European Conference on Computational Fluid Dynamics
ECCOMAS CFD 2006
P. Wesseling, E. Oñate and J. Périaux (Eds)

ASPECTS OF GOAL-ORIENTED MODEL-ERROR ESTIMATION IN CONVECTION-DIFFUSION PROBLEMS

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Key words: Model error, hierarchical modelling, goal-oriented error estimation, dual-weighted residual method, convection-diffusion problems.

Abstract. *For goal-oriented model adaptation a model-error estimator is required to drive the adaptation process. In recent years publications have appeared on the dual-weighted residual (DWR) method in the application of model-error estimation in output functionals. In this paper we study the application of the DWR method for convection-diffusion problems where hierarchical models are of different type. Omitting the diffusion operator often results in a singular perturbation problem considering the model residual in the limit of vanishing diffusion. This is caused by the change of mathematical type of the model equations and therefore the applied boundary conditions.*

In this work we show how a model error estimator is developed for steady and unsteady convection-diffusion problems. It is found that a weak formulation and weakly imposing boundary and initial conditions leads to a dual-weighted model-error estimator that also incorporates boundary residuals.

1 INTRODUCTION

The goal of CFD computations in engineering is to compute certain quantities of interest that are functionals of the solution, e.g. lift and drag. For this one can choose a suitable fluid-flow model from the class of hierarchical models in which the most simple model is also the cheapest in the sense of CPU-time. However, a cheap model also results in a lower accuracy of the quantities of interest. Model adaptation is expected to save CPU time in problems requiring a large number of CFD computations where a prescribed accuracy of the functional has to be achieved. To drive a model-adaptation algorithm a suitable goal-oriented model-error estimator is required, which is the subject of this research.

A general approach for deriving a goal-oriented error estimator in finite element approximations has been developed by Becker and Rannacher [1] and is referred to as the dual-weighted residual (DWR) method. This work has been extended by Oden and Prudhomme [8] for goal-oriented model-error estimation in computational mechanics. So far, the DWR method has been applied to problems where the model complexity varies, for instance, due to different forms of constitutive relations or modified properties of the medium considered. In all these cases the hierarchical models are of the same mathematical type, e.g., they are all elliptic partial differential equations. Examples are the modelling of heterogeneous materials [8, 9] and structural mechanics [10]. Also in work on (steady) flow(-type) problems [2, 3, 8], the hierarchical models are all of the same mathematical type. In the steady incompressible flow example by Oden and Prudhomme [8] the incompressible Navier-Stokes equations are approximated by the Stokes equations in which the convective term is neglected. In convection-diffusion problems considered by Braack and Ern [2, 3] the level of sophistication is determined by the diffusion model, by applying Fick's law as an approximation of a more accurate multicomponent diffusion model. In both cases the problem remains elliptic such that the same boundary conditions apply to both models.

Approximating the convection-diffusion problem by omitting the diffusion in the model is a more rigorous model simplification. Such a simplification is common in engineering: many flow problems are solved using the Euler equations, which are obtained when in the Navier-Stokes equations diffusion and heat conduction are omitted. Since in this case the highest order derivative is omitted in the equations, the mathematical type changes. In case of the unsteady equations, e.g., the type changes from parabolic to hyperbolic. For these problems special attention needs to be payed to constructing the dual problem and the model-error estimator. This is explained as follows.

In flow-type problems where the diffusion term (controlled by the diffusion parameter μ) is omitted in the approximating model $B_0(u_0, q) = F_0(q)$ with respect to the sophisticated model $B(u, q) = F(q)$, the model equation changes type. This means that the sophisticated problem is not similar to the approximating model in the limit of $\mu \to 0$:

$$\lim_{\mu \to 0} B(u, q) \neq B_0(u, q), \ \forall u, q \in U. \tag{1}$$

These kinds of problems are recognised as singular perturbation problems: the solution of the Navier-Stokes equations for the limit of zero viscosity is not equal to the solution of the Euler equations. The application of the DWR-method for goal-oriented model-error estimation in singular perturbation problems is not that straightforward as in regular problems. In singular perturbation problems the DWR method fails when boundary residuals are not taken into account as will be illustrated in this paper.

In the present work we show that imposing initial and boundary conditions weakly in the problem formulations and modifying the residual estimator leads to a suitable goal-oriented model-error estimator for convection-diffusion problems by the DWR method. We illustrate the method, the derivation of the proper adjoint problem and the limitations

of the DWR method when using the approximating adjoint for problems governed by the linear convection-diffusion equation. In this problem the approximating model is obtained by neglecting the diffusive term in the convection-diffusion equation such that the convection equation remains.

2 The DWR method for convection-diffusion problems

In the present work we give an overview of the DWR framework as it is applied to a linear convection-diffusion problem. In this problem the approximating model is governed by neglecting the diffusive term in the convection-diffusion equation (the *fine* model) such that the convection equation (the *coarse* model) remains. The unsteady convection-diffusion equation is of parabolic type and the convection equation is of hyperbolic type. Therefore the fine model requires boundary conditions on the inflow- and outflow boundaries (independent of the value of the diffusion coefficient) and the coarse model only requires an inflow boundary condition. In case of a Dirichlet outflow boundary, this results in a residual (a singular perturbation) on the outflow boundary, even for vanishing diffusion in the fine model.

2.1 The fine model

Consider the linear convection-diffusion equation on $(x,t) \in (0,1) \times (0,T)$:

$$u_t + a u_x - \mu u_{xx} = 0, \quad x \in (0,1),\ t \in (0,T), \tag{2}$$

with a the constant convective velocity and $\mu > 0$ the diffusion coefficient. The initial condition is $u(x,0) = u^0(x)$ from which the boundary conditions are found: $u(0,t) = u_L(t)$ and $u(1,t) = u_R(t)$, written as u_L and u_R, respectively. The weak form of the problem is found by introducing a test function q without imposing restrictions for q on the boundaries and at $t = 0$ and performing integration by parts after which the boundary and initial conditions are substituted:

$$\begin{aligned}
&B(u,q) = F(q), \quad \forall q \in V \Leftrightarrow \\
&\int_0^T \int_0^1 (u_t q + a u_x q + \mu u_x q_x) dx dt - \int_0^T \mu u_x q|_0^1 dt + \int_0^T \mu u(0,t) q_x(0,t) dt - \\
&\int_0^T \mu u(1,t) q_x(1,t) dt + \int_0^1 u(x,0) q(x,0) dx + \int_0^T a u(0,t) q(0,t) dt - \int_0^T a u(1,t) q(1,t) dt = \\
&\int_0^T \mu u_L(t) q_x(0,t) dt - \int_0^T \mu u_R(t) q_x(1,t) dt + \int_0^1 u^0(x) q(x,0) dx + \\
&\int_0^T a u_L(t) q(0,t) dt - \int_0^T a u_R(t) q(1,t) dt, \quad \forall q \in V,
\end{aligned} \tag{3}$$

with U and V suitable Banach spaces. It is mentioned that the integrals $\int_0^T a u(0,t) q(0,t) dt$ and $\int_0^T a u(1,t) q(1,t) dt$ are usually not included in the weak form. In this case we de-

cided to leave both terms in, since they will be required for deriving the goal-oriented error-estimator.

Suppose we are interested in evaluating the functional $Q(u(x,T))$ from the solution u of (3). Such an evaluation can be formulated as solving the (trivial!) constrained optimisation problem for $u \in U$ (see [1]):

Find $u \in U$ such that:

$$Q(u) = \inf_{v \in M} Q(v), \tag{4}$$

where $M = \{v \in U; B(v;q) = F(q), \forall q \in V\}$.

The minimum u corresponds to the stationary point $(u,p) \in U \times V$ of the Lagrangian (or modified functional):

$$L(u,p) := Q(u) + F(p) - B(u,p), \tag{5}$$

with p the influence function or adjoint variable. We assume that $L(u,p)$ is bounded by assuming a constant C exists such that:

$$|L(u,p)| \leq C||u||_U||p||_V. \tag{6}$$

For the stationary point (u,p) applies that small perturbations in u and p lead to insignificantly small perturbations in the Lagrangian $L(u,p)$:

$$L'((u,p);(v,q)) = 0, \quad \forall (v,q) \in U \times V. \tag{7}$$

Here v indicates the variation in the direction of u and q the variation in the direction of p. Furthermore, by taking the derivative of Eq. (5) we also have:

$$L'((u,p);(v,q)) = Q'(u;v) - B'(v,p) + F(q) - B(u,q), \quad \forall (v,q) \in U \times V, \tag{8}$$

where the semicolon indicates that Q might be non-linear in u. We seek $(u,p) \in U \times V$ such that:

$$B(u,q) = F(q), \quad \forall q \in V, \tag{9}$$

$$B'(v,p) = Q'(u;v), \quad \forall v \in U. \tag{10}$$

These equations are the primal and dual problem, respectively. Since the dual initial and boundary conditions depend on the quantity of interest considered, we continue for a specific choice of the $Q(u)$.

In case we are interested in the quantity of interest $Q(u) = \int_0^1 u(x,T)dx$ we find for (10) through performing integration by parts:

$$B'(v,p) = Q'(u;v), \quad \forall v \in U \Leftrightarrow$$
$$\int_0^T \int_0^1 (-vp_t - avp_x + \mu v_x p_x)dxdt - \int_0^T \mu v p_x|_0^1 dt - \int_0^T \mu v_x p|_0^1 dt + \int_0^1 v(x,T)p(x,T)dx = \int_0^1 v(x,T)dx, \tag{11}$$

where boundary terms and the initial condition have cancelled. Since Eq. (11) must hold for all v the initial and boundary conditions for the dual problem are given by:

$$\int_0^1 v(x,T)p(x,T)dx = \int_0^1 v(x,T)dx \quad \Rightarrow \quad p(x,T) = 1, \tag{12}$$

$$\int_0^T \mu v_x p|_0^1 dt = 0 \quad \Rightarrow \quad p(0,t) = p(1,t) = 0. \tag{13}$$

These initial and boundary conditions are applied to solve the dual problem:

$$\int_0^T \int_0^1 (-vp_t - avp_x + \mu v_x p_x)dxdt - \int_0^T \mu v p_x|_0^1 dt = 0. \tag{14}$$

Furthermore Eq. (11) shows that the dual problem is solved backwards in time with the dual initial condition $p(x,T) = 1$.

In strong form the dual problem to be solved is:

$$\begin{aligned} -p_t - ap_x - \mu p_{xx} = 0, \quad & \forall (x,t) \in (0,1) \times (0,T), \\ p(x,T) = 1, \quad & \forall x \in (0,1), \\ p(0,t) = 0, \quad & \forall t \in (0,T), \\ p(1,t) = 0, \quad & \forall t \in (0,T). \end{aligned} \tag{15}$$

2.2 The coarse model problem

Suppose that solving the fine model problem is too hard or expensive and therefore we want to approximate it by the coarse model. Omitting the diffusion term in the fine model (2) is a rigorous but common approximation. In many engineering flow problems the diffusion coefficient is a small parameter and often omitted, e.g. in the Euler equations with respect to the Navier-Stokes equations. The model-error is defined as $e_0 = u - u_0$ with u_0 the solution of the approximating model. The coarse model equation in strong form is given by:

$$u_{0t} + au_{0x} = 0, \quad x \in (0,1), t \in (0,T), \tag{16}$$

with the same initial condition as the fine model problem: $u_0(x,0) = u^0(x)$. Considering only sufficiently smooth solutions of Eq. (16) we assume $u_0 \in U$. For arbitrary a the boundary conditions need to be defined such that a boundary condition is given only at an inflow boundary (incoming characteristic $dx/dt = a$). With $a > 0$ we require $u_0(0,t) = u_L(t)$ and in case of $a < 0$ we require $u_0(1,t) = u_R(t)$. In the weak form this is

achieved by modifying the implementation of the boundary conditions:

$$B_0(u_0,q) = F_0(q), \quad \forall q \in V \Leftrightarrow$$
$$\int_0^T \int_0^1 u_{0t}q + au_{0x}q dx dt + \int_0^1 u_0(x,0)q(x,0)dx + \int_0^T a^+ u_0(0,t)q(0,t)dt -$$
$$\int_0^T a^- u_0(1,t)q(1,t)dt = \int_0^1 u^0(x)q(x,0)dx +$$
$$\int_0^T a^+ u_L(t)q(0,t)dt - \int_0^T a^- u_R(t)q(1,t)dt, \quad \forall q \in V, \quad (17)$$

where a^+ and a^- are defined as:

$$a^+ = \max(a,0), \quad (18a)$$
$$a^- = \min(a,0). \quad (18b)$$

Please notice that $F_0(q) \neq F(q)$ (compare Eq. (17) and (3)) due to weakly imposing the boundary and initial conditions. When the hierarchical models are of equal mathematical type we would have $F_0(q) = F(q)$. Since the boundary condition and the initial condition are imposed weakly, we do not need to constrain q to be zero at $x = 0$ and $t = 0$.

In a similar way as for the fine dual problem in the previous section we can derive the coarse dual problem:

$$B_0'(v,p_0) = Q'(u_0;v), \ \forall v \in U, \quad (19)$$

with p_0 the coarse-model influence function or coarse-adjoint variable. With the quantity of interest $Q(u) = \int_0^1 u(x,T)dx$ we find for Eq. (19):

$$B_0'(v,p_0) = Q'(u_0;v), \ \forall v \in U, \ \Leftrightarrow$$
$$\int_0^T \int_\Omega v(-p_{0_t} - ap_{0_x}) \ dx \ dt + \int_0^1 v(x,T)p_0(x,T)dx - \int_0^T (a-a^+)v(0,t)p_0(0,t)dt +$$
$$\int_0^T (a-a^-)v(1,t)p_0(1,t)dt = \int_0^1 v(x,T)dx, \ \forall v \in U. \quad (20)$$

The dual model error is $\epsilon_0 = p - p_0$. For $a > 0$, $a - a^- = a$ and $a - a^+ = 0$, then Eq. (20) reduces to:

$$\int_0^T \int_0^1 v(-p_{0_t} - ap_{0_x}) \ dx \ dt + \int_0^1 v(x,T)p_0(x,T)dx + \int_0^T av(1,t)p_0(1,t)dt =$$
$$\int_0^1 v(x,T)dx. \quad (21)$$

Since Eq. (21) has to hold for all $v \in U$ we find as dual initial condition $p_0(x,T) = 1$ and dual boundary condition $p_0(1,t) = 0$ showing that the boundary condition in the

coarse dual problem swaps to the other boundary $x = 1$ with respect to the primal boundary condition. To conclude, the (homogeneous) coarse dual equation with initial and boundary conditions in strong form is given by:

$$\begin{aligned} -p_{0t} - ap_{0x} = 0, \quad & \forall (x,t) \in (0,1) \times (0,T), \\ p_0(x,T) = 1, \quad & \forall x \in (0,1), \\ p_0(1,t) = 0, \quad & \forall x \in (0,T). \end{aligned} \tag{22}$$

For $a < 0$ a similar procedure can be followed and one would find that the dual boundary condition moves to the boundary $x = 0$ with the condition: $p_0(0,t) = 0$.

2.3 The error estimator

When the fine or coarse adjoint solution is computed by solving (11) or (20), respectively, the model error in the functional $Q(u_0)$ using the approximating solution can be computed. Therefore first the following residual functionals are defined:

$$R(u_0, q) = F(q) - B(u_0, q), \quad q \in V, \tag{23}$$

$$\bar{R}(u_0; p_0, v) = Q'(u_0; v) - B'(v, p_0), \quad v \in U, \tag{24}$$

which are the primal and dual residuals, respectively. A relation between the model error in the quantity of interest, $Q(u) - Q(u_0)$, and the residual functionals (23) is given by the following a posteriori error representation according to THEOREM 1 in Oden and Prudhomme [8]:

$$Q(u) - Q(u_0) = R(u_0, p_0) + \frac{1}{2}(R(u_0, \epsilon_0) + \bar{R}(u_0; p_0, e_0)) + r(e_0, \epsilon_0) \tag{25}$$

where $\epsilon_0 = p - p_0$ is the dual error and $r(e_0, \epsilon_0)$ contains integral remainders of order three:

$$r(e_0, \epsilon_0) = \frac{1}{2} \int_0^1 Q'''(u_0 + se_0; e_0, e_0, e_0) ds. \tag{26}$$

This term is zero for a quantity of interest which is linear or quadratic in u. A proof for this error representation can be found in Oden and Prudhomme [8]. A relation between the primal and dual residual is easily found by rewriting the dual residual:

$$\begin{aligned} \bar{R}(u_0; p_0, v) &= Q'(u_0; v) - B'(v, p_0) \\ &= Q'(u_0; v) - Q'(u; v) + Q'(u; v) - B'(v, p_0) \\ &= -[Q'(u; v) - Q'(u_0; v)] + Q'(u; v) - B'(v, p_0). \end{aligned} \tag{27}$$

For the term between square brackets we use the following (exact) Taylor expansion with integral remainder:

$$Q'(u; v) - Q'(u_0; v) = Q'(u_0 + e_0; v) - Q'(u_0; v) = \int_0^1 Q''(u_0 + se_0; e_0, v) ds. \tag{28}$$

Furthermore we have $B'(v,p) = Q'(u;v)$ from Eq. (10) such that we obtain:

$$\begin{aligned} \bar{R}(u_0;p_0,v) &= -\int_0^1 Q''(u_0+se_0;e_0,v)ds + B'(v,p) - B'(v,p_0). \\ &= -\int_0^1 Q''(u_0+se_0;e_0,v)ds + B'(v,\epsilon_0). \end{aligned} \tag{29}$$

Using $B(u,q) = F(q)$ (Eq. (3)) we can write the primal residual (23) as:

$$R(u_0,q) = B(u,q) - B(u_0,q) = B(u-u_0,q) = B(e_0,q). \tag{30}$$

For a linear problem one can find through integration by parts that the following relation holds:

$$B(e_0,q) = B'(e_0,q). \tag{31}$$

Using this in Eq. (30) and taking $q = \epsilon_0$ in (30) and $v = e_0$ in (29) gives the relation between the primal and dual residual:

$$\bar{R}(u_0;p_0,e_0) = R(u_0,\epsilon_0) - \int_0^1 Q''(u_0+se_0;e_0,e_0)ds. \tag{32}$$

This allows to write for (25):

$$\begin{aligned} Q(u) - Q(u_0) &= R(u_0,p_0) + R(u_0,\epsilon_0) - \frac{1}{2}\int_0^1 Q''(u_0+se_0;e_0,e_0)ds \\ &+ r(e_0,\epsilon_0) \\ &= R(u_0,p_0) + R(u_0,\epsilon_0) + O(e_0^2) \\ &= R(u_0,p) + O(e_0^2), \end{aligned} \tag{33}$$

with the residual $R(\cdot,\cdot)$ given in Eq. (23). For linear quantities of interest we have the exact a posteriori error representation:

$$Q(u) - Q(u_0) = R(u_0,p_0) + R(u_0,\epsilon_0) = R(u_0,p). \tag{34}$$

In case of non-linear problems, the integral remainders in (32) and $r(e_0,\epsilon_0)$ also have contributions from the operator B (see [8]).

Since we have $B_0(u_0,p) - F_0(p) = 0$ we can add it to (33):

$$\begin{aligned} Q(u) - Q(u_0) &= R(u_0,p) + O(e_0^2) = \\ &= F(p) - B(u_0,p) + B_0(u_0,p) - F_0(p) + O(e_0^2), \end{aligned} \tag{35}$$

which allows to split the contributions in the estimator into a contribution from the inner domain $(0,1)\times(0,T)$: $B_0(u_0,p) - B(u_0,p)$ and a contribution from the boundaries: $F_0(p) - F(p)$.

To emphasise the importance of inclusion of boundary terms we first derive the estimator in case the boundary conditions are imposed strongly such that we have $F_0(p) = F(p)$. This is followed by a derivation of the error estimator in case boundary conditions are imposed weakly. In the examples we illustrate the difference between both estimators. A linear quantity of interest is considered below, such that the error representation (34) holds.

2.3.1 Error estimator for strongly imposed boundary conditions

Suppose we did not impose initial and boundary conditions weakly as in the fine model (3) and the coarse model (17). We then would have the fine model as:

$$B(u,q) = F(q) \Leftrightarrow \int_0^T \int_\Omega (u_t q + a u_x q + \mu u_x q_x) dx dt = 0, \tag{36}$$

(where $q(0,t) = q(1,t) = 0$ in the strong form) and the coarse model:

$$B_0(u_0,q) = F_0(q) \Leftrightarrow \int_0^T \int_\Omega u_{0t} q + a u_{0x} q dx dt = 0. \tag{37}$$

Since we have now in fact $F(q) = F_0(q) = 0$ the model-error estimator (35) reduces to (in case of a linear quantity of interest):

$$\begin{aligned} Q(u) - Q(u_0) = B_0(u_0,p) - B(u_0,p) = \\ = \int_0^T \int_\Omega u_{0t} p + a u_{0x} p dx dt - \int_0^T \int_\Omega (u_{0t} p + a u_{0x} p + \mu u_{0x} p_x) dx dt = \\ - \mu \int_0^T \int_\Omega u_{0x} p_x dx dt. \end{aligned} \tag{38}$$

The resulting residual is an inner product of the derivatives of the coarse model solution and the adjoint solution on the space-time domain weighted by the diffusion coefficient μ.

2.3.2 Error estimator for weakly imposed boundary conditions

Now we derive the estimator for the models where initial and boundary conditions are imposed weakly. From Eq. (35) we find:

$$\begin{aligned} R(u_0,p) = B_0(u_0,p) - B(u_0,p) - (F_0(p) - F(p)) = \\ \int_0^T \int_\Omega \mu u_{0x} p_x dx dt + \int_0^T \mu u_{0x} p|_0^1 dt - \int_0^T \mu (u_R(t) - u_0(1,t)) p_x(1,t) dt + \\ \int_0^T \mu (u_L(t) - u_0(0,t)) p_x(0,t) dt - \int_0^T (a - a^-)(u_R(t) - u_0(1,t)) p(1,t) dt + \\ \int_0^T (a - a^+)(u_L(t) - u_0(0,t)) p(0,t) dt, \end{aligned} \tag{39}$$

where contributions from the inner domain and the boundaries are separated in 'convective' (involving a) and 'diffusive' contributions (involving μ):

In case $a > 0$ we have $a - a^+ = 0$ and $a - a^- = a$, so that equation (39) reduces to:

$$R(u_0, p) = -\int_0^T \int_\Omega \mu u_{0x} p_x dx dt + \int_0^T \mu u_{0x} p|_0^1 dt - \int_0^T \mu(u_R(t) - u_0(1,t)) p_x(1,t) dt + \int_0^T \mu(u_L(t) - u_0(0,t)) p_x(0,t) dt - \int_0^T a(u_R(t) - u_0(1,t)) p(1,t) dt. \quad (40)$$

In this equation the convective contribution is restricted to the outflow boundary ($x = 1$). In fact, writing $a - a^+$ and $a - a^-$ in (39) is somewhat superfluous since the boundary conditions for the coarse and fine model are equal at inflow boundaries, so the boundary residual is zero (here: $u_L(t) - u_0(0,t) = 0$). As a result we could write a instead of $a - a^-$ and $a - a^+$ in the general estimator (39). The same can be done for $a < 0$ which yields that a convective boundary contribution remains at the outflow boundary $x = 0$.

Comparing the estimator (39) for the weakly imposed boundary conditions with the estimator (38) derived for the case when boundary conditions are imposed strongly, shows that imposing the boundary conditions weakly in the model equations results in an estimator that incorporates boundary residuals besides the inner contribution. We will show in an example with a linear quantity of interest a case where the contribution in the interior of the computational domain is zero but the boundary contribution takes care of a correct computation of the error $Q(u) - Q(u_0)$. In this case 'correct' means that the error estimator is exact for a linear quantity of interest using the fine adjoint.

2.4 A computationally efficient error estimator

One can imagine that solving the coarse primal problem and the fine dual problem required to compute the estimator as given in Eq. (39) or (40) is equally expensive in the sense of CPU time (in case of linear problems) as solving the coarse and fine primal problem and computing $Q(u) - Q(u_0)$ directly. Therefore it is common, see [8, 2, 10], to approximate the error estimator, solving the coarse dual problem instead, and to compute only the residual term involving the coarse dual solution, as in Eq. (25). Moreover, to drive a model adaptation algorithm it is sufficient to have a reasonably accurate estimate of the error by using:

$$Q(u) - Q(u_0) \approx R(u_0, p_0). \quad (41)$$

For the linear convection diffusion problem described above where p_0 is the solution

of (22) we have:

$$R(u_0,p_0) = -\int_0^T \int_\Omega \mu u_{0x} p_{0x} dx dt - \int_0^T \mu(u_R(t) - u_0(1,t)) p_{0x}(1,t) dt + \int_0^T \mu(u_L(t) - u_0(0,t)) p_{0x}(0,t) dt. \quad (42)$$

In the following sections both analytical and numerical examples are given in which both fine-adjoint and coarse-adjoint based estimators are computed and compared.

3 Example of a steady problem

In this section the goal-oriented model-error estimator is illustrated for the steady linear convection-diffusion equation. We want to evaluate the quantity of interest $Q(u) = \int_\Omega u dx$ from the solution of the following problem on $\Omega = (0,1)$:

$$a u_x - \mu u_{xx} = 0, \quad x \in \Omega, \quad (43a)$$
$$u(0) = u_L = 0, \quad (43b)$$
$$u(1) = u_R = 1. \quad (43c)$$

The equation is made dimensionless by scaling the variables and introducing the Péclet number:

$$\mathrm{Pe} = \frac{aL}{\mu},$$

where L is a length scale, in this case chosen equal to the length of the domain: $L = 1$. The Péclet number indicates the ratio between convection and diffusion in a problem and is usually large in engineering flow problems. In terms of the Péclet number, Eq. (43) becomes:

$$u_x - \frac{1}{\mathrm{Pe}} u_{xx} = 0. \quad (44)$$

In weak form this is written as:

$$B(u,q) = F(q) \Rightarrow \int_\Omega (u_x q + \frac{1}{\mathrm{Pe}} u_x q_x) dx - \frac{1}{\mathrm{Pe}} u_x q|_0^1 + \frac{1}{\mathrm{Pe}} u(0) q_x(0) - \frac{1}{\mathrm{Pe}} u(1) q_x(1) + u(0) q(0) - u(1) q(1) = -\frac{1}{\mathrm{Pe}} u_R q_x(1) - u_R q(1). \quad (45)$$

The analytical solution in terms of the Péclet number, is given by:

$$u(x) = \frac{-1 + e^{\mathrm{Pe}x}}{-1 + e^{\mathrm{Pe}}}. \quad (46)$$

For $a = 1$ and three values of μ the primal fine solution is given in figure 1. The quantity

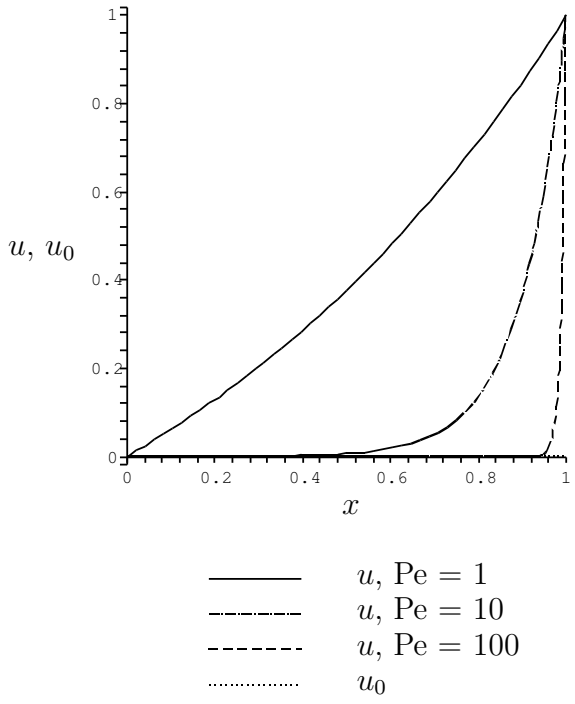


Figure 1: Fine and coarse model solutions, steady example.

of interest is then given by:

$$Q(u) = \int_\Omega u dx = \frac{e^{\mathrm{Pe}} - 1 - \mathrm{Pe}}{\mathrm{Pe}(-1 + e^{\mathrm{Pe}})}. \tag{47}$$

Now we want to evaluate the quantity of interest based on the approximating model in which the diffusion is neglected:

$$a u_x = 0, \quad x \in \Omega, \tag{48a}$$
$$u(0) = 0, \tag{48b}$$

or in weak form:

$$B_0(u_0, q) = F_0(q) \Rightarrow \int_\Omega a u_{0x} q dx + a u_0(0) q(0) = a u_L q(0), \ a > 0. \tag{49}$$

The solution of this problem is trivial: $u_0(x) = 0$, so we have for the quantity of interest $Q(u_0) = 0$. Neglecting the second order derivative means that only one boundary condition is required at the inflow boundary ($x = 0$ for $a > 0$). On the inner domain the limit of the fine model solution for vanishing diffusion $\mu \to 0$ (meaning $1/Pe \to 0$), is equal to

the coarse model solution:

$$\lim_{1/\mathrm{Pe}\to 0} u(x) = u_0(x),\ \forall x \in (0,1).$$

On the boundary, however, this is not the case:

$$\lim_{1/\mathrm{Pe}\to 0} u(1) \neq u_0(1),$$

showing we are dealing with a singular perturbation problem.

To estimate the model error in the quantity of interest $Q(u_0)$ by the DWR method we first derive the dual problems. The fine dual problem in weak form is given by:

$$B'(v,p) = Q(v) \Rightarrow \int_\Omega (-vp_x + \frac{1}{\mathrm{Pe}} v_x p_x)dx - \frac{1}{\mathrm{Pe}} vp_x|_0^1 - \frac{1}{\mathrm{Pe}} v_x(1)p(1) + \frac{1}{\mathrm{Pe}} v_x(0)p(0) = \int_\Omega v dx. \quad (50)$$

Since this has to hold for all v the boundary conditions are: $p(0) = p(1) = 0$. The fine dual solution is then:

$$p(x) = -\frac{e^{\mathrm{Pe}(1-x)} - x(1+e^{\mathrm{Pe}}) - e^{\mathrm{Pe}}}{a(-1+e^{\mathrm{Pe}})}. \quad (51)$$

For the coarse dual problem we have:

$$B_0'(v,p_0) = Q(v) \Rightarrow \int_\Omega -avp_{0_x} dx + av(1)p_0(1) = \int_\Omega v dx. \quad (52)$$

Since (52) has to hold for all v we arrive at the dual equation $-ap_{0_x} = 1$ with the boundary condition $p_0(1) = 0$ of which the solution is given by $p_0(x) = (1-x)/a$. This solution is shown together with the solution of the fine adjoint problem for $a > 0$ and three values of Pe in Figure 2.

Figure 2 illustrates that the dual problem is also a singular perturbation problem. The fine dual solution approaches the coarse adjoint solution on $(0,1)$ for $1/\mathrm{Pe} \to 0$, but on the dual outflow boundary a residual remains: $\lim_{1/\mathrm{Pe}\to 0} p(0) \neq p_0(0)$.

Now we can evaluate the residual estimator based on the fine and coarse dual solutions according to Eq. (39) for the steady case. For the fine adjoint-based estimator we obtain using $u_L - u_0(0) = 0$, $p(0) = p(1) = 0$, $u_R = 1$, $u_0(1) = 0$ and the fact that u_0 is constant on $(0,1)$:

$$\begin{aligned} R(u_0,p) &= B_0(u_0,p) - B(u_0,p) - (F_0(p) - F(p)) \quad (53)\\ &= \int_\Omega \mu u_{0x} p dx - \mu(u_R - u_0(1))p_x(1) + \mu(u_L - u_0(0))p_x(0) - \\ &\quad a(u_R - u_0(1))p(1) \\ &= -\mu(u_R - u_0(1))p_x(1) \\ &= -\mu(1-0)\Big(\frac{-e^{\mathrm{Pe}} + 1 + \mathrm{Pe}}{\mu \mathrm{Pe}(-1+e^{\mathrm{Pe}})}\Big) = \frac{1}{Pe} - \frac{1}{-1+e^{Pe}}. \end{aligned}$$

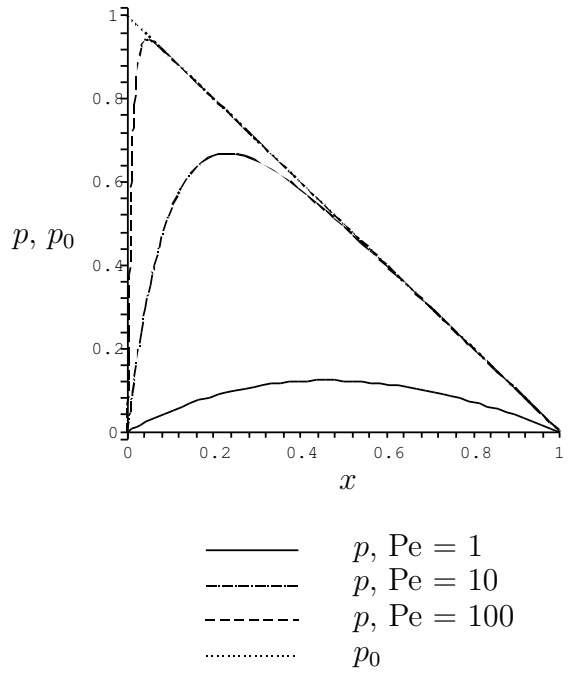


Figure 2: Fine and coarse dual solutions, steady example.

Comparing the result of (53) with the exact error $Q(u) - Q(u_0) = Q(u)$ in Eq. (47), it shows that this estimator is exact. Eq. (53) also illustrates the importance of the explicit inclusion of boundary contributions in the error estimator: the inner domain contribution (the first integral in (39)) is zero, so using expression (38) yields a zero model-error estimate. The residual estimator $R(u_0, p)$ is fully determined by the boundary contribution $-\mu(u_R - u_0(1))p_x(1)$.

Similarly we find for the coarse adjoint-weighted estimator by neglecting the dual error $\epsilon_0 = p - p_0$ and using $u_L - u_0(0) = 0$, $u_R = 1$, $u_0(1) = 0$, $p_0(1) = 0$, $p_{0_x}(1) = -1/a$ and u_0 being constant on $(0, 1)$:

$$\begin{aligned} R(u_0, p_0) &= B_0(u_0, p_0) - B(u_0, p_0) - (F_0(p_0) - F(p_0)) \\ &= -\mu(u_R - u_0(1))p_{0_x}(1) \\ &= \frac{1}{\mathrm{Pe}}. \end{aligned} \tag{54}$$

Also the coarse adjoint-weighted estimator (54) has a contribution exclusively from the boundary in this example. Both fine and coarse adjoint-weighted estimators are shown in Figure 3 for $a = 1$ together with the exact error $Q(u) - Q(u_0)$. For $\mu \lessapprox .3$ the difference between both estimators is negligible and for larger μ the coarse-adjoint weighted estimator over-estimates the exact error. This over-estimation makes the estimator more suitable for adaptation purposes than under-estimation.

Comparing Eq. (54) with Eq. (53) tells us that for large Péclet numbers the fine adjoint-weighted estimator converges to the coarse adjoint-weighted estimator and that both estimators are of $O(\frac{1}{Pe})$:

$$\lim_{\mathrm{Pe}\to\infty} R(u_0, p) = \lim_{\mathrm{Pe}\to\infty} \frac{1}{\mathrm{Pe}} = R(u_0, p_0). \tag{55}$$

This is due to the derivative of $p(x)$ which gives $\lim_{1/Pe\to 0} p_x(1) = p_{0x}(1)$, see also Figure 2. For small Pe the real error is over-estimated by $R(u_0, p_0)$.

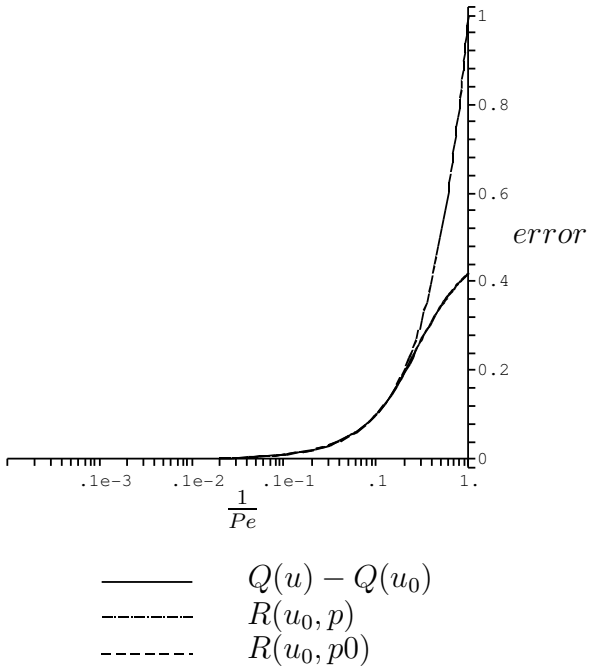


Figure 3: Real error and estimators based on fine and coarse dual solution ($a = 1$), Example 1.

4 Example of an unsteady problem

In this section numerical results are given for an example of the unsteady convection-diffusion equation on $(x, t) \in (0, 1) \times (0, 0.5)$. A Galerkin spectral element code in space-time formulation is used to approximate the primal and dual solutions. The case with a linear integral quantity of interest $Q(u) = \int_\Omega u dx$ as discussed in the previous sections is studied. For the first quantity of interest the estimator should be exact using the fine adjoint as weighting function. A fixed convective velocity $a = 1$ is used and the initial condition used is given by the following function:

$$u^0(x) = 1 - \cos \pi x, \;\; x \in [0, 1]. \tag{56}$$

The boundary conditions for the fine model (2) are derived from the initial condition: $u(0) = u^0(0) = 0$ and $u(1) = u^0(1) = 2$ and the boundary condition for the approximating model (16) with $a > 0$ is $u_0(0) = u^0(0) = 0$. For both quantities of interest the goal-oriented error estimators $R(u_0, p)$ and $R(u_0, p_0)$ are evaluated for different values of the diffusion coefficient μ.

4.1 The Galerkin spectral element model

For the numerical approximation by the Galerkin spectral element method (Galerkin SEM) the domain $(x,t) \in (0,1) \times (0,0.5)$ is divided into space-time slaps Ω_n which are again divided into N_{el} non-overlapping sub domains Ω_e:

$$\Omega_n = \bigcup_{e=1}^{N_{el}} \Omega_e.$$

With the finite dimensional subspace $U^h \subset U$ with basis ϕ_i, the approximating solution $u^h \in U^h$ (as well as the dual solution $p^h \in U^h$) can be written as:

$$u^h(x,t) = \sum_{e=1}^{N_{el}} \sum_{p=1}^{P+1} u_p^e \phi_p(x,t). \tag{57}$$

For the basis functions ϕ_i two-dimensional Lagrangian basis functions through the Gauss-Lobatto-Legandre nodes (see [4, 5, 7]) are used, based on the element coordinates $\vec{\xi} = (\xi, \eta)$ defined as the standard element $[-1,1]^2$. The order of the polynomials are indicated by P and Q for the order in space and time, respectively, so the elemental degree of freedom is $(P+1)(Q+1)$.

Numerical integration Numerical integration is performed through Gauss-Lobatto quadrature based on the Gauss-Lobatto-Legendre roots. The weights for numerical integration are the corresponding Gauss-Lobatto-Legendre weights (GLL-weights). Gauss-Lobatto quadrature is exact for polynomials up to degree $2P-1$. The evaluation of an integral in one dimension, for example in ξ, using Gaussian quadrature is done through the finite summation:

$$\int_{-1}^{1} f(\xi) d\xi \approx \sum_{p=1}^{P+1} w_p f(\xi_p), \tag{58}$$

where w_p is the GLL-weight and ξ_p the p-th GLL-point. To evaluate the integral in global coordinates (x,t) Eq. (58) is multiplied by the determinant of the mapping from the physical domain to the standard element.

In constructing the spectral element matrices as well as the computation of the model error the inner product of two functions needs to be evaluated over an elemental region

Ω_e. To do so, the inner product of two functions $u(x,t)$ and $v(x,t)$ is also computed using Gauss-Lobatto quadrature:

$$\begin{aligned}(u,v)_{\Omega_e} &= \int\int_{\Omega_e} u(\xi,\eta)v(\xi,\eta)|J^e|d\xi d\eta \\ &\approx \sum_{p=1}^{P+1}\sum_{q=1}^{Q+1} w_p w_q u(\xi_p,\eta_q)v(\xi_p,\eta_q)|J^e_{pq}| = \vec{u}^T\mathbf{W}\vec{v},\end{aligned} \tag{59}$$

where $\vec{u}$ and $\vec{v}$ are the vectors containing the values of u and v evaluated in the GLL-roots and $|J^e_{pq}|$ is the Jacobian determinant evaluated in (ξ_p,η_q) of element Ω_e required for the mapping from the local coordinates $\vec{\xi}$ to global coordinates (x,t). The diagonal weight matrix $\mathbf{W}$ contains the GLL-weights w_p and w_q:

$$\mathbf{W}_{ii} = w_p w_q |J^e_{pq}|, \quad i=(q-1)(P+1)+p,\ 1\le i\le (P+1)(Q+1). \tag{60}$$

The order of the numerical integration through Gaussian quadrature is chosen equal to the order of the polynomial expansion in (57).

Numerical differentiation Differentiation of u^h (and p^h) with respect to the global coordinates x and t is achieved by applying the differentiation matrices D_x and D_t which are defined in terms of the local coordinates ξ and η by:

$$D_x = \Lambda\Big(\frac{\partial\xi}{\partial x}\Big)D_\xi \tag{61a}$$

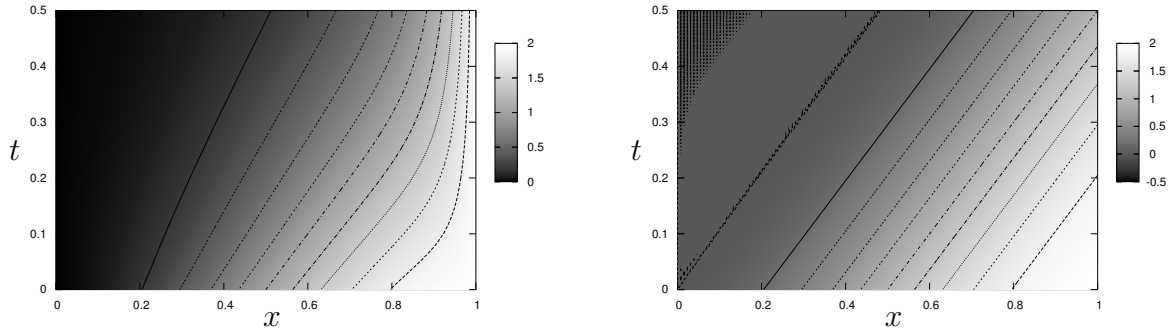
$$D_t = \Lambda\Big(\frac{\partial\eta}{\partial t}\Big)D_\eta, \tag{61b}$$

where $\Lambda(\cdot)$ is a diagonal matrix that evaluates the function between brackets at the GLL-points. The local differentiation matrices D_ξ and D_η contain the derivatives of the Lagrange interpolants through the GLL-points with respect to the local coordinates ξ and η, respectively. For more details on Spectral Element Methods the reader is referred to, e.g., [4, 5, 7].

Stabilisation of convection equation Since Galerkin is unstable for convection (dominated) problems a SUPG stabilisation [6] in space-time is applied with a stabilisation parameter $\tau = h^2$.

The solutions of the primal fine and coarse models (2) and (16) respectively, for the given initial solution (56) are shown in figure 4. These solutions are computed with 128 elements of second order in space and time. For the time steps we used a CFL number of .5. The diffusion coefficient used for the solution in Figure 4(a) is $\mu = .1$ such that, with $a = 1$, the Péclet number is 10. The boundary layer at boundary $x = 1$ becomes thicker/thinner with increasing/decreasing μ. As can be seen in Figure 4 the solution

of the approximating convection equation clearly lacks the presence of a boundary layer. The scales of both images differ somewhat since small overshoots exist in the convection solution. Due to the applied SUPG the overshoots are non-increasing in time.



(a) Fine model solution, $\mu = .1$.

(b) Coarse model solution.

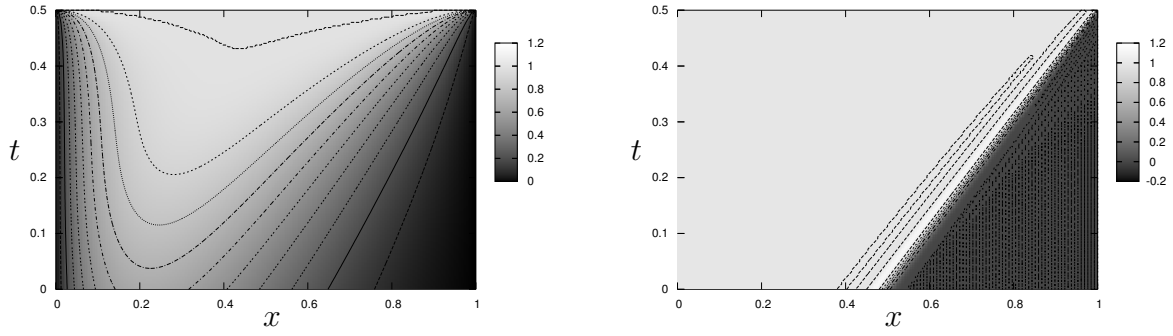
Figure 4: Solutions of the fine and coarse model, $N_{el} = 128$, $P = 2$, $Q = 2$.

4.2 Error estimator for $Q(u) = \int_\Omega u dx$

In Sections 2.1 and 2.2 the fine and coarse dual problems are derived for the linear integral quantity of interest $Q(u) = \int_\Omega u dx$ (for which the residual estimator $R(u_0, p)$ should be exact (apart from numerical effects). The dual initial and boundary conditions are given in Eq. (15) and Eq. (22) for the fine and coarse dual problem, respectively.

The fine and coarse dual solutions on $(x, t) \in (0, 1) \times (0, 0.5)$ are shown in Figure 5. The solutions shown are again computed with 128 elements, $P = Q = 2$. Please note that the dual problem is solved backwards in time and therefore $p(x, T) = 1,\ x \in (0, 1)$ is the dual initial solution. In the dual convection-diffusion solution (the *fine* dual solution), Figure 5(a), a boundary layer is visible at the dual outflow boundary $x = 0$ and the discontinuity introduced at $x = 1$ is smeared out by the diffusion. The dual convection solution (the *coarse* dual solution) in Figure 5(b) clearly lacks diffusion (apart from artificial diffusion from the SUPG) and the discontinuity is transported into the domain. The scales from both plots in Figure 5 differ slightly due to the overshoots in the coarse dual (convection) solution which are stable in time due to the SUPG stabilisation.

The error estimator in general form for a convection-diffusion problem on $(x, t) \in (0, 1) \times (0, T)$ is given by Eq. (39). Since for the problem considered the boundary condition for the coarse model is equal to the fine model boundary condition: $u_0(0, t) = u_L(t)$, the residual contributions on $x = 0$ are zero. Furthermore, both the second and the



(a) Fine dual solution, $\mu = .1$.

(b) Coarse dual solution.

Figure 5: Dual solutions of the fine and coarse model, $N_{el} = 128$, $P = 2$, $Q = 2$.

last integral in Eq. (39) are zero. Due to the homogeneous adjoint boundary conditions $p(0,t) = p(1,t) = 0$ estimator (39) reduces to:

$$R(u_0, p) = -\int_0^T \int_\Omega \mu u_{0x} p_x dx dt - \int_0^T \mu(u_R(t) - u_0(1,t)) p_x(1,t) dt. \tag{62}$$

4.2.1 The discrete error estimator

Using numerical integration and differentiation as given in Eq.s (59) and (61) the error estimator (62) is approximated in a discrete way where e indicates the element on time-level k:

$$\begin{aligned} R(u_0^h, p^h) \;=\; & -\mu \sum_{k=1}^{n} \sum_{e=1}^{N_{el}} (\mathbf{D}_x \vec{u}_0^h)^T|_e^k \mathbf{W}^k (\mathbf{D}_x \vec{p}^h)|_e^k - \\ & \mu \sum_{k=1}^{n} \sum_{q=1}^{Q+1} w_q \Big(\vec{u}_R - \vec{u}_0^h(\xi_{P+1}, \eta_q)|_{N_{el}^k} \Big) \vec{p}_x^h(\xi_{P+1}, \eta_q)|_{N_{el}^k} \frac{\partial y}{\partial \eta}|_{N_{el}^k}, \end{aligned} \tag{63}$$

where $\vec{u}_R$ is a vector with the boundary condition u_R in the GLL-roots at $\Omega_{N_{el}^k}(\xi_{P+1}, \eta_q)$, $\frac{\partial y}{\partial \eta}$ the determinant and $\vec{p}_x^h(\xi_{P+1}, \eta_q)|_{N_{el}}^k$ the vector with adjoint derivatives evaluated at the GLL-points on the right boundary (ξ_{P+1}, η) of element Ω_{Nel} at time-level k. For computations which are first-order accurate in time the GLL-points are on both right corners of the space-time element $\Omega_{N_{el}}$, or in local coordinates: $(1, -1)$ and $(1, 1)$. The derivative $\vec{p}_x^h(\xi_{P+1}, \eta_q)|_{N_{el}^k}$ is computed on element $\Omega_{N_{el}^k}$ at the corresponding time-level k

by:

$$\vec{p}_x^h(\xi_{P+1},\eta_q)|_{N_{el}} = \frac{\partial p^h}{\partial \xi}(\xi_{P+1},\eta_q)|_{N_{el}}\frac{\partial \xi}{\partial x}|_{N_{el}}, \tag{64}$$

where $i = q(P+1)$ and $1 < j < (Q+1)(P+1)$.

4.3 Results

The results are given for $\mu = 10^{-2}$ to 1 by the numerical approximation of the real error $Q(u^h) - Q(u_0^h)$, the estimated errors $R(u_0^h, p^h)$ and $R(u_0^h, p_0^h)$ and the two contributions to the estimator as given in Eq. (63). The quantity of interest is computed using the integration by Gaussian quadrature as in Eq. (58):

$$Q(u^h) = \sum_{e=1}^{N_{el}} \int_{-1}^{1} u^h(\xi,\eta_{Q+1})|_e d\xi \frac{\partial x}{\partial \xi} \approx \sum_{e=1}^{N_{el}}\sum_{p=1}^{P+1} w_p u^h(\xi_p,\eta_{Q+1})|_e \frac{\partial x}{\partial \xi}|_{N_{el}}. \tag{65}$$

Furthermore, also the efficiency index is used to indicate the quality of the estimator. A numerical approximation of the efficiency index is computed by:

$$I_{eff} = \frac{R(u_0^h, p^h)}{Q(u^h) - Q(u_0^h)}. \tag{66}$$

The dual problem for the case described in this section with $Q(u) = \int_\Omega u dx$ is derived in Section 2 and is subject to homogeneous boundary conditions $p(0,t) = p(1,t) = 0$. Together with the dual initial condition $p(x,T) = 1,\ \forall x \in (0,1)$ this means a discontinuity is introduced at the boundaries. For the convection-diffusion problem we experience numerical difficulties. Discontinuities do not exist in the solution space of problems with a diffusion operator (this is in fact a non-physical situation). It is, however, important to have a good approximation of the boundary values since the error estimator requires the derivative of the dual solution at the boundary $x = 1$, see Eq. (62). Increasing the order P of the elements does not improve the resolution of the solution. To maintain the situation that we have an infinite boundary derivative $p_x^h(1,T)$ but to make the initial condition more smooth (or in other words: more 'diffusion' friendly), the values of the initial condition are modified on the elements neighbouring the boundaries by a numerical 'boundary fix'. Instead of the value $p^h(\xi_p,T) = 1$ $(p = 1 \ldots P)$ the values in the Gauss-Lobatto points are computed according to a circle with its centre in $\vec{\xi} = (-1,\eta)$. This is illustrated in Figure 6 for the right boundary element of order $P = 4$ in space. Due to this modification of the initial adjoint values at the boundary elements the derivative of the adjoint at the boundaries $p_x(0,T)$ and $p_x(1,T)$ are infinite. Furthermore the oscillations of the polynomials are reduced since the jump from the boundary point to the neighbouring point of the element is eliminated.

The approximation to the real error $Q(u^h) - Q(u_0^h)$ and the estimated errors by $R(u_0^h, p^h)$ and $R(u_0^h, p_0^h)$ are shown in Figure 7 for $N_{el} = 128$ elements and $P = Q = 2$. Also the

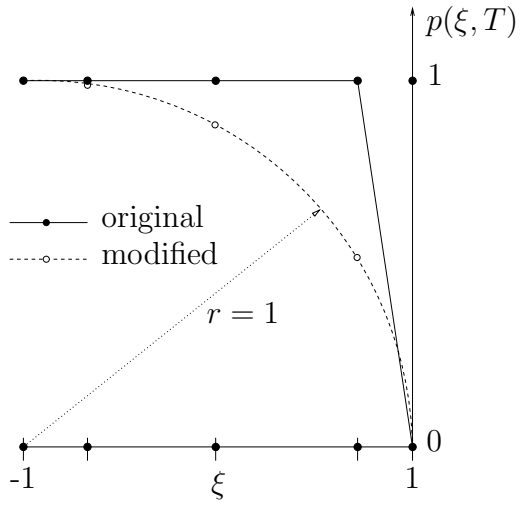
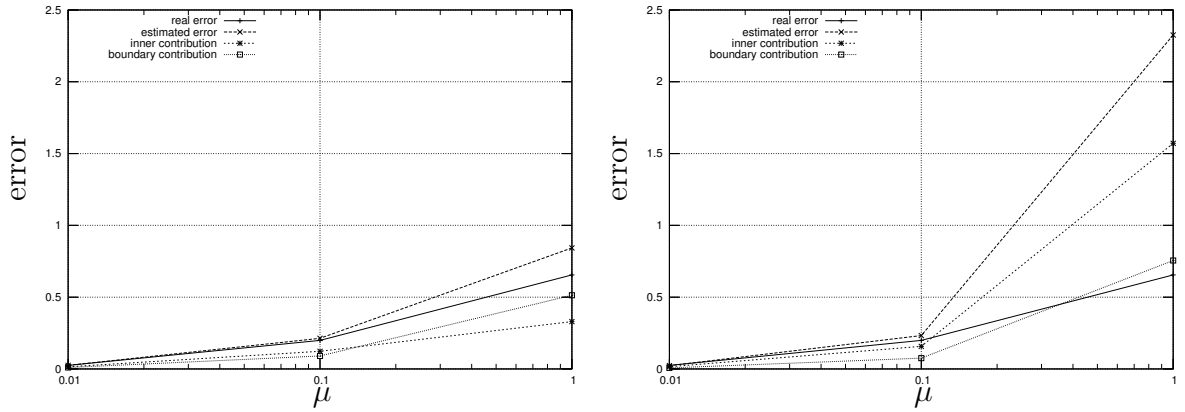


Figure 6: Original and modified initial adjoint solution at GLL-points of boundary element, $P = 4$.

absolute value of the individual contributions to the estimator from the inner domain and the boundaries are shown. Figure 7(a) shows that the boundary contribution has a significant contribution in the estimator. The coarse adjoint-weighted estimator $R(u_0^h, p_0^h)$ for $\mu = 1$ is heavily over-estimated, even by the inner domain contribution only. This over-estimation can be expected though, since in the steady analytical case the real error is over-estimated as well for large μ, see Figure 3 (remind that Pe$= aL/\mu$ with $a = L = 1$).



(a) $R(u_0^h, p^h)$.

(b) $R(u_0^h, p_0^h)$.

Figure 7: Exact and estimated errors, $N_{el} = 128$, $P = Q = 2$.

The efficiency index is given for both fine and coarse adjoint-weighted estimators, in figure 8 with h-refinement and in figure 9 for P-refinement. Both figures show the quality of the fine and coarse adjoint-based estimators with respect to the computed exact error:

since $R(u_0, p)$ is exact in the linear case the numerical approximation $R(u_0^h, p^h)$ should be close to one, see figure 8(a). Only for $\mu = 1$ there is a slight deviation which moves closer to one for increasing order P and Q. This affects an accurate computation of the derivate (64) at the boundary $p_x^h(1,t)$ required in the estimator (63). Even with the 'fix' described above the estimator is still not exact.

It is found that the coarse adjoint-based estimator $R(u_0^h, p_0^h)$ is a good approximation of the real error for $\mu \leq .1$, see figures 8(b) and 9(b). For $\mu = 1$ the error is highly over-estimated by the coarse adjoint-based estimator $R(u_0^h, p_0^h)$, although the over-estimation decreases for increasing order P and Q, see figure 9(b). The trend of over-estimation of the coarse adjoint based estimator for increasing μ is also found in the steady example in section 3 for a comparable quantity of interest $Q(u) = \int_\Omega u dx$, see Figure 3.

Furthermore, Figure 8 shows that the coarse adjoint-weighted estimator depends less on the element size h than the fine adjoint-weighted estimator. This is explained by the absence of boundary layers in the coarse adjoint solution. Therefore the accuracy of the solution is not influenced by a good or bad resolution of the boundary layers. As mentioned before the efficiency (or practical applicability) of the DWR requires the use of the coarse adjoint. In this example the coarse adjoint-weighted estimator is found to be a useful and reliable estimator, since:

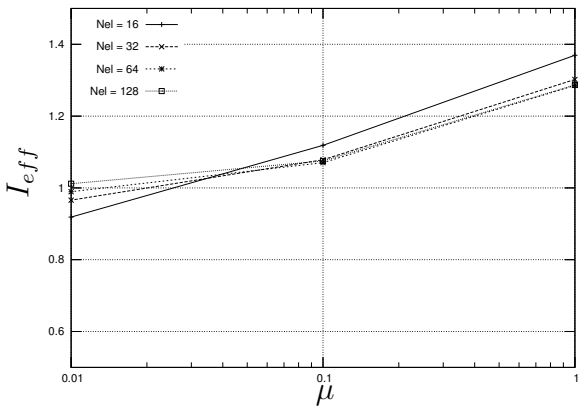
- it gives a good approximation for $\mu \lessapprox 1$,
- it shows a low mesh dependence,
- it over-estimates the real error.

The latter makes the coarse adjoint-weighted estimator more useful as driving criterion in an adaptation algorithm than under-estimation of the real error. Under-estimation might cause the adaptation process to stop too early due to which the required accuracy of the quantity of interest might not be achieved.

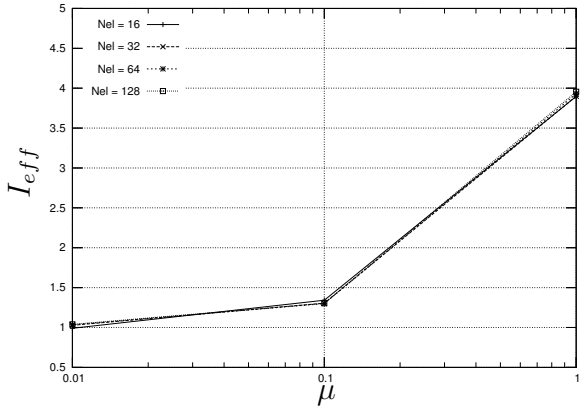
5 Conclusions

An approach has been presented for using the Dual-Weighted Residual method for goal-oriented model-error estimation in convection-diffusion problems where the diffusion term is omitted in the coarse model. In that case we are dealing with singular perturbation problems in the limit of a vanishing diffusion coefficient since the highest order derivative is omitted. Due to this change in mathematical character of the problem the required boundary conditions change and consequently boundary residuals arise between the fine and coarse model solutions on the outflow boundary.

By imposing the boundary conditions weakly in the problem formulation an estimator according the DWR method is obtained for $Q(u) - Q(u_0)$ that includes both inner domain and boundary contributions. In the goal-oriented model-error estimator according to the DWR method we have contributions from the diffusion as well as the convection operator.

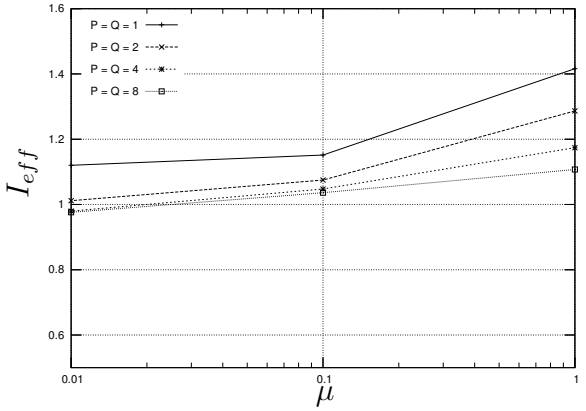


(a) h-Refined I_{eff} for $R(u_0^h, p^h)$.

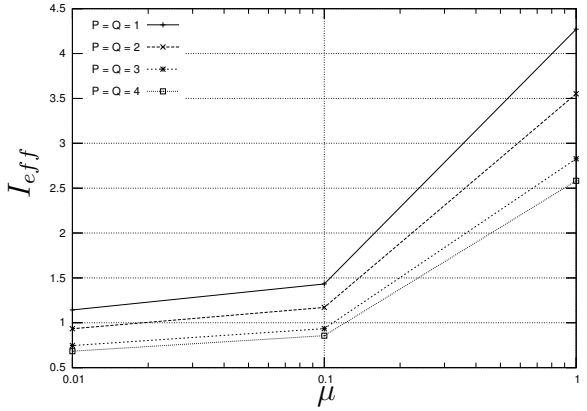


(b) h-Refined I_{eff} for $R(u_0^h, p_0^h)$.

Figure 8: h-Refinement for efficiency index of $R(u_0, p)$ and $R(u_0, p_0)$, $P = Q = 2$.



(a) P-refined I_{eff} for $R(u_0^h, p^h)$.



(b) P-refined I_{eff} for $R(u_0^h, p_0^h)$.

Figure 9: P-Refinement for efficiency index of $R(u_0, p)$ and $R(u_0, p_0)$, $N = 128$.

The boundary contribution in the model-error estimator has a significant contribution: in the steady (analytical) example the boundary contribution is in fact the only contribution. However, in the boundary contribution the boundary residual is weighted by the adjoint derivative which means that in numerical problems an accurate approximation is required of the adjoint derivative at the boundary. For the dual convection-diffusion problem this is complicated in case the adjoint boundary conditions are zero while the initial adjoint solution is not: this introduces a discontinuity at the boundary. A numerical fix of the initial adjoint solution is applied which improves the approximation of the

adjoint derivative.

Inherent to the efficiency of the DWR method is the use of the coarse adjoint as weighting function in the residual estimator. Especially in linear problems where solving the fine dual problem requires equal numerical effort as the fine primal problem (in non-linear problems the linearised fine dual problem is free of Newton-type linearisations).

As illustrated in the numerical examples computed using a Galerkin SEM applying the DWR method in unsteady problems is fairly expensive since the dual problem needs to be solved on the whole space-time domain. In a model adaptation procedure this would imply that after evaluating the quantity of interest based on the coarse model solution the dual problem has to be solved back in time to $t = 0$.

An advantage of the use of the coarse adjoint instead of the fine adjoint as weighting function is that in neither the primal nor the dual problem physical diffusion is present such that no mesh refinement is required to capture possible boundary layers. For the examples treated in this paper the coarse-adjoint based estimator is a good approximation of the fine adjoint based estimator and also of the real error.

Acknowledgements

The authors are grateful to Serge Prudhomme (The University of Texas at Austin) for useful comments and Bart de Maerschalck (Delft University of Technology/VKI Brussels) for providing the spectral element code.

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