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Large-eddy simulation subgrid modelling using neural networks

Robin Stoffer[1], Caspar van Leeuwen[2], Damian Podareanu[2], Valeriu Codreanu[2], Menno Veerman[1], and Chiel van Heerwaarden[1]

[1]Meteorology and Air Quality Group, Wageningen University, Wageningen, The Netherlands (robin.stoffer@wur.nl)

[2]SURFsara, Amsterdam, The Netherlands

Large-eddy simulation (LES) is an often used technique in the geosciences to simulate turbulent oceanic and atmospheric flows. In LES, the effects of the unresolved turbulence scales on the resolved scales (via the Reynolds stress tensor) have to be parameterized with subgrid models. These subgrid models usually require strong assumptions about the relationship between the resolved flow fields and the Reynolds stress tensor, which are often violated in reality and potentially hamper their accuracy.

In this study, using the finite-difference computational fluid dynamics code MicroHH (v2.0) and turbulent channel flow as a test case (friction Reynolds number Re_τ 590), we incorporated and tested a newly emerging subgrid modelling approach that does not require those assumptions. Instead, it relies on neural networks that are highly non-linear and flexible. Similar to currently used subgrid models, we designed our neural networks such that they can be applied locally in the grid domain: at each grid point the neural networks receive as an input the locally resolved flow fields (u,v,w), rather than the full flow fields. As an output, the neural networks give the Reynolds stress tensor at the considered grid point. This local application integrates well with our simulation code, and is necessary to run our code in parallel within distributed memory systems.

To allow our neural networks to learn the relationship between the specified input and output, we created a training dataset that contains ~10.000.000 samples of corresponding inputs and outputs. We derived those samples directly from high-resolution 3D direct numerical simulation (DNS) snapshots of turbulent flow fields. Since the DNS explicitly resolves all the relevant turbulence scales, by downsampling the DNS we were able to derive both the Reynolds stress tensor and the corresponding lower-resolution flow fields typical for LES. In this calculation, we took into account both the discretization and interpolation errors introduced by the finite staggered LES grid. Subsequently, using these samples we optimized the parameters of the neural networks to minimize the difference between the predicted and the 'true' output derived from DNS.

After that, we tested the performance of our neural networks in two different ways:

- A priori or offline testing, where we used a withheld part of the training dataset (10%) to test the capability of the neural networks to correctly predict the Reynolds stress tensor for data not used to optimize its parameters. We found that the neural networks were, in general, well able to predict the correct values.

- A posteriori or online testing, where we incorporated our neural networks directly into our LES. To keep the total involved computational effort feasible, we strongly enhanced the prediction speed of the neural network by relying on highly optimized matrix-vector libraries. The full successful integration of the neural networks within LES remains challenging though, mainly because the neural networks tend to introduce numerical instability into the LES. We are currently investigating ways to minimize this instability, while maintaining the high accuracy in the a priori test and the high prediction speed.