Generalized three-dimensional characteristic boundary conditions for unstructured grids

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1. Introduction

Within the framework of aeroacoustic simulations, two main approaches may be adopted to tackle the particularly difficult problem of predicting direct or indirect noise generation and propagation: (a) indirect noise evaluation by means of incompressible solvers coupled with models based on the acoustic analogy or (b) direct noise evaluation using fully compressible solvers. Both these solutions present a number of interesting features and the ideal tool is difficult to identify. The former approach may be less demanding in terms of transparent boundary conditions, but the latter is clearly a more flexible tool under more stringent compressibility requirements.

With regard to the compressible solvers, in particular, when dealing with aeroacoustic computations, the use of high-order schemes may be a *conditio sine qua non* to prevent the numerical error from spoiling the solution in terms of noise propagation. From this point of view, the use of structured codes is particularly attractive because of the relatively high flexibility that structured stencils offer to increase numerical accuracy. Nonetheless, unstructured solvers are often the best solution when dealing with geometries sa complex as those typically representative of practical engineering applications.

Moreover, the solution of the fully compressible Navier-Stokes equations requires transparent boundary conditions in order to properly evacuate the noise generated within the computational domain without significant numerical reflection. Among the different ways to address the development of transparent boundary conditions, those based on the propagation of characteristic waves have the intrinsic advantage of being naturally more easily adaptable to the case in which, for instance, a certain acoustic feedback is required due to some known source of noise reflection from regions “outside” the actual computational domain.

The following sections present a brief overview regarding the implementation of characteristic boundary conditions on the unstructured CDP code developed at CTR Stanford (Mahesh *et al.* 2004; Ham & Iaccarino 2004; Moureau *et al.* 2005, 2007).

2. The 3D-NSCBC procedure

Inspired by the work by Yoo *et al.* (2005); Yoo & Im (2007), Three-dimensional Navier-Stokes Characteristic Boundary Conditions (3D-NSCBC) (Lodato *et al.* 2008*a*) represented the natural evolution of the relevant mono-dimensional counterpart (Poinsot & Lele 1992).

If even in the most simple academic test cases, the complex nature, and spectrum, of the flow field resulting from Direct and Large-Eddy Simulations (DNS and LES, respectively), makes the Locally One-Dimensional and Inviscid (LODI) hypothesis (Poinsot & Lele 1992) too stringent to correctly represent the flow at the boundary, by contrast, the introduction of transverse gradients in the boundary plane may pose additional problems of wave coupling at edges and corners belonging to different boundary planes. These interface regions, which are seldom addressed in the literature, are indeed a key ingredient of efficient boundary treatments, as is the case, for instance, when using structured computational grids. Hence, a systematic procedure to solve the wave coupling mechanism over edges and corners was developed (Lodato *et al.* 2008*a*). The increased level of control over relaxed quantities, which may be achieved by accounting for chemical source terms in the computation of incoming characteristic waves, allowed the simulation of tubular-shaped flames crossing the boundary (Lodato *et al.* 2008*b*).

Note that the implementation of the original NSCBC procedure with the LODI assumption can be "easily" accomplished regardless of whether the computational grid is structured, whereas the introduction of transverse convection and pressure gradient over boundary faces and the relevant solution of wave coupling problems on edges and corners make the 3D-NSCBC procedure particularly suited for structured codes with easily accessible topological structures. However, its implementation on unstructured solvers is considerably more challenging, as will be briefly detailed in the next section.

3. Extending the 3D-NSCBC to unstructured solvers

We present a brief introduction to the mathematical framework from which these characteristic boundary conditions are derived, before describing the ongoing activities focused on the extension of the 3D-NSCBC procedure to the CDP unstructured code,. We consider the Navier-Stokes equations for a calorically perfect gas with the relevant equation of state:

$$\partial_t \rho + \partial_j(\rho u_j) = 0, \tag{3.1}$$

$$\partial_t(\rho u_i) + \partial_j\left[\rho u_i u_j + \delta_{ij} p - 2\mu A_{ij}\right] = 0, \tag{3.2}$$

$$\partial_t(\rho e) + \partial_j\left[\left(\rho e + p\right)u_j - 2\mu u_k A_{jk} - \tfrac{\mu c_p}{Pr}\partial_j T\right] = 0, \tag{3.3}$$

$$p = \rho R T = (\gamma - 1)\left[\rho e - \tfrac{1}{2}\rho u_k u_k\right], \tag{3.4}$$

where ρ is the density, u_i is the i-th component of the velocity vector, p is the pressure, μ is the dynamic viscosity, A_{ij} is the deviator of the velocity gradient tensor, e is the total energy (thermal + kinetic), c_p is the specific heat at constant pressure, Pr is the Prandtl number, T is the temperature, R is the gas constant and γ is the specific heat ratio. The above transport equations may be conveniently written in compact form as

$$\partial_t \boldsymbol{U} + \partial_j \boldsymbol{F}^j + \partial_j \boldsymbol{D}^j = 0, \tag{3.5}$$

where $\boldsymbol{U} = \begin{pmatrix}\rho & \rho u_1 & \rho u_2 & \rho u_3 & \rho e\end{pmatrix}^{\mathrm{T}}$ represents the vector of conservative variables, whereas $\boldsymbol{F}^j$ and $\boldsymbol{D}^j$ are the flux vectors and viscous terms, respectively. In order to transform the above equation in characteristic form, this is first written in quasi-linear form,

$$\partial_t \boldsymbol{U} + \boldsymbol{A}^j \partial_j \boldsymbol{U} + \partial_j \boldsymbol{D}^j = 0; \tag{3.6}$$

then the relevant formulation in primitive variables $\boldsymbol{\mathcal{U}}$ is derived resorting to the Jacobian $\boldsymbol{P} = \partial \boldsymbol{U}/\partial \boldsymbol{\mathcal{U}}$,

$$\partial_t \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{A}}^j \partial_j \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{D}} = 0, \tag{3.7}$$

with $\boldsymbol{\mathcal{A}}^j = \boldsymbol{P}^{-1}\boldsymbol{A}^j\boldsymbol{P}$ and $\boldsymbol{\mathcal{D}} = \boldsymbol{P}^{-1}\partial_j \boldsymbol{D}^j$; finally, the non-conservative Jacobian matrices $\boldsymbol{\mathcal{A}}^j$ (Hirsch 1990; Thompson 1987, 1990) are diagonalized. In this way, conservation laws are reformulated such that their dependency on characteristic waves becomes explicit.

In the particular application to unstructured grids, the orientation of boundary faces may generally not be aligned with the axes of the reference frame. Moreover, the orientation of boundary elements themselves may differ from cell to cell. Hence, a local reference frame change is a necessary step toward generalization of the method to unstructured grids. Defining a local orthonormal base of coordinates ξ, η, ζ and applying the chain rule to Eq. (3.7), the generalized system (using, for convenience, a slightly different notation) becomes

$$\partial_t \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{A}}' \partial_\xi \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{B}}' \partial_\eta \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{C}}' \partial_\zeta \boldsymbol{\mathcal{U}} + \boldsymbol{\mathcal{D}}' = 0, \tag{3.8}$$

where

$$\boldsymbol{\mathcal{A}}' = \boldsymbol{A}^j \xi_j, \quad \boldsymbol{\mathcal{B}}' = \boldsymbol{A}^j \eta_j, \quad \text{and} \quad \boldsymbol{\mathcal{C}}' = \boldsymbol{A}^j \zeta_j, \tag{3.9}$$

with ξ_j, η_j and ζ_j the cosines of the local orthonormal reference frame with respect to the global one and $\boldsymbol{\mathcal{D}}'$ the transformed viscous term.

If the axis ξ is orthogonal to the boundary element face under consideration, the transformed non-conservative Jacobian matrix $\boldsymbol{\mathcal{A}}'$ is then diagonalized by the transformation matrix $\boldsymbol{S}$ (*i.e.*, $\boldsymbol{\mathcal{A}}' = \boldsymbol{S}\boldsymbol{\Lambda}\boldsymbol{S}^{-1}$), with

$$\boldsymbol{S} = \begin{pmatrix} \rho/(2a) & 1 & 0 & 0 & \rho/(2a) \\ -\xi_1/2 & 0 & -\xi_3 & \xi_2 & \xi_1/2 \\ -\xi_2/2 & 0 & -\xi_2\xi_3/\xi_1 & -(\xi_1^2+\xi_3^2)/\xi_1 & \xi_2/2 \\ -\xi_3/2 & 0 & (\xi_1^2+\xi_2^2)/\xi_1 & \xi_2\xi_3/\xi_1 & \xi_3/2 \\ \rho a/2 & 0 & 0 & 0 & \rho a/2 \end{pmatrix}, \tag{3.10}$$

$$\boldsymbol{S}^{-1} = \begin{pmatrix} 0 & -\xi_1 & -\xi_2 & -\xi_3 & 1/(\rho a) \\ 1 & 0 & 0 & 0 & -1/a^2 \\ 0 & -\xi_3 & 0 & \xi_1 & 0 \\ 0 & \xi_2 & -\xi_1 & 0 & 0 \\ 0 & \xi_1 & \xi_2 & \xi_3 & 1/(\rho a) \end{pmatrix}, \tag{3.11}$$

and $\boldsymbol{\Lambda} = \mathrm{diag}(u_j\xi_j - a,\, u_j\xi_j,\, u_j\xi_j,\, u_j\xi_j,\, u_j\xi_j + a)$. From this point on, in the simplest case of planar boundaries (*i.e.*, each given boundary face is composed of boundary elements with the same orientation), the 3D-NSCBC formulation can basically be followed without any major difference, with the characteristic wave amplitude variations and the relevant transverse terms defined as

$$\boldsymbol{\mathcal{L}} = \boldsymbol{\Lambda}\boldsymbol{S}^{-1} \partial_\xi \boldsymbol{\mathcal{U}}, \quad \text{and} \quad \boldsymbol{\mathcal{T}} = -\boldsymbol{\mathcal{B}}' \partial_\eta \boldsymbol{\mathcal{U}} - \boldsymbol{\mathcal{C}}' \partial_\zeta \boldsymbol{\mathcal{U}}. \tag{3.12}$$

For numerical implementation of this method on unstructured grids, some additional difficulties need to be addressed. In the most general case of non-planar boundaries, each boundary cell element may have different orientation; hence it may be difficult to derive a proper numerical scheme, able to determine the transverse terms while fully respecting the right domains of influence in terms of wave propagation. Moreover, such a scheme would necessitate topological information regarding neighbor boundary faces that, at present, needs to be provided in the perspective of multiprocessor computations.

Each boundary value must be integrated in time using Eq. (3.8), hence resorting to a finite difference (FD) scheme in contrast to the finite volume (FV) scheme used in the interior domain. If, on the one hand, FD and FV schemes may be seen to be equivalent up to the second order over structured regular stencils (Ducros *et al.* 2000), on the other hand this equivalence may no longer be rigorous over irregular boundaries. Indeed, the 3D-NSCBC procedure is extremely sensitive to the numerical computation of transverse terms (or transverse fluxes), hence the necessity of an accurate scheme to handle those terms, at least when the boundary surface is not characterized by regions of strong curvature.

This point is actually under study, and a local polynomial reconstruction of the solution in order to evaluate transverse gradients is being assessed for planar and curved boundaries.

4. Time-dependent boundary conditions

As mentioned, the use of compressible solvers to directly solve for noise propagation requires, in general, non-reflecting boundary conditions. This is always the case when the computational domain represents a portion of an open unconfined physical domain. Conversely, in many practical applications, reflection from the boundary needs to be present and well controlled (*e.g.*, in the design of gas turbine combustors subject to reflection from the turbine end).

When spectral transfer functions relating to incoming and reflected waves are available for the region located downstream of the computational domain, reflected signals can be evaluated, provided that acoustic, entropy and vorticity waves can be clearly identified. Moreover, once the reflected waves are computed, the boundary conditions should be designed to easily accept prescribed incoming signals.

In this regard, characteristic boundary conditions represent a natural choice as they directly solve for the waves propagated back and forth through the boundary plane. With reference to Eq. (3.12), the different waves crossing the boundary are immediately identified as

$$\mathcal{L}_{1,5} = \lambda_{1,5}\left[\tfrac{1}{\rho a}\partial_\xi p \mp \left(\xi_1\partial_\xi u_1 + \xi_2\partial_\xi u_2 + \xi_3\partial_\xi u_3\right)\right] \qquad \text{(acoustic)}, \tag{4.1}$$

$$\mathcal{L}_2 = \lambda_2\left[\partial_\xi \rho - \tfrac{1}{a^2}\partial_\xi p\right] \qquad \text{(entropy)}, \tag{4.2}$$

$$\mathcal{L}_3 = \lambda_3\left[\xi_1\partial_\xi u_3 - \xi_3\partial_\xi u_1\right] \qquad \text{(vorticity)}, \tag{4.3}$$

$$\mathcal{L}_4 = \lambda_4\left[\xi_2\partial_\xi u_1 - \xi_1\partial_\xi u_2\right] \qquad \text{(vorticity)}. \tag{4.4}$$

In principle, the spectral representation of outgoing waves can be used as an input to the spectral transfer function of the downstream region, whereas the reflected acoustic signal can be transformed back in physical space and prescribed as an incoming wave in the characteristic boundary condition. In practice, we deal with discrete time signals generated during the simulation, and the computation of the relevant spectral representation may need some special care. However, specification of an incoming discrete time signal on a relaxed subsonic inflow condition based on the 3D-NSCBC procedure has already been successfully tested (Lodato *et al.* 2009) in the particular case of inlet turbulence specification by means of a digital filtered correlated random noise (Klein *et al.* 2003).

The work in progress includes evaluation of possible two-way coupling between the three-dimensional characteristic boundary conditions and methods to approximate the transfer functions relevant to regions which are outside the actual computational domain.

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