CFD4 - Assignment
Data-driven modelling of subgrid scale turbulent kinetic energy

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LES simulations require closure

- In LES
  - Filtering of the Navier-Stokes equations $\tilde{\cdot}$ and decomposition $(u = \tilde{u} + u'')$

$$\mathcal{N}\left(\widetilde{\tilde{u} + u''}\right) \rightarrow (\tilde{u} \cdot \nabla)\,\tilde{u} + \nabla\tilde{p} - \nu\nabla^2\,\tilde{u} + \boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}''\boldsymbol{u}''} = 0$$

(Subgrid) Reynolds stress $\tau_{ij} = \langle \boldsymbol{u}'\boldsymbol{u}' \rangle$ or $\widetilde{u''u''}$ require closure

Reynolds stress closure historically relied on physical intuition

- Many existing models for τ_{ij}
  - Eddy viscosity assumption $\tau_{ij} \approx \frac{2}{3} k \delta_{ij} - \nu_T (\nabla_j U_i + \nabla_i U_j)$
    - Algebraic models
    - Spalart-Allmaras, …
    - $k - \epsilon$, $k - \omega$, …
    - Smagorinsky model (for LES)
    - …

Even with physical intuition, model calibration still necessary

- Let's take the $k-\epsilon$ model, intuition-based transport equations

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k U_i)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right)+2\mu_t S_{ij}S_{ij}-\rho\epsilon$$

$$\frac{\partial(\rho \epsilon)}{\partial t}+\frac{\partial(\rho \epsilon U_i)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial x_j}\right)+C_{1\epsilon}\frac{\epsilon}{k}2\mu_t S_{ij}S_{ij}-C_{2\epsilon}\rho\frac{\epsilon^2}{k}$$

$$\rightarrow \mu_t=\rho C_\mu\frac{k^2}{\epsilon}$$

5 parameters to "fit" $C_\mu, \sigma_k, \sigma_\epsilon, C_{1\epsilon}, C_{2\epsilon}$

See for example Launder & Sharma 1974 for "standard" values (values calibrated for a low Re flow around spinning disk)

[Launder & Sharma, Let. Heat. Mass. Tsf., 1974]

Can we do more than just model calibration?

- Compared to 1970s:
  - Availability of high-resolution datasets
  - “Exact” Reynolds stress could be extracted
  - Can we leverage that?

The “promise” of data-driven modelling

“[Data] has historically been used to calibrate simple engineering models […]

with the availability of large […] datasets researchers have begun to explore methods to systematically inform turbulence models with data. […]

[…] by exploiting foundational knowledge in turbulence modeling and physical constraints, data-driven approaches can yield useful predictive models.”

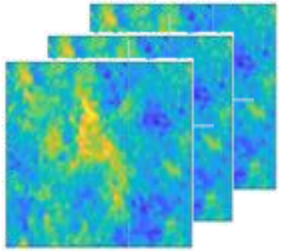
→ How can we leverage (high-fidelity) data to improve the modelling of turbulence?

[Duraisamy et al., Annu. Rev. Fluids., 2019]

From high-fidelity data to RANS/LES-like data

- Postprocessing of high-fidelity simulations

DNS



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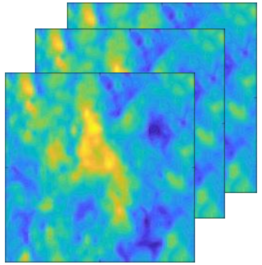
Filtering/Averaging



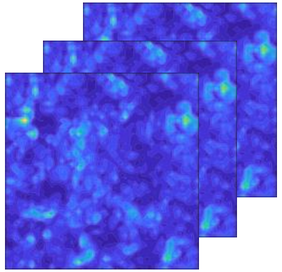
LES/RANS-like fields

$\tilde{u} = \int_{\Omega} u(\xi, t) G(x - \xi; \Delta) d\xi$ or $\langle u \rangle$

$u' = u - \langle u \rangle$ then averaging

$u'' = u - \tilde{u}$ then filtering

→ From DNS: dataset that has "resolved" and "unresolved" quantities

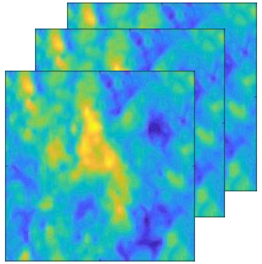


"Exact" closure term

$\tau_{ij} = \widetilde{u_i'' u_j''}$ or $\langle u_i' u_j' \rangle$

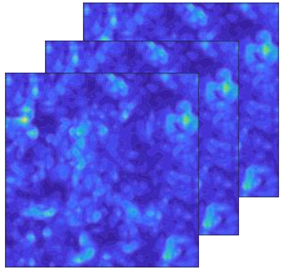
Note: similar process can be done starting from LES for RANS

Data-driven turbulence modelling: finding accurate link between resolved/unresolved



LES/RANS-like fields

$\xrightarrow{\mathcal{F}_\theta\,?}$



“Exact” closure term

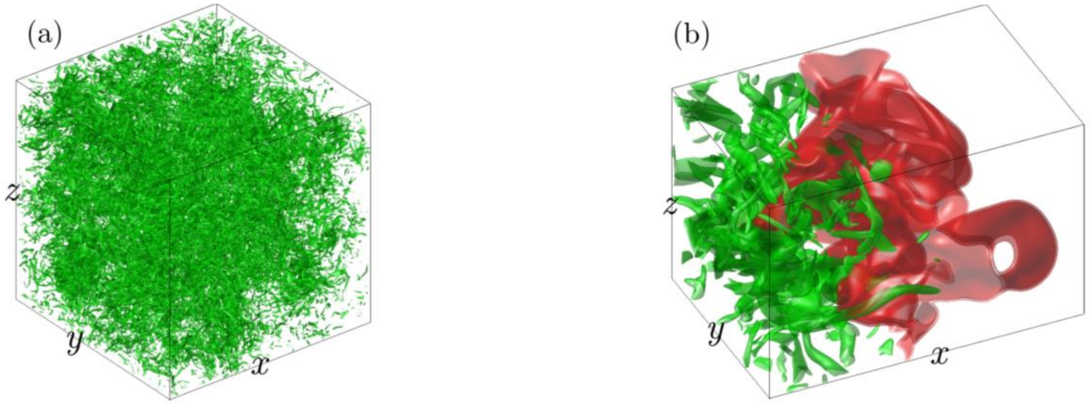
$\tau_{ij} = \widetilde{u_i'' u_j''}$ or $\langle u_i' u_j' \rangle$

$\tilde{u} = \int_\Omega u(\xi, t) G(x - \xi; \Delta) d\xi$ or $\langle u \rangle$

- Different methods depending on:
  - Choice of “functional form” $\mathcal{F}_\theta$ (symbolic regression, neural networks, random forest, …)

Objectives of the assignment

- Develop a NN-based turbulence model for k_{sgs} (subgrid scale kinetic energy)
- You are provided with two cases:
  - Homogeneous isotropic turbulence
  - Turbulence statistically planar flame
  - Dataset already filtered at different filtered sizes



Objectives of the assignment

- Notebook provided: indicates how to read the dataset
- Check the performance of your train NN-based model on the different filter sizes/across the two cases
- **No need to develop a BNN-based model**

Some useful formulas

- Existing models of subgrid kinetic energy are often related to ($\widehat{\cdot}$: test filtering operation):
  - Pope's model: $k_{sgs} \approx C_p \left| \widetilde{\boldsymbol{u}} - \widehat{\widetilde{\boldsymbol{u}}} \right|^2$
  - Bardina's model: $k_{sgs} \approx C_b \left| \widehat{\widetilde{\boldsymbol{u}} \cdot \widetilde{\boldsymbol{u}}} - \widehat{\widetilde{\boldsymbol{u}}} \cdot \widehat{\widetilde{\boldsymbol{u}}} \right|$
  - LDD model: $k_{sgs} \approx C_m |\Delta^2 \nabla \widetilde{\boldsymbol{u}} : \nabla \widetilde{\boldsymbol{u}}|$

See for more models: I. Langella, N.A.K. Doan, N. Swaminathan, Study of subgrid-scale velocity models for reacting and nonreacting flows, Phys. Rev. Fluids. 3 (2018) 1–24. https://doi.org/10.1103/PhysRevFluids.3.054602.