Eulerian models for the description of polydisperse sprays: from fundamental issues to industrial applications and HPC

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The modeling and simulation of multiphase reacting flows covers a large spectrum of applications ranging from combustion in automobile and aeronautical engines to atmospheric pollution as well as biomedical engineering. In the framework of this seminar, we will mainly focus on a disperse liquid phase carried by a gaseous flow field which can be either laminar or turbulent; however, this spray can be polydisperse, that is constituted of droplets with a large size spectrum. Thus, such flows involve a large range of temporal and spatial scales which have to be resolved in order to capture the dynamics of the phenomena and provide reliable and eventually predictive simulation tools. Even if the power of the computer resources regularly increases, such very stiff problems can lead to serious numerical difficulties and prevent efficient multi-dimensional simulations.

The purpose of this seminar is to introduce to the Eulerian modeling of polydisperse evaporating spray for various applications, that is the disperse liquid phase carried by a gaseous flow field is modeled by "fluid" conservation equations. Such an approach is very competitive for real applications since it has strong ability for optimization on parallel architectures and leads to an easy coupling with the gaseous flow field resolution.

We will show that all the necessary steps in order to develop a new generation of computational code have to be designed at the same time with a high level of coherence: mathematical modeling through Eulerian moment methods, development of new dedicated stable and accurate numerical methods, implementation of optimized algorithms as well as verification and validations of both model and methods using other codes and experimental measurements.

We will introduce both a new class of models and their mathematical analysis for the direct numerical simulation of spray dynamics, even in the presence of coalescence and break-up, as well as a set of dedicated numerical methods and prove that such an approach has the ability, once validated, to lead to high performance computing on parallel architectures. We will finally present a synthesis of recent contributions, which aim at: 1- on the one side transferring the proposed models into identified codes for industrial applications in the fields of solid propulsion, aeronautical and automotive engines, 2- on the other side extending the previous work to turbulent flows where some scales can not be resolved and have to be modeled, and where some dedicated numerical methods have to be designed.

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Predicting the performance of fusion plasmas in terms of amplification factor, namely the ratio of the fusion power over the injected power, is among the key challenges in fusion plasma physics. In this perspective, turbulence and heat transport need being modeled within the most accurate theoretical framework, using first-principle non-linear simulation tools. The gyrokinetic equation for each species, coupled to Maxwell’s equations are an appropriate self-consistent description of this problem. A new class of global full-f codes has recently emerged, solving the gyrokinetic equation for the entire distribution function on a large radial domain of the tokamak and using some prescribed external heat source [1]. Such simulations are extremely challenging and require state-of-the-art high performance computing (HPC).

The non-linear global full-f gyrokinetic 5D code GYSELA, which focuses on the electrostatic toroidal branch of the Ion Temperature Gradient driven turbulence with adiabatic electrons, is one of them. One particularity of the code is to solve the self-consistent problem on a fixed grid with a Backward Semi-Lagrangian scheme [2]. Despite the non-locality of this method, the new two-ion-species version of the code has been successfully ported on BlueGene architecture with a relative efficiency of 91% on 458 752 cores (weak scaling). The hybrid OpenMP/MPI parallelization which allows to obtain such performance will be detailed. One mid-term objective is to implement kinetic electrons in the code. This will need an increase of the mesh size by a factor of the order of 103 and need a decrease of the algorithm time step by a factor 10. Present simulations already require petascale computing resources. We will discuss the various approaches we currently investigate to prepare the code for our exascale future needs.