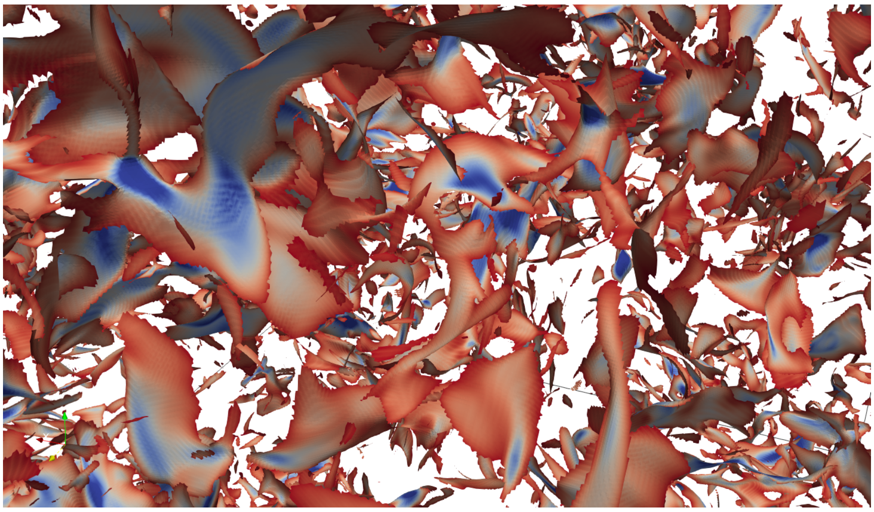
Master Thesis Research Project Proposal

Machine-learning-assisted turbulence modeling in dense gas flows

Ecole Centrale de Lyon / LMFA



Shocklets in turbulence colored by the divergence of the velocity field. ANR-EDGES

Context

Dense gases are characterized by their unusual thermodynamic behavior when their pressure, temperature and density are close to the saturation curve in the vicinity of the critical point. In this region, the fundamental derivative defined as $\Gamma = 1 + \frac{\rho}{c}\frac{\partial c}{\partial \rho}|_s$,with ρ the density, c the speed of sound and s the entropy, is lower than unity for dense gases. As a consequence, and in opposition to the perfect gas behavior, the speed of sound decreases with the density. Because of their molecular complexity, associated with a large molar mass and large heat capacities, some dense gases can reach thermodynamic states in which their fundamental derivative becomes even negative. Such fluids are known as "BZT" dense gases, where BZT stands for "Bethe-Zel'dovich-Thompson" to acknowledge the three researchers who first predicted the existence of such gases (Bethe, 1942 ; Zeldovich, 1966 ; Thompson, 1971). There are multiple consequences for the existence of a negative fundamental derivative thermodynamic region. Those have been studied in great details by Cramer and Kluwick (Cramer, 1984). Among the specific features of dense gas flows, one in particular has raised the interest of the research and industrial community : in supersonic turbulent flows of dense gases, compression shockwave amplitude is decreased by an order of magnitude when compared to the perfect gas prediction. This classical type of shock can even be suppressed in flows of dense gases if the thermodynamic variables remain within the BZT inversion region where the fundamental derivative becomes negative.

Dense gases, some of them BZT fluids, are used as working fluids in Organic Rankine Cycle (ORC) engineering systems harvesting thermodynamic cycles for the recovery of fatal heat. These ORC systems experience an accelerated development under the combined effect of the increase of the energy price and of the public awareness of climate issues (see Figure 1). Companies developing such systems face numerous challenges among which some come from a lack of basic knowledge regarding the turbulent flows of dense gases in expanders. Indeed, to obtain efficient turbomachinery systems, numerous prototypes are designed on the basis of computer simulations also known as Computational Fluid Dynamics (CFD) predictions before being tested. Today, Reynolds Averaged Navier-Stokes (RANS) simulations have become a usual tool in the design phase of these machines, but the turbulence models upon which they rely were all developed in the context of perfect gases. Dura Galiana et al. (Dura, 2016 ; Dura, 2017) show using Large Eddy Simulation that in an ORC turbine stage, the losses due to viscous effects can represent up to two third of the total losses. They also find that dense gas effects tend to increase losses in supersonic wake flows. Since turbulence models determine the accurate prediction of friction losses at the walls and in the blades' wakes, it is essential to assess their relevance in the framework of dense gas flows and to revisit them if necessary.

Figure 1 – Concentration solar panel Organic Rankine Cycle (Crédit STG international)

Numerous publications have shown the limitations of Reynolds Averaged Navier Stokes (RANS) turbulence models (Breuer, 2003), which have difficulties, even in the case of perfect gases, to reproduce phenomena such as boundary layer separation. To meet current challenges, Large Eddy Simulation (LES) has been proposed to simulate the largest structures of the turbulent spectrum and only model the smallest ones. Perfect gas LES impact on current industrial applications has been growing during the last decade and it would be of clear interest to directly rely on such a CFD approach to also address dense gas turbulent flows in expanders.

Unfortunately, there are currently no available turbulence closure models tailored to dense gases neither for statistical approaches such as RANS nor for unsteady ones such as LES. Preliminary results obtained by the authors even suggest that available LES models, all developed in the framework of perfect gases, fail to reproduce important features of the turbulence in dense gas flows (Giauque, 2017).

In 2018, a Young Researcher Project has been granted to our group at LMFA by Agence Nationale de la Recherche (ANR) to analyze the fundamental behavior of compressible turbulence in dense gas (DG) flows and to transfer this knowledge to the field of ORC turbine flow modeling. Since then, Direct Numerical Simulation (DNS) has been used to build an extensive database of turbulent DG flows. The database comprises decaying Homogeneous Isotropic Turbulence (HIT) (Giauque, 2017), forced HIT (Giauque, 2020, see Figure 2), mixing layer (Vadrot, 2020) and supersonic channel flow. Using this database and following Vreman's (Vreman, 1995) methodology, our research team currently concentrates its efforts on providing turbulence closure models to the dense gas flow community in general and to the ORC designer community in particular.

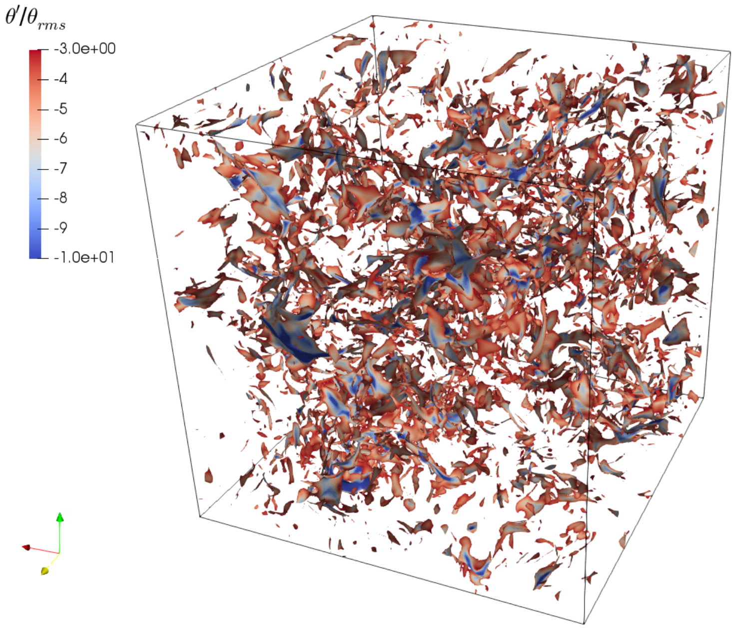


FIGURE 2 – Shocklets in turbulence colored by the divergence of the velocity field

Objectives and Methodology

The Master student will be part of this modeling research effort dedicated to turbulence closure for LES and RANS in the context of dense gas flows. The strategy that will be followed in this Master will largely rely on the notions of Optimal Estimator (Balarac, 2008) and of Uncertainty Quantification (Sudret, 2008). The notion of optimal estimator arises from the decomposition that one can make of the modeling error. Following Vollant (Vollant, 2015), if one wants to model a given term T using a model denoted τ, the error e_q can be split as follows :

$$e_q = \underbrace{\left\langle (T - < T|\phi >)^2 \right\rangle}_{e_{ir}} + \underbrace{\left\langle (< T|\phi > - \tau)^2 \right\rangle}_{e_r}$$

where $< T|\phi >$ is the conditional average of the term T to be modeled by the set of variables ϕ chosen to represent it in the model τ. The main advantage of such a decomposition is that it clearly shows that once the set of variables ϕ has been chosen, there is no way for the model to perform better than the optimal estimator $< T|\phi >$ which provides the irreducible part of the error e_{ir}. As a consequence to this statement, one should recognize that modeling a turbulence closure term requires to first choose on physical analysis principles the best set of variables on which the model should be built (Papoulis, 2002).

One this set is chosen, given the large choice of possible combinations for the model variables, modern techniques such as artificial neural networks (ANN) or Generative adversarial networks (GAN) will be used with profit during the course of the Master in order to identify the precise formula to be used for each statistical (RANS) or subgrid-scale (LES) model. Together with the best variables combination for the model, these methods will also provide the coefficients to be used in order to minimize the reducible error (er) both in terms of functional error (best energy transfer) and structural error (best representation of the sgs structures).

At this stage, the Master student will tackle the issue of robustness of the turbulence model. This can be done using the notion of polynomial chaos expansion (Congedo, 2011) for the turbulent kinetic energy (or any other macroscopic quantity of interest), adding variance (treated as uncertainties) to the coefficients of the model. Doing so, one introduces at the core of the modeling strategy the fact that the best model constants are the ones reducing the reducible error but also having the smallest influence on the final result.

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Master thesis advisors

Christophe Corre (Full Professor ECL) :

Christophe Corre graduated in Engineering from Ecole nationale supérieure de techniques avancées (ENSTA), holds a Master from Ecole nationale supérieure d'arts et métiers (ENSAM) and an accreditation to supervise research from Paris-VI University. He was successively Assistant Professor at ENSAM Paris and the SINUMEF/DynFluid Laboratory (numerical simulation in fluid mechanics) and Professor at Ecole nationale supérieure de l' énergie, l'eau et l'environnement (ENSE33) in Grenoble and at the Laboratory of Geophysical and Industrial Flows. He joined Ecole Centrale de Lyon and the Fluid Mechanics and Acoustics Laboratory (LMFA) in 2014 within the Turbulence and Stability research group. His teaching activities address the numerical simulation of flows and engineering optimization. His research activities cover three main areas : (1) the development of efficient methods for the simulation of hydrodynamic or aerodynamic flows, (2) the robust simulation of complex (two-phase, non-Newtonian, dense gases) flows, and (3) the analysis and optimization of flows including uncertainties.

Alexis Giauque (Assistant Professor ECL) :

During his Master thesis at CERFACS (2003-2007) with Prof. Poinsot, Alexis Giauque has led and participated to the development of large eddy simulation in the context of reactive flow and more specifically to the long lasting research effort trying to model thermoacoustic instabilities in realistic geometries. During his post-doctoral study at Stanford University (2007-2009), the author has engaged with Prof. H. Pitsch in theoretical developments to use advanced acoustics analogies for the modeling of combustion noise. At Onera (2009-2013), the author was part of the numerical aeroacoustics department. He helped develop a new re- search team on the topic of combustion noise. During this period, he supervised three Master thesis students and a Master thesis student in collaboration with Prof. S. Ducruix at Ecole centrale de Paris. Since 2013, the coordinator holds an assistant professor position at Ecole Centrale de Lyon. He is part of the LMFA turbomachinery research team and focuses his research on Large Eddy Simulation of secondary flows in realistic geometries. Since 2016, he has also started a new research initiative aiming at the precise modeling of turbulence in the context of turbulent dense gas flows for ORC turbomachinery applications. From this experience, the author has gathered significant expertise in both numerical and theoretical modeling of acoustics and its interactions with turbulent and entropy fluctuations in the sense of Kovasnay's decomposition. He has also become an expert in the development of massively parallel solvers used in various institutions such as AVBP, CEDRE, elsA and Turb'Flow.

Thanks to this expertise, he is regularly reviewing articles for international peer-reviewed journals and has been reviewing calls for research projects by the FRAE.

Profile

This Master thesis research project (starting date April 2021) will be carried out in the Fluid Mechanics and Acoustics Laboratory (LMFA) at Ecole Centrale de Lyon (ECL). Since it involves both physical modeling of turbulence and numerical developments in machine learning, technical skills in fluid mechanics and applied mathematics are expected from the applicant. A marked taste for modeling and physical analysis in fluids will be an asset. Depending mostly on the academic performance of the candidate, a PhD thesis in the research group on the same topic will be considered.
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