Exploratory Data Analysis of Turbulent Flows

Using Proper Orthogonal Decomposition and Dynamic Mode Decomposition.

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Abstract— **Large Eddy Simulations (LES) contains 3D instantaneous velocity fields as well as passive scalar concentration field describing the coherent flow structures. The study of coherent flow structures has a major impact on the mixing of the fuel and the oxidizer. The analysis of these structures in a turbulent jet is essential in understanding the fundamentals of fluid dynamics. Therefore there is a need for methods that can identify and analyze these structures. In this paper, we use machine-learning methods such as Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD) to analyze the coherent flow structures. We used 2D LES of subsonic jets as our data, with Reynolds number corresponding to Re: 6000 (low pressure) , 10,000 (medium pressure), and 13,000 (high pressure). Results for POD modes and DMD modes are discussed and compared.**

Keywords- POD, DMD, Proper Orthogonal Decomposition, Dynamic Mode Decomposition, LES, Turbulence.

I. Introduction

Today one of the major problems of oil based energy and transport sectors is exhaust gas emissions. Re- searchers are searching for ways to reduce the emission. Therefore, alternative fuels such as Natural Gas (NG) are of great interest. However, the shift from oil based fuels to alternative fuels takes several decades. Therefore, further research is needed on the Internal Combustion Engine (ICE). ICE is involved with extreme fluid velocities. Hence the Reynolds number of the flow is also substantial indicating the presence of turbulence. In fluid dynamics, turbulence or turbulent flow is a flow regime characterized by chaotic and stochastic fluid property changes. This includes low momentum diffusion, high momentum convection, and a rapid variation of pressure and velocity in space and time. In other words, turbulent flows are characterized by fluctuating velocity fields. These fluctuations mix transported quantities such as momentum, energy, and species concentration. Turbulence plays an important role when modeling the combustion process in the combustion chamber.

To gain a deeper understanding on combustion process and turbulence, machine-learning methods can be utilized. This field allows computers to adopt behaviors based on training data. These methods recognizes complex patterns and makes intelligent decisions based on data [2]. This techniques include: reduced order models or dimensionality reduction methods, statistical, and machine vision methods. Dimensionality reduction is a technique used to find a reduced order model on a given data. Such a technique includes feature selection and feature extraction methods. Feature selection is based on selecting a subset of variables which best define the data, whereas feature extraction transforms the data from high-dimensional space to a space of fewer dimensions [2]. The data transformation may be linear, as in Proper Orthogonal Decomposition (POD) [7] and Dynamic Mode Decomposition (DMD) [10] [8].

From the literature, it is expected that POD and DMD would be good methods for analyzing the flow structures. For example, a paper by Perrin et. al [7] used POD to obtain phase averaged turbulence properties for flow past a cylinder. In highly turbulent flows, the coherent flow structures are difficult to identify due to the combination of organized and chaotic fluctuating motions. Using POD analysis it is shown in [4], that von Karman vortices can be reproduced within the first few modes. POD has been used as a tool for the comparison of Particle Image Velocimetry (PIV) and Light Eddy Simulation(LES) data in [5] and it is also shown that POD modes have a good qualitative agreement between PIV and LES. A paper by Schmidt et. al [9], used DMD to a sequence of flow images of a slow jet entering quiescent fluid showcased the detection of dynamically relevant coherent structures that play an important role in characterizing the fluid behavior over processed time interval.

To identify the coherent flow structures caused by the turbulence, we study 3 cases of Large Eddy Simulations (LES) of subsonic jets with Reynolds number corresponding to Re: 6000, 10,000, and 13,000. LES is a novel numerical method that can be used to carry out the fluid dynamics simulations of turbulent flows using fine numerical resolution. By utilizing LES, a highly realistic turbulent fluid dynamics can be produced. The secret lies in the high level accuracy of the LES method. Hence coherent flow structures as seen in the experiments can be reproduced in simulations. The purpose of the simulations is to shed further light into the mixing process of Natural Gas (NG) and air. A long standing problem in this kind of simulations is the random and strongly transient nature of the jet data. The randomness of the data hides the underlying coherent flow structures of the jet which are expected to be of importance when trying to explain the jet behavior and possible cycle to cycle variations in Direct Injection (DI) NG engines. It is worth to do POD and DMD analysis and there by shed further light into this problem. These simulations were carried out by V.Vuorinen and the simulations are described in [12]. The motivation for this simulations lies in ICE applications where NG, i.e Methane (C H4) is considered to be the best alternative fuel for conventional diesel fuels. There are advantages and disadvantages in using NG. Advantages may be significant reduction of N Ox and soot emissions which are the most unwanted diesel emissions. The disadvantages are considered very harmful to the environment as the incomplete combustion of NG releases CH_4 into the atmosphere which is a harmful greenhouse gas. The experiments study the role of the injection pressure in the jet mixing. The simulations carried out by V.Vuorinen show that the turbulent structures in the beginning of the simulations produce a rolling tip vortex and also a growing Kelvin-Helmholz instability and at the later time the initially laminar flow becomes turbulent.

The objectives of the paper is as follows:

- POD and DMD is implemented with Matlab and used to analyze LES of subsonic data.
- The potential of POD and DMD in the ICE applications is shown.
- Results for POD and DMD are discussed and compared. The organization of this report is as follows:

In section 2 we study the computational methods for POD and DMD. Section 3 deals with the experiments and implementation details. Finally, conclusions are drawn and further research directions are discussed in section 4. This section is a part of the paper written for ICLASS conference [14].

II. Computational Methods

In this section we study about KLD, POD and DMD methods.

A. The Karhunen-Loeve Decomposition (KLD)

POD is known by various names like KLD, Principle Componant Analysis (PCA) and Singular Value Decompostion (SVD). It has various applications in other fields such as Information retreival[13]. In the context of turbulent flows, POD is a series of fluid variable representation. This theory is best described in [4]. For simplicity we consider it to be a scalar $x(t)$. It can be kinetic energy, concentration, pressure or temperature. $x(t)$ can be represented in the form

$$\hat{x}(t) = \sum_{n=1}^{\infty} c_n \varphi_n(t) \quad 0 < t < T \tag{1}$$

where $\varphi_n(t)$ is a set of orthonormal basis functions on the interval $(0, T)$. Mathematically this requires

$$\int_0^T \varphi_n(t)\varphi_n^*(t)dt = \delta(n-m) \tag{2}$$

and the coefficients c_n are random variables (when dealing with random processes like turbulence) given by

$$c_n = \int_0^T x(t)\varphi_n^*(t)dt \tag{3}$$

The POD method uses a set of basis functions such that the mean square error of the projections is minimised.

$$< [x(t) - \hat{x}(t)]^2 > 0 \quad 0 < t < T \tag{4}$$

To obtain the POD modes, the following eigenvalue problem needs to be solved.

$$\int_0^T R(t_1, t_2)\varphi_(t_2)dt_2 = \lambda\varphi(t_1) \quad 0 < t < T \tag{5}$$

where $R(t_1, t_2)$ is the auto-covariance of the fluid variable, $x(t)$. The basis function φ_n are the eigenvectors and the coefficients c_n are related to the eigenvalues λ_n by

$$< c_n c_m^* >= \lambda_n \delta(n-m) \tag{6}$$

From the above formula POD modes can be calculated. The eigenvalues of each POD mode represents energy contained in each mode. The magnitudes of the eigenvalues are in decreasing order such that $\lambda_n > \lambda_{n+1}$.

B. Method of Snapshots

The POD was first introduced in the field of Computational Fluid Dynamics (CFD) by Lumley [1]. The present day analysis uses method of snapshots introduced by Sirovich [11]. Here each LES data at a particular interval of time, interpolated on a uniform grid is considered to be one snapshot. This method was introduced to reduce the POD computations. To compute the POD using the Eq. 5 requires solving $n \times n$ eigenvalue problem. The main problem is the calculation of autocovariance matrix R. Snapshots method proposes that autocovariance matrix can be approximated by a summation of 'Snapshots'.

$$R_{ij} = \frac{1}{M}\sum_{n=1}^{M} x_i^n x_j^n \tag{7}$$

The snapshots are assumed to be distanced by a time or a spacial distance greater than the corelation time or distance. Nowadays this method has become extremely popular [3][4][6]. Its use in certain flows are questionable however, due to its assumption of the snapshots being uncorrelated. This discussion is briefly explained in [4].

C. Dynamic Mode Decomposition (DMD)

The mathematics underlying the extraction of dynamic information from time-resolved snapshots of LES data is closely related to the idea underlying the Arnoldi algorithm. Starting point of the Arnoldi algorithm is a equence of vectors (spanning a Krylov subspace K) of the form We assume v_j denotes each flow field. A sequence of N is writen as :

$$V_1^N = [v_1 v_2 v_3 v_4 \cdots v_N] \tag{8}$$

A linear mapping from one snapshot to another is assummed.

$$V_1^N = [v_1 A v_1 A^2 v_1 A^3 v_1 \cdots A^{N-1} v_1] \tag{9}$$

This can be further more taken as constant over the data sequence as:

$$v_{j+1} = A v_j \tag{10}$$

By the linear combination of available data fields, we have a standard Arlondi iteration problem.

$$A v_i^{N-1} \approx v_i^{N-1} S \tag{11}$$

where S is a companion matrix that simply shifts the snapshots 1 through $N-1$ and approximates the last snapshot N by a linear combination of previous $N-1$ snapshots. Hence this procedure will result in the low dimensional system matrix "S". We solve the "S" matrix problem using eigenvalue analysis and obtain eigen values. It is known that eigen values of S, approximate some of the eigen values of the full system A. The associated eigenvectors of S provide the coefficients of the linear combination that is necessary to express the modal structure with in the snapshot basis. S matrix is calculated as follows:

$$S = R^{-1} Q^H v_N \tag{12}$$

where Q^H is the complex conjugate transpose of Q from the QR-decomposition of V_1^{N-1}.

III. Experiments and Implementation

Here we discuss the Experimental and implementation details of POD and DMD on LES of subsonic jet data.

A. Pre-Processing

We consider LES of low pressure and medium pressure as the data. Each pressure case has 2 fields: 1) Velocity and 2) Concentration. As part of experiments, snapshot matrix X is constructed at first. Let U, V and Z be the velocity components:

$$X = [U^1 U^2 U^3 \cdots U^N] = \begin{pmatrix} U_1^1 & U_1^2 & \dots & U_1^N \\ \vdots & \vdots & \vdots & \vdots \\ U_M^1 & U_M^2 & \dots & U_M^N \\ V_1^1 & V_1^2 & \dots & V_1^N \\ \vdots & \vdots & \vdots & \vdots \\ V_M^1 & V_M^2 & \dots & V_M^N \\ Z_1^1 & Z_1^2 & \dots & Z_1^N \\ \vdots & \vdots & \vdots & \vdots \\ Z_M^1 & Z_M^2 & \dots & Z_M^N \end{pmatrix} \tag{13}$$

Let Ps be the scalar concentration component:

$$X = [Ps^1 Ps^2 Ps^3 \cdots Ps^N] = \begin{pmatrix} Ps_1^1 & Ps_1^2 & \dots & Ps_1^N \\ \vdots & \vdots & \vdots & \vdots \\ Ps_M^1 & Ps_M^2 & \dots & Ps_M^N \end{pmatrix}$$

B. Implementation of POD

The fluctuating velocity matrix U is calculated by substracting the mean velocities from the individual snapshots. Then the autocovariance matrix is computed as:

$$C = U^T U \tag{15}$$

The eigenvalue problem for the matrix reads as follows:

$$CA^i = \lambda^i A^i \tag{16}$$

The eigenvectors are arranged according to the decreasing order of eigenvalues reflecting the energies in different POD modes.

$$\lambda^1 > \lambda^2 > \lambda^3 > \lambda^4 > \cdots \lambda^N = 0. \tag{17}$$

Using the ordered eigenvectors the POD modes are constructed.

$$\phi^i = \frac{\sum_{n=1}^{N} A_n^i U^n}{\left\| \sum_{n=1}^{N} A_n^i U^n \right\|}, \quad i = 1, 2, \cdots, N. \tag{18}$$

C. Implementation of DMD

Calculation of fluctuating velocity matrix is not needed. But the snapshot matrix is divided into two parts.

$$V_1^{n-1} = [v_1 v_2 v_3 \cdots v_{n-1}] \tag{19}$$

$$V_2^n = [v_2 v_3 v_4 \cdots v_n] \tag{20}$$

QR decomposition in economy mode is performed as :

$$[Q, R] = qr(V_1^{n-1}, 0). \tag{21}$$

Companion matrix S is calculated as :

$$S = R^{-1} Q^H V_2^n. \tag{22}$$

The eigen value analysis is computed on S matrix

$$[X, D] = eig(S) \tag{23}$$

The dynamic mode spectrum is computed as :

$$\lambda_j = log(D_{jj}) / \delta t. \tag{24}$$

δt , is the time interval between the snapshots. The Dynamic modes can be computed as follows:

$$DM_j = V_i^{N-1} X(:, j) \tag{25}$$

where X is the original snapshot matrix. DMD contains details regarding the coherent structures and their temporal evolution as well. Since matrix A is needed is of no need at any point of implementation. [8].

IV. Results and Discussions

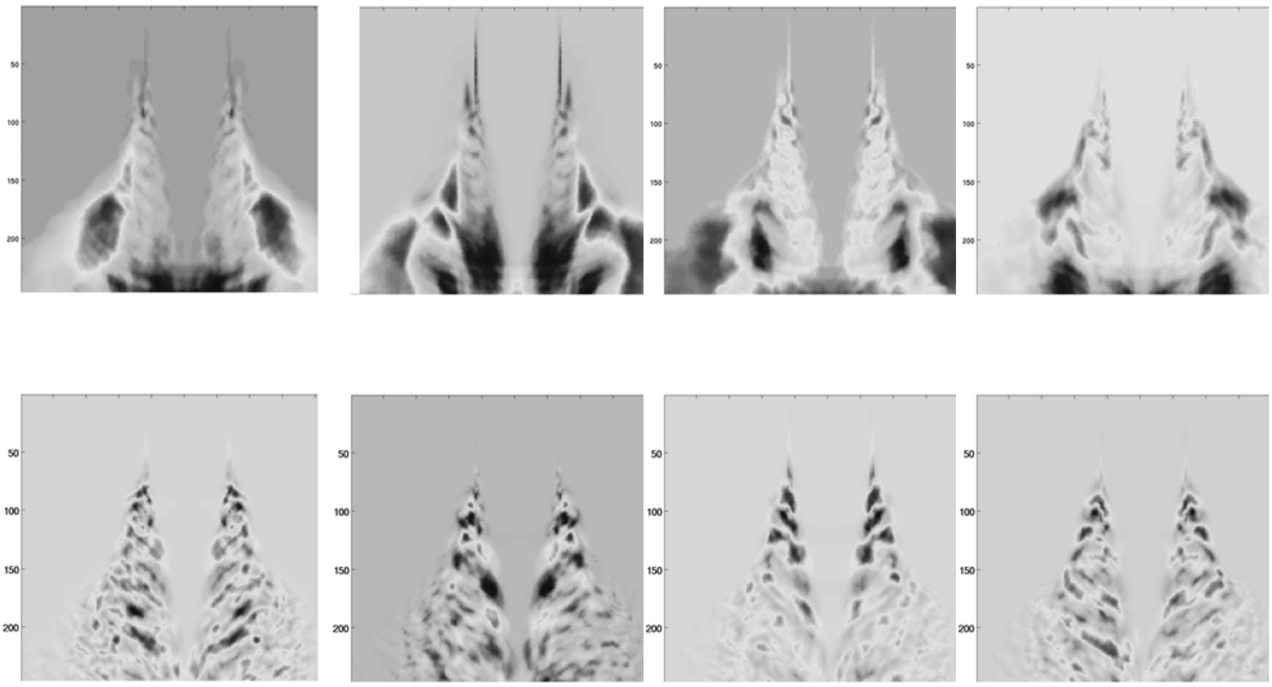

Figure 1: Comparison of first 4 POD modes (top) and DMD modes (bottom) for low pressure LES gas jet concentration field

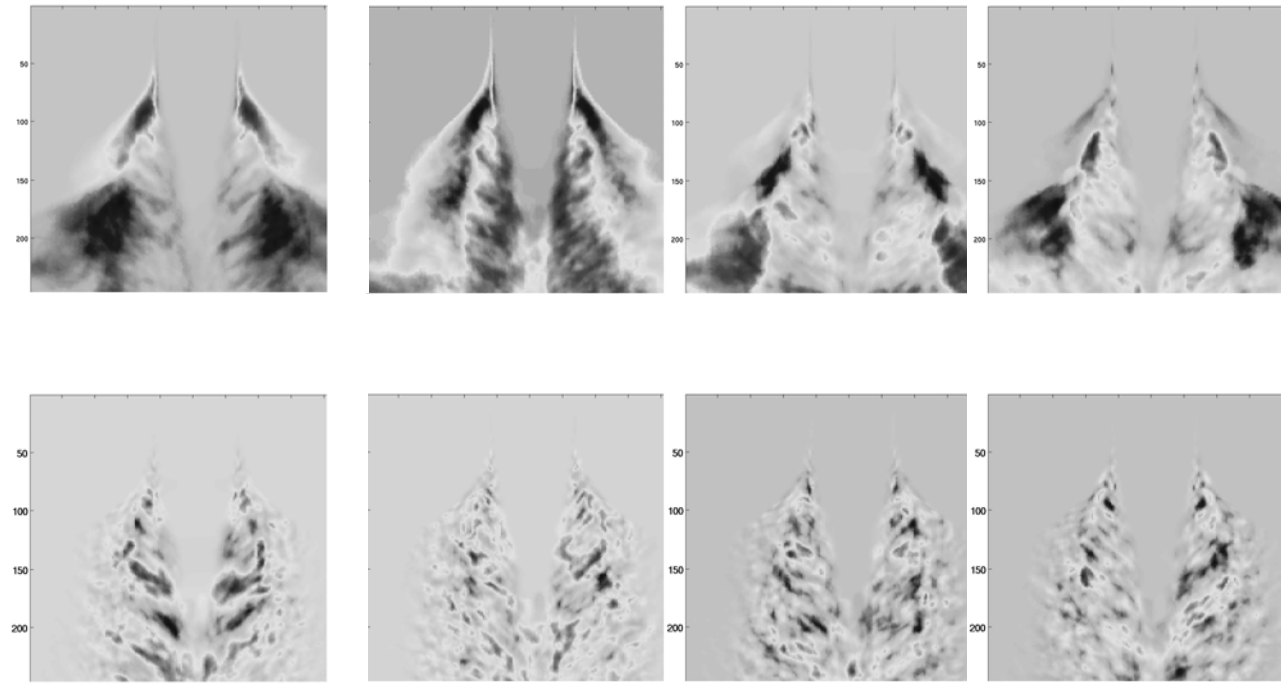

Figure 2: Comparison of first 4 POD modes (top) and DMD modes (bottom) for medium pressure LES gas jet concentration field.

The POD modes are the optimal decomposition for the flow and captures large scale structures or a large scale behaviour. Total kinetic energy is contained within the first few POD modes. Generally 95% of the total kinetic energy is used and the average flow field is described in the first n POD modes. Dynamic modes represents the perturbation dynamics and captures characteristic pattern located near the shear layer. DMD spectrum quantatively describes the jet behaviour. Higher the dynamic modes higher the is the frequency.

From the Figure 1 and Figure 2, it is observed from POD modes, that there is a formation of symmetric structures of Kelvin Helmholz instability. But from Dynamic modes, the Kelvin Helmholz instability is clearly visible. The second dynamic mode shows a characteristic pattern located near the shear layer, which represents the roll-up of the symmetric vortex sheet in Figure 1. The first and third mode depict small scale structures near the nozzle exit region.

From the Figure 3 and Figure 4, it is observed that due to breaking up of potential core and transition of the turbulence and interactions between the opposite sides of the jet (shear-layer) the ladder structures are formed. We can also see the increase of ring type structures in the shear-layer of the jet with the increase in the pressure.

POD and DMD methods can be utilised for analysing the LES data. The power of PODs fast convergence allows for a large scale structures to be isolated from the small scale structures in the turbulence. This would help in analysing the flow field in different ways. From the figures 1,2,3, and 4, POD and DMD methods are shown as a powerful numerical tools, for use in turbulent flows. The ability to maximize the kinetic energy of the flow with a miminal number of modes shows PODs strength in the analysis of the coherent flow structures and reduced order modelling.The DMD method has a clear advantages over POD, as it strives for a representation of the dominant flow features with in a temporal orthogonal framework, while POD is based on a spatial orthogonal framework.

From the Figure 5 the eigenvalues of S represent the mapping between subsequent snapshots: unstable eigenvalues are given by a modulus greater than one (i.e., are located outside the unit disk) [8]; stable eigenvalues have a modulus less than one (i.e., can be found inside the unit disk) [8]. For applications in fluid dynamics, it is common to transform the eigenvalues of S using a logarithmic mapping, after which the unsta-ble (stable) eigenvalues have a positive (negative) real part [8], see Figure 5. The procedural steps for computing the dynamic mode decomposition are given in section 3.

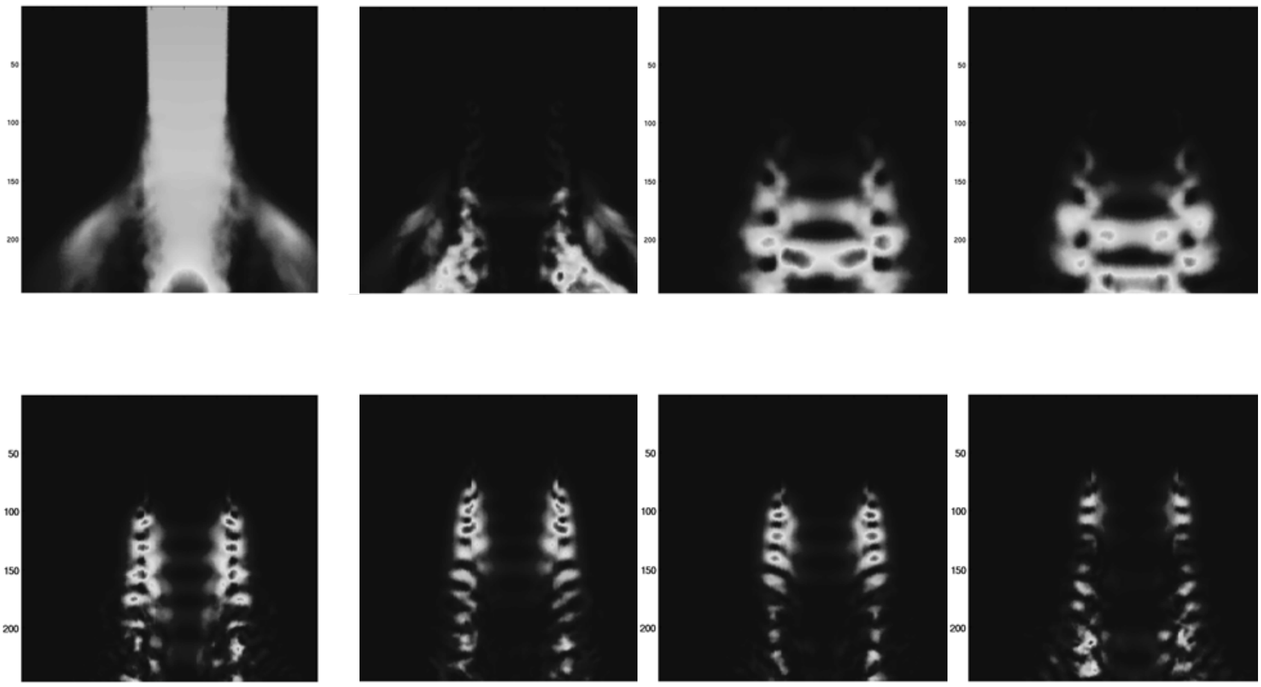

Figure 3: Comparison of first 4 POD modes (top) and DMD modes (bottom) for low pressure LES gas jet velocity field.

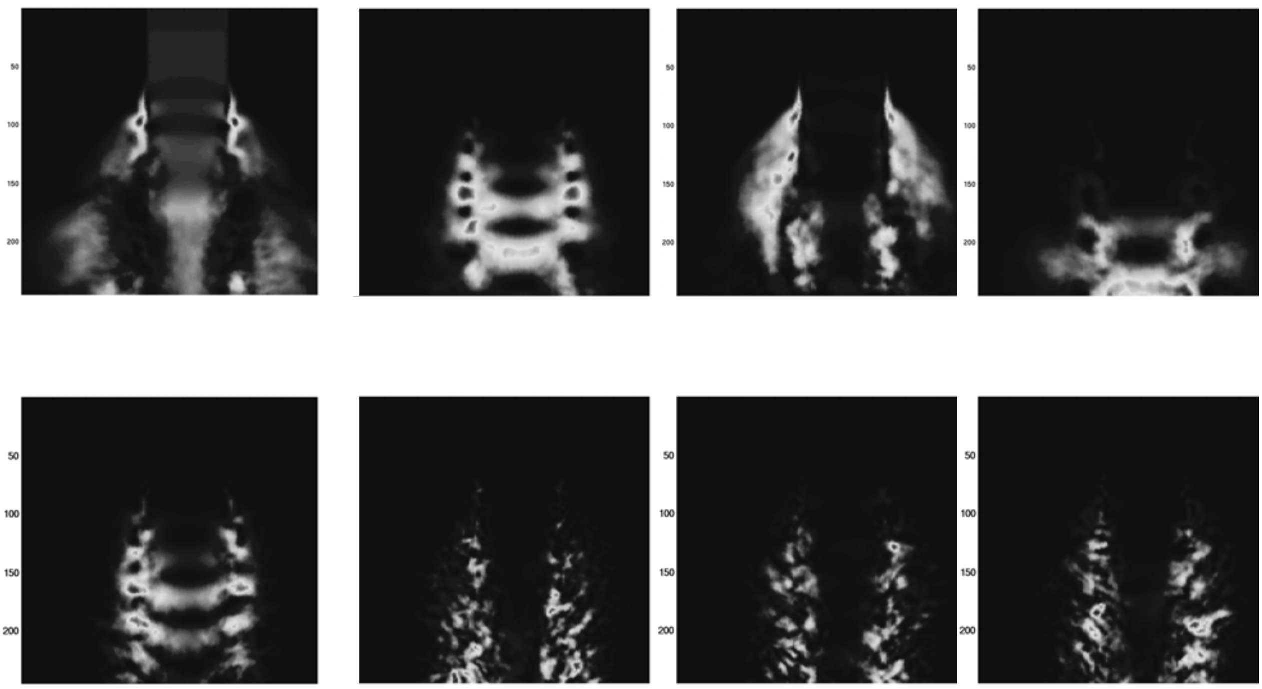

Figure 4: Comparison of first 4 POD modes (top) and DMD modes (bottom) for medium pressure LES gas jet velocity field.

Therefore, this paper summerizes that POD and DMD methods will provide the experimentalist with solid tools, in quantifying important mechanisms in time resolved measurements of fluid dynamics. It is hoped that DMD and POD methods help in further understanding of fundamental fluid processes.

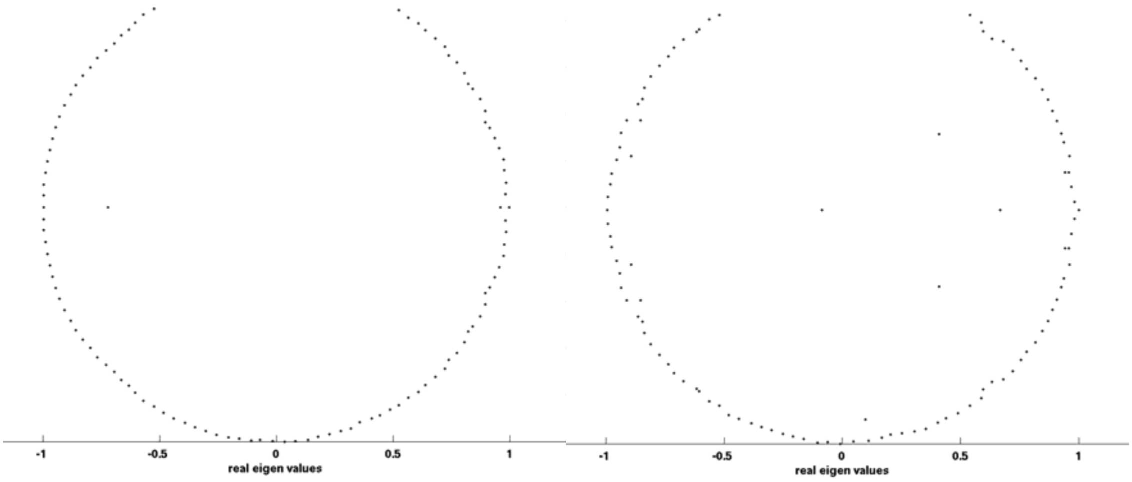

Figure 5: Eigenvalues of DMD for low pressure (left) and medium pressure (right) concentration field.

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