Assessment of LES quality measures using the error landscape approach

Markus Klein[1], Johan Meyers[2], and Bernard J. Geurts[3]

[1] Institute for Energy and Powerplant Technology, Technical University of Darmstadt, Petersenstrasse 30, 64297 Darmstadt, Germany kleinm@ekt.tu-darmstadt.de
[2] FWO – Vlaanderen (Science Foundation – Flanders); Department of Mechanical Engineering, Katholieke Universiteit Leuven Celestijnenlaan 300A, B3001 Leuven, Belgium Johan.Meyers@Mech.KULeuven.be
[3] Mathematical Sciences, Faculty EEMCS, University of Twente P.O. Box 217, 7500 AE Enschede, The Netherlands b.j.geurts@utwente.nl

Summary. A large-eddy simulation database of homogeneous isotropic decaying turbulence is used to assess four different LES quality measures that have been proposed in the literature. The Smagorinsky subgrid model was adopted and the eddy-viscosity 'parameter' C_S and the grid spacing h were varied systematically. It is shown that two methods qualitatively predict the basic features of an error landscape including an optimal refinement trajectory. These methods are based on variants of Richardson extrapolation and assume that the numerical error and the modelling error scale with a power of the mesh size. Hence they require the combination of simulations on several grids. The results illustrate that an approximate optimal refinement strategy can be constructed based on LES output only, without the need for DNS data. Comparison with the full error landscape shows the suitability of the different methods in the error assessment for homogeneous turbulence. The ratio of the estimated turbulent kinetic energy error and the 'true' turbulent kinetic energy error calculated from DNS is studied for different Smagorinsky parameters and different grid sizes. The behaviour of this quantity for decreasing mesh size gives further insight into the reliability of these methods.

Key words: Large-eddy Simulation, Quality, Assessment Measures, Error Landscape

1 Introduction

Due to considerable progress of the Large Eddy Simulation (LES) technique combined with a steady increase in computing power, more and more complex flow problems become computationally tractable. Nevertheless, some fundamental problems of the LES formalism remain unsolved. In particular, the application of LES demands for reliable quality assessment procedures.

Numerical and modeling errors have been extensively studied in the past [17, 8, 5, 10, 3, 11] and the investigations led to a better understanding of their interaction and their impact. Several authors attempted to define indices of quality, or error estimators in order to judge the reliability of a given LES. For an overview see, e.g. [1].

Meyers et al. [10, 13] proposed a method to assess LES using a database of pre-computed cases in order to obtain an overview of the error behaviour in the form of so-called error landscapes. In the illustration of this method DNS data of decaying homogeneous isotropic turbulence was adopted yielding a well-defined error surface as a function of grid resolution $N = 1/h$ and model parameter C_S. Though this method yields interesting insights in error-behaviour of LES, it is an *a posteriori* approach, requiring a large number of large-eddy simulations. An alternative was recently proposed by Geurts and Meyers [6] in which an optimal Smagorinsky constant was determined iteratively, at fixed resolution. This method was shown to require about 5 complete large-eddy simulations to reach an accurate estimate of the optimal Smagorinsky parameter. It was illustrated using an error-measure defined relative to DNS data.

This paper explores the possibility of substituting the calculation of the 'true' error, with an estimated simulation error. We investigate estimates in terms of LES data only, and study to what extent an independent 'self-consistent' error-control can be arrived at. The error landscape approach is subsequently used as a tool to assess the quality measures themselves.

2 Error landscapes

The different error estimators considered in this paper are evaluated using a LES and DNS database consisting of more than 100 simulations of decaying homogeneous isotropic turbulence, recorded at two different Taylor Reynolds numbers $Re_\lambda = 50, 100$ [10]. The following grid resolutions 24^3, 32^3, 40^3, 48^3, 56^3, 64^3, 80^3, 96^3, 128^3 have been used together with 20 different settings for the Smagorinksy parameter in the range from 0.0 to 0.2840.

Meyers et al. [10, 11] consider the time integrated relative turbulent kinetic energy deviation between LES and DNS as an error measure. We propose an analogous measure, in terms of LES data. In the current study, the time-averaging is replaced by averaging over two instants in time $t = 0.5, 1.0$.

Given DNS data for the decay of the turbulent kinetic energy, an error-measure can be defined as:

$$\delta_E(N, C_s) = \left[\frac{\sum_{t=0.5,1.0} \left(E_{LES}(t, N, C_s) - E_{DNS}(t)\right)^2}{\sum_{t=0.5,1.0} E_{DNS}(t)^2} \right]^{1/2}, \qquad (1)$$

For any LES at given N and C_S this yields an impression of the relative error.

Using the error estimators introduced in section 3 the presumed deviation based on these estimators can be defined in analogy to (1). We make two alterations: first, the difference between E_{LES} and E_{DNS} is replaced by one of the error estimators introduced below, and second, we normalize the error-measure with a reference value E_{ref} that can be obtained from LES instead of the DNS data as in (1). One could for example think of replacing E_{ref} with $E_{LES}(t, N_{ref}, C_{s,ref})$ or with a value $E_{LES}(t)$ extrapolated from the finest available LES grids. Since this is a normalization, this will only affect to global level of the results, but not the shape of the estimated errors as function of N and C_s. For the purpose of illustration of the method, equation (2) is in this work normalized with the DNS value.

These two steps can be criticized in many ways and their generality and robustness is not established, but at least the principle provides an operational error assessment that can be directly confronted with the full error-landscape procedure based on (1). In detail, we estimate:

$$D(N, C_s) = \left[\frac{\sum_{t=0.5,1.0} E_{est}(t, N, C_s)^2}{\sum_{t=0.5,1.0} E_{ref}(t, N, C_s)^2} \right]^{1/2} \tag{2}$$

Based on these definitions simulation errors can be shown in the form of so called error landscapes [10, 11] and an optimal refinement strategy can be identified as the Smagorinsky coefficient $\widehat{C}_s(N)$ for which the error $\delta_E(N, C_s)$ or D is minimal. As an example figure 1 shows the error landscapes for $\delta_E(N, C_s)$ for $Re_\lambda = 50$ (left) and $Re_\lambda = 100$ (right) together with the optimal refinement strategy (bold line).

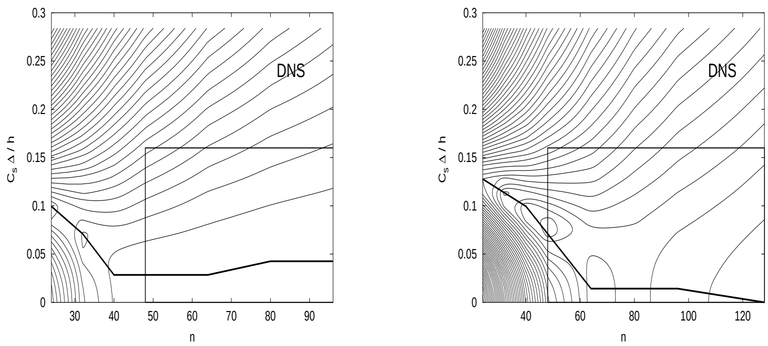

Fig. 1. Error landscapes for $\delta_E(N, C_s)$ obtained from DNS for $Re_\lambda = 50$ (left) and $Re_\lambda = 100$ (right). The bold line represents the optimal refinement strategy. The box in the figures encloses the parameter range where the error estimators have been evaluated in section 4.

3 LES Quality measures

Roache [15] gives the following taxonomy for obtaining information for error estimates in the context of RANS simulations. These also apply to LES and are summarized as follows:.

1. Additional solutions of the governing equations on other grids
   Grid refinement / coarsening / other unrelated grids
2. Additional solutions of governing equations on the same grid
   Higher / lower order accuracy solutions
3. Auxiliary PDE solutions on the same grid
   Solution of an error equation
4. Auxiliary algebraic evaluations on the same grid; surrogate estimators
   Non conservation of higher order moments (e.g. turbulent kinetic energy), methods developed for grid adaption, convergence of higher order quadratures (e.g. evaluation of a drag coefficient) etc.

This paper focuses on methods which can be applied to the decaying homogeneous isotropic turbulence database established in [10, 13]. We will not consider methods belonging to category 2 or 3. Instead, we focus on four error estimators from category 1 and 4. We restrict ourselves to estimating the turbulent kinetic energy error $E_{DNS} - E_{LES}$ following [1, 2, 4, 7]. It is important to remark that this is a difference between the kinetic energy in the unfiltered reference DNS and the LES. By formally defining a LES filter (denoted here with an overline), $E_{DNS} - E_{LES}$ may be further split into $E_{sgs} = E_{DNS} - E_{\overline{DNS}}$ and $E_{\overline{DNS}} - E_{LES}$ (where $E_{\overline{DNS}}$ is the energy in the filtered DNS). It is the latter difference that is usually defined as the LES simulation error on the kinetic energy [3, 10, 17]. However, for the Smagorinsky model (and many other models), the LES filter is not explicitly defined in the computational method, and implicitly related to the computational mesh at best. Hence, in practice the formal LES filter remains a mathematical abstraction, which makes a precise definition of $E_{DNS} - E_{\overline{DNS}}$ ambiguous.

Therefore, the error estimation methods in Refs. [1, 2, 4, 7] follow a more pragmatic approach, i.e. they lump E_{sgs} and $E_{\overline{DNS}} - E_{LES}$ together, trying to estimate the combined term. This may be supported by two empirical observations. First of all, in order to guarantee a good LES prediction, a sufficient amount of energy should be resolved on the computational mesh (e.g., Celik et al. [2] proscribes at least 80%). Hence, E_{sgs} should remain small, and may be included in an error estimation. Secondly, for the Smagorinsky model, it was observed that differences in the formal LES filter definition in the calculation of $E_{\overline{DNS}} - E_{LES}$ (including a 'no-filter' case) did not lead to appreciable differences in the overal shape of the error-landscape, and only the absolute levels of the error shifted [10]. Obviously, this observation should be handled with care when other subgrid-scale models are considered.

In the current study, two methods estimate $E_{DNS} - E_{LES}$ based on the turbulent viscosity ν_t obtained during the simulation and hence do not account for numerical errors unless ν_t is modifed for this purpose. The other two methods use information from additional simulations in order to calculate the error estimate based on variants of Richardson extrapolation.

Similar to the subgrid activity parameter $\langle\epsilon_t\rangle/(\langle\epsilon_t\rangle + \langle\epsilon_\mu\rangle)$ introduced by Geurts and Fröhlich [5], the E_{LESIQ_ν} relates the turbulent viscosity to the laminar viscosity using the following expression (Celik et al. [2]):

$$LESIQ_\nu = \frac{1}{1 + 0.05\left(\frac{\langle\nu+\nu_t\rangle}{\nu}\right)^{0.53}} \tag{3}$$

The LESIQ$_\nu$ is a dimensionless number between zero and one. The constants are calibrated in such a way that the index behaves similar to the ratio of resolved to total turbulent kinetic energy, i.e. $\mathrm{E}^{LES}/\mathrm{E}^{DNS}$. An index of quality greater than 0.8 is considered a good LES, 0.95 and higher is considered as DNS [2]. To make it comparable to the other error measures given below, a modified expression (4) is used in this work:

$$E^{est}_{LESIQ_\nu} = \left[1 - \frac{1}{1 + 0.05\left(\frac{\langle\nu+\nu_t\rangle}{\nu}\right)^{0.53}}\right] \cdot E_{DNS} \tag{4}$$

Another frequently used approach for evaluating the subgrid-scale turbulent kinetic energy based on the turbulent viscosity and the filter width Δ is due to Lilly [9],

$$E^{est}_{Lilly} = \nu_t^2 \Big/ (c\Delta)^2, \quad c = 0.094 \tag{5}$$

The LES Index of quality E_{LESIQ} proposed by Celik et al. [2] is based on Richardson extrapolation assuming that the scaling exponents m, n for modelling and numerical error are known and coincide.

$$E^{est}_{LESIQ} = \frac{|E_2 - E_1|}{1 - \beta^n} \tag{6}$$

Two simulations have to be performed on computational grids with grid spacing h resp. βh. The LES turbulent kinetic energy on these two grids is denoted E_1 and E_2.

The evaluation of the error using the sytemactic grid and model variation E_{SGMV} approach [7, 4] is based on three simulations. One standard LES solution, a second LES on a different grid and a third LES using a modified model parameter. It is assumed that the numerical error and the modelling error scale with the mesh size h like $c_n h^n$ resp. $c_m h^m$. The subgrid scale turbulent kinetic engergy is than estimated as:

$$E^{est}_{SGMV} = \left|\frac{(E_3 - E_1)}{(1-\alpha)}\right| + \left|\frac{(E_2 - E_1) - (E_3 - E_1)\frac{(1-\beta^m)}{(1-\alpha)}}{1 - \beta^n}\right| \tag{7}$$

Here E_1 is the standard LES solution, E_2 the coarse grid LES solution and E_3 the LES solution on the standard LES grid, but with a modified model parameter, i.e., $C^2_{S,3} = \alpha\ C^2_{S,1}$. Especially for higher Reynolds number flows $\alpha > 1$ is suggested in order to avoid numerical stability problems. The 1D grid coarsening factor is again denoted by β. Since the method is designed for practical applications grid coarsening is proposed. A value of beta too close to one is not recommended in the context of Richardson extrapolation [15], a value higher than 2 is not of much interest. Throughout, we adopt $\alpha = 4$ and $\beta = 2$. The scaling exponent of the numerical error has been set to $n = 2$. This is based on the fact that a fully second order numerical scheme was used to generate the DNS database. The scaling for the modeling error was set to $m = 2/3$ which is identical to the theoretical prediction [16, 14]. For more details see [1, 4] and the references therein.

4 Assessment of LES Quality measures

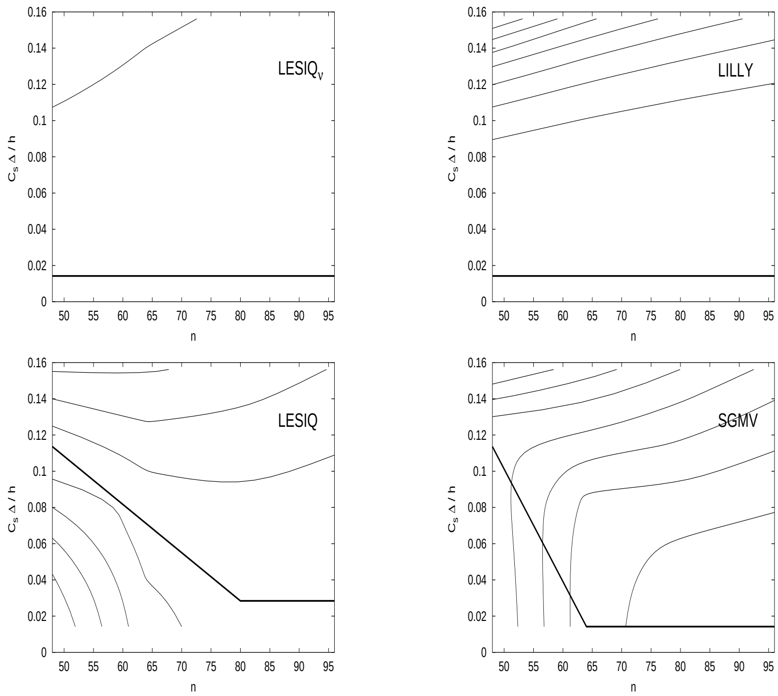

Fig. 2. Error landscapes for $D(N, C_s)$ calculated from 4 different error estimators for$Re_\lambda = 50$. The bold line represents the optimal refinement strategy.

In this section we combine the error landscape approach with the error estimators introduced above, in order to assess their quality and reliability. The SGMV method requires three simulations in order to evaluate the estimated error. In view of the enormous amount of possible combinations to select three LES runs from the database presented in section 2 the following choice has been made: *(i)* only grid coarsening by a factor of two is considered. *(ii)* for the model variation the model parameter is increased by a factor of four. In case the database did not contain an exact factor four increase, a deviation of up to 25 % was allowed. This implies that the estimated error is only available for grid resolution 48^3 or higher. Based on these two criteria all possible combinations of three simulations have been choosen from the database to estimate the simulation error for the SGMV method. The same cases were used for the other error estimators. This serves as the basis for the comparison. It is important to note that the systematic grid and model variation as well as the LESIQ can also be used for values of β less than two. Alternatively also grid refinement, i.e. $\beta < 1$ would be possible. Another option would be to perform the LES simulation with the modified model parameter on the coarse grid instead of the fine grid and certainly the value of α could be changed as well. The presentation of all these variations is however beyond the scope of this work and left for future discussions.

In the remainder of this section we assess the four error estimators using the following guidelines:

- An optimal refinement trajectory can be approximated
- The ratio of estimated and true error $D(N, C_s)/\delta_E(N, C_s)$ should be as close as possible to unity, or in general a constant value, depending on the reference E_{ref} which is employed. As a minimum requirement this is at least expected for small mesh sizes.
- Overestimation of error, i.e. conservatism, is preferred over underestimation of error.

Approximative error landscapes

Figures 2 and 3 show the error landscapes for $D(N, C_s)$ calculated from the estimators given in (4)-(7) for $Re_\lambda = 50$ resp. $Re_\lambda = 100$. We compare these with the error landscape for $\delta_E(N, C_s)$ obtained by using a DNS as point of reference, see figure 1. We included The true error landscapes in figure 1 defined relative to DNS data include a window indicating the parameter range in which the error-estimators have been assessed. Note that the horizontal and vertical scales differ. It can be observed that the systematic grid and model variation (SGMV) and the LES index of quality (LESIQ) are able to capture some characteristics of the actual error landscape obtained via DNS. Particularly these two error estimators are capable to predict an optimal refinement strategy as defined in [10]. This is in contrast to E_{LESIQ_ν} and E_{Lilly} which

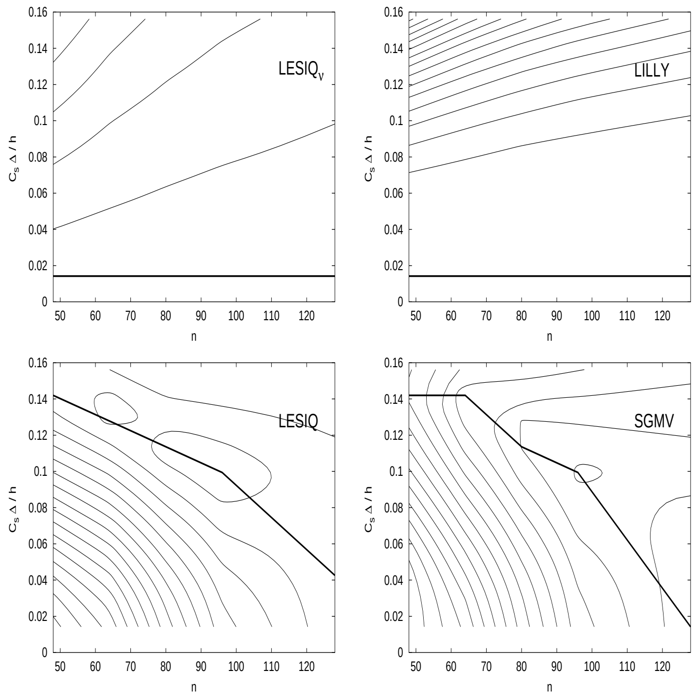

Fig. 3. Error landscapes for $D(N, C_s)$ calculated from 4 different error estimators for $Re_\lambda = 100$. The bold line represents the optimal refinement strategy.

are based on a single grid calculation. Here the predicted error basically decreases with the model parameter, hence the optimal model parameter would be zero.

Convergence of error estimators

In addition to the error landscapes it is interesting to investigate the magnitude of $D(N, C_s)$ to $\delta_E(N, C_s)$. Ideally the ratio of both quantities should be as close as possible to one. Due to the fact that the assumption of an assymptotic convergence behavior might not always be fullfilled, larger deviations are expected on coarser grids. However as a minimum requirement $D(N, C_s)/\delta_E(N, C_s)$ should approach unity for decreasing mesh size. Figures 4 and 5 show, for different but fixed model parameters, the ratio of the estimated error and true error $D(N, C_s)/\delta_E(N, C_s)$ for the four different approaches and the two Reynolds numbers. Note the double logarithmic plot.

The following observations can be made:

- $LESIQ_\nu$ diverges from unity for decreasing mesh size, i.e. the error estimate gets worse on finer grids.
- Lilly's approach underpredicts the error considerably. This is consistent with the findings in [7]. For a constant Smagorinsky parameter the estimated error does not converge towards the true error for decreasing mesh size.
- $LESIQ$ and $SGMV$ converge towards the true error for decreasing mesh size. Bigger discrepancies arise especially from unrealistic low model parameters. Note that the dash-dotted lines correspond to $C_s < 1.0$.
- The $LESIQ$ has a tendency to underpredict the error at coarse mesh sizes.
- The SGMV shows a more conservative error estimation behaviour. This is due to the fact that modelling and numerical error are treated separately and that the estimated error is the sum of their absolute values.
- The database consists of many simulations using rahter unphysical model parameters. For $C_s = 0.156$, a value close to the theoretical expecations for isotropic decaying turbulence, especially Lilly's approach and the SGMV show a good performace with $0.5 \leq D(N, C_s)/\delta_E(N, C_s) \leq 2.0$.

5 Conclusion

A large-eddy simulation database of homogeneous isotropic decaying turbulence has been used to assess the following LES quality measures ranging from single grid to three simulation studies: The LESIQ$_\nu$, Lilly's approach to estimate the subgrid scale turbulent kinetic energy, the LES index of quality based on Richardson extrapolation and the systematic grid and model variation (SGMV). The results suggest that only by performing additional simulations on different grids the basic features of an an error landscape, including an optimal refinement trajectory, can be captured. Among these two methods, i.e. LESIQ and SGMV, the systematic grid and model variation provides for the configuration under consideration a more conservative error estimate.

The extension of the present work to different spatial discretization schemes [12] as well as the consideration of other flow propeties as error measures [13] is part of the work in progress. The application of the systematic grid and model variation and the LESIQ to more complex flow configurations has been discussed in the literature, see [1] for an overview.

Acknowledgment

Financial support by the DFG (German Research Council) SFB568 is gratefully acknowledged.

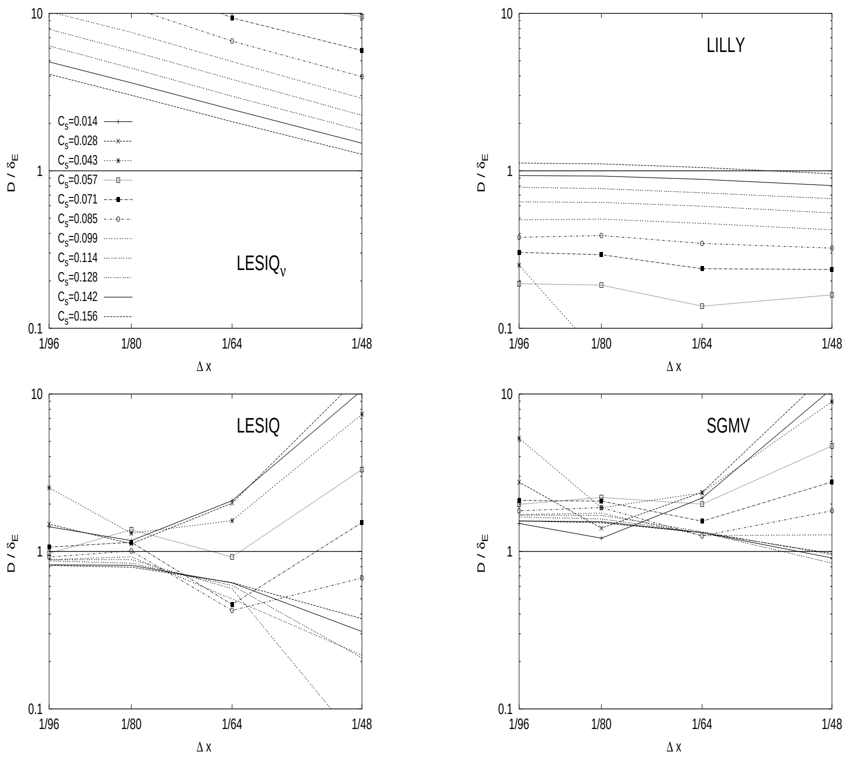

Fig. 4. Estimated error divided by true error plotted against grid resolution for different Smagorinsky parameters at $Re_\lambda = 50$.

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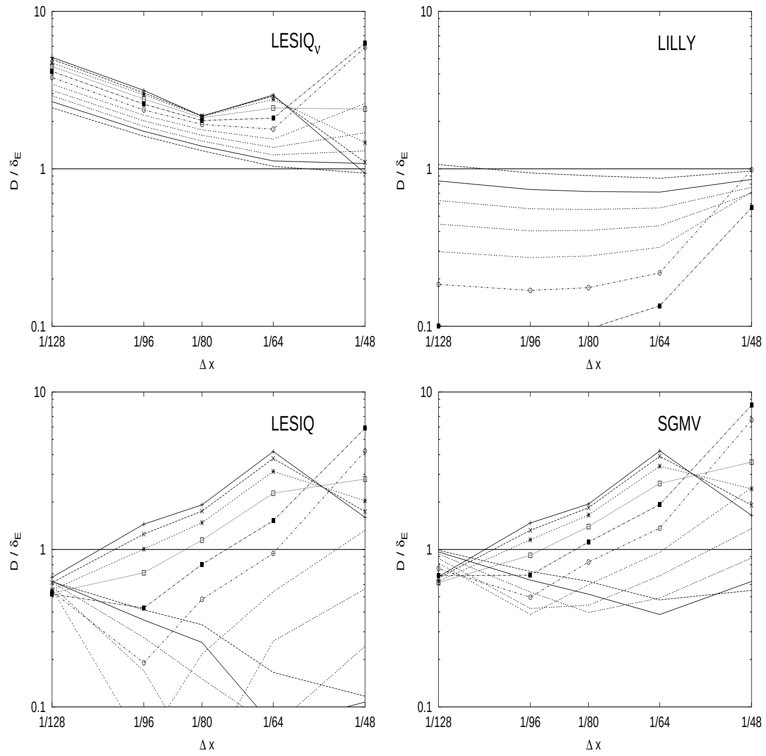

Fig. 5. Estimated error divided by true error plotted against grid resolution for different Smagorinsky parameters at $Re_\lambda = 100$ (see legend in figure 4)

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