An Assessment of Models in Large Eddy Simulation

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Abstract. This paper presents a numerical comparison between a rational LES model introduced by Galdi and Layton (2000) and a classical LES model. The new LES model is based on a rational approximation of the Fourier transform of the Gaussian filter while the classical LES model uses a Taylor polynomial approximation. The numerical experiments for the 2D driven cavity test problem show a clear improvement in solution quality for the rational LES model. This improvement is consistent with the new closure approximation which provides better attenuation of high frequencies.

Subject Classifications: AMS(MOS): 76F65, 76M10.
Key Words: Turbulence, Navier-Stokes Equations, Large Eddy Simulation.

1 Introduction.

Large Eddy simulation (LES) is currently one of the most promising approaches for simulation of turbulent flows (at high Reynolds numbers). In contrast to direct numerical simulation (DNS), it aims to catch the main flow features on coarser meshes than those necessary to resolve all important length scales. Many models have been developed for large eddy simulation (surveyed, for example, in Sagaut [Sag98] and Aldama [Ald90]). In this report we aim to begin a careful comparison and assessment of these models. Such a comparison is, of course, complicated by the uncertainties and instabilities of the underlying turbulent flow. For this reason, herein we are basing our comparisons on the behaviour of

(i) the flow's kinetic energy in the large eddies,

(ii) the deviation of the predictions of the LES model at moderate Reynolds number (Re) from a flow field calculated by resolving the Navier-Stokes equations,

(iii) at higher Re, a comparison of aspects of a "coarse mesh-high Re simulation" with those same aspects of a fine mesh simulation which agree across different models.

To this end, we have selected the driven cavity problem, which is perhaps the most popular test problem in computational fluid dynamics. The driven cavity does have reported difficulties with initial transients when an impulsive start is used ($\mathbf{u}(\mathbf{x}, t) \equiv 0$) Gresho and Sani [GS98], [GS00].

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We were careful to do all test with both an impulsive start and with a fully developed flow as initial condition to control for this effect.

By focusing on the above-detailed global flow behaviour, we feel that we can provide a reliable comparison between several LES models. We report simulations using the Smagorinsky model and a Galerkin finite element method (FEM) simulation of the Navier–Stokes equations to facilitate the main comparison of this report, which is between two LES models (described next). The Galerkin FEM approximation is under diffused, Tobiska [Tob95], and the Smagorinsky model is well-known to be over diffused, see Mohammadi and Pironneau [MP94]. Thus, a good LES model should, in some sense, be intermediate between these two.

The first main LES model we consider evolved from work of Leonard [Leo74] and Clark, Ferziger and Reynolds [CFR79]. Since its derivation (given in Section 2) is based on a truncated Taylor polynomial approximation in wave number space, we shall call this the "Taylor LES model". The second main model's derivation (also reviewed in Section 2) follows a similar path but is based instead on a Padé approximation – giving the "rational LES model".

Basing our comparison herein upon more global quantities, which can be more reliably calculated, has led to some interesting conclusions. The most important conclusion is that the Taylor LES model can exhibit a considerable blow up of kinetic energy and should be replaced by the rational LES model. To our knowledge, no computational tests of the driven cavity has ever reported finite time blow up of the computed solutions kinetic energy. Thus, these results provide strong evidence that the Taylor LES model is not appropriate. The evidence is not conclusive, because the mathematical theory of the driven cavity is much less clear, since the solution $\mathbf{u}$ is discontinuous on the boundary, $\nabla\mathbf{u}$ is not in the Sobolev space $L^2(\Omega)$ and standard theory of the Navier–Stokes equations does not apply.

In Section 2 we present the features of the true large eddies in the flow, being the local spatial averages. Section 2 also presents the two main models. Section 3 presents the experimental results and Section 4 the conclusions.

2 Mathematical Properties of the Models.

This section briefly presents a traditional Taylor LES model (introduced by Clark, Ferziger and Reynolds in [CFR79], analyzed mathematically by Coletti in [Col98], and numerically by Cantekin, Westerink and Luettich in [CWJ94]), and the new rational LES model introduced by Galdi and Layton in [GL00], pointing out the essential difference in their derivation.

Consider an incompressible viscous fluid flowing in a bounded domain Ω in $\mathbb{R}^d, d = 2, 3$, and driven by body forces and/or boundary velocities. In nondimensionalized terms, its velocity $\mathbf{u}$ and pressure p are solutions of the Navier-Stokes equations, given by:

$$\begin{array}{rcll} \dfrac{\partial \mathbf{u}}{\partial t} - \mathrm{Re}^{-1}\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p & = & \mathbf{f} & \text{in } \Omega\times(0,T], \\ \nabla\cdot\mathbf{u} & = & 0 & \text{in } \Omega\times(0,T], \\ \mathbf{u}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{u} & = & \mathbf{g} & \text{on } \partial\Omega, \end{array} \tag{1}$$

where $\int_\Omega p(\mathbf{x})d\mathbf{x} = 0,\ \nabla\cdot\mathbf{u}_0 = 0$ and $\int_{\partial\Omega}\mathbf{g}\cdot\hat{\mathbf{n}}\ ds = 0$. The spatial averages are obtained through convolution with a space filter; one common filter, which we select herein, is the Gaussian filter:

$$g_\delta(\mathbf{x}) := \left(\frac{\gamma}{\pi}\right)^{3/2}\frac{1}{\delta^3}\exp\left(-\gamma\frac{||\mathbf{x}||_2^2}{\delta^2}\right),$$

where γ is a constant (often $\gamma = 6$, and this is the value we are using herein) and δ is the averaging radius and $||\mathbf{x}||_2$ the Euclidean norm of $\mathbf{x}$. Extending all variables appropriately outside Ω, the convolution $\overline{\mathbf{u}} = g_\delta * \mathbf{u}$ represents the eddies of size $O(\delta)$ or larger. For constant filter width δ, differentiation and convolution commute. Thus, applying this averaging operator to the

Navier-Stokes equations gives the set of space-filtered Navier-Stokes equations:

$$\begin{aligned}
\frac{\partial \overline{\mathbf{u}}}{\partial t} - \mathrm{Re}^{-1}\Delta\overline{\mathbf{u}} + \nabla\cdot(\overline{\mathbf{u}\mathbf{u}}) + \nabla\overline{p} &= \overline{\mathbf{f}} && \text{in } \Omega,\\
\nabla\cdot\overline{\mathbf{u}} &= 0 && \text{in } \Omega\\
\overline{\mathbf{u}}(x,0) &= \overline{\mathbf{u}}_0(x) && \text{in } \Omega,\\
\overline{\mathbf{u}}(x,t) &= (g_\delta * \mathbf{u})(x,t) && \text{on } \partial\Omega.
\end{aligned} \tag{2}$$

This system cannot be solved directly due to the well known closure problem. Continuum models used for LES are an approximation to $\overline{\mathbf{u}}$ in (2). Thus, it is worthwhile to consider the essential properties of solutions of (2) which we seek (in so far as possible) to retain in solutions of LES models.

Proposition 2.1 *Let $(\mathbf{u}(\mathbf{x},t), p(\mathbf{x},t))$ be a weak solution (see [Gal94]) of the Navier-Stokes equations and let $\mathbf{u}$ and p continued by zero outside Ω. Then,*

(i) $\overline{\mathbf{u}}(\mathbf{x},t)$ is infinitely differentiable in space, $\overline{\mathbf{u}}$ in $C^\infty(\Omega)$,

(ii) $\overline{\mathbf{u}} \to \mathbf{u}$ in $L^2(\Omega)$ as $\delta \to 0$,

(iii) the kinetic energy in $\overline{\mathbf{u}}$ is bounded by that of $\mathbf{u}$:

$$\frac{1}{2}\int_\Omega |\,\overline{\mathbf{u}}\,|^2\,dx \le \frac{1}{2}\int_\Omega |\,\mathbf{u}\,|^2\,dx \le C(Re, \mathbf{f}, \mathbf{u}_0) < \infty.$$

Proof: (i) and (ii) follow by standard properties of convolution operators while (iii) follows from Young's inequality for convolutions:

$$\begin{aligned}
\frac{1}{2}\int_\Omega |\,\overline{\mathbf{u}}\,|^2\,dx &\le \frac{1}{2}\int_{\mathbb{R}^d} |\,\overline{\mathbf{u}}\,|^2\,dx \le \frac{1}{2}\int_{\mathbb{R}^d} |\,\mathbf{u}\,|^2\,dx = \frac{1}{2}\int_\Omega |\,\mathbf{u}\,|^2\,dx\\
&\le C(Re, \mathbf{f}, \mathbf{u}_0) < \infty
\end{aligned}$$

□

To perform a large eddy simulation, closure in (2) must be addressed to obtain a system whose solution approximates $(\overline{\mathbf{u}}, \overline{p})$. Many approximations to the Reynolds stress tensor are possible see, e.g., Aldama [Ald90], Sagaut [Sag98]. Proposition 2.1 gives a quantitative criterion for comparing different models: if the global kinetic energy in the model approximating $\overline{\mathbf{u}}$ is significantly larger than that of a Galerkin FEM approximation to $\mathbf{u}$, the model needs to be reconsidered. Further, the distribution of energy is also important. By Proposition 2.1 (i) it should be concentrated in the low frequencies with corresponding attenuation of high frequencies.

With this in mind, consider the closure problem in (2). Writing $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$, we get:

$$\overline{\mathbf{u}\mathbf{u}} = \overline{(\overline{\mathbf{u}} + \mathbf{u}')(\overline{\mathbf{u}} + \mathbf{u}')} = \overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}} + \overline{\overline{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\overline{\mathbf{u}}} + \overline{\mathbf{u}'\mathbf{u}'} \tag{3}$$

Equation (3) is a decomposition of the averaged nonlinear interactions into "resolved scales", $\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}}$, "cross terms", $\overline{\overline{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\overline{\mathbf{u}}}$ describing the interaction of large and small eddies, and the "subgrid scale" term $\overline{\mathbf{u}'\mathbf{u}'}$, describing the effects of the interaction of small eddies on the mean flow. A formal asymptotic expansion reveals their relative sizes for smooth functions:

$$\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}} = O(1), \quad \overline{\overline{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\overline{\mathbf{u}}} = O(\delta^2), \quad \text{and } \overline{\mathbf{u}'\mathbf{u}'} = O(\delta^4). \tag{4}$$

This formal expansion gives insight into the selection of subgrid scale models. If the subgrid scale model for $\nabla\cdot(\overline{\mathbf{u}'\mathbf{u}'})$ is $O(\delta^2)$ on the smooth components of the flow, then it is not a faithful model of turbulent fluctuations. An $O(\delta^2)$ subgrid scale model will dominate the model of the *larger* cross terms in calculations. Accordingly, it is important to perform experiments in which the subgrid scale model is either absent or exceedingly small to test the model of the cross terms.

The modeling technique used in the derivation of the Taylor LES model is employing closure approximation in Fourier space in (3) following, e.g., Leonard [Leo74], and Aldama [Ald90]. For example, for the first term on the right hand side of (3), we have:

$$\mathcal{F}(\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}}) = \hat{g_\delta} * \mathcal{F}(\overline{\mathbf{u}}\,\overline{\mathbf{u}}) = \hat{g_\delta}(\hat{\overline{\mathbf{u}}} * \hat{\overline{\mathbf{u}}}) = e^{-\frac{\delta^2}{4\gamma}||\mathbf{k}||_2^2}(\hat{\overline{\mathbf{u}}} * \hat{\overline{\mathbf{u}}}),$$

where $\mathbf{k}$ is the $\mathbf{k}$–Fourier mode of $\mathbf{u}$. Using a Taylor series approximation to the exponential here gives:

$$\mathcal{F}(\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}}) = \left(1 - \frac{\delta^2}{4\gamma}||\mathbf{k}||_2^2\right)(\hat{\overline{\mathbf{u}}} * \hat{\overline{\mathbf{u}}}) + O(\delta^4).$$

Proceeding in a similar manner for the other three terms, dropping all terms (formally) of order $O(\delta^4)$ or higher, and then taking the inverse Fourier transform (see [Ald90] for details), we get a traditional space-filtered Taylor LES model used in many studies, e.g., [Ald90], [Col98], [CWJ94] etc.:

$$\begin{array}{rcll} \frac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta\mathbf{w} + \nabla\cdot(\mathbf{w}\mathbf{w}) + \nabla q & & & \\ +\nabla\cdot\left(\frac{\delta^2}{2\gamma}\nabla\mathbf{w}\nabla\mathbf{w}\right) & = & \bar{\mathbf{f}} & \text{in } \Omega\times(0,T], \\ \nabla\cdot\mathbf{w} & = & 0 & \text{in } \Omega\times(0,T], \\ \mathbf{w}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{w}(\mathbf{x},t) & = & (g_\delta * \mathbf{u})(\mathbf{x},t) & \text{on } \partial\Omega, \end{array} \tag{5}$$

where $(\mathbf{w}, q)$ is an approximation to $(\overline{\mathbf{u}}, \overline{p})$ and $(\nabla\mathbf{w}\nabla\mathbf{w})_{i,j}$ is shorthand for $\sum_l \frac{\partial \mathbf{w}_i}{\partial \mathbf{x}_l}\frac{\partial \mathbf{w}_j}{\partial \mathbf{x}_l}$ and model the cross terms in (3). The turbulent fluctuations $\overline{\mathbf{u}'\mathbf{u}'}$ in (3) are usually modeled by a Smagorinsky [Sma63] term of the form

$$C_s\delta^2||\mathbb{D}(\overline{\mathbf{u}})||\mathbb{D}(\overline{\mathbf{u}}) \tag{6}$$

which is added to the left hand side of (5). Here

$$\mathbb{D}(\overline{\mathbf{u}}) = (d_{ij})_{i,j=1,\dots,d} := \frac{1}{2}\left(\nabla\overline{\mathbf{u}} + (\nabla\overline{\mathbf{u}})^t\right)$$

is the deformation tensor associated with $\overline{\mathbf{u}}$ and

$$||\mathbb{D}(\overline{\mathbf{u}})|| = \left(\sum_{i,j=1}^{d} d_{ij}^2\right)^{1/2}.$$

Thus, the Taylor LES model becomes:

$$\begin{array}{rcll} \frac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta\mathbf{w} + \nabla\cdot(\mathbf{w}\mathbf{w}) + \nabla q & & & \\ +\nabla\cdot\left(\frac{\delta^2}{2\gamma}\nabla\mathbf{w}\nabla\mathbf{w}\right) - \nabla\cdot(C_s\delta^2||\mathbb{D}(\mathbf{w})||\mathbb{D}(\mathbf{w})) & = & \bar{\mathbf{f}} & \text{in } \Omega\times(0,T], \\ \nabla\cdot\mathbf{w} & = & 0 & \text{in } \Omega\times(0,T], \\ \mathbf{w}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{w}(\mathbf{x},t) & = & (g_\delta * \mathbf{u})(\mathbf{x},t) & \text{on } \partial\Omega. \end{array} \tag{7}$$

A basic theory of existence of weak solutions for this model has recently been provided by Coletti [Col98]. For large data, this theory has one pivotal condition: the constant C_s has to be large enough such that the Smagorinsky model dominates the other nonlinear terms. This condition is questionable in view of (4).

The Taylor series approximation used in the derivation of the above model is, however, inconsistent with Proposition 2.1 (i)'s required attenuation of high frequencies in $\overline{\mathbf{u}}$. It actually increases the high wave number components (large $||\mathbf{k}||_2$), whereas the original function $\hat{g_\delta} = e^{-\frac{\delta^2}{4\gamma}||\mathbf{k}||_2^2}$ decreases the high wave number components, see Figure 1.

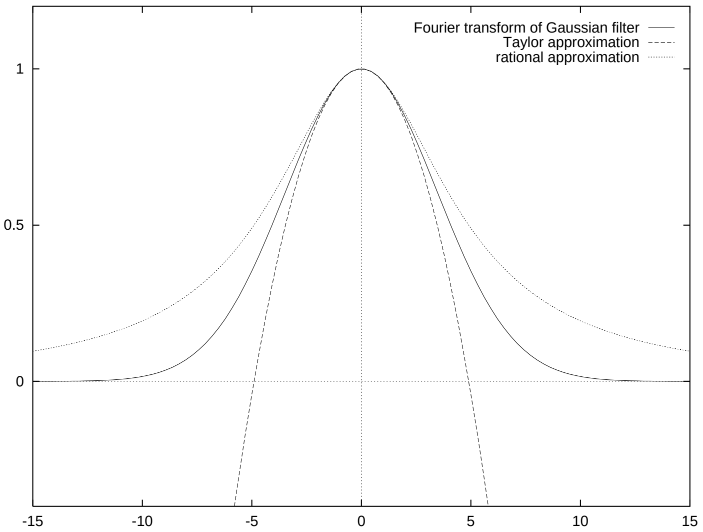


Figure 1: Taylor and rational approximation of the Fourier transform of the Gaussian filter.

This incorrect stimulation of high frequencies plays an important role in numerical calculations at high Reynolds numbers, since increasing the high wave number components (large $||\mathbf{k}||_2$) in the Fourier space is equivalent to increasing the small scales (small $||\mathbf{x}||_2$) in the physical space ($\mathbb{R}^d$). We believe that this is the true cause of the need for powerful dissipative mechanisms, such as the $O(\delta^2)$ Smagorinsky model for $\overline{\mathbf{u}'\mathbf{u}'}$.

Motivated by the above observation, Galdi and Layton proposed in [GL00] a modified model which is consistent with the required attenuation of high frequencies in $\overline{\mathbf{u}}$. This model is based upon a rational approximation to $\hat{g_\delta}$, such as the (0,1) Padé:

$$\hat{g_\delta} = e^{-\frac{\delta^2}{4\gamma}||\mathbf{k}||_2^2} = \frac{1}{1+\frac{\delta^2}{4\gamma}||\mathbf{k}||_2^2} + O(\delta^4).$$

The resulting model is given by:

$$\begin{array}{rcll} \multicolumn{2}{l}{\dfrac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta \mathbf{w} + \nabla\cdot(\mathbf{w}\mathbf{w}) + \nabla q} & & \\ +\nabla\cdot\left[\left(-\dfrac{\delta^2}{4\gamma}\Delta + I\right)^{-1}\left(\dfrac{\delta^2}{2\gamma}\nabla\mathbf{w}\nabla\mathbf{w}\right)\right] & = & \bar{\mathbf{f}} & \text{in } \Omega\times(0,T], \\ \nabla\cdot\mathbf{w} & = & 0 & \text{in } \Omega\times(0,T], \\ \mathbf{w}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{w}(\mathbf{x},t) & = & (g_\delta * \mathbf{u})(\mathbf{x},t) & \text{on } \partial\Omega, \end{array}$$

Actually, there are two natural variants of this model:

1) rational approximation model with auxiliary problem, where the inverse operator is calculated directly, solving a discrete elliptic problem,

2) rational approximation model with convolution, where the smoothing operator $\left(-\frac{\delta^2}{4\gamma}\Delta + I\right)^{-1}$ is replaced by direct convolution with the Gaussian filter.

Our goal here is to compare and contrast the Taylor and the classical LES model. Accordingly, all algorithmic choices not associated with the closure problem will be taken the same. Thus, we shall also use the Smagorinsky model (6) for the turbulent fluctuations in the rational model as in (7). Thus, the rational LES model with auxiliary problem we consider is:

$$
\begin{array}{rcll}
\multicolumn{4}{l}{\dfrac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta \mathbf{w} + \nabla \cdot (\mathbf{w}\mathbf{w}) + \nabla q} \\
\multicolumn{4}{l}{+\nabla \cdot \left[\left(-\dfrac{\delta^2}{4\gamma}\Delta + I \right)^{-1} \left(\dfrac{\delta^2}{2\gamma} \nabla \mathbf{w} \nabla \mathbf{w} \right) \right]} \\
-\nabla \cdot (C_s \delta^2 \|\mathbb{D}(\mathbf{w})\| \mathbb{D}(\mathbf{w})) & = & \bar{\mathbf{f}} & \text{in } \Omega \times (0,T], \\
\nabla \cdot \mathbf{w} & = & 0 & \text{in } \Omega \times (0,T], \\
\mathbf{w}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\
\mathbf{w}(\mathbf{x},t) & = & (g_\delta * \mathbf{u})(\mathbf{x},t) & \text{on } \partial\Omega.
\end{array}
\tag{8}
$$

In the rational LES model with convolution, the first equation of (8) is replaced by

$$
\begin{array}{c}
\dfrac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta \mathbf{w} + \nabla \cdot (\mathbf{w}\mathbf{w}) + \nabla q \\
+\nabla \cdot \left[g_\delta * \left(\dfrac{\delta^2}{2\gamma} \nabla \mathbf{w} \nabla \mathbf{w} \right) \right] - \nabla \cdot (C_s \delta^2 \|\mathbb{D}(\mathbf{w})\| \mathbb{D}(\mathbf{w})) \quad = \quad \bar{\mathbf{f}} \quad \text{in } \Omega \times (0,T],
\end{array}
\tag{9}
$$

where the convolution is approximated numerically.

Last, we consider the pure Smagorinsky model [Sma63] which is also common and popular due to its simplicity and good stability properties:

$$
\begin{array}{rcll}
\multicolumn{4}{l}{\dfrac{\partial \mathbf{w}}{\partial t} - \mathrm{Re}^{-1}\Delta \mathbf{w} + \nabla \cdot (\mathbf{w}\mathbf{w}) + \nabla q} \\
-\nabla \cdot (C_s \delta^2 \|\mathbb{D}(\mathbf{w})\| \mathbb{D}(\mathbf{w})) & = & \bar{\mathbf{f}} & \text{in } \Omega \times (0,T], \\
\nabla \cdot \mathbf{w} & = & 0 & \text{in } \Omega \times (0,T], \\
\mathbf{w}(\mathbf{x},0) & = & \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \\
\mathbf{w}(\mathbf{x},t) & = & (g_\delta * \mathbf{u})(\mathbf{x},t) & \text{on } \partial\Omega.
\end{array}
\tag{10}
$$

3 The Numerical Studies

Based on Section 2, the usual Galerkin finite element method for the Navier–Stokes equations (1), the Taylor LES model (7), the two variants of the rational LES model (8), (9) and the Smagorinsky model (10) are compared using the two–dimensional driven cavity problem.

This problem is given by $\Omega = (0,1)^2$, the boundary conditions $\mathbf{w} = (1,0)$ for $0 < x < 1, y = 1$, homogeneous Dirichlet boundary conditions at the other boundaries, and $\mathbf{f} = \mathbf{0}$. The driven cavity problem is a classical test example used in a number of papers, e.g. Cantekin, Westerink and Luettich Jr.. [CWJ94] and Coletti [Col98]. The incompatibility of the boundary conditions at the corners $(0,1)$ and $(1,1)$ leads to a non–smooth solution such that in general analytical results, such as Proposition 2.1, do not hold. Also, an appropriate initial condition for the time dependent problem is not agreed upon in the literature. For all models, we have tried to use a, so–called, impulsive start in our computations, i.e. the velocity inside the domain is chosen zero at the beginning. Investigations by Gresho and Sani [GS98], [GS00] show that an impulsive start can create a quickly decaying but nonphysical transient in the solution of an incompressible flow problem. For this reason, we repeated the tests which failed with the impulsive start also with other initial conditions to make sure that their failure is not caused by the impulsive start.

We did computations for a low Reynolds number flow ($Re = 400$) and a high Reynolds number flow ($Re = 10000$). Results for comparison are available for both Reynolds numbers in Ghia, Ghia and Shin[GGS82]. All LES models are applied without turbulent viscosity for $Re = 400$ ($C_s = 0$ in (6)) and with $C_s = 0.01$ in the tests for $Re = 10000$. The pure Smagorinsky model (10) was applied also with $C_s = 0.01$.

First, the Navier–Stokes equations are discretized in time by the fractional–step–θ–scheme, e.g. see Bristeau, Glowinsky and Periaux [BGP87], which is analyzed for the time dependent Navier–Stokes equations by Kloucek and Rys [KR94]. This implicit scheme is of second order accuracy, more stable than the Crank–Nicolson scheme and is currently considered “best” on the basis of accuracy and reliability, e.g. see Turek [Tur99] or Rannacher [Ran00]. Unless mentioned otherwise, all computations were carried out with the equidistant time step $\Delta t = 0.01$.

The equations in each time step are discretized by the so–called (Gresho and Sani [GS00]) Q_2/P_{-1} finite element, i.e. the velocity is approximated by continuous piecewise biquadratics and the pressure by discontinuous linears. This conforming pair of finite element spaces fulfils the inf–sup or Babuška–Brezzi stability condition. It is currently considered the most stable and best performing element for finite element discretizations of Navier–Stokes equations, e.g. see Fortin [For93] or Gresho and Sani [GS00]. In addition, it has been proven to be superior to other pairs of finite elements in a recent study for a benchmark problem for laminar flows [JM00]. All computations were carried out on equidistant grids with squares of size $h \times h$. We used the deformation tensor formulation

$$2(\mathbb{D}(\mathbf{w}), \mathbb{D}(\mathbf{v}))$$

as variational form of the viscous term.

The fractional–step–θ–scheme divides each time step in three sub time steps. In each sub time step, a nonlinear saddle point problem has to be solved. All terms in the Galerkin finite element method of the Navier–Stokes equations and of the Smagorinsky model are treated always fully nonlinear. In the LES models, the convective term and the Smagorinsky term (10) are also treated implicitly whereas the additional term coming from the LES models is computed in each sub time step before the nonlinear iteration and it is not changed within this iteration. The linear problems are solved by a coupled multigrid method with Vanka–type smoothers as studied numerically e.g. in John and Tobiska [JT00] or John and Matthies [JM00]. These algorithmic choices are currently considered best in terms of reliability, stability and accuracy in finite element CFD.

We present results for the mesh widths $h = 1/16$, $h = 1/32$ and $h = 1/64$. The corresponding number of degrees of freedom (d.o.f.) in space are given in Table 1. If not mentioned otherwise, the averaging radius δ is chosen to be the diameter of the mesh cell, i.e. the longest distance of two of its vertices, which is $\delta = \sqrt{2}h$.

Besides the kinetic energy of the computed solution $\mathbf{w}_h$, we consider also the H^1–semi norm

$$\left(\int_\Omega \nabla \mathbf{w}_h^2 dx\right)^{1/2}.$$

The H^1–semi norm is closely related to the rate of viscous dissipation of the flow and thus another interesting measure of the global energy balance.

All computations were carried out with the code MooNMD [BJMS00].

Table 1: Mesh widths and degrees of freedom (d.o.f.).

mesh width	velocity d.o.f.	pressure d.o.f.	total d.o.f.
1/16	2 178	768	2 946
1/32	8 450	3 072	11 522
1/64	33 282	12 288	45 570

3.1 The low Reynolds number flow

One property of a good LES model is that its use in a laminar or low Reynolds number flow results in a solution which is very close to the solution obtained by solving the Navier–Stokes equations. All models in our study show a very similar behaviour with respect to the kinetic energy and the H^1–semi norm of the computed solutions, see Figures 2, 3 and Tables 2 - 5 (the pictures for the other mesh sizes look very similar to those presented here). This result is not consistent with the conclusions in Coletti [Col98] that the Taylor LES model does not give satisfying results for the driven cavity problem with $Re = 400$ and the P_2/P_1 spatial finite element discretization

(Taylor/Hood) on a triangular mesh. Since the most essential difference between both studies are the finite element spaces, the Q_2/P_{-1} element seems to have a better stabilization effect on the Taylor LES model than the P_2/P_1 finite element.

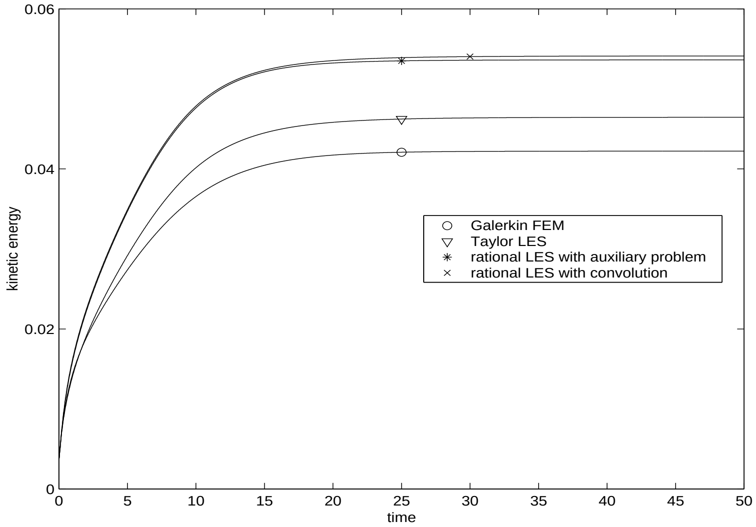


Figure 2: Kinetic energy, $Re = 400$, $h = 1/16$, $\delta = \sqrt{2}/16$.

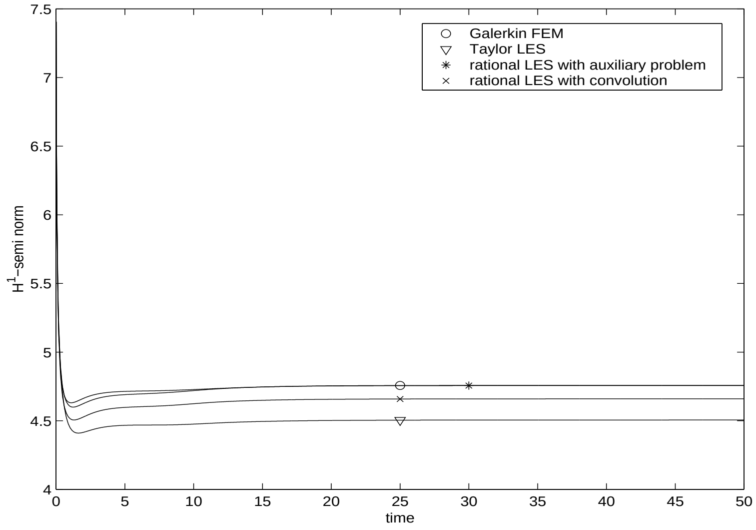


Figure 3: H^1–semi norm, $Re = 400$, $h = 1/16$, $\delta = \sqrt{2}/16$.

Table 2: Kinetic energy for the stationary state, $Re = 400$. Note, the kinetic energy balance of all models is comparable in the low Reynolds number case.

model	$h = 1/16$	$h = 1/32$	$h = 1/64$
Galerkin FEM	4.221643e-2	4.092915e-2	4.082648e-2
Taylor LES model	4.644998e-2	4.337106e-2	4.162151e-2
rational LES with auxiliary problem	5.362197e-2	4.354168e-2	4.156234e-2
rational LES with convolution	5.410823e-2	4.377640e-2	4.160454e-2

Table 3: H^1–semi norm for the stationary state, $Re = 400$.

model	$h = 1/16$	$h = 1/32$	$h = 1/64$
Galerkin FEM	4.758018	5.010872	5.284203
Taylor LES model	4.505765	4.876411	5.232359
rational LES with auxiliary problem	4.756212	4.967851	5.257608
rational LES with convolution	4.659970	4.920823	5.241819

Table 4: Difference in L^2–norm to Galerkin FEM solution of the Navier–Stokes equations, $Re = 400$.

model	$h = 1/16$	$h = 1/32$	$h = 1/64$
Taylor LES model	4.875961e-2	1.827302e-2	5.417927e-3
rational LES with auxiliary problem	5.074473e-2	1.395288e-2	1.866429e-3
rational LES with convolution	5.661102e-2	1.576287e-2	4.600475e-3

Table 5: Difference in H^1–semi norm to Galerkin FEM solution of the Navier–Stokes equations, $Re = 400$.

model	$h = 1/16$	$h = 1/32$	$h = 1/64$
Taylor LES model	1.996393e+0	1.133348e+0	6.001845e-1
rational LES with auxiliary problem	8.116643e-1	3.687168e-1	1.208750e-1
rational LES with convolution	9.719111e-1	4.734631e-1	2.626503e-1

3.2 The high Reynolds number flow

3.2.1 The Blow Up of the Taylor LES Model

Simulations with the Taylor LES model with Smagorinsky type turbulent viscosity of form (6) blow up in finite time for $RE = 10000$, see Figures 6 - 12. Table 6 shows that a refinement of the spatial mesh does not prevent the blow up. A reduction of the time step on the same mesh level prevents the blow up but on the next finer mesh level the model blows up again. The scalings in Table 6 show that this does not occur as a function only of $\Delta t/\Delta x$, i.e., the blow up is not related to a simple CFL–type condition. When solving the driven cavity with an impulsive start, Gresho and Sani [GS98] have shown that there is an initial, non–physical transient that makes small time approximate solutions questionable. This small time transient did not influence the blow up behaviour because the same behaviour was observed when starting instead with fully developed flows as initial condition. Indeed, when we used the solutions of the other models for $h = 1/64$ at $T = 1000$ as initial conditions, see right lower picture in Figure 8 for the Galerkin FEM of the Navier–Stokes equations, the Taylor LES model blew up within only few time steps, see Figures 4 and 5! Thus, the impulsive start is not responsible for the failing of the Taylor LES model.

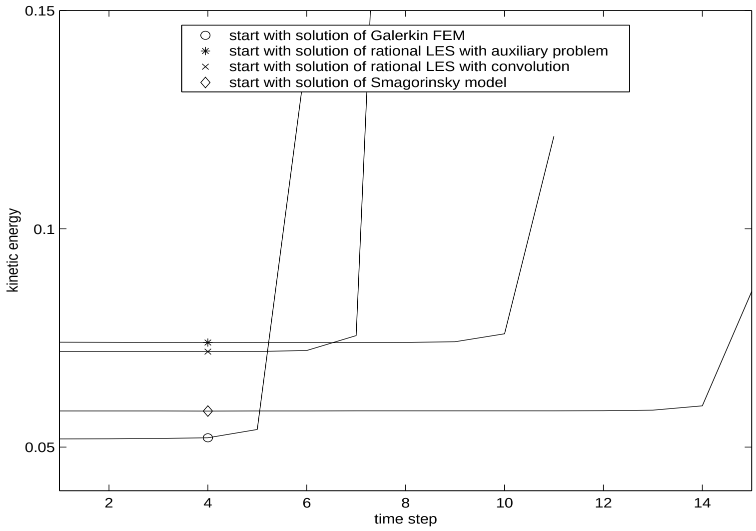


Figure 4: Blow up of Taylor LES model starting with various fully developed flow fields as starting conditions at $t = 1000$, $h = 1/64$, $\delta = \sqrt{2}/64$, $Re = 10000$. Note that the blow up does not depend on using an impulsive start.

Table 6: Blow up times for Taylor LES model, $Re = 10000$, $\delta = \sqrt{2}/64$. Note that the blow up behaviour changes if δ is fixed and Δt and h are reduced.

Δt	$h = 1/64$	$h = 1/128$
10^{-1}	$2\,10^{-1}$	10^{-1}
10^{-2}	$19\,10^{-2}$	$2\,10^{-2}$
10^{-3}	no blow up	$8\,10^{-3}$
10^{-4}	no blow up	$239\,10^{-4}$

The failure of the Taylor LES model is consistent with results reported by Coletti [Col98]. He reports blow up of this model for $RE = 10000$ and the P_2/P_1 finite element discretization. In other calculations, we have observed the same for the Taylor/Hood finite element on a quadrilateral grid

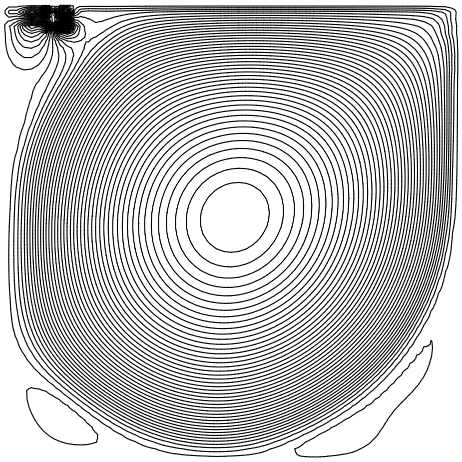


Figure 5: Streamlines of Taylor LES model solution just before blow up (time step 15 starting with the Smagorinsky model solution).

(Q_2/Q_1). Thus, it seems clear that the Taylor LES model for large eddies does indeed stimulate rather than attenuate small eddies and it does not work in its unmodified form.

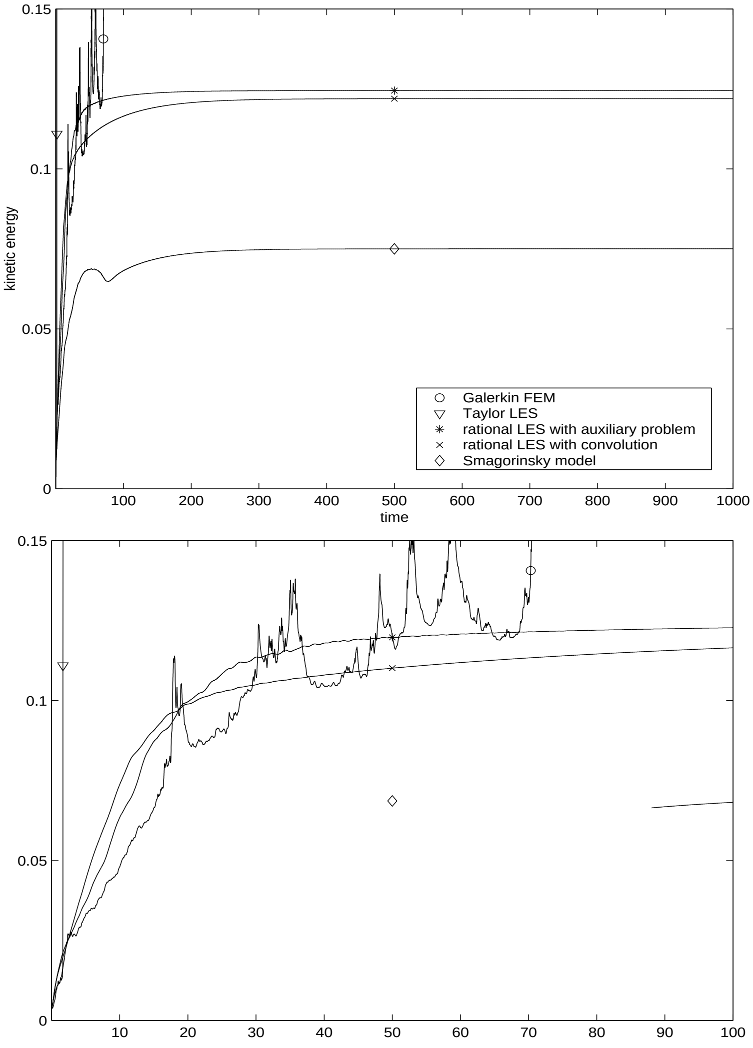
3.2.2 The Behaviour of the Rational LES Model

For the rational LES model with the auxiliary problem and the rational LES model with convolution, both with turbulent viscosity of type (6), the kinetic energy behaves consistently for all parameters in contrast to the Taylor LES model, see Figures 6 - 12. Both variants of the rational LES model give similar results for the global energy balance for all tests. From the computational point of view, we found that the regularization using the auxiliary problem is cheaper than performing a convolution.

The computations for the mesh widths $h = 1/16$ reflect best the normal condition for the numerical simulation of turbulent flows which is a very coarse mesh compared to the Reynolds number. The results in Figures 6 and 7 show the blow up of the Galerkin FEM for the Navier–Stokes equations and the Taylor LES model. A comparison of the computed flow fields with the flow field of the Galerkin FEM of the Navier–Stokes equations on a much finer grid, Figure 8, shows that the solutions of the rational LES model are reasonable whereas the Smagorinsky model is overly diffusive.

The energy balance of the solutions obtained with the Galerkin FEM for the Navier–Stokes equations is considerably different for $h = 1/32$ and $h = 1/64$. This indicates that the discretization error in space is still relatively large. The kinetic energy of the discrete solutions in all models decreases for finer meshes. For $h = 1/32$, the kinetic energy of the solution with the Galerkin FEM of the Navier–Stokes equation is larger than for the solution of the Galerkin FEM of the Smagorinsky model whereas the situation for $h = 1/64$ is vice versa. The kinetic energy of the solutions for both types of the rational LES was always somewhat larger than for the solutions of the Galerkin FEM of the Navier–Stokes equations and the Smagorinsky model.

Both variants of the rational LES model as well as the Smagorinsky model show a smoothing effect on the discrete solution. This can be seen from the fact that the H^1–semi norms of the discrete solutions is considerably smaller than for the discrete solution obtained with the Galerkin FEM of the Navier–Stokes equations, Figures 10 and 12. This can be expected since the solution of the LES models approximates $g_\delta * \mathbf{u}$ which is $C^\infty(\mathbb{R}^d)^d, d = 2, 3$, for any $\mathbf{u}$ having bounded kinetic energy.


0.15
0.1
0.05
0
kinetic energy
100
200
300
400
500
600
700
800
900
1000
time
○ Galerkin FEM
▽ Taylor LES
✳ rational LES with auxiliary problem
× rational LES with convolution
◇ Smagorinsky model
0.15
0.1
0.05
0
10
20
30
40
50
60
70
80
90
100