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Adjoint based model adaptation for a linear problem

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SUMMARY

In aerospace engineering CFD is often applied to obtain values for quantities of interest which are global functionals of the solution. To optimise the balance between accuracy of the computed functional and CPU time we focus on dual-weighted adaptive hierarchical modelling of fluid flow. In this paper we study estimation of the model error in a quantity of interest and present an adaptive modelling strategy to meet the required accuracy for a quantity of interest in a linear elliptic model problem.

KEY WORDS: Model error, model adaptation, dual-weighted-residual method

INTRODUCTION

In aerospace engineering Computational Fluid Dynamics (CFD) is often applied to obtain values for quantities of interest which are global functionals of the (discrete) solution. Examples are the lift, drag and aerodynamic moments. These quantities may be used to compute control and stability derivatives necessary in flight simulation models for flight simulators, which is our ultimate application. The required accuracy of the stability and control derivatives and the large number of computations required to cover the complete flight envelope of an aircraft are conflicting demands. In the class of hierarchical fluid flow models the sophisticated models, e.g. (Reynolds-Averaged) Navier-Stokes, are suitable to obtain accurate values for output functionals but are computing intensive. As alternatives we have cheaper but less sophisticated models such as potential flow methods.

To optimise the ratio of accuracy of the output functional and CPU time we focus on dual-weighted adaptive hierarchical modelling of fluid flow. The dual-weighted residual method, first introduced by Becker and Rannacher [1] for *a posteriori* discretisation error control, couples the model residual (or discretisation residual in the original case) to the output functional by the dual or adjoint variables (the weights). This coupling provides us with an estimate for the

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model error in the output functional. This requires the solution of an adjoint problem. The main theory on model error estimation and adaptive methods for hierarchical modelling in computational mechanics has been formulated by Oden and others in [4, 5, 6, 7]. A combined model and mesh adaptation strategy can be found in [2].

In this work we present an adaptive modelling algorithm and apply it as a first step toward application in fluid flow problems, to a linear 1-D elliptic model problem of which exact primal and dual solutions exist. The quality of the model error estimator and the use of the estimator as a correction on the computed output functional are studied. Furthermore, the influence of a tolerance parameter on the adaptive model algorithm in a discrete setting is analysed.

MODEL ERROR ESTIMATION IN LINEAR PROBLEMS

Based on the work of Oden and Prudhomme [4] we give a brief summary of the estimator in case of a linear problem. Consider a continuous linear model on Ω governed by a linear differential operator L, representing a *sophisticated* or *fine* model, and a sourceterm f:

$$Lu = f, \quad u \in \mathbf{V}, \tag{1}$$

with $\mathbf{V}$ a suitable normed function space. We want to evaluate the linear (or linearised) functional $Q(u) = \langle g, u \rangle$ from the solution of (1), with g a density function associated with $Q(\cdot)$ and $\langle \cdot, \cdot \rangle$ representing an inner product on $\mathbf{V}$. The Lagrangian system corresponding to the constrained minimisation problem of minimising $Q(u)$ subject to $Lu = f$, results in the adjoint equation:

$$L^* p = g, \quad p \in \mathbf{V}. \tag{2}$$

The fine model equations (1) and (2) can be approximated by the *coarse* model equations, indicated by the subscript 0, given by:

$$L_0 u_0 = f \quad \text{and} \quad L_0^* p_0 = g, \quad u_0, p_0 \in \mathbf{V}_0. \tag{3}$$

where u_0 corresponds to an approximation of u if $\mathbf{V}_0 = \mathbf{V}$ (which we assume further). The model error in Q is now given by the following expression, with $e_0 = u - u_0$ and $\epsilon_0 = p - p_0$ the primal and dual errors, respectively:

$$\begin{aligned} Q(u) - Q(u_0) = Q(e_0) = \langle g, u - u_0 \rangle = \langle L^* p, u - u_0 \rangle = \\ = \langle p, f - Lu_0 \rangle = \langle p_0, f - Lu_0 \rangle + \langle \epsilon_0, f - Lu_0 \rangle. \end{aligned} \tag{4}$$

Since it is not economical to solve the fine dual problem, we have split the estimator in (4) in a model residual $f - Lu_0$ weighted by a computable coarse dual variable p_0 and by a dual error ϵ_0. The latter term can be ignored for adaptation purposes or estimated. A bound on the estimate for the dual error contribution $\langle \epsilon_0, f - Lu_0 \rangle$ in (4) can be derived using the norms of the primal and dual residuals denoted by Λ and Λ^*, respectively, and the smallest singular value of L, λ_m^L:

$$|\langle \epsilon_0, f - Lu_0 \rangle| = |\langle L^*(p - p_0), L^{-1}(f - Lu_0) \rangle| \leq |(\lambda_m^L)^{-1}| \, \|\Lambda^*\| \, \|\Lambda\|. \tag{5}$$

For this, the singular value has to be estimated by, for instance, computing the Rayleigh quotient. Finally, the estimated error from (4) can be used as a correction on the computed coarse output functional $Q(u_0)$ by:

$$Q_c(u_0, e_0) = Q(u_0) + Q(e_0). \tag{6}$$

DISCRETE APPROACH AND ADAPTATION ALGORITHM

For 'real life' engineering problems we apply a discrete approach to solve the problem given by the equations (1) and (2), and to the model error estimator (4). This introduces a discretisation error. With $u_0^h \in \mathbf{V}^h \subset \mathbf{V}$ the discrete approximation of u_0, the contributions from model error and discretisation error can be separated according to:

$$Q(u) - Q(u_0^h) = Q(e_0^h) = [Q(u) - Q(u_0)] + [Q(u_0) - Q(u_0^h)]. \tag{7}$$

In the present study we concentrate on adaptive modelling and leave mesh adaptation as a topic for further research (see also [2] for combined mesh and model adaptation). $Q(e_0^h)$ is estimated by the simplest, computationally inexpensive, formulation by using only the coarse dual solution as weight, so $Q(e_0^h) \approx \tilde{Q}(e_0^h) = \langle p_0, f - Lu_0 \rangle$. In the discrete approach with N the number of the degrees of freedom and $L_{i,j}$ the discrete representation of the differential operator, we compute the coarse model contribution of equation (4) by:

$$Q(u) - Q(u_0^h) \approx \tilde{Q}(e_0^h) = \sum_{i=1}^{N} p_{0\,i}^h \Lambda_i^h = \sum_{i=1}^{N} p_{0\,i}^h \sum_{j=1}^{N} (f_i - L_{i,j} u_{0\,j}^h). \tag{8}$$

For the model adaptation algorithm a localisation of the (estimated) model error is required, which is achieved by considering the individual contribution of each element in (8), indicated by e_Q^l.

Model adaptation algorithm

The implemented model adaptation strategy is inspired by the work of Oden and Vemaganti [6] on goal-oriented adaptive modelling of heterogeneous materials, and is given in the following scheme:

`do while` $|\tilde{Q}(e_0^h)| > \alpha_{\text{tol}} |Q(u_0^h)|$

- `compute approximate solutions` u_0^h `and` p_0^h
- `estimate the global model error` $\tilde{Q}(e_0^h)$
- `determine contribution of individual elements` e_Q^l
- `if` $|e_Q^l| > \frac{1}{N} \beta_{\text{tol}} |\tilde{Q}(e_0^h)|$
  - `refine model of element` l
  - `re-assemble the global matrix`

The estimated model error is compared to the estimated value of the output functional multiplied with a global tolerance parameter α_{tol} which is set by the user. A posteriori, the model error can be given with respect to the corrected output functional $Q_c(u_0^h, e_0^h)$.

When the individual contribution of each element to the global error estimator exceeds the local threshold the model in the corresponding element is refined. A suitable choice of β_{tol} is problem dependent. In the model problem we investigate the influence of β_{tol}. A small value of β_{tol} minimises the number of adaptation loops and a large value minimises the size of sub-domain(s) in which the fine model is applied.

RESULTS FOR A MODEL PROBLEM

The linear model problem consists of a 1-D Helmholtz equation as fine model and a 1-D Poisson equation as coarse model on $\Omega = [0,1]$. For the discrete approach the problem has been discretised by means of finite elements with continuous linear elements. The Helmholtz equation on the unit interval is given by:

$$Lu := -u_{xx} + k^2 u = 0, \quad x \in \Omega, \quad u \in \{\mathrm{C}^2, u(0) = 0, u(1) = 1\}, \tag{9}$$

with $k \in \mathbf{R}^+$ a parameter determining the difference between the models. A special case is $k = 0$, resulting in the coarse model Poisson equation denoted by L_0. The details and exact solutions of the primal and dual equations can be found in [3]. Since the equations are self-adjoint, we use the same matrix to compute the primal and dual solutions. The considered output functional $Q(u) = \langle g, u \rangle$ is the integral of u over Ω (i.e. $g = 1$).

Numerical tests are performed with $N = 10$ for β_{tol}=0.5, 1.0, 1.5, $k = 2$ (giving $Q(u) = .38080...$) and a global error tolerance level $\alpha_{\text{tol}} = 0.05$. The results of the error estimator together with the exact error and the adaptation algorithm are given in table I. In figure 1 the discrete approximated primal solutions during the computations for β_{tol}=1 are shown together with the exact fine and coarse model solution. The effectivity index I_{eff} is defined as $I_{\text{eff}} = \tilde{Q}(e_0^h)/Q(e_0)$ and L/L_0 is the ratio of number of Helmholtz over number of Poisson elements.

β_{tol}	run	L/L_0	$Q(u_0^h)$	$\tilde{Q}(e_0^h)$	$Q(e_0)$	$Q(u) - Q_c(u_0^h, e_0^h)$	I_{eff}
-	0	0	0.5	-1.6500e-01	-1.1920e-01	4.5797e-02	1.38
0.5	1	.8	0.38481	-4.2573e-03	-4.0111e-03	2.4615e-04	1.06
1.0	1	.6	0.39404	-1.3039e-02	-1.2330e-02	1.1187e-04	1.06
1.5	1	.3	0.43038	-5.8524e-02	-4.9587e-02	8.9373e-03	1.18
	2	.6	0.39313	-1.3039e-02	-1.2330e-02	7.0879e-04	1.06

Table I. Model error estimation and effectivity for α_{tol}=0.05, $\beta_{\text{tol}} = 0.5$, 1, 1.5 (k=2).

Comparison of the results for different β_{tol} from table I shows that with $\beta_{\text{tol}} = 0.5$ and 1 the prescribed accuracy is obtained after one adaptation step, but with $\beta_{\text{tol}} = 0.5$ more elements are refined to the fine model. Although this model problem does not illustrate the CPU time savings when model adaptivity is applied one can understand that in large-scale 3-D problems, adapting 60 or 80% of the domain may imply a significant difference in CPU time. Computations with $\beta_{\text{tol}} = 1.5$ require 2 adaptation steps to meet the required tolerance and therefore one can conclude that $\beta_{\text{tol}} = 1.5$ is too high (the same number of elements are refined as in the case of $\beta_{\text{tol}} = 1$, but 2 adaptation steps are required). In this case $\beta_{\text{tol}} = 1.0$ is most effective.

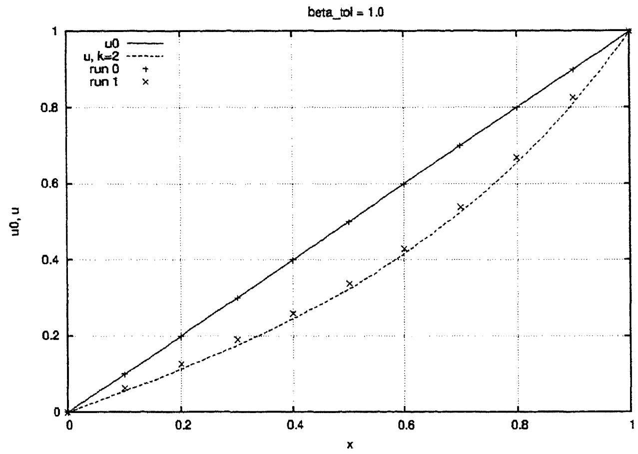

Figure 1. Primal solution during adaptation for β_{tol}=1 (k=2).

In addition, table I shows that using the estimated error as a posteriori correction on Q gives a large gain in accuracy of the computed output functional. The exact error after correction, $Q(u) - Q_c(u_0^h, e_0^h)$, drops at least one order of magnitude.

Table I shows that the quality of the estimator $\tilde{Q}(e_0^h)$ increases (the effectivity index approaches 1) after model adaptation. This is due to transformation of coarse model elements into fine model elements (i.e. p_0^h approaches p^h) resulting in a more accurate model error estimator. Observation shows that using the corrected output functional $Q_c(u_0^h, e_0^h)$ in the adaptation algorithm instead of $Q(u_0^h)$ does not result in better performance of the adaptation algorithm due to strong over-estimation of $\tilde{Q}(e_0^h)$ in the first step.

Discretisation error

In this model problem the discretisation error $Q(u_0) - Q(u_0^h)$ (in the second column of table II) is two orders of magnitude smaller than the estimated model error $\tilde{Q}(e_0^h)$ (as well as the exact $Q(e_0) = -0.11920...$) in case of N=10 and four orders of magnitude lower with N=100 (without model refinement). However, after model adaptation the order of magnitude of the model error gets closer to the discretisation error. This illustrates the importance combined model and mesh adaptation. The estimate $\tilde{Q}(e_0^h)$ seems to become 'worse' with increasing number of elements, but this is caused by the better approximation of the (over-predicting) coarse model error estimate $\langle p_0, \Lambda \rangle = -1/6$ (see [3] for details on the model problem).

N	$Q(u_0) - Q(u_0^h)$	$\tilde{Q}(e_0^h)$	$\lvert\langle \epsilon_0, \Lambda \rangle\rvert$	$\lvert(\lambda_m^L)^{-1}\rvert \, \lVert\Lambda^{*h}\rVert \, \lVert\Lambda^h\rVert$	$I_{\text{eff}}^{(1)}$	$I_{\text{eff}}^{(2)}$
10	1.2685e-03	-1.6500e-01	4.74637e-02	6.1851e-02	1.30	0.87
100	1.2693e-05	-1.6665e-01	4.74637e-02	6.0811e-02	1.28	0.89

Table II. Discretisation error and bound of $\langle \epsilon_0, \Lambda \rangle$.

Estimate of the dual error contribution

Although adaptation using the coarse dual-weighted estimator $\tilde{Q}(e_0^h)$ works satisfactory for this model problem, we investigate the bound of $\langle \epsilon_0, \Lambda \rangle$ by (5), since for large-scale 3-D problems using only the coarse dual-weighted estimator as in (8) might not be sufficient accurate for adaptation purposes. Table II shows the effectivity indexes for the bound and for the 'total estimate', i.e. $\tilde{Q}(e_0^h)$ plus the computed bound, which are, respectively, given by:

$$I_{\text{eff}}^{(1)} = \frac{|(\lambda_m^L)^{-1}| \, \|\Lambda^{*h}\| \, \|\Lambda^h\|}{|\langle \epsilon_0, \Lambda \rangle|} \quad \text{and} \quad I_{\text{eff}}^{(2)} = \frac{\tilde{Q}(e_0^h) + |(\lambda_m^L)^{-1}| \, \|\Lambda^*\| \, \|\Lambda\|}{Q(e_0)}.$$

As can be seen in table II the computed bound (8) over-predicts the dual error contribution and is therefore not suitable to be used in the adaptation algorithm in this case. In addition, the computation of the smallest singular for large-scale 3-D problems value will be complicated and computing intensive. Therefore, computing the estimate of the dual error contribution by (8) is not a suitable method to improve the model error estimator $\tilde{Q}(e_0^h)$.

CONCLUSIONS AND PERSPECTIVES

We have studied a dual-weighted model error estimator for an output functional and a corresponding adaptive modelling algorithm. The error estimator based on the coarse dual solution as weight for the model residual and the adaptation algorithm were implemented in a discrete 1-D linear elliptic problem. The coarse model dual solution is found to be sufficient for adaptation purposes. A bound of the dual error contribution $\langle \epsilon_0, \Lambda \rangle$ does not improve the initial total error estimator for this problem, as shown by the effectivity index. The effect of the local adaptation tolerance parameter β_{tol} on the adaptation algorithm has been studied. An optimal value for the linear elliptic model problem of $\beta_{\text{tol}} = 1$ was found. In that case adaptation is most efficient in terms of accuracy of the output functional and CPU time. A posteriori correction of the computed output functional $Q(u_0^h)$ using the error estimator shows a significant gain in accuracy in the estimate of $Q(u)$.

In future research we will focus on model error estimation and adaptive modelling in unsteady non-linear problems in a finite volume formulation 2 and 3 dimensions.

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