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MODEL ERROR ESTIMATION IN GLOBAL FUNCTIONALS BASED ON ADJOINT FORMULATION

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Abstract. *In aerospace engineering Computational Fluid Dynamics (CFD) is often applied to obtain values for quantities of interest which are global functionals of the solution of the CFD computation. For instance the lift, drag and control- and stability derivatives necessary in flight simulation models for flight simulators. In the application for flight simulation models it would require years of performing CFD computations to generate such a model. One way of reducing the computational time is to apply a mathematical fluid flow model which is sufficiently sophisticated to compute the quantity of interest with the required accuracy. The ultimate goal is to apply a model adaptive strategy which adapts the 'coarse' mathematical model (in parts of the computational domain) to a more sophisticated model when the modelling error in the quantity of interest is too large. This approach requires the application of adjoint techniques to couple the local modelling errors to the global quantity of interest. In this paper we study global modelling error estimation in a quantity of interest by a dual weighted residual method, as described in [2], to a simple linear, scalar model problem of which the analytical solutions are known exactly.*

1 INTRODUCTION

In aerospace engineering mathematical models for fluid flows with different levels of sophistication are being used: full-potential, Euler and (Reynold-Averaged) Navier-Stokes. The user of Computational Fluid Dynamics (CFD) codes judges what model is most appropriate based on the required accuracy and the efficiency. Choices are mostly based on a-priori knowledge of the flow and efficiency of the available codes. In CFD computations the main source of errors in the solution are discretisation errors due to the applied discretisation scheme and modelling errors due to the use of less sophisticated mathematical models. Verification and validation are generally applied to quantify the discretisation and modelling error, respectively. Moreover, engineers are mostly interested in specific quantities of interest which are global functionals of the solution of the mathematical flow model (such as lift and drag). When the solution of a less sophisticated (or 'coarse') model is sufficient to compute the quantity of interest with acceptable accuracy, the engineer will choose to use the coarse model from the point of view of efficiency. Therefore the ultimate goal is to adapt the flow model to obtain the desired accuracy of the quantities of interest efficiently. This requires estimation of the modelling error in the quantity of interest. In this paper we study the estimation of the modelling error in a quantity of interest by using the framework developed in [2] for an abstract variational problem. A linear scalar model problem is chosen to gain insight in the effectiveness and limits of the method.

2 THE MODEL PROBLEM: HELMHOLTZ VS. POISSON EQUATION

We take a Helmholtz-type equation and a Poisson-type equation to describe the same phenomenon and define the Helmholtz-type equation as the 'fine' model and the Poisson-type equation as the 'coarse' model. For both problems we take exactly the same Dirichlet boundary conditions[1] (In the remainder of this paper, the Helmholtz- and Poisson-type equation are shortly called the Helmholtz and Poisson equation, respectively). The Helmholtz equation on the unit interval is given by:

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

with L the Helmholtz differential operator and $k \in \mathbf{R}^+$ a parameter which will be used to simulate the difference between both models (the larger k the 'coarser' the approximation of the Helmholtz equation by the Poisson equation). The Poisson equation is given by:

$$L_0 u_0 := -u_{0xx} = 0 \quad x \in (0,1), \quad u_0(x) \in \{C^2, u_0(0) = 0, u_0(1) = 1\}, \tag{2}$$

with L_0 the Poisson differential operator. The quantity of interest, further called output functional, Q in our model problem is also linear and is chosen to be:

[1] In more complicated problems the fine model may require additional boundary conditions.

$$Q(u) = \int_0^1 u(x)dx. \tag{3}$$

3 EXACT MODELLING ERROR

To check the results of the modelling error estimation by adjoint formulation, to be described in the next section, we first compute the exact modelling error using the exact solutions of the Helmholtz and Poisson equation, (1) and (2), respectively:

$$u(x) = \frac{e^{kx} - e^{-kx}}{e^k - e^{-k}} \tag{4}$$

and

$$u_0(x) = x. \tag{5}$$

For $k = 1, 2, 4$ the solutions are shown in figure 1. In case of $k = 1$ the values of Q for the fine and coarse model are $Q(u) = .46212...$ and $Q(u_0) = \frac{1}{2}$, respectively.

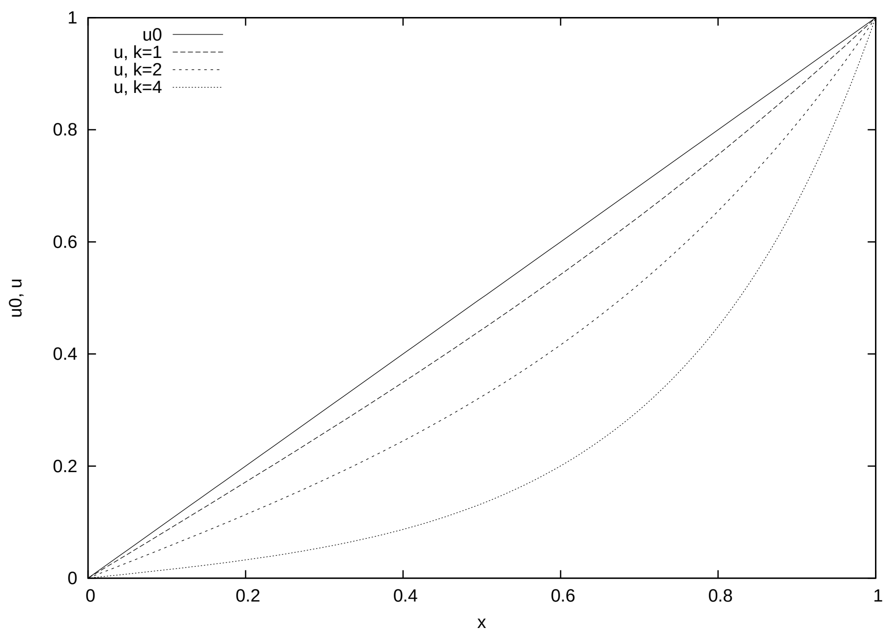

Figure 1: Coarse and fine model solution (for $k = 1, 2, 4$)

The modelling error in the output functional is given by:

$$Q(u) - Q(u_0).$$

The exact modelling error $Q(u) - Q(u_0) = Q(u - u_0)$ is given by the following integral:

$$\int_0^1 \left(\frac{e^{kx} - e^{-kx}}{e^k - e^{-k}} - x \right) dx = \frac{1}{k} \frac{e^{kx} + e^{-kx}}{e^k - e^{-k}} - \frac{1}{2} x^2 |_0^1 = \frac{e^k + e^{-k} - 2}{k(e^k - e^{-k})} - \frac{1}{2}.$$

4 DUAL FORMULATION OF THE PROBLEM

In general the output functional Q may consist of an integral over the domain Ω and over the boundary of the domain $\partial\Omega$:

$$Q = \langle g, u \rangle_\Omega + \langle h, Cu \rangle_{\partial\Omega} \tag{6}$$

where $\langle \cdot, \cdot \rangle$ denotes an integral inner product over Ω or $\partial\Omega$:

$$\langle a, b \rangle_\Omega = \int_\Omega ab \; d\Omega \quad \text{and} \quad \langle a, b \rangle_{\partial\Omega} = \int_{\partial\Omega} ab \; d\partial\Omega.$$

In order to define the corresponding dual problem we formally set u and p in a Hilbert subspace $\mathbf{H}$ of $L^2(0,1)$ so the inner product $\langle p, Lu \rangle$ is finite $\forall \; p \in \mathbf{H}$ and u satisfying the boundary conditions $Bu = e$, as given in (1). The corresponding dual form of the output functional becomes now:

$$Q = \langle p, f \rangle_\Omega + \langle C^* p, e \rangle_{\partial\Omega} \tag{7}$$

with f the right hand side of the primal problem $Lu = f$ and given that $L^* p = g$ on Ω and that the dual boundary conditions $B^* p = h$ are satisfied. The general adjoint identity to be satisfied is found by the equivalence of the primal and dual form of Q as shown in Giles and Pierce [1]:

$$\langle p, Lu \rangle_\Omega + \langle C^* p, Bu \rangle_{\partial\Omega} = \langle L^* p, u \rangle_\Omega + \langle B^* p, Cu \rangle_{\partial\Omega}. \tag{8}$$

The specific form of (8) for the Helmholtz equation is found by integration by parts of $\langle p, Lu \rangle$ and yields:

$$\langle p, Lu \rangle = \int_0^1 p(-u_{xx} + k^2 u) dx = \int_0^1 u(-p_{xx} + k^2 p) dx - p u_x |_0^1 + p_x u |_0^1. \tag{9}$$

We can directly find the adjoint equation $L^* p = g$ from (9):

$$L^* p := -p_{xx} + k^2 p = 1, \quad x \in (0,1), \qquad \forall \; p \in \mathbf{H}. \tag{10}$$

Identity (9) can also be written with the boundary terms in vector form:

$$\langle p, Lu\rangle - \langle L^* p, u\rangle = [\mathbf{pAu}]_0^1 \tag{11}$$

with

$$\mathbf{u} = \begin{pmatrix} u \\ u_x \end{pmatrix}, \qquad \mathbf{p} = \begin{pmatrix} p \\ p_x \end{pmatrix}$$

and

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

The primal boundary conditions are written in terms of $\mathbf{u}$ at both boundaries:

$$Bu = u \equiv \mathbf{Bu} = e, \quad \mathbf{B} \equiv (1\ 0),$$

with $e = 0$ on $x = 0$ and $e = 1$ on $x = 1$. Furthermore we find from identity (9):

$$Cu = u_x \equiv \mathbf{Cu}, \quad \mathbf{C} \equiv (0\ 1).$$

For identity (11) to satisfy (8) we have to find $\mathbf{B}^*$ and $\mathbf{C}^*$ on each boundary $\partial\Omega$ such that

$$\mathbf{A} = \mathbf{B}^{*T}\mathbf{C} - \mathbf{C}^{*T}\mathbf{B}. \tag{12}$$

Since Bu and Cu are the same on both boundaries, also $\mathbf{B}^*$ and $\mathbf{C}^*$ are the same on $x = 0$ and $x = 1$. Equation (12) is solved by:

$$\begin{pmatrix} -\mathbf{C}^* \\ \hline \mathbf{B}^* \end{pmatrix} = \begin{pmatrix} \mathbf{C} \\ \hline \mathbf{B} \end{pmatrix}^T \mathbf{A}^T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{13}$$

and hence $B^*p = -p$ and $C^*p = -p_x$ at both $x = 0$ and $x = 1$. With $B^*p = h$ and $h = 0$ the boundary conditions for the dual problem become:

$$-p(0) = -p(1) = 0 \quad \Rightarrow \quad p(0) = p(1) = 0.$$

The functional Q is found by substituting C^*p for both boundaries into equation (7) remembering that $f = 0$:

$$Q = \langle C^* p, e\rangle_{\partial\Omega} = -p_x u|_0^1 = -p_x(1). \tag{14}$$

This result is an interesting aspect of the dual formulation of the output functional: in the primal case Q depends on the integral over the whole domain $\Omega = (0, 1)$ and in the dual case Q depends solely on the derivative of the adjoint variable at one of the boundaries.

The solution of the adjoint equation (10) together with the dual boundary conditions $p(0) = p(1) = 0$ is given by:

$$p(x) = \frac{1}{k^2}\left(\frac{e^{-k}-1}{e^k-e^{-k}}e^{kx} + \frac{1-e^k}{e^k-e^{-k}}e^{-kx} + 1\right). \tag{15}$$

Therefore Q can now be written as:

$$Q = -p_x(1) = \frac{1}{k}\frac{2-e^k-e^{-k}}{e^k-e^{-k}}, \tag{16}$$

which, for $k = 1$ becomes $Q = .46212...$, which is exactly equal to the value obtained by substituting (4) into (3).

For the coarse model equation we can follow the same procedure to define the coarse model dual problem, resulting in:

$$L_0^* p_0 := -p_{0_{xx}} = 1, \quad x \in (0,1), \qquad \forall\ p_0 \in \mathbf{H}, \tag{17}$$

with again $p_0(0) = p_0(1) = 0$ as boundary conditions. The coarse model dual solution is now:

$$p_0(x) = -\frac{1}{2}x^2 + \frac{1}{2}x. \tag{18}$$

The dual solutions of the fine and coarse model equations are given in figure 2 for $k = 1, 2, 4$.

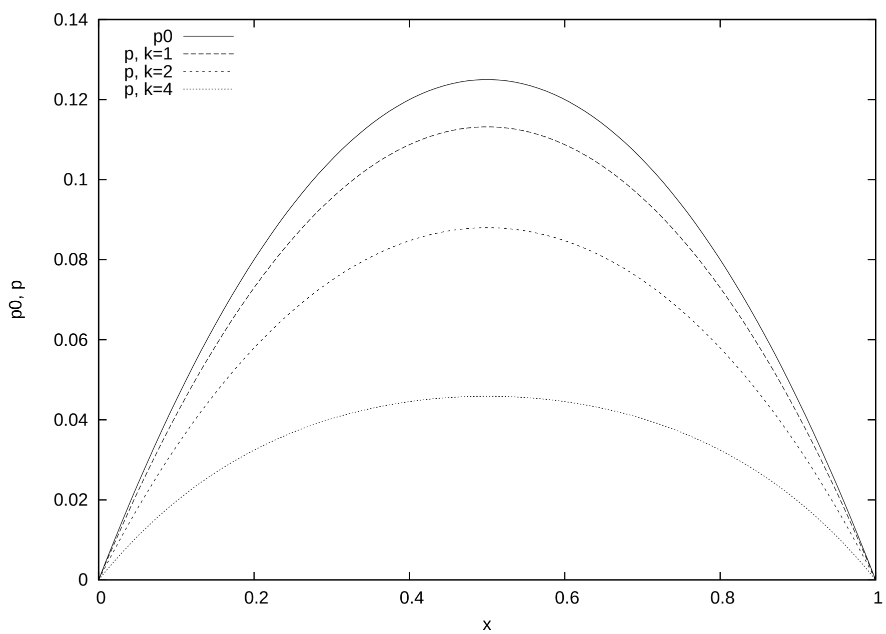

Figure 2: Coarse and fine model dual solutions (for $k = 1, 2, 4$)

Based on the coarse model equations a similar expression can be derived for the output functional Q as (16):

$$Q = -p_{0x}(1) = \frac{1}{2}, \tag{19}$$

which is equal to the integral of $u_0(x) = x$ over $[0, 1]$.

5 ERROR ESTIMATION BY ADJOINT FORMULATION

The modelling error in the output functional, $Q(u) - Q(u_0)$, can also be estimated based on dual weighted residuals, as described in [2]. The idea is that only coarse model primal and dual solutions are directly available and other terms involving error estimation by adjoint formulation are estimated. Since we know all fine as well as coarse model primal and dual solutions we are, however, able to exactly compute the involving terms.

5.1 Derivation of dual weighted modelling error

Oden and Prudhomme [2] derive a relation for $Q(u) - Q(u_0)$ for the constrained minimisation problem:

$$\text{Find } u \in \mathbf{V} \text{ such that } Q(u) = \inf_{v \in M} Q(v), \tag{20}$$

where

$$M = \{v \in \mathbf{V}; \mathcal{B}(v; q) = F(q), \forall\, q \in \mathbf{V}\}$$

with $\mathcal{B}(\cdot;\cdot)$ a coercive and continuous semi-linear form defined on the Banach space $\mathbf{V}$ and $F(\cdot)$ a continuous linear functional on $\mathbf{V}$. The solution u to (20) corresponds to a saddle point $(u, p) \in \mathbf{V} \times \mathbf{V}$ of the Lagrangian:

$$L(u, p) = Q(u) + F(p) - \mathcal{B}(u; p), \tag{21}$$

with p the influence function or adjoint variable. Now suppose that u and p are solutions of (21) and apply small perturbations $\varepsilon_1 \tilde{u}$ and $\varepsilon_2 \tilde{p}$ to u and p. Since we are looking for a stationary point, we have:

$$\lim_{\varepsilon_1, \varepsilon_2 \to 0} [L(u + \varepsilon_1 \tilde{u}, p + \varepsilon_2 \tilde{p}) - L(u, p)] = 0. \tag{22}$$

This results in the following two equations:

$$\begin{aligned} \mathcal{B}(u; \tilde{p}) &= F(\tilde{p}), \qquad \forall\, \tilde{p} \in \mathbf{V}, \\ \mathcal{B}'(u; \tilde{u}, p) &= Q'(u; \tilde{u}), \qquad \forall\, \tilde{u} \in \mathbf{V} \end{aligned} \tag{23}$$

where the first equation is the primal problem and the second equation the dual or adjoint problem. The same procedure is followed for the approximating coarse model, resulting in:

$$\begin{aligned} \mathcal{B}_0(u_0;\tilde{p}) &= F(\tilde{p}), \qquad \forall\ \tilde{p} \in \mathbf{V_0}, \\ \mathcal{B}_0'(u_0;\tilde{u},p_0) &= Q'(u_0;\tilde{u}), \qquad \forall\ \tilde{u} \in \mathbf{V_0}, \end{aligned} \tag{24}$$

with p_0 the coarse-model adjoint variable. Now, the degree to which (u_0, p_0) fails to satisfy the fine problem (23) is characterised by the residual functionals:

$$\begin{aligned} R(u_0;\tilde{p}) &= F(\tilde{p}) - \mathcal{B}(u_0;\tilde{p}), \qquad \forall\ \tilde{p} \in \mathbf{V} \\ \bar{R}(u_0,p_0;\tilde{u}) &= Q'(u_0;\tilde{u}) - \mathcal{B}'(u_0;\tilde{u},p_0), \qquad \forall\ \tilde{u} \in \mathbf{V}. \end{aligned} \tag{25}$$

With the primal and dual errors given by:

$$e_0 = u - u_0 \quad \text{and} \quad \epsilon_0 = p - p_0. \tag{26}$$

Oden and Prudhomme [2] give the following relation for $Q(u) - Q(u_0)$ in terms of the primal and dual solutions and errors:

$$Q(u) - Q(u_0) = R(u_0;p_0) + R(u_0;\epsilon_0) + \frac{1}{2}\Delta R + r(e_0,\epsilon_0), \tag{27}$$

with $\Delta R = \bar{R}(u_0,p_0;e_0) - R(u_0,\epsilon_0)$ and $r(e_0,\epsilon_0)$ a residual term based on Taylor expansions with integral remainders for functionals, see also [2]. According to Oden and Prudhomme, these last two terms can be neglected when the errors e_0 and ϵ_0 are sufficiently small. Since the operators L and L_0 in our model problem are linear operators these terms are exactly zero.

5.2 Application to the Helmholtz-Poisson problem

Applying this to the Helmholtz-Poisson problem we obtain as primal fine-model equation in weak form:

$$\mathcal{B}(u;\tilde{p}) = \int_0^1 \left(\frac{du}{dx}\frac{d\tilde{p}}{dx} + k^2 u\tilde{p} \right) dx = 0, \qquad \forall\ \tilde{p} \in \mathbf{H} \tag{28}$$

with $\tilde{p} = 0$ on the boundaries and for the fine model dual equation:

$$\mathcal{B}'(u;\tilde{u},p) = Q'(u;\tilde{u}) \to \int_0^1 \left(\frac{d\tilde{u}}{dx}\frac{dp}{dx} + k^2 \tilde{u}p \right) dx = -\int_0^1 \tilde{u}dx, \qquad \forall\ \tilde{u} \in \mathbf{H} \tag{29}$$

with $\tilde{u} = 0$ on the boundaries. Since the equations (1) and (2) are linear, as well as the functional Q, the explicit dependence of B' and Q' on u disappears.

As coarse model equations we obtain:

$$\mathcal{B}_0(u_0; \tilde{p}) = \int_0^1 \left(\frac{du_0}{dx} \frac{d\tilde{p}}{dx} \right) dx = 0, \qquad \forall\ \tilde{p} \in \mathbf{H} \tag{30}$$

and for the coarse model dual equation:

$$\mathcal{B}_0'(u_0; \tilde{u}, p_0) = Q'(u_0; \tilde{u}) \rightarrow \int_0^1 \left(\frac{d\tilde{u}}{dx} \frac{dp_0}{dx} \right) dx = -\int_0^1 \tilde{u} dx \qquad \forall\ \tilde{u} \in \mathbf{H}. \tag{31}$$

The first residual term in (25) is given by:

$$R(u_0; \tilde{p}) = F(\tilde{p}) - \mathcal{B}(u_0; \tilde{p}) = -\mathcal{B}(u_0; \tilde{p}). \tag{32}$$

Since $\mathcal{B}_0(u_0; \tilde{p}) = 0$ in our case, we can also write:

$$R(u_0; \tilde{p}) = -\mathcal{B}(u_0; \tilde{p}) + \mathcal{B}_0(u_0; \tilde{p}). \tag{33}$$

Using (28), (30) now results in the following relation for the residual term:

$$R(u_0; \tilde{p}) = -\int_0^1 \left(\frac{du_0}{dx} \frac{d\tilde{p}}{dx} + \ k^2 u_0 \tilde{p} \right) dx + \int_0^1 \left(\frac{du_0}{dx} \frac{d\tilde{p}}{dx} \right) dx \ = -\int_0^1 k^2 u_0 \tilde{p} dx. \tag{34}$$

Now the first term of (27) can be calculated by using the coarse model primal and dual solutions (5) and (18), respectively:

$$R(u_0; p_0) = -\int_0^1 k^2 u_0 p_0 dx = -\int_0^1 k^2 x \frac{1}{2}(x - x^2) dx = -\frac{1}{24} k^2. \tag{35}$$

For the second term in (27) we can write:

$$R(u_0; \epsilon_0) = -\int_0^1 k^2 u_0 \epsilon_0 dx. \tag{36}$$

Taking (35) and (36) together and using (26) gives:

$$R(u_0; p_0) + R(u_0; \epsilon_0) = -\int_0^1 k^2 u_0 p dx = R(u_0; p), \tag{37}$$

which becomes:

$$R(u_0, p) = -\int_0^1 k^2 x \left(\frac{1}{k^2} \left(\frac{e^{-k} - 1}{e^k - e^{-k}} e^{kx} + \frac{1 - e^k}{e^k - e^{-k}} e^{-kx} + 1 \right) \right) dx = \tag{38}$$
$$= \frac{e^k + e^{-k} - 2}{k(e^k - e^{-k})} - \frac{1}{2}$$

This result is equal to the exact error given in (6) which confirms that the last two terms in (27) are indeed zero in our model problem.

5.3 A more common approach

When we want to determine $Q(u) - Q(u_0)$ we can also derive a relation by using the form of (6):

$$\begin{aligned} Q(u) - Q(u_0) = \langle g, u\rangle_\Omega + \langle h, Cu\rangle_{\partial\Omega} - \langle g, u_0\rangle_\Omega - \langle h, Cu_0\rangle_{\partial\Omega} &= \\ \langle g, u - u_0\rangle_\Omega + \langle h, Cu - Cu_0\rangle_{\partial\Omega} &= \\ \langle L^* p, u - u_0\rangle_\Omega + \langle B^* p, C(u - u_0)\rangle_{\partial\Omega} &= \\ \langle p, L(u - u_0)\rangle_\Omega + \langle C^* p, B(u - u_0)\rangle_{\partial\Omega} &= \\ \langle p, f - Lu_0\rangle_\Omega + \langle C^* p, e - Bu_0\rangle_{\partial\Omega}&. \end{aligned} \tag{39}$$

Applying this to our model problem and using that the fine-model and coarse-model primal boundary conditions are equal, $Bu = B_0u_0 = Bu_0 \rightarrow e - Bu_0 = 0$, we find:

$$Q(e_0) = \langle p, -Lu_0\rangle_\Omega = \langle p_0, -Lu_0\rangle_\Omega + \langle \epsilon_0, -Lu_0\rangle_\Omega, \tag{40}$$

where we split the result in a term existing of the (in general) computable coarse model primal and dual solutions and the unknown dual error ϵ_0. Equation (40) shows that to compute the modelling error the coarse model solution needs to be substituted into the fine model equation:

$$Lu_0 = -u_{0xx} + k^2 u_0 = k^2 x.$$

This residual is now weighted with the exact dual solution p to estimate the modelling error:

$$\begin{aligned} Q(e_0) = \langle p, -Lu_0\rangle_\Omega = \int_0^1 p(-k^2 x)dx = \\ = \int_0^1 \left(\frac{1}{k^2} \left(\frac{e^{-k} - 1}{e^k - e^{-k}} e^{kx} + \frac{1 - e^k}{e^k - e^{-k}} e^{-kx} + 1 \right) (-k^2 x) \right) dx = \frac{e^k + e^{-k} - 2}{k(e^k - e^{-k})} - \frac{1}{2} \end{aligned} \tag{41}$$

which is equal to the exact error (6) and shows the same result as equation (38) found by the using the framework of [2].

In case the dual error ϵ_0 is small, we can omit the last term of (40) and use p_0 to weight the residual Lu_0:

$$Q(e_0) = \langle p_0, -Lu_0\rangle_\Omega = \int_0^1 p_0(-k^2 x)dx = -\int_0^1 k^2 x \frac{1}{2}(x - x^2)dx = -\frac{1}{24}k^2, \tag{42}$$

which is exactly the result of equation (35).

6 RESULTS OF DUAL WEIGHTED ESTIMATION VS. EXACT ERROR

As described in section 5.1 the first two terms in (27) are sufficient when e_0 and ϵ_0 are 'small'. To verify the accuracy of the modelling error estimate by using (35) (and (42)) we can make e_0 and ϵ_0 smaller or bigger by modifying k. Increasing k means the coarse model solution will differ more from the fine model solution, in other words: e_0 and ϵ_0 will also increase. The accuracy of the estimator (35) is illustrated in figure 3 in which one can see that the estimator converges to the exact error for $k \to 0$.

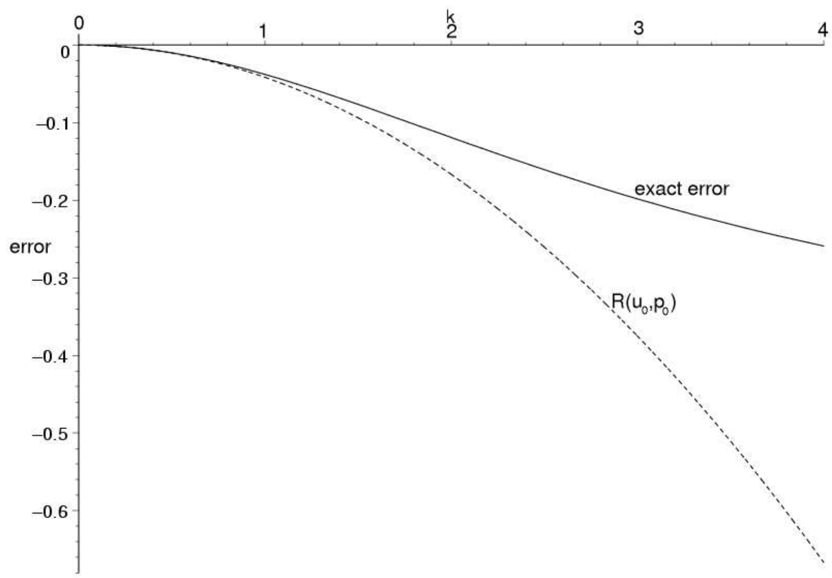

Figure 3: The error estimators and exact error as function of k

In table 1 the exact as well as estimated modelling errors are given for some values of k.

k	e_{ex}	$R(u_0;p_0)$
.5	-.01016	-.01042
1	-.03788	-.04167
2	-.11920	-.16667
4	-.25899	-.66667

Table 1: Exact (e_{ex}) and estimated modelling error in Q for $k = .5, 1, 2, 4$

Table 1 shows that for k =.5 and 1 the estimation is acceptable (within 10%) but for $k = 2$ the estimation by $R(u_0, p_0)$ differ from the exact error 40%. This illustrates the importance to find an appropriate estimator for ϵ, since the exact adjoint solution is not available. Moreover we want to avoid computing the exact adjoint solution, otherwise the whole idea of estimating the modelling error would be useless since the required computational time could also be used to solve the fine model problem. In our model problem the adjoint error ϵ_0 can be computed exactly since the differential operators L and L_0 are linear and no error is introduced by linearisation to obtain the adjoint equations.

7 CONCLUSIONS

The use of dual weighted residuals to estimate the modelling error in a global quantity of interest is shown to be exact in case of linear equations when using the fine-model adjoint solution the dual weight. However, since in practical applications we only want to compute the coarse model dual solution this requires the estimation of the dual error ϵ. Furthermore, in case of non-linear equations, linearisation will also introduce errors and may require the computation of additional terms in the estimation of the error in the quantity of interest as derived by Oden and Prudhomme [2]. Further study will focus on estimating ϵ_0 necessary in (27). Once we have a reliable modelling error estimator for a class of fluid flow models we can use it in a model adaptive strategy in order to efficiently compute the quantity of interest.

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