OPTIMIZATION OF AN IMPLICIT SUBGRID-SCALE MODEL FOR LES

S. Hickel*, S. Franz*, N.A. Adams*, P. Koumoutsakos**
*Dresden University of Technology, Institute of Fluid Mechanics, 010162 Dresden, Germany
**ETH Zürich, Institute of Computational Sciences, Switzerland

Summary We give a summary of the derivation of an implicit subgrid-scale model for LES which is obtained from a new approach for the approximation of hyperbolic conservation laws. Adaptive local deconvolution is performed using a quasi-linear solution-adaptive combination of local interpolation polynomials. The physical flux function is substituted by a suitable numerical flux function. The truncation error has physical significance and effectively acts as subgrid-scale model. It can be determined by a modified-differential-equation analysis and is adjustable through free parameters. Computational results for Burgers equation show that the model with parameters identified by evolutionary optimization give significantly better results than other models.

INTRODUCTION

The key idea of implicit subgrid-scale (SGS) modeling is that the truncation error of an under-resolved discretization can be utilized to model the effects of the unresolved scales. In order to reveal the connection of implicit to explicit SGS models the differential equation has to be analysed [1, e.g.]. Without loss of generality we initially focus on a generic scalar conservation law $\partial_t u + \partial_x F(u) = 0$. The finite-volume semi-discretization

$$\partial_t \bar{u}_N + G * \partial_x F_N(u_N) = \varepsilon_{SGS} \tag{1}$$

is based on applying an explicit spatial filtering $\bar{u} = G * u$, where G is the top-hat function with the spatial averaging scale h. The grid function $\bar{u}_N = \{\bar{u}_j\}$ results from the spectrally accurate projection $\bar{u}_j \approx \bar{u}(x_j)$. The cutoff frequency $\xi_C = \pi/\Delta$ is linked to the spatial grid spacing Δ and to the spatial filter scale $h = \Delta$. In the case of LES, characterized by (under-resolved) finite grid spacing, a non-closed subgrid-scale error $\varepsilon_{SGS} = G * \partial_x F_N(u_N) - G * \partial_x F_N(u)$ remains on the right hand side due to the nonlinearity of $F(u)$. Common practice is to close (1) by an explicit model of the SGS stresses τ which approximates $\varepsilon_{SGS} = -\partial_x \tau$.

CONSTRUCTION OF THE IMPLICIT SGS MODEL

As shown in [2] it is desirable to exploit the deconvolved solution $u_N = G^{-1} * \bar{u}_N$. Since the used top-hat filter is not fully invertible the application of any approximate inverse $\tilde{u}_N = \tilde{G}_N^{-1} * \bar{u}_N$ results in an additional error term. Finally, we replace the physical flux function by a more suitable numerical flux function $\tilde{F}_N$. If the resulting cumulative numerical truncation error $\varepsilon_N = G * \partial_x F_N(u_N) - G * \partial_x \tilde{F}_N(\tilde{G}_N^{-1} * \bar{u}_N)$ approximates ε_{SGS}, the implicit SGS model contained in the numerical discretization

$$\partial_t \bar{u}_N + G * \partial_x \tilde{F}_N(\tilde{u}_N) = 0 \tag{2}$$

substitutes the explicit model. Thus the construction of an implicit SGS model amounts to devise an appropriate adaptive deconvolution operator and a suitable numerical flux function. Consistently with the framing finite-volume approach, the top-hat filtering of the one-dimensional flux divergence in (2) returns the difference of the flux trough the cell faces $x_{j\mp 1/2}$, while the filtered solution $\bar{u}_N$ is known at the cell centers only. Following the suggestion in [3] intended for Essentially-Non-Oscillatory (ENO) schemes, the required reconstruction of point values of the deconvolved solution can be determined by the interpolation polynomials $u(x_{j\pm 1/2}) = \sum_{l=0}^{k-1} c^{\mp}_{j,k,r,l} \bar{u}_N(x_{j-r+l}) + \mathcal{O}(h^k)$, where the coefficients $c^{\mp}_{j,k,r,l}$ contain the grid-dependend deconvolution and interpolation operator which can be computed with a rule given by [3]. The shift $r = 0, \ldots, (k-1)$ characterises the treated stencil. The main idea of weighted ENO is the linear combination of reconstructions of a single order $k \equiv K$ to obtain a approximation of order $2K - 1$ in smooth regions. We extend this scheme by also including the computationally cheaper reconstructions of order $k = 1, \ldots, K$

$$\tilde{u}_N^{\mp}(x_{j\pm 1/2}) = \sum_{k=1}^{K} \sum_{r=0}^{k-1} \omega^{\mp}_{k,r}(x_j) p^{\mp}_{k,r}(x_{j\pm 1/2}) \qquad \text{with} \qquad p^{\mp}_{k,r}(x_{j\pm 1/2}) = \sum_{l=0}^{k-1} c^{\mp}_{j,k,r,l} \bar{u}_N(x_{j-r+l}). \tag{3}$$

Since highest possible order of accuracy is not required, free parameters can be introduced. The weights $\omega^{\mp}_{k,r}(x_j)$ are computed from a solution-dependend function $\beta_{k,r}(x_j)$ which is used as smoothness measure and from a set of constant parameters $\gamma^{\mp}_{k,r}$ which denote stencil-selection preferences in particular allow to adjust the truncation error [4] .

REPRODUCTION OF EXPLICIT SGS MODELS

Since the model should depend on the kind of nonlinearity, the following analysis is limited to the viscous Burgers equation $F(u) = u^2/2 - 1/Re\ \partial_x u$, which is the relevant model for the Navier-Stokes equation. As mentioned above, the dominating terms of the implicit SGS model are identified by comparing the modified differential equation (2) with the exact LES equation (1). The model parameters can be adjusted in order to reproduce approved explicit SGS models. We found a set of parameters for $K = 3$ that matches with the standard Smagorinsky model $-\partial_x \tau = 2C_S h^2 |\partial_x \bar{u}| \partial_x^2 \bar{u}$ up to order $\mathcal{O}\left(h^3\right)$

$$\varepsilon_N = 2\,C_S\,\left|\partial_x \bar{u}\right|\,\partial_x^2 \bar{u}\,h^2 - \frac{1}{6}\,C_S\,\left|\partial_x \bar{u}\right|\,\partial_x^4 \bar{u}\,h^4 + \mathcal{O}\left(h^6\right)\ . \tag{4}$$

For validation, simulations of statistically forced and decaying turbulence of the viscous Burgers equation were performed with this implicit model. In both cases we observe a good agreement with the reference data computed with a de-aliased spectral discretization where the Smagorinsky SGS model is added explicitly (Fig. 1).

OPTIMIZATION OF THE IMPLICIT SGS MODEL

If computations with the implicit model produce results of comparable quality as common explicit models, the benefit is in the implicit character which removes computational overheads of explicit SGS models. Other parameters, however, may yield much better results than those matched to explicit models. In order to identify them, one has to evaluate the implicit model by defining a cost function for every test case. For the stochastically forced Burgers equation a suitable criterion is the grade of agreement of the inertial range of the time-averaged energy spectrum with theoretical predictions. There are, however, two major difficulties: First the dependency of parameters and spectra is unknown, and second, the effects of random forcing result in an ambiguous cost function. Therefore traditional optimization strategies are not applicable. The idea of Evolutionary Optimization (EO) adopts concepts with random components as selection, recombination and mutation [5]. The application on the above mentioned test case shows nearly monotone convergence which slows down after 200 generations and leads to a set of parameters that results in the effective model

$$\varepsilon_N = \left(-0.11108\,\left(\partial_x^2 \bar{u} \partial_x \bar{u} + \partial_x^3 \bar{u} \bar{u}\right) + 0.66667\,|\partial_x \bar{u}| \partial_x^2 \bar{u}\right)\,h^2 + \mathcal{O}\left(h^4\right)\ . \tag{5}$$

Computational results for stochastically forced Burgers equation show that these model parameters give significantly better results than parameters from other models (Fig. 1).

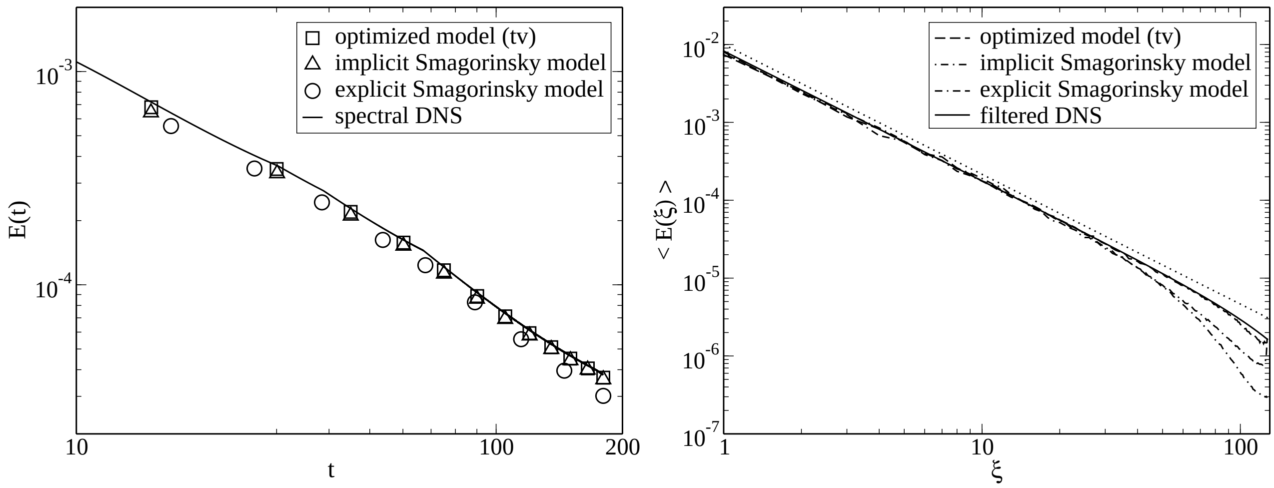

Figure 1. *Left:* decaying turbulence: temporal evolution of total energy; *Right:* forced turbulence: time-averaged energy spectra

CONCLUSIONS

Subgrid-scale model and discretization of a conservation law can be merged. Systematical optimization of the presented implicit SGS model results in an superior model, which has been successfully applied to the one-dimensional Burgers equation. The extension of the optimization to three-dimensional Navier-Stokes equation is subject of ongoing work.

References

[1] Margolin, L.G. ; Rider, W.J. (2002) A rationale for implicid turbulence modelling. Int. J. Numer. Meth. Fluids 39 : 821-841
[2] Adams, N.A. ; Stolz, S. (2002) A subgrid-scale deconvolution approach for shock capturing. J. Comput. Phys. 178 : 391-426
[3] Shu, C.W. (1997) Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws. Technical Report 97-65, NASA Langley Research Center, Hampton, Virginia
[4] Adams, N.A. ; Hickel, S. ; Franz, S. (2004) Implicit subgrid-scale modeling by adaplive deconvolution. J. Comput. Phys. (in press)
[5] Beasley, D. ; Bull, D., Martin, R. (1993) Overview of Genetic Algorithms Part I and II. University Computing