ParCFD'2020
32^{nd} International Conference on Parallel Computational Fluid Dynamics
May-11-13 2020, Nice FRANCE

A DYNAMIC LOAD BALANCE STRATEGY FOR ADDRESSING CHEMICAL REACTIONS IN COMBUSTION PROBLEMS

D. Mira*, A. Surapaneni*, G. Ramírez*, V. López*, Eduardo J. Pérez-Sánchez*, R. Borrell*, O. Lehmkuhl*, M. García-Gasulla*, G. Houzeaux*

* Barcelona Supercomputing Center
Department of Computer Applications in Science and Engineering
08034 Barcelona, Spain
e-mail: daniel.mira@bsc.es, web page: https://www.bsc.es

Key words: combustion, chemical reactions, load balancing, hybrid parallelization

Abstract. The more stringent emissions regulations in the automotive and aircraft industries are forcing the combustion systems to operate with low emissions and increased efficiency. The formation of pollutants is directly linked to the local conditions of the combustion process, and it is influenced not only by the thermodynamic conditions within the combustion chamber, but also by the level of mixing, heat transfer and residence time. The prediction of pollutant formation at engine-relevant conditions is a major challenge in the community, as some pollutants like soot are governed by the kinetics processes that require detailed descriptions of the chemical evolution of the flow.

The use of detailed chemistry in reacting flow simulations involving turbulent flows still represents a major challenge. It can occur that the chemical scales can be of the same size as the turbulent length scales, and the interactions between these two has to be considered. This can be a difficult task when a detailed mechanism is employed as it is required to account for fast and slow chemical reactions. The slow reactions are usually responsible of controlling the chemical evolution of the reaction process, while the fast reactions are important to ensure the correct radical pool involved in the combustion process. This disparity in chemical scales introduces stiffness in the computation of the species consumption rates and makes this calculation highly costly. The application of detailed chemistry in direct numerical simulation (DNS) and large-eddy simulations (LES) results in low performance if the chemical problem is not addressed with load balance techniques. In fact, chemical reactions usually take place in thin layers that represent small portions of the computational domain, so the overall computational cost of the time step can be dominated by the cells performing source term integrations.

The present study is dedicated to analyse this problem and provide dynamic load balance strategies using a dynamic load balancing library in the context of a hybrid MPI/OpenMP approach. This library is used on the top of OpenMP pragmas in order to continuously exploit all the resources available at the node level, thus increasing the load balance and the efficiency of the parallelisation with MPI.