Deep Learning for Efficient Reconstruction of High-Resolution Turbulent DNS Data

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Within the domain of Computational Fluid Dynamics, Direct Numerical Simulation (DNS) is used to obtain highly accurate numerical solutions for fluid flows. However, this approach for numerically solving the Navier-Stokes equations is extremely computationally expensive mostly due to the requirement of greatly refined grids. Large Eddy Simulation (LES) presents a more computationally efficient approach for solving fluid flows on lower-resolution (LR) grids but results in an overall reduction in solution fidelity. Through this paper, we introduce a novel deep learning framework SR-DNS Net, which aims to mitigate this inherent trade-off between solution fidelity and computational complexity by leveraging deep learning techniques used in image super-resolution. Using our model, we wish to learn the mapping from a coarser LR solution to a refined high-resolution (HR) DNS solution so as to eliminate the need for DNS simulations on highly refined grids. Our model efficiently reconstructs the high-fidelity DNS data from the LES like low-resolution solutions while yielding good reconstruction metrics. Thus our implementation improves the solution accuracy of LR solutions while incurring only a marginal increase in computational cost required for deploying the trained deep learning model.

1. Introduction

Direct Numerical Simulation (DNS) is a highly accurate but expensive method for computationally solving the Navier-Stokes equations. Thus, even with the apparent fidelity benefits and the advent of modern computing, DNS has still not seen widespread adoption within the industry and the CFD community. On the other hand, Large Eddy Simulation (LES) which yields a spatially filtered approximation of the DNS results has much higher adoption within the industry and community in general. Solving on lower resolution grids like the ones used in LES, captures only the larger scale turbulent flows. It yields only a coarse approximation of the solution and subsequently requires much less computation. However, it also has some obvious drawbacks. LES solutions need augmentation via sub-grid scale (SGS) modelling in order to preserve unresolved small-scale physical processes. This results in a reduction in overall solution fidelity compared to DNS solutions. Herein lies the inherent trade-off between solution fidelity and computational complexity that CFD researchers and practitioners constantly grapple with. Through this paper, we suggest a novel machine learning (ML) based approach to mitigate this trade-off by ensuring high solution fidelity while keeping the computational overhead at a minimum.

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Recently, machine learning especially deep learning has shown great promise in several interesting applications within the disciplines of computer vision and data driven modelling. Within fluid dynamics, deep learning has seen particular interest with applications to the field of turbulence modelling [Kutz 2017]. Using machine learning, novel turbulence models have been developed for RANS simulations [Ling et al 2016]. Additionally, machine learning has been used for developing closure models for CFD simulations [Beck et al 2019; Maulik & San 2017; Maulik et al 2019; Gamahara & Hattori 2017; Bode et al 2019]. ML architectures like convolutional auto-encoders (CAE) and Long Short-Term Memory (LSTMs) have shown great success in reduced order modelling (ROM) of fluid flows. Such architectures are replacing and augmenting conventional dimensionality reduction techniques such as Principal Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD) for developing reduced order models [Maulik et al 2020; Mohan & Gaitonde 2018; Lee & Carlberg 2020; Gonzalez & Balajewicz 2018].

Through this paper, we aim to translate the novel advancements in machine learning to the domain of CFD. For this, we make use of deep neural networks to learn a mapping from the coarser LES like solutions to the refined DNS solutions. Such an ML network enables the reconstruction of high-frequency features that cannot be captured by the coarser low-resolution solutions, thereby eliminating the need for using empirical sub-grid scale models for turbulence. Most importantly, by learning a complex and highly non-linear mapping between the low and high fidelity CFD simulations, massive savings in computational cost can be obtained. In fact, computational run times would decrease by orders of magnitude and would make the use of high fidelity CFD solutions more enticing.

On close analysis of this problem it is apparent that it is analogous to up-scaling a low-resolution image to a high-resolution image (Super Resolution). So for our application, the result from a lower fidelity solver can be treated as the LR input whereas the HR output would approximate the DNS solution. Various ML architectures have continuously improved the Single Image Super Resolution (SISR) performance, particularly in terms of Peak Signal to Noise Ratio (PSNR) and the Structural Similarity Metric (SSIM).

Some of the earliest works in SISR used a convolutional neural network (CNN) based approach such as SRCNN [Dong et al 2015]. Next, deeper CNN architectures were developed which incorporated residual blocks [He et al 2016] that significantly boosted the performance of conventional CNNs. Since then, several different implementations of residual blocks have shown improvement in certain aspects where previous models were shown to be lacking. DenseNets [Tong et al 2017] and Residual Dense Blocks (RDB) [Zhang et al 2018] are examples of this. More recently, Generative Adverserial Network (GAN) based methods like SRGAN [Ledig et al 2017] and Enhanced SRGAN [Wang et al 2018] have been able to produce sharp and highly perceptually accurate images.

All the architectures described above are highly effective in image reconstruction but are too heavily focused on attaining the best reconstruction metrics. Consequently, these architectures have large network sizes and are significantly lacking in terms of computational efficiency. Due to their large number of parameters, these networks consume a lot of computational resources. Also, these large networks take really long to train and are notoriously hard to converge. These flaws in above mentioned networks render them unsuitable for use with CFD solvers where fast turnaround times are of the essence. So, in order to develop a framework for the efficient reconstruction of DNS data from LR data, an architecture is required which can yield decent reconstruction metrics while minimizing the network size at the same time.
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Recently, ML models have also been used for upscaling of low-resolution CFD data. Bode et al. (2019) and Fukami et al. (2018) are good examples of this. However, these implementations have shortcomings in certain key areas that we aim to address through our implementation. Reconstruction performed by Bode et al. (2019) uses a GAN based model for upscaling which has several computational efficiency based downsides. The implementation by Fukami et al. (2018) utilises a simple CNN and hence lacks in depth and complexity. It doesn’t make use of residual blocks which results in an overall reduction in reconstruction performance.

Thus through this paper, we present SR-DNS Net, a deep learning framework which presents the possibility of upscaling low fidelity LR solutions to high fidelity DNS solutions in a computationally efficient manner.

2. Dataset

For training our model and evaluating its performance we utilise the Isotropic Forced Turbulence data-set from the Johns Hopkins Turbulence Database (JHTDB) (Li et al. 2008). This dataset contains direct numerical simulation (DNS) results for the Forced Isotropic Turbulence problem having a computational domain with $1,024^3$ nodes. The Navier-Stokes equation for this problem is solved using the pseudo-spectral method and the Taylor-scale Reynolds number for this simulation fluctuates around $Re \approx 433$. In order to create low-resolution datasets, the DNS data is filtered using a box-filter (Equation 2.1) of 3 different filter widths ($\Delta$). This results in the loss of high-frequency features and yields spatially filtered data just like in the case of a solution obtained on a coarser grid (figure 1). Three different filter widths ($\Delta = 11, \Delta = 21$ & $\Delta = 41$) are used to create a spectrum of low-resolution data. This helps in analysing and validating the model’s reconstruction performance on a wide range of low-resolution data. Depending on the degree of refinement or ($\Delta$), the three datasets are referred as Low Resolution - Fine (LR-Fine), Low - Resolution Medium (LR-Medium) and Low - Resolution Coarse (LR-Coarse).

$$\frac{1}{\Delta^3} \cdot \sum_{i=n-\delta}^{n+\delta} \sum_{j=n-\delta}^{n+\delta} \sum_{k=n-\delta}^{n+\delta} f(x_i, y_j, z_k)$$

(2.1)

where $n = \text{int}(\frac{x'}{\Delta x}) = \text{int}(\frac{y'}{\Delta y}) = \text{int}(\frac{z'}{\Delta z})$ and $\delta = \text{int}(\frac{\Delta}{2\Delta x})$
3D velocity data is sampled from the entire computational domain \((1024 \times 1024 \times 1024)\) over a duration of 10 seconds with the data being queried only at intervals of 0.1 seconds. The sampled data is then divided into separate channels of \(x, y\) and \(z\) velocities within 2 dimensional regions of \(64 \times 64\) pixels. This segmentation is necessary for limiting the machine learning model to a manageable size given our computational constraints. Thus each of the 3 final datasets consist of 50,000 \(64 \times 64\) DNS and LR snapshots from the JHUTDB Forced Isotropic Turbulence Dataset. Finally, dataset augmentation is performed by randomly flipping the corresponding snapshots about the \(X\) and \(Y\) axes. This improves model training by increasing the number of training samples without storing additional CFD data on memory.

3. Methodology

To perform the reconstruction of the HR turbulent data we utilise a machine learning (ML) model which in its crux is just a function approximator with learnable parameters \(f\). Given, the LR CFD data as input the machine learning model tries to generate a non-linear function mapping which can most closely generate the HR CFD data as its output. The learning aspect of the model occurs via iteratively updating the function parameters. This update is based on the back propagation of the error between the ground truth \(y\) and the function prediction \(f(w, \theta)\) to the function parameters. Thus, the problem reduces down to finding the function parameters \(\theta\) that can minimize the error between the ground truth and the prediction (Equation 3.1).

\[
\theta = \arg\min_\theta \epsilon(y, f(w, \theta)) \quad (3.1)
\]

\[
\theta = \arg\min_\theta \|y - f(w, \theta)\|_1
\]

*Here, the error \(\epsilon\) is evaluated using the L1 loss metric*

Given the similarity of our task with single image super resolution problems, ML models that performed well in the area were examined. Additionally, an additional constraint in terms of computational complexity was applied to narrow down the ML architecture subspace. Based on these constraints, Generative Adversarial Network (GAN) based SISR models were deemed infeasible. GAN based SR models have large model sizes due to the presence of two independently trainable networks within namely the generator and discriminator. Moreover, GANs and their instability during training has been well documented \cite{Salimans2016}. GANs also have a propensity for running into convergence oscillations, mode collapse and vanishing gradients due to unbalanced training.

Given the above stated constraints and considerations, implementing deep CNNs with residual blocks (ResNets) emerged as the obvious choice. But again, the large number of trainable parameters associated with residual blocks severely bogged down the network’s performance. Thus, we had to identify a CNN with the capabilities of ResNets minus the massive computational overhead. Here, Mobilenets come to the fore by maintaining the network complexity while using only a fraction of the computational resources of ResNets \cite{Howard2017, Sandler2018}. This is because, MobileNets were developed to be used for performing real-time image segmentation on embedded systems and mobile devices. To achieve this, MobileNets make use of Inverted Residuals layers with Linear Bottlenecks instead of the regular Residual Blocks. These layers boost performance by replacing conventional convolutions with depthwise convolutions \cite{Szegedy2015}.
Thus, using inspiration from the highly efficient MobileNet Architecture, we replaced the residual blocks with Inverted Residual Blocks with Linear Bottlenecks. This change yielded a significant improvement in training times (table 2) compared to a ResNet and a GAN based architecture being used previously, while maintaining almost equivalent performance. Nonetheless, in order to achieve a high-quality reconstruction a very deep neural network was still required. So, a network with 16 inverted residual blocks was implemented. However, such deep networks tend to encounter the problem of vanishing gradients. To tackle this, we introduced a skip connection within the architecture (figure 2). This ensured that the error was able to backpropagate through to the initial convolutional layers without diminishing significantly.

Another important consideration in deciding the network architecture was deciding between 2D and 3D convolutions. While working with the isotropic 3D DNS data, the convolution operation can be performed in the form of 3D volume convolutions across the computational volume or by performing 2D convolutions on 2D slices (snapshots) of the velocity data. The downside of using 2D convolutions instead of 3D convolutions is the loss of spatial correlation in the direction that has been collapsed. However, performing 2D convolutions instead of 3D convolutions brings about a significant reduction in the number of trainable parameters. In the end given our constraints, we decided to utilise 2D convolutions for our application.

Next, for the upsampling operation in our architecture a Pixel-Shuffle layer (Shi et al. 2016) was used which provided a performance boost compared to a conventional deconvolution upsampling. Pixel-Shuffle is highly efficient in up-sampling images and can decrease the computational complexity of the network logarithmically in the image dimension compared to the conventional convolutional methods. Furthermore, We experimented with different loss metrics for evaluating the error. We found that the MAE (L1) loss yielded significantly better results compared to MSE (L2). The model trained on the L1 was found to be less susceptible to getting stuck in local minimas, something which was quite prevalent when using L2 as the loss metric. This difference in performance can be attributed the formulation of the loss metrics themselves. The slope of the L2 error is large away from the origin but it quickly diminishes to zero near the origin. Whereas, L1 has a constant slope throughout its domain, even in the regions adjacent to the origin. Thus, using an L1 loss we can attain marginal gains even when the error value tends to zero.

Our Network uses the Adam (Kingma & Ba 2014) optimizer with default parameters along with a learning rate scheduler to speed up model convergence. We also implement early stopping to identify the most suitable model for reconstruction by reducing overfitting. Finally, to train and deploy the deep learning model we used a system with an
| Dataset     | Metric | LR Input | Recon. | DNS   | %Improv. |
|-------------|--------|----------|--------|-------|----------|
| LR Fine     | PSNR   | 20.831 dB| 22.948 dB| ∞     | 10.163   |
| (∆ = 11)    | SSIM   | 0.894    | 0.915  | 1     | 2.349    |
| LR Medium   | PSNR   | 16.924 dB| 20.032 dB| ∞     | 18.634   |
| (∆ = 21)    | SSIM   | 0.817    | 0.884  | 1     | 8.201    |
| LR Coarse   | PSNR   | 13.713 dB| 17.268 dB| ∞     | 25.924   |
| (∆ = 41)    | SSIM   | 0.657    | 0.755  | 1     | 14.916   |

Table 1: Comparison of metrics between the LR Input, Reconstruction and Ground Truth(DNS) data on the test set

![Graph](image.png)

Figure 3: PSNR(a) and SSIM(b) metrics for super resolution reconstruction on different LR datasets

Intel Core I9-9900K processor with 16GB of RAM and an NVIDIA GeForce RTX 2080 Ti GPU with 11GB of VRAM.

4. Results

To determine the efficacy of our ML model, we evaluated the performance of our model on three datasets with varying levels of coarseness. So, comparison based on metrics such as Peak Signal to Noise Ratio (PSNR) and Structural Similarity Index Metric (SSIM) was carried out. PSNR is the ratio of the peak signal power to the noise(MSE) in the image. It is used to compare the quality of reconstruction in terms of pixel-wise accuracy. Since it is inversely related to MSE, higher PSNR values correspond to better reconstruction. SSIM is used to evaluate the perceptual or perceived similarity between two images on a scale from 0 to 1 with 1 representing perfect perceptual similarity.

Our network significantly improves the PSNR and SSIM values of the LR data in all three datasets (table 1, figure 3). This super-resolution enhancement is also apparent on visual inspection of the reconstruction results as shown in figure 4.

In terms of fluid dynamics based metrics, there is good agreement between the DNS and the reconstructed values. On unseen test datasets, our model only slightly under predicts the kinetic energy and average turbulent velocity values (figure 5, figure 6) while showing marked improvement in kinetic energy correlation when compared to the
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Figure 4: Comparison of velocity reconstruction results on samples from the 3 different Low-resolution Test Datasets. a) LR-Fine Dataset; b) LR-Medium Dataset; c) LR-Coarse Dataset. SR-DNS Net yields good reconstruction results as can be seen by the similarity between the reconstruction (Prediction) and the ground truth (Target). The mean absolute error for the reconstructed kinetic energy values is clearly less than the MAE for the Low-resolution data (figure 5). Also, the vorticity distribution plots show good agreement between the reconstruction and the ground truth values on all three datasets. From figure 7, it can be seen that the probability distribution functions of vorticity on the LR-Fine dataset almost exactly overlaps with the ground truth values. Moreover, the reconstruction on LR-Medium is also decent while the probability distribution on the LR-coarse dataset is slightly concentrated towards the origin (figure 7) which was expected. Additionally, the distribution of the average turbulent velocity (figure 6) yielded similar trends with best reconstruction results on the fine LR dataset followed by medium LR and coarse LR. Furthermore, even on visual inspection of the up-sampling, differences between the reconstruction and the ground truth are almost imperceptible for the LR-Fine dataset (figure 4). However, slight differences become
Table 2: Comparison of training and inference times between a CNN ResNet, ESRGAN and SR-DNS Net with comparable reconstruction performance. Training is performed on 50k images. Inference times are evaluated on a single image. A pretrained model for ESRGAN was used to compare reconstruction performance during inference.

| Mode         | CNN (ResNet)     | SR-DNS Net       | ESRGAN       |
|--------------|------------------|------------------|--------------|
| Training     | 368s per epoch   | 286s per epoch   | Pre-trained  |
| Inference    | $5.39 \times 10^{-3}$s | $4.77 \times 10^{-3}$s | $3.76 \times 10^{-2}$s |

Figure 5: MAE of Kinetic Energy for LR(left) and Reconstruction(right) Test Datasets. a) LR-Fine Dataset; b) LR-Medium Dataset; c) LR-Coarse Dataset. Observe the reduction in MAE on the reconstruction plots compared to low-resolution inputs.

more and more apparent as the low-resolution input decreases in its level of refinement. Nonetheless, SR-DNS Net is able to inject meaningful sub-grid scale turbulence even on the very coarse LR input data. Finally, by replacing the residual blocks in the network with Inverted Residual blocks and using Pixel Shuffle deconvolution, we observe a significant performance improvement in terms of training and inference times (table 2).
Figure 6: Comparison of Average Turbulent Velocity Distribution between reconstruction and the ground truth (DNS) on the test datasets. Notice the high degree of overlap between the blue and orange markers along with slight offset in the average values.

Figure 7: Comparison between vorticity probability distribution for the ground truth (DNS) and the reconstruction on the different test sets.
5. Conclusions

A deep learning model (SR-DNS Net) has been developed and deployed to perform super-resolution based reconstruction of turbulent DNS data from the low-resolution LES like data. The model yields a significant improvement in terms of image similarity metrics (PSNR and SSIM) between snapshots of the reconstruction and the LR input. Furthermore, the model provides a highly accurate reconstruction of key flow metrics such as turbulent velocity, vorticity and kinetic energy for the isotropic homogeneous turbulence test case. To further validate the model’s efficacy, it has been tested on 3 datasets with varying levels of coarseness (LR-Fine, LR-Medium and LR-Coarse). Using SR-DNS Net, a mapping between the coarser LR data and the refined DNS data was successfully learned. This learning was subsequently injected into future CFD simulations (test data) to improve its fidelity. This proves that future simulations could be performed on much coarser grids with the high frequency features being introduced via the super resolution reconstruction. Our framework thereby facilitates the use of coarser grids for performing high fidelity CFD simulations. Thus SR-DNS Net has the potential to greatly reduce the massive computational overhead usually associated with high fidelity CFD solutions. Additionally, our model is able to inject meaningful sub-grid scale turbulence to CFD simulations performed on coarse grids. Hence, by mapping the LES like LR solution directly to DNS, SR-DNS Net can potentially eliminate the need for sub-optimal empirical models for sub-grid scale turbulence. Finally, our network makes use of a highly computationally efficient deep learning architecture which greatly improves its training and deployment times. In conclusion, our research serves as an important initial step towards demonstrating the effectiveness and future potential of such super-resolution based reconstruction models. Such models can efficiently increase solution fidelity of CFD simulations while mostly mitigating the associated computational costs.

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7. Declaration of Interests

The authors report no conflict of interest.

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