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PREDICTION OF CYCLIC COMBUSTION VARIABILITY IN INTERNAL COMBUSTION ENGINES VIA COUPLED 1D-3D LES METHOD

B. ROUX*, J. BOHBOT*, Q. H. TRAN* AND P. SAGAUT†

* IFP Énergies nouvelles
1 & 4 avenue de Bois-Préau 92852 Rueil-Malmaison Cedex, France
e-mail: benjamin.roux@ifpen.fr, www.ifpenergiesnouvelles.fr

†Institut Jean le Rond d'Alembert, UMR CNRS 7190, Université Pierre et Marie Curie
4 place Jussieu, 75252 Paris Cedex 05, France
e-mail: pierre.sagaut@upmc.fr, www.dalembert.upmc.fr

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Abstract. The capability of Large Eddy Simulation (LES) to predict cycle-to-cycle variations in internal combustion engine has been assessed. Previous works pointed out a lack of data for the definition of boundary conditions. System simulation or one-dimensional CFD have already been used to generate boundary conditions for engine simulations [4]. The goal of present work is to develop an approach using LES to capture the detailed features of the complex reactive flow in the combustion chamber of an engine while accounting for its interaction with the flow and acoustics in the complete engine system. Three coupling methods based on the exchange of conservative, primitive and characteristic variables are developed and assessed on one-dimensional test cases; the method relying on primitive variables is selected. Then it is validated over 1D/3D coupling on duct flow and motored engine computation.

1 INTRODUCTION

Environmental constraints aiming at the reduction of the production of carbon dioxide in transportation have become an important factor. Furthermore, European norms on pollutant emissions of motor vehicles are more and more stringent. To overcome these increasing constraints the development of innovative engine concepts is necessary. Among them, exhaust gas recycling (EGR), direct injection (DI), stratified combustion, lean combustion, downsizing and forced induction are widely used and transform the engines in complex systems sensitive to cycle-to-cycle variations (CCV) and abnormal combustion such as knock and rumble. Experimental studies have shown that these technologies increase CCV already present and can lead to unstable engines [1,2]. In this context, predictive simulations of cycle-to-cycle variations in the engine are particularly interesting.

System simulations and classical Reynolds Averaged Navier-Stokes (RANS) are commonly used but are not able to predict CCV by nature. The increase of computational power and the need for a more accurate tool make Large Eddy Simulation (LES) attractive. Recent works have shown the capability of LES to predict cycle to cycle variations. First, in [10,11], a few fired cycles are computed on a mono-cylinder IC engine and have shown cycle-to-cycle variations. Later work [3] has shown that LES is able to reproduce good quantitative CCV but not enough cycles were computed for statistical convergence. In both studies only the cylinders and portion of intake and exhaust ducts which are close to the cylinder were simulated. They have pointed out a lack of data for the definition of boundary conditions. A database dedicated to LES studies of CCV in spark ignited engines has been created in [7]. Multi-cycle computations on this database [12,13,14] concluded that the velocity field at ignition is crucial in the CCV process and have shown LES quantitative prediction of stability in an engine bench. These computations including the whole bench, intake and exhaust ducts with their plenum are achieved on an academic engine which are impossible to do for an industrial engine with forced induction or EGR. System simulation has been used to define boundary conditions in ducts near the cylinder in [4] but the use of one way coupling does not allow to take into account the effects of CCV on the entire system. A strong or two-way coupling permits to compute the entire engine system at different level of precision and take into account elements that are impossible to simulate in LES such as turbocharger and EGR valve.

The aim of this work is to develop an approach using LES to simulate in detail the complex reactive flow in the combustion chamber and its close vicinity, while accounting for its interaction with the flow and acoustics in the complete engine system. To do so, a coupled 1D/3D LES method is developed between the one-dimensional in-house code Flow1D and the 3D solver AVBP [29]. The middleware OpenPalm [30] is used to couple these two codes for high performance computing. Three coupling methods, respectively based on exchange of primitive, conservative [5] and characteristic [6] variables across the interface, have been implemented. First, they have been compared in 1D/1D test cases (de Laval nozzle, Sod shock tube and acoustic wave propagation). Then 1D/3D computation of an exhaust line have been carried out. Finally, the first calculations of a motored (without combustion) engine system are presented and compared with results from system simulation.

2 MULTI-CYCLE LES OF INTERNAL COMBUSTION ENGINE

The massively parallel code AVBP is used to perform LES. AVBP solves compressible, reactive and multi-species Navier-Stokes equations on unstructured hybrid meshes using cell-vertex finite-volume method [16]. The centered second-order Lax-Wendroff numerical scheme [17] is used to explicitly advance the solution in time with low numerical diffusion. The time-step is limited by acoustic CFL number. This kind of scheme generates spurious oscillation if there are high rates of change in the flow field and is stabilized by second and fourth-order viscosity. The subgrid-scale stresses are modeled by a classical Smagorinsky model [18]. The mesh movement is managed by Arbitrary Lagrangian Eulerian method combined with Conditioned Temporal Interpolation technique [20] and shock generated by valves displacement is handled by hyper-viscosity [19]. The Navier-Stoke characteristic boundary conditions (NSCBC) method [6] is used to define boundary conditions and turbulent boundary layer is modeled by an isothermal logarithmic wall law [21]. Furthermore a new coupling boundary condition has been implemented in AVBP and is described in the next section.

Full multi-cycle approach is used in this study to examine CCV. Consecutive cycles are computed and first cycles are dismissed due to a high dependency at the initial conditions. A sufficiently large number of cycles have to be computed to yield converged statistical quantities. Another approach, perturbed single-cycle, consists in computing the same cycle several times with different perturbations at each realization [32]. It allows computing only a part of the cycle which decreases the computational time but the results are highly dependent on the imposed perturbation.

3 DEVELOPMENT OF THE 1D/3D COUPLING APPROACH

In the literature, studies present 1D/3D coupling that can be classified into four main techniques. The first performs the coupling by directly transferring flow field variables [22,23,24]. In the second type of method, the cells at the coupling interface are updated using Godunov method by means of a Riemann solver [25,26]. The third solution, consisting in the use of the method of characteristics [27], is particularly interesting because it provides the exact solution if the hypotheses are satisfied and AVBP already uses boundary conditions of this type. At last, iterative methods (each scheme reiterates until the coupling condition is completed) have been used in [28] on incompressible fluid systems. The large meshes used in the present work for LES and the CFL constraint condemn this method. Notice that only [22] deals with LES.

In this section two coupling methods directly transferring either primitive or conservative variables are developed. A third technique, based on the method of characteristic is implemented on the basis of the variables used in [6].

3.1 Flow1D solver

In order to investigate the coupled methodology, the Flow1D solver has been developed to perform academic tests on numerical scheme and different coupling approach. Flow1D code solves the Euler equations for an ideal gas with null thermal conductance in a variable cross section duct. Two numerical schemes are available: the two step Lax-Wendroff (LW2S) proposed by Richtmyer and Morton [9] modified by Basset et al. to take into account source terms [8] and the AVBP Lax-Wendroff Cell-Vertex reduced to 1D (LWCV). The LW2S scheme is stabilized by a flux limiter due to Davis [15] whereas LWCV have second and fourth order artificial viscosity. Both scheme are explicit, second order in time and space and time advancement is limited by the CFL criterion. As in AVBP, the boundary conditions used are the NSCBC [6].

3.2 Coupling strategies

As mentioned previously, both solvers are explicit, second order accurate with CFL criterion. Solved equations and numerical schemes are different but the main difference is the dimension. From a software point of view, the middleware OpenPalm is used to achieve parallel execution and communication of the programs on HPC cluster.

The first two methods are performed by a special boundary condition for both codes. The values at the boundary of one domain are obtained by picking up values on the internal nodes of the other domain. Variables transferred from three-dimensional domain to one-dimensional one are volume weighted averaged and those doing the opposite are set constant along the section. When the variables to be exchanged are the primitive ones, one more step is necessary: they are obtained via the equation of state, then exchanged, then transformed back into conservative ones. This is time consuming but it has been shown in [5] that this is better in case of different mixture properties in the domains. All this process is independent from the direction of the flow.

The second technique transfers characteristic variables which represent the waves crossing the boundary. Some of the waves are propagating inside the computational domain and others are propagating out of it. The outgoing waves are computed from inside the domain and the ingoing ones cannot be computed. In this coupling we use the fact that the ingoing waves of one domain are the outgoing of the other domain. Thus all waves are computed from the inside of one domain or the other and conservative variables are computed from characteristic ones.

Coupling interface should be placed where the flow is supposed to be uniform along the section.

3.3 One-dimensional validations on academic tests.

In order to validate the three coupling methods on both numerical schemes, they are applied to different problems whose analytical solutions exist. The first one is the classical Sod shock tube. The next test case is a Laval nozzle. Propagation of acoustic impulse is then investigated.

The simulations are achieved on 1D/1D coupling between Flow1D using the LW2S scheme and Flow1D with the LWCV scheme.

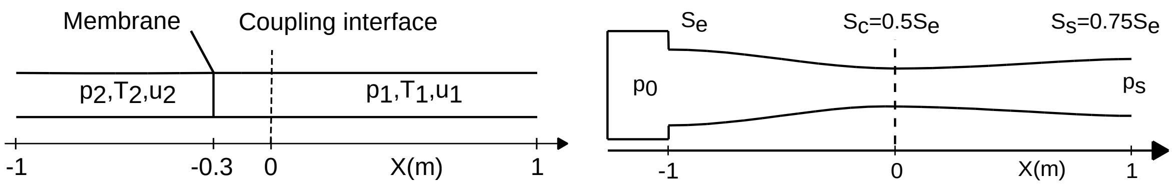

Figure 1: Scheme of the Sod's shock tube (left) and the converging diverging nozzle (right).

The shock tube is a two-meter long duct with constant section and opened end. A membrane separates the left part from the right one. The pressure is higher on the left than on the right, temperature is constant and velocity null. At time zero, the membrane vanishes and flow starts. The tube is discretized in 800 cells. The nozzle consists in an infinite volume plenum at pressure p_0 connected to a converging and a diverging part. The outflow pressure is controlled to obtain three different flow regimes. The mesh of the nozzle contains 200 cells. The coupling interface is always at zero on the *x*-axis.

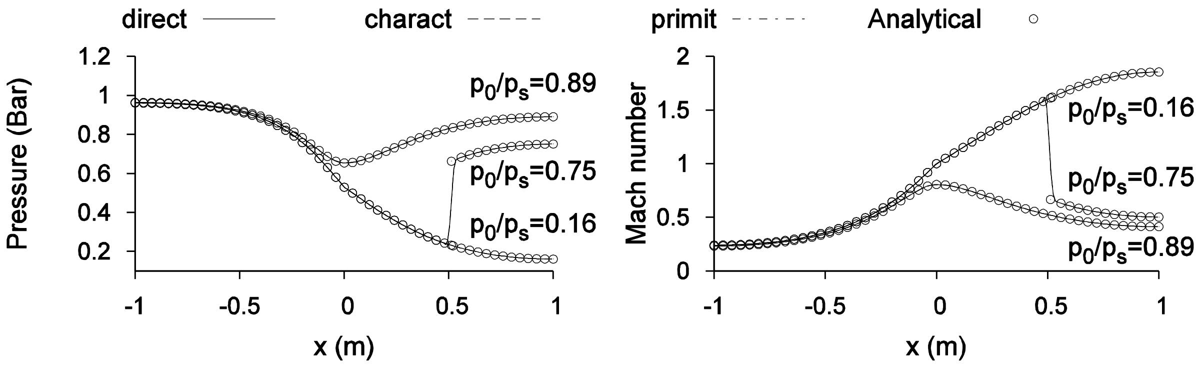

Figure 2: Comparison between the coupled computations and the analytical solutions on a de Laval nozzle.

The results on the nozzle displayed in Figure 2. We observe a good agreement for both flow regimes. The different coupling methods cannot be distinguished.

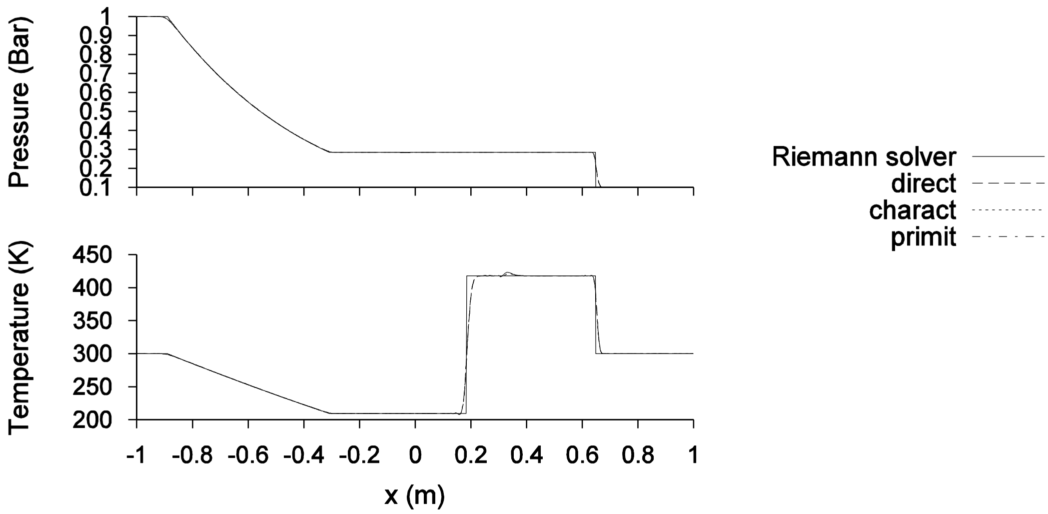

Figure 3: Results of the coupled methods and an exact Riemann solver on Sod's shock tube.

Figure 3 shows concordance of the solution on the Sod shock tube. Shock and contact discontinuity are smoothed and the small peak that appears on temperature is due to the numerical errors when the shock cross the interface. The reference for the computation of the error is the result of a 1D uncoupled simulation with coarse grid then the L^2-norm

$$\|f\|_{L^2} = \int_{-\infty}^{+\infty} f^2(x)\, dx \tag{1}$$

is computed and presented in Figure 4.

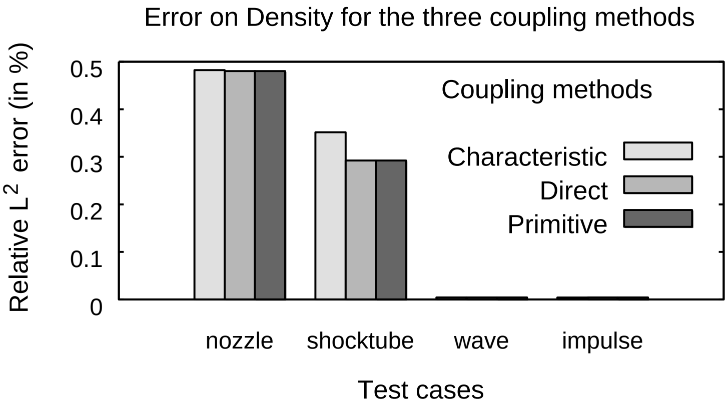

Figure 4: Summary of the 1D/1D validations

The results obtained and the analytical solutions are well correlated. The three coupling methods give close results. At this stage, it is hard to determine which one is the most efficient to engine simulations.

To this purpose, we consider an issue we will encounter in future reactive computation: Flow1D can transport three “modeled” chemical species. These “modeled” species are air, burnt gases and fuel. On another hand, AVBP uses more than eight chemical species when performing combustion simulation. Although the equations of state are the same and gas properties are computed similarly we can have differences in the computation of the pressure of the mixture as in [5]. The specific heat of a mixture composed of N species labeled by subscript k is computed via

$$C_p(T) = \sum_{k=1}^{N} Y_k C_{p,k}(T) \tag{2}$$

and is dependent on the concentration of each individual specie Y_k. The chemical reactions modify the concentrations creating discontinuity through the interface.

Errors in the specific heat ratio are modeled by forcing a different value of the specific heat ratio from a side of the interface to the other.

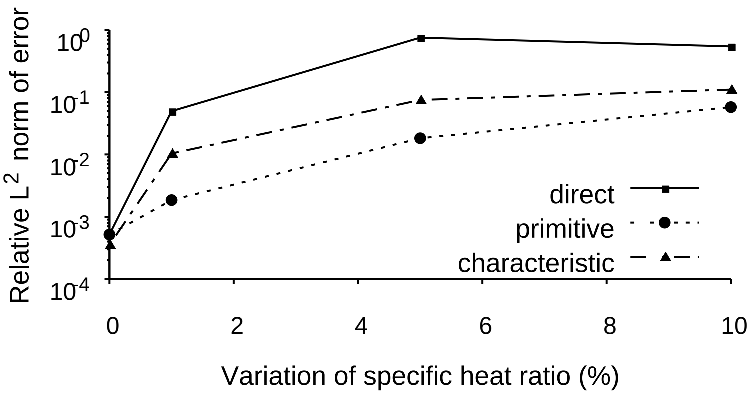

Figure 5: Error on density with respect to specific heat ratio variations across the interface on the nozzle test case

The results are compared to a constant specific heat ratio case to compute the error as this represents the ideal case in which no deviation may be observed. Figure 5 shows that the error is less important for the coupling by primitive variables. Thus this method will be used in the following analyses.

3.4 1D/3D cases

Coupling between the Flow1D code and AVBP on a pipe flow have been carried out. The first test case is the Sod shock tube presented Figure 6. The results of the computations in Figure 7 are consistent with the analytical results obtained via an exact Riemann solver.

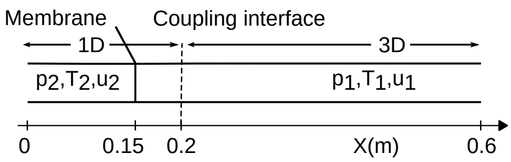

Figure 6: Scheme of the 1D/3D shock tube

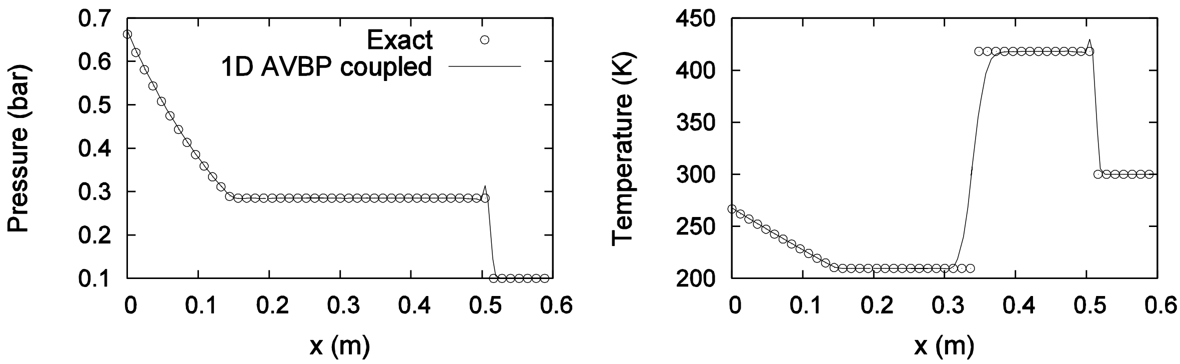

Figure 7: Results of the 1D/3D coupled computation and an exact Riemann solver on Sod's shock tube.

The acoustic waves being very important in the engine ducts, the coupling methods are then validated on propagation of acoustic impulses and waves. Figure 8 shows the numerical set-up of the simulations. An acoustic impulse generated by a Gaussian velocity disturbance enters the domain in E at 1 ms and propagates through the three domains.

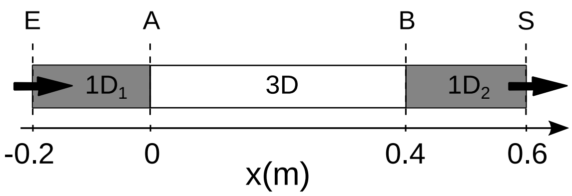

Figure 8: Scheme of the impulse test rig

The results are shown in Figure 9, where we can see a good agreement between the coupled case and the analytical results of the linear acoustic. The impulse is slightly damped and we notice no reflection of the impulse at the interface A while a 1% reflection is present at the interface B.

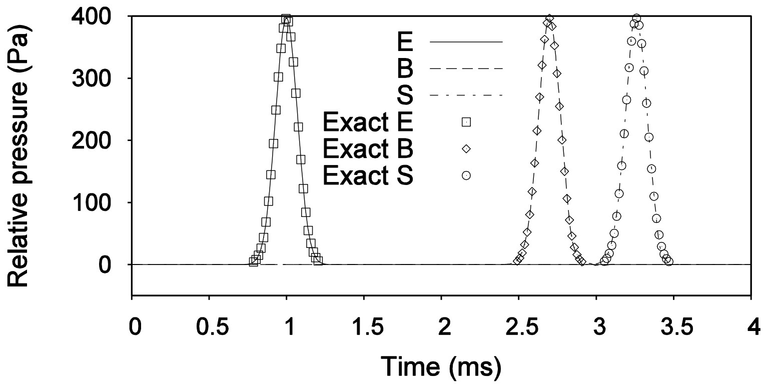

Figure 9: Results of the coupled 1D/3D impulse test and the analytical result from linear acoustic

In the third computation, sine acoustic wave with frequencies and amplitudes close to the values in an exhaust duct are introduced into the coupled tube at E.

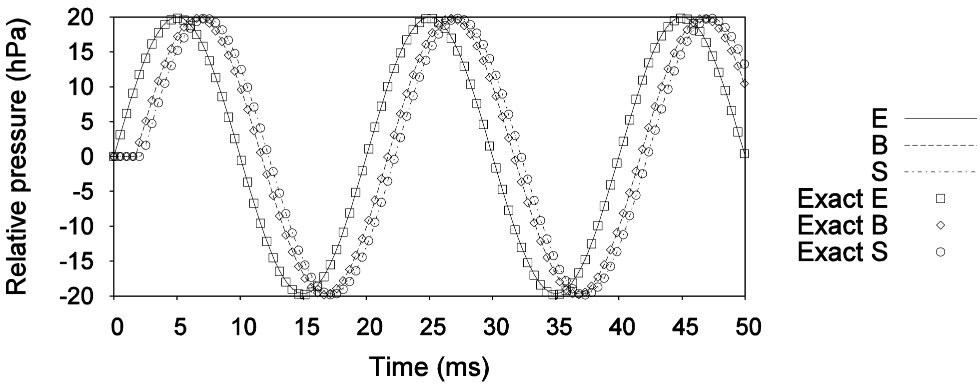

Figure 10: Results of the 1D/3D coupling on the 50Hz wave compared to the linear acoustic predictions

Temporal evolution of the relative pressure is plotted in Figure 10. The solution computed with 1D/3D primitive coupling method concord with the analytical solution of the linear acoustic. The frequency at the outlet is preserved, the signal is in phase, not damped and no reflection is present.

4 INTERNAL COMBUSTION ENGINE SIMULATION

In this part, computations on a motored engine are investigated. The mesh of the engine is presented in Figure 11**.** The coupling interface is positioned far enough from the cylinder and the bends to ensure the homogeneity of the flow in the section. A cycle consists of 41 meshes between 1.9 to 9.6 million of tetrahedral cells, solution are interpolated from a mesh to another by a piecewise linear interpolation.

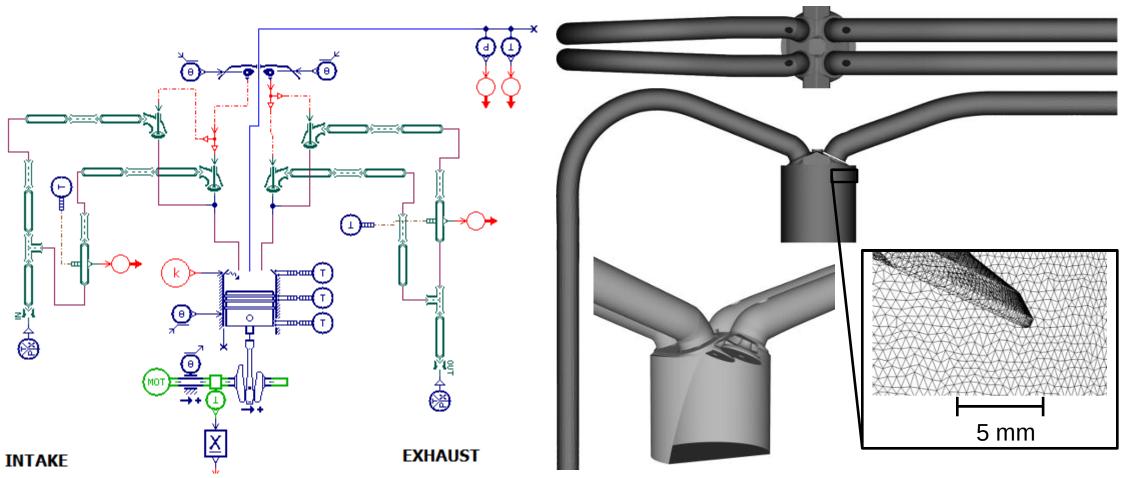

Figure 11: System simulation sketch of the engine (left) and mesh of the cylinder and neighboring ducts (right)

The grid in the cylinder has to be coarse enough to resolve 90% of the turbulent kinetic energy (Δx < 0.8mm) to ensure a good quality of LES results. The characteristics and the timing of the engine are summarized in Table 1. To validate the simulations, the coupled 1D/3D computations are compared to system simulation results obtained via the commercial code LMS Image.Lab AMESim [31]. The boundary conditions of the 1D domain are purely reflective NSCBC imposed pressure and temperature. Six consecutive cycles have been computed, each one took 38h on 256 Intel SandyBridge cores. The use of two coupling boundary condition on a mesh increases the computational time by 20%.

Table 1: Characteristics of the SGEmac engine

	Unity	Values		Unity	Values
Number of cylinders	-	1	Engine speed	rpm	1200
Number of valves	-	4	Exhaust temp.	K	300
Compression ratio	-	9.9	Exhaust press.	bar	1.01
Bore	mm	82	Intake temp.	K	295
Stroke	mm	83.5	Intake press.	bar	0.44
Connecting rod length	mm	144	Wall temp.	K	300
Intake Valve Opening (IVO)	CAD	350			
Intake Valve Closing (IVC)	CAD	-120			
Exhaust Valve Opening (EVO)	CAD	120			
Exhaust Valve Closing (EVC)	CAD	-350			

The results are shown in Figure 12 and Figure 13. The maximal pressure in the cylinder is well estimated and the pressure during exhaust phase does not fit well but such an error is acceptable and come from the thermic of the exhaust. The pressure in the intake is well reproduced by the coupled simulations in term of amplitude and frequency. The exhaust pressure is close to system simulation one except on the peaks.

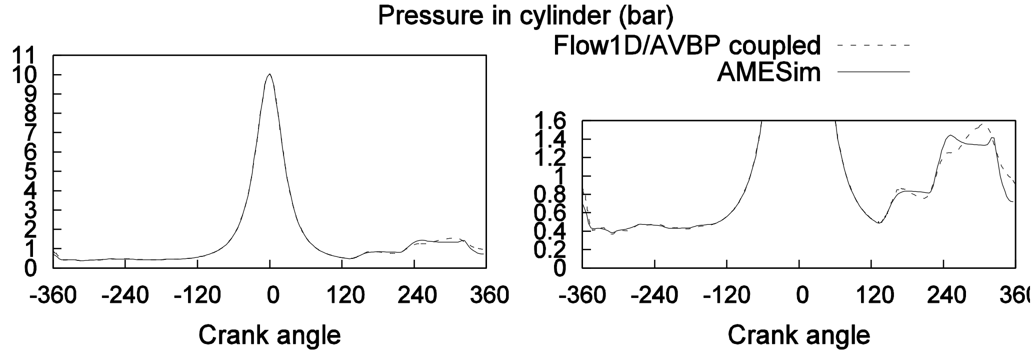

Figure 12: Pressure in cylinder

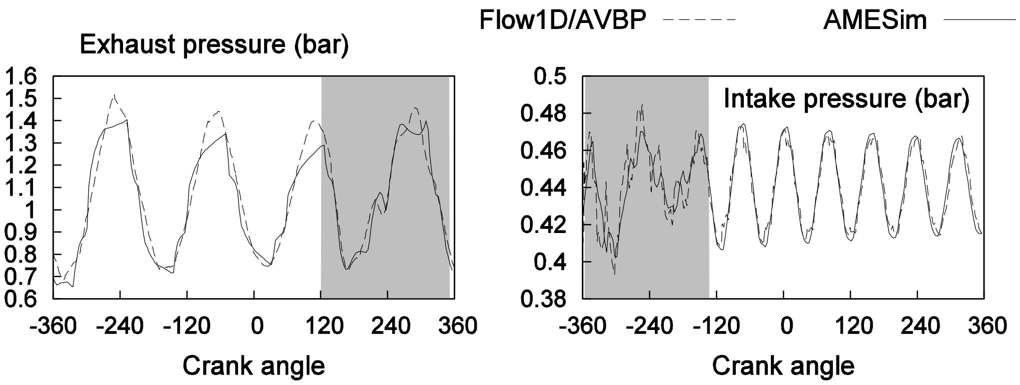

Figure 13: Pressure in the exhaust and in the intake

5 CONCLUSION

Three coupling methods have been developed and validated over one-dimensional test cases for which analytical solutions are known. The interface strategy based on primitive variables has been preferred to achieve engine computation and is tested on a 1D/3D pipe due to its capability to handle discontinuities in the gas properties. These computations on duct acoustic have shown good agreement with the linear acoustic. Finally, coupled simulations on a motored engine are compared to system simulations. The agreement between system simulations and coupled computations shows that the latter could be applied on complex industrial engines out of reach via full LES simulations.

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