streamwise plane. Solid and dash contour lines are positive and negative, respectively.
The extra mode has lower kurtosis so ICA is not able to find it. The association of the corrected modes 7 and 10 after rotation increases from (DC=0.76, FC=0.69) to (DC=0.93, FC=0.97) while the interaction of either with mode 12 decreases from (DC=0.77, FC=0.66) to a maximum of 0.07. Thus, ICA certainly enhances modal distinction compared to the original modes but further improvement based on the temporal behavior of the coefficients is possible.

Despite the reasonable explanation for the last mode group, more sophisticated interactions may exist. POD coefficients of corrected modes 24, 25, 28, and 30 (Figure 5.19) which previously was shown to be associated (figures 5.16, 5.14c, and 5.14d) does not reveal any three-dimensional rotational that reduces the complexity of the sub-space. Higher dimensions can be counter intuitive so investigation without proper analytical tools can be cumbersome or fruitless. Two major speculations could be proposed for future works; either a better sub-space can be formed if other modes are combined, or the coordinate system of the bases does not allow further dimensional reduction. Since this mode group is in an uncertainty range that contains many other modes, it is possible that including other modes reveals a rotational direction that provides better decomposition of the mode groups. However, including more modes without having proper analytical tool of finding a preferred rotation only increases the complexity. Another possibility is that the average of selected modes could be used as Pinier [113] described in his analysis of the free jet. Since the goal of this thesis is not to develop a physical understanding of the flow, this discussion is left open for future works.

A time-resolved dataset can use the Modal Corrections, traveling wave criteria, and the Energy-Ratios from the previous chapter to find the most interesting time range regarding desired modal interactions. Figures 5.20 and 5.21 shows the incremental clarity acquired by the developed methods compared to the use of raw POD coefficients. The coefficients and ERs of both plot are illustrated with white when
Figure 5.17: Corrected POD coefficients of modes 7, 10, and 12 of pipe flow in streamwise plane.
Figure 5.18: Rotated POD modes to increase modal interaction. CM: Corrected Mode, RM: Rotated Mode after correction, k: kurtosis. Solid and dash contour lines are positive and negative, respectively.
Figure 5.19: Corrected POD coefficients of modes 24, 25, 28, and 30 of pipe flow in streamwise plane.
they are close to zero and black otherwise. Since the original POD modes are global, they can obscure the modal interactions in order to compensate for locality. For example, reconstructions with the first two modes in the range $0 < tU/D < 5$ have a dominant structure only near the top wall, so the coefficients of the second mode are higher. However, this mode has non-zero values close to the lower wall, so the coefficients of original mode 1 have to be negative. This modal interaction becomes more complicated in the range $39 < tU/D < 68$. On the other hand, the corrected coefficients show a more sensible representation. In the time range $0 < tU/D < 5$ only the first corrected mode is non-zero which clearly shows same event has not occurred close to the lower wall. The behavior of the corrected coefficients in the time range $39 < tU/D < 68$ also shows the reconstruction is more dominant near the top wall. However, understanding the modal behavior of traveling waves, specifically when more than 2 modes are involved, can be very difficult from the coefficient plots.

Using the traveling wave criteria and ER to group the modal behaviors can ease their understanding significantly and be less error prone. The original and corrected Energy-Ratios plotted in Figure 5.21 are selected using the traveling wave criteria when the association is mutual and more than 0.5. Comparing the original Energy-Ratios in Figure 5.21a to the coefficients in Figure 5.20 shows the importance of ER. Although the original coefficients of modes 5 and 6 are non-zero in a wide time range, the ER shows their behavior can be observed best in the vicinity of $tU/D = 20$. Comparing the ER of original and corrected modes (figures 5.21a and 5.21b) again shows the disadvantage of, and probably misinterpretation caused by, using the original modes. In time range $24 < tU/D < 29$, the ER of the original modes 3 and 4 has a peak which suggests the reconstruction will be dominant near the lower wall. However, the corrected ER indicates that dynamics of this instances is mostly described by modes 5 and 6 which are close to the upper wall. Moreover, the ER of associated modes can be used to study the spatial interaction of different
groups. For example, Figure 5.21b shows that the dynamics of instances in the time range \(58 < tU/D < 63\) are distributed between mode groups (1), (5,6), and (8,9,11) which are all close to the upper wall.

As a final remark, performance of DF and FC should be compared. All the plots show that DC is less susceptible to noise as predicted. Equation 5.14 states that the noise level is reduced by the frequency of the derivative coefficient. Figures 5.14 and 5.15 show that the lower left corner of DC always has less noise than FC. The noise on the top right corner does not decrease, as it is connected to the derivative of the lower mode, but is also not considerably more than FC. In the light of less noise and reasonable agreement of both traveling wave methods, only the Frequency Criteria will be used for the next section.

5.5.2 Channel and Pipe Flow Cross-stream Plane

Modes in the cross-stream planes are normally harder to interpret as the structure may not have a clear translational behavior in this plane. The original modes of cross-stream planes (figures 5.22 and 5.25) are more complex than the streamwise plane, nonetheless, display the same global behavior. Despite occasional partial low values (modes 1, 6 of pipe and 3, 5, 6 of channel flow) near wall regions are strongly related. The globality of the original POD modes increases quickly in higher modes for both flows. Although the first 9 modes of pipe flow have similar shapes (five azimuthal sign changes), none of them appears as a phase shifted version of one another which is unexpected. Mode 15 and 16 are the first mode pair that have similar shapes with a phase shift but they do not express a traveling wave (DC=0.05,FC=0.06). This is notable as it shows a practical case where the phase shift in the mode shape is not indicative of a traveling wave. Another uncommon feature of the cross-flow plane is the large scale of modes 17 and its phase shifted version (mode 18 shown later in Figure 5.28) which shows the most energetic forms do not always have largest scale.
Figure 5.20: Original and corrected coefficients and POD modes of pipe flow.
Figure 5.21: Time history of POD original and corrected coefficients and their Energy-Ratios.
This is expected as most energetic structures occur near the wall. Again, these two modes do not associate to form a traveling wave. Inspecting the original modes of the channel flow did not reveal any modes that resemble each other with a phase shift, neither larger structures were found in higher modes.

The corrected modes of the cross-stream plane of the pipe flow show better locality, as expected. Figure 5.24 shows that first 9 modes of the streamwise velocity component are conveniently localized to be silent in a significant part of the domain but maintain some overlap. Similar to the streamwise plane, higher modes become less local as modes 10 to 12 show. Modes 13 and 14 (not shown) are also similar to modes 10 to 12 but with a rotation which demonstrates better consistency in the corrected modes. The size of the non-silent part of these modes has clearly increased compared to the previous modes. Although the two mode groups (1-9) and (10-14) show local structures with similar shapes and rotations (or phase shifts), they are not interacting to form traveling waves. The low-dimensional reconstruction with modes 1 to 9 shows the structure can simultaneously move in azimuthally opposite directions and mostly fluctuate in place rather than azimuthal translations. The next mode group with similar shapes are modes (15,16) and (17,18). Neither the shape nor the association of original modes change after correction. The globality of the modes does not persist for all the higher modes but rather becomes sporadic similar to the streamwise plane.

The cross-stream plane of the channel flow does not indicate similarities to the pipe flow (Figure 5.23). The original mode groups (1,2) and (3,4) loosely each other with a phase shift in parts of the domain. The modes of the first group has a reasonable similarity near the lower wall. The resemblance within the second group only exists close to the top wall. Moreover, many other modes with similar structure sizes can be found (for example modes 5 to 7). So these modes cannot be grouped to be representative of a structure without correction and investigating the association
Figure 5.22: Streamwise velocity component of the pipe flow original POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.23: Streamwise velocity component of the channel flow original POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.24: Streamwise velocity component of the pipe flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively.
The correction of the cross-stream plane of channel flow (Figure 5.25) is not as successful as the stream-wise plane or the cross-stream of the pipe flow. Although modes are mostly localized, the interaction of the opposite walls are not removed similar to the stream-wise plane or the cross-stream plane of the pipe flow. Mode groups (3,5), (1,2,4), and (9,10) indicate phase shifts to a lesser degree than the original modes. However, the decreased number of similar modes with a phase shift may not be important in this plane since the modal interactions are insignificant as will be shown later. The span-wise locality is not enhanced as strong as for the pipe flow but becomes more obvious in higher modes. In general, neither original nor the corrected modes of the pipe and channel flow do not show any similarities in this plane. Again, the reason for the poor performance compared to the pipe flow could be the fewer number of samples.

It should be noted that POD analysis of this plane also supports the outcome of Chapter 3 that POD modes are not harmonic functions in the homogeneous direction. The numerical simulations do not have the noise or uncertainty of experimental measurement to deviate the POD modes. The azimuthal and translational symmetry of the pipe and channel flow are perfect to the order of round-off errors, nevertheless the lower modes do not resemble harmonic functions but combinations of them, like the analytical example. This is more clear in the corrected modes 1 to 9 for the pipe flow where a large number of length scales are very similar. The shape of these modes suggests a combination of harmonic functions and a Gaussian-like distribution which can only be explained by including many harmonic functions.

Exploring the modal energies in this plane (Figure 5.26) endorses the difficulty of using the Scree method from Chapter 4. The original energy levels are very close with multiple small abrupt drops so the Scree method cannot be used confidently. Visual inspection of the energy content in the pipe flow reveals possible mode groups
Figure 5.25: Streamwise velocity component of the channel flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively.
((1-9), (10-14), (15-18), (19,20)) with similar trends in their energy. The progressive isolating method, used to group non-overlapping modes, has selected the same modes. The original energy content of the channel flow does not show any apparent group of modes which can be selected, mainly due to the higher eigenvalue uncertainty. In both cases, the correction has changed the energy levels to be more even within each group. Although this is contradictory to the optimality notion of POD, but it should be recalled that the true values of eigenvalues are not known. Also the modes in the same uncertainty range usually have close length scales, so a more even distribution of energy is plausible. The correction increases the energy gap between the mode groups which helps the selection of modes for low-dimensional reconstruction.

The association levels in cross-stream plane are very low and dispersed among many modes due to the complexity of the modes as Figure 5.27 shows. The reason is likely that a structure with rotation axis aligned with streamwise direction induces counter-rotating structures in its neighborhood with similar scales and temporal characteristics. So all such structures are projected on the same modes. As a result, the non-linear behavior cannot be linearly decomposed in a small number of modes. Subsequently, the original association maps (figures 5.27a and 5.27b) does not show many high peaks, but many smaller interactions in the order of 0.1. The correction of the channel flow modes does not improve the modal association (Figure 5.27d). The association map of the pipe flow indicates a weak multi-modal interaction between modes 17, 18, 41, 44, 45, and 49 which in total constitutes 4.2% of the kinetic energy.

The corrected association of pipe flow represents a more comprehensible behavior. The modal interactions is more pronounced in mode groups (17,40,63) and (18,43,47). Inspection of the coefficients in three dimensions did not reveal any better rotation of basis as in the previous section. The reason could be because the mutual association is dominantly limited to two modes per group which are (17,40) and (18,43). The streamwise velocity component of corrected modes (Figure 5.28)
Figure 5.26: Relative energy contents of the first original and corrected 40 modes in cross-stream plane. Top: pipe, bottom: channel.
Figure 5.27: Association map of original and corrected POD modes of pipe and channel flow in the cross-stream plane by DC. Pure black and white are perfect and no associations, respectively.
does not show any prevalent association. However, the cross-stream velocity components indicate a horizontal and a vertical secondary flow in mode groups (17,40) and (18,43), respectively, which pushes the flow from the pipe center toward the wall and induces a counter flow close to the walls. The quiver plots (Figure 5.29) reveal the modal interaction of the first group is a continuous transition between stronger and weaker core of the secondary flow (a beating wave). The other mode group also shows the same behavior in the vertical direction as can be inferred from Figure 5.28. It should be noted that such interactions cannot be discovered with other traveling wave methods as the two modes do not represent the traveling of a structure. The near zero interaction between the two mode groups means the secondary flow does not have a circular rotation but rather an irregular behavior in the azimuthal direction.

The modal interaction of the two aforementioned groups has a crucial notion that should be considered with caution. The higher modes should necessarily not be excluded from analysis because of their lower energy. Most of the lower modes are dominated by the modes where the main flow direction is significant. The cross-stream components which may have dynamic importance could be found in higher modes with lower energy due to their nature. The low energy of these modes does not mean dynamical insignificance as Figure 5.30 shows, instantaneously these 4 modes can contain up to 20% of the dynamics despite the average 4.2% energy. Additionally, interpreting the modal interactions should be wary of weaker associations. In this case, each group of modes has a third mode which weakly interacts with the other modes. When the association levels are close, all combination of the modes should be investigated. The third mode is excluded here as the association level is about half of the other modes and a physical interpretation of the flow is not the goal of this thesis.
Figure 5.28: Velocity components of pipe flow corrected POD modes in cross-stream plane. Solid and dash contour lines are positive and negative, respectively.
Figure 5.29: Cross-stream velocity components of pipe flow corrected POD modes in cross-stream plane.
Figure 5.30: Combined Energy-Ratio of modes 17, 18, 40, and 43 of pipe flow in cross-stream plane.

5.6 Conclusion

This chapter presented a detailed study on the impact of traveling waves on POD. The main challenges to uncovering modal interactions are the presence of noise, improper frame of reference, and the globality of the modes. It was shown that the global behavior of the modes is mostly an artifact of degenerate eigenvalues which is inevitable in practice due to uncertainty of eigenvalues. A method was developed to increase locality of the modes by mitigating inter-modal dependency. The numerical test function and practical example of the pipe and channel flow in the streamwise plane portrayed the enhanced effect of Modal Correction. The independent regions of the flow do not interact and the expected symmetry of the modes has been increased. Moreover, the similarity of the POD modes of the pipe and channel flow increased in the streamwise plane. This is of paramount importance as the previous evidence suggests both flow have streak-like structures near walls.

The other contribution of this chapter is development of two methods to uncover the modal interactions. The methods, called Frequency and Derivative Criteria, are
based on well-established Granger-causality. The superiority of developed methods is their *a posteriori* use of POD coefficients without any assumptions on the number of the interacting modes or their spatial shapes. The performance of both methods in the numerical test function and the streamwise plane of simulations proves their strength. The association maps, further show that Modal Corrections truly decreases the inter-modal dependency as the modal interactions become stronger, limited to fewer number of modes, and symmetric as expected. Association maps of simulations in the cross-stream plane did not find modal interactions as strong as in the streamwise plane due to the complicated behavior of the structures in this plane which cannot be linearly decomposed in a small number of modes. Nonetheless, the association map of the pipe flow in the cross-stream plane finds two group of modes which resemble a secondary flow. The symmetry of the mode shapes and their interaction at such high mode number with very low energy content shows the reliability of the developed criteria.

Lastly, the Energy-Ratio method developed in the previous chapter demonstrated the instantaneous importance of higher modes. Such modes with insignificant average energy could instantaneously hold significant dynamics up to 4 or 5 times their average energy. Unearthing the importance of such modes by searching random instances is virtually impossible but the Energy-Ratio provides a clear measure.
Chapter 6

POD Coefficient Based Sequencing

6.1 Introduction

The purpose of this chapter is to develop a method that takes advantage of the "curse of dimensionality" to provide the most probable sequences of instances. The "curse of dimensionality" is the exponential rise in the required number of samples to represent the space by increasing the dimensions. For example a line ($d = 1$) limited to the range $[-1, 1]$ needs only $10^d = 10$ points to be uniformly sampled at a distance of 0.1, but a cube ($d = 3$) limited to $[-1, 1]^3$ needs $10^d = 1000$ points. It is evident that the high-dimensional spaces in fluid mechanics ($d = O(10^3)$ for dense experimental methods such as PIV and $d = O(10^6)$ for numerical simulations) are tremendously under-sampled regardless of the number of instances. Decomposition methods, such as Fourier or POD transforms, reduce the dimensionality of the space but not to the extent where the number of samples represent the whole subspace. However, the physically attainable instances are on the surface of a manifold (which is a hyper-ellipsoid), not the lattice of the space. The coefficients are the right eigenvectors of the SVD problem multiplied by the eigenvalues as explained in Chapter 2. Since the eigenvectors are orthonormal, each right eigenvector (which is the normalized
POD coefficient of an instance) has a unit length. Thus the normalized coefficient space is a hyper-sphere. Multiplication by eigenvalues scales the hyper-sphere in each dimension to be a hyper-ellipsoid. However, the surface of this manifold is still intractable with the limited number of samples. Projection onto lower dimensions increases the number of effective samples at the cost of entangling the manifold. Therefore, given the proper number of dimensions is chosen, the subspace has enough samples on the manifold and is not entangled so as to be obscured, then the dynamics of the system could be understood.

As an over-simplified example for the sake of illustration, consider the helical trajectory of Figure 6.1. The black line represents the true trajectory of the system in all available dimensions which is randomly sampled by blue dots. All the dynamics of the system cannot be recovered as the three-dimensional space is under-sampled but the projection on a two-dimensional space (green dots) is well-represented. It is clear in this simple example that the dynamics of the two-dimensional space is a circle but such visual investigation is obviously not feasible in higher dimensions (even as low as four). Moreover, there is no guarantee that the low-dimensional space is uniformly sampled or the distance of two consecutive samples are small enough so the transition between them could be understood. In other words, if three instances of the flow are known to be just one eddy-turn-over-time apart, the transition between them remains unknown. Given a sequence of the samples in the low-dimensional space is available, then the knowledge gained from finely sampled regions could be used to interpolate the missing instances in the under-sampled regions. In this example, the green dot on the lower left part of the two-dimensional plane is more distant to the other nodes but the circle-like behavior can be understood from its neighbors. The red line of this example has been produced with the methods developed in this chapter but more complex examples will be presented.

The existence of the hyper-ellipsoid has an immediate notable outcome; the re-
alizable instances can align with any POD mode (even the noise beyond p50). The impracticality of such instances reveals that not all the surface of the manifold is physically plausible. At least, the poles of the noise dimensions can be excluded. However in lower-dimensions, this is not the case. An extreme example is the low-dimensional space with two modes where the reconstructions can align reasonably with one of the modes. Increasing the dimension of the subspace decreases the possibility of such alignment. If the coherent structures are recoverable with a small number of modes, then physical instances are plausible where the low-dimensional reconstruction resembles a single mode which is contrary to the conclusion of Kevlahan et al. [80]. Despite the asymmetric definition, the space formed by Kevlahan et al.’s test function \((a + bx) \exp(-x^2)\) has symmetric points \((a = 0 \text{ or } b = 0)\) and POD correctly finds such points to present the most optimal bases. The erroneous conclusion was drawn because their test function has no temporal evolution to assure samples resolve the space properly. In practice, the alignment of the instances and modes can occur in low-dimensional reconstructions with more than reasonable number of modes. A good example is the uncanny similarity of the right column of Figure 2.11 (reconstructed with 13 modes) and the first POD mode of the corresponding case in Figure 2.9.

The layout of this chapter is by introducing the method in Section 6.2 and then validating its assumptions in Section 6.3. Section 6.2 starts by deriving the relation between the distances and angle changes in the coefficient space to time difference and momentum of the instances in the physical space, respectively. Next, the methodology is developed, based on established rules, to find the most probable sequences in the low-dimensional space. To refine the sequences, a proper interpolation method is demonstrated to provide fine resolution of the transition between instances in a sequence. Then, Section 6.3 assesses the validity of the rules and provides the guidelines to maintain them in a low-dimensional space using the pipe and channel flow...
databases from Chapter 5. Finally, Section 6.4 uses the pipe flow simulation from Chapter 5 to assess the performance of the Sequencing method on time-resolved data with different sampling rates as well as comparing a sequence from independent set to time-resolved data.

### 6.2 Sequencing Method

To find the possible pathways between instances, first the relation between POD coefficients and the physics of the flow should be understood. Since sequences are built by incremental changes in the POD space, the difference between the coefficients of two instances will be the building block. As low-dimensional reconstruction is the multiplication of the coefficients and modes, so the difference in POD space is related to changes of velocity in physical space. The discretized momentum change ($\Delta P$) of a single measurement point can be written as:

$$\Delta P(x) \Delta t = \rho [u(t_1) - u(t_0)]$$

$$= \rho \sum_{n=1}^{N} [a_n(t_1) - a_n(t_0)] \phi_n(x)$$

For an incompressible flow, the magnitude of the momentum change over the whole domain can be calculated by integrating the dot product of the above equation by itself:

$$\int (\Delta P \cdot \Delta P) d^2x / \rho^2 = \int \sum_{n=1}^{N} [a_n(t_1) - a_n(t_0)] \phi_n \sum_{m=1}^{N} [a_m(t_1) - a_m(t_0)] \phi_m dx$$

$$= \int \sum_{n=1}^{N} \sum_{m=1}^{N} [a_n(t_1) - a_n(t_0)] [a_m(t_1) - a_m(t_0)] \phi_n \phi_m dx$$

$$= \sum_{n=1}^{N} \sum_{m=1}^{N} [a_n(t_1) - a_n(t_0)] [a_m(t_1) - a_m(t_0)] \int \phi_n \phi_m dx$$
Figure 6.1: Example of extracting low-dimensional dynamics from an under-sampled high-dimensional space.
The integral on the right hand side of the last equation reduces to Dirac’s delta so the equation can be simplified:

\[
\int (\Delta P \cdot \Delta P) \Delta t^2 / \rho^2 \, dx = \sum_{n=1}^{N} [a_n(t_1) - a_n(t_0)]^2 = \|A_i - A_j\|^2
\]  

(6.1)

Which shows the distance of two POD coefficients is related to the magnitude of the total momentum change in time. Hence, proximity of two instance in the POD coefficient space is a measure of their similarity. In other words, two snapshots with closer POD coefficients are more likely to occur sequentially than two snapshots that are further apart. This is, in fact, intuitive because POD transformation is only a unitary rotation.

The rate of the momentum change can be measured by projecting \(\Delta P\) of two successive instances onto each other:

\[
(\Delta P_{t_1} \cdot \Delta P_{t_0}) \Delta t^2 / \rho^2 = [u(t_1) - u(t_0)] \cdot [u(t_2) - u(t_1)]
= \sum_{n=1}^{N} [a_n(t_1) - a_n(t_0)] \phi_n \sum_{m=1}^{N} [a_m(t_2) - a_m(t_1)] \phi_m
= \sum_{n=1}^{N} \sum_{m=1}^{N} [a_n(t_1) - a_n(t_0)] [a_m(t_2) - a_m(t_1)] \phi_n \phi_m
\]

Averaging the momentum change over the whole domain, reduces the last term to Dirac’s Delta function:

\[
\frac{\int \Delta P_{t_1} \cdot \Delta P_{t_0} \Delta t^2 / \rho^2 \, dx}{\int \, dx} = \sum_{n=1}^{N} [a_n(t_1) - a_n(t_0)] [a_n(t_2) - a_n(t_1)]
\]

This can be normalized in vector form as:

\[
\frac{\int \Delta P_{t_1} \cdot \Delta P_{t_0} \, dx}{\sqrt{\int \Delta P_{t_1} \cdot \Delta P_{t_1} \, dx} \sqrt{\int \Delta P_{t_0} \cdot \Delta P_{t_0} \, dx}} = \frac{\|A(t_1) - A(t_0)\| \cdot [A(t_2) - A(t_1)]}{\|A(t_2) - A(t_1)\| \|A(t_1) - A(t_0)\|}
\]
Rewriting with indices of three sequential instances $i, j, m$:

$$\cos(\theta_{ijm}) = \frac{(A_j - A_i) \cdot (A_m - A_j)}{\|A_j - A_i\| \|A_m - A_j\|}$$  \hspace{1cm} (6.2)$$

So the angle formed by three POD coefficients is related to the average rate of momentum changes; the larger angle in coefficient space, the larger rate of average momentum changes. This angle should be close to zero for infinitesimal time steps.

For coarser time steps (yet fine enough to be considered time-resolved), it is safe to assume the changes of this angle over time are small and continuous. This criteria will be referred to as differentiability. The differentiability condition means if on average the flow is accelerating between two known instances in the sequence, the next logical instance is most likely one that maintains the same rate. If other instances with different rate of acceleration are physically possible, they will be collected by other sequences.

This criteria can be illustrated better using Figure 6.2. The plot is changes of one velocity component measured at one location over time. If points $i, j$ are the last two in a sequence and $m_1$ to $m_3$ are candidates of the next point, without a priori knowledge of the applied forces to the domain, it is safest to assume that the next point in the sequence is $m_3$. The other outcome of the differentiability condition is better insight into limitations of the angles in the coefficient space. Because of the time continuum, the next point of the sequence cannot be on the left hand side of the dotted line which limits the maximum angle in the coefficient space. In the case of infinitesimal time steps, a $180^\circ$ in Figure 6.2 at point $j$ means infinite force on the fluid element. Since equation 6.2 is averaged over the domain, such angle appears when all measurement points experience infinite force which is physically impossible.

The integration over the domain is beneficial in two more ways. The first, is the expected Probability Distribution Function (PDF) of both the distance and angles between the POD coefficients. The momentum change in every point can be
considered a random variable with arbitrary PDF. According to the Central Limit Theorem, summing all the random variables over the domain means the distance and angles between the subsequent instances is normally distribution. Second, if the flow has a homogeneous direction, the integrals on the left hand side of equations 6.2 and 6.1 are constant. So the distances and angles between subsequent instances in the coefficient space are constant in time.

The sequence starts by using the differentiability property at the surface of the confining hyper-ellipsoid. In the full space, the trajectory of a sequence is always tangential to the hyper-ellipsoid. A low-dimensional projection is still confined to a hyper-ellipsoid (imagine projecting points on a sphere to a 2D plane). Given there are adequate number of samples in the dataset to produce a meaningful sequence, at least one pathway should be tangential to the confining hyper-ellipsoid due to differentiability property. This is not satisfied only when a sequence is truncated by the confining manifold (time-resolved measurements have a starting point) which does not pose a problem to the Sequencing Method. Thus, the goal is to find two points near the confining hyper-ellipsoid.

To fulfill the established points, the sequence starts with a pair that meet three conditions. First, the average of the coefficient vector length should be as large
as possible to ensure they are close to the confining hyper-ellipsoid. Second, the difference between their coefficient vector length should be minimal to ensure they are tangential to the confining hyper-ellipsoid. Third, their distance should be as small as possible to satisfy the differentiability. To fortify the third condition and avoid outliers, the samples are filtered to retain only pairs that are mutually closest neighbors. Then all conditions are examined on instances $i$ and $j$ of a pair by their Energy-Measure (EM) defined as:

$$em_{ij} = \frac{\|a_i\| + \|a_j\|}{\epsilon + |\|a_i\| - \|a_j\||}$$

(6.3)

Each pair can be used to search for a sequence of instances as multiple contact points are possible. The first sequence uses the pair with the highest EM as it is closer to the ellipsoid boundaries. If a pair is collected by a sequence, it will not be used to start another sequence as it already is on a probable pathway. Other forms of EM can be defined but equation 6.3 proved to be both stable and computationally efficient.

Once the starting points of the sequence are found, then the next instance is a point in close proximity that satisfies the differentiability. The candidates are the $k$ closest instances to one end of the sequence which are not collected by it. As explained before, the angles between the candidates and the last two points should be similar to the angle between last three points in the sequence (reference angle). The measure of angle (equation 6.2) is most favorable at its highest, meanwhile the instances with smaller distance are preferred, so one measure should be mapped. Considering the better known restrictions on the cosine of the angle and its limited domain, its mapping will be used as a weight to distances. The mapping function should be large at unphysical $cos(\theta_{ijm}) = -1$ and minimum at the reference angle.
The selected function in this study is:

\[ w_d(x) = |x - \frac{1 + x_{ref}}{2}| + b \]

\[ w(x) = w_d e^{w_d^2} \] (6.4)

The bias \( b \) determines the strength of weighting. Naturally, \( x_{ref} = 1 \) at the start of the sequence. Since maintaining \( x_{ref} < 1 \) is unstable during many instances of the sequence, it is averaged with 1 in the weighting function. So the measuring factor of neighbor \( m \) is:

\[ d_w = ||A_j - A_m|| w(\cos(\theta_{ijm})) \] (6.5)

The neighbor instance which has the least weighted distance will be added to the sequence. The number of selected neighbors \( k \) is the square root of the number of samples \( \sqrt{S} \) as a general guideline from K Nearest Neighbors method [91].

The last piece is to stop the sequence appropriately when no proper candidate is available. Knowing the PDF of distances is normal, the search stops when the distance of the best candidate is larger than the 95 percentile distances of the \( k \) neighbor points (including the instances in the sequence).

To study the sequences, a smooth transition between the instances is necessary. Regardless of sample number, regions of the coefficient space attributed to rare events may not have sufficient samples to mimic a time-resolved transition. The most reasonable choice is interpolating based on time as it is the only independent variable of POD coefficients (equation 2.5 for space-only POD). For example if a PIV system has reasonably high sampling rate, then the time difference between two snapshots are known and can be used as interpolation parameter. In a sequence from non-time-resolved data, there is no information about time but the correspondence of time difference and distances in the POD space, as explained before, can be used. The length of the curve defined by the sequence in the coefficient space can be
considered as interpolation parameter. Suppose $A_i$ is the POD coefficient of instance $i$ in a sequence with $M$ instances ($i = 1, ..., M, \ M < S$), then the interpolation parameter can be calculated as:

$$\zeta_i = \begin{cases} 
\sum_{j=2}^{i} \| a_j - a_{j-1} \|, & i > 1 \\
0, & i = 0 
\end{cases} \quad (6.6)$$

If the measured field is stationary and has a homogeneous field, then interpolated instances mimic a measurement with constant time change. In flows with no homogeneous directions, the transition is perceptible but any time-related calculations are not reliable.

Due to the missing information in a non-time-resolved dataset, the Sequencing Method has its limitations which should be considered. The sequences cannot reveal the direction of temporal evolution. For example, a traveling wave might look as if it is propagating backward. Researchers must then choose a direction based on available information such as the velocity field or the movement of the structures. Also as a consequence of the stochastic nature of turbulence and dimensionality reduction, there can be multiple ways the flow reaches a certain instance in the low-dimensional space. Thus, the algorithm finds many sequences with possible overlaps. For an unbiased understanding of the energy transfer from a group of modes, all the sequences with overlapping instances should be studied.

The reader should be aware that the Sequencing Method only limits the physically possible transition between the instances, but neither all sequences are meaningful nor do they describe all the dynamics. As a simple example, consider two circles in a two-dimensional plane that are connected at a single point. The underlying dynamics can have a multitude of possibilities how the trajectory moves between the circles, but the method either sequences each circle individually with an overlap, or finds a single sequence that moves from one circle to the other only once.
The result of the Sequencing Method on the numerical test function are shown in Figure 6.3. The top plot shows the original test function in time without any noise which is desired to be acquired. The middle figure has shuffled instances to mimic a non-time-resolved measurement with added noise (as discussed in Chapter 4). Other sampling methods have also been used to simulate the non-time-resolved measurements, such as random, large time interval, and dropping random samples from a time-resolved dataset which showed similar success. Due to the perfect periodicity of the test function, sequencing result of all the sampling methods are the similar. The low-dimensional reconstruction of a sample sequence using 7 modes, shown in the third figure, illustrates the strength of the method when applied to a mechanism with perfect periodicity.

6.3 Assessment and Guidelines

Both fully developed pipe and channel flows have a homogeneous direction in the streamwise and cross-stream planes, so the distance and angle between consecutive instances of the time-resolved case should be constant based on Section 6.2. The distances of POD coefficients with different number of modes are fairly constant for pipe flow in the streamwise plane as shown in Figure 6.4. A straight line is not observed as the distances in the sampled data are sections of the discretized curve. Distances decrease in lower dimensions, needless to say, because the projected vectors have a smaller length than the original ones. The summary of both flows and planes in table 6.1 shows that the standard deviation increases in lower dimensions. Thereby, a reliable interpolation needs sufficient number of dimensions to calculate the interpolation parameter.

The next assessment is the constant angle in the POD coefficient space. As Figure 6.5 shows, the streamwise plane of the pipe flow supports the expectations
Figure 6.3: Sequencing of low-dimensional reconstruction of test function $u_5$. 

---

Original test function ($u_5$)

Added noise, shuffled

Sorted, low-dimensional
Figure 6.4: Distance between instances in original POD coefficient space of pipe flow in streamwise plane with different mode numbers.

Table 6.1: Distance of instances in POD coefficient space with different number of modes.

<table>
<thead>
<tr>
<th>modes</th>
<th>Pipe stream mean</th>
<th>std%</th>
<th>Pipe cross mean</th>
<th>std%</th>
<th>Channel stream mean</th>
<th>std%</th>
<th>Channel cross mean</th>
<th>std%</th>
</tr>
</thead>
<tbody>
<tr>
<td>all</td>
<td>0.62</td>
<td>9.4</td>
<td>0.23</td>
<td>9.1</td>
<td>0.027</td>
<td>8.3</td>
<td>0.020</td>
<td>8.2</td>
</tr>
<tr>
<td>p50</td>
<td>0.57</td>
<td>9.3</td>
<td>0.23</td>
<td>9.4</td>
<td>0.021</td>
<td>9.0</td>
<td>0.017</td>
<td>8.7</td>
</tr>
<tr>
<td>p95</td>
<td>0.47</td>
<td>10.2</td>
<td>0.21</td>
<td>10.0</td>
<td>0.013</td>
<td>10.8</td>
<td>0.012</td>
<td>10.0</td>
</tr>
<tr>
<td>p100</td>
<td>0.45</td>
<td>10.4</td>
<td>0.21</td>
<td>10.2</td>
<td>0.011</td>
<td>11.2</td>
<td>0.012</td>
<td>10.4</td>
</tr>
<tr>
<td>1-12</td>
<td>0.06</td>
<td>25.3</td>
<td>0.07</td>
<td>23.3</td>
<td>0.003</td>
<td>25.7</td>
<td>0.004</td>
<td>23.4</td>
</tr>
<tr>
<td>3-6</td>
<td>0.04</td>
<td>32.8</td>
<td>0.04</td>
<td>40.6</td>
<td>0.001</td>
<td>37.7</td>
<td>0.002</td>
<td>38.8</td>
</tr>
</tbody>
</table>
Figure 6.5: Angle change in POD coefficient space with fine (top) and coarse (bottom) time steps.

reasonably when time-resolved data are used, regardless of number of dimensions. The trajectory of the full-dimensional space has a constant concavity of about $\pi/6$. Decreasing the dimensionality leads to smaller angles which is desirable for the Sequencing Method. A slower sampling rate ($\Delta tU/D \approx 0.2$) increases the angle in the coefficient space, meaning the trajectory has circular behavior on the surface of the high-dimensional hyper-ellipsoid. Nonetheless, the angles are reasonably constant in lower dimensions.

The summary of the angles on both planes and flows in table 6.2 confirms the same behavior. The cosine of mean of angles increases in both planes by reducing the
dimensionality but the asymptotic value is smaller than 1 in the absence of traveling wave (cross-stream planes). Since with an infinitesimal time step, the angles should approach zero for any physical flow, it can be inferred that the current sampling rate is not sufficient for the cross-stream planes. The standard deviation of cosine of angles are reasonable unless the subspace is very small (3 modes). Requiring faster sampling rate is the cause of higher standard deviation in the cross-stream plane.

The effect of sampling rate on the cosine of angles, summarized in table 6.3, indicates that the more complex flows need larger number of samples for effective sequencing. The reported values are measured using all dimensions, except the last row where 12 modes are used with a sampling rate of $\Delta tu/D \approx 0.24$. The mean of cosine of angles decreases unfavorably but consistently in all cases by decreasing the sampling rate. Even so, the mean of cosine of angles is sufficiently high, with low STD, in the streamwise plane when 12 modes are used. Unfortunately, this is not the case for the cross-stream plane. The low mean and high STD suggests the trajectory of the coefficients of cross-stream planes are not as organized as the streamwise plane. In conclusion, the requirements of the Sequencing Method are satisfied better when traveling waves are present in the flow, otherwise a very high number of samples are required.

Assessment of interpolations has two steps; the extent of interpolation validity for different sampling rate, and effectiveness of POD distance as the interpolation parameter. The time-resolved data are under-sampled with three different sampling rates ($\Delta tU/D = 0.96, 1.93, 3.86$), then the intermediate instances are interpolated using time as the interpolation parameter (Figure 6.6). The interpolated data shows an acceptable consistency with the time-resolved coefficients when $\Delta tU/D = 0.96$. Sharp peaks and high frequency changes are lost in higher modes only occasionally. Sampling with two eddy-turn-over-time captures the general behavior of mode 6, and to some extent mode 19 but only retains the very low frequencies in mode
Table 6.2: Cosine of angle between three consecutive instances in POD coefficient space with different number of modes.

<table>
<thead>
<tr>
<th>modes</th>
<th>Pipe</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>stream</td>
<td>cross</td>
</tr>
<tr>
<td></td>
<td>mean</td>
<td>std%</td>
</tr>
<tr>
<td>all</td>
<td>0.86</td>
<td>0.6</td>
</tr>
<tr>
<td>p50</td>
<td>0.88</td>
<td>0.6</td>
</tr>
<tr>
<td>p95</td>
<td>0.90</td>
<td>0.7</td>
</tr>
<tr>
<td>p100</td>
<td>0.91</td>
<td>0.7</td>
</tr>
<tr>
<td>1-12</td>
<td>0.99</td>
<td>0.3</td>
</tr>
<tr>
<td>3-6</td>
<td>1.00</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Table 6.3: Cosine of angle between three consecutive instances in POD coefficient space with all modes and different temporal resolution. The last row has 12 modes with the sampling of the row above it.

<table>
<thead>
<tr>
<th>∆(tU/D)</th>
<th>Pipe</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>stream</td>
<td>cross</td>
</tr>
<tr>
<td></td>
<td>mean</td>
<td>std%</td>
</tr>
<tr>
<td>0.05</td>
<td>0.86</td>
<td>0.6</td>
</tr>
<tr>
<td>0.14</td>
<td>0.52</td>
<td>3.1</td>
</tr>
<tr>
<td>0.19</td>
<td>0.12</td>
<td>22.1</td>
</tr>
<tr>
<td>0.24</td>
<td>-0.2</td>
<td>17.6</td>
</tr>
<tr>
<td>1-12</td>
<td>0.89</td>
<td>4.1</td>
</tr>
</tbody>
</table>
12. The smallest sampling rate results in considerable aliasing of modes 6 and 19, and captures the low frequencies in mode 12. Although the coefficients of higher modes generally tend to have higher frequency behavior, the figure shows modes with closer energy content (beyond the uncertainty range) can exhibit unexpected behavior. Nonetheless, the reliability of interpolation decreases as the sampling rate is decreased which is corresponding to the distance of the coefficients in the POD space.

Next, the coefficient of mode 19 and sampling rate $\Delta tU/D = 1.93$ is estimated with different interpolation parameters (Figure 6.7). As mentioned in previous section, the best parameter is time but the distances in the coefficient space should also be equivalent. The correspondence of distance in coefficient space and time is proved when all the POD dimensions are used, but the figure shows the distance based on lower dimensions are also valid. The modes beyond p50 are dominated by noise omitting them has minimal effect on the distance. Using the distance in a sub-space with 19 modes as the interpolation parameter also has a tremendous consistency with time. In the span of the time-resolved dataset, only three peaks are misrepresented. Consistency of distances in sub-spaces and time as interpolation parameter validates that distance in POD space and time are corresponding, hence interpolation in POD space provides good enough approximation after Sequencing Method. It should be noted that if very small number of modes (such as 3) are used, then the correspondence is not reliable anymore. Thus even though the Sequencing Method might use only 4 modes, the interpolation should be calculated based on higher number of modes.
Figure 6.6: Interpolated POD coefficients of streamwise plane of pipe flow with spline method for different sampling rates ($tU/D$ is Eddy-turn-over time).
Figure 6.7: Interpolated time-resolved POD coefficients of mode 19 ($\Delta t U/D = 1.93$) by time, distance in 19 modes, and distance in P50 modes.

6.4 Validation

To validate the Sequencing Method, first it is applied to time-resolved pipe flow data which are under-sampled and then shuffled. Figures 6.8 to 6.11 illustrates the Sequencing Method results with 3, 6, 12, and 19 modes. Each row indicates one output of the Sequencing Method where the vertical bars and dots (best distinguishable at the top of the plots) are instances collected or excluded by the sequence, respectively. The color of bars indicates the order of the instances from dark blue at the start to yellow at the end while the true order is from left to right. Since the Sequencing Method is agnostic to the true order, the main objective is to find the correct sequence of instances, so a continuous color change in plot means successful sequencing. For example, the lowest row is the illustration of the original time-resolved data for reference which transitions smoothly from left to right. Each figure has 5 different sampling rates and only the five longest sequences are shown, when applicable. As the sampling rate decreases from bottom to top of each figure, the distance between the instances increase.

Considering the complexity of the fully turbulent pipe flow, 3 modes (Figure
6.8) is an example of inadequate number of modes for the Sequencing Method. Nevertheless, the shuffled time-resolved data are perfectly sequenced for much of the data as the second row from the bottom shows. As mentioned, the direction of the sequences are not detectable so the last portion of this case is reversed. Correct sequences have been found for considerable portions even for sampling rates as slow as $\Delta t U/D = 0.241$. Further under-sampling leads to sparse distribution in the sub-space which is insufficient for proper sequencing. Nonetheless, the method finds the correct order in small sections that span up to 5 eddy-turn-over-time.

The performance of the Sequencing Method is increased tremendously by using 6 or 12 modes (figures 6.9 and 6.10). The perfect sequence is found for sampling rates $\Delta t U/D = 0.048$ and 0.145 in both figures. Again, this sequence is reversed in Figure 6.9 but only the order of instances is of importance. Sequences with 6 modes and $\Delta t U/D = 0.241, 0.482$ are mostly correct but have discontinuities. The reason is that the low-dimensional projection of distant instances could be similar. Such similarities can be disentangled by increasing the dimensionality as confirmed by the perfect sequences with 12 modes. The effect of insufficient samples with the lowest sampling rate exacerbates by increasing dimensions, as is observable in both figures. The sampling rate $\Delta t U/D = 0.482$ does not have enough samples when 19 modes are used (Figure 6.11). Thus, smaller portions of the sequences are correct as compared with lower dimensions.

Proving the performance of the Sequencing Method for an independent dataset is a much more difficult task as there is no \textit{a priori} understanding of the general dynamics. To address this, a combination of the time-resolved and independent datasets are used. The coefficients of two consecutive instances which have high Energy-Ratio for the first 6 modes (Figure 5.8) are chosen from the time-resolved dataset and appended to the coefficients of the independent set to act as reference instances. Since the selected coefficients could be buried in the sub-space, they are
Figure 6.8: Sequencing time-resolved pipe flow data with 3 Modes and different sampling rates.
Figure 6.9: Sequencing time-resolved pipe flow data with 6 Modes and different sampling rates.
Figure 6.10: Sequencing time-resolved pipe flow data with 12 Modes and different sampling rates.
Figure 6.11: Sequencing time-resolved pipe flow data with 19 Modes and different sampling rates.
used as initial points for the Sequencing Method with the first 6 modes. Due to the chaotic nature of turbulent flows, the same event almost never occurs twice. Thus the expectation is not a perfect match, but similar dynamics occur between the time-resolved trajectory and sequenced instances in the vicinity of the reference instances. Figures 6.12 and 6.13 compare the time-resolved and sequenced POD coefficients for two different pairs of initial instances. The black dots are the output of the sequence while the other dots are from time-resolved set that are color coded with their ER. The black lines are splines interpolated to sequence outputs and the abscissa is centered on the first reference point. All the modes other than 2 and 4 show a very good agreement of the trend of coefficients for the first pair of initial points (Figure 6.12). The misrepresentation of mode 2 could be attributed to its low ER as indicated by its color. The wrong behavior of mode 4 is due to the independent nature of the modes near the top and lower wall which means similar combination of the structures near the opposite walls has not occurred in the independent dataset. As explained, this is inevitable due to the nature of turbulent flows.

The next set of initial points shows better performance (Figure 6.13). The sequence matches the time-resolved set in Modes 3, 5, and 6 very closely. The trend of sequenced instances emulates the correct trends but with different magnitudes. So the dynamics of the flow is captured but with wrong magnitudes. The interpolation of mode 1 is distorted due to the reference points. The low ER of mode 2 indicates its wrong trend is unimportant as it does not affect the total dynamics of the instances.

Comparing the low-dimensional reconstruction of this sequence with the reference set in Figure 6.14 illustrates the strength of the method better. Each row depicts the reference time-resolved instance and the corresponding interpolated reconstruction from the sequence. The interpolation parameter is calculated using p50 which is 731 modes. The structures near the upper wall are matched impeccably as their corresponding modes are 5 and 6 which have close levels and trends (Figure
6.13). The structures near the lower wall, which are dominantly tied to modes 3 and 4 (Figure 5.8), are presenting wrong trends up to $tU/D = -0.48$ due to the wrong level of mode 4 which is illustrated in Figure 6.13. The mitigated inaccuracy of mode 4 after the reference point is clear in the reconstruction of the instances. In summary, the Sequencing Method proved to be able to provide a meaningful sequence of instances from an independent dataset.

Lastly, the Sequencing Method has been applied to the non-time-resolved velocity measurements of turbulent jet flow outlined in chapter 2 to demonstrate the performance of the method in experimental measurements of a high Reynolds number flow. The Sequencing Method and reconstruction has been conducted with 12 modes, then the interpolation is refined iteratively until the total length of the n-dimensional trajectory is converged to less than 1%. For the sake of brevity, every fifth instance of the sequence are plotted in Figure 6.15 where the order is from left to right and top to bottom. Since the temporal information is lost, it is not possible to label the instances with pseudo-time labels like in Figure 6.14. The data is captured at sampling rate of 10 Hz, which is far from time-resolved, but the reconstructed instances show a physically plausible sequence with smooth transition between them. Although these measurements are at $x/D = 10$, there is some similarity to Citrinit and George’s [22] 138 simultaneous hot-wire POD investigation in the jet.

6.5 Conclusion

In conclusion, the Sequencing Method developed in this chapter provides a guideline to better analyze the underlying dynamics of independent datasets. The physical significance of the distances and angles in the POD coefficient space are presented analytically for the first time. The connection between the distances and angles of POD coefficients respectively with time difference and rate of momentum change is
Figure 6.12: Sequenced and time-resolved POD coefficients of first 6 modes of pipe flow. The reference instance is at $tU/D = 28$. 

184
Figure 6.13: Sequenced and time-resolved POD coefficients of first 6 modes of pipe flow. The reference instance is at $tU/D = 66$. 
Figure 6.14: Time-resolved and sequenced instances (with first 6 modes) from pipe flow. The reference instance is at $tU/D = 66$. 
Figure 6.14 (cont.): Time-resolved and sequenced instances (with first 6 modes) from pipe flow. The reference instance is at $tU/D = 66$.  

187
Figure 6.15: Sample sequence of streamwise velocity component of jet flow in cross-stream plane. The sequence has been down-sampled by showing one out of every 5 instances.
Figure 6.15 (cont.): Sample sequence of streamwise velocity component of jet flow in cross-stream plane. The sequence has been down-sampled by showing one out of every 5 instances.
used along with the basic properties of POD to develop the Sequencing Method. The developed method provides probable transition between independent instances in a low-dimensional space that sheds lights on the underlying dynamics of the system. The performance of the method is tested using two different approaches. The under-sampled time-resolved data were sequenced perfectly when the proper number of modes is used. A portion of the time-resolved velocity field was successfully reproduced from independent dataset.

The parametric interpolation method can be used in semi-time-resolved data as well as to refine the sequences. Modern experimental setups such as time-resolved PIV that can provide a refined temporal sampling are limited to very small spaces in addition to their high cost. Although, cheaper systems, capable of high sampling rate, are becoming more popular, there will always be a limit on sampling speeds, as higher Reynolds numbers and more complicated flows are explored. The interpolation method can be used for this temporally coarse data to yield a better transition between instances. More importantly, the connection between distances in POD space and time differences provides an interpolation parameter to refine the sequences from independent dataset where the temporal information are non-existent.
Chapter 7

Conclusion

The objectives of this thesis was to revisit the concepts and develop guidelines or methodologies for a better understanding of POD analysis\(^1\). The kernel choice and equivalency of POD and the Fourier decomposition in the homogeneous direction are examined rigorously to determine proper practices. Guidelines for the cut-off mode number are introduced in the context of fluid mechanics and new criteria were developed to filter proper instances in a low-dimensional space. The behavior of POD modes with respect to traveling waves are analyzed to prepare the ground for reliable detection methods which can capture multi-modal interactions. The performance of traveling wave criteria is enhanced when the original POD modes are corrected to have better locality. Finally, a novel Sequencing Method was developed to find physically plausible sequences of instances in the low-dimensional space with meaningful transition between them.

A general form of the base matrix was developed to embed the inner product of the space into the data. The advantage is that the Jacobian of the coordinate system or quadrature of the grid will no longer complicate the application of different variations. This is of paramount importance as many advanced extensions of POD

\(^1\)The Python source code and modules for the first 5 chapters are available at https://github.com/Mahdi-Hosseinali/pyPOD
are developed in other fields without consideration of such matrices. So efficient numerical packages (often open source) can be used in the fluid mechanics context with minimal effort.

The base matrix could be defined in many ways, the most two common being scalar and vectorial. The scalar kernel is no longer as popular, thanks to the computational power of modern computers and improved instrumentation, but has been used in much previous research. Thus it is important to know the limitations of each kernel. The analytical analysis of the right kernels formed by each choice shows that modes and, to a lesser degree, reconstructions of the scalar kernel are coordinate system dependent as well as been affected by interpolation. On the other hand, the vectorial kernel is invariant under coordinate system transformation and less susceptible to errors of interpolation. If modes and reconstructions are used to enable the understanding of coherent structures, they should be coordinate system invariant like the structures. The vectorial kernel should be used when possible, and the change of coordinate system or interpolation should be avoided as they either introduce no better insight or affect the kinetic energy of the system.

Another common choice of implementation in the POD process is using Fourier-POD in the presence of homogeneous directions instead of applying POD to all dimensions. It was shown by the analytical POD solution of an analytical test function that the equivalence of POD and Fourier transform is not always true in a finite domain. Despite the validity of Fourier transform in the homogeneous direction, it leads to many practical difficulties which can be avoided by using a full dimensional POD. The most important problem with Fourier-POD is the inconsistency of the kernels which is scalar in the Fourier transform and almost always vectorial in POD. As proved, the scalar modes are not the best representations of physical structures, so POD analysis on such unsound grounds is not the most suitable choice. This can be avoided by using vectorial and modified base matrix which is invariant to
coordinate systems and easy to implement.

The development of new methods for proper and easy interpretation of the POD modes and their reconstruction is one of the main outcomes of this thesis. Understanding the underlying dynamics of the flow using any decomposition method has two steps; selection of the low-dimensional space and best instances to represent the dynamics. However, these two are hardly separable as all the modes representing moving structures should be retained in the low-dimensional space. The Frequency and Derivative Criteria, developed here, are successful in finding such groups of modes. Furthermore, the eigenvalue uncertainty and ICA are used to reduce the degeneracy and produce modes with enhanced locality. This post-processing of the modes generated better perception of traveling waves by more understandable interactions between modes. Despite the outstanding improvement, the Modal Correction is open for further research. The Monte-Carlo and rule-N methods provide a basis to discard the modes dominated by noise which is helpful when structures are dominant. Additionally, the Denoising Technique is developed that can be used when a selected subspace is over-sampled.

Lastly, the Energy-Ratio and the Sequencing Method are developed as alternatives to the previously random selection of the low-dimensionally reconstructed realizations. The ER is an instantaneous measure of retained dynamics in the low-dimensional space. The ER is substantial because it excludes the instances which have lost most of their dynamics in the low-dimensional reconstruction, and also can show if a high mode number has dynamical significance. Additionally, the application of ER on groups of traveling waves after Modal Correction, provides a fast and reliable measure to find the best instances of a time-resolved data where the desired modes are interacting. For non-time-resolved datasets, the developed Sequencing Method finds the most probable sequences that could be extracted from the data. To understand the transition between instances, the proper selection of
the interpolation parameter was also examined.

As a final remark, the developed methods improve our ability to extract, and ultimately to better understand coherent structures, but the techniques are not necessarily limited to the context of fluid mechanics. For example, the modified base matrix should be used in dimensional reduction of any dataset measured on physical points. The Denoising Technique can be applied to large datasets to produce a tractable set for faster exploratory data analysis and development of initial models. The ER can be used by any other decomposition method such as the Fourier transform. The traveling wave criteria discovers the dependencies in any temporal signals such as stock market price fluctuations. The Modal Correction method follows the eigenvalue based problems regardless of the kernel definition (such as advective mode decomposition). Finally, the Sequencing Method provides a ground to understand the progressive dynamics of any dataset that has reasonable number of samples of repetitive events such as medical images or recommender systems.
Chapter 8

Future Work

This chapter is a summary of possible further improvement of the developed methods. Further progress could be attained by revisiting the fundamental equations of POD deeper than in this thesis. The increasing popularity of high fidelity numerical simulations provide a tremendous amount of data, such as simultaneous pressure and velocity field. Although a vast amount of research has been dedicated to POD analysis on pressure, it has never been coupled with velocity in POD analysis. The recommendation is to investigate the possibility of using pressure as the forcing function in the Fredholm integral (equation 2.2).

The application of rule-N to spatially dense datasets is straightforward, but the effective number of samples in spatially sparse datasets could be improved. The fast sampling rate of modern acquisition systems can produce a large amount of data in a short period of time, so datasets of size $O(10^4)$ statistically independent samples are very common. As a result, the uncertainty ranges become negligible and the Monte-Carlo band collapses to a line. However, it is unlikely that few spatial point can have such large amount of numerically independent samples with underlying dynamics. The methods in Section 4.3 finds the effective sample size only when two successive samples are correlated. The recommendation is iterative use of the
Denoising Technique and Monte-Carlo to ensure all samples are truly independent.

The performance of the correction method in Chapter 5 is reasonable, but requires further refinement. The simplest improvement is the definition of the eigenvalue uncertainty. Currently, it only factors in the sampling uncertainty but not any other sources. The instrumental and system uncertainty should also be included. Isolating the groups of modes for ICA is not very reliable in higher modes so other methods should also be examined. Finally, a better rotation of each corrected mode group could be found using the coefficients.

Further understanding of modal interactions using the Derivative Criteria outlined in Chapter 5 is also possible. Since the method is based on the idea of Granger-Causality, an analytical relation between DC and Granger-Causality should be possible. The asymmetric and negative signs of the association map could shed more light in the direction of energy transfer. Lastly, with proper analysis, the convection speed of structures could be measured using the convex of their phase plot which would be more informative than convection speeds measured using two-point cross-correlations.

The traveling wave criteria developed herein are capable of finding convective and beating structures but their performance in absolute instability remains unknown. Further work that examines the ability of the method in this context can be constructive for future developments.

Many improvements could be developed in the Sequencing Method. As of now, there is no \textit{a priori} information about the proper number of modes or if the number of samples are adequate for such subspace. A methodological examination of the overlap in sequences would be a major improvement. Finally, the cosine of the angle of POD coefficients filters the data to a cone, other methods to satisfy the differentiability method should also be investigated.
Bibliography


213


Appendix A

Coordinate System

Transformation Example

Section 2.5 analytically proves that the scalar kernel is coordinate system dependent, while the vectorial kernel is invariant (for any isometric transformation). This appendix is a simpler example of transformation from Cartesian to polar coordinates. The Cartesian velocity components can be converted to polar coordinate system as:

\[
\begin{align*}
    u_r &= +u \cos(\alpha) + v \sin(\alpha) \\
    u_\theta &= -u \sin(\alpha) + v \cos(\alpha) \\
    u_z &= w
\end{align*}
\]

Here, \(u, v, w\) are the Cartesian velocity components, \(u_r, u_\theta, u_z\) are the polar velocity components, and \(\alpha\) is the angle between the radial axis of the polar coordinates and the horizontal axis of the Cartesian coordinates. A single element of the vectorial auto-correlation kernel (kernel of the Method of Snapshots) in Cartesian and polar
coordinates is defined as:

\[ K(x, y, z) = \Sigma_{i=1}^{N} [u^i u^j + v^i v^j + w^i w^j] \]

\[ K(\theta, r, z) = \Sigma_{i=1}^{N} [u^r u^j + u^\theta u^\theta + w^i w^j] \]

Proving that each term of the summation are equal for both kernels means that all the modes, coefficients, eigenvalues, and reconstructions are invariant of coordinate system.

\[
\begin{align*}
&u^i r^i + u^\theta u^\theta + w^i w^j = [u^i \cos(\alpha) + v^i \sin(\alpha)] [u^j \cos(\alpha) + v^j \sin(\alpha)] \\
&\quad + [u^i \sin(\alpha) + v^i \cos(\alpha)] [-u^j \sin(\alpha) + v^j \cos(\alpha)] \\
&\quad + w^i w^j \\
&= [u^i u^j \cos^2(\alpha) + v^i v^j \sin^2(\alpha) + (u^i v^j + v^i u^j) \sin(\alpha) \cos(\alpha)] \\
&\quad + [u^i u^j \sin^2(\alpha) + v^i v^j \cos^2(\alpha) - (u^i v^j + v^i u^j) \sin(\alpha) \cos(\alpha)] \\
&\quad + [w^i w^j] \\
&= [u^i u^j + v^i v^j](\sin^2(\alpha) + \cos^2(\alpha)) \\
&\quad + \sin(\alpha) \cos(\alpha)[(u^i v^j + v^i u^j) - (u^i v^j + v^i u^j)] \\
&\quad + w^i w^j \\
&= u^i u^j + v^i v^j + w^i w^j
\end{align*}
\]

Which shows that the vectorial auto-correlation kernel is independent of the coordinate system. In the case of the scalar kernel, the terms of the summations for the kernel definition of each scalar are the three underlined equations, where the transformation coefficients \( \sin(\alpha), \cos(\alpha) \) are not canceled. So the scalar kernels and
subsequently modes, coefficients, eigenvalues, and reconstructions will be coordinate system dependent. In simple language, the summation terms of the vectorial kernel are the inner product of physical vectors, so the value is independent of the coordinate system. However, the inner products are calculated only on a projection in the case of the scalar kernel which is dependent on the coordinate system and not physical.
Appendix B

Analytical Solution of Fredholm Integral Equation

B.1 Solution Method

The Fredholm integral equation (2.3) will be solved analytically by the use of kernel degeneracy [156]. A degenerate kernel can be expressed as a sum of multiplications separated by each dimension:

\[ K(x, x') = \sum_j m_j(x)n_j(x') \]

replacing the degenerate form in the Fredholm integral equation 2.2, reordering the summation and integral, and moving the \( x' \) invariant term outside of the integration yields:

\[ \lambda \psi = \sum_j m_j(x) \int n_j(x')\psi(x')dx' \quad (B.1) \]

The integrals can be solved analytically:

\[ c_j = \int n_j(x')\psi(x')dx' \quad (B.2) \]
Replacing \( c_j \) constants into equation B.1 shows that eigenfunctions can be expressed as a sum:

\[
\lambda \psi(x) = \sum_j c_j m_j(x)
\]  

(B.3)

Changing the dummy index of B.3 and replacing it into equation B.2, then changing the order of summation and integration results in:

\[
\lambda c_i = \sum_j c_j a_{ij}
\]

\[
a_{ij} = \int m_i(x)n_j(x)dx
\]

which is a linear system of eigenfunctions and can be solved analytically. Substituting the eigenfunctions of this system in equation B.3 determines the eigenfunctions of the system.

Averaging the kernel over the samples can be achieved analytically by temporal integration, so the kernel will be:

\[
K(x, x') = \int_t u(x, t)u(x', t)dt
\]

Averaging over the blocks that have same period as every term of the test functions result in the same function. Block lengths other than an integer multiplication of the test function’s period leads to the windowing effect explained in Chapter 3. Since the focus of the study is not the windowing effect, the former will be used. The Fourier transform of Fung’s estimation 3.1 in time has the general form:

\[
F[u(x, t)](x, \omega) = \sum_{n=-N}^{N} \sum_{p=-P}^{P} S_{n,p} \exp i(k_n x)[\delta(\omega - m) + \delta(\omega + m)]
\]

where \( S_{n,p} = A_{n,p} + iB_{n,p} \) is the complex form of the original equation 3.1 and \( \delta \) is
Dirac’s delta function. Finally POD will be solved for every $\omega = \pm m$ individually:

$$K(x, x', m) = \sum_{n=-N}^{N} S_{n,p} \exp(i k_n x) \sum_{q=-N}^{N} S_{q,p} \exp(-i k_m x)$$

$$\sum_{n=-N}^{N} \sum_{q=-N}^{N} S_{q,p} S_{n,p} \exp(i k_q x) \exp(-i k_n x)$$

### B.2 Solution of Test Functions

The following are the time-averaged kernel solution for all the test functions and POD-Fourier in space and time for test function $u3$ only. For simplicity the dummy variable $x'$ has been replaced to $y$ in the kernel definition.

Solution of test function $u1$ (3.2):

$$K(x, y) = \sin(ax) \sin(ay) + \cos(ax) \cos(ay)$$

$$m_j = \left[ \begin{array}{c} \sin(ax) \\ \cos(ax) \end{array} \right], n_j = \left[ \begin{array}{c} \sin(ax) \\ \cos(ax) \end{array} \right], a_{ij} = \left[ \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right]$$

$$\Lambda = \left[ \begin{array}{c} 1 \\ 1 \end{array} \right], \quad \phi = \left[ \begin{array}{c} \sin(ax) \\ \cos(ax) \end{array} \right]$$

Solution of test function $u2$ (3.3):

$$K(x, y) = c^2 \cos(a(x-y)) + 2c \sin(a(x+y)) + \cos(a(x-y))$$

$$m_j = \left[ \begin{array}{c} \sin(ax) \\ \cos(ax) \end{array} \right], n_j = \left[ \begin{array}{c} c^2 \sin(ax) + 2c \cos(ax) + \sin(ax) \\ c^2 \cos(ax) + 2c \sin(ax) + \cos(ax) \end{array} \right], a_{ij} = \left[ \begin{array}{cc} c^2 + 1 & 2c \\ 2c & c^2 + 1 \end{array} \right]$$

$$\Lambda = \left[ \begin{array}{c} (c + 1)^2 \\ (c - 1)^2 \end{array} \right], \quad \phi = \left[ \begin{array}{c} \sin(ax) + \cos(ax) \\ \sin(ax) - \cos(ax) \end{array} \right]$$
Time averaged solution of test function $u_3$ (3.4):

$$K(x, y) = 2c \sin (a (x + y)) + 2d \sin (b (x + y))$$

$$+ (c + d) (\sin (ax + by) + \sin (ay + bx))$$

$$+ (c^2 + 1) \cos (a (x - y)) + (d^2 + 1) \cos (b (x - y))$$

$$+ (cd + 1) (\cos (ax - by) + \cos (ay - bx))$$

$$m_j = \begin{bmatrix} \sin (ax) \\ \cos (ax) \end{bmatrix},$$

$$n_j = \begin{bmatrix} 2c \cos (ax) + (c + d) \cos (bx) + (c^2 + 1) \sin (ax) + (cd + 1) \sin (bx) \\ 2d \cos (bx) + (c + d) \cos (ax) + (d^2 + 1) \sin (bx) + (cd + 1) \sin (ax) \\ 2c \sin (ax) + (c + d) \sin (bx) + (c^2 + 1) \cos (ax) + (cd + 1) \cos (bx) \\ 2d \sin (bx) + (c + d) \sin (ax) + (d^2 + 1) \cos (bx) + (cd + 1) \cos (ax) \end{bmatrix}$$

$$a_{ij} = \begin{bmatrix} c^2 + 1 & cd + 1 & 2c & c + d \\ cd + 1 & d^2 + 1 & c + d & 2d \\ 2c & c + d & c^2 + 1 & cd + 1 \\ c + d & 2d & cd + 1 & d^2 + 1 \end{bmatrix}$$

$$\Lambda = \begin{bmatrix} (c + 1)^2 + (d + 1)^2 \\ (c - 1)^2 + (d - 1)^2 \end{bmatrix}, \quad \phi = \begin{bmatrix} \frac{c-1}{d-1} [\cos(ax) - \sin(ax)] + \cos(bx) - \sin(bx) \\ \frac{c+1}{d+1} [\cos(ax) + \sin(ax)] + \cos(bx) + \sin(bx) \end{bmatrix}$$

Even though $m_j, n_j$ have four elements, two of the eigenvalues of $a_{ij}$ are zero which reduces the degree of freedom of this matrix.
Solution of test function $u_4 (3.5)$:

$$K(x, y) = 2c \sin (a (x + y)) + 2d \sin (b (x + y))$$
$$+ (c^2 + 1) \cos (a (x - y)) + (d^2 + 1) \cos (b (x - y))$$

$$m_j = \begin{bmatrix} \sin (ax) \\ \cos (ax) \end{bmatrix}, n_j = \begin{bmatrix} 2c \cos (ax) + (c^2 + 1) \sin (ax) \\ 2d \cos (bx) + (d^2 + 1) \sin (bx) \\ 2c \sin (ax) + (c^2 + 1) \cos (ax) \\ 2d \sin (bx) + (d^2 + 1) \cos (bx) \end{bmatrix},$$

$$a_{ij} = \begin{bmatrix} c^2 + 1 & 0 & 2c & 0 \\ 0 & d^2 + 1 & 0 & 2d \\ 2c & 0 & c^2 + 1 & 0 \\ 0 & 2d & 0 & d^2 + 1 \end{bmatrix},$$

$$\Lambda = \begin{bmatrix} (c + 1)^2 \\ (d + 1)^2 \\ (c - 1)^2 \\ (d - 1)^2 \end{bmatrix}, \quad \phi = \begin{bmatrix} \sin(ax) + \cos(ax) \\ \sin(bx) + \cos(bx) \\ \sin(ax) - \cos(ax) \\ \sin(bx) - \cos(bx) \end{bmatrix}.$$
Fourier modes are:

\[
K(x, y) \bigg|_{\omega = 1} = c^2 e^{-ia(x-y)} + d^2 e^{-ib(x-y)} + cd \left( e^{i(ax+by)} + e^{i(ay-bx)} \right) \\
+ c \left( e^{i(-ax-by)} + e^{i(ay-bx)} \right) + d \left( e^{i(ax+by)} + e^{-i(ay+bx)} \right) \\
+ e^{i(ax-by)} + e^{i(-ay+bx)} + c \left( e^{i(x-y)} + e^{ib(x-y)} \right) \\
+ 2d \cos(b(x + y)) + 2c \cos(a(x + y))
\]

\[
K(x, y) \bigg|_{\omega = -1} = c^2 e^{-ia(x-y)} + d^2 e^{-ib(x-y)} + cd \left( e^{i(ax+by)} + e^{i(ay-bx)} \right) \\
- c \left( e^{-i(ax+by)} + e^{i(ay-bx)} \right) + d \left( e^{i(ax+by)} + e^{i(ay-bx)} \right) \\
+ e^{ia(x-y)} + e^{ib(x-y)} - e^{i(ax-by)} - e^{i(by-ax)} \\
+ 2c \cos(a(x + y)) - 2d \cos(b(x + y))
\]

The separated parts of the kernel and the respective coefficient matrix are omitted for brevity. The eigenvalues of negative and positive kernel are equal and the corresponding eigenfunctions are complex.

\[
\lambda_{-\omega, \omega} = 2 \left( c^2 + d^2 + 2 \right)
\]

\[
\phi_{\omega} = \frac{2 \cos (ax)}{d + 1} \frac{d}{d + 1} \left( c + 1 \right) + 2 \cos (bx) + \frac{2i \sin (ax)}{d + 1} \frac{d}{d + 1} \left( 1 - c \right) + \frac{2i \sin (bx)}{d + 1} \frac{d}{d + 1} \left( 1 - d \right)
\]

\[
\phi_{-\omega} = \frac{2 \cos (ax)}{d - 1} \frac{d}{d - 1} \left( c + 1 \right) + 2 \cos (bx) + \frac{2i \sin (ax)}{d - 1} \frac{d}{d - 1} \left( 1 - c \right) - \frac{2i \sin (bx)}{d - 1} \frac{d}{d - 1} \left( 1 + d \right)
\]
Appendix C

Discrete Fourier Transform of a Normal Random Variable

This derivation is taken from an answer on dsp.stackexchange.com provided by DanielSank. Three basic properties of random variables are used: The probability distribution of a scaled random variable ($Y = aX$) is:

$$P_Y(y) = \frac{1}{a}P_X(y/a)$$  \hspace{1cm} (C.1)

PDF of sum of random variables ($Z = X + Y$) is the convolution of their PDFs:

$$P_Z(z) = (P_X \otimes P_Y)(z)$$  \hspace{1cm} (C.2)

Fourier transform of convolution is equal to multiplication of Fourier transforms:

$$\int (f \otimes g)(x)e^{-ikx}dx = \left(\int f(x)e^{-ikx}dx\right)\left(\int g(x)e^{-ikx}dx\right)$$  \hspace{1cm} (C.3)

The sequence of the sampled noise ($x_n$) is assumed to be uncorrelated and has Gaussian distribution for every sample with standard deviation $\sigma$, so its PDF is
denoted as \( P_{x_n}(x) = G_\sigma \). Discrete Fourier Transform (DFT) of the series is:

\[
X_k = \frac{1}{N} \sum_{n=0}^{N-1} x_n e^{-i2\pi nk/N} \tag{C.4}
\]

Considering only the real part:

\[
\Re X_k = \frac{1}{N} \sum_{n=0}^{N-1} x_n \cos(2\pi nk/N) \tag{C.5}
\]

The cosine function is a deterministic coefficient on each term, so using equation C.1 it can be simplified as:

\[
y_n = \frac{x_n}{N} \cos(2\pi nk/N)
\]

\[
P_{y_n}(y) = \frac{N}{\cos(2\pi nk/N)} G_\sigma \left( \frac{yN}{\cos(2\pi nk/N)} \right) = G_{\sigma c_{n,k}/N}(y)
\]

\[
c_{n,k} \equiv \cos(2\pi nk/N)
\]

Using above and the second rule (C.2), the PDF of the real part of the transformation (equation C.5) can be rewritten as:

\[
P_{\Re X_k}(x) = (G_{\sigma c_{0,k}} \otimes G_{\sigma c_{1,k}} \cdots \otimes G_{\sigma c_{N-1,k}})(x)
\]

The multiple convolution is not possible to be done in its current form, so rule 3 (equation C.3) will be used, noting the Fourier transform of a Gaussian function is
also Gaussian with width $1/\sigma$:

\[
F(P_{RX_k})(\nu) = \Pi_{n=0}^{N-1} F(G_{\sigma c_{n,k}/N})
\]

\[
= \Pi_{n=0}^{N-1} G_{N/\sigma c_{n,k}}
\]

\[
= \Pi_{n=0}^{N-1} \sqrt{\frac{\sigma^2 c_{n,k}^2}{2\pi N^2}} \exp \left[ -\frac{\nu^2}{2(N^2/\sigma^2 c_{n,k}^2)} \right]
\]

\[
= \left( \frac{\sigma^2}{2\pi N^2} \right)^{N/2} \left( \Pi_{n=0}^{N-1} c_{n,k} \right) \exp \left[ -\frac{\nu^2}{2N^2 \sigma^2 \Sigma_{n=0}^{N-1} c_{n,k}^2} \right]
\]

The coefficients of the exponential function are independent of $\nu$ and act as a normalization factor. Also the sum inside the exponential is $N/2$, so the simplified equation can be written as:

\[
F(P_{RX_k})(\nu) \propto \exp \left[ -\frac{\nu^2}{2N} \frac{1}{\sigma^2} \right]
\]

\[
= G \sqrt{2N/\sigma^2}
\]

therefore:

\[
P_{RX_k} = G \sigma / \sqrt{2N}
\]
Appendix D

Jacobian Matrix for Cloud of Points

The area related to each point is calculated by first triangulating the cloud of data points for example using Delauny method\(^1\). The triangles which are outside of the domain (centroids are average of points) should be removed in case of concave field. Next, the circumcenter of each triangle is calculated which is the intersection of the bisection of edges\(^2\). Then the area contributed to each node is the sum of two triangles formed by edge bisection point, corner, and circumcenter as show in figure D.1. The area could be calculated by the outer product of the vectors which connects the corner to circumcenter and bisection\(^3\). The vectorial notation does not need any further consideration when the circumcenter is outside or on the edges. For example, the area contributed to node 0 is:

\(^1\)\text{tris} = \text{pyPOD.utilities.triangulatePoints(ps)} \text{ where ps is an array of points with each dimension as a column.}

\(^2\)This step is done in the module automatically.

\(^3\)\text{Q} = \text{pyPOD.utilities.calcA(ps, tris)} \text{ where Q is the coefficient matrix regardless of the coordinate system.}
Figure D.1: Annotation of triangle to calculate area contributed to each node.

\[ A_0 = \frac{1}{2} \frac{d_{20}}{2} \times d_{c0} + \frac{1}{2} \frac{d_{01}}{2} \times d_{c0} \]

\[ = \frac{d_{20} \times d_{c0} + d_{01} \times d_{c0}}{4} \]
Vita

Candidate’s full name: Mahdi Hosseinali

Universities attended:
B.Sc. of Mechanical Engineering in Heat Transfer and Fluid Flow from University of Tabriz: 2004-2009
M.Sc. of Mechanical Engineering in Thermo Fluids from AmirKabir University of Technology: 2010-2013

Publications:
M. Hosseinali, S. Wilkins, A.A. Akbari, G. Holloway, J.W. Hall, “POD Analysis of Flow Behind a Four-Wing Vortex Generator”, APS March meeting, 2015, Boston, USA.
M. Hosseinali, J.W. Hall, “Revisit on Proper Orthogonal Decomposition Methods Classic-Snapshot”, APS March meeting, 2015, Boston, USA.