Subgrid-scale representations for neural network based closure models for turbulent flows

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1 Problem

In turbulence modelling, and more particularly in the LES framework, we are concerned with finding a suitable closure model to represent the effect of the unresolved subgrid-scales on the larger/resolved scales. In recent years, the scientific computing community has started to gravitate towards machine learning techniques to attempt to solve this issue. However, stability and abidance by physical structure of the resulting closure models is still an open problem.

2 Preliminaries

2.1 Discretizing PDEs

In this project we deal with PDEs of the following type:

$$\frac{\partial u}{\partial t} = f(u), \tag{1}$$

which describe the evolution of some initial fluid velocity field $u(x, t = 0) = u_0$ in space $x \in \Omega$ and time t. The right-hand side (RHS) f is typically derived from underlying physical conservation laws. In order to solve such a PDE on a computer we discretize in space to obtain a set of ODEs:

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = f_h(\mathbf{u}), \tag{2}$$

where $\mathbf{u} \in \mathbb{R}^N$ approximates $\mathbf{u}$ on a grid (with grid-spacing h) and f_h is an approximation of the continuous operators in f. The problem is that in the case of turbulent flows we require N to be large, resulting in high computational costs [1].

2.2 Filtering

To resolve this issue we apply a spatial averaging filter to the solution:

$$\bar{\mathbf{u}} = \mathbf{W}\mathbf{u}, \tag{3}$$

where multiplication by $\mathbf{W} \in \mathbb{R}^{I \times N}$ reduces the degrees of freedom in the system from N to I. However, we still require knowledge of the high-resolution approximation $\mathbf{u}$ to evolve the averaged system in time [1]:

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = \mathbf{W} f_h(\mathbf{u}). \tag{4}$$

To circumvent this we rewrite this to

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f_H(\bar{\mathbf{u}}) + \underbrace{(\mathbf{W} f_h(\mathbf{u}) - f_H(\bar{\mathbf{u}}))}_{:=\mathbf{c}}, \tag{5}$$

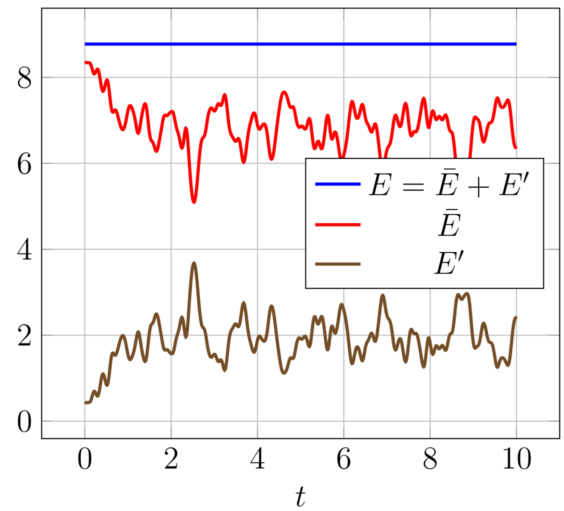

Figure 1: Decomposition of kinetic energy E into $\bar{E}$ and E'.

where f_H represents a coarse discretization of the PDE. The commutator error $\mathbf{c}(\mathbf{u})$ is referred to as the closure term. The goal is now to model this closure term by some approximation $\tilde{\mathbf{c}}(\bar{\mathbf{u}})$ s.t.

$$\tilde{\mathbf{c}}(\bar{\mathbf{u}}) \approx \mathbf{c}(\mathbf{u}). \tag{6}$$

In this way we do not require knowledge of the high-resolution approximation to "close" the averaged system of ODEs s.t. we lower the degrees of freedom and in turn alleviate the computional burden.

2.3 Machine learning solution

Machine learning algorithms, more specifically neural networks, can readily be applied to model this closure term [2–6] which transform the set of ODEs to

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f_H(\bar{\mathbf{u}}) + \mathrm{NN}(\bar{\mathbf{u}}) \tag{7}$$

with $\mathrm{NN}(\bar{\mathbf{u}})$ being the output of a neural network. The neural network is trained by minimizing the error w.r.t. high-resolution reference data. However, these hybrid classical + neural network approaches can lead to unstable simulations, as the neural network is unaware of physical conservation laws. In ongoing work attempt resolve by building kinetic energy conservation into the neural network.

2.4 Energy conservation

To achieve this, we first show that we can split the kinetic energy into a resolved $\bar{E}$ and unresolved E' part:

$$E = \bar{E}(\bar{\mathbf{u}}) + E'(\mathbf{u}'), \tag{8}$$

where $\mathbf{u}' \in \mathbb{R}^N$ is everything that is filtered out by multiplying $\mathbf{u}$ with $\mathbf{W}$. We refer to $\mathbf{u}'$ as the subgrid-scale (SGS) content and to E' as the SGS energy. This changes the energy-conservation condition to

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}\bar{E}}{\mathrm{d}t} + \frac{\mathrm{d}E'}{\mathrm{d}t} = 0. \tag{9}$$

This decomposition is shown in Figure 1 for a high-resolution simulation of the Korteweg-de Vries equation [7]. To circumvent the need for the full $\mathbf{u}'$ in this conservation law we introduce a set of SGS variables $\mathbf{s} \in \mathbb{R}^I$ which approximate the SGS energy on the coarse grid as

$$E' \approx \frac{H}{2}\mathbf{s}^T\mathbf{s}, \tag{10}$$

where H is the grid-spacing for the uniform coarse grid. The result is an approximated kinetic energy conservation condition

$$\frac{\mathrm{d}\bar{E}}{\mathrm{d}t} + \frac{H}{2}\frac{\mathrm{d}\mathbf{s}^T\mathbf{s}}{\mathrm{d}t} = 0. \tag{11}$$

Both $\bar{\mathbf{u}}$ and $\mathbf{s}$ are evolved in time using our newly developed skew-symmetric neural network architecture that ensures that this condition is satisfied, yielding stability.

Currently, these SGS variables are constructed by applying a linear filter, learned from high-resolution simulations, to $\mathbf{u}'$ which compresses the SGS content onto the coarse grid reducing the degrees of freedom of the system from N to $2I$.

3 Objectives & project outline

For this project we are mainly interested in gaining more understanding of both the theoretical and practical aspects of the SGS variables. We therefore propose the following outline of the project:

- Literature study on: partial differential equations, computational fluid mechanics, closure modelling, machine learning [2–5, 8, 9].
- Theoretical study on the SGS variables: What do they represent?
- Suggest new forms for the SGS variables, e.g. neural networks.
- Possibly suggest new neural network architectures (or non-data-driven approaches, linear models etc.) for the closure model, derived from energy arguments.
- Implement SGS variables and compare performance for the convection-diffusion equation.
- If everything goes well: Burgers equation, Korteweg-de Vries equation, possibly Navier-Stokes.

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