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Short note

Towards improved boundary conditions for the DNS and LES of turbulent subsonic flows

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The purpose of this note is to extend the outflow boundary condition treatment of previous work [1] to include viscous and thermal conduction effects.

We consider a problem defined on $\mathbb{R}^n$, and examine a boundary whose normal points in the x_α direction. The NSCBC [2] approach decomposes the α-direction flux term of the Navier–Stokes equations into

$$\frac{\partial}{\partial t}(\mathbf{U}) + \mathbf{S}_\alpha^{-1}\mathbf{L}_\alpha \frac{\partial}{\partial x_\alpha}(\mathbf{U}) + \sum_{\substack{i=1 \\ i\neq\alpha}}^{n} \mathbf{P}^{-1}(\mathbf{F}_i)_\mathbf{U} \frac{\partial}{\partial x_i}(\mathbf{U}) = \mathbf{P}^{-1}\mathbf{C}, \tag{1}$$

where $\mathbf{L}_\alpha = \{L_1, L_2, \ldots, L_{n+2}\}^\mathrm{T}$ is the vector of *characteristic wave amplitude variations* (or *amplitudes* hereafter), $\mathbf{U}$ is a vector of primitive variables, $\mathbf{P}$ is a transformation matrix relating primitive and conserved quantities, $\mathbf{F}_i$ is the flux vector, and $\mathbf{S}_\alpha$ is the matrix of left eigenvalues of $\mathbf{P}^{-1}(\mathbf{F}_\alpha)_\mathbf{U}$. There is no summation over Greek indices. The amplitude vector is associated with $n+2$ eigenvalues: a left-going and a right-going acoustic amplitude (denoted L_1 and L_{n+2} and propagating with speeds $u-a$ and $u+a$, respectively), and n degenerate eigenvectors with propagation speed u representing convective transport.

We set $n=2$ here, and consider a flow with spanwise periodicity and a bulk velocity of u_b m/s. For an outflow located on the right-hand face of the domain, we have previously shown [1] that a new non-reflecting boundary condition for equation set 1 of the form

$$L_1 = L_4 + (\gamma-1)T\sqrt{\frac{\rho}{\gamma p}}\left(v\frac{\partial u}{\partial y} - u_\mathrm{b}\frac{\partial u}{\partial x}\right) - (\gamma-1)T(\Delta^{(1)}), \tag{2}$$

does not introduce the spurious pressure oscillations associated with the NSCBC/LODI approach. $\Delta^{(1)}$ is referred to as an *acoustic divergence*.

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In deriving Eq. (2), we have assumed that the flow physics evolve on two disjoint families of length scales: *inertial* scales and *acoustic* scales. To separate these effects, we non-dimensionalize Eq. (1) and introduce a low Mach number expansion for each of the dependent variables [3] (i.e. $p = p^{(0)} + Mp^{(1)} + O(M^2)$ for pressure, where M is a suitably defined Mach number). We denote the inertial length scales as $\widehat{x}_i$ and the acoustic length scales as $\xi_i = M\hat{x}_i$, and assume the two to be mutually independent. The derivatives appearing in the dimensionless form of Eq. (1) can then be written as [4]

$$\left.\frac{\partial}{\partial x}\right|_{M,t} = \frac{\partial}{\partial \hat{x}} + M\frac{\partial}{\partial \xi}. \tag{3}$$

The final step in the current approach is to make these substitutions into the definitions of the amplitudes themselves. In so doing, the non-reflecting boundary condition proposed by Hedstrom [5] is seen to set all orders of the amplitude definitions to zero. In contrast, the current approach allows us to retain the inertial elements of the amplitudes while still allowing transparent acoustic wave treatment.

Using the previous definitions, the acoustic term appearing in Eq. (2), is then defined as

$$\Delta^{(1)} = \frac{\partial u_i^{(0)}}{\partial \xi_i}. \tag{4}$$

We define the *total divergence* as $\Delta \equiv \partial u_i/\partial x_i$ and assume that it can be calculated during a simulation using some approximate numerical scheme. $\Delta^{(1)}$ can be related to the dimensionless form Δ by introducing the low Mach number decomposition to obtain

$$\Delta = \Delta^{(0)} + M\Delta^{(1)} + O(M^2) \tag{5}$$

$$\Delta^{(0)} \equiv \frac{\partial u_i^{(0)}}{\partial \hat{x}_i}, \tag{6}$$

where $\Delta^{(0)}$ is referred to as the *inertial* divergence. For cold, low Mach number problems, we have $\Delta^{(0)} = 0$ (the flow is solenoidal) and the acoustic divergence can be obtained immediately from Δ. As the parity between $\Delta^{(1)}$ and Δ is only true for cold flows, a more general prescription for $\Delta^{(0)}$ is required for flows with strong thermal gradients.

$\Delta^{(0)}$ can be estimated through the pressure transport equation [6]:

$$\frac{\partial p}{\partial t} + u_k\frac{\partial p}{\partial x_k} + \gamma p\left(\frac{\partial u_k}{\partial x_k}\right) = \tau_{ik}\frac{\partial u_i}{\partial x_k} + (\gamma - 1)\frac{\partial}{\partial x_k}\left(\lambda\frac{\partial T}{\partial x_k}\right). \tag{7}$$

Inserting the low Mach number expansion into the dimensionless form of Eq. (7), and decomposing the derivatives according to Eq. (3), we find that, to leading order:

$$\frac{\partial p^{(0)}}{\partial t} = -\gamma p^{(0)}\Delta^{(0)} + \frac{1}{Re\ Pr}\frac{\partial}{\partial \hat{x}_k}\left(\lambda\frac{\partial T^{(0)}}{\partial \hat{x}_k}\right). \tag{8}$$

For problems involving large thermal gradients, we assume that $T^{(0)} = T^{(0)}(\hat{x}_i, t)$, and $\rho^{(0)} = \rho^{(0)}(\hat{x}_i, t)$. This assumption is exact if the temperature and density gradients are produced by combustion. The leading orders of the momentum equations provide $p^{(0)} = \text{const.}$ (providing the flow experiences no bulk compression) and $p^{(1)} = p^{(1)}(\xi_i, t)$ [4]. It is straightforward to show that viscosity is an $O(M^2)$ term and has no effect on the two leading order terms of the pressure equation; it can therefore influence neither $\Delta^{(0)}$ nor $\Delta^{(1)}$ and we conclude then that the expression derived for $\Delta^{(1)}$ in [1] for requires no modification to include purely viscous effects.

For more general flows at low Mach number on open domains and without bulk compression, the thermodynamic pressure is constant in time and space. It follows from Eq. (8) that to leading order, the inertial divergence in fully dimensional form can be approximated by

$$\Delta^{(0)} \simeq \frac{\gamma - 1}{\gamma p}\frac{\partial}{\partial x_k}\left(\lambda\frac{\partial T}{\partial x_k}\right).$$

As in the inviscid case, the momentum equation is used to relate the incoming and outgoing amplitudes. For the Navier–Stokes equations, the viscous terms must be included, and we therefore modify Eq. (2) (in fully dimensional form)

$$\begin{aligned} L_1 &= L_4 - (\gamma-1)T\sqrt{\frac{\rho}{\gamma p}}\left(\left(\frac{\partial\tau_{yx}}{\partial x}+\frac{\partial\tau_{yy}}{\partial y}+u_{\mathrm{b}}\frac{\partial u}{\partial x}-v\frac{\partial u}{\partial y}\right)+\sqrt{\frac{\gamma p}{\rho}}\Delta^{(1)}\right) \\ \Delta^{(1)} &\simeq \Delta - \frac{(\gamma-1)}{\gamma p}\frac{\partial}{\partial x_k}\left(\lambda\frac{\partial T}{\partial x_k}\right), \end{aligned} \tag{9}$$

where both Δ and the thermal conduction terms are calculated by using some approximate numerical scheme such as compact finite differences [7].

The acoustic transparency of the boundary conditions and their performance with respect to turbulent outflows has been established for cold viscous flows [8], where they have been found to have the same excellent non-reflective behaviour as their inviscid counterparts. The inclusion of viscous terms on the outflow appears to have little effect on the pressure field over the whole domain. This is consistent with the fact that viscous terms are $O(M^2)$ and are thus attached to the inertial components of the flow. As such, they are convected at the same speed as the entropy and vorticity waves. Provided the flow contains no strong recirculation at the outflow, then any errors arising from an incorrect viscous flux specification will be convected out of the domain without influencing the solution.

Fig. 1a–d shows the pressure evolution for two hot (~600 K) co-rotating vortices leaving a computational domain that is 7.5 mm square in size. This configuration was chosen for two reasons; (a) there is an inertial

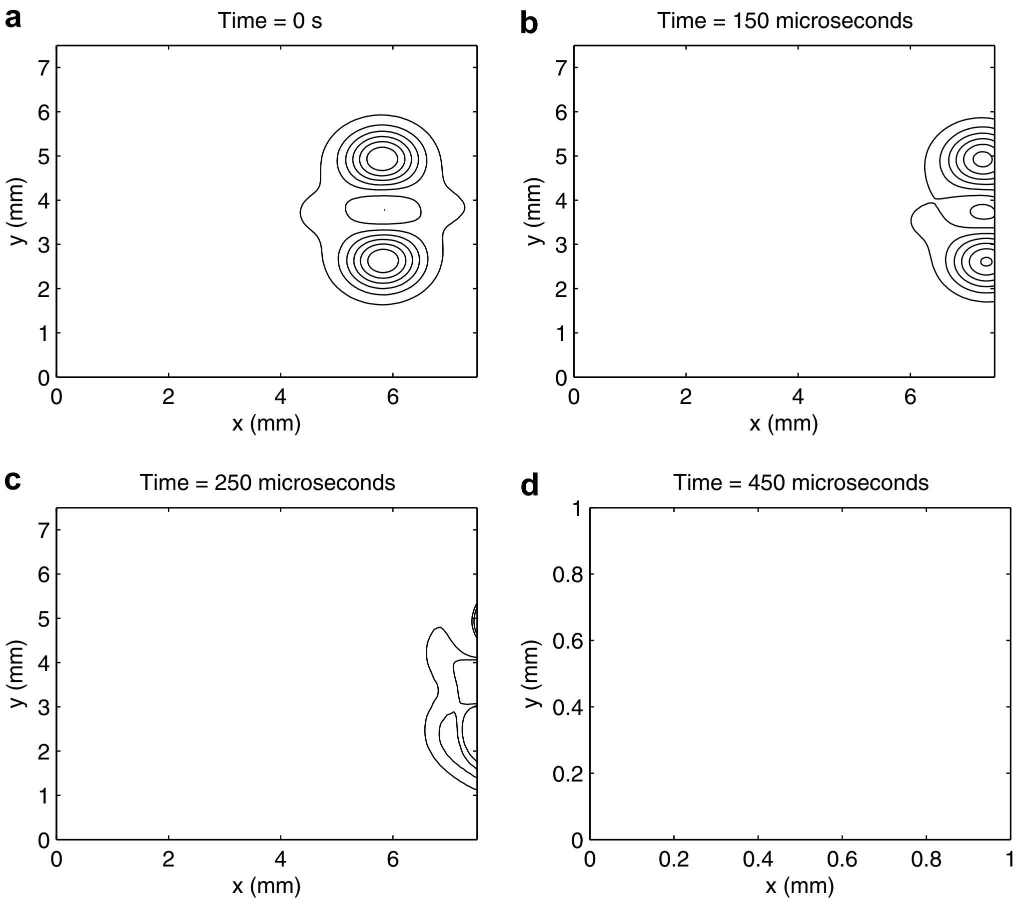

Fig. 1. Contour plots of pressure for twin co-rotating vortices approaching a revised non-reflecting outflow. Centres of vortices are heated to 600 K. The pressure range satisfied $-15\ \mathrm{N/m^2} \leqslant p - p^{(0)} \leqslant 5\ \mathrm{N/m^2}$ throughout the simulation.

evolution in the flow, arising from the two vortices wrapping asymmetrically around each other as the flow develops and; (b) acoustic transients emerge from the initial conditions and conduction effects. The mean flow speed u_b was set to 10 m/s, and the two vortices were initialized using a stream function approach with a radius set to 8% of the domain size. The ambient temperature was set at 300 K and, with the assumption that the pressure was initially constant at $p^{(0)} = 101{,}325\ \mathrm{N/m^2}$, the density was calculated using the thermal equation of state. The thermal conductivity was calculated using [9]

$$\lambda = 2.58 \times 10^{-5} \times c_p \left(\frac{T}{300}\right)^{0.7}.$$

For the inlet, a fixed velocity, non reflecting condition was imposed [1].

To obtain a reference solution, we doubled the streamwise length of the computational domain and applied standard non-reflecting boundary conditions to the outflow. The vortex pair was allowed to propagate through the extended domain, with the simulation terminating before the vortices approached the outflow boundary. The reference solution was taken as the left half of the extended domain, and was compared to the solution obtained using the new boundary conditions.

As can be seen from Fig. 1a–d, there is no significant distortion in the pressure distribution arising from the boundary conditions. As the vortices wrap around each other, the resultant asymmetry in the pressure field is well captured. This result is a considerable improvement on the solution calculated using the NSCBC approach. Results from the latter are given in Fig. 2a–d. In the figures, the contours have been restricted

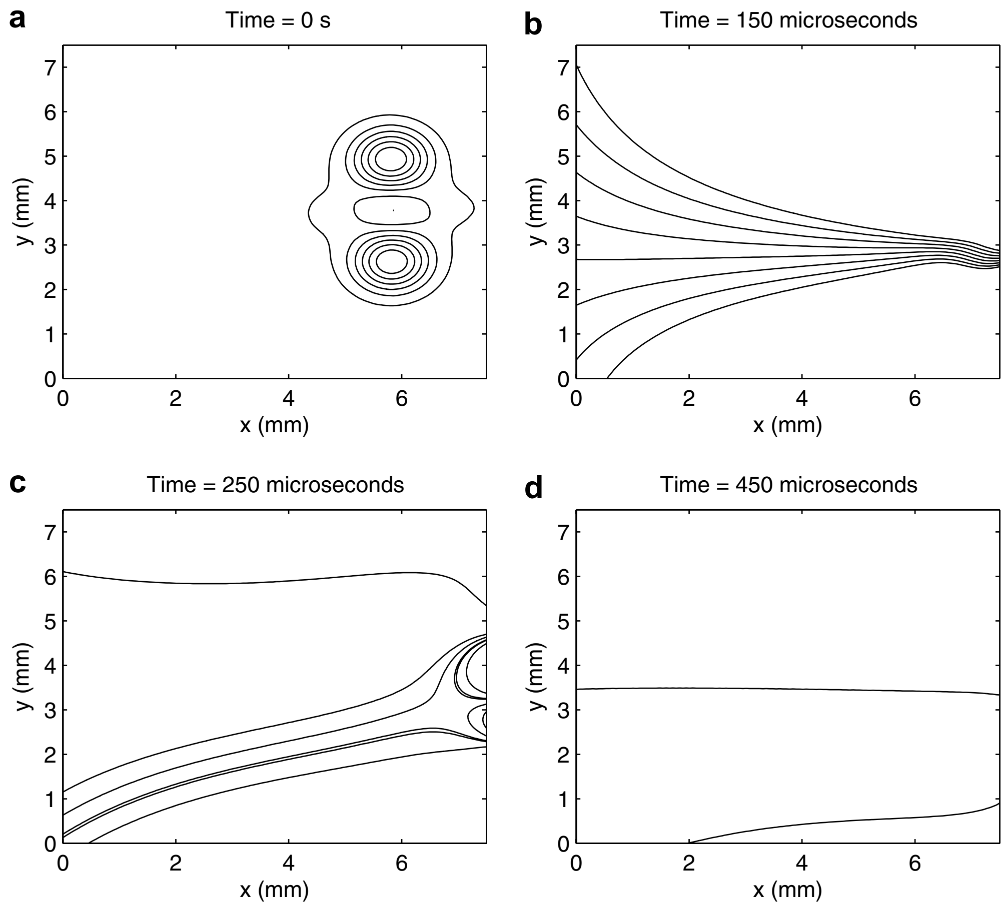

Fig. 2. Contour plots of twin co-rotating vortices approaching a standard non-reflecting outflow. Centres of vortices are heated to 600 K. The pressure range satisfied $-120\ \mathrm{N/m^2} \leqslant p - p^{(0)} \leqslant 70\ \mathrm{N/m^2}$ throughout the simulation.

to the same range as those in Fig. 1a–d. The pressure history of the two solutions is given in Fig. 3, where a normalized pressure difference, defined as

$$\frac{\|p(\mathbf{x},t)-p_{\mathrm{ref}}(\mathbf{x},t)\|_2}{\|p_{\mathrm{ref}}(\mathbf{x},0)-p^{(0)}\|_2},$$

is plotted as a function of time. We recall that p_{ref} is taken from the left half of the extended benchmark solution domain. We observe that throughout the simulation, the solution obtained with the new boundary conditions remains close to the benchmark. Conversely, in the NSCBC case there are considerable transients in the solution and, in the worst instance, the normalized pressure difference is about an order of magnitude larger than that obtained using the new approach.

The differences between the solution obtained with the new treatment and the benchmark appear to be related to differences in the treatment of viscous and momentum boundary conditions. The importance of correct viscous flux specification for reacting flows has been explored by Sutherland and Kennedy [10]. In this case, the condition imposed on the heat flux vector is likely to have the dominant effect on the flow. This is due to the fact that the viscosity has only an $O(M^2)$ influence in the pressure distribution, while conduction is leading order. The net effect of the thermal conduction boundary condition will depend on the mean flow speed; as the mean flow decreases, the larger relative influence of viscous transport will have greater influence on the pressure. This is true of all boundary condition treatments derived from the method of characteristics.

The new approach provides a significantly better treatment of the pressure field for viscous conducting flows than do many previous characteristics based methods. The new treatment is able to deal with flows comprising inhomogeneous high temperature regions without inducing spurious effects. The scheme appears to be

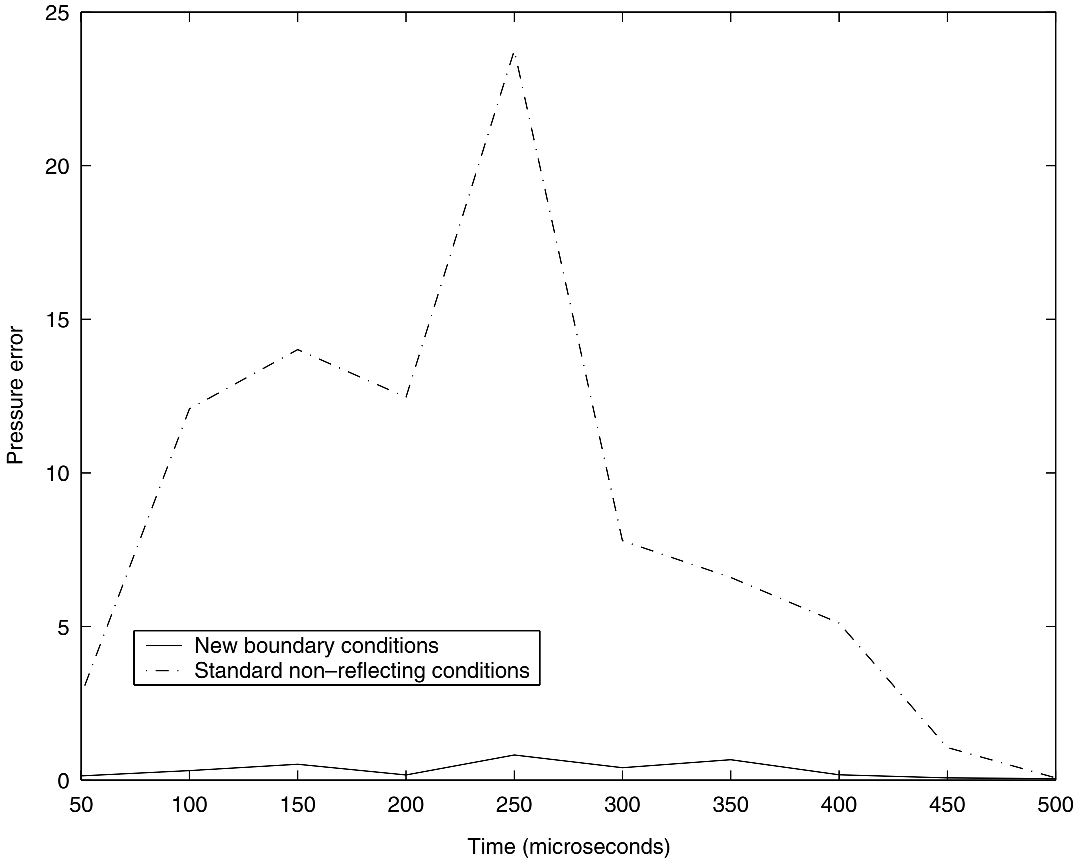

Fig. 3. Time evolution of the normalised pressure difference for: (—) the new boundary condition and (· – ·) the standard non-reflecting condition.

stable for long time integration periods. Future work will examine further improvements of the method by (a) reducing the (very small) pressure drift associated with characteristics-based methods, (b) further reducing the effects of the viscous boundary conditions on the pressure field and (c) extending the treatment to incorporate chemical reactions.

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