On LES outflow conditions for integrated LES-RANS computations

By **J. U. Schlüter** AND **X. Wu**

1. Motivation and objectives

For the numerical prediction of turbulent flows of industrial relevance two approaches are currently in use. One is based on the Reynolds-Averaged Navier Stokes (RANS) approach, which computes essentially an ensemble-average of the flow and uses a turbulence model to approximate all scales of turbulence. The other approach is that of Large-Eddy Simulations (LES), where the large scales of motion are resolved in time and space and only the smallest scales are modeled. Although LES is considered the more accurate approach, its application to a number of flow applications is prohibited by the increased computational costs. One way to combine both methods is the integrated LES-RANS approach, where two separate flow solvers, one RANS flow solver and one LES flow solver, are executed simultaneously, each computing a portion of a given domain (Schlüter *et al.* 2003; Schlüter *et al.* 2004a). This approach has been used for the computation of flows in gas turbines (Schlüter *et al.* 2004b; Schlüter *et al.* 2004c; Schlüter *et al.* 2004d). In these previous studies of flows in complex geometries, the RANS domain is upstream of the LES domain, and hence the LES has to use the RANS data to define its inflow.

For the following study we want to concentrate on the reverse case, where the LES domain is upstream of the RANS domain. The RANS solver receives flow data from the LES solver to define its inflow boundary conditions. In return, the upstream LES solver has to receive flow information from the downstream RANS flow solver. This last step is necessary in order to take into account the influence of the downstream flow development onto the flow in the LES domain. In previous years, we have developed LES outflow boundary conditions for integrated LES-RANS computations and tested these using a structured LES flow solver (Schlüter *et al.* 2002; Schlüter *et al.* 2004e). It has been demonstrated that the downstream flow can have a significant effect on the upstream flow features, and we have shown that the previously developed method of body forces can transfer the necessary flow information to the LES domain.

Here, we first recapitulate the method of body forces for integrated LES-RANS computations. We will then elaborate on the determination of the body force constant. Finally, we will report the implementation and validation of this method for unstructured flow solvers.

2. Body force method

In integrated LES-RANS computations we consider overlapping grids between the upstream LES and the downstream RANS. In the LES portion of the overlap region we can use virtual body forces to drive the LES solution to a RANS solution delivered by the downstream flow solver. This body force is employed on the right hand side of the momentum equations.

$$F_i(\mathbf{x}) = \sigma\left(\overline{u}_{i,\text{RANS}}(\mathbf{x}) - \overline{u}_{i,\text{LES}}(\mathbf{x})\right) . \tag{2.1}$$

In Eq.(2.1) $\overline{u}_{i,\text{RANS}}$ is the vector of target velocities obtained from the RANS computation, $\overline{u}_{i,\text{LES}}$ is the vector of time-averaged velocities from the LES computation, and σ is a the body force constant.

This body force term is defined using a temporal mean velocity of the LES solution. This temporal mean can be determined by a trailing time-window over which the LES solution is time-averaged. This allows to correct the mean velocity of the LES solution while allowing for temporal fluctuations due to fine scale turbulence. This preserves the resolved turbulence in the body force volume.

The choice of σ controls the characteristic response time of the LES solution to a change in the outlet boundary condition. If σ tends to zero, the body force becomes essentially ineffective resulting in a drift of the outflow mean velocity profile towards the unforced solution. High values of σ lead to faster change to the desired velocity field, but may lead to numerical instabilities.

3. Estimation of body force constant σ

Previously, we gave a crude estimate for σ from the bulk velocity and the length of the forcing region (Schlüter *et al.* 2002). We now want to provide a more accurate estimate for the choice of σ. This is carried out using a 1D analysis of the stationary Euler equations:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} + \sigma(\langle\bar{u}\rangle_{\text{RANS}} - \langle\bar{u}\rangle_{\text{LES}}) . \tag{3.1}$$

To simplify the equation, we assume a zero pressure gradient and a constant convection velocity u_B. Furthermore, we assume that the flow is stationary, which makes $\langle\bar{u}\rangle_{\text{LES}} = u$. With $\langle\bar{u}\rangle_{\text{RANS}} = u_t$, the target velocity Eq. 3.1 becomes:

$$u_B\frac{\partial u}{\partial x} = \sigma(u_t - u) . \tag{3.2}$$

This ordinary differential equation can be solved analytically and leads to the following expression for u:

$$u(x) = u_t + (u_0 - u_t)\exp\left(-\frac{\sigma}{u_B}x\right) \tag{3.3}$$

with u_0 being the velocity at the beginning of the forcing region.

We now want to determine σ so that at the end of the forcing region ($x = l_F$) the velocity difference is smaller than the relative error

$$\epsilon = \frac{|u(l_F) - u_t|}{u_t} . \tag{3.4}$$

Then, Eq. 3.3 leads to

$$\sigma_{\min} = \frac{u_B}{l_F}\ln\left(\frac{|u_0 - u_t|}{\epsilon u_t}\right) . \tag{3.5}$$

Although this estimate for σ ensures the accuracy of the approach for steady flows, in truly unsteady coupled computations a higher value for σ should be used in order to decrease the time-lag in which the flow solution adjusts to the target velocity obtained from an unsteady downstream computation.

On the upper end, σ is limited by numerical stability considerations. Here, it is useful

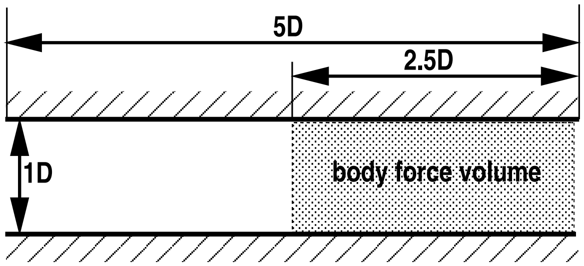

FIGURE 1. Geometry of the pipe test-case

to write σ as an inverse time-scale τ_F. The upper limit is then defined corresponding to the CFL-condition:

$$\sigma_{\max} = \left(\frac{1}{\tau_{\mathrm{F}}}\right)_{\max} = \frac{u_{\mathrm{c}}}{\Delta x_{\mathrm{F}}} \tag{3.6}$$

with Δx_{F} being the size of the smallest cell in the forcing region and u_{c} is the local convection velocity in this cell.

4. Assessment of body force constant

In the following section we want to assess the influence of this constant. For this purpose we consider a pipe flow with diameter D, and length $5D$. The virtual body force is applied in a volume of length $2.5\,D$ at the end of the pipe flow and is used to force the flow to a solution which would not naturally occur in this flow. This setup corresponds to the original investigation of the body force method (Schlüter *et al.* 2001).

For this investigation we use a structured LES flow solver (Pierce & Moin 1998). The flow solver solves the filtered momentum equations with a low-Mach number assumption on an axisymmetric structured mesh. A second-order finite-volume scheme on a staggered grid is used (Akselvoll & Moin 1996). The subgrid stresses are approximated with an eddy-viscosity approach. The eddy viscosity is determined by a dynamic procedure (Germano *et al.* 1991; Moin *et al* 1991). For numerical purposes a convective boundary condition is applied at the outlet plane of the LES domain.

The mesh for the pipe flow consists of 128×32×64 cells. We consider a laminar flow at Reynolds-number $Re = 1000$.

Fig. 2 shows the results for a series of computations. The solid-crossed line shows the parabolic inlet profile corresponding to the solution of a fully-developed pipe flow. Without forcing, this would be the solution at any downstream location in the pipe. The circles denote an arbitrarily-chosen velocity profile, with the same mass flow rate as the inlet profile, which is to be matched at the outlet. Considering these two velocity profiles as the initial and the target velocity. For a desired accuracy of 1% ($\epsilon = 0.01$) this leads to:

$$\sigma_{\min} = \frac{1.0}{2.5} \cdot \ln\left(\frac{|2.0 - 0.75|}{0.01 \cdot 0.75}\right) = 2.05 \tag{4.1}$$

and

$$\sigma_{\max} = \frac{1.0}{\frac{5.0}{128}} = 25.6 \tag{4.2}$$

In order to show the robustness of the method to the choice of σ, several computations were performed with varying σ. Fig. 2 shows that with increasing σ the accordance of

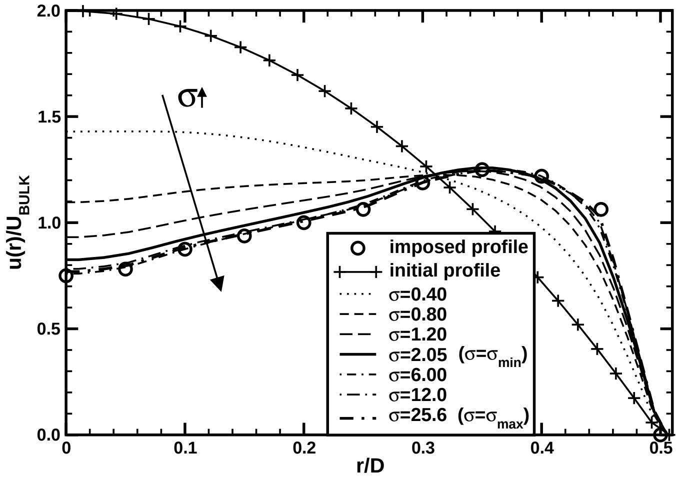

FIGURE 2. Laminar pipe flow: profiles of axial velocity at the outlet ($x/D = 5.0$) in dependance of body force constant σ. Solid lines with crosses: inlet profile. Symbols: imposed profiles. All other lines: LES solution at the outlet plane using different values of σ.

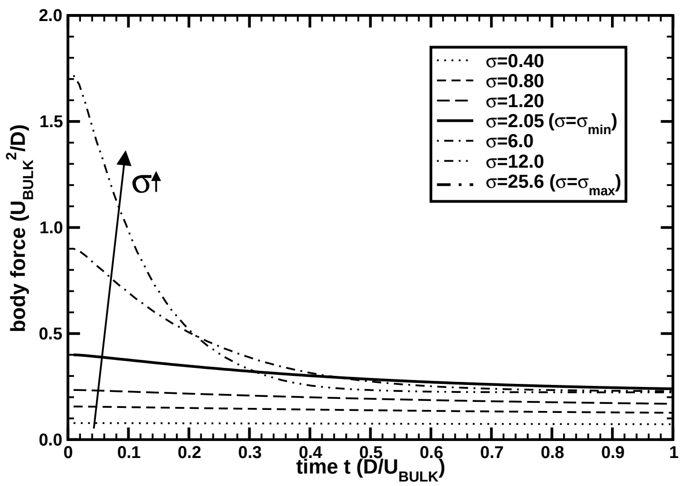

FIGURE 3. Laminar pipe flow: temporal development of body force in the outlet plane in dependance of body force constant σ.

the LES solution with the imposed profile improves. The solutions using $\sigma \geq \sigma_{\rm min}$ show satisfactory results. Computations using a $\sigma = 35.0 > \sigma_{\rm max}$ resulted in a diverging solution.

The temporal development of the body force dependent on the σ is shown in Fig. 3. Here, the spatial average of the body force in the outlet plane is computed and normalized with the bulk velocity and the diameter. Above the minimum σ the body force converges to the same residual body force that is needed to uphold the enforced velocity distribution. A higher body force allows the solution to converge in a shorter period of time.

5. Body force method for unstructured flow solvers

In order to prepare for integrated LES-RANS simulations of complex geometries, we implemented and validated the body force method in the unstructured LES flow solver CDP. Even though the underlying organization of an unstructured LES solver is more complex than a structured LES code, the local nature of the definition of the boundary treatment requires little additional work in for the porting process to unstructured solvers.

The LES flow solver used for this study is the CDP code (Ham *et al.* 2003; Moin & Apte 2004). The filtered momentum equations are solved on a cell-centered unstructured mesh and are second-order accurate. An implicit time-advancement is applied. The subgrid stresses are modeled with a dynamic procedure.

We want to validate the flow solver and the body force method on a swirl flow. Swirl is an important feature in combustor fluid dynamics, since it determines the mixing behavior as well as the evolving pressure field in the combustor. Its complexity and sensitivity to small changes makes it a challenging test-case.

The considered test-case corresponds to that of the experimental investigation of Dellenback *et al.* (Dellenback 1986; Dellenback *et al.* 1988). The geometry is a pipe with a sudden axisymmetric expansion with a ratio in diameters of 1:2 leading to a area ratio of 1:4. The Reynolds-number is $Re = 30,000$ and the swirl number $S = 0.6$ with S defined as:

$$S = \frac{1}{R}\frac{\int_0^R r^2 \langle\bar{u}\rangle_x \langle\bar{u}\rangle_\phi \, dr}{\int_0^R r \langle\bar{u}\rangle_x^2 \, dr}, \tag{5.1}$$

where u_x is the axial velocity component, u_ϕ the azimuthal velocity component, and R the radius of the nozzle. The LES inflow in the simulation was generated by using a swirling pipe flow database (Pierce & Moin 1998).

First, we will compute a reference LES solution using a computational domain sufficiently large to simulate this flow. This geometry will reach from $x/D = -0.5$ to $x/D = 10$ with the origin of the coordinate system at the center of the expansion. The comparison with experimental data will demonstrate the accuracy of the LES solver.

Then, we will compute a smaller domain by truncating the flow domain behind the expansion at $x/D = 1.5$. We will show that this domain is not sufficiently large to simulate this flow, since the influence of the outlet will disturb the flow solution.

Next, we will use a body force volume from $x/D = 1.1$ to $x/D = 1.5$ to drive the LES solution to the mean flow field as determined by the reference solution. We will show that the body force method is able to simulate the effect of the downstream domain.

Two different methods are used to determine the time-averaged LES solution $\overline{u}_{i,\text{LES}}$ for Eq. 2.1. The first method uses an overall time-average using all available time-steps. This is the most accurate description for $\overline{u}_{i,\text{LES}}$ for a statistically steady flow. However, we want to apply the integrated LES-RANS approach also to statistically unsteady flows. Hence, we will also use an average over a trailing time-window to determine $\overline{u}_{i,\text{LES}}$, which allows for unsteadiness in the target solution.

Figure 4 shows the results of the reference solution. The LES solution (solid lines) matches well with the experimental data (symbols).

Figure 5 shows the axial velocity component for the simulations with the truncated domain. We can see that the simulations using a truncated domain without the body force (dashed lines) is disturbed by the proximity of the outflow and deviates from the reference solution. Using a body force (dotted lines and dashed dotted lines) corrects this

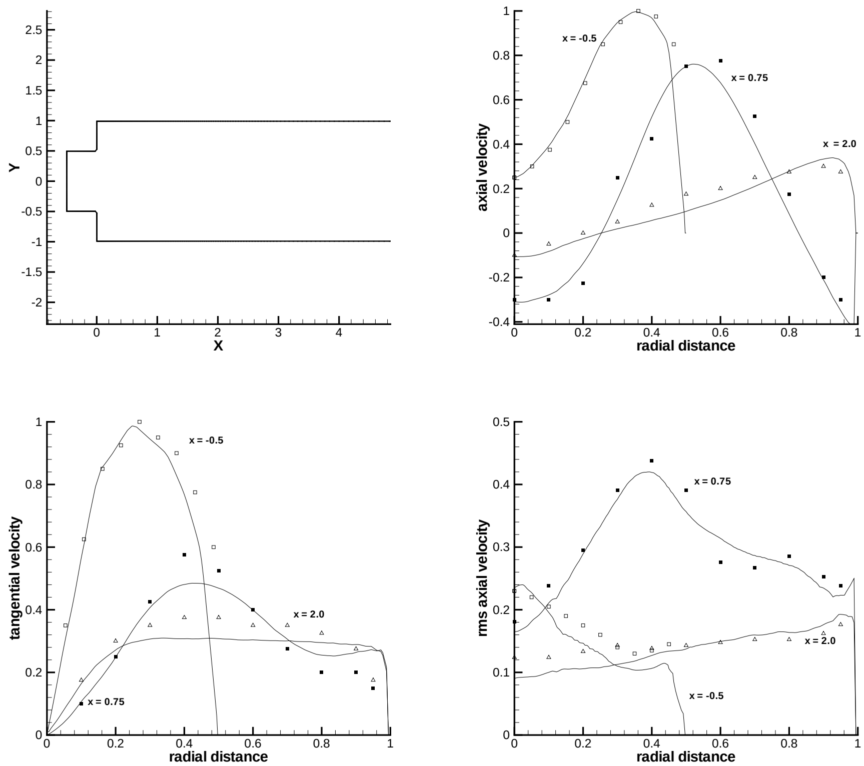

FIGURE 4. Geometry and velocities of a swirling flow through an sudden 1:2 axisymmetric expansion. Reference test case using sufficiently large computational domain. Symbols: experimental data. Solid lines: LES.

behavior and the solution tends towards the reference solution. We can also determine that the use of a trailing time-window for the determination of $\overline{u}_{i,\mathrm{LES}}$ is as accurate as the use of the overall mean.

Figure 6 shows the tangential velocity component for these simulations. The effect of the domain truncation and the correction using a body force are even more apparent.

The results demonstrate that the influence of the downstream flow development on the upstream flow can be simulated using the body force method.

6. Conclusions

For integrated LES-RANS simulations the body force method has been previously developed in order to modify the LES outflow to take the flow development downstream of the LES domain into account.

Here, we gave an estimate for the body force constant σ based on a 1D Euler analysis. We tested the influence of the body force constant on a simple test-case. Furthermore, we implemented the body force method into an unstructured LES solver. The implementation allows to move towards the computation of complex geometries with the integrated LES-RANS approach.

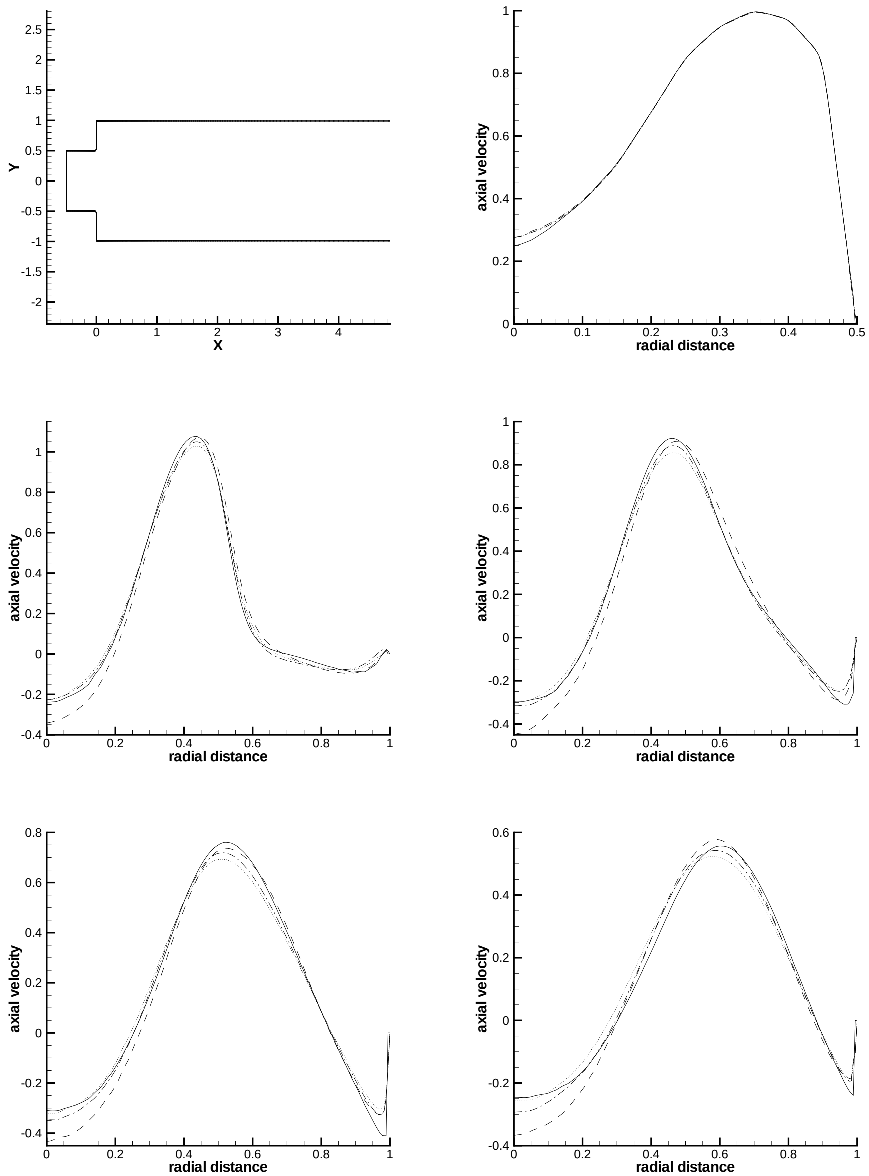

FIGURE 5. Influence of body force on flow development: axial velocity component Solid lines: reference solution using full geometry. Dashed lines: geometry truncated at x=1.5, no body force used. Dotted lines: geometry truncated at x=1.5 using body force scheme with trailing time window. Dash-dotted lines: geometry truncated at x=1.5 using body force scheme without trailing time window. Results are for x=-0.49, 0.25, 0.5,0.75 and 1.0, respectively (row major).

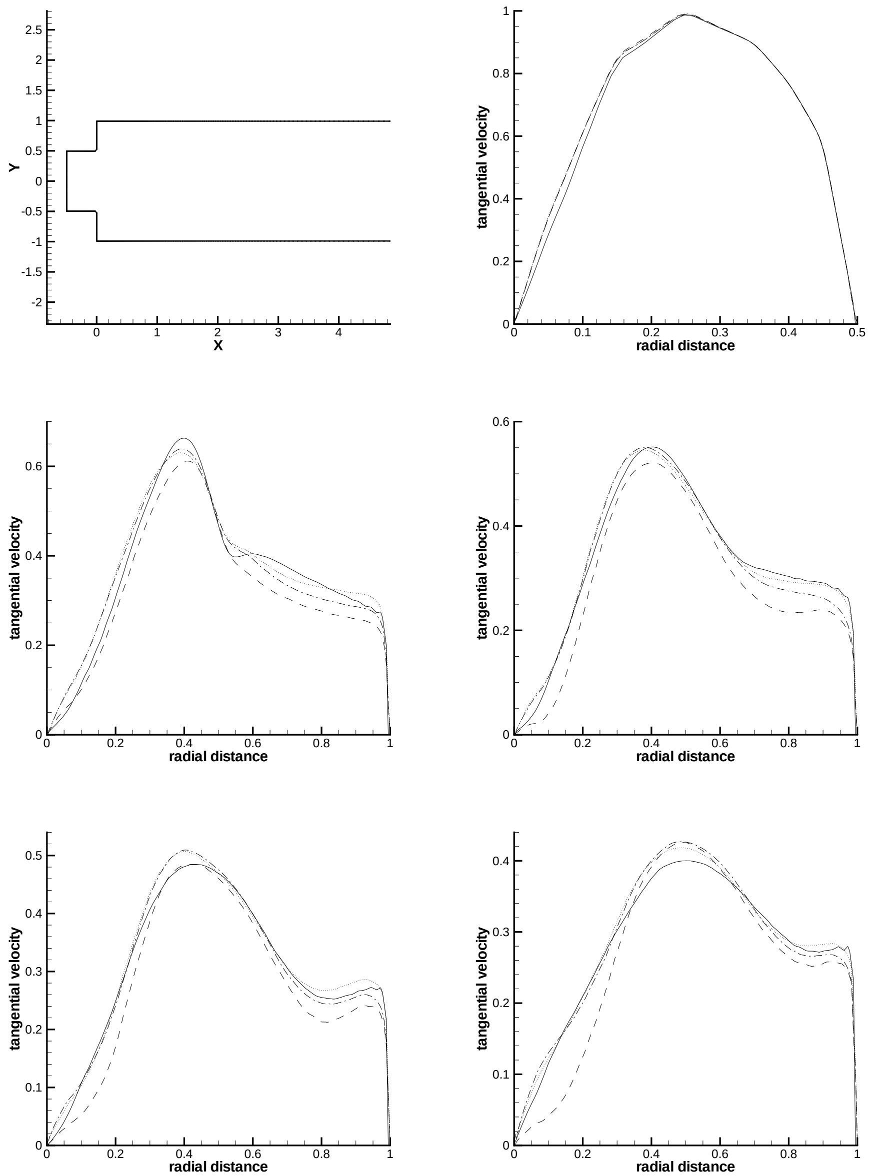

FIGURE 6. Influence of body force on flow development: azimuthal velocity component Solid lines: reference solution using full geometry. Dashed lines: geometry truncated at x=1.5, no body force used. Dotted lines: geometry truncated at x=1.5 using body force scheme with trailing time window. Dash-dotted lines: geometry truncated at x=1.5 using body force scheme without trailing time window. Results are for x=-0.49, 0.25, 0.5,0.75 and 1.0, respectively (row major).

These are important steps toward the use of integrated LES-RANS to applications of industrial relevance.

7. Acknowledgments

We wish to thank the US Department of Energy for the support under the ASC program.

We want to thank Dr. Frank Ham for the support using the LES flow solver CDP.

REFERENCES

AKSELVOLL, K., & MOIN, P. 1996 Large-eddy simulation of turbulent confined coannular jets. *J. of Fluid Mech.*, **315**, 387–411.

DELLENBACK, P. A., METZGER, D. E. & NEITZEL, G. P 1988 Measurements in turbulent swirling flow through an abrupt axisymmetric expansion. *AIAA J.*, **26**, 669-681.

DELLENBACK, P. A. 1986 *Heat transfer and velocity measurements in turbulent swirling flows through an abrupt axisymmetric expansion.* PhD thesis, Arizona State University.

GERMANO, M., PIOMELLI, U., MOIN, P. & CABOT, W., 1991 A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids* A **(3)**, 1760-1765.

HAM, F., APTE, S., IACCARINO, G., WU, X., HERRMANN, M., CONSTANTINESCU, G., MAHESH, K., MOIN, P. 2003 Unstructured LES of reacting multiphase flows in realistic gas turbine combustors. *CTR Annual Research Briefs*, pages 139–160, 2004. Center for Turbulence Research, Stanford.

MOIN, P., SQUIRES, K., CABOT, W. & LEE, S. 1991 A dynamic subgrid-scale model for compressible turbulence and scalar transport. *Phys. Fluids*, A **(3)**, 2746-2757.

MOIN, P., APTE, S. 2004 Large-eddy simulation of realistic gas turbine combustors. *AIAA Paper*, (AIAA 2004-0330), January 2004.

SCHLÜTER, J. U., PITSCH, H. 2001 Consistent boundary conditions for integrated LES/RANS simulations: LES outflow conditions. *CTR Annual Research Briefs*, pages 19–30, 2001. Center for Turbulence Research, Stanford.

SCHLÜTER, J. U., PITSCH, H., MOIN, P., 2002 Consistent boundary conditions for integrated LES/RANS simulations: LES outflow conditions. *AIAA paper* 2002-3121

SCHLÜTER, J., SHANKARAN, S., KIM, S., PITSCH, H., ALONSO, J. J., 2003 Towards multi-component analysis of gas turbines by CFD: integration of RANS and LES flow solvers. *ASME paper*, (ASME GT2003-38350), 2003. ASME Turbo Expo 2003, June 16-19, 2003, Atlanta, GA.

SCHLÜTER, J. U., WU, X., KIM, S., ALONSO, J. J., PITSCH, H. 2004A A framework for coupling Reynolds-averaged with large eddy simulations for gas turbine applications. *Journal of Fluids Engineering*, submitted, 2004.

SCHLÜTER, J. U., WU, X., KIM, S., ALONSO, J. J., PITSCH, H. 2004B Integrated RANS-LES computations of gas turbines: Compressor-diffuser. *AIAA Paper*, (AIAA 2004-0369), January 2004.

SCHLÜTER, J. U., WU, X., KIM, S., ALONSO, J. J., PITSCH, H. 2004C Coupled RANS-LES Computation of a Compressor and Combustor in a Gas Turbine Engine. *AIAA Paper*, (AIAA 2004-3417), July 2004.

Schlüter, J. U., Wu, X., Kim, S., Alonso, J. J., Pitsch, H. 2004d Integrated RANS-LES of a realistic compressor and combustor in a gas turbine engine *CTR Annual Research Briefs*, 2004. Center for Turbulence Research, Stanford.

Schlüter, J. U., Pitsch, H., Moin, P., 2004e Outflow conditions for integrated Large-Eddy simulation/Reynolds-averaged Navier-Stokes simulations. *AIAA J.* accepted, to appear 2004.

Pierce, C. D. & Moin, P. 1998 Method for generating equilibrium swirling inflow conditions. *AIAA J.*, **36**, 1325-1327.