Super-Resolution-based Subfilter Modeling for Interfacial Flows

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Abstract

Super-resolution tools have been originally invented for image super-resolution but are also increasingly used for improving scientific simulations or data-storage. Examples range from cosmology to urban prediction. One particular network framework, physics-informed enhanced super-resolution generative adversarial networks (PIESRGANs), has been shown to be a powerful tool for subfilter modeling. This work extends large-eddy simulation (LES) subfilter modelling with PIESRGAN for turbulence to interfacial flows. For that, a database of temporal jets is employed and used for training of the network. A priori and a posteriori results are presented. It is shown that the PIESRGAN modeling approach gives highly accurate results and even predicts droplet dynamics on coarse meshes correctly.

Keywords

Super-Resolution, Interfacial Flow, Large-Eddy Simulation.

Introduction

Many industrial flows feature multiple phases, such as one liquid and one gaseous phase, call interfacial flows. The computation of liquid/gas systems is numerically challenging for multiple reasons. One reason is the density ratio, which leads to problematic mass conservation errors if the interface between both phases is not accurately predicted. Therefore, interface tracking and capturing approaches have been developed for many years. Prominent examples are level set (LS) and volume of fluid (VoF) or combined approaches. While LS is known to accurately predict the interface geometry, VoF gives good results with respect to mass conservation.

One known issue of LS/VoF is the mesh dependency, i. e., the breakup of the liquid phase is typically slower on coarser meshes. This is especially a problem in simulations of complex systems, for which usually not all areas can be resolved sufficiently. One way to deal with underresolved simulations is large-eddy simulation (LES), originally developed to accurately model the effect of turbulence. A filter is used to decouple the larger and small flow scales, equations are only solved for the larger flow scales, and subfilter models are used to estimate the effect of the small flow scales on the larger flow scales. This assumes that turbulence is universal on the small scales, which is often a good assumption.

A similar approach is used in this work for interfacial flow. The unclosed terms in the transport equations for LS and VoF are closed by an AI super-resolution technique, called physics-informed enhanced super-resolution generative adversarial network (PIESRGAN) [1, 2, 3, 4]. This data-driven approach is trained with coupled LS/VoF data, and it is shown that it is able to accurately predict the droplet dynamics on coarser meshes.

Data

Direct numerical simulations (DNSs) of a temporal jet configuration were used to study modeling of interface-driven effects in two-phase flows in this work. All jets have a bulk Reynolds number (Re) of 5000 and a viscosity ratio (VR) of 40. The Weber number (We) and the density ratio (DR) vary by a factor of 20 between realizations in order to study the sensitivity of the interface with respect to these parameters. As larger Weber numbers require higher spatial resolution, up to about eight billion cells were used for the largest DNS. All DNSs were performed using an in-house code, which solves the incompressible Navier-Stokes equations along with multiphysics effects with structured finite differences of arbitrary order. For prediction of the interface, a 3-D unsplit coupled level set/volume of fluid (3DU-CLSVOF) scheme considering surface tension [5] and a second-order accurate, monotonicity preserving Lagrange-remap solver [6] were used.

Methods

PIESRGAN [7] uses a GAN, which is trained with subboxes of DNS data to minimize a target loss function. The loss function is given as

$$\mathcal{L} = \beta_1 L_{\text{adversarial}} + \beta_2 L_{\text{pixel}} + \beta_3 L_{\text{gradient}} + \beta_4 L_{\text{physics}}, \tag{1}$$

where β_1 to β_4 are coefficients weighting the different loss term contributions with $\sum_i \beta_i = 1$. The adversarial loss is the discriminator/generator relativistic adversarial loss [8], which measures both how well the generator is able to create accurate reconstructed data compared to the fully resolved data and how well the discriminator is able to identify fake data. The pixel loss and the gradient loss are defined using the mean-squared error (MSE) of the quantity and its gradient, respectively. The physics loss enforces physically motivated conditions, such as the conservation of mass as well as the velocity and pressure conditions at the interface.
The network architecture is sketched in Fig. 1. The generator heavily uses 3-D CNN layers (Conv3D) [9] combined with leaky rectified linear unit (LeakyReLU) layers for activation [10]. The residual in residual dense block (RRDB), which was introduced for ESRGAN, is essential for the performance of state-of-the-art super-resolution. It replaced the residual block (RB) employed in previous architectures and contains fundamental architectural elements such as residual dense blocks (RDBs) with skip-connections. A residual scaling factor β_{RSF} helps to avoid instabilities in the forward and backward propagation. RDBs use dense connections inside. The output from each layer within the dense block (DB) is sent to all the following layers. The discriminator network is simpler. It inherits basic CNN layers (Conv3D) combined with LeakyReLU layers for activation with and without batch normalization (BN). The final layers contain a fully connected layer with LeakyReLU and dropout with dropout factor β_{dropout}.

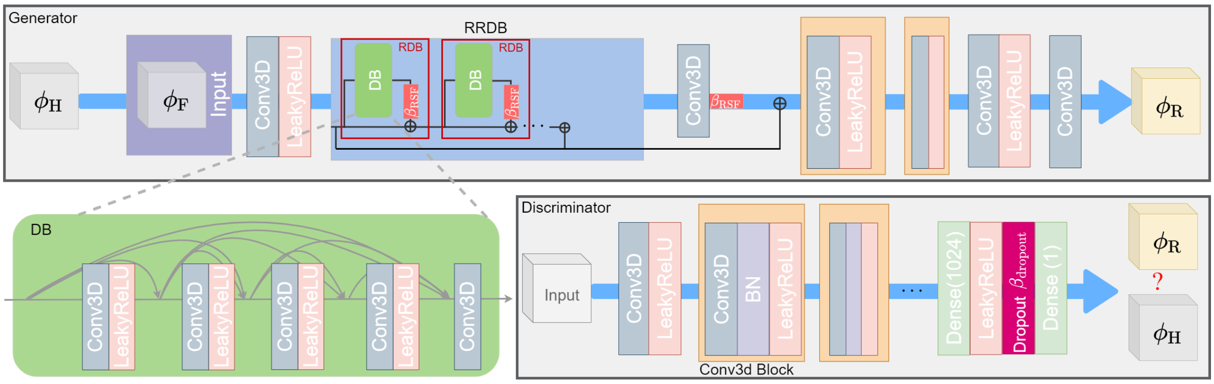

Figure 1. Sketch of PIESRGAN. "H" denotes high-fidelity data, such as DNS data, "F" are corresponding filtered data, and "R" are the reconstructed data. The components are: Conv3D - 3D Convolutional Layer, LeakyReLU - Activation Function, DB - Dense Block, RDB - Residual Dense Block, RRDB - Residual in Residual Dense Block, β_{RSF} - Residual Scaling Factor, BN - Batch Normalization, Dense - Fully Connected Layer, Dropout - Regularization Component, β_{dropout} - Dropout Factor. Image from [11].

The solution algorithm in every time step starting with the LES solution Φ^n_{LES} at time step n reads:

1. Use the PIESRGAN to reconstruct Φ^n_{R} from Φ^n_{LES}.
2. Use Φ^n_{R} to estimate the unclosed terms Ψ^n_{LES} in the LES equations of Φ by evaluating the local terms with Φ^n_{R} and applying a filter operator.
3. Use Ψ^n_{LES} and Φ^n_{LES} to advance the LES equations of Φ to Φ^{n+1}_{LES}.

Results and Discussion

To show the quality of the developed method, the temporally evolving planar jet setup is used, which was also used for training. A priori and a posteriori results are presented.

A priori

The a priori test uses data at one time step, filters the data, and reconstructs the data with PIESRGAN. The filtered mesh, which was chosen, used half of the cells per direction compared to the DNS mesh. The results are shown in Fig. 2. The visual agreement is very good.

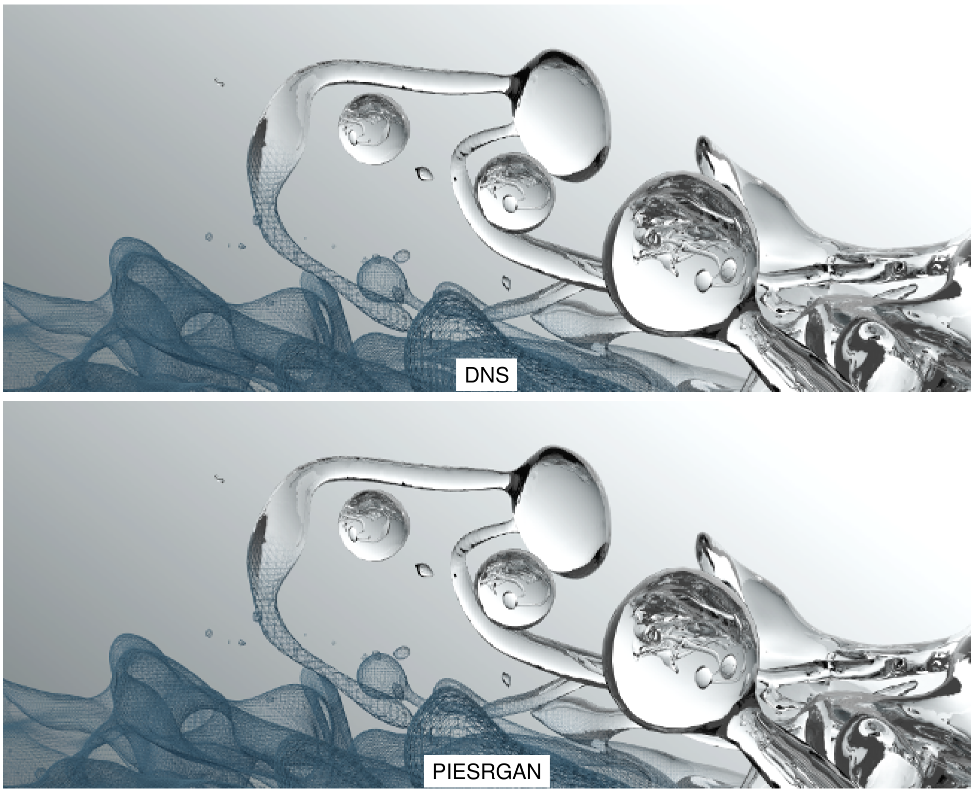

Figure 2. A priori results for the VoF field shown for DNS and reconstructed data.

A posteriori

The droplet, which is formed and already visible in the a priori visualization, is tracked over time with DNS and LES with a coarser mesh. The result is shown in Fig. 3. Again, the visual agreement is very good. Without model, the breakup on the coarser mesh would be slower.

Conclusions

This short paper introduces PIESRGAN for interfacial flow. The method is explained and demonstrated by means of a temporally evolving planar jet. The prediction accuracy of PIESRGAN is very good, and it is able to eliminate mesh dependency of breakup simulations.

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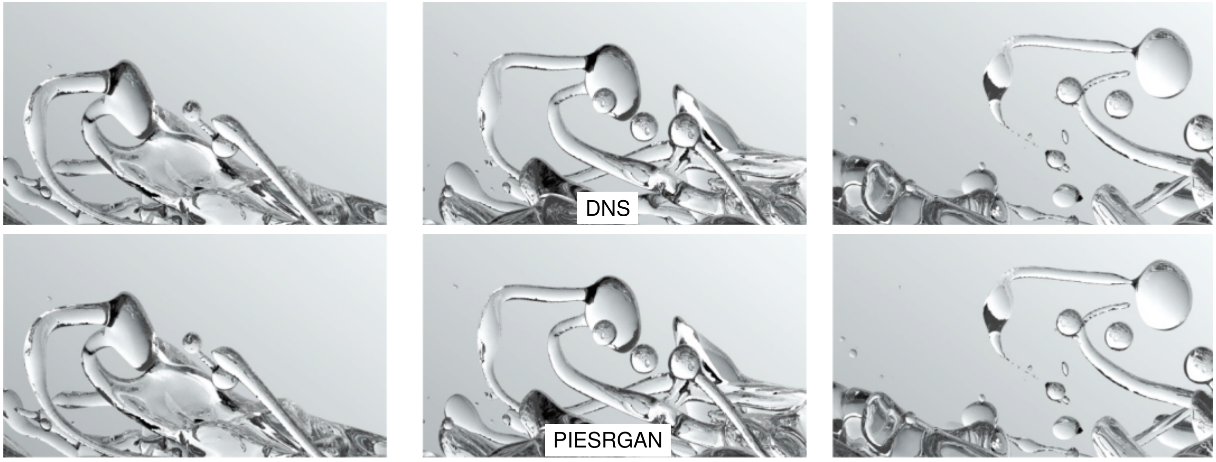

Figure 3. A prosteriori results for the VoF field shown for DNS and LES.

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