Center of Excellence in Combustion

D4.1 - Concept Plan for Methodologies

[Version 1.3]

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Outline

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1. Introduction

The Center of Excellence in Combustion (CoEC) was born out of the European Union's need to move towards decarbonization in the power generation and transportation sectors with the aim to achieve net-zero greenhouse gas (GHG) emissions by 2050 [1]. Indeed, global energy demand is increasing every year and most of this energy is produced by burning fossil fuels. To overcome this drawback, growth in the use of sustainable fuels, such as biofuels, hydrogen, or Power-to-X (P2X) based on ”e-fuels” is envisioned in the short future. Therefore, there is a clear need to develop advanced simulation software to assist in this transition.

Combustion is a complex multi-physics and multi-scale problem, so it is necessary to understand the physics behind the burning process of these new fuels in order to identify the technological developments for the new generation of combustors so they operate more efficiently and with fewer emissions. Numerical simulations are an essential tool for this purpose and, considering the increase in computational power over the past years, an evaluation of physical models and numerical methods is required [2].

The accurate simulation of turbulent combustion in realistic configurations is extremely demanding in terms of computational resources. A transition towards exascale architectures in High-Performance Computing (HPC) systems is foreseen, where numerical simulations will play an increasingly important role in the design of new, more complex, and less polluting combustion systems [3]. This will nonetheless happen only if the Computational Fluid Dynamics (CFD) codes and existing algorithms re optimize or new models are developed in order to harness the computational power that will be available.

This work package (WP4) aims to enhance and develop simulation methodologies enabled by the use of (pre-)Exascale systems, with the focus on the applications defined by the Exascale Challenge Demonstrators (ECD) in WP7.

The main and general objectives are:

- To develop numerical strategies and optimize the existing models for the simulation of combustion in realistic and canonical configurations, so that they will take advantage of the features and power of the exascale architectures.
- To develop error estimators for dynamic mesh adaptation and optimize the existing algorithms for the study of combustion in the Eulerian-Lagrangian framework.
- To develop new thermo-chemical models and solvers with a high degree of accuracy and a low computational cost.
- To optimize the existing models or develop highly-parallel algorithms for the particle transport in the Euler-Euler and the Euler-Lagrange frameworks.

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For this reason, this work package will be divided into four tasks:

1. High-order methods for reactive and multi-phase flows: The goal is to develop high-order spatial and temporal discretization formulations. The numerical methods developed in this task will be the prerequisite step for the developments conducted in WP5 and will be tested on the simulations performed in the WP7.

2. Error estimators for dynamic mesh adaptation in the Eulerian-Lagrangian framework: The Adaptive Mesh Refinement (AMR) techniques allow for having a local refinement around the flame zone. However, this might be challenging in spray flames, because spray droplets might be mainly localized around this zone. This task aims to develop an error estimator to allow for having a double-constrained load-balancing. This task is mainly linked to the developments from WP5 and will be tested on the WP7 benchmarks.

3. Adaptive chemistry and UQ of chemistry reduction: The development of more accurate and optimized chemistry models will allow better prediction of pollutant emissions, such as NOx and CO. These two species are of special importance since their slow chemical rates make their prediction models very complicated. The objectives of this task are to develop and implement adaptive chemistry allowing to use the most appropriate and computationally efficient chemical kinetics mechanism on-the-fly, and to realize innovative solvers for the stiff systems of Ordinary Differential Equations (ODEs) representing the chemistry that will be efficiently coupled with the CFD solvers. The developments of this task will be tested on the benchmarks of WP7.

4. Euler-Euler and Euler-Lagrange methods for particle transport: The objective is to develop robust algorithms able to perform high-fidelity simulations with a high degree of accuracy to gain a deeper understanding of the fundamental processes occurring in multiphase flows. For instance, on the spray combustion side it will be focused on transport and evaporation of the fuel liquid droplets, while in particulate matter, it will focus on the formation and transport of soot and aerosols. The developments of this task will be tested on a selected case of the WP7.

The development of those methodologies will significantly improve the simulation capacity of the flagship codes from the consortium.

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2. Combustion methodologies

2.1 High-order methods for reactive and multi-phase flows

2.1.1 Background

The participant institutions involved in this task are the Aristotle University of Thessaloniki (**AUTH**) jointly with the Eidgenössische Technische Hochschule Zürich (**ETHZ**), the Barcelona Supercomputing Center (**BSC**), and Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (**CERFACS**). In this task, high-order algorithms will be developed for an accurate description of the combustion process as well as all its underlying phenomena. These algorithms will be developed in the hexahedral spectral-elements-based codes **Nek5000** and **NekRS** [4] from AUTH & ETHZ, the finite element-based code **Alya** [5] from BSC, both using the low-Mach number approach for reacting turbulent flows, and the spectral-differences based, fully compressible code **Jaguar** [6] from CERFACS.

2.1.2 Aims

The present High-order methods for reactive and multi-phase flows task aims at developing algorithms for high-order methods that allow the use of high resolution only in the neighborhood of the thin reaction zones. These algorithms include dynamic relocation of grid points following the flame movement (r-refinement), overlapping grids, and adaptive h-p mesh refinement methods. Note also that, artificial or entropic viscosity methods for enhanced stability in reactive simulations and minimization of over- and undershoots in scalar fields will be investigated.

The choice and the formulation of such methods is particularly challenging for Exascale computing architectures and the goal is to establish ground rules for the optimal design of numerical schemes for Exascale-type simulations.

Thus, according to the capabilities and specific interests of each partner:

- AUTH & ETHZ will focus on the implementation of new algorithms on r-adaptivity in Nek5000 and NekRS as well as optimizing the already existing domain-decomposition-based iterative solvers. An evaluation of the convergence issues with the overlapping grid approach will be carried out. To be able to study internal combustion engine geometries following the piston and valve motions, the arbitrary Lagrangian-Eulerian mesh motion will be implemented, using high-order spectral interpolation. Finally, the Artificial Viscosity Method will be implemented in NekRS to avoid over- and undershoot in scalar fields.

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- BSC's objective is to develop a high-order combustion solver based on the use of quadratic and cubic elements. To do that, the low-Mach number and the flamelet solvers will be extended to be used with quadratic and cubic elements and entropy-stable methods. Finally, the solver will be integrated with Adaptive-Mesh Refinement technique to explore the possibilities of mesh adaptation in a high-order elements framework.
- CERFACS's main goal is to prove the capability of the Jaguar code with spectral differences to predict reacting flows in large-scale high-fidelity combustion simulations.

2.1.3 Strategy

Two main strategies will be followed. On the one hand, AUTH/ETHZ and BSC will select, test, and compare **splitting approaches for thermochemistry** in their respective codes (Nek, Alya). They will also jointly investigate **artificial/entropic viscosity methods** for enhanced stability and minimization of over and undershoots in scalar fields.

On the other hand, AUTH/ETHZ and CERFACS will discuss the suitability of the application of adaptive approaches for high-order methods (static or dynamic refinement), will assess the high-order instabilities related to h-p refinement due to the flame movement when going from high-to-low resolution and will exchange expertise on h-p methods. For this purpose, cases with increasing complexity will be proposed extending from simple 1D and 2D laminar flames to 3D turbulent flames.

To validate the developments achieved in this task, tests will be performed on common benchmark cases. AUTH & ETHZ, will perform Direct Numerical Simulation (**DNS**) to study flame propagation in turbulent spherically propagating flames in open and close domains [7], in collaboration with RWTH and TUe. BSC and CERFACS will also participate in this study to assess the accuracy and performance of the high-order methods developed in Alya and Jaguar, respectively. Moreover, the VOLVO bluff-body flame [8] will be also investigated by BSC and CERFACS.

2.1.4 Expected outcomes

The expected outcome of this task is to demonstrate the validity and performance of high-order methods in turbulent reacting flows simulations. Two major achievements are intended:

- Algorithms that allow the dynamic relocation of grid points that follow the flame movement, i.e. r-refinement, the use of overlapping grids, and adaptive h-p mesh refinement methods.

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- The development of artificial or entropic viscosity methods for enhanced stability in the computations of scalar fields in reactive simulations.

2.2 Error estimators for dynamic mesh adaptation in the Eulerian-Lagrangian framework

2.2.1 Background

The participanting institutions in this task are the *Barcelona Supercomputing Center* (**BSC**), and the *Complexe de Recherche Interprofessionnel de Aérothermochimie – Unité Mixte de Recherche du Centre National de la Recherche Scientifique* (**CORIA – CNRS**). Both partners will perform Large-Eddy Simulations (**LES**), using the Euler-Lagrange (**E-L**) approach of turbulent spray flames. While BSC will model chemistry effects by a tabulated chemistry approach, CORIA-CNRS will use a finite-rate chemistry description. The discretization of the Partial Differential Equations (PDEs) of Navier Stokes is done by the Finite-Element Method (FEM) in **Alya** [5], the BSC code, and the Finite-Volume Method (FVM) in **YALES2** [9]**,** the CORIA-CNRS code. Both codes are capable of working with unstructured meshes and complex geometries using the low-Mach number assumption and beyond second-order space and time schemes for scalars and momentum transport.

2.2.2 Aims

The main objective of this task is to further develop the AMR methodology and adaptation criteria for the study of two-phase flows in the Euler-Lagrange framework. Moreover, both partners will work on the development of error estimators for dynamic mesh adaptation in the Finite Element and Finite Volume formulations. To this end, both teams will work together on this topic and compare the different strategies.

2.2.3 Strategy

The strategy chosen in this task is based on building up the capabilities of the codes in a step-by-step process. Common test cases will be used to evaluate accuracy and performance of the codes. The first test case corresponds to a simple 2D hydrogen-air premixed Bunsen flame and then this will be extended to a 3D spray configuration, still to be defined.

2.2.4 Expected outcomes

From this task, we expect to obtain two codes fully capable of using dynamic mesh adaptation in reacting two-phase flows, with high parallel performance and degree of accuracy.

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2.3 Adaptive chemistry and UQ of chemistry reduction

2.3.1 Background

The participant institutions on this task are the *Aristotle University of Thessaloniki* (**AUTH**) jointly with the *Eidgenössische Technische Hochschule Zürich* (**ETHZ**), the *Barcelona Supercomputing Center* (**BSC**) and the *Rheinisch-Westfälische Technische Hochschule Aachen* (**RWTH**). The partners are expected to develop together a library in order to address two of the main issues regarding the combustion on exascale computing: minimize the dimension of the chemistry problem and introduce innovative methodologies for its solution. The library will be first developed for the codes of the groups involved in the task (**Nek5000** and **NekRS** [4], the AUTH & ETHZ code**; Alya** [5], the BSC code; and **CIAO** [10] the RWTH code), and will later be made available to all partners in CoEC.

2.3.2 Aims

This task focuses on building an efficient solution to the chemistry problem in the context of exascale computations of reacting turbulent flows with both DNS and LES methodologies. The aim of this task is two-fold: (i) reduce the size of chemical kinetics mechanisms through the development and optimization of methodologies for the on-the-fly reduction of these mechanisms; (ii) develop and optimize ODE solvers based on semi-implicit methods and able to take advantage of GPU technology.

The realization of adaptive on-the-fly reduction of the chemical kinetics mechanisms has for objective to drastically reduce the number of degrees-of-freedom needed for the accurate simulation of the combustion process including pollutants and particulate matter. In addition, the innovative solvers will be coupled with splitting algorithms in the flow solver. To drastically reduce the computational time keeping high accuracy. The methodologies developed will be included in a library that will be available for all CoEC partners. The success of this task will affect the realization of the WP7 and consequently the ECDs.

The targets of this task will be pursued by the partners involved in a complementary fashion.

- AUTH & ETHZ will develop the semi-implicit ODE solver integrator for the stiff system of equations resulting from the chemical source term. This step will first be accomplished within the Nek5000 framework and then distributed to all CoEC partners.
- BSC & RWTH will focus on the development and implementation of dynamic adaptive chemistry methods with the final aim to use finite-rate chemistry instead of a tabulated simplification.

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2.3.3 Strategy

As stated above, the works realized by the partners involved in this task are complementary. The partners will attack the different aims following the strategies here elucidated:

- AUTH & ETHZ will implement high-order time splitting schemes and investigate the performance and accuracy of different integrators for each physical or chemical subprocess (convection, diffusion and chemical source term). This will be done first in the current CPU version of the low Mach reactive flow solver and subsequently in the next-generation CPU/GPU version of the spectral element solver NekRS.

The steps that will be performed in T4.3 are as follows:

  - Study the performance and accuracy of different high-order splitting schemes (i.e. Strang-type, balanced, steady-state preserving)
  - Investigate different combinations of time integration schemes for the corresponding terms (convection, diffusion, chemical source term)
  - Investigate how the different chemistry descriptions can be coupled in the interface regions
  - Develop efficient and scalable GPU-friendly kernels for the computation of thermodynamic and transport properties and chemical source terms
  - Implement the most accurate scheme first in Nek5000 and subsequently in NekRS to address load balancing and other performance issues

- BSC will focus on the realization of dynamic adaptive chemistry (DAC) methods into the in-house low-Mach solver, Alya, with to finite-rate chemistry, through the following steps:
  - Develop a framework for DAC including optimizations based on correlated (CO)-DAC and Tabulated-DAC (TDAC).
  - Realization of chemistry reduction based on Path Flux Analysis (PFA) [11] and Reaction Flow Analysis (RFA) [12].
- RWTH will also focus on the realization of dynamic adaptive chemistry methods into the in-house low-Mach solver with to finite-rate chemistry (CIAO), following a complementary approach which includes the following steps:
  - Clustering of the computational domain into sub-region having a homogeneous combustion regime and stage. This step consists of the development of an unsupervised artificial intelligence network that will be

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trained on a set of databases of multi-regimes flames (premixed, diffusion and autoignition) [13].

- Implementation of the Directed Relation Graph with Error Propagation (DRGEP) methodology [14] into the in-house code FlameMaster [15] for the realization of reduced mechanisms.
- Targeting of the model reduction criteria in order to realize a reduced mechanism for each of the cluster present in the computational domain.
- Integration of the methodologies developed above into CIAO.

The first benchmark test for this task is a laminar tri-branchial flame (multi-regime) of Dimethyl ether (DME) and air [16]. This test presents complex characteristics in terms of the size of the chemical kinetics mechanisms and interaction between the thermo-diffusive and chemical phenomena, while the computational cost remains low. When the methodologies developed will become mature enough in terms of reliability and accuracy, more challenging tests will be performed to assess the computational efficiency. These are turbulent spherically propagating flames in open spherical and in closed cylindrical domains [7], turbulent propagating flames (e.g. slot or jet burners) [17]. The final application is still to be discussed, among WP4 and the WPs (particularly WP7) and the ECDs that will benefit from the library produced. The ones under consideration are: the Cambridge RQL burner [18], DLR hydrogen-enriched natural gas burners [19], and the Coria Rouen Spray burner (CRSB) [20] for spray flames with soot formation.

2.3.4 Expected outcomes

The expected outcome from this task is a realization of a library for exascale computing of the chemistry problem for the CoEC flagship codes. The library will include two main aspects:

1. Algorithms for the on-the-fly reduction of the chemical kinetics mechanisms according to different strategies as detailed above
2. Realization of high-accuracy semi-implicit ODEs for stiff problems.

2.4 Euler-Euler and Euler-Lagrange methods for particle transport

2.4.1 Background

The participating institutions in this task are the *Aristotle University of Thessaloniki* (**AUTH**) jointly with the *Eidgenössische Technische Hochschule Zürich* (**ETHZ**), the *Barcelona Supercomputing Center* (**BSC**), the *Complexe de Recherche Interprofessionnel de Aérothermochimie – Unité Mixte de Recherche du Centre National de la Recherche Scientifique* (**CORIA – CNRS**), *Technical University of Darmstädt* (**TUDa**), the *Rheinisch-*

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Westfälische Technische Hochschule Aachen (**RWTH**), and the *University of Cambridge* (**UCAM**). Each partner is expected to develop a specific capability of their code for a given application, therefore, a wide variety of computational methods will be used. The discretization of the Navier-Stokes Partial Differential Equations (PDEs) is done by the Finite-Element Method (FEM) in **Alya** [5], the BSC code, the Finite-Volume Method (FVM) in **YALES2** [9], **OpenFoam** [21], and **CLIO** [22], the CORIA-CNRS, TUDa and the UCAM codes, respectively, the Hexahedral Spectral Elements (SEM) approach in **Nek5000** and **NekRS** [4], the AUTH & ETHZ code, and the Finite-Difference Method in **CIAO** [10], the RWTH code. All codes use the low-Mach number assumption and at least second-order space and time schemes for scalars and momentum transport.

2.4.2 Aims

The long-term objective of this task is to develop and optimize extremely parallel algorithms for the multiphase flow calculations, mainly for liquid-gas, solid-gas and liquid-solid-gas multiphysics problems. These flow problems may be either the spray produced by fuel injection or particulate matter, such as soot or aerosols. The gas-phase will be studied with the Eulerian approach. For the dispersed phase two techniques are used: the Lagrangian approach coupled with the Eulerian approach, henceforth called the **E-L** approach, and the Eulerian approach coupled with the Eulerian gas phase, hereinafter referred as to **E-E** approach.

Another target of this task is to develop new algorithms and solvers and to further improve and optimize the already existing algorithms for particle transport (liquid and solid) in multiphase flow problems.

- AUTH & ETHZ will test the validity of the GPU-targetting code NekRS for combustion, which has already been validated for non-reacting flows. They will also focus on the optimization of Nek5000 to better capture the flame propagation in open and closed systems. Besides, they will implement the *Method of Moments with Interpolative Closure* (**MOMIC**) [23] and the *Hybrid Method of Moments* (**HMOM**) [24] for particulate matter in Nek5000.
- BSC will focus on soot formation using the *Discrete Sectional Method* (**DSM**) [25] and aims to create a stand-alone soot model library for GPUs.
- CORIA-CNRS's objective is to profile, improve and optimize the E-L model for spray flames. They will focus on vectorization and the improvement of relocalization for the Lagrangian part with load balancing algorithms.
- UCAM will focus on the development of new models for dissipation in spray flames and the optimization of the chemistry transport. They will also implement the *Doubly Conditioned Moment Closure* (**DCMC**) [26] combustion model for the study of dual-fuel and jet-ignited natural gas reciprocating

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engines. Moreover, they will develop the required capabilities to predict soot emissions.

- TUDa will focus on the profiling and optimization of the Eulerian-Lagrangian framework for spray simulations. A reference test case will be defined to assess the performance of the E-L method and load-balancing will be explored within the project.
- RWTH will focus on the optimization and scalability of the E-L model for spray. Recent updates further improve the accuracy of the methodology implemented in terms of conservation properties. Besides, the computational performance of the overall E-L method will be optimized for the exascale architecture.

2.4.3 Strategy

On the one hand, the spray will be investigated using the E-L method by CORIA-CNRS, TUD, RWTH and UCAM. All partners will perform LES. In YALES2 and CIAO detailed chemistry effects will be taken into account based on reduced chemistry obtained through the methodologies developed in Task 4.3, while in CLIO a Conditional Moment Closure (CMC) and DCMC for LES is adopted. TUDa will use a tabulated chemistry approach with the flame thickening strategy or the Probability Density Function (PDF)-based methods coupled to the Quadrature-based Moment Methods (QMOM) [27,28] to describe particle size distribution for soot.
On the other hand, particulate matter will also be studied by AUTH & ETHZ, BSC, RWTH and UCAM. AUTH & ETHZ will perform DNS with an E-E approach using the MOMIC and the Hybrid Method of Moments HMOM. The BSC will perform LES using an E-E approach based on the DSM with tabulated chemistry methods for gaseous and spray flames. Finally, the UCAM will use CMC and DCMC based combustion models for LES using an E-L approach for spray flames with soot formation.
To test the developments and the optimizations of each code, several benchmarks are available. Two main configurations will be investigated in this task that will be linked to ECDs in WP7. For gaseous sooting flames, the Cambridge RQL flame [18] will be evaluated using DNS and LES. Likewise, the CRSB [20] test case which was specifically designed to address spray flames with soot formation. Apart from these two test cases, each partner will also perform simulations on particular cases to test both, spray flame and particulate matter.

2.4.4 Expected outcomes

The expected outcomes from this task can be divided into two main parts:

1. To obtain fully optimized algorithms for the study of multi-physics combustion for the CoEC flagship codes. This will prepare the codes to address the ECDs on (pre)Exascale architectures.

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2. To assess and compare different strategies for the study of spray flames and soot formation using E-E and E-L frameworks. This activity will permit the evaluation of the different methodologies in terms of accuracy and performance and provide guidelines and recommendations for best practice modeling strategies for particle transport.

3. Conclusion

To meet European Union requirements on pollutant emissions, it is necessary to have a better understanding of the underlying processes featured in combustion systems. The study of combustion, which is a highly complex multiphysics problem, requires increasingly powerful numerical tools. Therefore, the transition towards exascale architectures is necessary. In this new paradigm, where increased computing power is becoming available, it is necessary to revise and develop new methodologies that cope hardware transition with numerical methods and software transition, i.e., CFD codes must be optimized for the best performance in these new architectures. This work-package (WP4) will be focused on the development of new models and the optimization of existing algorithms for the numerical simulation of turbulent combustion. For this purpose, the work has been divided into 4 main tasks:

- Task 4.1 consists of the development of high-order numerical methods for the study of multiphase reactive flows.
- Task 4.2 focuses on the optimization of dynamic mesh adaptation algorithms together with the development of error estimators in the Euler-Lagrange framework for spray combustion.
- Task 4.3 aims to develop more accurate and optimized chemistry models, such as dynamically adaptive chemistry, and ad-hoc numerical solvers which will not only improve the computational performances but also the prediction of pollutant emissions.
- Task 4.4 focuses on the development of models for particle transport, either for the study of spray, which includes its transport and evaporation, or the study of particulate matter such as soot, which includes its formation and transport. These models will be developed for the E-L or E-L framework.

All these tasks will be highly related to the developments carried out in task WP5 and tested and validated in WP7.

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