European Conference on Computational Fluid Dynamics
ECCOMAS CFD 2006
P. Wesseling, E. Oñate and J. Périaux (Eds)

A NUMERICAL INVESTIGATION OF THE BOUNDARY COMMUTATION ERROR IN LARGE EDDY SIMULATION

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Key words: Large eddy simulation, boundary conditions, boundary commutation error, approximate deconvolution, finite element method

Abstract. *The boundary commutation error in large eddy simulation is studied numerically. It is shown that an accurate representation of the boundary commutation error has an important role in a reliable large eddy simulation of wall bounded flows. The numerical experiments in this paper are conducted for a 2D channel flow.*

1 INTRODUCTION

One of the main challenges for Large Eddy Simulation (LES) is specification of efficient, general boundary conditions for the filtered variables.[6,16,20] There are essentially two ways to treat boundary conditions in LES.[18] The first is to decrease the filter width to zero at the boundaries. This popular approach, known as Near Wall Resolution (NWR),[18] captures the important flow features near the boundary, but has high computational cost since it requires a fine mesh near the wall. The second is referred to as Near Wall Modeling (NWM).[18] The NWM boundary conditions are developed by using boundary layer theory. Although more ad-hoc (and problem specific), the discretization near boundaries can remain coarse. Hence, the NWM approach is a better candidate for LES of realistic turbulent flows.

When using the NWM, however, filtering through the boundaries of the computational domain is usually employed. This introduces a boundary integral term that needs to be added to the equations for the space-filtered variables. This new term, called *Boundary Commutation Error (BCE)*,[6] was investigated from a theoretical point of view in.[12] There it was proved that the BCE term can be significant and should be included for reliable NWM.

This paper presents a numerical investigation of the BCE. The numerical experiments are carried out for the 2D channel flow test problem. It is demonstrated that neglecting the BCE term yields inaccurate numerical results.

2 THE BOUNDARY COMMUTATION ERROR

In the case of an incompressible fluid, the non-dimensionalized form of the Navier-Stokes equations (NSE) is

$$\begin{aligned} \boldsymbol{u}_t - Re^{-1}\Delta \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\,\boldsymbol{u} + \nabla p &= \boldsymbol{f}, \quad \text{in } \Omega, & (1)\\ \nabla\cdot\boldsymbol{u} &= 0, \quad \text{in } \Omega, & (2)\\ \boldsymbol{u} &= 0, \quad \text{on } \partial\Omega. & (3) \end{aligned}$$

where $\boldsymbol{u}$ is the velocity, p is the pressure, and $Re := U\,L/\nu$ is the Reynolds number, defined as the ratio between the product of a characteristic length-scale L and a characteristic velocity U, and the kinematic viscosity ν.

The equations for the filtered variables $\overline{\mathbf{u}} := g_\delta * \mathbf{u}$ and $\overline{p} := g_\delta * p$ in LES are obtained by convolving the NSE (1)–(3) with a rapidly decaying spatial filter g_δ. When filtering in a bounded computational domain Ω, one needs to extend the flow variables outside the computational domain,[6,12] since the convolution integral is computed over the entire $\mathbb{R}^3$. This extension is inherently *non-smooth*, since the unavailable exact solution inside Ω would be needed for a smooth extension. Because of this non-smooth extension, the following term, called the boundary commutation error,[7,12,13,22] needs to be added to the right-hand side of (1):

$$\int_{\partial\Omega} g_\delta(\mathbf{x}-\mathbf{s})\ \left[Re^{-1}\nabla\mathbf{u}(\mathbf{s})\ \mathbf{n}(\mathbf{s}) - p(\mathbf{s})\ \mathbf{n}(\mathbf{s})\right]\, d\mathbf{s}, \qquad \mathbf{x}\in\Omega. \tag{4}$$

In (4), $\mathbf{n}(\mathbf{s})$ is the outward unit normal vector to $\partial\Omega$ at the point $\mathbf{s}\in\partial\Omega$.

In,[12] an exquisite theoretical investigation was carried out. In particular, it was shown that the BCE term (4) is significant and should be included in the LES model. In this paper, a numerical investigation of the role of the BCE term in NWM is performed.

It is interesting to note that recently, there have been some interesting developments in the numerical approximation of the boundary commutation error.

In[11] the following approach was proposed: To estimate the shear stresses, a buffer region outside the wall was included in the computational domain. In this region, the velocities were set to zero, and the wall stress was determined to minimize the kinetic energy in the buffer region. The resulting system can be thought of as an LES version of embedded boundary techniques. The approach has been tested in turbulent channel flow simulations, with good results.

A different approach has been recently proposed in.[8] The *approximate deconvolution*[1,21] approach was used to approximate the boundary commutation error. The approximate deconvolution is using the mathematical properties of the particular spatial filter g_δ and the numerical approximation of $\overline{\mathbf{u}}$ to obtain an *approximation* of (some of) the subfilter-scale information contained in $\mathbf{u}-\overline{\mathbf{u}}$. The applications that would probably benefit most from this approach would be those in which the boundary conditions are time-dependent (such as in a flow control setting).

Another approach uses statistics of turbulent channel flow simulations to approximate the BCE.[5] Finally, a term similar to the BCE was approximated numerically in the context of multiphase flow computations.[17]

3 NUMERICAL EXPERIMENTS

3.1 The Numerical Method

The numerical experiments in this paper have been carried out by using *ViTLES*, the Virginia Tech Large Eddy Simulator, a *parallel, finite element* computational platform for the numerical validation of CFD and LES models.

For the spatial discretization, the computational domain is decomposed in a collection of non-overlapping triangles (in 2D) or tetrahedra (in 3D). The traditional Taylor-Hood finite element pair (continuous quadratic velocities and continuous linear pressures) which satisfies the discrete inf-sup condition[9] were used.

For the time discretization, the second-order accurate, unconditionally stable Crank-Nicolson scheme[10] was employed. Thus, for each time step, the following nonlinear system of equations is solved:

$$\begin{aligned} & \frac{\mathbf{u}^{k+1}-\mathbf{u}^{k}}{\Delta t} - \theta\nabla\cdot\left(2Re^{-1}\nabla^{s}\mathbf{u}^{k+1}\right) + \theta(\mathbf{u}^{k+1}\cdot\nabla)\mathbf{u}^{k+1} + \theta\nabla p^{k+1} \qquad (5) \\ = \;& (1-\theta)\nabla\cdot\left(2Re^{-1}\nabla^{s}\mathbf{u}^{k}\right) - (1-\theta)(\mathbf{u}^{k}\cdot\nabla)\mathbf{u}^{k} - (1-\theta)\nabla p^{k} + \theta\mathbf{f}^{k+1} + (1-\theta)\mathbf{f}^{k}, \end{aligned}$$

where $(\mathbf{u}^{k+1}, p^{k+1}, \mathbf{f}^{k+1})$ and $(\mathbf{u}^{k}, p^{k}, \mathbf{f}^{k})$ are the velocity, pressure, and forcing vectors at the current and previous time-step, respectively, $\theta=\frac{1}{2}$ for Crank-Nicolson, and Δt is the time-step.

The incompressibility constraint $\nabla\cdot\mathbf{u}=0$ in the Navier-Stokes equations is relaxed by using the penalty method [10,14,19]

$$\varepsilon p_{\varepsilon} + \nabla\cdot\mathbf{u}_{\varepsilon} = 0, \qquad (6)$$

where ε is a small parameter. It can be proved that[14]

$$|\mathbf{u}-\mathbf{u}_{\varepsilon}|_{1} + ||p-p_{\varepsilon}||_{0} \leq C\,\varepsilon.$$

In our computations, we used $\varepsilon=0.001$. The time discretization for the penalty method reads

$$\varepsilon p^{k+1} + \nabla\cdot\mathbf{u}^{k+1} = \varepsilon p^{k},$$

where the $k+1$ superscript denotes the current time step, and the k superscript denotes the previous time step. In this form, the penalty method resembles the artificial compressibility method,[10,14] the augmented lagrangian method,[19] or the iterated penalty method.[14]

A Newton iteration scheme was used to solve the nonlinear system at each time step. The scheme implemented in ViTLES explicitly constructs approximations of the Jacobians rather than calculating the actual Jacobian matrix. Such a scheme provides rapid computational implementation, and is easily transportable in the sense of applicability to a number of physical problems. In view of (5) and (6), at each time-step the following equation is solved:

$$R(\mathbf{u}^{k+1}, p^{k+1}) = \mathbf{0},$$

where

$$\begin{aligned} & R(\mathbf{u}^{k+1}, p^{k+1}) \\ := \ & (\mathbf{u}^{k+1} - \theta \Delta t \nabla \cdot (2Re^{-1} \nabla^s \mathbf{u}^{k+1}) + \theta \Delta t (\mathbf{u}^{k+1} \cdot \nabla) \mathbf{u}^{k+1} + \theta \Delta t \nabla p^{k+1} + R_k, \\ & \nabla \cdot \mathbf{u}^{k+1} + \varepsilon p^{k+1} - \varepsilon p^k), \end{aligned} \tag{7}$$

and R_k is the part of $R(\mathbf{u}^{k+1}, p^{k+1})$ that depends only on $\mathbf{u}^k$ and p^k:

$$R_k := -\mathbf{u}^k - (1-\theta)\Delta t \nabla \cdot (2Re^{-1} \nabla^s \mathbf{u}^k) + (1-\theta)\Delta t (\mathbf{u}^k \cdot \nabla)\mathbf{u}^k + (1-\theta)\Delta t \nabla p^k.$$

The Newton iteration $(\mathbf{u}^n, p^n)$ will yield an approximation to $(\mathbf{u}^{k+1}, p^{k+1})$, where n is the Newton iteration number. Thus, Newton's method for $R(\mathbf{u}^n, p^n) = \mathbf{0}$ reads

$$R'(\mathbf{u}^n, p^n)(\mathbf{u}^{n+1} - \mathbf{u}^n, p^{n+1} - p^n) = -R(\mathbf{u}^n, p^n),$$

where

$$[R'(\mathbf{u}^n, p^n)]_{ij} := \frac{\partial R_i(\mathbf{u}^n, p^n)}{\partial (\mathbf{u}^n, p^n)_j}$$

is the Jacobian of R. We explicitly construct the approximation to R', element by element, from a sequence of finite differences

$$[R'(\mathbf{u}^n, p^n)]_{ij} \approx \frac{R_i((\mathbf{u}^n, p^n) + h\mathbf{e}_j) - R_i((\mathbf{u}^n, p^n)}{h},$$

where h is the differencing parameter and $\mathbf{e}_j$ is the j-th unit vector. The explicit construction of the approximation to the Jacobian instead of using matrix-free Jacobian vector products is advantageous in sensitivity computations.

ViTLES is written on top of PETSc (the portable, extensible toolkit for scientific computing) developed at Argonne National Laboratory.[2–4] ViTLES makes use of MPI, linpack and the blas. ADIC, the automatic differentiation tool,[15] was also used to compute Jacobians. This allowed an efficient implementation of closure modeling and sensitivity analysis. Routines have been developed to convert ViTLES format to several visualization routines including Tecplot, VTK and VU.

3.2 2D channel flow

For the 2D channel flow, the following computational choices were made: The computational domain was $\Omega = (0.0, 1.0) \times (0, 10) \subset \mathbf{R}^2$. Dirichlet boundary conditions at the inlet ($x = 0.0$), on top ($y = 1.0$) and bottom ($y = 0.0$), and "do-nothing" boundary conditions (i.e., $(-p\mathbb{I} + 2Re^{-1}\nabla^s \mathbf{u}) \cdot \mathbf{n} = 0$) at the outlet ($x = 10$) were used. The boundary conditions and the forcing term have been chosen so that the system (u, v, p) defined by

$$\begin{aligned} u(x,y) &= \sin(\pi\, t)\,[\sin(\pi\, y) + 0.2\,\sin(9\,\pi\, y)], \\ v(x,y) &= 0.0, \\ p(x,y) &= 0.0, \end{aligned}$$

satisfy the Navier-Stokes equations (1)–(3). This choice results in homogeneous boundary conditions on top and bottom, and an inflow profile consisting of a "small wave number component" ($\sin(\pi\, y)$) on which a "high wave number component" ($\sin(9\,\pi\, y)$) was superimposed. The exact solution was used as initial condition.

A coarse nonuniform mesh of size $h = 0.5$, a small time-step $\Delta t = 10^{-3}$, and a small penalty parameter $\varepsilon = 10^{-4}$ in the penalty method were used. The nonlinear system at each time-step was solved with a Newton iteration up to an Euclidian norm of the residual vector less than 10^{-4}. The final time was $T = 2.0$ (i.e., 2000 time-steps). A filter radius $\delta = 0.4$ was used. This relatively large value for δ increased the effect of the BCE term on the numerical results. A $Re = 1$ was also used.

It is clear that, since we have an exact solution and a low Re, this flow is *not* turbulent. We chose this setting, however, because we wanted to assess carefully the effect of the BCE on the numerical results. Its effect is apparent at a fundamental level. Indeed, the BCE is essential in filtering *any* type of partial differential equation on a bounded domain,[6] not only in LES of turbulent flows. Obviously, a real turbulent flow numerical investigation of the BCE term is needed and will be carried out in a future study.

3.3 Numerical results

We have run two different set of numerical experiments. All the parameters were the same in the two tests, with one exception: In the first test, the BCE term (4) was *not* used, whereas in the second test the exact BCE term (4) was used.

It is clear from Figure 3.3 that neglecting the BCE term yields inaccurate results. Indeed, the sign of the pressure gradient is *wrong* – the pressure gradient acts in the opposite direction of the flow. By including the BCE term, however, the pressure gradient points in the right direction. (The magnitude of the pressure gradient is inaccurate, however, for the second test, but this is not unexpected at the coarse, LES-like spatial discretization $h = 0.5$ used.)

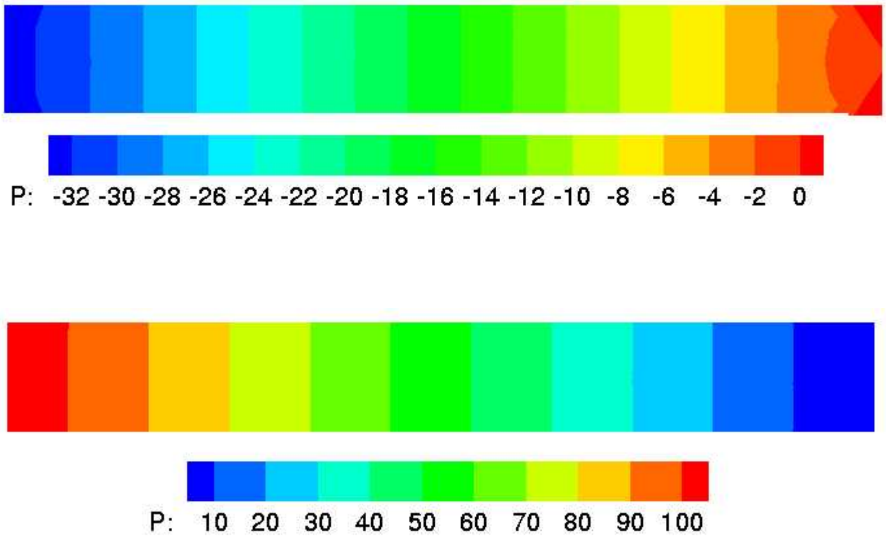

Figure 1: Pressure approximations in 2D channel flow: without BCE (top); and with BCE (bottom).

4 CONCLUSIONS AND FUTURE WORK

The boundary commutation error in large eddy simulation was studied numerically. It was shown that an accurate representation of the boundary commutation error has an important role in a reliable large eddy simulation of wall bounded flows. Specifically, in the numerical simulation of 2D channel flows, discarding the boundary commutation error yields inaccurate results - the pressure gradient is pointing in the opposite direction of the flow.

The approximate deconvolution approach in[8] to approximate the boundary commutation error was used successfully in a simplified linear setting. Extending this approach to a realistic turbulent flow will be carried out in a future study.

Acknowledgments. The support of AFOSR grants F49620-00-1-0299, F49620-03-1-0243, and FA9550-05-1-0449 and NSF grants DMS-0209309, DMS-0322852, and DMS-0513542 is gratefully acknowledged.

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