Towards Subgrid-Scale Turbulence Modeling in Dense Gas Flows

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3rd Non-Ideal Compressible
Fluid Dynamics Conference
Delft NL
29-30/10/2020

Context and motivations

- **ORC industry** looks toward **more CFD based designs**
- **Turbulence** is known to be **at the origin of** a significant amount of the **turbine losses (see Wheeler's team work)**
- **No dedicated turbulence model exists for dense gas flows.**

→ French Research Agency (ANR)
Young Researcher project
EDGES

EDGES Program (2018-2022)

- **Context: A few words on EDGES Program (2018-2022)**
  - **A DNS database for the analysis of turbulence in DG flows**

- A bit of theory: Turbulence subgrid-scale (sgs) terms in DG flows and the issue of total energy

- Analysis of sgs terms in HIT and mixing layer
  - The example of sgs pressure

- Towards modeling of sgs pressure
  - Correlation based model
  - Neural network model

- Conclusion

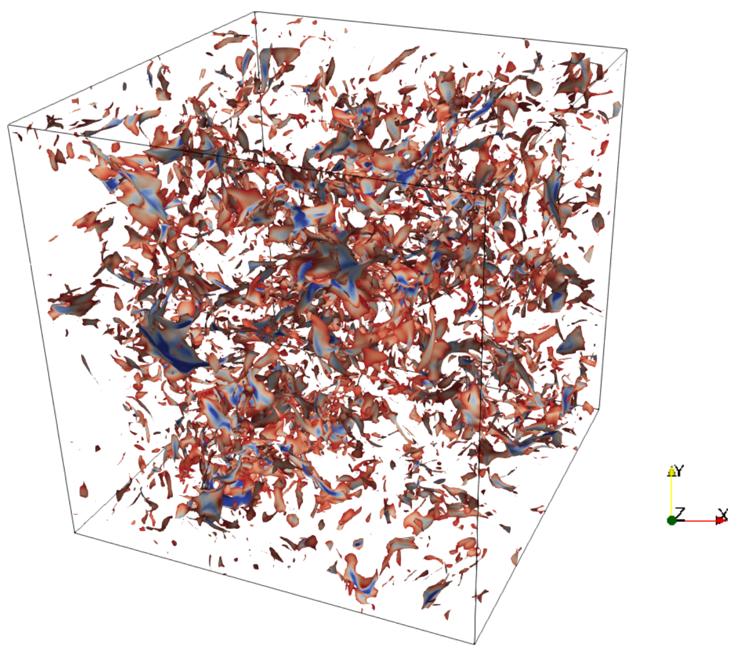
Context and motivations

- The ANR Young Researcher EDGES project (2018-2022):
  - 4 researchers over 4 years

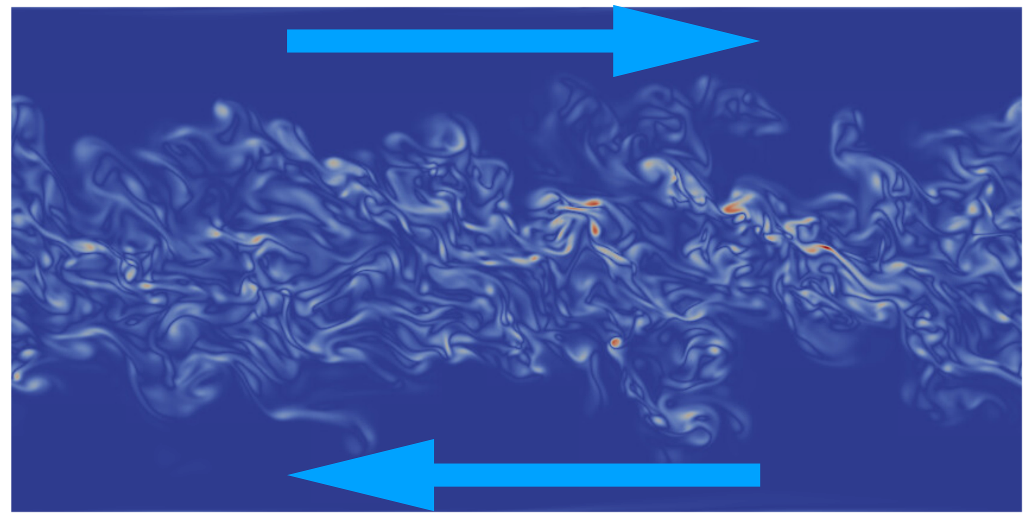
- WP1 : Production of a DNS database of turbulent dense gas flows
- WP2 : A-priori analysis of LES and RANS turbulence closure models
- **WP3 : Development of new models for RANS and LES methods**
- WP4 : LES and RANS simulation of a realistic ORC turbine (a-posteriori validation)

A DNS database for the analysis of turbulence in DG flows

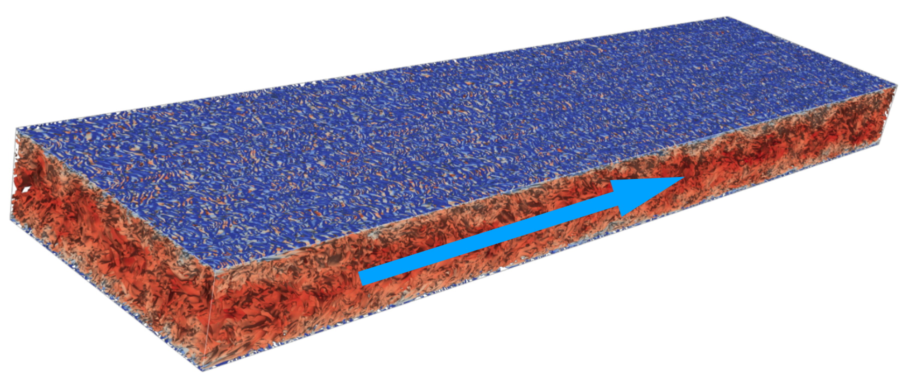
- Forced and free HIT
  (Giauque et al., JoT 2020)



- Mixing Layers (Vadrot et al., JFM 2020)
  (Vadrot et al., 2021 submitted to JFM)



- Channel flows
  Grand challenge TGCC
  (P Errante)



Outline

- Context: A few words on EDGES Program (2018-2022)
  - A DNS database for the analysis of turbulence in DG flows

- **A bit of theory: Subgrid-scale (sgs) terms in DG flows and the issue of total energy**

- Analysis of sgs terms in HIT and mixing layer
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- Towards modeling of sgs pressure
  - Regression model
  - Neural network model

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The issue of total energy in LES (a debate from the 90's)

- When filtered, total energy in a perfect gas (PG) writes as

$$\bar{\rho}\tilde{E} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i + \frac{\tau_{ii}}{2}$$

- Which shows that even in PG, when Vreman (1995) writes a transport equation for

$$\bar{\rho}\hat{E} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i$$

it is not a conservation equation because some energy lies at the subgrid-scale

$\bar{f}$ Reynolds average

$\tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}}$ Favre average

$\hat{f} = f(\bar{\rho}, \tilde{u}_i, \tilde{E})$ Quantity computed using only filtered fields

The issue of total energy in LES (a debate from the 90's)

- The fact is, not many people care and most often one assumes that since

$$\frac{1}{2}(\widetilde{u_i u_i} - \tilde{u}_i \tilde{u}_i) \ll \widetilde{E_{int}} \implies \tilde{E} \approx \hat{E}$$

- The main reason is that given the simplicity of the EoS equation, the following equalities stand

$$\bar{\rho}\tilde{E}_{int} = \frac{\bar{p}}{\gamma - 1} = C_v \bar{\rho} \tilde{T}$$

In PG, thermodynamics does not care about filtering and the difference for total energy only lies in sgs velocity correlations $\frac{1}{2}(\widetilde{u_i u_i} - \tilde{u}_i \tilde{u}_i)$

The issue of total energy in LES in dense gas

- In dense gas, internal energy is influenced by the filtering

$$\tilde{E} \neq E(\bar{\rho}, \bar{P})$$

- or equivalently

$$\bar{P} \neq P(\bar{\rho}, \tilde{E})$$

In DG, thermodynamics is influenced by the filtering

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- **A-priori analysis of sgs terms in HIT and mixing layer**
  - **The example of the momentum equation and sgs pressure**
- Towards modeling of sgs pressure
  - Regression models
  - Neural network model
- Conclusion

Analysis of sgs terms in HIT and mixing layer

- To illustrate our results will now concentrate on the momentum equation

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} = -\frac{\partial \hat{p}}{\partial x_i} - \frac{\partial(\bar{p}-\hat{p})}{\partial x_i} + \frac{\partial \hat{\tau}_{ij}}{\partial x_j} + \frac{\partial(\bar{\tau}_{ij}-\hat{\tau}_{ij})}{\partial x_j} - \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} - \frac{\partial \bar{\rho}(\widetilde{u_i u_j}-\tilde{u}_i\tilde{u}_j)}{\partial x_j}$$

Pressure: Main

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Tau: Main

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Convective: Main

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Convective: sgs

Analysis of sgs terms in HIT and mixing layer

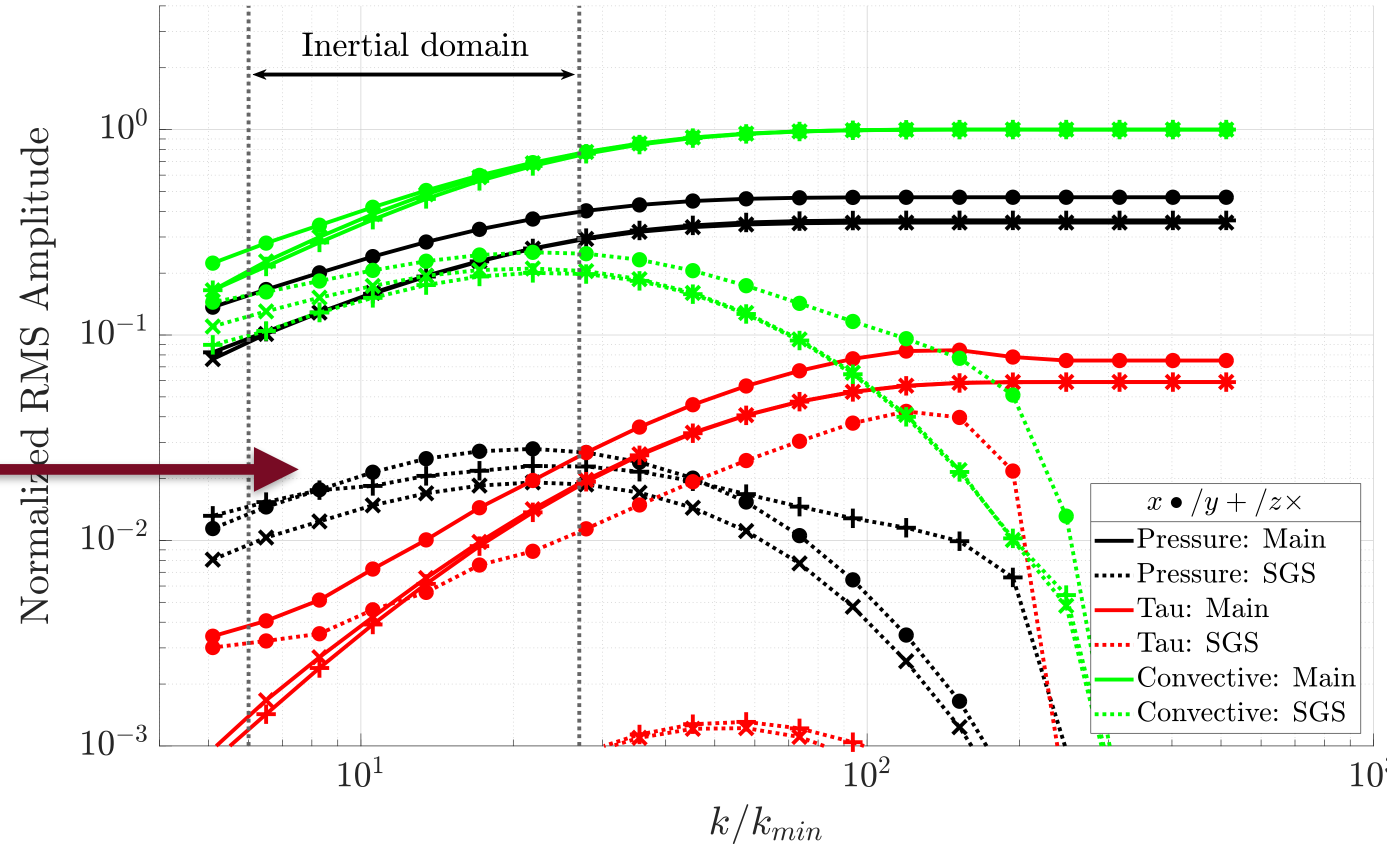
- To determine the importance of the different terms in the momentum equation, we filter the DNS fields between :
  - $k = k_{min}$ which corresponds to a very large scale filter of size L
  - $k = k_{max}$ which corresponds to no filtering (scale is equal to $2\Delta x$)
- Note that in this case $\bar{f}, \tilde{f}, \hat{f}$ should be denoted $\bar{f}^k, \tilde{f}^k, \hat{f}^k$

Analysis of sgs terms in HIT and mixing layer

- We finally compute the rms amplitude of each term in the volume for each filtering wavenumber.

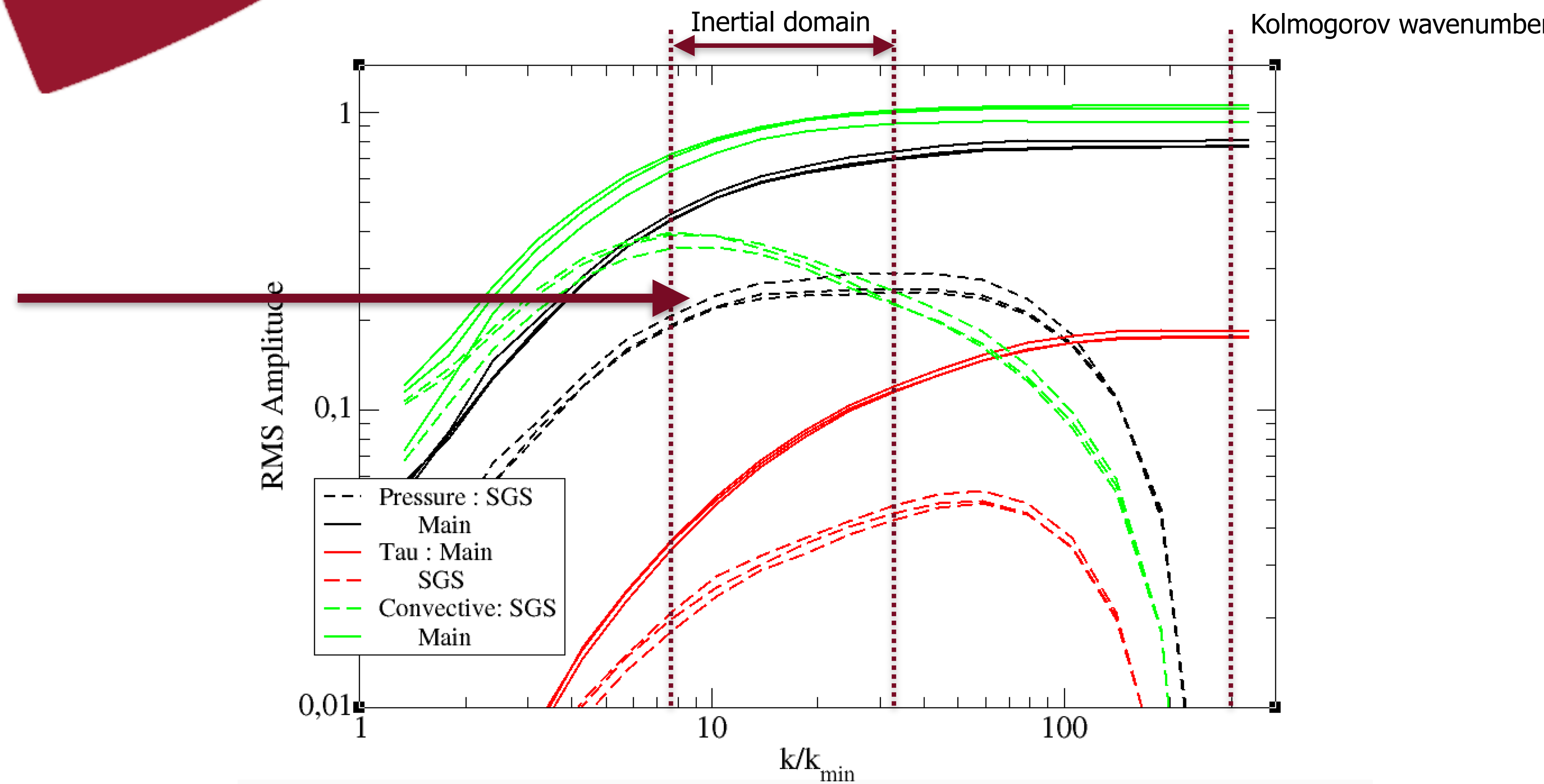
$$\text{Pressure main term} = \left(\left\langle \left[\frac{\partial \hat{p}}{\partial x_i} \right]^2 \right\rangle_V - \left\langle \frac{\partial \hat{p}}{\partial x_i} \right\rangle_V^2 \right)^{1/2}$$

DG sgs terms- Mixing layer



- The pressure sgs term is larger than the main resolved viscous term

DG sgs terms- HIT



- The pressure sgs term is of the order of the usual convective sgs term!

The example of sgs pressure in HIT

- We now concentrate on the subgrid-scale pressure in HIT.

$$p_{sgs} = \bar{p} - \hat{p}\left(\bar{\rho}, \overline{\rho E}\right)$$

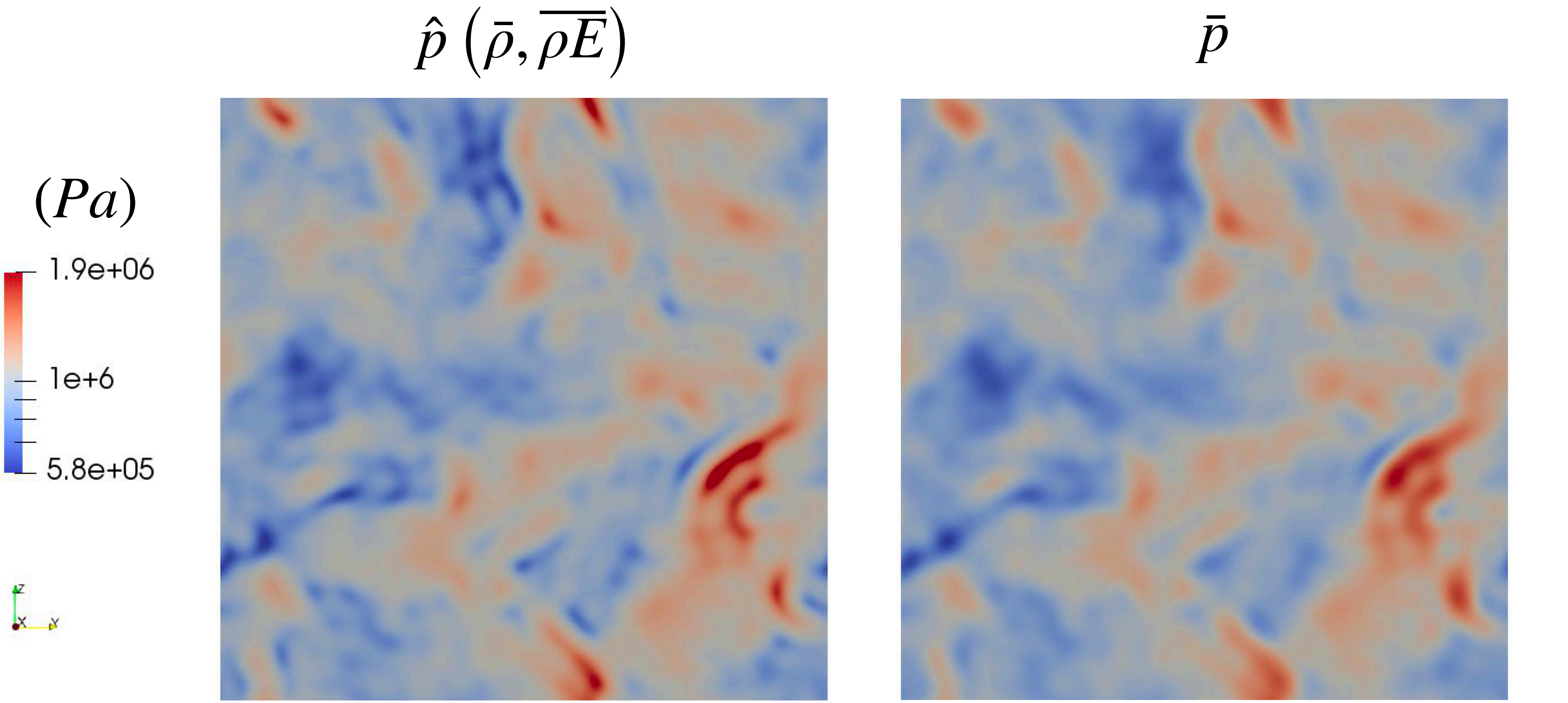
- p_{sgs} changes with the filter size. We choose

$$l = L/15 \equiv k/k_{min} = 15$$

as it lies in the inertial range of turbulence where stronger correlations between filtered fields and sgs fields are expected

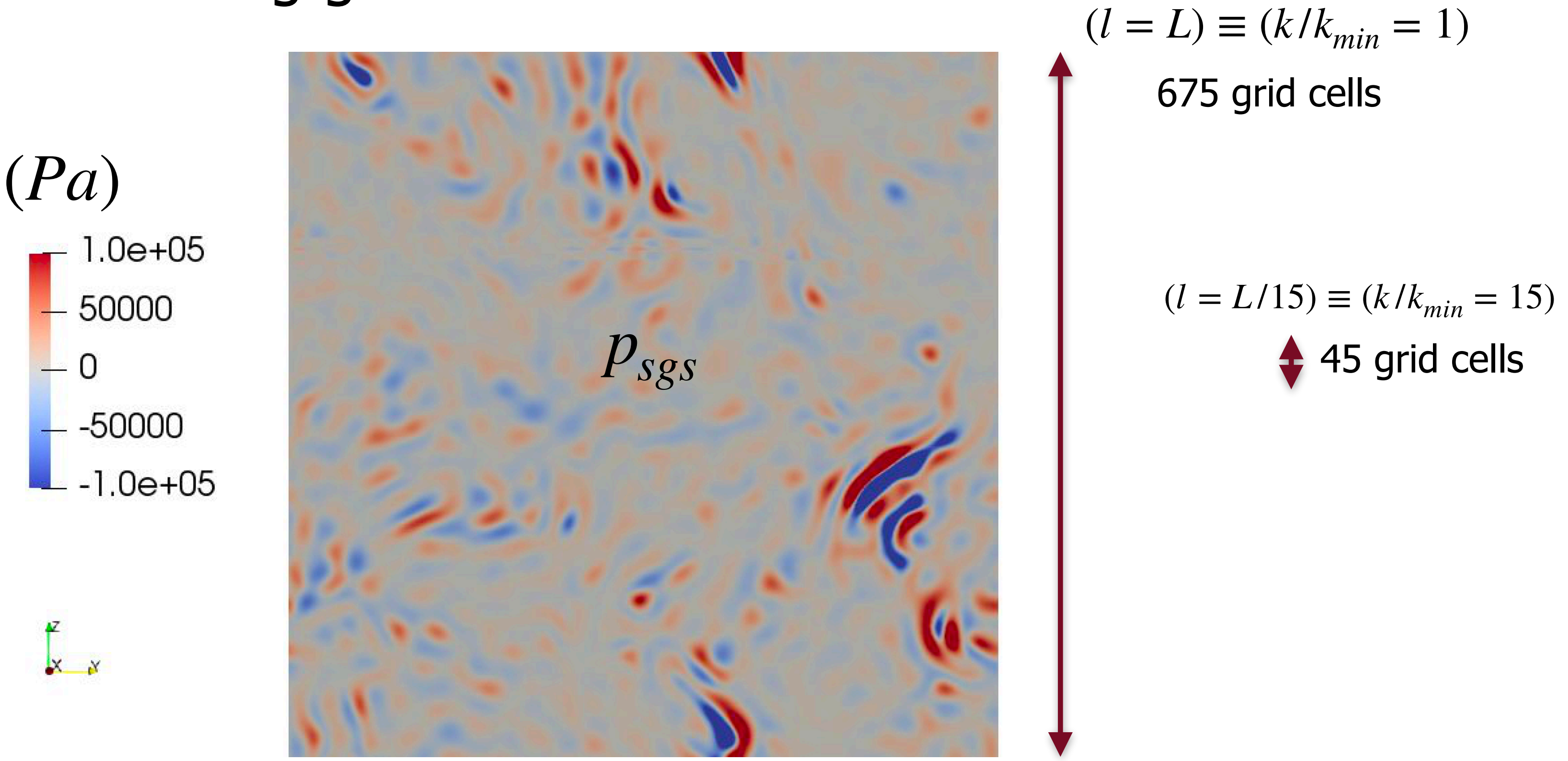
The example of sgs pressure in HIT

- $\hat{p}\left(\bar{\rho}, \overline{\rho E}\right)$ shows differences with $\bar{p}$ especially in regions of strong gradients which are more sensitive to the filtering



The example of sgs pressure in HIT

- As expected p_{sgs} character length lies below the filtering size. Yet structures of larger sizes also appear related to region of strong gradients.



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  - **Neural network model**
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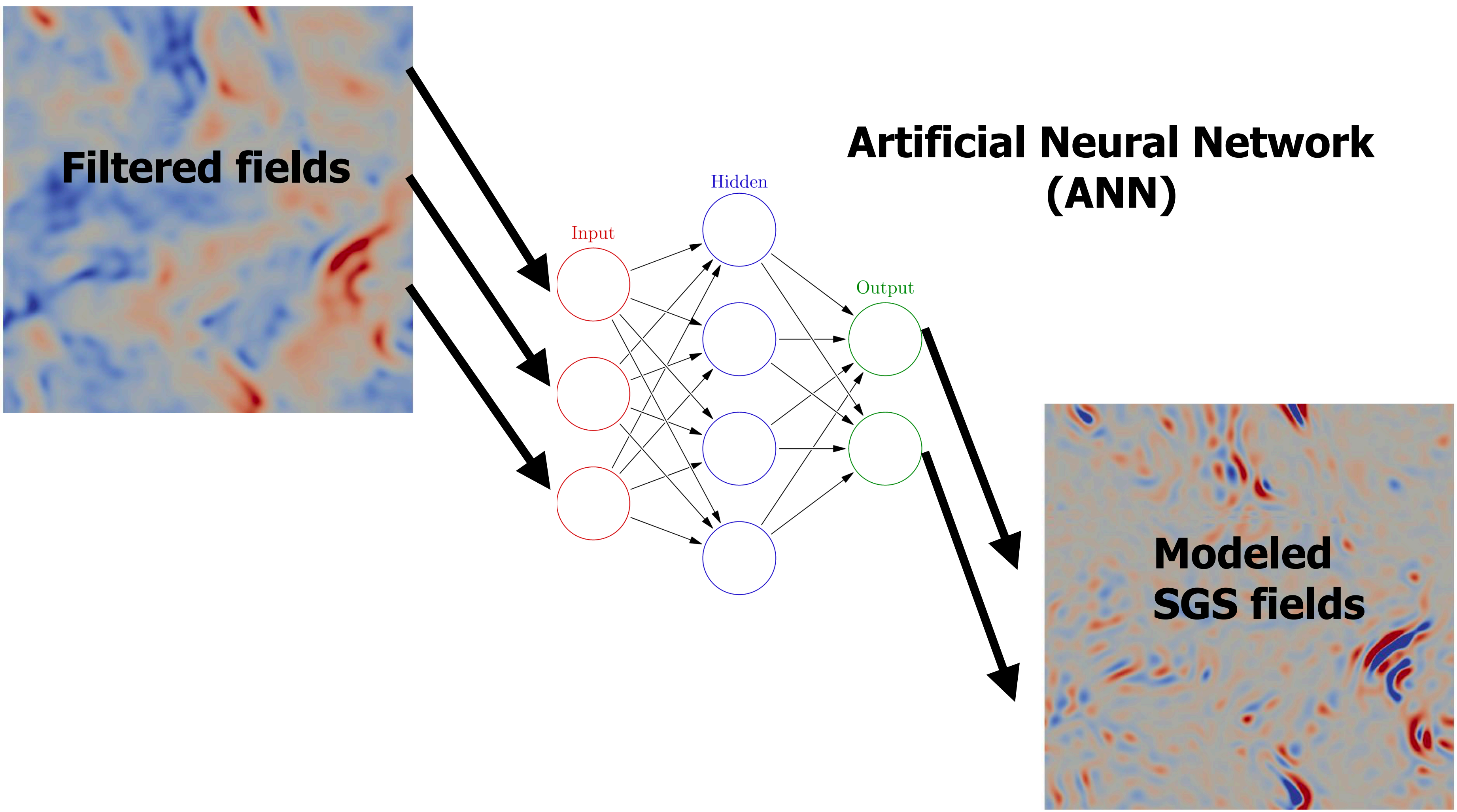
Towards modeling of sgs pressure — Constraints

- **Constraints** are imposed to the modeling strategy:
  - Only quantities accessible to the future LES are used as inputs.
    - **Only filtered fields are used as inputs**
  - The model should be invariant by translation and rotation
    - **Only variables independent of the coordinate system are used**
  - To be efficient, the model should be local in space and time
    - **No history** is taken into account
    - The model at location x is obtained from fields at the same location x (**no space convolution**)
  - The model should be as independent as possible from the types of flows present in the DNS database.
    - **All datasets** (HIT, Mixing layer, Channel) **will be used during training**

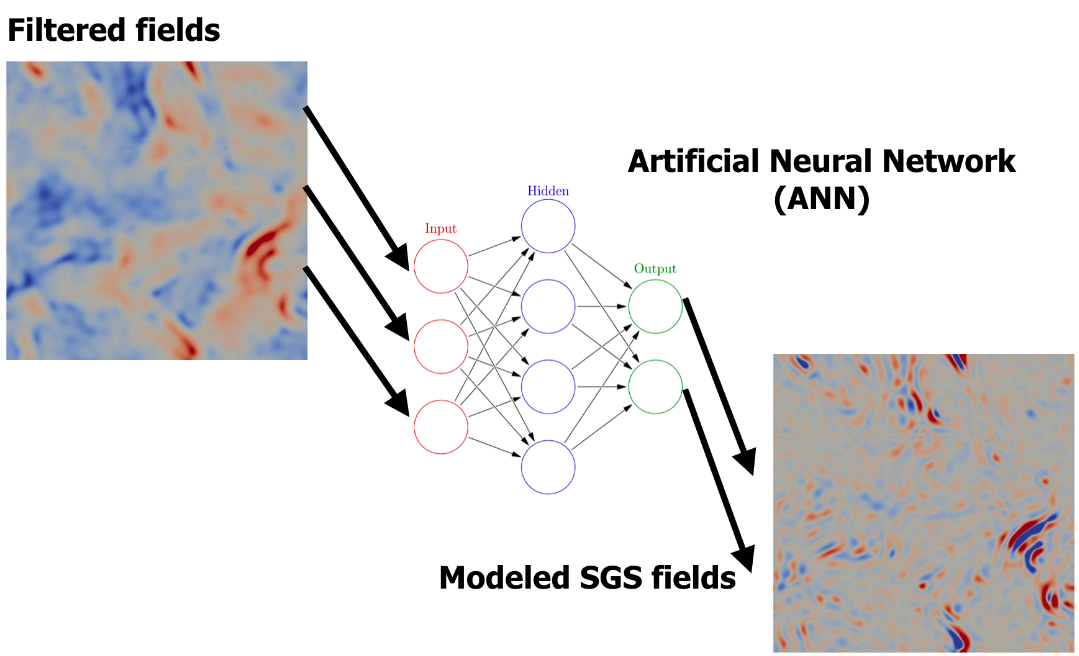
Towards modeling of sgs pressure — Machine Learning



Towards modeling of sgs pressure — ANN example

- Let’s switch to Jupyter and see how ANN regression for sgs fields prediction can be easily implemented using tensorflow?

  - For those interested in the notebook, feel free to contact me!



Towards modeling of sgs pressure — ANN example

- Using Parallel libraries, larger networks and large database (300M points), the correlation improves to 0.95 and R2 to 0.9.
- R2 of 0.9 means that 90% of the variance of the sgs term can be explained by the filtered fields.

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Model Performance:
Correlation:  0.9569431616360217
R2:  0.9066780541374565
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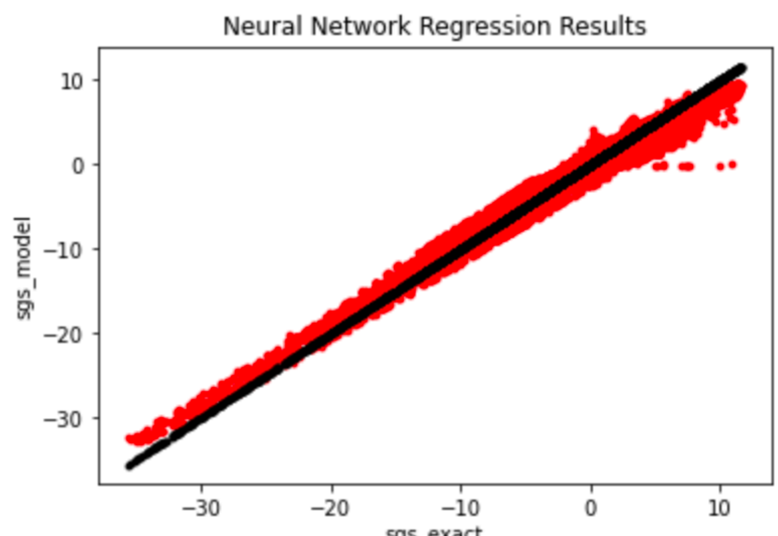

Towards modeling of sgs pressure — Incoming challenges

- (WIP) further HPC implementation of the ANN training and optimize the architecture
- (TBD) Cross case (HIT, Mixing Layer, Channel) training and validation
- (TBD) Feature simplification using only the most influential parameters (network pruning using output of random forest)

- a-posteriori validation thanks to available experimental results!

Thank you for your attention

Questions?