D4.5 COMPUTATIONAL PERFORMANCE ANALYSIS
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Author	Eduardo J. Pérez Sánchez (BSC)
Contributor(s)	Ruud Eggels (RR), Federica Ferraro (TUDa), Christian Hasse (TUDa)
Reviewer	Daniel Mira Martínez (BSC)
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Change Log

Version	Author	Description of Change
V0.1	Eduardo J. Pérez Sánchez	Initial draft
V0.2	Daniel Mira	Full review
V1.0	Ruud Eggels, Federica Ferraro, Christian Hasse	Final version

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1. Executive Summary

This document provides a summary of the current performance of the models from the different consortium members codes that have been implemented during the project or are essential for the simulations to be accomplished in the project. The results gathered in this document have been mainly obtained recently in the Preparatory Access 2010PA5720 from PRACE (Partnership for Advanced Computing in Europe) which extended from 12/4/2021 to 12/6/2021. Therefore, results are representative for the production simulations scheduled during next months. A continuous work is being developed to improve the performance of the models and, in consequence, such performance is susceptible of being further improved in the incoming weeks.

2. Introduction

A large effort has been dedicated by the members of the consortium to develop and implement the turbulent combustion and soot models to accurately simulate and predict soot in terms of chemical evolution and particle formation. However, this accuracy has to come along with a high performance of the codes to obtain results in a reasonable amount of time and make the CFD (Computational Fluid Dynamics) competitive and applicable to relevant and realistic problems. Due to the intensive computation, the problems faced in CFD simulations for combustion are CPU-bound and, therefore, only strong scalability analysis has been carried out. In the following, the summary of the main results for the different codes and models are described.

3. Description of the models and the codes

The models and codes that will be used in the production simulations for the project and for which the scalability analysis has been carried out are described.

3.1 Combustion and soot models

The following combustion models have been considered:

- Flamelet Generated Manifold (FGM) model (van Oijen and de Goey, 2000): where the thermochemical structure of the flame is tabulated in a pre-processing stage and several controlling variables are transported with the flow equations. The flame structure is recovered from look-up tables reducing substantially the computational cost.
- Conditional Moment Closure (CMC) model (Klimenko and Bilger, (1999)): species mass fractions conditioned to the mixture fraction are solved, resulting in a robust, accurate, but expensive method for turbulent combustion.

The following soot models have been considered:

- Discrete Sectional Method (DSM) (Gelbard et al., 1980; Blacha et al., 2012) :the Particle Size Distribution (PSD) is approximated by partitioning the range of soot volume particles in several bins or sections inside which properties for soot are considered constant. From such properties the soot mass for each section is transported.
- Extended Quadrature Method of Moments (EQMOM) (Yuan at el., 2012; Salenbauch et al. 2019): to reduce the computational cost involved in transporting the sections, in the EQMOM low-order moments of the PSD are transported and an approximated PSD is reconstructed.

3.2 CFD codes

The following codes have been analysed:

- Alya: the multi-physics code Alya has been developed at BSC and belongs to the PRACE Benchmark Suite for HPC applications. Alya is based on the Finite Element Method (FEM), has been highly optimized and tested independently in most of the European supercomputer platforms and applied to a wide range of engineering problems with noticeable and successful results (Vázquez et al., 2016), e.g.: it has been recently tested in the context of Center of Excellence in Engineering EXCELLERAT (www.excellerat.eu) in 48k CPUS in problems of reacting sprays of 1 billion cells in MareNostrum 4. Alya is written in Fortran and uses a master-slave strategy using hybrid parallelization MPI/OpenMP. Regarding the combustion models, both the flamelet and CMC models are implemented in Alya while the DSM model for soot is coded too. Regarding the computational methods, an explicit Runge-Kutta scheme with temporal 3rd order discretization and a second order discretization in space is used to solve the momentum and scalar transport. Moreover, for continuity and momentum, a low-dissipation scheme for low Mach number reacting flow based on the fractional step algorithm with a third order temporal scheme is used (Both et al., 2020). For CMC chemistry is integrated with Cantera using the CVODE algorithm while flamelet tables are used to look up thermochemical variables when running with the FGM model.

- OpenFOAM: OpenFOAM is a free, open-source CFD software written in C++ for HPC applications, based on the Finite Volume Method (FVM), that has a large user base across most areas of engineering and science, from both commercial and academic organizations. The present OpenFOAM code is an extended in-house version from TUDa in which the flamelet-progress variable combustion model is implemented using flamelet look-up tables (FLUTs) including premixed and non-premixed flamelet configurations and the EQMOM model is applied for modeling the soot formation and evolution. The flamelet tables are saved and read in hdf5 format, which is advantageous in terms of memory requirement. OpenFOAM uses MPI for parallelization. Finally, to note that the code has been recently tested for combustion problems in the context of Center of Excellence in Combustion CoEC (www.coec-project.eu).

- PRECISE-UNS: PRECISE-UNS is a FVM code written in Fortran developed by Rolls Royce based on a pressure correction method for both incompressible as well as compressible flows that uses second-order discretization in space and time. The Flamelet Generated Manifold (FGM) and detailed reaction combustion models are available in combination with presumed, but also with the Eulerian stochastic field Probability Density function closure methods for chemistry-turbulence interaction. The detailed chemistry is integrated with an in-house developed highly efficient method, making use of inline chemistry and analytically derived Jacobians. PRECISE-UNS is parallelized based on domain decomposition using Parmetis and/or Scotch and by the use of standards OpenMPI and Intel MPI. The variables are solved sequentially using an AGMG or the Hypre solver. PRECISE-UNS scalability has been tested and demonstrated on Archer and STFC Hartree Centre (UK), and also has been used on PRACE machines.

The main characteristics of the codes are described in the table.

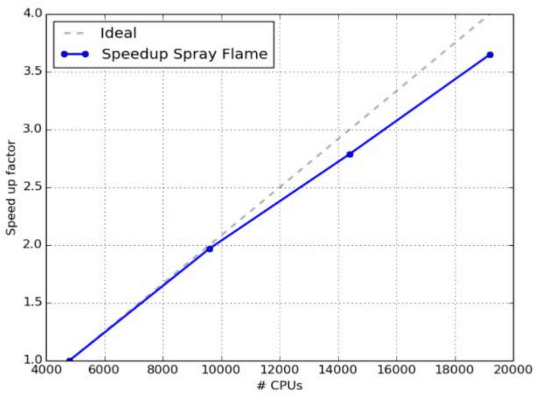
	Alya	**OpenFOAM**	**PRECISE-UNS**
Computational Method	FEM	FVM	FVM
Kind of parallelism	OpenMP and MPI	MPI	MPI
Programming language	Fortran	C++	Fortran
Combustion models	FGM and CMC	FGM	FGM
Soot models	DSM	EQMOM	2-equation

Table 1. Main characteristics of the CFD codes used in ESTiMatE project.

4. Strong scalability analysis

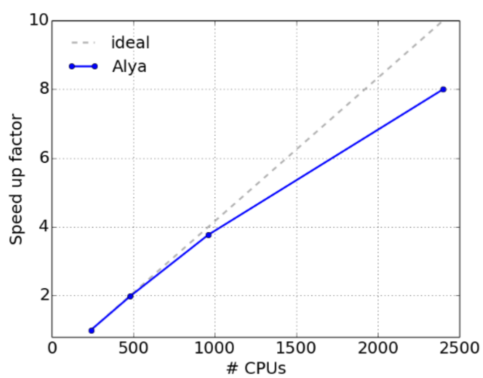
The strong scalability analysis for the aforementioned codes is shown in the following figures and more specific information is gathered in the tables.

- Alya:
  - FGM model:
    Strong scaling curve for the FGM method of a spray flame in a swirl stabilized burner with 1 billion cells and 200k particles:



Number of cores	Wall clock time	Speed-up	Efficiency (%)
4800	27,7	1,00	100,0
9600	14,1	1,97	98,5
14400	9,9	2,78	92,9
19200	7,6	3,65	91,2

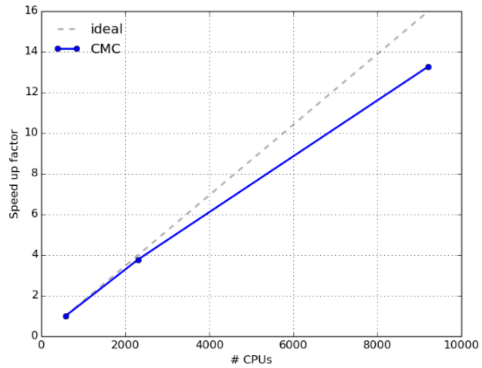
  - FGM model coupled to the DSM soot model[1]:
    Strong scaling curve for the FGM method coupled to the DSM soot model implemented in Alya for a RQL burner with 57M elements:



Number of cores	Wall clock time	Speed-up	Efficiency (%)
240	20,0	1,00	100,0
480	10,1	1,98	99,0
960	5,3	3,77	94,3
2400	2,5	8,00	80,0

[1] Wall clock time refers to the average value per time step.

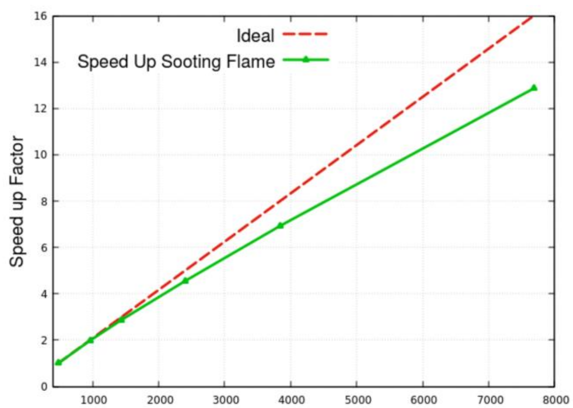
- CMC model[2]: Strong scalability for CMC model for a RQL burner with 57M elements and 25 mixture fraction levels.



Number of cores	Wall clock time	Speed-up	Efficiency (%)
576	591,0	1,00	100,0
2304	156,3	3,78	94,5
9216	44,5	13,28	83

- OpenFOAM

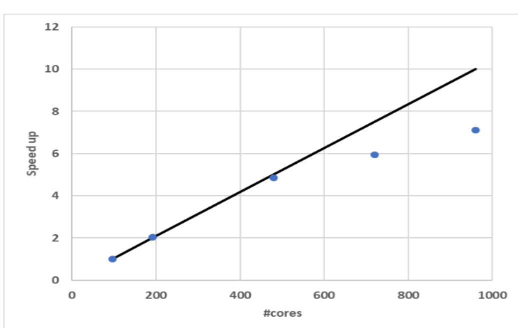
  Strong scaling curve for FGM with soot model calculations:



Number of cores	Wall clock time	Speed-up	Efficiency (%)
480	1037,0	1,00	100,0
960	523,7	1,98	99,0
1440	361,3	2,87	95,7
2400	228,0	4,55	91,0
3840	149,6	6,93	86,6
7680	80,6	12,86	80,4

- PRECISE-UNS

  Strong scaling curve for the FGM method:



Number of cores	Wall clock time	Speed-up	Efficiency (%)
96	5415	1,0	100,0
192	2649	2,04	102,0
480	1119	4,84	96,8
720	913	5,93	79,1
960	763	7,10	71,0

[2] For this model the wall clock time refers to the average value per time step.

In general, the performance is satisfactory and fulfills the expectations. It is worth mentioning that the decay in performance with high number of cores is mainly due to a low load per subdomain. In general, the parallel performance of the codes is satisfactory for the application cases considered in the project ESTiMatE and the codes can now be used in production runs. These results have helped to understand certain aspects of the models and to confirm an adequate implementation of the models in terms of use of resources as well as that they can be used for production simulations. Moreover, with the help of these results some aspects will be carefully analysed to intend to reduce the computational cost and further improve the performance of the models.

5. Conclusions

Fulfilling the objectives posed in the project ESTiMaTE requires the use of advanced combustion and soot models in codes that show high performances and excellent scalability. In this report the main results regarding scalability for the three CFD codes used in the project in conjunction with the models to be applied in production simulations are gathered showing that their performance is fairly satisfactory. Moreover, thanks to this study some aspects of the implementations have been identified with potential to enhance the performance of the models.
In conclusion, it is considered that the current study is a guarantee to successfully cope with the simulations scheduled in the project and, therefore, give response to the need of better understanding the physical phenomena involved in soot formation, its evolution at aero-engine operation and how is affected by the Turbulence-Chemistry Interaction (TCI) of the combustion models, concerns that motivated the creation of the ESTiMatE project.

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