

Hyper-Parameter analysis of Deep Auto Encoder for Flow Prediction

A PROJECT REPORT

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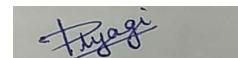
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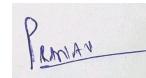
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CANDIDATE'S DECLARATION

We, Prakrit Tyagi, Pranav Bahl, Roll No's – 2K17/ME/163, 2K17/ME/164 students of B.Tech (Mechanical Engineering), hereby declare that the project Dissertation titled “Hyper-Parameter analysis of Deep Auto Encoder for Flow Prediction” which is submitted by us to the Department of Mechanical Engineering, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of degree of Bachelor of Technology, is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.



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Place: Delhi

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CERTIFICATE

I hereby certify that the Project Dissertation titled “Hyper-Parameter analysis of Deep Auto Encoder for Flow Prediction” which is submitted by Prakrit Tyagi, Pranav Bahl, Roll No’s – 2K17/ME/163, 2K17/ME/164, Mechanical, Production and Industrial Department ,Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Bachelor of Technology, is a record of the project work carried out by the students under my supervision. To the best of my knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.



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Abstract

Reducing the order of the system from high order dynamical space to a low dimensional subspace has been a challenging task and the models that achieve this are referred to Reduced Order Models (ROMs). Linear Projection methods have been used extensively in the past for building such ROMs, some common examples are POD,DMD etc. Though they have been successful in modelling several non-linear scenarios, their usage limits their applications pertaining to complex High order dynamical systems efficiently. In this study we aim to make use of advancement made in the field of Deep Learning to build a DL based ROM. We aim to probe the impact of hyper-parameters pertaining to flow prediction using deep autoencoders built with the help of artificial neural network. The parameters for our study that were used here were three different network sizes and two data sizes to compare the performance in flow prediction. Dataset for the Vorticity was generated using in-compressible URANS CFD solver icoFoam in an open-source CFD toolbox OpenFOAM. Von-Karman Vortex Street at Reynolds' number 100 around a bi-dimensional cylinder was simulated for our study.

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List of Symbols

r	Radius
v	Velocity
p	Ambient Pressure
α	Rate of momentum
η	adaptation step
W	Weight
w^t	State of vector at time t
e	Error
θ_ϕ	Network Parameters of decoder
θ_ψ	Network Parameters of encoder
ζ	Bottleneck Layer
ho	Output values
hi	Input values
θ_j	Threshold values
whi	Weighted correction between neuron i of the input layer and neuron j of the hidden layer
who	Weighted correction between neuron j of the hidden layer and neuron k of the output layer
N_{input}	Input parameters
N_{hidden}	Number of units in hidden layer
$N_{classes}$	Number of output of the problem
exp	Exponent
i_j	Input features
o	Output features

Chapter 1

INTRODUCTION

Advances in Machine Learning over the past decade has made it a popular field among the scientific community. It has found wide range of applications in fields such as robotics, neurobiology, economics and financial prediction, system dynamic modeling, prediction, etc.. A large role played in the explosive growth of machine learning is of availability of data and increase in computing resources which has yielded a reliable technique that has found plethora of applications.

In the era of computing, simulation has become essential for scientific progress. It plays an important role in decision making through prediction, helps in design by simulating a model over time and presents results for analysis, thus to achieve accurate simulation results a great emphasis is placed on model reliability. To achieve this it is necessary to use high spatial-temporal resolution models of the system for computation. This can be computationally expensive requiring hundreds of computing cores and time consuming making it unsuitable for real time applications requiring quick feedback.

Simulation is essentially for solving partial differential equations through iterative algorithms (deterministic or heuristic) by incorporating conditions. The models of systems used in simulations are essentially group of partial differential equations known as full order model (FOM). Full order model if used will be computationally expensive therefore reduced order model (ROM) is a technique aim at replacing the FOM by a reduced order model (ROM), which has a lower dimension but still able to describe the model of the problem described by the FOM. The basic assumption underlying the construction of such a ROM is that the solution of a PDE, lies on a low-dimensional set embedded in this space. This ROM is used to solve for solution in low dimension and then the solution is increased to FOM dimensions. This technique can be solved using a special type of artificial neural network called Deep Autoencoder. The neural network structure is such that it is able to reduce the dimension of the input and then reverse the dimension again. This has various application, in particular it is able to solve non-linear problems through

composition of hidden layer and thus not restrict us to linear spaces.

Autoencoder is a neural network than can learn to imitate its input and output the same input data. Here we make use of an Auto-encoder Neural Net to learn the spatial and temporal distribution of flow and give satisfactory results with low error when compared to CFD results. This is a slight deviation from general usage of autoencoder and our efforts are to make use of advancements that have been made in the Neural networks or Deep Learning methods to build an efficient ROM (Reduced order Model) that would be able to capture the High Order Dynamics effectively and represent it in reduced latent space capturing the essential features and thereby reconstructing high order snapshot for the next time step. This paper presents results for comparisons with different hyper-parameters. Three different network sizes are used and following this different data sizes were used for training and comparison was made among them. Below is the generalized mathematical foundation of our model which presents the w^{t+1} predicted vectorized state, the model and its parameters $\varphi(\cdot; \theta_\varphi)$ and the input to the model i.e. the current time step w_t . 'e' represents the error term generated by model corresponding to the actual true state, hence predicted state is represented as \hat{w}^{t+1} and the True state as w^{t+1} .

$$w^{t+1} = \varphi(w_t; \theta_\varphi) + e \quad (1.1)$$

$$e = w^{t+1} - \hat{w}^{t+1} \quad (1.2)$$

The report is organised as follows. The literature review is presented in **Chapter 2: Literature Review**. The problem formulation and Methodology is described in **Chapter 3: Methodology**. The evaluation of results are presented in **Chapter 4: Results** and conclusions are presented in **Chapter 5: Conclusion**.

Chapter 2

LITERATURE REVIEW

Advances in Machine Learning techniques has made its usage reliable and economical and opened plethora of applications in fields of robotics , neuro science, economic and financial prediction, system dynamic modeling and prediction etc.. Autoencoder is one such technique which learns by itself to represent large data in reduced form. This is advantageous as using low dimensional data for analysis and calculation is efficient, computationally economical and reduces cost. Therefore this technique has found extensive usage in flow reconstruction, reduced-order modeling [1], prediction of fluid flow dynamical system [2] and flow prediction [3].

Computational fluid dynamics is the go to technique for simulating fluid flow but it is computationally expensive and if a users has inadequate resources, he/she will find it difficult to simulate and innovate. However, CFD has found its application across various engineering disciplines such as Aerospace industry, Heating and Ventilation applications, Flows corresponding to cardiovascular operation, Fluid machinery etc [4]. The need for such simulation often requires very high temporal and spatial resolution and hence the high order dynamics are simulated using Full-order-Models (FOMs) which are various numerical methods such as Finite Volume Method (FVM), Finite Element Method (FEM) etc. which are based on the governing equations (Partial Differential Equations). These models hence hinders its use in Multi-query [5, 6] scenarios which require rapid simulation result generation. The application of building large scale dynamical systems to simulate highly complex and non-linear flows seems to be failing in its use without taking a lot of computational burden. Hence there is an inherent need to represent higher order dynamics in reduced representations, which could be further used to evolve dynamics and when required can be reconstruct back to it's high-order form. These techniques are often referred to as Reduced-order-Models (ROMs) and many academicians have made their contributions in the past to model such techniques [7, 8, 9, 10]. Building ROMs is not an easy task, since the models doesn't perform well in situations where the dynamical systems are complex since the parameters aren't robust enough. There are various projection based

methods which have been introduced in the past which makes use of linear basis to form basis functions with help of snapshots generated using FOMs. These methods have found its acceptance among many researchers, such as Proper Orthogonal Decomposition(POD) [11, 12, 13], Dynamic mode Decomposition(DMD) [14, 15], Koopman Theory [16, 17] etc.

Proper Orthogonal Decomposition method is a method to decompose a physical vector field representing a physical phenomenon into a composition of deterministic functions that each reflect some part of total fluctuating kinetic energy. Through this method the hope is to find obscure hidden structures in any phenomenon that are difficult to observe and define. Dynamic mode Decomposition is similarly to POD i.e it is used to analyse dynamics of complex non-linear phenomenon that are difficult to observe and define. If given a temporal set of data, DMD computes a set of modes each of which is associated with a fixed oscillation frequency and decay/growth rate. These set of modes with their parameters help in extracting information about dynamics. Koopman Theory is an formulation of study of dynamical system through data-driven analysis. Provided a set of time-series data that is arranged in a vector space the Koopman operator gives a linear transformation of this vector. It can be seen a lifting of the dynamics from the state space into the space of observables.

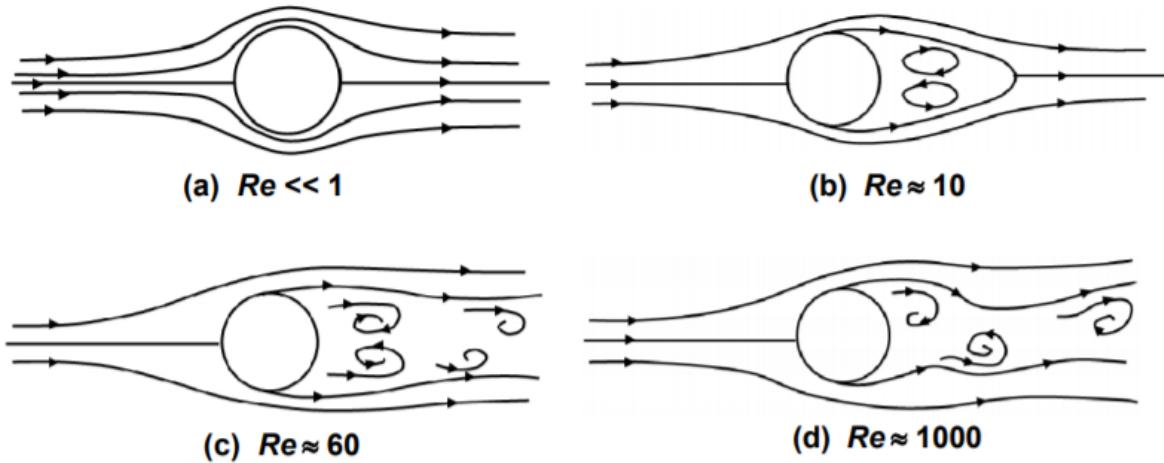


Figure 2.1: Flow pattern generated around a cylinder for different reynolds number

In this project we aim to estimate the spatial and temporal distribution of flow around a cylinder. Flow around a cylinder generates intriguing pattern in the wake of the cylinder. This is a popular phenomenon to simulate and test your algorithms. Flow patterns generated around a circular cylinder immersed in a uniform flow are shown in figure 2.1 [18].

A Kármán vortex street (or a von Kármán vortex street) is a repeating pattern of swirling vortices, caused by a process known as vortex shedding. It is formed in the wake of the flow around a bluff body. When the Reynold's number exceeds about 30,

the two vortices formed behind the body gets stretched and are washed down. At the place of these two vortices, two new are formed and the process continues. The shape of every streamline is symmetrical not only around the cylinder's upper to lower side, but also around its front to rear. Karman gave the explanation for this phenomenon and according to him there are two possible configuration of the vortex trail i.e. symmetrical and the staggered configuration. Formation is dependent on Reynold's number of the flow, as the Reynolds number increases, the length of the vortex increases, at less than 5 Re no shedding, 5 to about 40 Re fixed symmetrical vortex, above 90 Re alternating vortices shedding starts. As shown in figure 2.1 the vortex The frequency of the shedding is directly proportional to the Dimensionless quantity "Strouhal Number" The Von Karman vortex streets are as a consequence of Strouhal instability, which occurs on the transition between laminar and turbulent flows. Thus, this instability is linked with the Reynolds dimensionless number which determines the stability and the flow type. The variation of strouhal number versus reynolds number is shown in figure 3.3 [19]

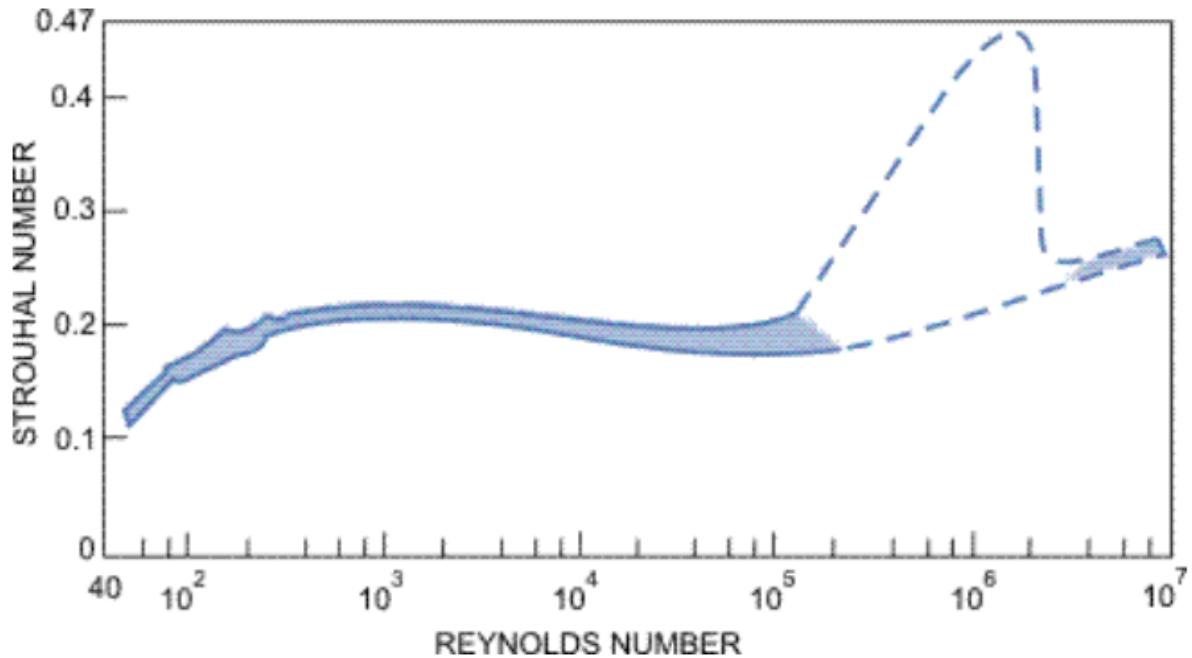


Figure 2.2: Strouhal number versus Reynolds number for flow around a cylinder

Chapter 3

METHODOLOGY

3.1 Bi-dimensional Flow Around Cylinder

3.1.1 Case Description

The analysis is based on the flow around a bluff body i.e. 2d circular cylinder. The specifics of the given case presented here is the two-dimensional or bi-dimensional mathematical modelling of laminar flow around this body which is in-compressible in nature. The model generated is made possible with the help of OpenFOAM version 7 tool-box. The mesh generated here for our case has specific high-resolution on the targeted areas wherein the effects of viscous nature is more dominant. The computational fluid dynamics (CFD) simulations are generated here for Reynolds Number 100, and visible vortices within the flow can be seen in the form of vortex shedding. We have constantly maintained decent qualitative metrics for our simulation case such as Mesh quality, Courant Number etc. Given the correct initial conditions for our simulation case , OpenFOAM have been able to accurately model our case of 2D Von Karman Vortex Shedding with correct Strouhal Number.

3.1.2 Hypotheses

The following are the hypotheses considered for our case of simulation, which comprehends the simplicity or straight-forwardness of our problem with respect to extremely complex Non-Linear problems.

1. The flow is Incompressible in nature, with no variations in the density.
2. The flow is Laminar in nature, with no lateral mixing of fluid layers.
3. The fluid is newtonian in nature.

4. The flow is 2-Dimensional in nature, with no gradients in the z-direction.
5. The gravitational effects on our fluid flow is negligible.

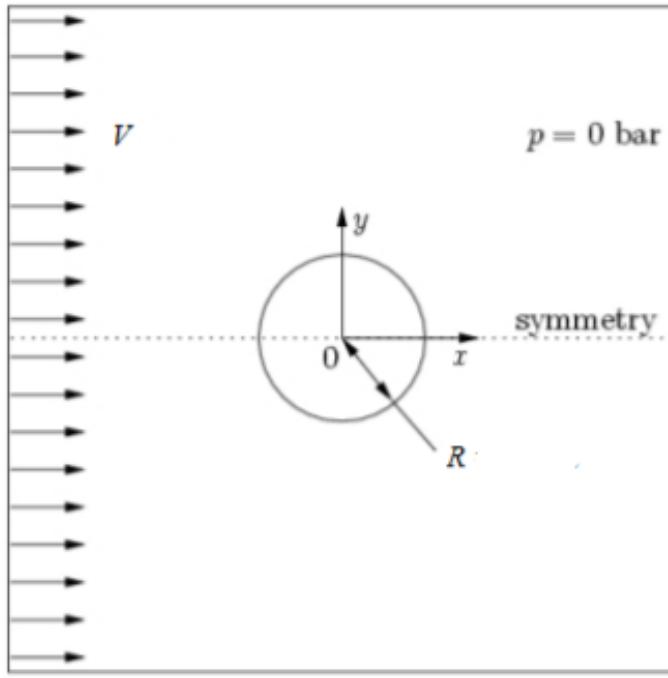


Figure 3.1: Domain Description

3.1.3 Case Setup

The CFD setup generated here makes use of bluff body which is 2-Dimensional in nature and represents physically a circular object placed in a flow. The diameter of the circular object is 0.1 m and the velocity of the flow from the inlet is of constant speed 1 m/s, following which the outlet is kept at Ambient condition of the pressure. The solution for the simulation is not an analytical one and henceforth the behaviour of the flow is governed by the governing equations of the system and the dimensionless number representation corresponding to the problem. The fluidic behaviour is high Non-linear in nature and the dependency of the system is dependent on the Reynolds number of the flow. The viscous behavior of the fluid can be observed wherein the boundary layer detachment is seen as an existential phenomena because of the adverse pressure gradient. A widely known phenomenon takes place due to the symmetry of the system i.e. Von karman vortex street, which is observable in the form of alternate shedding of the vortices behind the body. The dimensionless number associated with the shedding of these vortices is Strouhal Number.

1. The Continuity Equation :

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (3.1)$$

2. The Momentum Equation :

$$\frac{\partial u}{\partial \tau} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = - \frac{\partial p}{\partial x} + \frac{1}{Re} \left(\frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} \right) \quad (3.2)$$

$$\frac{\partial v}{\partial \tau} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = - \frac{\partial p}{\partial y} + \frac{1}{Re} \left[\frac{\partial^2 v}{\partial^2 x} + \frac{\partial^2 v}{\partial^2 y} \right] \quad (3.3)$$

3. The Reynolds Number :

$$Re = \frac{\rho V L}{\mu} \quad (3.4)$$

4. The Strouhal Number :

$$St = \frac{wD}{2\pi U} \quad (3.5)$$

As stated above the CFD modelling of the problem defined was done using OpenFOAM. The solver that was used here under the regime of the tool-box is called icoFoam. The icoFoam solver used here is an incompressible solver of the Navier-Stokes equations and the method involved in solving these equations is called Pressure Implicit with Splitting Operator - PISO Algorithm. This solver has proved to be an efficient and accurate solver for such kind of problems before as well.

3.1.4 Computational Mesh

The mesh was generated here to cater the problem defined as above. The bidimensional cylinder here has a diameter of 0.1 metre with the flow of fluid coming from the $+x$ direction and leaving at an Ambient pressure at the outlet. The order of the problem has dependency on the size of the boundary layer and corresponding to this, certain sections of the mesh were created with high-resolution discretizations. The theoretical version of such discretization strategy often refers to using equally sized grid-points and small enough to capture relevant features.

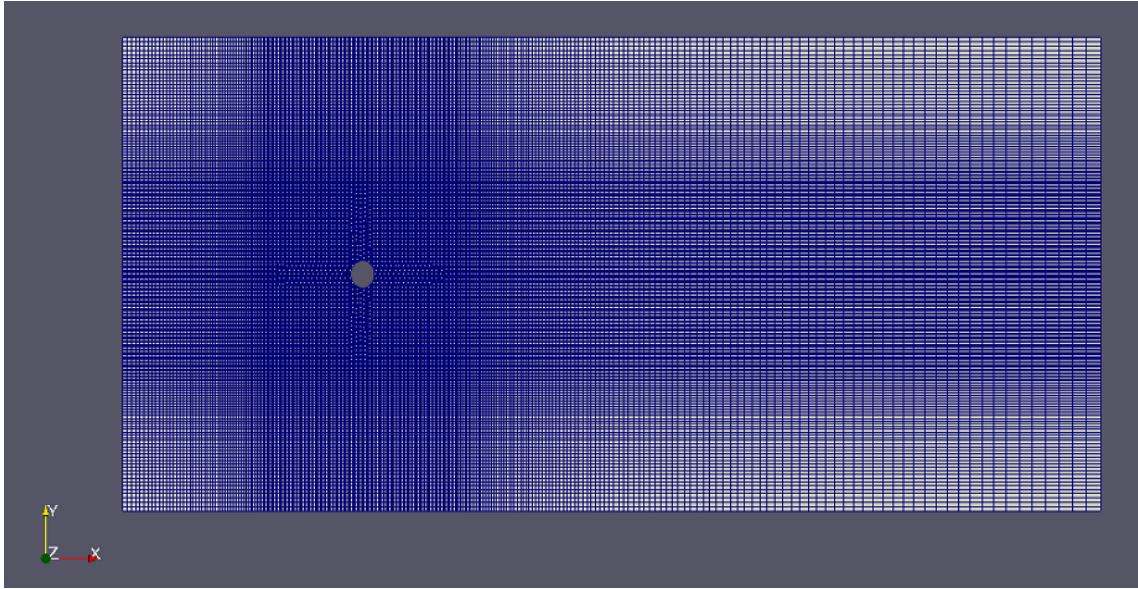


Figure 3.2: Computational Mesh

Since to enhance the computational burden from the system we make use of the variation in resolution, without compromising on losing of relevant features. The fineness of the mesh around the cylinder is more than the other spatial-domain since it needs to capture the boundary layer prevalent features. The blockMeshDict in the directory /system is used to generate /constant/PolyMesh for mesh. The following mesh has been defined with the help of six different patches i.e. Top, Bottom, Inlet, Outlet, Cylinder and FrontAndBack of the respective domain. The development of the fine mesh around the cylinder was done using feature arc instruction of the blockMesh utility. The cylinder patch was defined as wall and FrontAndBack patch was defined as empty for the sake of bi-dimensionality of the problem. The patch instruction were passed for the inlet and the outlet section of the problem and as such no information is specified since then we can use it for instructing the flow at specified initial conditions. As discussed before the resolution of the mesh around the cylinder is increased as for efficient capturing of the boundary layer and hence fluid elements near edges which are smaller are restricted as a consequence.

3.1.5 Computational Model

The description of the model used in our case could be fundamentally drawn from the files situated at directories /0 and /constant and /system. The discussion of these respective files would be made in the consequent sections explaining the descriptions of the models and their usage. The files are corresponding to the version 7 of OpenFOAM CFD tool-Box. In the /0 directory the files that are present are the files corresponding to the /0/p

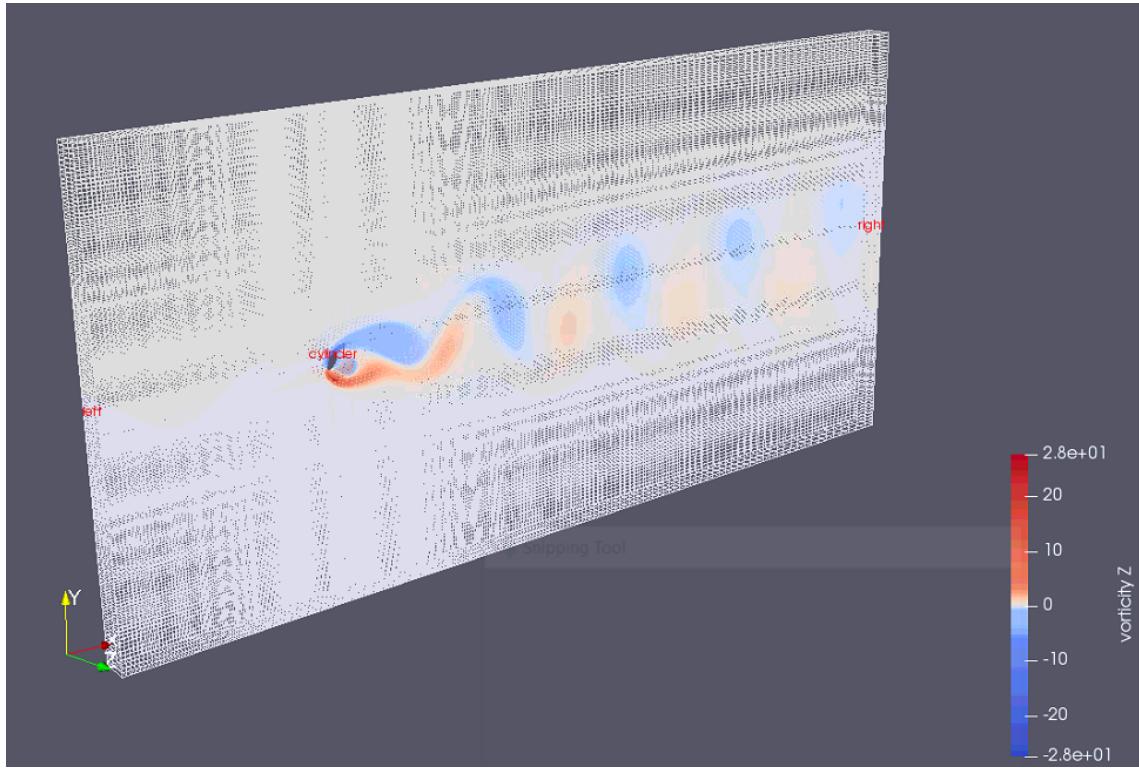


Figure 3.3: Vorticity data on Computational Mesh Wireframe

and $/0/U$ and hence as the name suggests contains the information corresponding to initial conditions of the respective boundaries. The following is the bifurcations made :

1. Patch : Top and Bottom - symmetryPlane condition
2. Patch : Front and Back - empty condition
3. Patch : Inlet and Outlet - freeStreamPressure condition

The patch freeStreamPressure leads to the constant setting of the inlet with the negligible gradient with the corresponding outlet hence providing an absolute critical environment for the flow of the fluid. The next file which contains the initial conditions for the velocity contains information corresponding to the uniform velocity directed from the $-x$ direction of the spatial domain to the $+x$ direction of the domain. The internalField term inside the file contains the information corresponding the quantitative measure of the uniform velocity to be given as the input. The dynamic viscosity of the fluid is adjusted as such that the inlet velocity with its value form the required Reynolds number of 100. Again the conditions corresponding to the boundaries were made as follows :

1. Patch - Top and Bottom - symmetryPlane Condition
2. Patch - Front and Back - empty Condition

3. Patch - Cylinder - noSlip Condition

The empty condition as usual has been used here to direct the system to a bi-dimensional form and the cylinder has been initiated here with the noSlip condition of OpenFOAM so as to direct zero velocity at this patch through-out leading to the formation of a boundary layer. The next file corresponding to the modelling of the system are /constant. There are two files namely in this directory i.e. /constant/RASProperties and /constant/transportProperties. The file RASProperties as the name suggests is used to define the Reynolds Averaged Model and can be used to flag the model to be used in the case of simulation. Since our simulation setup corresponds to the laminar flow, we set the system by writing the flag as laminar. The constantly printing of the coefficients can also be adjusted here. The next file that we have in this directory is transportProperties which contains the information corresponding to the property of the fluid i.e. kinematic viscosity which is dynamic viscosity divided by the density of the fluid and can be altered to adjust the Reynolds number. Next in the queue comes the /system directory which contains the files that directs the code to run in a particular way. /system/controlDict implements the code to run with a certain time-step and controls the total iterations to run for the simulation and also has the command over the writing of the data. The solver is also to be mentioned in this file i.e. for our case icoFoam. We set the time-step accordingly for the system taking help of the courant number. The start-time of the simulation is kept as 0 and final as 10 seconds. The simulation start is also kept as the start-time at the starting and as latest-time in the middle of simulations. The write-interval option is also presented in the controlDict file, and can be set accordingly. /system/fvSchemes file directs the cfd code to use which schemes whether it be discretization schemes or the interpolation schemes. GaussLinearOrthogonal function has been used for the laplacian schemes section. The file /system/fvSolutions contains which solvers to use for solving the CFD problem. The solver for the velocity section used here is PBiCG and the pre-conditioner used corresponding to it is DILU. Since PISO solver is used here hence we have nNonOrthogonalCorrectors at constant value 3 which helps in getting more features get captured by our simulation.

3.1.6 Dataset

The cylinder has a diameter of a unit along with its distance corresponding to the centre from the inlet is 8 units and from the outlet is 25 units. Boundary conditions of the domain corresponds to the unit velocity from inlet and pressure of 0 at the outlet. A no-slip BC has been initiated for the circular body. The simulation carried out here is of Unsteady RANS simulation using OpenFOAM. The solver used here is icoFoam which is

an incompressible Navier-stokes solver. There is an inherent need for extracting relevant features/information from the corresponding data-set and hence we only concentrate our study around the formation of vortices and its shedding, henceforth we look forward to cut-out the part of the data for relevant understanding of the system. The cut-out stretch that has been proposed here contains the spatial domain with stretch in the y-direction from - 2 unit to the + 2 unit and following this in the x-direction the stretch starts from 0 unit to +16 unit. The following cut-out stretch has data in an unstructured form and hence a MATLAB code was written to use linear-interpolant to distribute data uniformly in the space and thereby facilitating in even distribution of weights and biases throughout domain. The uniformly distributed data has data has quantitative features of 80 points in the y-domain and 320 points in the x-direction and the data used here is Z-Vorticity data. Other from the computation of the rate of the flow and the wall shear stress calculation the vorticity of the fluid can be generated with the help of OpenFOAM utility. The vorticity of the fluid can be presented as a pseudovector field that comprehends the circular motion of the fluid locally with respect to some reference point. The vorticity of the fluid can be represented mathematically as below, which basically the curl of the velocity field.

$$\begin{aligned}\vec{\omega} &= \nabla \times \vec{v} = \left(\frac{\partial}{\partial x} \quad \frac{\partial}{\partial y} \quad \frac{\partial}{\partial z} \right) \times (v_x \quad v_y \quad v_z) \\ &= \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z} \quad \frac{\partial v_x}{\partial z} - \frac{\partial v_z}{\partial x} \quad \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} \right)\end{aligned}$$

Figure 3.4: Mathematical representation of Vorticity

As suggested our current case is a 2-Dimensional or bi-dimensional flow the curl of the velocity field will be with respect to the x-direction and the y-direction and hence curl would automatically mean the magnitude of the vector to be in the z-direction and hence the vectors are perpendicular to the state of the system.

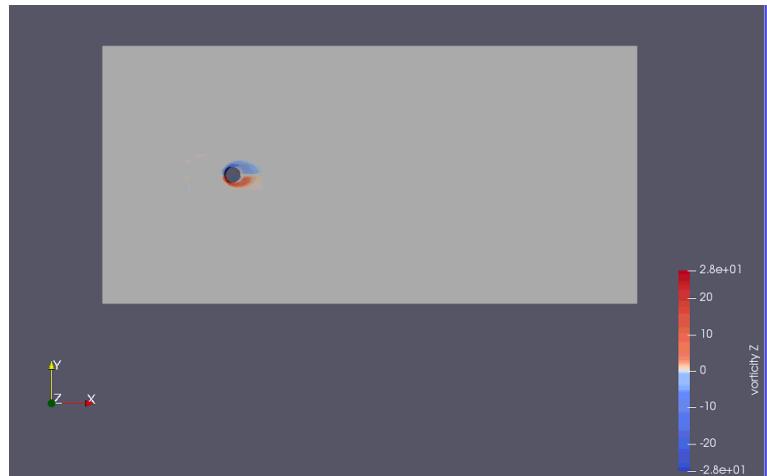


Figure 3.5: Vorticity contour plot: Von Karman Street (time step 10)

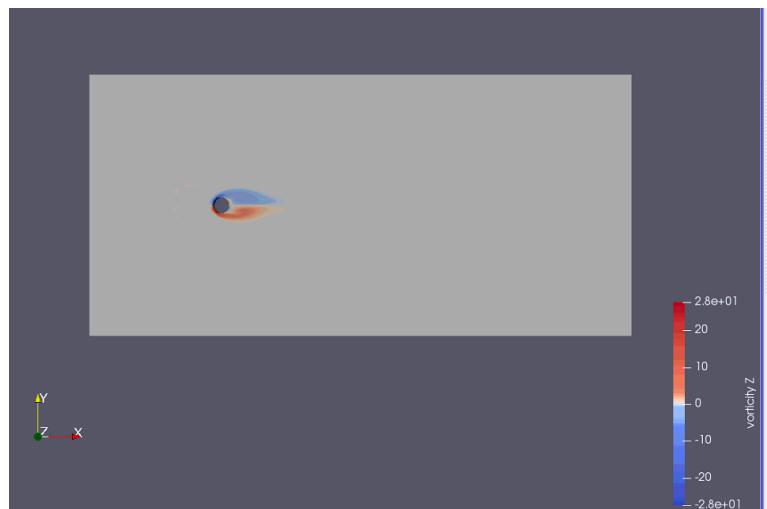


Figure 3.6: Vorticity contour plot: Von Karman Street (time step 20)

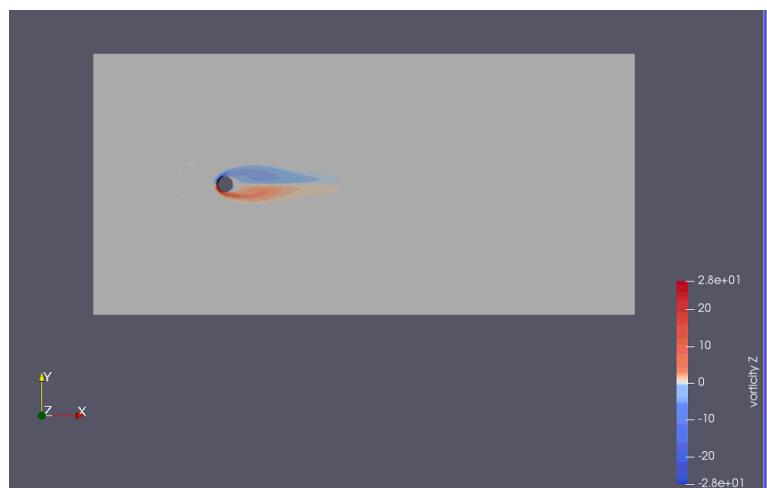


Figure 3.7: Vorticity contour plot: Von Karman Street (time step 30)

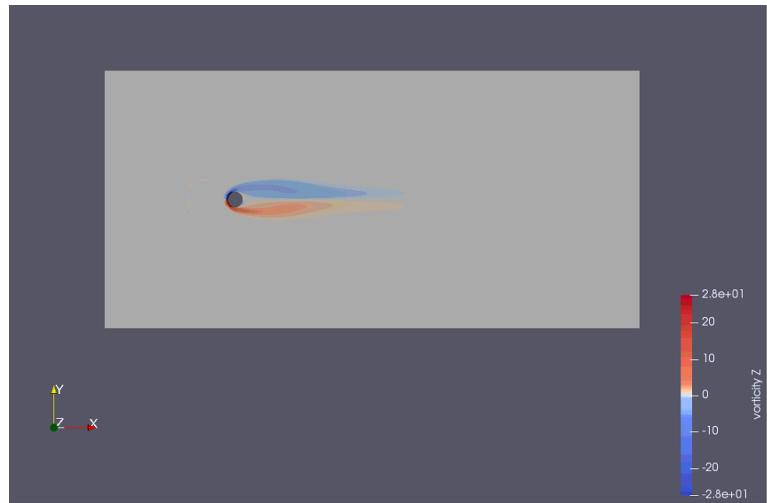


Figure 3.8: Vorticity contour plot: Von Karman Street (time step 40)

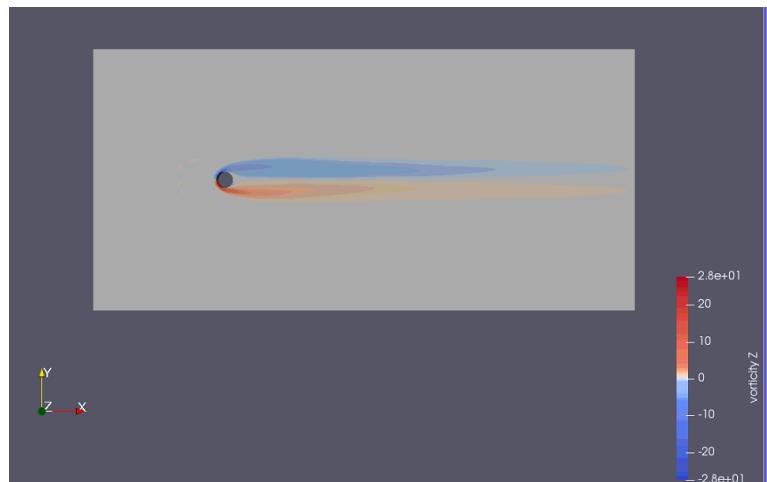


Figure 3.9: Vorticity contour plot: Von Karman Street (time step 50)

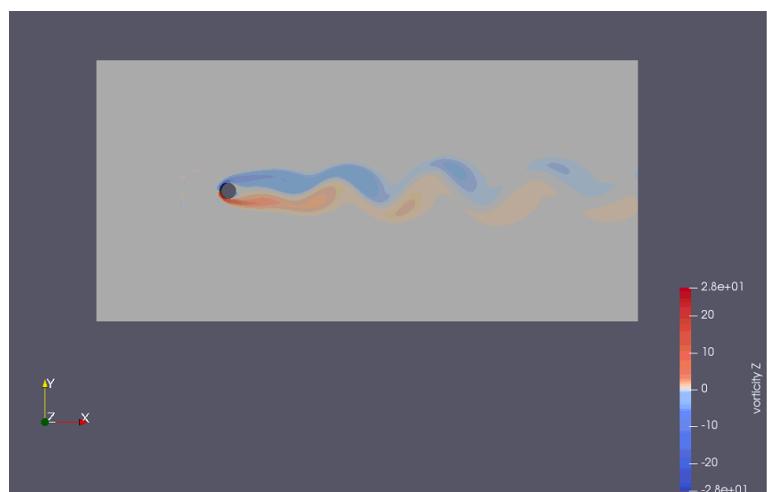


Figure 3.10: Vorticity contour plot: Von Karman Street (time step 60)

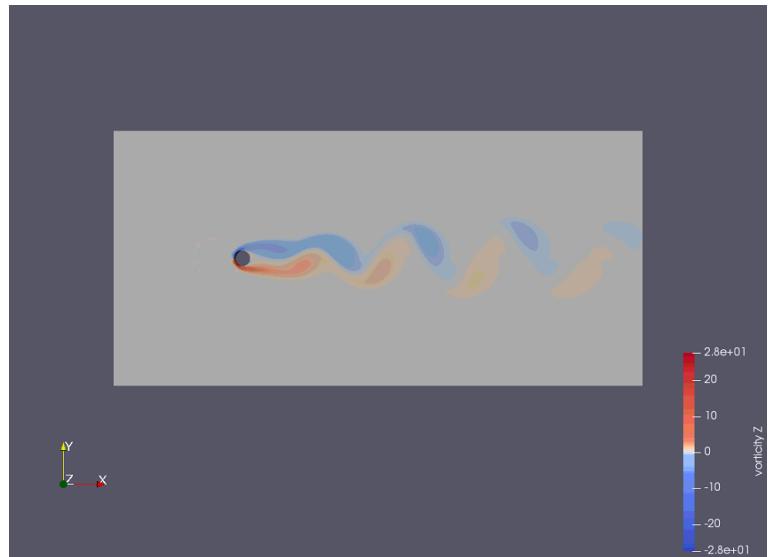


Figure 3.11: Vorticity contour plot: Von Karman Street (time step 70)

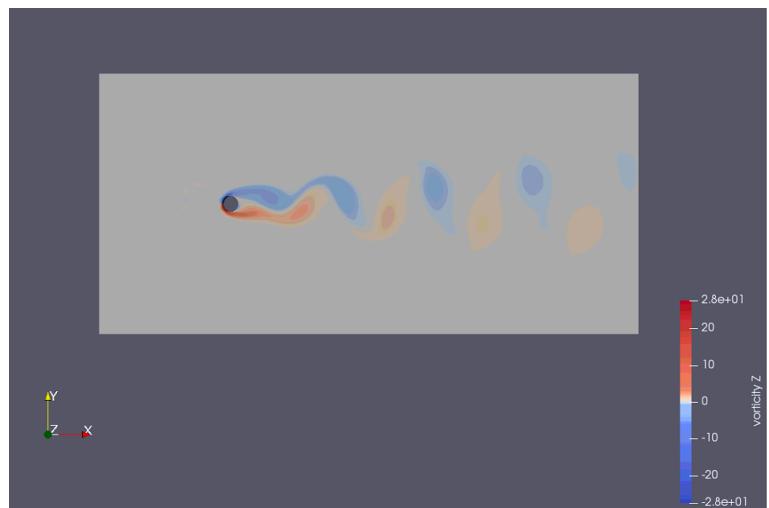


Figure 3.12: Vorticity contour plot: Von Karman Street (time step 80)

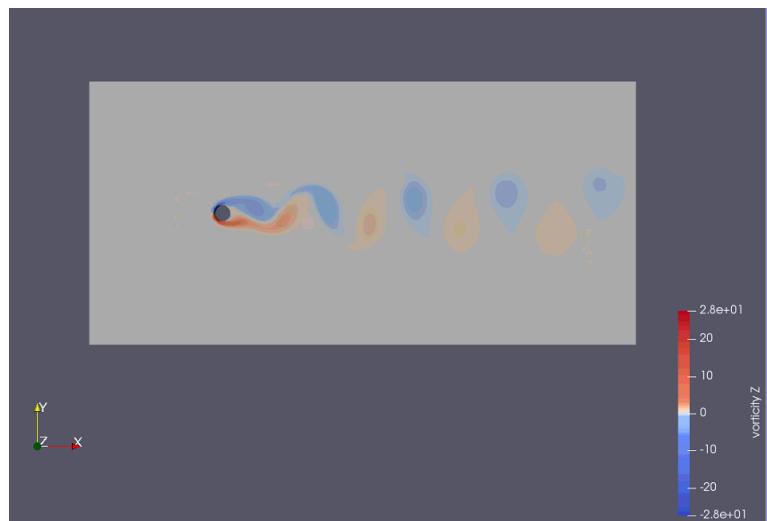


Figure 3.13: Vorticity contour plot: Von Karman Street (time step 90)

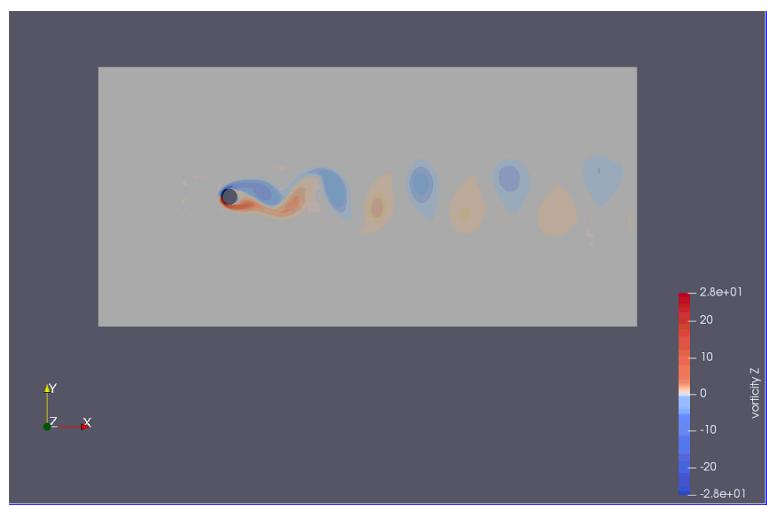


Figure 3.14: Vorticity contour plot: Von Karman Street (time step 100)

3.2 NOAA OISST V2 - Sea Surface Temp. Dataset

As the proof of concept and generalization of our machine learning technique, we test our approach on another well-known highly-nonlinear data i.e. Sea Surface Temperature (SST) dataset. SST Data is made publicly available and uploaded by the Physical Sciences Division at National Oceanic and Atmospheric Administration (NOAA). The data is made available by the respective organization after the analysis of in-situ and satellite observation of the Sea surface temperature by the help of ship-buoys and expensive satellites. The resolution of the data available corresponding to the variable ‘time’ or as we call it the temporal resolution of the data is Weekly data, Monthly data and monthly long-term mean data. The resolution corresponding corresponding to the spatial domain is of 1 deg latitude and 1 deg longitude, which translates to 180 x 360 grid points. Since our earth constitutes of 360 deg longitude and 180 deg latitude the above described data covers all the spatial domain of the earth along with the sea and the surface. The surface data here is represented as a large number meaning no existential sea surface temperature. In this study we make use of weekly mean data from the year 1990 on-wards. This resolution for the temporal dependency was used since the time-steps corresponding to other temporal resolution were either in very large quantity or else in shortage for the training of the model. The data is said to be centred around Wednesday for this period, meaning the features corresponding to the whole week were centered for a single point in the time space.

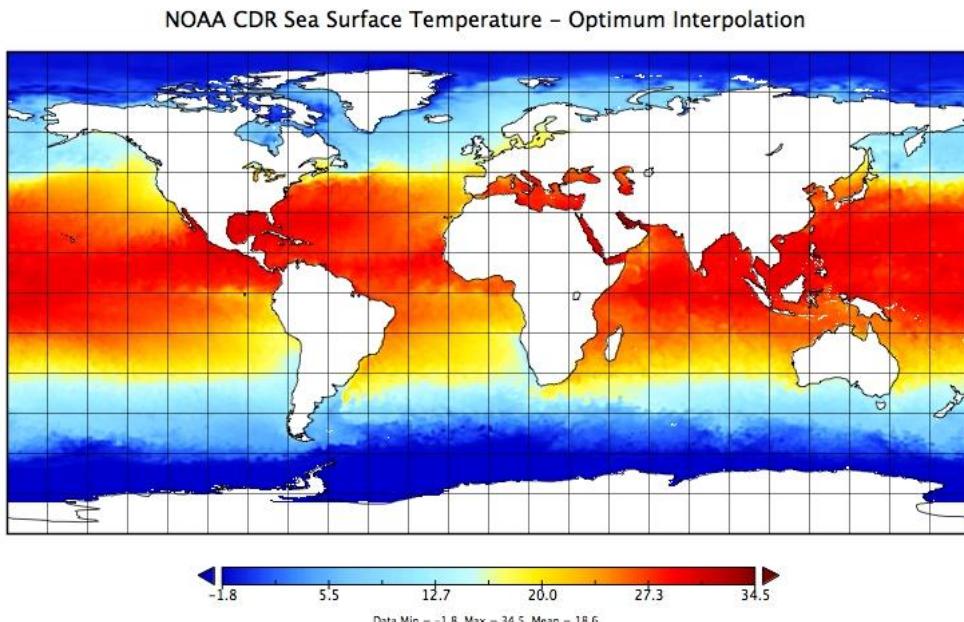


Figure 3.15: Representation of Sea surface temperature contour plot

Data for initial 400 weeks was chosen as the training data-set for our machine learning model. Following 100 weeks data was chosen as validation data-set for recommending the system as valid for its application to the real world data for predicting, and following 200 weeks of the data was used for the testing of the model's accuracy. The problem description here is to reconstruct the SST data on the time-step $t+1$ with the input to the model at time-step at t , henceforth making an model recursively predicting the next time-steps.

3.3 Machine Learning

3.3.1 Introduction

This section will briefly cover the specifics related to machine learning algorithm and how do they function. The increase in the existential use of data-driven algorithm over the course of whole globe has increased dramatically, the one good reason for the following could be the huge rise in the production of data. The focus of this subject is to study and analyse the data generated and develop algorithms that can help in understanding such data. The primary task defined is to find a function that can map the input features X to output Y i.e. the predictions of the function. Machine learning tasks can be classified into different sites of applications such as classification problem or prediction of the state, irrespective of the application the accuracy of the system is to be measured and calibrated accordingly. Hence there has to be a performance measure that has to be present for an algorithm to develop the model as accurate as possible. Machine learning techniques are often subdivided on the basis of the optimization problem or the kind of training required to optimize the algorithm's weights and biases. These are called namely, Supervised method of learning, Unsupervised method of Learning and Reinforcement strategy for learning. The first case of supervised methodology as the name suggests makes use of the data-set that are labeled in nature i.e. a corresponding has a particular output. Such techniques are made use of wherein the input to the model and output to the model are available in large quantities and the focus is on reducing the error between the predicted output by the model to the respective input. Next in the queue come the unsupervised learning technique, which makes use of unlabeled data-sets that has no input-output pair to reduce some error associated with the predicted state, rather the focus is more on the discovering of the similarity or cluster formation among the data and seek useful information out of it. Reinforcement techniques are rather based on the feedback-loop of the system wherein the function is trained on the whole ideology of reward based system , as every action has its own set of consequence. The amount of

the data around us is tremendous and it is the prerogative of the system to derive useful information/inferences out of it. In today's age of Internet, Internet of Things, Sensors etc every hour unimaginable amount of data is generated. Hence there is an inherent need for developing algorithms that helps us understand Non-linear complex phenomena of the world accurately.

3.3.2 Neural Networks

Neurons

This section will present intricate details pertaining to modern day deep learning technique known as Neural Networks that are artificially generated. The discussion starts with inheriting the design of the biological neurons that are present in the human brain. These biological neurons are said be extensively interconnected and forms the basic cell for processing the information presented. They are composed of the biological terms associated as follows, dendrites, soma and the axon. Each of these have their own function associated with respect to the biological entity i.e. in case of dendrites they send electrical signals to soma with the help of extremely dense interconnected branches.

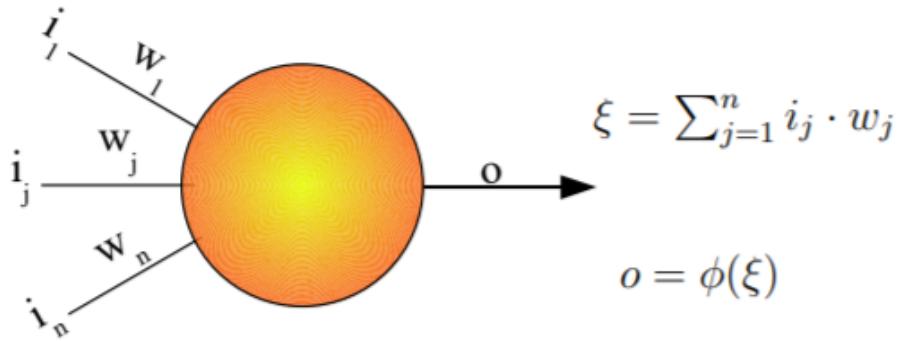


Figure 3.16: Artificial Neuron Structure

All the information is processed in the Central part of the neuron i.e. soma , the activity next performed by axon is to take away signal from the soma. Similar is the way that an artificial neuron is generated i.e. some input features are given to a artificial neuron and the function is to output a data after the processing of the input data. The working is presented in the most simple form that is the input data is multiplied by the weight they hold to the answer processed and also if an extra bias associated, for that an additional term. The whole processed data after this is passed onto the activation function, which is

a source for adding non-linearity in the system. Without the advent or use of activation function it isn't possible for the system to add non-linearity in the problem and hence a linear function is what will be left in the end. There have been several instances in the past that has shown that single layer of the neuron can depict or approximate any kind of a function with a certain level of accuracy.

$$\phi_{sig}(\xi) = \frac{1}{1 + \exp(-\xi)} \quad (3.6)$$

$$\phi_{id}(\xi) = \xi \quad (3.7)$$

$$\phi_{step}(\xi) = \begin{cases} 1, & \xi > 0 \\ 0, & \text{otherwise,} \end{cases} \quad (3.8)$$

Optimization Algorithm

The optimization problem posed on the algorithm is of a popularly known algorithm i.e. Back-propagation algorithm. The fundamental required necessity for the algorithm is a derivative based function. As the derivative is calculated as parameter to reach near the global optimum. Several Activation function used here are corresponding to the differentiable functions such as the sigmoid function, ReLU, Tanh etc.

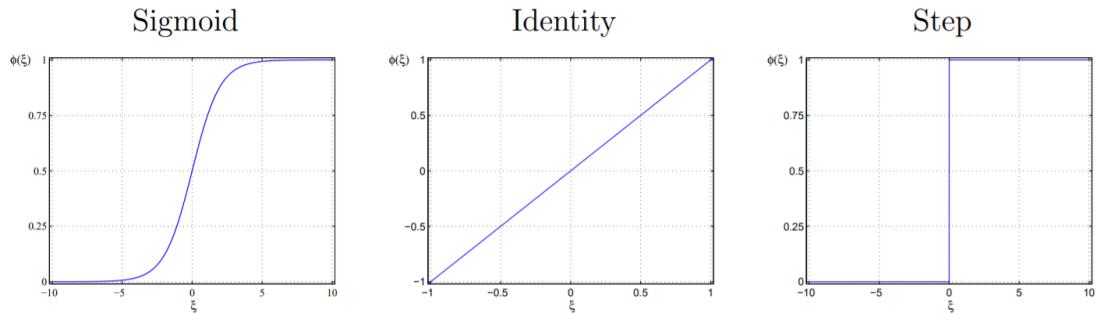


Figure 3.17: Activation Functions : Sigmoid, Identity and Step (From left to right)

The activation functions to be used are corresponding to the kind of application we intend to apply it for, example if the value is corresponding to true or false and henceforth sigmoid function would be used to limit the value between 0 and 1. For tanh, varied data is required for normalized value between 1 and -1. The common problem pertaining to both of these problem is the fact that the curve for the function near the end has infinitely

small values which leads to very small updating of the given function's weight. This leads to very popular choice of the activation function i.e. ReLU that helps in rapid simulation rates and higher computational efficiency pertaining to easy update of the given weights of the system.

3.3.3 ANN : Artificial Neural Network

This section contains the information pertaining to the network topology of the multi-layer network with layers of neurons connected with respect to each other and the processing of the information takes place between the layers, adding extra non-linearity to the system along with enhancing the complexity of the data-driven model to better capture the system relevant features. There are three components to this type of network namely, the first layer then the hidden layer following which there is an output layer. The input layer processes the input to the system wherein the number of neurons used here is equal to the number of the features. Following this we tend to make use of the input information processed to pass on the information to the hidden layers thereby increasing processing the information even-more and hence-forth modelling our complex function.

The output layer is the one which hence collects the information from the processed output of the hidden layers in the action and hence the output layer is the one that finally processes and outputs the data in the number of features expected out of the model in the number of output neurons. The process of calibrating the weights of the system in order to make the model is done with the help of training procedure. The process begins with the random initialization of the weights and thereby the back-propagation and the gradient-descent algorithm comes in and the weights and the biases are updated accordingly. The below are the respective equations presented wherein the weights are multiplied with the respective features and the bias is added. Following this the activation function is applied to the system of output and results are derived.

$$ii_i = io_i = x_i \quad (3.9)$$

$$hi_j = \sum_{i=1}^{Ninputs} wih_{i,j} \cdot x_i + \theta_j \quad (3.10)$$

$$ho_j = \frac{1}{1 + \exp(-hi_j)} \quad (3.11)$$

Here now comes our discussion pertaining to the updating of the system of equations with their respective weights with the help of the Back-propagation which is essentially applied in almost all the supervised trained algorithm. The process essentially contains a minimization or optimization problem of a error function associated with the input and the output of the system. The true output is essentially compared with predicted output and residual generated is used for the back-propagation algorithm. The following are the systems of equation which are used to implement this. Below are the given weight adjustment strategy adopted. The adaptation rate and the momentum rate has been mentioned in the given problem.

$$Error(x) = \frac{1}{2} \cdot \sum_{c=1}^{N_c} (d_c(x) - y_c(x))^2 \quad (3.12)$$

$$W(t+1) = W(t) - \eta \frac{\partial Error}{\partial W}(t) + \alpha \cdot (W(t) - W(t-1)) \quad (3.13)$$

$$\frac{\partial Error}{\partial W}(t) = \frac{\partial Error}{\partial who_{j,k}}(t) = -\delta_k \cdot ho_j \quad (3.14)$$

$$\delta_k = (d_k - y_k) \cdot (1 - y_k) \cdot y_k \quad (3.15)$$

$$\frac{\partial Error}{\partial W}(t) = \frac{\partial Error}{\partial wih_{i,j}}(t) = - \left(h0_j \cdot (1 - ho_j) \cdot \sum_{h=1}^{N_{output}} \delta \cdot who_{j,h} \right) \cdot x_i \quad (3.16)$$

The following are applied to the the data-sets that majoritarian are divided into three major parts that is the training set, Validation set and the test set. The training set is essentially used to calibrate or update the weights of the system and the Validation set is hence used for selection of the best network configuration to be applied to the generalized schemes. Finally the test set is used to refer the accuracy of the model crated here. Essentially the part of the data used as Training set and the Validation set are known as Learning set of the data and the rest is Test set. The major problem with network that may propose over-fitting at times because of the added non-linearity. Hence regularization of the model is to be done or the complexity of the system needs to be reduced by reducing the network's neurons per-say.

3.3.4 Proposed Approach

In this section, we will put forward the details of the framework for Deep Learning based model which can be used as a Reduced Order Model for predicting future time steps of the High Order Model with less computational efforts. The model is based on a Linear Auto-encoder approach which makes use of encoder and decoder architecture for reducing the number of computational nodes. The approach is used to learn the reduced latent subspace through a non-linear approach which helps in reducing the loss of information with comparison to its counterparts such as Proper Orthogonal Decomposition (POD), DMD, Petrov-Galerkin approach etc. which on other hand uses linear approach for the aforementioned function. Training of the model uses vectorized form of data $\tau = [\tau_1, \tau_2, \tau_3, \dots, \tau_n] \in N_t$ which represents the data over t time steps. The state vector represented as $w \in N_w$ and predicted data as $\tau = [\tau_1 + 1, \tau_2 + 1, \tau_3 + 1, \dots]$. The expression of the predicted state variable at time step "t+1" is as presented below.



Figure 3.18: Auto-encoder Architecture

$$\zeta = \psi(w_t; \theta_\psi) \quad (3.17)$$

$$\phi(\zeta) = \hat{w}^{t+1} \quad (3.18)$$

$$\hat{w}^{t+1} = \phi(\psi(w_t; \theta_\psi); \theta_\phi) \quad (3.19)$$

Where the $\phi(\cdot; \theta_\phi)$ represents the decoder network which projects the reduced latent space back to the original high order space with θ_ϕ being its network parameters to optimize. The $\psi(w_t; \theta_\psi)$ network represents the encoder which reduces the previous time step's high order data to a nonlinear reduced subspace with θ_ψ being the network parameters to optimize. We present in the paper following using this architecture that non-linear approach to project is an efficient method in comparison to it's counter-parts. The optimization of the network has been carried out using Mean Squared Error (MSE) approach for the optimization of the network parameters. The mathematical formulation has been presented below, wherein the "e" represents the difference between the predicted and the true state vector.

$$\alpha = \min \frac{1}{N-1} \sum_{n=0}^{N-1} \|e\|_2^2 \quad (3.20)$$

$$\alpha = \min \frac{1}{N-1} \sum_{n=0}^{N-1} \|w^{t+1} - \phi(\psi(w_t))\|_2^2 \quad (3.21)$$

The Auto-encoder approach as stated in this paper involves the use of a deep neural network containing neurons which in the first place are reduced as moving in the forward layers and then increased, so as to reconstruct the next time step. There are two split parts which are referred to as encoder and decoder wherein the encoder compresses the data, thereby performing the function of a Reduced-order-Model and then the decoder reconstructing the reduced state back to the high order output. During the training phase of the architecture, input to the encoder is the vectorized form of the flow-field at the time step "t" and the label corresponding to the output of the decoder is the vectorized form of the flow field at time step "t+1". The Auto-encoder architecture mentioned in the paper has 5 layers of neural network with 3 hidden layers and 3rd layer being the bottleneck layer. The activation function used here for the purpose of adding non-linearity to the ANN was chosen as ReLU. Linear activation is used in the end layer for predicting the vectorized form of the fluid flow prediction. ReLU has been used here since it is computationally less expensive. The mathematical formulation of ReLU function has been presented below.

$$F(x) = \text{Max}(0, x) \quad (3.22)$$

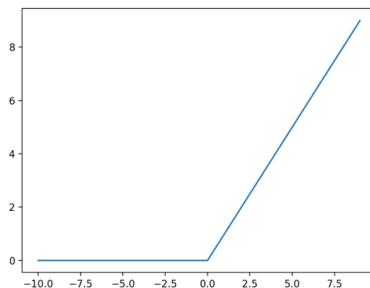


Figure 3.19: ReLU Activation Function

The training of the network has been carried out with the help of ADAM Optimizer with a learning rate of 0.01. The parameters corresponding to encoder and decoder are represented as θ_ψ and θ_ϕ which are optimized with the help of ADAM algorithm. For regularization of the network we use L^2 regularization to eradicate the possibility of overfitting. Weight decay of 0.5 have been used here so as to regularize the network.

Chapter 4

RESULTS and DISCUSSION

4.1 Effect of Network size

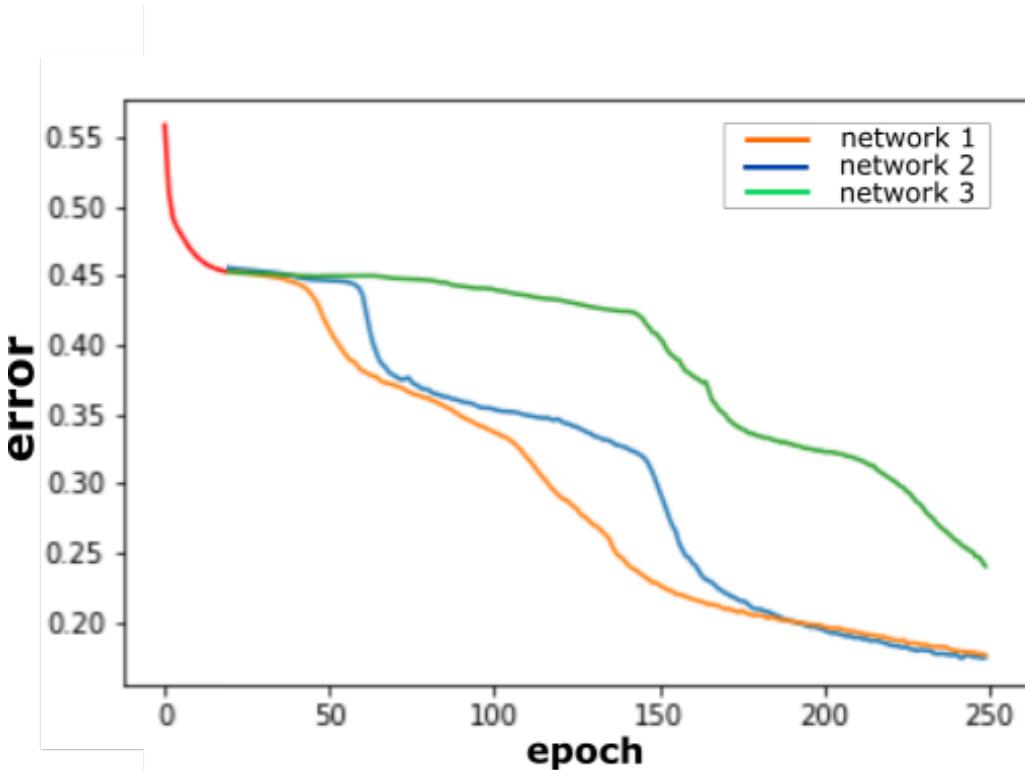


Figure 4.1: Effect of Network Size

In this section we present the effect of network size during training. Three network architecture were chosen with hidden layers as given network:1 [200,100,200], network:2[100,50,100] , network:3 [50,25,50] .The data set of Von Karman street was used in training process. The data size contained 400 time steps and each architecture was trained on it. Vorticity data at 25600 data points was used as input. The number of epoch $n_{epoch} = 250$. It can be seen in fig:4.1 that as the network size was increased i.e

neuron were increased in the hidden layer the training error decreased sharply in case of network one (orange) and in case of network three (green) it decrease sharply in initial epochs but then on it got stuck in local minimum and the error decreased very slowly, this is due to under-fitting.

We also tested this for Sea Surface Temperature data set and found the same result.

4.2 Effect of Training Data size

In this section we present the effect of data size during training. The data set of Von Karman street was used in training process. Two data sizes were used with size one having 921 time steps and size two having 400 timestamps for the training set. Vorticity data at 25600 data points was used as input. The number of epoch $n_{epoch} = 250$. It can be seen in fig:4.2 that with training with larger data size fig:4.2a the error decreased rapidly but with smaller data size fig:4.2b the error plateaued because it got stuck locally. Below from fig fig:4.3 to fig:4.6 is spatial representation of predicted output compared with true values in the case data size two for Von Karman flow and from fig:4.7 to fig:4.10 is spatial representation of predicted output compared with true values for Sea surface temperature data set.

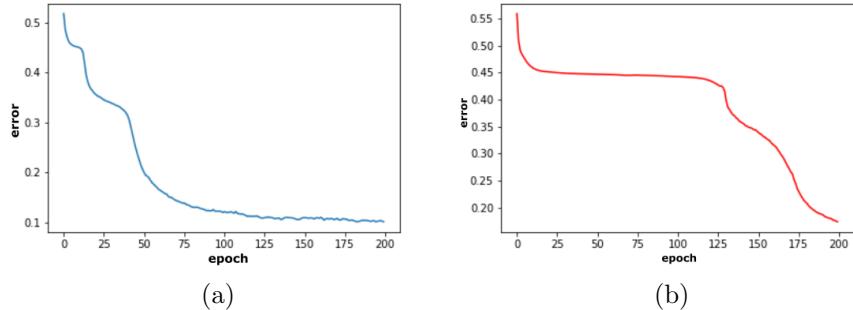


Figure 4.2: Effect of data size: (a) plot for data size one (b) plot for data size two

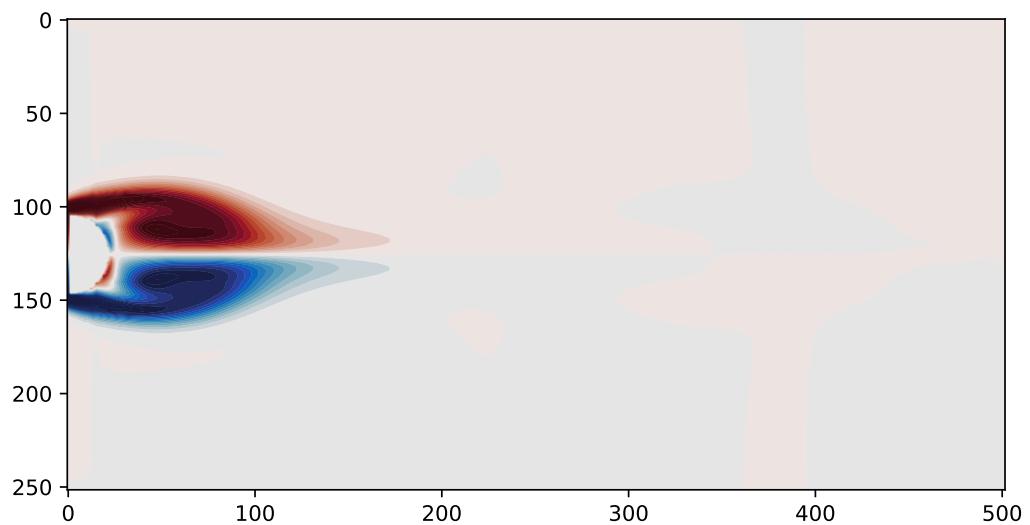


Figure 4.3: True Value of vorticity at time step 5

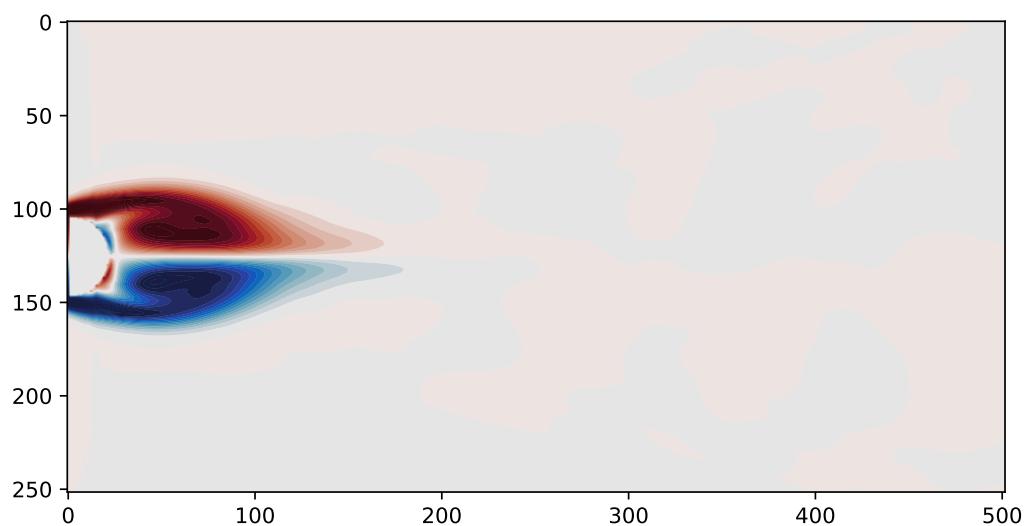


Figure 4.4: Predicted Value of vorticity at time step 5

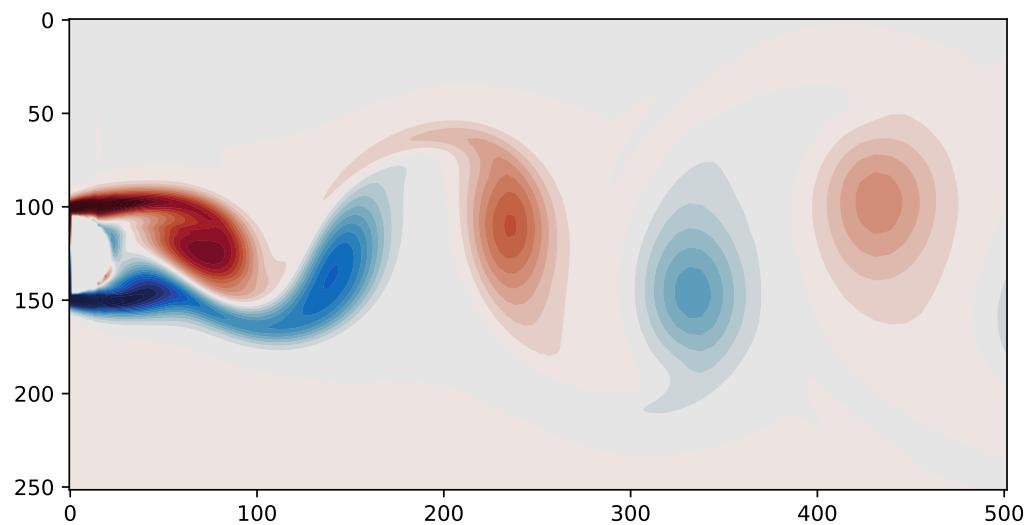


Figure 4.5: True Value of vorticity at time step 50

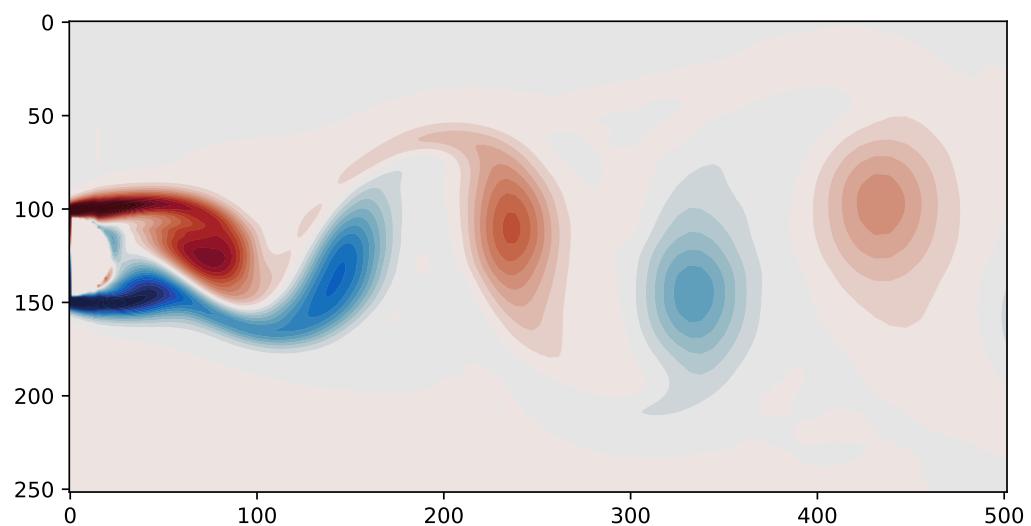


Figure 4.6: Predicted Value of vorticity at time step 50

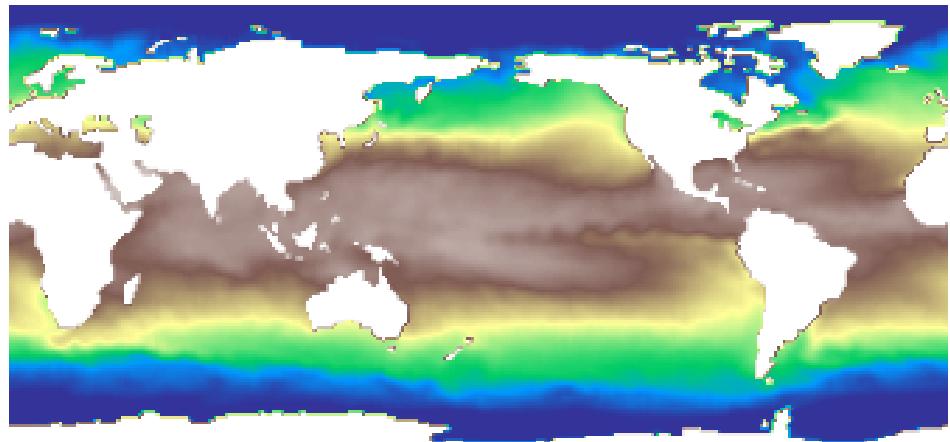


Figure 4.7: True Value of Sea surface temperature at time step 5

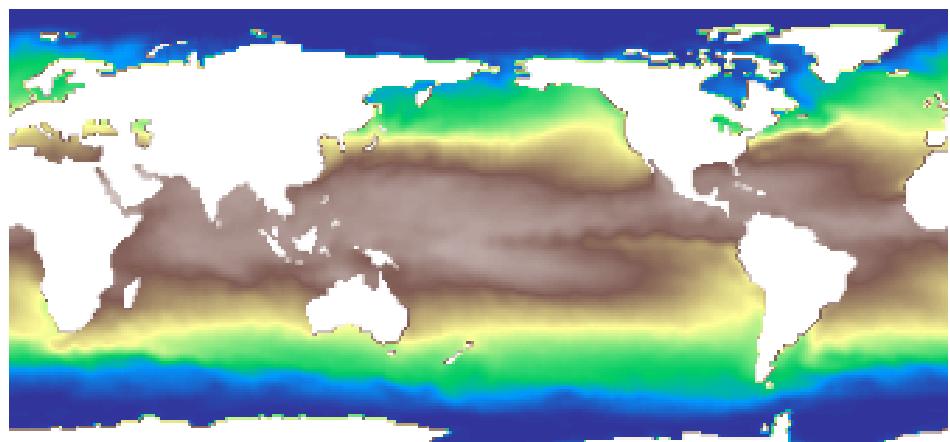


Figure 4.8: Predicted Value of Sea surface temperature at time step 5

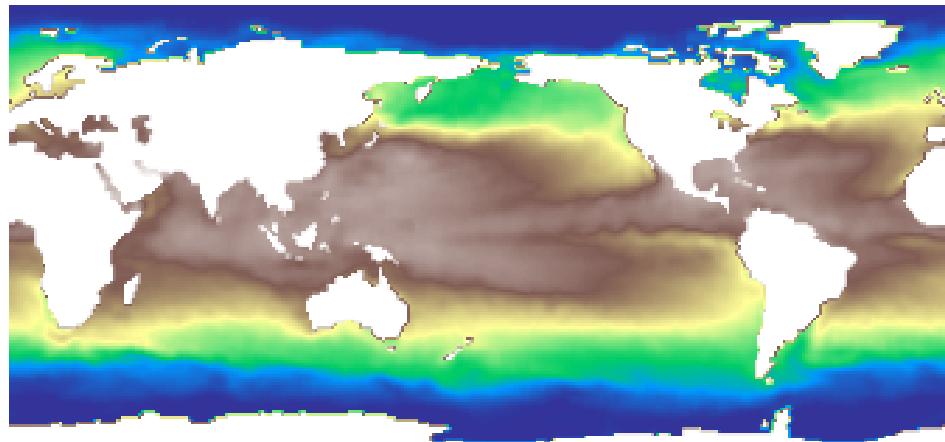


Figure 4.9: True Value of Sea surface temperature at time step 50

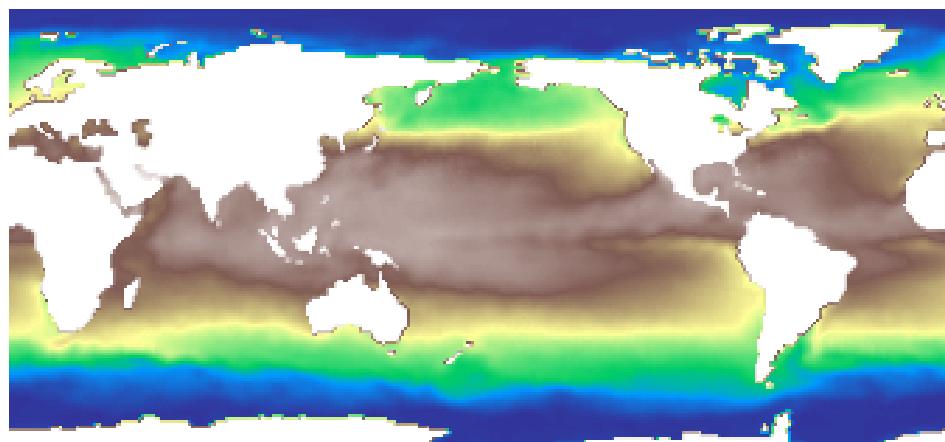


Figure 4.10: Predicted Value of Sea surface temperature at time step 50

Chapter 5

CONCLUSION AND FUTURE SCOPE

This paper presents the Hyper-parameters comparison between different Auto-encoder architectures and there comparison pertaining to each other. This paper presents a Deep learning based Reduced order Model (ROM) which is expected to reduce the losses in the information and extract only relevant data in the bottleneck layer so as to reconstruct the high order dynamics efficiently from the reduced state. We were successful in coding and simulating the encoder algorithm through cloud service provided by google (google colab). The training time was practical and the dataset was of normal size making the solution feasible. We have made comparison between network architectures wherein the following conclusion was made, i.e. the training error sharply decreased as we increased the network size, which has its underlying reason for added non-linearity in the network but also leads to a relatively more computationally expensive model to its counter-part architecture. Following this we also make comparison between increased size of dataset and lower amount of dataset which were generated with the help of different time-steps. It was seen and concluded that a larger dataset helped in converging to the solution much rapidly and easily in comparison to the shorter dataset. The numerical Accuracy of Deep learning Autoencoder is of order of magnitude higher than that provided by linear ROMs.

As for the future scope of the project instead of using artificial neural network we can use conversational neural network and work out the same problems. Combining this machine learning method with something more deterministic can we future work, where we can combine neural network power of approximating functions with physical dynamical equations to achieve convergence and to solve problems that have non-linear equations describing their motion. This way we can aim to reduce computation time to train the neural network and get better accurate results.

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Hyper-Parameter Analysis of Deep Auto Encoder for Flow Prediction

Prakrit Tyagi, Pranav Bahl and B B Arora

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Hyper-Parameter analysis of Deep Auto Encoder for Flow Prediction

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Abstract. Reducing the order of the system from high order dynamical space to a low dimensional subspace has been a challenging task and the models that achieve this are referred to Reduced Order Models (ROMs). Linear Projection methods have been used extensively in the past for building such ROMs, some common examples are POD,DMD etc. Though they have been successful in modelling several non-linear scenarios, their usage limits their applications pertaining to complex High order dynamical systems efficiently. In this study we aim to make use of advancement made in the field of Deep Learning to build a DL based ROM. We aim to probe the impact of hyper-parameters pertaining to flow prediction using deep autoencoders built with the help of artificial neural network. The parameters for our study that were used here were three different network sizes and two data sizes to compare the performance in flow prediction. Dataset for the Vorticity was generated using in-compressible URANS CFD solver icoFoam in an open-source CFD toolbox OpenFOAM. Von-Karman Vortex Street at Reynolds' number 100 around a bi-dimensional cylinder was simulated for our study.

Keywords: Deep Autoencoder · Von Karman Vortex Street · Hyper-parameters.

1 Introduction

Advances in Machine Learning techniques has made its usage reliable and economical and opened plethora of applications in fields of robotics , neuro science, economic and financial prediction, system dynamic modeling and prediction etc.. Autoencoder is one such technique which learns by itself to represent large data in reduced form. This is advantageous as using low dimensional data for analysis and calculation is efficient, computationally economical and reduces cost. Therefore this technique has found extensive usage in flow reconstruction, reduced-order modeling [1], prediction of fluid flow dynamical system [2] and flow prediction [3].

Computational fluid dynamics is the go to technique for simulating fluid flow but it is computationally expensive and if a users has inadequate resources, he/she will find it difficult to simulate and innovate. However, CFD has found its application across various engineering disciplines such as Aerospace industry, Heating and Ventilation applications, Flows corresponding to cardiovascular operation, Fluid machinery etc [4]. The need for such simulation often requires

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This is to enlighten you that the above manuscript has been appraised by the editors of LNME and is accepted for the **6th International Conference on Advanced Production and Industrial Engineering (ICAPIE)- 2021 to be held during June 18-19, 2021**. The paper is recommended for publication in **Lecture Notes in Mechanical Engineering (Scopus Indexed publication of Springer Nature), ISSN: 2195-4356**. The manuscript has been submitted to Springer in May 2021 and will be online during October 2021.

Finally, the team of CAPIER DTU and ICAPIE-2021 would like to extend congratulations to you.

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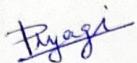
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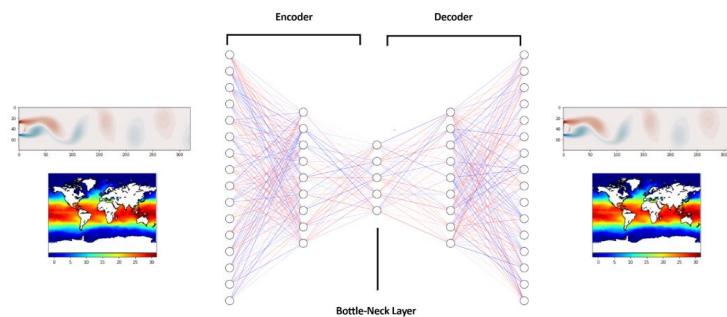
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Hyper-Parameter analysis of Deep Auto Encoder for Flow Prediction



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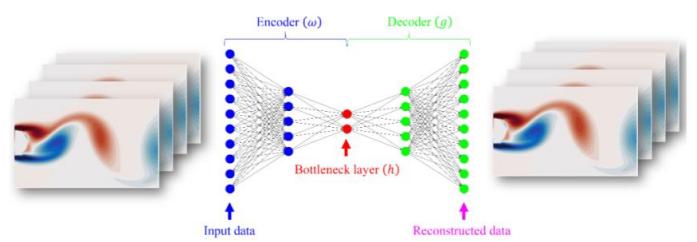
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Outline

- Motivation
- Problem Statement
- Formulation
- Results
- Conclusion

Motivation

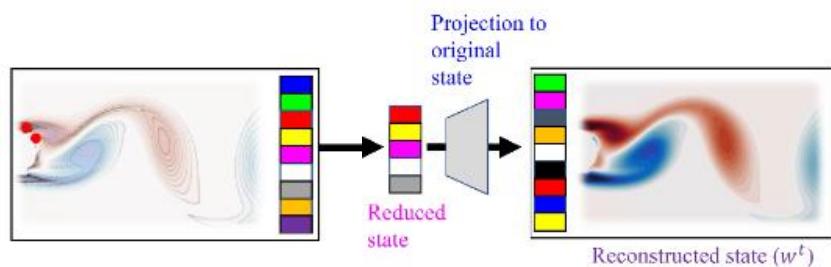
- Fluid Flow prediction is computationally expensive when using iterative algorithms for solving parametric equation.
- Explosion of data and available computation resource has made machine learning appealing.
- Machine learning can help solve most challenging nonlinear problems in feasible manner that classically take enormous amount of time and computation .
- Challenges:
 - Low availability of data
 - Data is noisy



Problem Statement

To analyse the effect of changing hyper-parameters values in accuracy of prediction.

- Consider a problem of predicting flow pattern if given information about existing condition, spatial and temporal features of flow.
- Autoencoder modelled with three hidden layer plus input and output layer is to be trained on vorticity data of flow around a cylinder and on sea surface temperature data.
- The trained model must be able to predict future flow pattern accurately.
- Compare results for each case of hyperparameters.



Formulation: Autoencoder

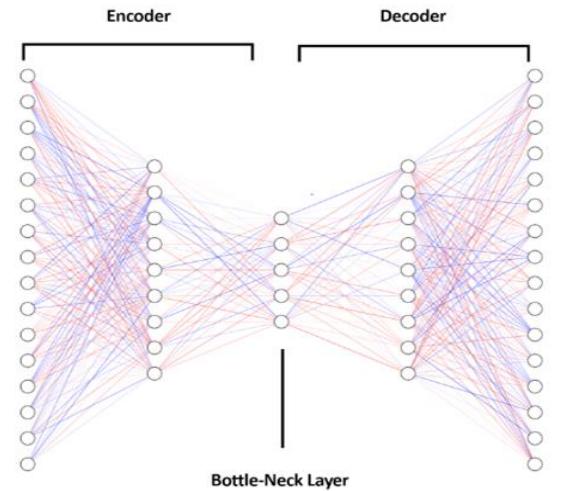
- Artificial Neural Network is a computational model consisting of various neurons or functional nodes.
- The input data is multiplied to corresponding weights and a bias is added following which an activation function is applied to the whole output of the neuron to add the nonlinearity to the function
- A loss function is decided at the end of the network as a means to optimize the parameters of the model.

Remark 1: A situation where $\mathbf{g}(\omega(\xi)) = \xi$ everywhere needs to be avoided [33]. In other words, the training algorithm is designed in such a way to restrict direct copying of the input.

Remark 2: In AE, the dimensionality of the latent space $\mathbf{h} \in \mathbb{R}^h$ is generally much smaller than the dimensionality of the input variable $\xi \in \mathbb{R}_N$, $h \ll N$. Therefore, \mathbf{h} can be thought of as a reduced-order representation of ξ .

Remark 3: When the decoder \mathbf{g} is linear, and \mathcal{L} is a mean-squared error, an AE learns to span the same subspace as principal component analysis.

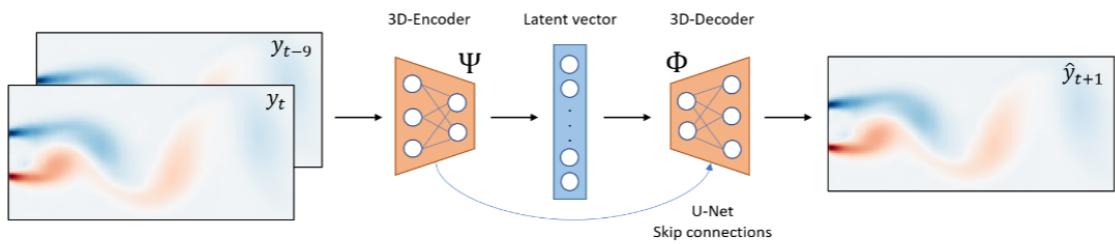
Remark 4: AE with nonlinear encoder ω and nonlinear decoder \mathbf{g} learns a nonlinear reduced-



$$\mathbf{h} = \omega(\xi), \hat{\xi} = \mathbf{g}(\mathbf{h}),$$

$$\alpha = \arg \min_{\alpha} \mathcal{L}(\xi_t, \mathbf{g}(\omega(\xi)); \alpha),$$

Formulation: Proposed Approach



Mapping Data from Input to the Reduced State and back to Original state

$$\phi(\zeta) = \hat{w}^{t+1} \quad \zeta = \psi(w_t; \theta_\psi)$$

Predicting the state of the vector from a given input

$$\hat{w}^{t+1} = \phi(\psi(w_t; \theta_\psi); \theta_\phi)$$

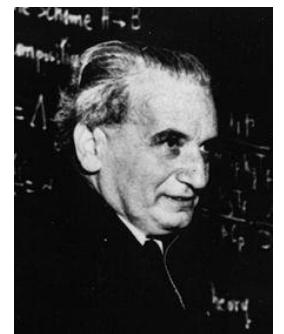
Relative Error : Quantitative Metric for measuring Accuracy

$$\alpha = \min \frac{1}{N-1} \sum_{n=0}^{N-1} \|e\|_2^2$$

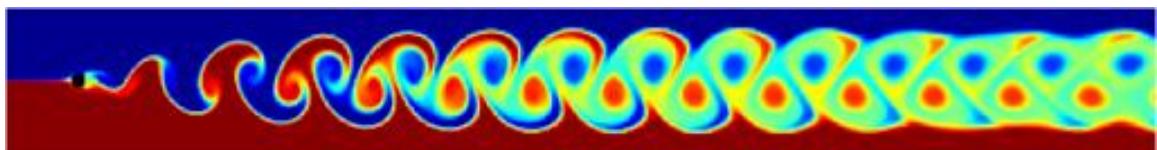
$$\alpha = \min \frac{1}{N-1} \sum_{n=0}^{N-1} \|w^{t+1} - \phi(\psi(w_t))\|_2^2$$

Von Karman Vortex Street

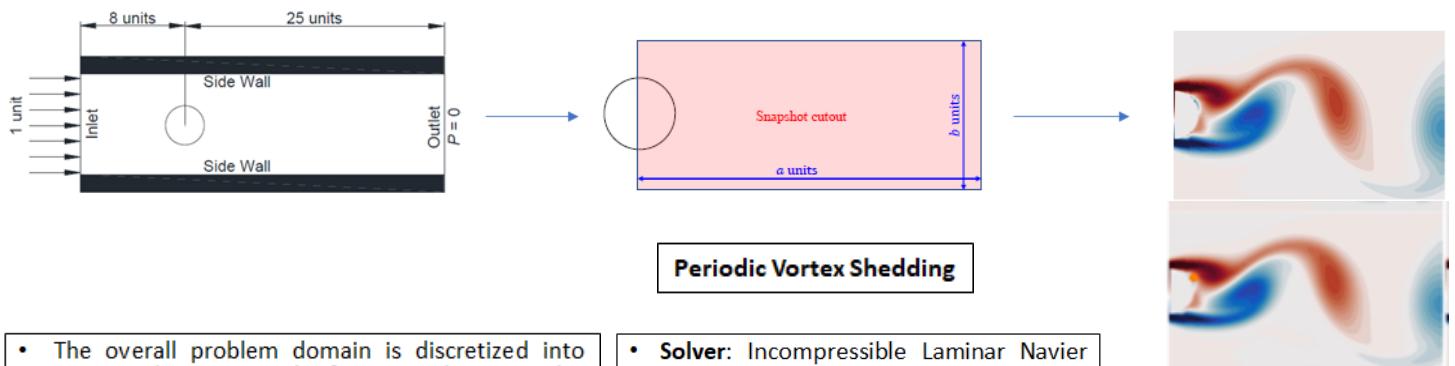
- 1) A Kármán vortex street (or a von Kármán vortex street) is a repeating pattern of swirling vortices, caused by a process known as vortex shedding. It is formed in the wake of the flow around a bluff body.
- 2) When the Reynold's number exceeds about 30, the two vortices formed behind the body gets stretched and are washed down. At the place of these two vortices, two new are formed and the process continues.
- 3) Karman gave the explanation for this phenomenon and according to him there are two possible configuration of the vortex trail i.e. symmetrical and the staggered configuration.
- 4) Formation is dependent on Reynold's number of the flow, less than 5 no shedding, 5 to about 40 fixed symmetrical vortex, above 90 alternating vortices shedding starts.
- 5) The frequency of the shedding is directly proportional to the Dimensionless quantity "Strouhal Number"



Theodore von Kármán



Numerical Experiment (OpenFOAM)



- The overall problem domain is discretized into 63420 elements with finer mesh near the cylinder. Time step $\delta t = 0.02$ units is considered.
- Training: 180 Snapshots ; Valid: 60 , Test: 60
- Separation b/w snapshots: $10 \delta t$
- Reynolds Number : 190
- $168 * 251$ points in X and Y direction
- $a = 6$ units ; $b = 4$ units

- Solver:** Incompressible Laminar Navier Stokes solver based on PISO Algorithm -- **IcoFoam** solver (OpenFOAM)
- No Slip boundary condition at body.
- Inlet Velocity : 1 unit ; Outlet Pressure: 0

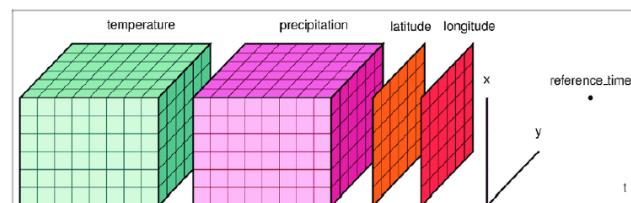
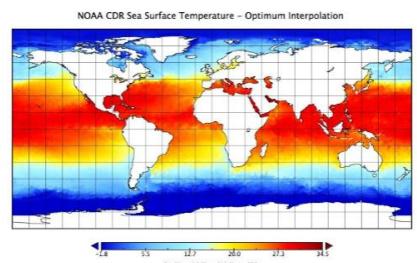
$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) - \nabla \cdot (\nu \nabla \mathbf{u}) &= -\nabla p \end{aligned}$$

Ref 1: Nirmal J. Nair and Andres Goza. Leveraging reduced-order models for state estimation using deep learning. *Journal of Fluid Mechanics*, 897:R1, 2020.

Ref 2: Kumar, Yash, Pranav Bahl, and Souvik Chakraborty. "State estimation with limited sensors-A deep learning based approach." *arXiv preprint arXiv:2101.11513* (2021).

Dataset : NOAA OISST V2 - Sea Surface Temperature

- 1) NOAA (OI) Sea Surface Temperature V2 data-set has been made publicly available by the Physical sciences division at NOAA.
- 2) The temporal resolutions available for the data-set are weekly, monthly and monthly long-term mean data.
- 3) The weekly-data is centered on Wednesday for the brief period of 1990-2020 and on Sunday for the period of 1981-1989.
- 4) The spatial resolution of the data is 1-deg latitude and 1-deg longitude leading to 180 x 360 grid points. This was chosen as the High Resolution Data.
- 5) The spatial resolution of the data 2-deg latitude and 2-deg longitude leading to 90 x 180 grid points was chosen as the Low Resolution Data.
- 6) Training 400 snapshots : Monthly data (1984 – 2021)
- 7) Training : 1500 snapshots : Weekly Data (1990 – 2021)



Simulation Results

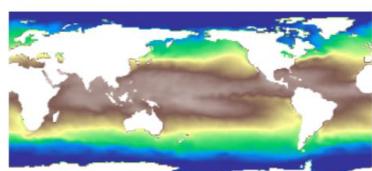


Figure 4.7: True Value of Sea surface temperature at time step 5

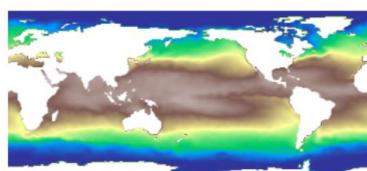


Figure 4.8: Predicted Value of Sea surface temperature at time step 5

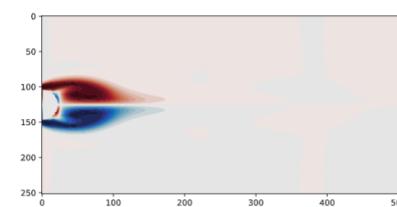


Figure 4.3: True Value of vorticity at time step 5

Figure 4.4: Predicted Value of vorticity at time step 5

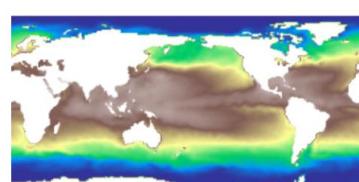


Figure 4.9: True Value of Sea surface temperature at time step 50

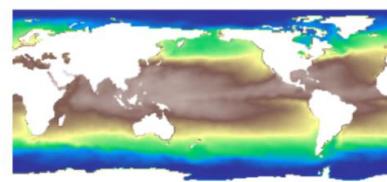


Figure 4.10: Predicted Value of Sea surface temperature at time step 50

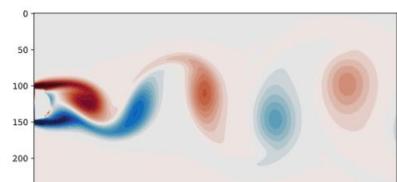
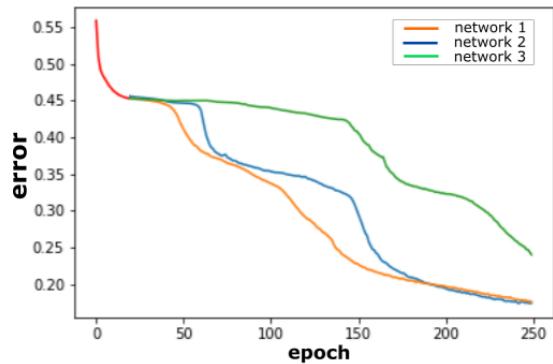


Figure 4.5: True Value of vorticity at time step 50

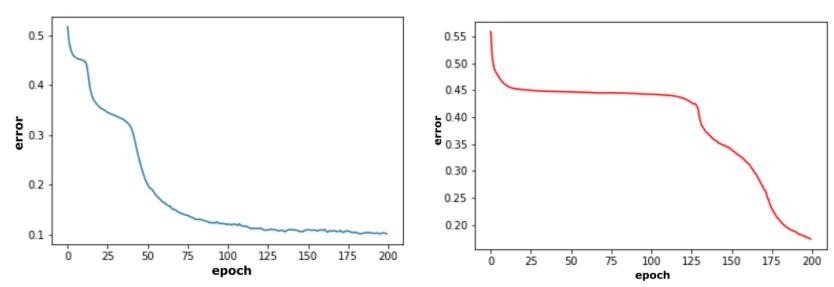
Figure 4.6: Predicted Value of vorticity at time step 50

Simulation Results

Effect of Network size



Effect of Data size



Conclusion and Future Work

We have made comparison between network architectures wherein the following conclusion was made,

- ❖ The training error sharply decreased as we increased the network size, which has its underlying reason for added non-linearity in the network but also leads to a relatively more computationally expensive model to its counterpart architecture.
- ❖ Following this we also make comparison between increased size of dataset and lower amount of dataset which were generated with the help of different time-steps. It was seen and concluded that a larger dataset helped in converging to the solution much rapidly and easily in comparison to the shorter dataset.
- ❖ Make use of autoencoder based 3D-UNets to generate reduced order models and to use this reduced state to predict future timesteps presents a novel and effective solution for reducing computational runtimes of CFD simulations.