AA-PINN: Attention Augmented Physics Informed Neural Networks

Abhinav Sagar
Vellore Institute of Technology
Vellore, Tamil Nadu, India
abhinavsagar4@gmail.com

Abstract

Physics Informed Neural Networks has been quite successful in modelling the complex nature of fluid flow. Computational Fluid Dynamics using parallel processing algorithms on GPUs have considerably reduced the time to solve the Navier Stokes Equations. CFD based approaches uses approximates to make the modelling easy but it comes at the cost of decrease in accuracy. In this paper, we propose an attention based network architecture named AA-PINN to model PDEs behind fluid flow. We use a combination of channel and spatial attention module. We propose a novel loss function which is more robust in handling the initial as well as boundary conditions imposed. Using evaluation metrics like RMSE, divergence and thermal kinetic energy, our network outperforms previous PINNs for modelling Navier Stokes and Burgers Equation.

1. Introduction

Computational Fluid Dynamics (CFD) has become the core technology behind every fluid simulation. Deep learning uses powerful information-processing algorithms for modeling, optimization, and control of fluids. Fluid mechanics has been traditionally concerned with big data, thus making deep learning an obvious choice in modelling the complexity. Neural Networks of late has been quite successful in understanding, predicting, optimizing, and controlling fluid flows. Some of the more complex problems in fluid mechanics, such as reduced-order modeling and shape optimization can be modelled as optimization and regression tasks.

Neural Network has proven to improve optimization performance and reduce convergence time drastically. Neural network is also used for turbulence modelling, dimensionality reduction, identifying low and high dimensional manifolds and understanding continuous and discrete flow regimes. Deep learning algorithms are able to take into account inherent complexity of the problem thus optimizing for the performance, robustness or convergence for complex tasks. It helps in providing a general purpose framework for interpretability, generalizability and explainability of the results achieved. Understanding the physics behind fluid flows is a complex problem which can be solved using neural networks by feeding lots of training data.

2. Related Work

Neural network to solve Reynolds Averaged Navier Stokes Equation was proposed by (Ling et al., 2016). The Reynolds stress term was modelled using DNS equation by (Wang et al., 2017). Neural network was used to model turbulent flows using Large Eddy simulation (Zhou et al., 2019). A convolutional neural network was used to model the velocity field over a cylinder (Jin et al., 2018). (Wu et al., 2020) proposed a similar CNN based method to model the unsteady flow in arbitrary fluid regimes. A thorough study of data driven methods using machine learning approaches for modelling the turbulence was studied by (Duraisamy et al., 2019).

(Brunton et al., 2020) also did a comprehensive study of machine learning approaches for modelling different kind of problems in fluid mechanics. (Raissi et al., 2017) proposed physics informed neural networks for solving nonlinear partial differential equations using neural network. This work was further improved in (Raissi et al., 2019). The theoretical exact solution of the 3d Navier Stokes equation was shown by (Ethier and Steinman, 1994). Deep feedforward neural networks was used (Lui and Wolf, 2019) for modelling complex flow regimes. CNN were used for making faster fluid simulation (Tompson et al., 2017).

A novel neural network was proposed for solving the function approximation and inverse PDE problems (Meng and Karniadakis, 2020). (Khoo et al., 2021) used neural network for solving parametric PDEs. (Meng et al., 2020) proposed a neural network for solving unsteady PDEs. Bayesian neural network was used to quantify the uncertainty while solving PDEs (Yang et al., 2021). Data driven approaches for solving PDEs was proposed by (Long et al., 2018) and (Long et al., 2019). c(Sirignano et al., 2020) used neural network for solving PDEs in the context of large-eddy simulation.

(Bar and Sochen, 2019) was one of the first works to use unsupervised learning for solving PDEs.

(Thuerey et al., 2020) proposed a deep learning approach for solving Reynolds-averaged Navier-Stokes equation around airfoils. Another approach for solving PDEs using deep learning was used (Miyanawala and Jaiman, 2017) in the context of unsteady wake flow dynamics. A comprehensive study of deep learning approaches for modelling and solving fluid mechanics problem was done by (Kutz, 2017). (Ranade et al., 2021) proposed a deep learning based solver for Navier–Stokes equations using finite volume discretization. Neural networks was used for solving incompressible Navier-Stokes equations (Jin et al., 2021). A method for predicting turbulent flows using deep learning was proposed by (Wang et al., 2020).

Our main contributions can be summarized as:

• A novel network architecture combining channel and spatial attention mechanism is used for modelling the inherent complexity in fluid flow problems.

• We train and test our network using a more robust loss function for solve PDEs behind incompressible Navier Stokes and Burgers Equation.

• Our network achieves better results than previous PINNs using commonly used evaluation metrics while still running at good enough speed.

3. Background

3.1. Navier Stokes Equation

The incompressible transient two dimensional Navier-Stokes equations for mass and momentum conservation are written as defined in the below set of equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu \nabla^2 u_x + g_x \tag{2}$$

$$u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu \nabla^2 u_y + g_y \tag{3}$$

in which u is the velocity field (with x and y components for 2 dimensional flows). A non-uniform steady-state flow condition is assumed, hence the accumulation term (time t dependence term) is dropped. Here g represents the gravitational acceleration and μ the dynamic viscosity of the fluid. The terms on the left-hand side of these equations represents the convective transport, whereas the terms on the right-hand side represents the pressure coupling and diffusive transport.

3.2. Momentum Equations

When the difference operators are expanded using uniform grid spacing h and time step k results in:

$$\begin{aligned} u_{i,j} - \frac{k\nu}{h^2}\left(u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i,j+1} + \right. \\ \left. u_{i+1,j} + \frac{k}{h}\left(\bar{u}^n_{i+1,j}\bar{u}_{i+1,j} - \bar{u}^n_{i,j}\bar{u}_{i,j}\right) + \frac{k}{h}\left(\bar{v}^n_{i,j}\widetilde{u}_{i,j} - \right. \right. \\ \left. \left. \bar{v}^n_{i,j-1}\widetilde{u}_{i,j-1} = u^n_{i,j} - \frac{k}{h}\left(p_{i+1,j} - p_{i,j}\right)\right) \end{aligned} \tag{4}$$

Where variables without superscripts denote advanced time level results to be computed. Using the formulas of the averages and collecting the terms results in equation below:

$$\begin{aligned} -A_1 u_{i-1,j} - A_2 u_{i,j-1} + A_3 u_{i,j} - A_4 u_{i,j+1} - \\ A_5 u_{i+1,j} = b_{i,j} - \frac{k}{h}\left(p_{i+1,j} - p_{i,j}\right) \end{aligned} \tag{5}$$

The various coefficients in the above equation are given using the set of equations as follows:

$$A_1 = \frac{k}{h}\left(\frac{\nu}{h} + \frac{1}{2}\bar{u}^n_{i,j}\right) \tag{6}$$

$$A_2 = \frac{k}{h}\left(\frac{\nu}{h} + \frac{1}{2}\bar{v}^n_{i,j-1}\right) \tag{7}$$

$$A_3 = 1 + 4\frac{k\nu}{h^2} + \frac{k}{2h}\left(\bar{u}^n_{i+1,j} - \bar{u}^n_{i,j} + \bar{v}^n_{i,j} - \bar{v}^n_{i,j-1}\right) \tag{8}$$

$$A_4 = \frac{k}{h}\left(\frac{\nu}{h} - \frac{1}{2}\bar{v}^n_{i,j}\right) \tag{9}$$

$$A_5 = \frac{k}{h}\left(\frac{\nu}{h} - \frac{1}{2}\bar{u}^n_{i+1,j}\right) \tag{10}$$

It is to be noted that in the continuous equations, we ignored effects of correction quantities in advective and diffusive terms. The u-component velocity correction can be written in the form as defined in Equation below:

$$u'_{i,j} = \frac{k}{A_3 h}\left(p'_{i,j} - p'_{i+1,j}\right) \tag{11}$$

We now present analogous results for the y-momentum equation. The v-component velocity correction can be written in the form as defined in Equation below:

$$v'_{i,j} = \frac{k}{B_3 h}\left(p'_{i,j} - p'_{i,j+1}\right) \tag{12}$$

3.3. Pressure Poisson Equation

By substituting the velocity corrections into the discrete continuity equation for grid cell (i, j) results in:

$$\frac{u_{i,j} - u_{i-1,j}}{h_x} + \frac{v_{i,j} - v_{i,j-1}}{h_y} = 0 \tag{13}$$

After substituting the decomposed velocity components, the above equation can be written as:

$$\frac{(u^* + u')_{i,j} - (u^* + u')_{i-1,j}}{h_x} + \frac{(v^* + v')_{i,j} - (v^* + v')_{i,j-1}}{h_y} = 0 \tag{14}$$

For simplicitiy, we set h_x = h_y = h, and rewrite this as:

$$\begin{aligned} -\frac{1}{A_{3,i-1,j}} p'_{i-1,j} - \frac{1}{B_{3,i,j-1}} p'_{i,j-1} + \left(\frac{1}{A_{3,i,j}} + \frac{1}{A_{3,i-1,j}} + \right. \\ \left. \frac{1}{B_{3,i,j}} + \frac{1}{B_{3,i,j-1}} \right) p'_{i,j} - \frac{1}{B_{3,i,j}} p'_{i,j+1} - \\ \frac{1}{A_{3,i,j}} p'_{i+1,j} = -\frac{h^2}{k} D^*_{i,j} \end{aligned} \tag{15}$$

It can alternatively written in a more compact form similar to that used for the momentum equations:

$$C_1 p'_{i-1,j} + C_2 p'_{i,j-1} + C_3 p'_{i,j} + C_4 p'_{i,j+1} + C_5 p'_{i+1,j} = d^*_{i,j} \tag{16}$$

The various coefficients in the above equation is defined as follows:

$$\begin{aligned} C_1 &\equiv \tfrac{1}{A_{3,i-1,j}}, \quad C_2 \equiv \tfrac{1}{B_{3,i,j-1}}, \\ C_3 &\equiv -\left(\tfrac{1}{A_{3,i,j}} + \tfrac{1}{A_{3,i-1,j}} + \tfrac{1}{B_{3,i,j}} + \tfrac{1}{B_{3,i,j-1}} \right) \\ C_4 &\equiv \tfrac{1}{B_{3,i,j}}, \quad C_5 \equiv \tfrac{1}{A_{3,i,j}}, \quad d^*_{i,j} \equiv \tfrac{h^2}{k} D^*_{i,j} \end{aligned} \tag{17}$$

3.4. Burger's Equation

In one space dimension, the Burger's equation along with Dirichlet boundary conditions is defined using the below set of equations:

$$\begin{aligned} &u_t + u u_x - (0.01/\pi) u_{xx} = 0, \quad x \in [-1, 1], \quad t \in [0, 1] \\ &u(0, x) = -\sin(\pi x) \\ &u(t, -1) = u(t, 1) = 0 \end{aligned} \tag{18}$$

Here, t^i_u, x^i_u, u_i N_u i=1 denotes the initial and boundary training data on $u(t, x)$ and t^i_f, x^i_f N_f i=1 denotes the collocations points for $f(t, x)$. The loss MSE_u corresponds to the initial and boundary data while MSE_f enforces the structure used by equation at a finite set of collocation points.

4. Method

4.1. Spatial Attention Module

The spatial attention module is used for capturing the spatial dependencies of the feature maps. The spatial attention (SA) module used in our network is defined below:

$$f_{SA}(x) = f_{sigmoid}\left(W_2\left(f_{ReLU}\left(W_1(x)\right)\right)\right) \tag{19}$$

where W_1 and W_2 denotes the first and second 1×1 convolution layer respectively, x denotes the input data, $f_{Sigmoid}$ denotes the sigmoid function, f_{ReLU} denotes the ReLu activation function.

The spatial attention module used in this work is shown in Figure 1:

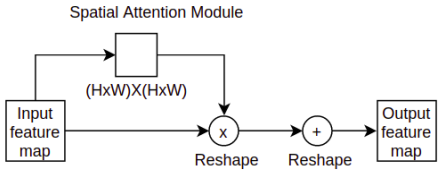

Figure 1. Details of our spatial attention module

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4.2. Channel Attention Module

The channel attention module is used for extracting high level multi-scale semantic information. The channel attention (CA) module used in our network is defined below:

$$f_{CA}(x) = f_{sigmoid}(W_2(f_{ReLU}(W_1 f^1_{AvgPool}(x)))) \tag{20}$$

where W_1 and W_2 denotes the first and second 1×1 convolution layer, x denotes the input data. $f^1_{AvgPool}$ denotes the global average pooling function, $f_{Sigmoid}$ denotes the Sigmoid function, f_{ReLU} denotes ReLU activation function.

The channel attention module used in this work is shown in Figure 2:

4.3. Network Architecture

We use deep convolutional neural network in this work. The input is the spatial and temporal co-ordinates of the points in the fluid flow domain. This information is propagated to three Residual blocks sequentially. In between the blocks, channel attention module is used to weight the usefulness of important features and spatial attention module is

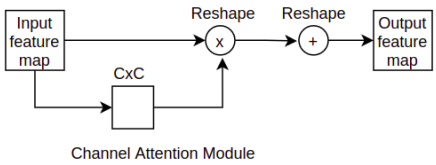

Figure 2. Details of our channel attention module

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used for modelling the inter-spatial relationship of features. Fusion operator is used to merge the individual features. The output is the spatio-temporal pressure and velocity fields predicted. The complete network architecture used in this work is shown in Figure 3:

4.4. Loss Functions

The MSE loss function is used for both the X and Y components of momentum equation which is defined as:

$$MSE_u = \frac{1}{N_u}\sum_{i=1}^{N_u}\left|u\left(t_u^i, x_u^i\right) - u^i\right|^2 \tag{21}$$

$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f}\left|f\left(t_f^i, x_f^i\right)\right|^2 \tag{22}$$

The shared parameters between the neural networks $u(t,x)$ and $f(t,x)$ can be learned by minimizing the mean squared error loss as defined using in the equation below:

$$MSE_t = \alpha MSE_u + \beta MSE_f \tag{23}$$

The weighting coefficients α and β are used to balance different terms of the loss function and accelerate convergence in the training process. The individual loss function terms L_e, L_b and L_i represent loss function components corresponding to the residual of the Navier-Stokes equations, the boundary conditions, and the initial conditions, respectively. The loss function is defined using the set of equations below:

$$L_e = \frac{1}{N_e}\sum_{i=1}^{4}\sum_{n=1}^{N_e}|e_{VPi}^n|^2 \tag{24}$$

$$L_b = \frac{1}{N_b}\sum_{n=1}^{N_b}|\mathbf{u}^n - \mathbf{u}_b^n|^2 \tag{25}$$

$$L_i = \frac{1}{N_i}\sum_{n=1}^{N_i}|\mathbf{u}^n - \mathbf{u}_i^n|^2 \tag{26}$$

Where N_b, N_i and N_e denote the number of training data for different terms. The above 3 terms can be combined to give:

$$L_t = \gamma L_e + \delta L_b + \rho L_i \tag{27}$$

The weighting coefficients γ, δ and ρ are used to balance different terms of the loss function and accelerate convergence in the training process. The complete loss function for training the parameters of our network is defined as follows:

$$L_{final} = MSE_t + L_t \tag{28}$$

4.5. Optimization Details

For a general gradient descent algorithm, the iterative formulation of the parameters of our network can be expressed as:

$$\begin{aligned}\theta^{(k+1)} = \theta^{(k)} - \eta\gamma\nabla_\theta L_e - \eta\delta\nabla_\theta L_b - \\ \eta\rho\nabla_\theta L_i - \eta\alpha\nabla_\theta MSE_u - \eta\beta\nabla_\theta MSE_f\end{aligned} \tag{29}$$

where θ denotes the parameters of the neural network, namely the weights of all the layers, k is the iteration step, and η is the learning rate.

4.6. Evaluation Metrics

Root Mean Square Error (RMSE) is the most popularly used metric for quantifying the prediction performance. The downside of using it is that it only measures indivdual pixel differences. There is a need to check whether the predictions are physically meaningful and preserve desired physical quantities, such as Turbulence Kinetic Energy and Divergence. In this work, we use following metrics for evaluation.

1. Root Mean Square Error: We calculate the RMSE of all predicted values from the ground truth for each pixel.

2. Divergence: We study about incompressible turbulent flows in this work, which means the divergence, δw, at each pixel should be zero. We use the average of absolute divergence over all pixels at each prediction step as an additional evaluation metric.

3. Turbulence Kinetic Energy: In fluid dynamics, turbulence kinetic energy is the mean kinetic energy per unit mass associated with eddies in turbulent flow. Physically, the turbulence kinetic energy is characterised by measured root mean square velocity fluctuations as defined by:

$$\left(\overline{(u')^2} + \overline{(v')^2}\right)/2, \quad \overline{(u')^2} = \frac{1}{T}\sum_{t=0}^{T}(u(t) - \bar{u})^2 \tag{30}$$

where t is the time step. We calculate the turbulence kinetic energy for each predicted sample of 100 velocity fields.

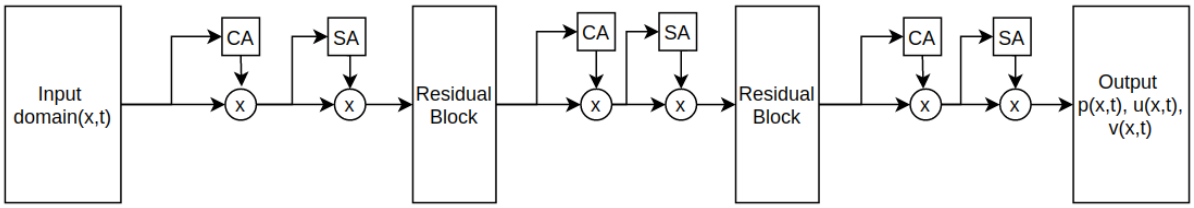

Figure 3. Illustration of our network architecture. A residual block denotes convolution, max pooling, relu activation function and batch normalization layer sequentially; CA and SA denotes channel and spatial attention module respectively; x denotes fusion operator.

4.7. Implementation Details

An adaptive optimization algorithm, Adam (Kingma and Ba, 2014), is used to optimize the loss function. The parameters of the neural networks are randomly initialized using the Xavier intitalization scheme. We simulate turbulent channel flow at $Re_\tau = 9.99 \times 10^2$ using our network. The time step value of 0.005 is used for evaluating the residuals our network. We feed the training data using mini-batches to train our network in this study. There are three parts in the input data corresponding to the initial conditions, the boundary conditions and the residuals of equations respectively. We place 100,000 points inside the domain and 25,000 points on the boundary sampled at each time step, and 150,000 points at the initial time step to determine the loss function. The total number of iterations in one training epoch used is 100. The hyper-parameter values are $\alpha = 100$, $\beta = 100$.

5. Results

The performance comparison of our network with previous state of the art is shown in Table 1:

The exact and learned dynamics solution for the Burgers equation using our network is shown in Figure 4:

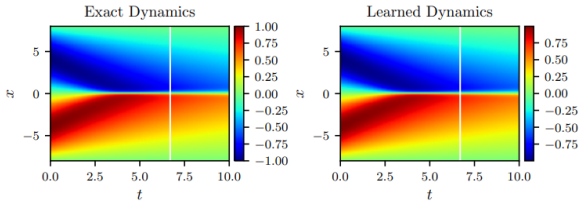

Figure 4. A solution of the Burger's equation (left panel) is compared to the corresponding solution of the learned partial differential equation (right panel).

The exact and learned dynamics solution for the Navier Stokes equation using our network is shown in Figure 5:

The actual and and the predicted dynamics of the velocity components u and v using our network at different timeframes is shown in Figure 6:

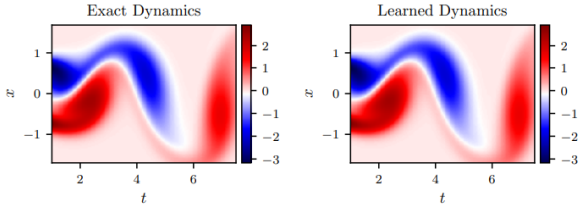

Figure 5. A solution of the Navier Stokes equation (left panel) is compared to the corresponding solution of the learned partial differential equation (right panel).

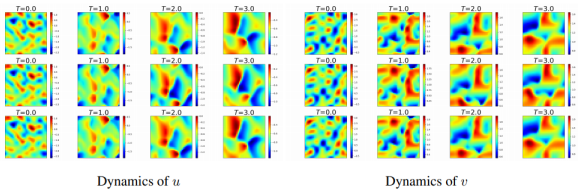

Figure 6. The first row shows the images of the true dynamics. The last two rows show the images of the predicted dynamics using our network.

5.1. Ablation Studies

A study of with and without using channel and spatial attention module on the performance is shown in Table 2:

6. Conclusions

In this paper, we present a attention based physics informed neural network named AA-PINN to simulate incompressible Navier Stokes and Burgers Equations. We formulate our network using Pressure-Velocity coupling. The spatial and temporal co-ordinates of the domain are input while instantaneous pressure and velocity fields are output. We use the initial and boundary conditions as supervised data-driven parts, while residual of the Navier-Stokes and Burgers equations as the unsupervised part in the loss function while training our network. We propose a more robust loss function to handle both the boundary conditions as well as initial conditions. We test the performance our network using RMSE, divergence and TKE as the evaluation metrics. We demonstrate our designed network is more robust while

Table 1. Comparion of SOTA networks using the number of parameters, the best number of input frames, the best number of accumulated errors for back-propogation and training time for one epoch.

Models	TF-net	U-net	GAN	ResNet	ConvLSTM	SST	DHPM	Ours
no of param(10^6)	15.9	25.0	26.1	21.2	11.8	49.9	2.12	**0.53**
input length	25	25	24	26	27	23	23	**20**
accumulated errors	4	6	5	5	4	5	5	**2**
time for one epoch(min)	**0.39**	0.57	0.73	1.68	45.6	0.95	4.591	0.72

Table 2. Ablation study using variations of spatial and channel attention modules.

Metrics	Only SA	Only CA	Both
number of parameters(10^6)	1.23	0.71	**0.53**
accumulated errors	5	3	**2**
time for one epoch(min)	1.05	1.16	**0.72**

modelling the complex flow physics. In the future, we would like to study the effect of attention mechanism for solving compressible and steady Navier Stokes Equations.

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