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Large Eddy simulation for engineering applications

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Abstract

In the field of fluid engineering, controlling turbulent flows remains a crucial problem. This paper presents a basis of numerical methods and turbulence models for the large Eddy simulation. Simulation results include the unsteady analyses of complex flows, such as the vortex dynamics of turbulent jets subject to inlet perturbations and the reacting flow with flame propagation in a gas–turbine combustor flow. Applications employing large Eddy simulation are emerging as one of the most important aspects of the “Frontier Simulation Software for Industrial Science” project for the next generation of fluid dynamic design and development.

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Keywords: Numerical simulation; Computational fluid dynamics; Large Eddy simulation; Turbulence

1. Introduction

Among various fields of science and technology, contributions from computational science appear particularly promising in the 21st century as a basis for technology evolution, social life safety, and environmental conservation. However, additional effort is needed to develop next generation software for high performance computing. For continuing research and development in fluid dynamics, a new innovative technology that can adapt well to the strict requirements and worldwide standards posed by recent environmental and energy concerns is needed. For this purpose, design optimization has been investigated for a variety of complicated conditions to aid in the development of a key technology based on the studies of three-dimensional unsteady features in fluid flows. This technique will not only be used for fundamental research, but also for practical industrial applications. Recent innovations in computer
technology have allowed for remarkable advances in computer-aided engineering (CAE), which enables more realistic numerical simulation and visualization and can be applied to three-dimensional unsteady analyses of fluid flows in a detailed and straightforward manner. The “Frontier Simulation Software for Industrial Science (FSIS)” project was started at Institute of Industrial Science (IIS), The University of Tokyo in 2002 as a proposal to the IT-program organized by the Ministry of Education, Culture, Sports, Science and Technology (Kobayashi, 2002). As one of the research topics under the FSIS project, high-performance simulation software named “FrontFlow” is developed for the next generation of fluid dynamics simulations. Turbulence remains a challenging problem for current CAE technology because it cannot be solved using universal numerical methods at a practical accuracy and cost due to a highly non-linear and unsteady phenomenon.

Therefore, this project aims to develop a standard simulation method for unsteady turbulent phenomena based on large Eddy simulation (LES), in which different scales in the turbulence are decoupled. LES with hundreds of million grids produces a sufficiently accurate simulation of unsteady turbulent phenomena for the advanced digital design of fluid engineering. LES is also capable of predicting complex problems with turbulence; combustion and multiphase flows in energy equipment and flow noise and fluid-induced vibration on a vehicle, turbo machine and structures. The basic concept of the proposed LES code is illustrated in Fig. 1. This paper presents advanced LES coupling research with multi-scale physics and discusses some examples of the method applied to engineering problems.

2. Fundamentals of large Eddy simulation

2.1. Turbulence models for LES

The governing equations for incompressible flows are the Navier–Stokes and continuity equations given by

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_i \partial x_j},$$

(1)
\[ \frac{\partial u_i}{\partial x_i} = 0. \]  

Here, \( u_i \) is the velocity component in the \( x_i \) direction \((i = 1, 2, 3)\), \( p \) is the pressure divided by the density, \( \nu \) is the kinematic viscosity, and \( t \) is the time. The summation rule is assumed for repeated indices.

In the LES of turbulent flow, the spatial filter function, \( G(x; \bar{\Lambda}) \), is introduced to separate the resolved field from the full field as

\[ \bar{f}(x, t) = \int G(x - x'; \bar{\Lambda}) f(x', t) \, d^3 x'. \]  

When the filter size \( \bar{\Lambda} \) is chosen as the grid resolution size, the subgrid-scale (SGS) of the fluctuation is removed from the grid-scale (GS) represented by the filtered value \( \bar{f} \). The typical filter functions for LES are Gaussian, tophat and sharp cutoff filters (Leonard, 1974). The expressions for these filter functions in the physical and wavenumber spaces are

Gaussian filter:
\[
G(x; \bar{\Lambda}) = \sqrt{\frac{6}{\pi \cdot \bar{\Lambda}^2}} \exp \left( -\frac{6x^2}{\bar{\Lambda}^2} \right), \quad G(k; \bar{\Lambda}) = \exp \left( -\frac{(\bar{\Lambda}^2k)^2}{24} \right),
\]  

Top-hat filter:
\[
G(x; \bar{\Lambda}) = \begin{cases} 
\frac{1}{\bar{\Lambda}} & (|x| \leq \frac{\bar{\Lambda}}{2}), \\
0 & (|x| > \frac{\bar{\Lambda}}{2}), 
\end{cases} \quad G(k; \bar{\Lambda}) = \sin \left( \frac{\bar{\Lambda}k}{2} \right),
\]  

Sharp cutoff filter:
\[
G(x; \bar{\Lambda}) = \frac{\sin \left( \frac{\pi x}{\bar{\Lambda}} \right)}{\pi x}, \quad G(k; \bar{\Lambda}) = \begin{cases} 
1 & (|k| \leq \frac{\pi}{\bar{\Lambda}}), \\
0 & (|k| > \frac{\pi}{\bar{\Lambda}}),
\end{cases}
\]

where \( k \) is the wavenumber.

The Gaussian filter has the same smooth form in both physical and wavenumber spaces. The tophat filter exhibits sharp edges in the physical space, while the cutoff filter exhibits sharp edges in the wavenumber space. The cutoff filter is typically used with the spectral method. The Gaussian filter or the tophat filter is used with the finite difference scheme, which is generally applied to practical simulations. Since the numerical simulations for fluid flow including LES are obtained as flow fields on a finite number of grids, the accuracy of the equations is affected by an additional discrete filtering effect. In recent studies, the basic equations for LES have been obtained by filtering the velocity field after discretizing the governing equations (Carati et al., 2001; Gullbrand and Chow, 2003) as

\[
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial C_{ij}}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tilde{\tau}_{ij}}{\partial x_j}, \quad (5)
\]
where the turbulent stress is defined as $\tau_{ij} = \overline{u_i u_j} - C_{ij}$ and $C_{ij} = \overline{\tilde{u}_i \tilde{u}_j}$. $\tilde{f}$ denotes a variable $f$ on a grid, and its filtered value is $\overline{\tilde{f}}$. Precisely speaking, each term in the governing equations is affected differently by the discretization with finite differences. The turbulent stress can be divided into two parts as

$$
\tau_{ij} = \tilde{\tau}_{ij} + B_{ij}, \quad \tilde{\tau}_{ij} = \overline{u_i u_j} - \overline{\tilde{u}_i \tilde{u}_j}, \quad B_{ij} = \overline{\tilde{u}_i \tilde{u}_j} - \overline{\tilde{u}_i \tilde{u}_j}.
$$

(7)

While the SGS stress $\tilde{\tau}_{ij}$ depends on scales beyond the resolution domain and requires an SGS model, the resolved sub-filter-scale stress $B_{ij}$ can theoretically be estimated by deconvolution procedure (Domaradzki and Saiki, 1997; Stolz and Adams, 1999). Fig. 2 shows the schematic partition of the velocity spectrum $E(u)$ of the turbulence. Here, $k_g$ is the wavenumber corresponding to the grid size. The difference between $E(u)$ and $E(\tilde{u})$ indicates the filtering effect and the discrepancy between $E(u)$ and $E(\tilde{u})$ depicts the effect of the numerical error. The spectral method (corresponding to the sharp cutoff filter) offers the ideal resolution and $E(\tilde{u})$ lies on $E(u)$ at wavenumbers lower than $k_g$. Until recently, the effects of filtering and discretization were not clear. However, it becomes apparent that the computational results of the LES are highly dependent on both the SGS stress model and numerical discretization method. The author’s research group has focused on these LES issues, including SGS modeling, the LES numerical method, and its applications since 1980’s. Some of the LES research conducted by the author’s group is presented in this paper. Note that $\overline{\tilde{u}_i}$ is hereafter rewritten as $\tilde{u}_i$ for simplicity.

The most popular SGS model is the Smagorinsky eddy viscosity model:

$$
\tau_{ij}^* = -2\nu_t \tilde{S}_{ij}, \quad \nu_t = (C_s \bar{S})^2 |\overline{\tilde{S}}|, \quad |\overline{\tilde{S}}| = (2 \tilde{S}_{ij} \tilde{S}_{ij})^{1/2}, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right).
$$

(8)
The superscript * represents the trace-free operator, $\tau_{ij}^* = \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk}$. The under-bar ___ denotes a tensor and the bracket || indicates its norm. $\Lambda$ is the filter length and the model parameter $Cs$ should be optimized according to a type of turbulent flow field ($0.1 \leq Cs \leq 0.23$). The near-wall correction is also required, and the Van Driest type wall damping function, $f_{VD} = 1 - \exp(-y^+ / 25)$, is traditionally introduced as $\Lambda \rightarrow \Lambda f_{VD}$ ($y^+ = u_+ y / v$ is the wall normal coordinate and $u_+$ is the wall friction velocity). Morinishi and Kobayashi (1991) constructed a variable length scale Smagorinsky model based on an analytically derived formulation (Yoshizawa, 1989) as

$$Cs = Cs_0 \left( 1 + C_A \frac{D |\vec{S}|}{Dt} \right), \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j}. \quad (9)$$

The model constants in Eq. (9) vary depending on the kind of turbulent flow fields. The dynamic procedure introduced by Germano et al. (1991) makes it possible to optimize the model constants dynamically and to remove the wall-damping function requirement. The model constants are dynamically specified through the Germano identity, which describes the relationship between subgrid and subtest fields, in conjunction with the least square minimization technique developed by Lilly (1992). However, the dynamic Smagorinsky model has some drawbacks. In particular, the model exhibits a strong dependence on the grid resolution and numerical instability in practical LES simulations.

These drawbacks appear to be caused by the eddy-viscosity formulation of the Smagorinsky model,

$$v_1 \propto \ell^2 / \tau, \quad (10a)$$

where $\ell = \Lambda$ and $\tau = 1 / |\vec{S}|$ are the SGS length and time scales. Yoshizawa et al. (1996) reformulated the SGS eddy viscosity as

$$v_1 \propto \ell u, \quad (10b)$$

where $u = \sqrt{(\bar{u}_i - \bar{u}_i)^2}$ is the SGS velocity scale. Tsubokura (2001) also reformulated the viscosity as

$$v_1 \propto u^2 \tau. \quad (10c)$$

These reformulations reduced the strong grid dependence of the LES results for the dynamic Smagorinsky model with finite difference codes. Furthermore, the addition of the scale-similarity model improves the anisotropic representation of the SGS stress. The modification formulation of the dynamic two-parameter mixed SGS model proposed by Morinishi and Vasilyev (2001) is described by

$$\tau_{ij}^* = -2v_1 \bar{S}_{ij} + C_L (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j)^*, \quad (11)$$

where $C_L$ is a model parameter. The dynamic SGS models require an additional grid filtering operation. Taniguchi (1995) proposed an approximate filtering technique using either a Gaussian or tophat filter for the dynamic SGS model on a finite difference grid as

$$\hat{f}_i = \bar{f}_i + \frac{r^2}{24} (\bar{f}_{i+1} - \bar{f}_i + \bar{f}_{i-1}), \quad \gamma = \hat{\Lambda} / h, \quad (12)$$

where $\hat{\Lambda}$ is the length of the additional filter, and $h$ is the grid size. In the filtering formulation, the subscript indicates the grid location ($f_i = f(x_0 + i h)$). Numerical instability occurs in dynamic SGS models if a smoothing technique is not introduced. However, the smoothing technique makes it difficult to apply
LES to practical problems. To overcome this problem, a non-dynamic eddy viscosity SGS model was proposed by Yoshizawa et al. (2000) as

\[ v_t = C_{VS} f_w \Delta u, \quad f_w = 1 - \exp \left( \frac{-C_W u}{|S|} \right)^2, \]  

(13)

where \( C_{VS} \) and \( C_W \) are model parameters.

The non-dynamic SGS model is suitable not only for channel flow but also for separated flow fields, since the wall friction velocity is not used in the wall-damping function. Neither the existing models nor the SGS models mentioned above explicitly account for the discretization effect on the governing LES equation. Recently, Morinishi and Vasilyev (2002) proposed a new dynamic procedure that introduces a vector level identity, which takes the effect of the numerical error into consideration.

2.2. Numerical methods for LES

The unsteady, three-dimensional turbulent simulations including LES are much less tolerant of numerical dissipation because it selectively removes energy from the dynamically important small-scale eddies. For this reason, non-dissipative central-difference schemes or spectral methods are usually preferred for LES simulations. The spectral method in conjunction with a dealiasing operation offers ideal spatial resolution but is too difficult to apply to practical problems. One promising method for LES applications is the energy conservative central finite difference scheme for convection in a staggered grid, although only the second-order version is known (Harlow and Welch, 1965),

\[ \frac{\partial u_j u_i}{\partial x_j} \approx \frac{\delta_1 u_j^{1x_j} u_i^{1x_j}}{\delta_1 x_j}. \]  

(14)

Here, \( u_j^{1x_j} \) and \( \delta_n u / \delta_n x_j \) are the interpolation and difference operators, respectively, with stencil \( n \) acting on \( u \) in the \( x_j \) direction. In the staggered grid, velocity components and pressure are located on cell faces and the center of the control volume, respectively. The convection (14) conserves kinetic energy in the inviscid limit provided that the continuity equation is discretized at the pressure point as

\[ \frac{\partial u_i}{\partial x_i} \approx \frac{\delta_1 u_i}{\delta_1 x_i} = 0. \]  

(15)

This is due to the fact that the finite difference scheme

\[ u_i \frac{\partial u_j u_i}{\partial x_j} = \frac{\partial u_j (u_i u_i)/2}{\partial x_j} + \frac{1}{2} u_i u_i \left( \frac{\partial u_j}{\partial x_j} \right) \]  

(16)

preserves the analytical conservative property of the convection term in a discrete sense.

The reduction of the numerical error, especially in the convection term, is as important as the SGS stress closure in real LES simulations, as shown in Fig. 2. However, the truncation error of the second-order finite difference scheme is the same order as the SGS stress, and at least a fourth-order accurate discretization method is necessary for reliable LES simulations. Morinishi et al. (1998) proposed fourth- and higher-order energy conservative staggered finite difference schemes, and offered a useful tool for unsteady turbulent simulations like LES and direct numerical simulation (DNS). The fourth-order energy
Fig. 3. Mean velocity profile of turbulent channel flow at $Re_\tau = 395$. The simulations are done without the SGS model at a poor grid resolution. Computational region size, $(2\pi h, 2h, 2\pi h/3)$; Grid number (32, 64, 32). The dashed and solid lines, and the triangles represent the results of second- and fourth-order finite differential methods, and pseudo-spectral method, respectively.

Conservative finite difference scheme for the convection term and the accompanied continuity discretization are

$$\frac{\partial u_j u_i}{\partial x_j} \approx \frac{9}{8} \frac{\delta_1 u_j^{4th} u_i^{-1} x_j}{\delta_1 x_j} - \frac{1}{8} \frac{\delta_3 u_j^{4th} u_i^{-3} x_j}{\delta_3 x_j}, \quad u_j^{4th} x_i = \frac{9}{8} u_1 x_i - \frac{1}{8} u_3 x_i,$$

(17)

$$\frac{\partial u_i}{\partial x_i} \approx \frac{9}{8} \frac{\delta_1 u_i}{\delta_1 x_i} - \frac{1}{8} \frac{\delta_3 u_i}{\delta_3 x_i} = 0,$$

(18)

where the superscript 4th means that the interpolated value $u_j^{4th,x_i}$ has 4th-order accuracy.

Fig. 3 shows the computational results for the mean velocity profile of turbulent channel flow without the SGS model using different discretization methods. The Reynolds number $Re_\tau$ based on the friction velocity and channel half width is 395, and the simulations are carried out at a poor grid resolution. The differences between the pseudo-spectral and the finite difference methods indicate the numerical errors due to the finite differences (corresponding to the region of numerical error in Fig. 2). The result apparently indicates the advantage of the fourth-order scheme over the second-order one. The energy conservative finite difference scheme has recently been extended to cylindrical coordinates with an excellent pole treatment (Morinishi et al., 2004). In Morinishi et al. (1998), the existing finite difference schemes in regular, staggered and collocated grid systems were analyzed and their conservative properties were also estimated. Based on this study, Kogaki et al. (1999) constructed a finite difference code for LES for practical use. After specifying the grid correspondence between physical and computational space, $\zeta^i = \zeta^i (x_1, x_2, x_3)$ and $x_i = x_i (\zeta^1, \zeta^2, \zeta^3)$ for $i = 1, 2, 3$, and estimating $\zeta^j = \partial \zeta^j / \partial x_i$ and the Jacobian of the transformation, $J = \partial (x_1, x_2, x_3) / \partial (\zeta^1, \zeta^2, \zeta^3)$, the governing equations of the LES with the SGS
eddy viscosity model are written as

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{1}{J} \frac{\partial \bar{U}^j \bar{u}_i}{\partial \xi^j} = - \zeta_j \frac{\partial \bar{P}}{\partial \xi^j} + \frac{1}{J} \frac{\partial}{\partial \xi^j} \left[ J \zeta_k (v + v_t) \left( \zeta^j \frac{\partial \bar{u}_i}{\partial \xi^k} + \zeta^j \frac{\partial \bar{u}_k}{\partial \xi^j} \right) \right],$$

(19)

$$\frac{1}{J} \frac{\partial J U^j}{\partial \xi^j} = 0,$$

(20)

where $\bar{U}^j = \zeta^j \bar{u}_i$ is the GS contravariant velocity component. In Eqs. (19) and (20), and related sentences, superscript and subscript indicate covariant and contravariant components on the curvilinear coordinates, respectively. The code is available for boundary fitted curvilinear structured grids. In order to analyze more complex flow geometries, finite element LES codes were also constructed for structured and unstructured grids by Kobayashi et al. (1994) and Tsubokura et al. (1995), respectively. The filtering technique for the finite element grid was proposed by Oshima et al. (1996).

2.3. Analysis of eddy structures in turbulence

The key characteristic of DNS and LES is that they can reproduce unsteady and three-dimensional turbulent eddies, contrary to the Reynolds-averaged Navier–Stokes (RANS) modeling in which only the mean values are obtained. In this section, the common problems encountered when analyzing three-dimensional turbulent eddy structures using DNS and LES is discussed. Turbulence contains various eddies with a wide range of length scales. Small eddies are more isotropic and their role in heat and mass transfer is only diffusive, while larger eddies bear the characteristic feature of the flow depending on the boundary conditions. Consequently, heat and mass transfer due to small eddies can be assessed rather easily because this physical process is supposed to be similar to molecular transport, while turbulence transport by larger eddies is more difficult to estimate a priori. This feature is important for LES turbulence modeling because it is still difficult to capture the three-dimensional small eddy structures precisely by experimental measurements in most practical cases.

As a typical case, the eddy structures of plane and round impinging turbulent jets (Tsubokura et al., 2003), in which coherent turbulent eddies play an important role in the turbulent heat and mass transfer processes, are analyzed. In fact, impinging jet flow is of great interest in industrial applications because it is often utilized to heat, cool or dry materials. This technique is highly utilized during material processing because the flow results in high heat and mass conductivity in the stagnation region. For the plane impinging jet case, Sutera et al. (1963,1965) proposed that the stretched vortex aligned parallel to the wall plays an important role in the heat transfer process. Yokobori et al. (1983) experimentally studied the plane impinging jet using a flow visualization technique and observed counter-rotating vortex pairs along the wall. The temperature distribution was measured and it was discovered that the high heat transfer rate is related to these counter-rotating twin vortices. Sakakibara et al. (2001) further studied the plane impinging jet using simultaneous measurements of velocity and temperature fields using digital particle image velocimetry (PIV) and laser-induced fluorescence. The results indicated that the counter-rotating vortex pairs are convected from an upstream location and stretched in the vicinity of the wall. These studies suggest the possibility of controlling the heat transfer on the stagnation by varying the eddy structures. In contrast to the plane jet, few studies have been conducted on the eddy structures in the stagnation region of a round impinging jet until recently (e.g., Satake and Kunugi, 1998). In this study,
attention is focused on the differences in the eddy structures of plane and round jets excited at the inlet, which may shed light on the possibility of heat transfer in the context of turbulent eddy control.

In both plane and round jet cases, the flat plate is mounted 10D away from the nozzle exit, where D is the width or diameter of the nozzles, and the flow impinges in a direction normal to the plate. The origin of the plane jet case is located at the middle of the stagnation line on the plate, where x, y, and z represent the transverse, wall-normal and spanwise directions in the Cartesian coordinate system, respectively. The origin of the round jet case is located at the stagnation point, where y is the axial (wall-normal), r is the radial and θ is the azimuthal direction in the cylindrical coordinate system. The total grid number is $N_x \times N_y \times N_z = 400 \times 100 \times 96$ in plane jet and $N_y \times N_r \times N_θ = 100 \times 150 \times 96$ in round jet.

The governing equations are given by the incompressible Navier–Stokes and continuity equations without any explicit turbulent models. In addition to these fluid motion equations, the transport equation for a passive scalar is also solved in order to investigate dispersion and mixing mechanisms, as well as to visualize the flow field (used as a virtual dye in numerical visualization). The governing equations are discretized using a finite difference scheme. All space derivatives are discretized using second-order central differences, so no artificial viscosity or upwind type schemes are employed for the convective term, while fully explicit time marching is conducted using a third-order Runge–Kutta scheme. The MAC method is adopted to address the coupling between the velocity and pressure. The resulting Poisson equation for pressure is solved by FFT for the statistically homogeneous direction, i.e. the spanwise or azimuthal direction, while the incomplete Cholesky decomposed conjugant gradient method is adopted for the other two inhomogeneous directions.

Transition or the evolution of jets is strongly affected by the inlet condition at the nozzle exit. In the present study, nozzle flows are not explicitly solved, but treated by prescribing an assumed velocity profile at the nozzle exit as the inlet boundary condition. A disturbance is artificially added to the assumed mean velocity profile on the nozzle exit plane in the form of an uniform sinusoidal profile in the streamwise direction at a Strouhal number $S_t = 0.4$ normalized by the inlet velocity $V_0$ and D, which is close to the natural unstable mode of the shear-layer for the present plane and round impinging jets.

In addition to the streamwise disturbance, a spatial periodic disturbance is added in the spanwise or azimuthal direction. This disturbance is a single sinusoidal wave with a wavelength of $\lambda$. The amplitudes of both the unsteady and the spatial disturbances are 0.5% of $V_0$. It should be noted that these disturbances are imposed only on the streamwise velocity. The number of waves in the spanwise or the azimuthal direction is varied to investigate how the disturbance affects the structures in the stagnation region of the impinging jets. Three wavenumbers, 3, 4 and 6, are considered. Because both the spanwise length of the plane jet and the circumference of the round jet are set equal to $\pi D$ at the nozzle exit, the imposed wavelengths of both plane and round jets are $\lambda = \pi D/3, \pi D/4, \pi D/6$, respectively. The resulting inlet profiles are given by

$$V(z, \theta, t)/V_0 = -\{1 - (2z/D)^8\} + 0.005 \sin(2\pi S_t t) + 0.005 \sin(2\pi z/\lambda_z), \quad (21a)$$

$$V(r, \theta, t)/V_0 = -\{1 - (2r/D)^8\} + 0.005 \sin(2\pi S_t t) + 0.005 \sin\left(\frac{\pi D}{\lambda_0} \theta\right). \quad (21b)$$

The Reynolds numbers $Re$, based on the width or diameter of the nozzle and the inlet velocity at the nozzle, results in 2000.
A convective boundary condition is adopted at the outflow plane while periodic conditions are used in the spanwise direction of the plane jet. A no-slip condition is applied at the wall and a passive scalar is set to unity at the nozzle outlet, while the normal gradient of the scalar is set to zero on the wall.

Figs. 4(a)–(f) show the instantaneous eddy structures and the scalar distribution images for several \((x, z)\) cross planes of a plane jet for different spanwise disturbances. As can be clearly seen, two-dimensional eddies roll up near the inlet, and exhibit a three-dimensional structure due to the growth of the spanwise disturbance as the flow evolves downstream. The scalar distribution in each image also shows that the development of the spanwise disturbance during the transition is strongly affected by the inlet spanwise forcing and that the wavenumber of the disturbances is exactly the same as the value imposed at the inlet (three, four and six waves from the left to the right).

The round impinging jet, on the other hand, follows a different tendency in regard to the development of the azimuthal disturbance, as shown in Fig. 5. In general, the transition process is the same as for the plane jet in the sense that eddies roll up around \(y/D = 6\) and a vortex ring develops three-dimensional structures as the flow moves downstream. However, the stability of the imposed azimuthal disturbance is different from the plane jet. When three or six waves are imposed at the inlet of the round jet, the scalar images close to the impinging plate show that six waves are produced for both cases (the same star-like scalar distributions containing six ridges can be seen in both (A) and (C)). However, when four waves
were imposed at the inlet, the disturbance was ultimately suppressed, as seen in (B). Due to the different sensitivities of the roll-up eddies to the azimuthal disturbance, the breakdown of the roll-up eddies in the six-wave case occurs a little closer to the inlet than the three-wave case. This tendency is more evident in the four-wave case, where a distinct development is not evident, and even after the impingement, the flow field is still somehow organized.

As before, all cases of the plane jet show a similar transition regardless of the spanwise disturbances unlike the round jet cases. Thus, in regard to the spanwise or azimuthal instability of a plane or a round impinging jet, the round jet has definite instability modes at $\lambda_0/\pi D = \frac{1}{3}$, while the plane jet shows a similar sensitivity to all tested modes and the three disturbances with wavelengths of $\lambda_x/\pi D = \frac{1}{3}$, $\frac{1}{4}$ and $\frac{1}{6}$ at the inlet are equally developed.

Another important difference in eddy structures is found in the stagnation region. To extract the organized eddy structures arising directly from the inlet temporal disturbance, we apply a phase-averaging technique. The averaging period is defined by a Kelvin–Helmholz instability wave for the inlet jet that is imposed as the inlet boundary condition. Fig. 6 displays the phase-averaged vorticity $\omega_x$ in the stagnation region of the plane jet. This figure shows the notable structures of the plane jet in the stagnation region, which are the elongated twin vortices in the transverse direction ($x$-direction). It is clear from these figures that the arrangement of these twin vortices in the stagnation region strongly depends on the inlet disturbance, and the number of pairs of these vortices is exactly the same as those for the spanwise disturbance wave inlet condition. This is the organized structure that was observed both experimentally.
and numerically in a previous study (e.g., Yokobori et al., 1983; Sakakibara et al., 2001; Tsubokura et al., 1998). In the round jets, twin vortices in the transverse direction ($r$-direction) in the stagnation region could not be identified.
3. LES of turbulent combustion flows

3.1. Modeling of turbulent combustion flows

This section introduces the LES of turbulent combustion flow that is typical complex problems in engineering applications. Conventional computer codes that use RANS approaches, such as the $k-\varepsilon$ model or the Reynolds stress model, have been widely used to design combustors. These approaches can predict relatively steady flow fields with sufficient accuracy and only a small computational cost. However, designers of combustion devices that use methods based on the RANS model face difficulties when solving the multi-scale physics and unsteady dynamics in turbulent combustion flows. DNS has been used to reveal fundamental processes of the combustion flows. However, its application is limited to microscopic phenomena. LES is an alternative approach that can directly analyze unsteady and complex interactions between turbulence and combustion in a practical object by using a model only for microscopic phenomena. The LES approach has been employed to predict a premixed turbulent flame in fundamental studies by previous researchers (Im and Lund, 1997; Park et al., 2000) and for the practical application of combustion flows (Taniguchi et al., 1999; Cannon et al., 2001). These studies have shown that the LES approach can be effectively applied to a thin laminar flamelet, which is a common model for turbulent combustion flows.

The aim of this section is to describe a numerical prediction for turbulent combustion flows of the engineering design using LES. In order to validate the numerical methods and models for a practical case of turbulent premixed combustion, an LES is designed and applied to the practical flow in a gas turbine system. Flame propagation and its interaction with turbulence fluctuation are also analyzed.

The turbulent premixed combustion is modeled using the laminar flamelet concept (Menon, 1992). This concept assumes that the turbulent flame is infinitely thin compared to the size of the turbulent structures and that it can be modeled by the motion of a flame surface separating unburnt and burnt gases with a laminar combustion speed $S_L$. The state of the flame propagation in LES is defined by the spatially filtered equation with index scalar $G$,

$$\frac{\partial G}{\partial t} + \frac{\partial u_j G}{\partial x_j} = S_L |\nabla G| - \frac{\partial}{\partial x_j} (u_j G - u_j G).$$  \hfill (22)

In this equation, $G$ increases from 0 in the unburned region to 1 in the burned region through the flame front. The flame position is assigned to the isosurface $G = G_0$, where $G_0$ denotes the initial flame position. The laminar flame speed $S_L$ generally depends on the “mixture fraction” $\xi$ (i.e. $S_L = S_L(\xi)$). The mixture fraction is defined as a mass fraction of an atom in the mixture gas normalized by the difference between those fractions in fuel gas and oxidizer gas. The governing equation of $\xi$ is also solved in addition to that of $G$.

The first term on the right-hand side of Eq. (22) cannot be calculated using only the GS solution in LES. When the turbulent combustion speed $S_T$ is introduced to evaluate the flame front acceleration in turbulence, that term is modeled as

$$S_L |\nabla G| = S_T |\nabla G|.$$  \hfill (23)
Here, the turbulent combustion speed $S_T$ is estimated by Yakhot’s model (1988) as

$$\frac{S_T}{S_L} = \exp \left[ \left( \frac{u'}{S_L} \right)^2 / \left( \frac{S_T}{S_L} \right)^2 \right], \quad u' = c_t \Delta |\overline{S}|,$$

where the SGS fluctuation $u'$ is evaluated by the LES filter with width $\Delta$ and strain rate level $|\overline{S}|$, based on the dimensional analysis under isotropic turbulence conditions. The parameter $C_t$ is set to be 0.15 in this study.

### 3.2. LES of premixed turbulent flame

The first example is the combustion flow behind a backward facing step (Park et al., 2000). This type of flow is a common test case for separated flow and it is a simplified model of the typical diffuser combustor for a gas turbine. Here, corresponding to the experiment performed by Pitz and Daily (1983), a propane–air premixed flow at an equivalence ratio $\phi = 0.57$ is introduced with inlet conditions of 13 m/s, 293 K and 1 atm pressure, and the bulk Reynolds number for the reacting condition is 22,100. The equivalence ratio $\phi$ is defined as a fuel-air mass ratio of the premixed gas condition normalized by that in the stoichiometric condition. The computational domain shown in Fig. 7 is divided into a Cartesian grid containing $247 \times 48 \times 20$ points in the $x$, $y$ and $z$ directions, respectively. The Smagorinsky model is employed in the LES momentum equation, while the turbulent flame propagation is simulated using the filtered $G$-equation (22) described in Section 3.1. The numerical methods are basically the same as those in Section 2.3.

Fig. 8 shows instantaneous iso-surfaces of streamwise velocity $u = 0$ for the reacting (right) and non-reacting (left) flows. The recirculation zone for each case is located on the underside of the iso-surface behind the backward facing step. The contours of the spanwise vorticity $\overline{\omega_z}$ on the center-plane are also displayed in Fig. 8. In the reacting case, the length of the recirculation zone is shorter and the maximum reverse velocity is larger due to the expansion of hot combustion gas and its higher kinetic viscosity. The LES combustion model successfully predicts these features; the predicted maximum reverse velocity $0.42 U_0$ and the length of the recirculation zone $4.4h$, agree well with those of the experimental data, which are $0.44 U_0$ and $4.5h$, respectively. The vortices gradually grow and move downstream at nearly the same convective velocity. In the reacting case, the velocity fluctuation and vorticity generally decrease, and their scales become smaller in the recirculation zone.
Fig. 8. The instantaneous iso-surface of streamwise velocity $u = 0$ and the contours of the spanwise vorticity on the center-plane for the reacting (right) and non-reacting (left) flows.

Fig. 9. Instantaneous contours of the normalized temperature (left) and reaction rate (right) on the center-plane.

Fig. 10. Time-averaged profiles of (a) streamwise velocity and (b) turbulent intensity at $x/h = 3$ and (c) temperature at $x/h = 3.5$. Lines and symbols represent the LES and experimental results, respectively, with black denoting the non-reacting case and red denoting the reacting case.

Fig. 9 shows the instantaneous temperature and reacting rate $\bar{\rho}_u S_T |\nabla \bar{G}|$ distributions on the center-plane. In the reacting case, the incoming fluid contains cold premixed reactants (293 K) that mix with the hot combustion products in the shear layer behind the step. Heat releases generally occur in the large-scale structures that form in the shear layer entraining cold reactants and hot products. Fig. 10 shows time-averaged profiles of the streamwise velocity, turbulent intensity and temperature in the section crossing
Fig. 11. Sequential series of instantaneous temperature and streamline from the LES of flame; time interval is 9.3 ms each from (a) to (h). Lines denote the streamlines, and red and blue colors indicate the burnt ($G = 1$) and unburnt gas ($G = 0$), respectively.

the recirculation zone. Here, the SGS component is assumed to be small enough to neglect its effect on the turbulent intensity. For both the reacting and non-reacting cases, the LES profiles agree well with the experimental data.

For better understanding of the flame propagation development process, a sequential series of flame snapshots are illustrated in Fig. 11. Calculations of the combustion flow are started from a fully developed non-reacting turbulent flow. Ignition is given by $G = 1$ at the backward facing step wall and $G = 0$ is assigned at all other regions as the initial combustion conditions in Fig. 11(a). The snapshots are captured every 9.3 ms from Figs. 11(a)–(h), and the premixed gas passed three-time length of the test combustor rig over a total of 0.07 s. Development of the vortices in the initial stages of the mixing layer is clearly evident, and they appear similar to the vortices of the reacting flow. The coalescence of eddies in the reacting flow can be seen. These observations suggest that heat release, which results in the expansion and increase in kinetic viscosity of the gas mixture in the mixing layer, does not considerably affect the vortex shedding behind the step.

3.3. LES of gas–turbine combustor flow

In order to validate the LES for an engineering problem, it is applied to a gas–turbine combustor flow of an axially staged annular combustor (Kobayashi, 2002; Tominaga et al., 2003), which was investigated experimentally by Tsuru et al. (2002). Recently, lean premixed combustion has become a key technology in the design of gas turbine combustors because it reduces harmful emissions, such as $\text{NO}_x$, with high cycle efficiency. Lean premixed combustion, however, has some problems including combustion oscillation or blowout, especially during power setting changes. These difficulties can be avoided by employing staged combustor geometry and controlling the output with a number of combustion areas. Efforts to counter the difficulties of lean premixed combustion require an understanding of the physics of a combustor. In
LES, most of turbulent diffusion effects, which often characterize the flow and affect flame propagation, should be precisely calculated as the GS components.

The model combustor built for the experiment is shown in Fig. 12. This test piece is a three-sector cutout model of a staged annular combustor that contains a total of 16 sectors. The pilot flame exists in the inner pilot stage and propagates to the outer main stage when a power setting is shifted to a higher level. The pilot nozzle has a double-swirler in order to generate a recirculation zone and to maintain the pilot flame. The main nozzle contains six twisting tubes in which the fuel and air are premixed. To protect the liner wall from hot burnt gases, a film-cooling method is used to lower the surface temperature. In the experiment, methane gas is chosen as the fuel, in light of the fact that it is difficult to predict combustion with liquid fuel spray. The premixed gas is pre-heated to 623 K in the combustion flow experiment. In the non-combustion flow experiment, the velocity distribution is measured by hot-wire anemometry, which employs an X-type probe to measure the axial and the circumferential velocity components simultaneously. In Fig. 12, \( z \), \( r \) and \( \theta \) represent the axial, radial, and circumferential coordinates, respectively. These are non-dimensionalized with regard to \( Z = 257 \text{ mm} \) (the total length of the liner), \( R = 382.5 \text{ mm} \) (the maximum radius of the outer liner), and \( \Theta = 22.5^\circ \) (the center angle of a sector), respectively.

In order to investigate the limitation of flame propagation from the pilot stage to the main stage, the equivalence ratio \( \phi_m \) at the exit of the main nozzle is measured when flame propagation occurs. The measurement procedure for \( \phi_m \) is as follows. First, a given amount of fuel is supplied only to the pilot nozzle. Then, after a stable flame is formed in the pilot stage, the fuel supply to the main nozzles is initiated and the amount is gradually increased to propagate the flame to the main stage. Finally, the igniting value of \( \phi_m \) is determined by measuring the value at the moment of flame propagation, which is detected as a sudden temperature rise of more than 300 K. The temperature is monitored by a thermocouple positioned near the exit of the main nozzles. This procedure is carried out several times for each value of \( \phi_p \), which represents the equivalence ratio at the exit of the pilot nozzle. The results are shown in Fig. 13. It should be noted that the igniting values \( \phi_m \) exhibit variations among several trials with the same \( \phi_p \) due to measurement errors and the instability of the flame propagation phenomenon.
In the present study, the computational domain is defined as a single sector of the combustor. The grid resolutions are $\Delta z = 0.00197Z \sim 0.021Z$, $\Delta r = 0.00564R$, and $\Delta \theta = 0.0167\theta$. The grid widths in the $r$ and $\theta$ directions correspond to about a 30th of the pilot nozzle diameter. This resolution corresponds to approximately 590,000 grid points. Assuming circumferential periodicity, we can generate the entire annular combustor geometry. The inlet velocity distribution from the pilot nozzle is determined using experimental results obtained by a stereo-PIV system at the nozzle exit. The premixed gas exiting the main nozzle is assumed to have a uniform velocity distribution. The liner wall boundaries, which are cooled by airflow through the cooling slots, are modeled as free-slip walls. A convective boundary condition is applied to the outlet boundary.

The flow settings for the calculations listed in Table 1 are the same as the physical conditions of the referenced experiment, except for the equivalence ratio. The fuel equivalence ratios for the flame propagation simulations are fixed in the two cases. In the non-reacting case experiment, flow characteristics are measured under room conditions, while the inlet flows in all calculations are pre-heated to obtain the same Reynolds number for easier comparison between the non-reacting and reacting cases.

In the calculations, LES with the G-equation for the flamelet model and the transport equation for the mixture fraction $\xi$ are conducted simultaneously. The governing equations are spatially discretized.
The LES for the non-combustion turbulent flow is first discussed. **Fig. 14** displays a three-dimensional view of the instantaneous distributions of the axial velocity in three sections. The predicted time-averaged velocity profiles on the centerlines of the sections are also compared with the experimental data in **Figs. 15 and 16**. The averaged values in the LES calculation are evaluated over 15,000 time-steps (30 ms). In the pilot stage shown in **Fig. 15**, the recirculation zone generated by the strong swirl is predicted as a negative value of axial velocity due to a gradient of the circumferential velocity. The LES results based on the LES code with a Boundary Fitted Coordinate scheme (Kogaki et al., 1999), which was coded in-house and well parallelized. A second-order central differential scheme was chosen, except for the convection terms of the scalars $G$ and $\xi$ where the QUICK scheme was applied to minimize numerical instability. The algorithm for time advancement is a fractional step method with a second-order Adams–Bashforth scheme and Crank–Nicolson scheme for the convection terms and diffusion terms, respectively.
agree well with the experimental data. In the main stage in Fig. 16, a weak recirculation is formed in the center of the twisted arrangement of the six tubes composing the main nozzle. The jets from the main nozzle produce a steep velocity gradient at the boundary between the pilot and main stages. The recirculation zone at the center of the jets is not observed clearly in the experimental data, although it has been predicted numerically for $r/R = 0.84 \sim 0.92$. The LES calculations predict a swirl flow at the same position. Because the inlet flows from the main nozzle are assumed to be steady and uniform, under-estimation of turbulent diffusion of the fluid momentum occurs, causing the over-estimation of the recirculation zone length and strength. The predicted value in the periodic one-sector model is relatively close to the experimental results for the practical evaluation of the mixing process in the pilot and main combustion stages.

Next, the reacting flow simulation is investigated using the $G$-equation flamelet model. The procedure for the LES calculation is as follows. First, the non-reacting flow is calculated to obtain a well-developed flow field and mixture fraction distribution, which is used as the initial conditions for the reacting case calculation. Scalar $G$ is defined as 0 (unburnt) at the inlet and wall boundary. $G$ is initially set to zero everywhere except for a small region behind the pilot fuel nozzle, where $G = 1$ (burnt) is set as the ignition point. Starting with these initial conditions, the $G$-equation calculations are conducted for the two fuel equivalence ratio cases described in Table 1 and plotted in Fig. 13. The experimental results reveal that flame propagation from the pilot stage to the main stage does not occur in the case of $\phi_m = 0.25$ and $\phi_p = 0.7$ (Case 1), but does occur in the case of $\phi_m = 0.6$ and $\phi_p = 0.7$ (Case 2).

In Fig. 17, the time evolutions of scalar $G$ on the central surface of the sector are illustrated at 4 ms intervals. The pilot stage is filled with burnt gas at 8 ms (4000 time-steps) after ignition. Because the mixture fraction equation predicts that the pilot gas fills the pilot stage, the flame behaviors in the stage are dominated by the pilot gas equivalence ratio $\phi_p$, which defines the flame propagation speed. Thus, the $G$ distributions indicating the flame front are almost the same for both fuel ratio cases with the same $\phi_p$. The flame fully develops into the main stage at 20 ms (10,000 time-steps) after ignition. The flames propagate into the main stage along two pathways. In one path, the flame propagates back from the downstream through the center of the swirl flow in the main stage. In the other path, a flame travels around the main nozzle jets, and then moves through the center of the main nozzle outlet between the twisting jets. The latter flame is held in the main stage recirculation zone.
In the richer fuel Case 2 ($\phi_m = 0.6$), the downstream flame merges with the flame that remains in the recirculation zone and then spreads stably throughout the whole sector. On the other hand, in leaner fuel Case 1 ($\phi_m = 0.25$), the burnt downstream gas also reaches the main stage recirculation zone, although it exists only intermittently due to instability of the flame. The results for Case 2 correlates well with the experimental data in the shaded area of Fig. 13. In this simulation, the predicted lean limit of the flame propagation to the main stage is smaller than the observed limitation in the experiments. In Case 2, the $G$ distribution in the center of the six main jets is not steep because the local burning velocity is slow compared to the turbulent velocity fluctuation. It is suspected that, in this region, the $G$ distribution represents the mixture of burnt and unburnt gases rather than the thin flame propagation. To predict the limit for the flame propagation with a higher accuracy, the $G$-equation model should be extended to include such a condition.

Fig. 18 shows the flame surface structures at 8 and 20 ms after the start of the reacting calculations for Case 2 ($\phi_m = 0.6$) and allows for the visualization of the flame propagation. The flame ignited in the
pilot stage spreads with a swirling flow. It propagates from the lower edge of the main fuel nozzle exit and finally forms a corn-shaped flame on the surfaces of the main stage jets.

These results indicate the capability of LES for the design of flame limit conditions of premixed combustion with a non-uniform fuel mixture rate in a staged combustor. The flame propagation mechanism can be simulated in the stable combustion cases detailed in this study. However, it should be noted that the incompressible flow and simplified boundary condition assumptions in this study cause numerical errors that could affect the prediction of mass and heat exchanges at the boundaries of the pilot and main stages. These assumptions could also lead to an inaccurate prediction of flame features, especially in Case 1 near the flammability limit condition. For a more precise and reliable prediction, the accuracy of flamelet models in lean burn turbulent flame should be improved, which is still an important problem. A database generated by direct numerical simulations considering accurate chemical reactions should be constructed to investigate advanced modeling.

4. Concluding remarks

The LES has been developed as a standard numerical method for unsteady turbulent phenomena. This paper has presented recent advances in the numerical methods and turbulence models for the LES and its related applications. In engineering fields, however, it is difficult to apply the LES to practical problems due to a shortage of software resources and validation studies compared to the Reynolds averaged approach that is widely accepted in engineering research and design facilities. In order to overcome such problems, a fundamental investigation of LES is necessary, especially for the accurate numerical methods and turbulence modeling of multi-scale and multi-physics problems. Applying these methods to practical engineering problems is also an important aspect of validating the LES. Frontier Simulation Software, which is available to the public, is expected to support researchers and engineers both in science and in industry. The software “FrontFlow” developed by the FSIS project is available at http://www.fsis.iis.u-tokyo.ac.jp/. LES research is expected to contribute to the advancement of computational fluid dynamics within the next generation.

References


