Boundary conditions and subgrid scale models for LES simulation of Internal Combustion Engines

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Abstract. The implementation and the combination of advanced boundary conditions and subgrid scale models for Large Eddy Simulations are presented. The goal is to perform reliable cold flow LES simulations in complex geometries, such as cylinder engines. In the paper, an inlet boundary condition for synthetic turbulence generation is combined with a fully non reflecting Navier Stokes Characteristic Boundary Condition (NSCBC) for the outlet and with the local Dynamic Smagorinsky subgrid scale model, that is not included in the official distribution of OpenFOAM®. Validation of the models has been performed separately on two steady state flow benches: a backward facing step geometry [1] and a simple IC engine geometry with one axed central valve [2]. The code developed has been included into LibICE®, a set of applications and libraries for multi-dimensional engine modeling based on the OpenFOAM® technology.

Key words: turbulence, Large Eddy Simulation, wall bounded flow, unstructured mesh, OpenFOAM®

INTRODUCTION

LES applied to ICE is potentially a reliable tool to simulate turbulent motion during gas exchange phase (swirl, tumble), fuel mixing and combustion, cyclic combustion variability. However, there are some known issues that cannot be neglected: boundary conditions in the LES code must be able both to properly handle acoustic waves and turbulence properties, solution of Navier Stokes (NS) equations in the unstructured meshes typically used for real-world cylinder heads may lead to have a high numerical dissipation that is comparable to \( \nu \). Also, when simulations of complex geometries such as in internal combustion engines are performed, the behavior of the eddy-viscosity models near a wall represents a second difficulty [3]. This paper is divided into two halves, one theoretical and one computational. In the first part, two boundary conditions, for synthetic turbulence generation at the inlet and for an acoustically non-reflecting outlet, are presented. The second part contains results from simulations, which display a wide range of interesting features. The anechoic boundary condition has been used and tested in a three-dimensional time-domain CFD approach, that have been employed to predict and analyze the acoustic attenuation performance of complex perforated muffler geometries, where strong 3D effects limit the validity of the use of one-dimensional models. Results from LES simulations using the inlet boundary condition and the SGS models implemented have been compared with experimental data on a backward facing step geometry [1]. Flow conditions were incompressible and fully turbulent and a separation region with recirculation was present; the influence of the inlet boundary conditions and of the subgrid models on the recirculation region characteristics and the overall flow quantities have been studied. Finally, to explore the suitability of this methodology for large-eddy simulation (LES) in reciprocating internal combustion engines, simulations on a simple cylinder configuration, also studied in [2], were carried out and LES velocities profiles were compared to LDA measurements.

DEVELOPMENT OF NSCBC IN LOCAL COORDINATES

In order to have a fully non-reflecting outlet boundary condition, that permits waves to pass through the boundaries without spurious reflections, the formulation of the characteristic treatment for Navier-Stokes equations (NSCBC) is needed. The NSCBC theory by Poinsot and Lele [4], originally suggested in Cartesian coordinates, has been extended to local coordinates. The resulting system of equations has been solved by a multistage time stepping scheme to improve the numerical performance. To transform the conservative system from a physical domain \((\xi, \eta, \zeta)\) to a computational domain \((x, y, z)\), a change of variables is required because, as it will be discussed later, the characteristic theory to include in the compressible subsonic Navier Stokes equations refers to a wave element that is perpendicular to the outlet domain. Being \( u_i \) (where

![Figure 1: For each cell face at the boundary end, a local reference frame \((\xi, \eta, \zeta)\) has been defined. Each reference frame has its origin in the cell face center and the vector \( \zeta \) is set as perpendicular to the cell face.](image-url)
\[ \mathbf{L} = \begin{bmatrix} \lambda_1 \left( \frac{\partial p}{\partial \eta} - \rho c \frac{\partial u_1}{\partial \eta} \right) \\ \lambda_2 \left( \frac{\partial^2 p}{\partial \eta^2} - \frac{\partial p}{\partial \eta} \right) \\ \lambda_3 \frac{\partial u_2}{\partial \eta} \\ \lambda_4 \frac{\partial u_3}{\partial \eta} \\ \lambda_5 \left( \frac{\partial p}{\partial \xi} + \rho c \frac{\partial u_1}{\partial \xi} \right) \end{bmatrix} \]

\( L_i \) are associated with each characteristic velocity \( \lambda_i \):

\[
\begin{cases} 
\lambda_1 = u_1 - c \\
\lambda_2 = \lambda_3 = \lambda_4 = u_1 \\
\lambda_5 = u_1 + c 
\end{cases}
\]

In particular, in (3), \( c \) is the local speed of sound, \( \lambda_1 \) and \( \lambda_5 \) are the velocity of sound waves moving along the positive and negative stream-wise direction, \( \lambda_2 \) is the velocity for entropy advection, while \( \lambda_3 \) and \( \lambda_4 \) are the velocity at which \( u_2 \) and \( u_3 \) are advected in the \( \xi \) direction.

Application of the LODI relations into the NS equations (anechoic b.c.)

The implementation of the non reflecting boundary condition to model an anechoic termination requires some caution. The NSCBC approach sets values for the wave amplitude variations in the viscous multi-dimensional case by examining a Local One Dimensional Inviscid (LODI) problem \[4\], where transverse, viscous and reaction terms are neglected:

\[
\begin{align*}
\frac{\partial p}{\partial t} + \frac{1}{c^2} &\left[ L_2 + \frac{1}{2} (L_5 + L_1) \right] = 0 \\
\frac{\partial \rho}{\partial t} + \frac{1}{2} (L_5 + L_1) &= 0 \\
\frac{\partial u_1}{\partial t} + \frac{1}{2pc} (L_5 - L_1) &= 0 \\
\frac{\partial u_2}{\partial t} + L_3 &= 0 \\
\frac{\partial u_3}{\partial t} + L_4 &= 0
\end{align*}
\]

For subsonic flows at the exit, the eigenvalue \( \lambda_1 = u_1 - c \) in (3) associated to the wave amplitude \( L_1 \) is negative and the disturbance travels inward the boundary at the speed of sound relative to the moving fluid. The application of the LODI relations into the Navier Stokes equations, that does not necessarily imply a hyperbolic nature of the system, is questionable. In particular, if the ingoing characteristic is set to zero (perfect anechoic condition), the problem results to be ill-posed and the information about the static pressure in the outer domain never feeds back into the computational domain \[6, 7, 8\]. For a well-posed problem \[6\], corrections must be added to the treatment of the non-reflecting NSCBC, that becomes therefore partially reflective. It is important to note that partial reflection also includes the contributions of spurious reflections caused by the numerical approximation of hyperbolic equations at the boundary \[9\]; this effect looks stronger if inviscid boundary conditions for the primitive variables are specified and if transverse terms in the equations are neglected. The acoustic theory proposed to characterize the actual reflection coefficient of numerical "non-reflecting" boundary condition using LRM (Linear Relaxation Method) proposed by Rudy and Strikwerda \[6\] has been applied to derive a formulation of the reflected characteristic in generalized coordinates \[10\]:

\[
L_1 = K \cdot (p - p_\infty) = \sigma \cdot \frac{1}{\sqrt{2 J \rho l}} (p - p_\infty) \tag{5}
\]

that has been included in Eq. (4). In Eq. (5), \( M \) is the local Mach number of the boundary cell, \( l \) is the characteristic length of the domain. The preferred range for constant \( \sigma \) is in the interval [0.1; \( \pi \)]. The difference \( L_5 - L_1 \) in Eq. (4) can be still calculated by one side upwind differencing.

Validation

The performance of non-reflecting boundary conditions can depend on a number of different factors \[11\]: the cut-off ratio, the ratio between frequency and wavelength (gas sound velocity), the angle of the incident waves relative to the boundary normal, the mean flow velocity, the damping constant \( \sigma \) of the LRM. The effect of these parameters on the performance of the boundary condition was investigated, for a fixed value of the damping constant \( \sigma \) in (5), that was set to 0.2. Tests were performed on the shock tube geometry shown Fig. 2: the gas modeled was air at ambient temperature (293 K), the pressure difference \( p_1 - p_2 \) between air at high and low pressure was 650 Pa, a non-reflecting boundary conditions was set at the open
end of the duct. The simulation time was set accurately to allow the compression wave front to completely cross the boundary and to avoid any interference between waves reflected by the other boundaries.

Figure 2: Schematic representation on the XY plane of the 3D shock-tube geometry. Initial pressure conditions: $p_1=100650\ \text{Pa}$, $p_2=100000\ \text{Pa}$.

For a fixed value of $K$ in Eq. (5) (which is the case in any computation), different frequencies of the signal are not reflected in the same way: usually, waves at high frequency will easily leave the computational domain ($R \to 0$) whereas low frequency waves will be strongly reflected.

The frequency that splits the different behavior of the boundary condition is the cut-off frequency ($f_c$), that separates reflected waves ($f < f_c$) by waves that will leave the domain ($f > f_c$). In terms of energy content, half of the acoustic energy is fed back into the computational domain at the frequency $f_c$. A reliable parameter to evaluate the performance of a non-reflecting boundary condition is the reflection coefficient $R$, that represents the permeability of the boundary towards low frequency waves and that can be calculated according to the characteristic theory as:

$$R(f, \alpha) = \frac{L_1(f, \alpha)}{L_5(f, \alpha)}$$  \hspace{1cm} (6)

The behavior of the reflection coefficient has been studied in a range of the incident pressure wave angle $\alpha$ in between 0 and 60 degrees. In Fig. 3, the amplitude of the wave reflection coefficient $|R|$ of Eq. (6) as a function of the frequency is analyzed. As expected, $R$ is higher at low frequency and constantly decreases in the low frequency range [0 600] Hz. Differences in magnitude for the reflection coefficient $R$ do not seem appreciable with different wave angles $\alpha$ for frequencies lower than 600 Hz. Beyond this value, the reflection coefficient generally increases with the wave angle. An exception has been found with a wave angle $\alpha = 60^\circ$. In this case, results look very similar to the case with a wave having normal incidence; the explanation of this unexpected behavior is still under investigation. From the frequency of about 600 Hz, the slope of $R$ becomes positive.

Figure 3: Magnitude $R$ of the numerical reflection coefficient with varying wave angles.

Figure 4: Transmission loss of different flow reverse chambers with zero mean flow [12]. Experimental data have been provided by AVL GmbH.

The boundary condition has been applied to model an anechoic termination, when simulations of acoustic silencers for internal combustion engines applications were carried out. The Transmission Loss for different configurations of silencers have been calculated and some results are depicted in Fig. 4. A more detailed description and an extensive validation of the approach is reported in [12].

SYNTHETIC TURBULENCE INLET B.C.

One of the possible way to have realistic turbulence at the inflow boundary of a LES domain is to superpose random fluctuations onto a mean velocity profile. However, care must be taken to meet some physical requirements, that would ensure turbulence is not destroyed by the Navier-Stokes solver and that it possess some properties of “real” turbulence. Therefore, synthetic fluctuations must be divergence-free, and they must have a specified spec-
ential energy content together with time- and space-correlation. This can be achieved by generating the fluctuating component as a sum of Fourier modes with wavenumbers $\kappa_1 \ldots \kappa_N$. Following the procedure developed by Davidson [13], the fluctuating component of velocity is calculated as:

$$u_i'(x_j) = 2 \sum_{n=1}^{N} \hat{u}^n \cos(\kappa_j x_j + \psi^n) \sigma_i^n$$  \hspace{1cm} (7)

Orientation in space of wavenumber vector $\kappa_j$ (as well as the phase angle $\psi^n$) is chosen randomly according to a predefined statistical distribution.

Solenoidality is enforced by generating velocity vectors $\sigma_i$ that lie on a plane orthogonal to $\kappa_j$. Spectral mode amplitude $\hat{u}^n$ is calculated according to a prescribed spectrum shape. In this work, a modified version of the Von Kármán energy spectrum is used:

$$E(\kappa) = \frac{A u_{rms}^2}{\kappa_c} \frac{(\kappa/\kappa_c)^4}{[1 + (\kappa/\kappa_c)^2]^{15/6}} \exp \left[-2(\kappa/\kappa_c)^2\right]$$  \hspace{1cm} (8)

where:

- $\kappa_c = \varepsilon^{1/4} \nu^{-3/4}$ is the maximum wavenumber, corresponding to Kolmogorov timescale
- $A = 1.456$ is a model’s constant
- $\kappa_c = 9\pi/55 \frac{A}{\mathcal{L}}$ is a function of the integral length-scale ($\mathcal{L}$).

Time correlation is obtained by applying Billson temporal filter [15] to the ‘raw’ fluctuations given by (7):

$$(u')^m = a (u')^{m-1} + b (u'')^m$$  \hspace{1cm} (9)

where ($T$ is the integral timescale):

$$a = \exp(-\Delta t/T), \quad b = \sqrt{1 - a^2}$$

The algorithm for synthetic turbulence generation is applied at each temporal integration step. The additional computational cost implied by the b.c. for synthetic turbulence generation has been estimated about 10% of the total simulation time.

### RESULTS

To explore the suitability of this methodology for large-eddy simulation (LES) in reciprocating internal combustion engines, the local dynamic Smagorinsky model [16] subgrid-scale model has been implemented in the OpenFOAM® technology. Results coming from LES simulations performed by using the implemented SGS model and implicit LES have been compared to experiments for two steady state flow benches: a backward facing step geometry [1] and a simple IC engine geometry with one axed central valve [2].

### Backward facing step

The configuration with a sudden expansion, the backward facing step (BFS), has been simulated to reproduce the first difficulty occurring in IC engines: the strong detachment due to the increase of the diameter between the intake ports and the cylinder. Figure 6 shows the domain used by Eaton et al [1] in the experiments. The turbulent boundary layer was generated by positioning two trips: the former was located on the step wall, the latter was located on the wall opposite to the step. Both trips were placed at the same distance from the step but their heights were different, so the boundary layer thickness was different on the step wall and on the wall opposite to the step. The results obtained with LES for mean velocity profiles, as well as for velocity fluctuations, have been quantitatively compared to the experimental LDA measurements [1] in terms of both mean and RMS velocities.

Figure 6: Schematic of the backward facing step geometry [1] simulated; $L1=0.4953$ m, $L2=0.127$ m, $W1=0.0762$ m, $W2=0.015$ m, $H1=0.0508$ m.

In the computations object of this paper, only a small portion of the domain of the BFS was modeled; the inlet channel length $L1$ was chosen to have fully developed flow near the step, while the outlet channel length $L2$ was supposed to be long enough to not be affected by the small numerical reflections coming by the outlet boundary condition. The fluid-dynamic information recorded by a RANS simulation on a precursor domain has been used to reconstruct the turbulent fluctuations at the boundary inlet by the synthetic turbulence inlet b.c. described above. An unsteady convective boundary condition has been used for the outlet. Periodic boundary conditions were set on the $z$-normal surfaces, while all the other surfaces of the domain were set as adiabatic walls.

Simulations were carried out on a fully structured mesh having about 800000 hexahedral cells both by implicit SGS models (where the dissipation is given by discretization er-
The local dynamic Smagorinsky SGS model. The algorithm, the local dynamic Smagorinsky SGS model.

ors of monotone convection algorithms) and by an explicit algorithm, the local dynamic Smagorinsky SGS model. Mean inlet velocity of the flow was 11.6 m/s (Re ≈ 50000) and the values of grid resolution were ∆x+ = 200, ∆y+ = 0.8, ∆z+ = 20, where x, y, z denote the streamwise, wall-normal and spanwise directions. No wall functions were used, the boundary layer was directly resolved at the walls. Despite grid resolution looked consistent with the guidelines from the literature on wall bounded flows [17], by Fig. 7 it is apparent how the mean velocity and the turbulent intensity were not properly captured, in particular in the vicinity of the walls; this has been found also on test performed on finer grids (up to 4M cells). Preliminary results shown here on the BFS geometry evidenced the need to implement a subgrid viscosity model that could improve the quality of the predictions on the cases shown in the paper.

Cold flow IC simulation

A simple IC engine geometry (consisting of a sudden expansion with ratio 3.5 and one axis-centered valve), reported in Fig. 8, has been also tested. Measurements of mean flow velocity and of velocity fluctuations (along the radial and tangential directions) were available on two planes located at a distance of 20 mm and 70 mm from the cylinder top, respectively. Similar studies on this configuration have already been done in [2].

In this work, two computational grids were used for the same geometry: the former was made of 1.4 million of cells, the latter had about 8 million of cells. Mean velocity at the inlet was 65 m/s and no explicit subgrid model has been applied (implicit LES); simulations with explicit SGS modeling are running at the time this paper is written.

Figure 7: Backward facing step geometry: comparison of the velocity profiles between the LES simulation and PIV measurements [1] at different locations along the streamwise direction; a-h) mean axial velocity i-r) mean axial velocity fluctuations.

Figure 8: Two-dimensional schematization for the axial symmetric piston-cylinder assembly of [2], including coordinate system.

Comparison of the current LES with LDA measurements are shown in Fig. 9. Quantities of graphs a-c are referred to the upper plane (20 mm below the cylinder top), while plots d-f are referred to the lower plane (70 mm below the cylinder top). Results have been averaged both in time, after a steady-state has been reached, and in space, along the circumferential direction. Mean velocities are captured rather well both by the coarse and the fine mesh in both planes. On the other hand, RMS of the fluctuating component of the velocity exhibits a significant deviation from the measured values, especially near the cylinder walls. The poor predictions in the wall region are most likely due to the insufficient resolution of the grid to solve the near-wall turbulence. Although it is difficult to study in detail the dynamics of the near-wall turbulence for such a complex case (no reference test-cases exist), it might be useful to evaluate the scaled mesh resolution at the wall as an index of spatial resolution. In the simulation using the 1.4 M grid, the scaled mesh sizes are: ∆x+ ≈ 200, n+ ≈ 10 and ∆x+ ≈ 500, while in the 8 M grid the resolution is...
\[ \Delta x_{tg}^+ \approx 100, \ n^+ \approx 5 \text{ and } \Delta x_{ax}^+ \approx 500, \] being \( n \) the wall-normal (radial) direction, \( x_{tg} \) the tangential coordinate and \( x_{ax} \) the axial coordinate. These high values indicate that the dissipation at the wall is not correctly evaluated, and this has a strong influence on the predictions of the fluctuating velocity components.

\[ \Delta x_{tg}^+ \approx 100, \ n^+ \approx 5 \text{ and } \Delta x_{ax}^+ \approx 500, \] being \( n \) the wall-normal (radial) direction, \( x_{tg} \) the tangential coordinate and \( x_{ax} \) the axial coordinate. These high values indicate that the dissipation at the wall is not correctly evaluated, and this has a strong influence on the predictions of the fluctuating velocity components.

Figure 9: Comparison of the velocity profiles between the LES simulation and the LDA measurements. Plane \( x = 20 \text{ mm} \): a) mean axial velocity b) mean axial velocity fluctuations c) mean tangential velocity fluctuations. Plane \( x = 70 \text{ mm} \): c) mean axial velocity d) mean axial velocity fluctuations e) mean tangential velocity fluctuations.

CONCLUSIONS

In this paper, LES simulations of a simple internal combustion engine geometry have been performed. First, boundary conditions for LES have been implemented and validated. Quantitative comparisons have been made between the experimental and numerical velocity profiles for different mesh sizes of the geometries tested. Turbulent fluctuations are not properly captured near the walls, where the turbulent viscosity looks underestimated. This error, that is more apparent with implicit LES, is still present with a refined mesh, because the grid resolution used was not high enough to directly resolve the boundary layer at the walls. On the other hand, proper grid resolution would lead to grids having a number of cells that would be too high for the available computational resources. To have a better prediction of the scaling at the wall, the dynamic Smagorinsky subgrid model has been implemented into the OpenFOAM® technology. Results on the BFS geometry show an improved agreement when the subgrid model is used, despite several tasks are still open; in particular, it is not really clear what is the minimum mesh refinement needed to conclude which kind of mesh is more appropriate for LES computation of internal combustion engine geometries. This topic is currently under investigation.

Recently, a Wall-Adapting Local Eddy-viscosity (WALE) subgrid scale model has been implemented in the OpenFOAM® technology. The WALE model is based on the square of the velocity gradient tensor and it accounts for the effects of both the strain and the rotation...
rate of the smallest resolved turbulent fluctuations and it recovers the proper $y^+$ near-wall scaling for the eddy viscosity without requiring dynamic pressure; hence, it is supposed to be a very reliable model for ICE simulation. Current research activity is involving the testing and the validation of this model on engine test cases.

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