Practical Quality Measures for Large-Eddy Simulation

S. E. Gant

Health and Safety Laboratory (HSL), Harpur Hill, Buxton, Derbyshire, UK
simon.gant@hsl.gov.uk

Large-Eddy Simulation (LES), Detached-Eddy Simulation (DES) and Scale-Adaptive Simulation (SAS) models are increasingly being used as engineering tools to predict complex flows where reference DNS or experimental data is not available. Frequently, the flow has not been studied previously and the required grid resolution is unknown. Industrial users studying these flows tend to be using commercial CFD codes and do not usually have access to high-performance computing facilities, making systematic grid-dependence studies unfeasible. There is a risk therefore that LES, DES and SAS simulations will be performed using overly coarse grids which may lead to unreliable predictions.

The present work surveys a number of practical techniques that provide a means of assessing the quality of the grid resolution. To examine the usefulness of these techniques, a choked gas release in a ventilated room is examined using DES and SAS. The grid resolution measures indicate that overall the grids used are relatively coarse. Both DES and SAS models are found to be in poor agreement with experimental data and show greater grid sensitivity compared to RANS results using the SST model. The work highlights the need for grid-dependence studies and the dangers of using coarse grids.

1 Introduction

There has been a steady increase in the use of LES for safety related studies in recent years. This has particularly been the case in the fire safety industry, largely due to the increasing popularity of the Fire Dynamics Simulator freeware [1]. A recent report by the OECD [2] has also recommended that LES is used in assessing nuclear reactor safety. In view of the current and future use of LES in safety critical applications there is a need for practical advice for CFD users on quality and trust issues with LES.

2 Grid Resolution Measures

A number of techniques have been suggested previously to assess the grid resolution in LES. Following Celik *et al.* [3], these can be classified into four groups: rules of thumb, techniques based on prior RANS results, single-grid estimators and multi-grid estimators.

Assessing the grid resolution using a RANS simulation prior to running a full LES has significant advantages since the computer runtime of a RANS simulation is typically an order of magnitude less than the equivalent LES. The RANS results can be used to examine the ratio of the filter width, Δ, to the integral turbulence length scale, $l_I = k^{3/2}/\varepsilon$. Recommended values are for the ratio l_I/Δ to be above 12 [4, 5]. Prior RANS simulations can also be used to assess near-wall cell sizes in terms of wall units.

Single-grid estimators include the ratio of the SGS to the laminar viscosity (ν_t/ν), the Relative Effective Viscosity Index [3], the ratio of the cell size to the Taylor microscale [6], the Subgrid Activity Parameter [7], the ratio of resolved to the total turbulent kinetic energy, k_{res}/k_{tot}, and analysis of power spectra. Recommended values of these parameters and examples of their use in the literature are given by Gant [8].

Multi-grid estimators include the "Index of Quality", LES_IQ_k of Celik *et al.* [9] and the systematic grid and model variation approach of Klein [10]. The former is based on Richardson extrapolation on the resolved turbulent kinetic energy, while the latter involves running three LES calculations: a standard LES, a coarse-grid LES and an LES with the SGS model constant modified.

Each of the above grid resolution measures has advantages and limitations. The RANS-based techniques are reliant upon the accuracy of the RANS model which may be a limiting factor in massively separated flows, for example. If the flow involves regions that are laminar, the turbulent length scale ratios from RANS simulations also become meaningless indicators. Celik *et al.* [9] noted that in most applied LES studies the turbulent viscosity is significantly larger than the molecular viscosity ($\nu_t \gg \nu$), and the subgrid activity parameter will therefore nearly always be close to unity. The fundamental problem with methods involving the resolved turbulent kinetic energy is that whereas k_{res} might be expected to increase as the grid is refined, it has been shown in mixing layers, jets and wakes [9, 10] that k_{res} can actually decrease. This implies that the resolved turbulent kinetic energy is not a reliable indicator of grid resolution. A number of the above approaches do not account for the numerical dissipation which in many situations is of the same order or even larger than the modelled dissipation. Turbulence spectra cannot easily be plotted over the entire flow field to produce, for example, contour plots of grid resolution quality. Furthermore, the slope of the concentration or temperature spectra is modified in buoyant flows, and in low Reynolds number flows a distinct inertial subrange may not exist. Finally, Brandt [11] has shown that multi-grid approaches based on Richardson extrapolation can produce misleading results due to the grid resolution not being within the asymptotic range.

3 Application

A continuous jet of methane gas released into a ventilated enclosure is modelled. The configuration was previously examined by HSL to assess the implications of new hazardous area classification legislation. The main interest in studying the flow is to predict the size of the flammable gas cloud. The room has internal dimensions $4 \times 4 \times 2.92$ m with two ventilation inlets and two outlets. The ventilation rate is 12 ach and the gas is released in one corner of the room at a rate of 0.86 g/s. A description of the experiments undertaken for this work is given by Ivings *et al.* [12].

Four different turbulence treatments are tested: steady RANS, unsteady RANS, SAS and DES. LES calculations could not be performed because of the nature of the high-speed jet flow. The steady and unsteady RANS calculations used the SST model and the DES model was the SST-based version of Strelets [13]. Both the SAS and DES models used a spatial discretization scheme that switched from upwind biased second-order to central differencing in regions where flow unsteadiness was resolved. All calculations were performed using the commercial code ANSYS-CFX11. Three unstructured computational grids were tested: coarse, medium and fine, comprising 224,000, 412,000 and 660,000 nodes respectively. Further details of the CFD model are given by Gant [8].

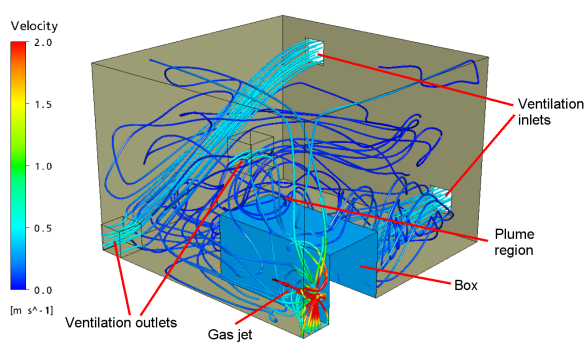

Fig. 1. Streamlines coloured by mean velocity

Figure 1 shows the predicted streamlines from a steady RANS simulation. The gas jet is confined within a narrow cavity in a corner of the room where the flow recirculates, giving rise to locally high gas concentrations. The buoyant gas then rises as a plume towards the ceiling.

Figure 2a shows the ratio of the integral turbulence length scale to the cell size, l_I/Δ, for the fine grid. The ratio is highest in the plume region with the fine mesh where it has a maximum value of 10. Elsewhere in the room the ratio falls to around 5 and in the predominantly laminar regions a value of one or less. This implies that even the fine grid is relatively coarse for LES.

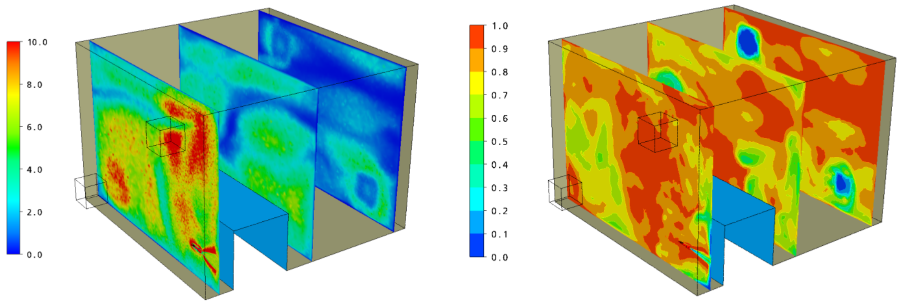

Fig. 2. a.) Ratio of the integral length scale to the cell size calculated using steady RANS on the fine grid (left); b.) Ratio of resolved to total turbulent kinetic energy for the DES (right)

The ratio of the resolved to the total turbulent kinetic energy (k_{res}/k_{tot}) is shown for the fine-grid DES in Figure 2b. The value of k_{tot} is calculated from the sum of the resolved and the modelled components, k_{res} and k_{mod}. The results show that the DES model resolves 70 to 90% of the turbulence energy in the majority of the plume region which suggests that the grid resolution is reasonable. Broadly similar results were obtained for the SAS model.

The ratio of the SGS to the laminar viscosity (ν_t/ν) for the DES model on the fine grid is around 15 to 40 in the plume region. Given that the turbulent Reynolds number here is around 2000, these value are high compared to the target value of around 20 suggested by Celik *et al.* [9]. In the DES calculations, the subgrid activity parameter was close to one across the majority of the room and showed relatively little sensitivity to the grid resolution.

The power spectral density based on the concentration fluctuations in the plume for the DES results showed the spectra decaying at high frequencies faster than the -5/3 power law with no clearly discernible inertial subrange. This appeared to be related to the relatively small separation of turbulent length scales and the influence of buoyancy effects.

The "Index of Quality", LES_IQ_k, based on Richardson extrapolation of the turbulent kinetic energy between the medium and fine grids produced values generally above 60% in the plume region although its value fluctuated significantly between neighbouring cells due to the non-smooth distribution of the ratio of cell sizes. At various points in the flow the LES_IQ_k value either exceeded a value of 100% or became negative.

Mean gas concentrations at 14 points in the room were recorded in the experiments. Figure 3a shows the discrepancy between the CFD and the measured values averaged over all the measurement positions. For the fine grid, the DES and SAS results have more than double the error of the URANS or RANS model predictions. The error diminishes as the grid is refined in the RANS results, whereas with the DES and SAS models the reverse trend is produced with the greatest error on the finest grid.

The predicted gas cloud volumes defined using the Vz criterion are shown in Figure 3b. The statistical uncertainty in the mean values is indicated by error bars which show the 95% confidence intervals. One of the claimed advantages of the SAS model is that it is less grid dependent than LES or DES since the model equations do not rely explicitly on the size of the grid cell. However, in the results shown in Figure 3b, the SAS model exhibits the greatest grid sensitivity of the four models tested.

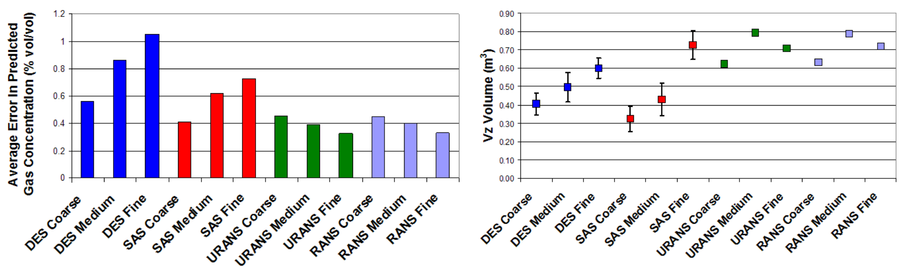

Fig. 3. a.) Average error between the CFD and experimental mean gas concentrations (left); b.) Mean Vz gas cloud volumes and their 95% confidence intervals (right).

4 Discussion & Conclusions

Overall, the various grid quality measures tested here indicate that the spatial resolution was barely adequate for LES. Some of the grid quality measures could not provide useful information in regions of the flow where the turbulence levels were very low. This was particularly an issue for the RANS-based approaches in laminar regions of the flow and the power spectral density in the plume. The ratio of the modelled to the total turbulent kinetic energy appeared to show that the grid resolution was reasonable, but this may have been overly optimistic since it did not take account of any numerical dissipation. The LES "Index of Quality" did not provide useful information and produced values that were less than zero and greater than 100%.

The relatively poor performance of the DES and SAS models is likely to have been a consequence of using overly coarse grids. It would have been useful to undertake simulations with finer grids to establish that DES predictions could produce accurate results. However, the fine-grid DES calculations took 134 CPU-days compared to around 8 CPU-days for the equivalent steady RANS calculation. The cost of undertaking well-resolved DES should not be underestimated, especially for industrial flows.

Although the SAS and DES models may be considered appropriate for modelling flows exhibiting large-scale oscillatory behaviour, the present work has shown that on relatively coarse grids these models can produce less reliable predictions and results that are more grid-dependent than a standard RANS model.

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