# An optimal control approach to adaptivity in computational fluid mechanics

# R. Becker\*, V. Heuveline and R. Rannacher

Institut für Angewandte Mathematik, University of Heidelberg, Im Neuenheimer Feld 294, 69120 Heidelberg, Germany

## SUMMARY

We consider a typical design cycle in computational fluid mechanics: First, an output value such as the drag coefficient is computed. Then, this value is optimized by varying certain control parameters. Finally, the stability of the resulting optimized flow is analysed. For each of these tasks, we derive *a posteriori* error estimators within a uniform framework based on the optimal control approach described in Becker and Rannacher (*Acta Numerica*, Iserles A (ed.). CUP: Cambridge, 2001; 1). These estimators are used for adaptive mesh refinement in order to increase the accuracy upto a given tolerance. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: finite elements; mesh adaptation; error control; optimal control; eigenvalue computation; hydrodynamic stability

## 1. INTRODUCTION

In this paper we present a general approach to *a posteriori* error estimation and automatic mesh adaptation in computational fluid mechanics. Traditionally, *a posteriori* error estimation in Galerkin finite element methods aims at estimating the error with respect to some natural 'energy norm' in terms of the localized 'residual' of the computed solution. This approach appears to be rather generic as it is based on the variational formulation of the problem and allows us to exploit inherent coercivity properties. However, in most applications the error in the 'energy norm' does not provide useful bounds on the errors in the quantities of real physical interest and the generated meshes may not be economical. A more versatile method for 'goal-oriented' adaptivity is obtained by using duality arguments common in the *a priori* error analysis ('Aubin-Nitsche trick'). In fact, the approximation of partial differential equations by discretization may be considered in the context of *model reduction* where a conceptually *infinite* dimensional model is approximated by a *finite* dimensional one. Controlling the error in such a process requires us to determine the influence factors of the local error

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<sup>\*</sup>Correspondence to: R. Becker, Institut für Angewandte Mathematik, Universitat Heidelberg, Im Neuenheimer Feld 293/294, D-61920, Heidelberg, Germany.

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indicators on the target quantity J(u). This suggests simultaneously considering the 'primal' error  $e_h = u - u_h$  and the 'dual' or 'adjoint' error  $e_h^* := z - z_h$ , which is common in the Euler– Lagrange approach of optimal control theory. This concept is easily realized for discretization by a Galerkin finite element method. Employing the natural Galerkin orthogonality, we can derive error representations of the form  $J(e_h) = \langle \rho(u_h), h^2 \omega^*(z) \rangle + \langle h^2 \omega(u), \rho^*(z_h) \rangle + R_h$ , in which primal and dual residuals  $\rho(u_h)$  and  $\rho^*(z_h)$  are mutually multiplied by dual and primal weights  $h^2 \omega^*(z)$  and  $h^2 \omega(u)$ . The remainder term  $R_h$  due to linearization is cubic in the errors and may be neglected. From these error representations, we derive local error indicators that are used to construct economical meshes for the particular purpose of the computation. This approach will be illustrated by several prototypical applications involving the differential operator  $\mathscr{A}(\cdot)$  governing the Navier–Stokes equations:

- 1. Computation of a quantity J(u) from the solution of  $\mathcal{A}(u) = f$ .
- 2. Minimization of J(u) w.r.t. some control q under the constraint  $\mathcal{A}(u) + Bq = f$ .
- 3. Determination of the stability of  $\hat{u}$  by solving the eigenvalue problem  $\mathscr{A}'(\hat{u})u = \lambda \mathscr{M}u$ .

All these problems can be treated within the same abstract framework that essentially uses arguments from elementary calculus. The material presented is based on results developed in References [1-4].

#### 2. FORMULATION OF THE FLOW PROBLEMS

For simplicity, the following presentation concentrates on applications that are related to the Navier–Stokes equations for modelling viscous, incompressible fluid flow. The same techniques can also be used for more complex situations of compressible flow involving temperature transport and chemical reactions (see References [5-7]).

#### 2.1. The boundary value problem

As an example, we consider the laminar flow around the cross-section of a cylinder in a 2D channel (with slightly displaced vertical position) as shown in Figure 1. This is a standard benchmark problem for which reference solutions are available [8]. The underlying model is the stationary Navier–Stokes system

$$\mathscr{A}(u) := -v\Delta v + v \cdot \nabla v + \nabla p = f, \quad \nabla \cdot v = 0 \tag{1}$$

for a pair  $u := \{v, p\}$ , where v is the velocity field, p the hydrostatic pressure, v the kinematic viscosity (density  $\rho \equiv 1$ ) and f a prescribed volume force (f = 0 in this case). At the boundary  $\partial \Omega$ , the usual non-slip condition  $v|_{\Gamma_{rigid}} = 0$  is imposed together with suitable inflow and free-stream outflow conditions  $v|_{\Gamma_{in}} = v^{in}$  and  $v\partial_n v - np|_{\Gamma_{out}} = 0$ , respectively. In the following, scalar and vector functions are both denoted by normal type and no distinction is made in the notation of the corresponding inner products and norms.

Quantities of physical interest are, for example, the drag and lift coefficients defined by

$$J_{\text{drag}} := \frac{2}{\bar{U}^2 D} \int_S n^{\mathrm{T}} \sigma(v, p) e_x \, \mathrm{d}s, \quad J_{\text{lift}} := \frac{2}{\bar{U}^2 D} \int_S n^{\mathrm{T}} \sigma(v, p) e_y \, \mathrm{d}s$$

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Figure 1. Configuration of the flow problems.

where S is the surface of the cylinder, D its diameter,  $\overline{U}$  the reference velocity and  $\sigma(v, p) = \frac{1}{2}v(\nabla v + \nabla v^{T}) + pI$  the stress force acting on S. In our example, the Reynolds number is  $Re = \overline{U}^2 D/v = 20$ , such that the flow is stationary. For evaluating the drag and lift coefficients, one usually uses equivalent volume-oriented formulas, see for example, Reference [9], e.g. for the drag:

$$J_{\text{drag}} = \frac{2}{\bar{U}^2 D} \int_{\Omega} \{ \sigma(v, p) \nabla \bar{e}_x + \nabla \cdot \sigma(v, p) \bar{e}_x \} \, \mathrm{d}x$$

where  $\bar{e}_x$  is an extension of  $e_x$  to the interior of  $\Omega$  with support along S. Notice that on the discrete level the two formulas differ. Theory and computation show that the volume formula yields significantly more accurate and robust approximations of the drag coefficient; see References [2, 10].

The finite element discretization of problem (1) is based on a variational formulation. We introduce the standard function spaces  $L := L^2(\Omega)$ ,  $\hat{H} := H^1(\Omega)^2$ ,  $H := \{v \in \hat{H} : v_{|\Gamma_{in} \cup \Gamma_{rigid}} = 0\}$ ,  $\hat{V} := \hat{H} \times L$  and  $V := H \times L$ . Further, for arguments  $u = \{v, p\}$ ,  $\varphi = \{\varphi^v, \varphi^p\} \in \hat{V}$ , we define a semi-linear form  $a(\cdot; \cdot)$  and a linear form  $f(\cdot)$  by

$$a(u;\varphi) := (\nabla u, \nabla \varphi^v) + (v \cdot \nabla v, \varphi^p) - (p, \nabla \cdot \varphi^v) + (\nabla \cdot v, \varphi^p), \quad f(\varphi) := (f, \varphi^v)$$

Then, the variational formulation of (1) seeks  $u \in V + \{\bar{v}^{in}, 0\}$  such that

$$a(u;\varphi) = f(\varphi) \quad \forall \varphi \in V \tag{2}$$

For discretizing this problem, we use a finite element method based on the quadrilateral  $Q_1/Q_1$ . Stokes element with globally continuous (piecewise isoparametric) bilinear shape functions for both unknowns, pressure and velocity. The corresponding finite element subspaces are denoted by  $L_h \subset L$ ,  $\hat{H}_h \subset \hat{H}$ ,  $H_h \subset H$ ,  $\hat{V}_h := \hat{H}_h \times L_h$  and  $V_h := H_h \times L_h$ , where  $h \in \mathbb{R}_+$  is the mesh size parameter. Further,  $v_h^{\text{in}} \in \hat{H}_h$  is a suitable interpolation of the boundary function  $v^{\text{in}}$ . This construction is motivated by the case of a polygonal domain  $\Omega$  for which the boundary  $\partial\Omega$  is exactly matched by the mesh domain  $\Omega_h := \bigcup \{T \in \mathbb{T}_h\}$ . In the case of a curved boundary (as in the above example) some standard modifications are necessary which are omitted here for the sake of brevity.

In order to obtain a stable discretization of (1) in these spaces with 'equal-order interpolation' of pressure and velocity, we use the least-squares technique proposed by Hughes *et al.* [11]. Following Hughes and Brooks [12], a similar approach is adopted for stabilizing the convection term. We use the approximation

$$\mathscr{S}(u)\varphi := v \cdot \nabla \varphi^v + \nabla \varphi^p$$

to the derivative  $\mathscr{A}'(u)$  for defining the stabilized form

$$a_{\delta}(u; \varphi) := a(u; \varphi) + (\mathscr{A}(u) - f, \mathscr{S}(u)\varphi)_{\delta}$$

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with the mesh-dependent inner product and norm

$$(\varphi,\psi)_{\delta} := \sum_{T \in \mathbb{T}_h} \delta_T(\varphi,\psi)_T, \quad \|\varphi\|_{\delta} = (\varphi,\varphi)_{\delta}^{1/2}$$

The stabilization parameter is chosen according to  $\delta_T = \alpha (vh_T^{-2}, \beta | v_h |_{T;\infty} h_T^{-1})^{-1}$  with the heuristic values  $\alpha = \frac{1}{12}, \beta = \frac{1}{6}$ . By definition, the stabilization parameter  $\delta$  explicitly depends on the solution  $v_h$ . However, in the following discussion this dependence will be neglected for simplicity. With this notation, the discrete Navier–Stokes problem determines  $u_h := \{v_h, p_h\} \in V_h + \{v_h^{\text{in}}, 0\}$  by

$$a_{\delta}(u_h;\varphi_h) = f(\varphi_h) \quad \forall \varphi_h \in V_h \tag{3}$$

This discretization is fully consistent with (1) in the sense that the continuous solution  $\hat{u}$  automatically satisfies (3). This implies 'Galerkin orthogonality'

$$a_{\delta}(u;\varphi_h) - a_{\delta}(u_h;\varphi_h) = 0, \quad \varphi_h \in V_h \tag{4}$$

which is an important ingredient of our approach to a posteriori error estimation.

## 2.2. The optimization problem

Next, we consider an optimization problem related to the boundary value problem introduced above. The goal is to minimize the 'cost-functional'  $J(u) := J_{drag}$  for  $u \in V + \{v^{in}, 0\}$ , under the equation constraint

$$\mathscr{A}(u) + \mathscr{B}q = f \tag{5}$$

where q is a 'boundary control' realized by imposing pressure values at the two openings  $\Gamma_1$ and  $\Gamma_2$ ; see the configuration shown in Figure 1. Since solving the state equation several times with good accuracy is expensive, the use of an economical discretization is indispensable. This leads us to the question of what degree of 'admissibility' of the approximate state  $u_h$  is needed for the optimization process. Our approach is based on the concept that the discretization of the state equation should be adapted according to the evaluation of the cost-functional  $J(\cdot)$ . The resulting 'optimal' controls  $q_h^{opt}$  and flow states  $u_h^{opt}$  usually satisfy the state equation (Navier– Stokes equations) only in a rather weak sense. This may raise concern about the physical relevance of this solution. However, the purpose of the 'model reduction' is only to minimize the costs of the optimization process. Once we have obtained a good optimal control  $q_h^{opt}$ , a more 'admissible' flow state may be generated by approximating the equation  $\mathscr{A}(u) = f - \mathscr{B} q_h^{opt}$  on a finer mesh. Usually, this 'post-processing' step is much cheaper compared to carrying out the whole optimization process on such a fine mesh.

Using the notation from above, the equation of state in variational form reads

$$a_{\delta}(u;\varphi) + b(q,\varphi) = f(\varphi) \quad \forall \varphi \in V \tag{6}$$

with the bilinear 'control form'  $b(q, \varphi) := -(q, n \cdot \varphi^v)_{\Gamma_Q}$ . The control q is chosen constant at the two components of the control boundary  $\Gamma_Q = \Gamma_1 \cup \Gamma_2$  and therefore spans a two-dimensional control space  $Q = \mathbb{R}^2$ . Hence, the solution space for the optimal control problem is  $\hat{V} \times \mathbb{R}^2 \times V$ .

In order to incorporate the optimization problem into our general approach to adaptivity, we will use the so-called 'indirect' method of optimization in which the problem is reformulated

into a boundary value problem by employing the Lagrange formalism. The optimal solution  $\{u^{\text{opt}}, q^{\text{opt}}\} \in \{V+u^{\text{in}}\} \times \mathbb{R}^2 \times V$  of the Lagrangian

$$L(x) = L(u, q, \lambda) := J(u) - a_{\delta}(u; \lambda) - b(q, \lambda) + f(\lambda)$$

on the space  $X := V \times V \times \mathbb{R}^2$ . The corresponding Euler–Lagrange system reads

$$a_{\delta}'(u; \varphi, \lambda) = J(\varphi) \quad \forall \varphi \in V$$

$$a_{\delta}(u; \psi) + b(q, \psi) = f(\psi) \quad \forall \psi \in V$$

$$b(\gamma, \lambda) = 0 \qquad \forall \gamma \in O$$
(7)

In this particular case, the adjoint variable  $\lambda$  and the state variable u are coupled only through the non-linearity in  $a_h(\cdot; \cdot)$ .

Now the discretization is applied to the Euler-Lagrange system (7), that is, we seek triples  $\{u_h, q_h, \lambda_h\} \in \{V_h + u_h^{in}\} \times \mathbb{R}^2 \times V_h$  such that

$$a_{\delta}'(u_{h};\varphi_{h},\lambda_{h}) = J(\varphi_{h}) \quad \forall \varphi_{h} \in V$$

$$a_{\delta}(u_{h};\psi_{h}) + b(q_{h},\psi_{h}) = f(\psi_{h}) \quad \forall \psi_{h} \in V_{h}$$

$$b(\chi_{h},\lambda_{h}) = 0 \qquad \forall \chi_{h} \in Q_{h}$$
(8)

For this approximation, an *a posteriori* estimate will be derived for the error with respect to the cost functional, that is  $J(u)-J(u_h)$ . We will see that with this natural choice, the resulting *a posteriori* error estimate will have a particularly simple structure.

#### 2.3. The eigenvalue problem

Finally, we may be interested in the stability of the optimal solution  $\hat{u} = \{\hat{v}, \hat{q}\}$  obtained in the preceding subsection. To this end, the classical 'linear' stability theory considers the eigenvalue problem of the linearization of (1) about  $\hat{u}$ ,

$$\mathscr{A}'(\hat{u})u := -v\Delta v + \hat{v} \cdot \nabla v + v \cdot \nabla \hat{v} + \nabla p = \lambda v, \quad \nabla \cdot v = 0$$
(9)

for non-trivial  $u := \{v, p\} \in V$  and  $\lambda \in \mathbb{C}$ , under the homogeneous boundary conditions  $v|_{\Gamma_{rigid} \cup \Gamma_{in}} = 0$  and  $v\partial_n v - pn|_{\Gamma_{out}} = 0$ . For  $\hat{v} \neq 0$  this eigenvalue problem is non-symmetric and may possess complex eigenvalues. Therefore, our analysis uses complex-valued functions and associated function spaces. If an eigenvalue of (9) has positive real part, then the base solution  $\hat{u}$  is unstable, otherwise it is said to by 'linearly stable'. However, 'linear stability' does not guarantee full 'non-linear' stability due to effects caused by the non-normality of the problem (9). A sufficient criterion for the  $L^2$ -boundedness of (non-stationary) perturbations is that all eigenvalues of the *symmetric* eigenvalue problem

$$-v\Delta v + \frac{1}{2}(\nabla \hat{v} + \nabla \hat{u}^{\mathrm{T}})v + \nabla p = \lambda v, \quad \nabla \cdot v = 0$$
<sup>(10)</sup>

are non-negative. This criterion is usually more restrictive than that of the 'linear stability' analysis, but it can also be used for non-stationary flows.

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Again, the finite element discretization of the eigenvalue problem (9) is based on its variational formulation. Corresponding to the base solution  $\hat{u}$ , we define the derivative form

$$a'(\hat{u};\psi,\varphi) := v(\nabla\psi^v,\nabla\varphi^v) + (\hat{v}\cdot\nabla\psi^v,\varphi^v) + (\psi^v\cdot\nabla\hat{v},\varphi^v) - (\psi^p,\nabla\cdot\varphi^v) + (\nabla\cdot\psi^v,\varphi^p)$$

and the bilinear form  $m(\psi, \varphi) := (\psi^v, \varphi^v)$ , for arguments  $\psi = \{\psi^v, \psi^p\}, \varphi = \{\varphi^v, \varphi^p\} \in V$ . Then, the eigenvalue problem seeks  $u = \{v, p\} \in V$  such that

$$a'(\hat{u}; u, \varphi) = \lambda m(u, \varphi) \quad \forall \varphi \in V \tag{11}$$

and  $m(u,u) = ||v||^2 = 1$ . Associated to the primal eigenfunction u, there is a 'dual' eigenfunction  $u^* = \{v^*, p^*\} \in V$  corresponding to  $\lambda$  that is determined by

$$a'(\hat{u};\varphi,u^*) = \lambda m(\varphi,u^*) \quad \forall \varphi \in V \tag{12}$$

The dual eigenfunction is usually normalized by  $m(u, u^*) = (v, v^*) = 1$ . However, this requires the eigenvalue  $\lambda$  to have defect zero. If  $m(u, u^*) = 0$ , the boundary value problem

$$a'(\hat{u};\tilde{u},\varphi) - \lambda m(\tilde{u},\varphi) = m(u,\varphi) \quad \forall \varphi \in V$$
(13)

possesses a solution  $\tilde{u} \in V$ , a so-called 'generalized eigenfunction', uniquely determined by the condition  $m(\tilde{u}, u) = 0$ . In this case the eigenvalue  $\lambda$  is said to have non-trivial 'defect'.

For discretizing the eigenvalue problem (11), we use the stabilized sesquilinear form

$$a_{\delta}'(\hat{u}; u_h, \varphi_h) := a'(\hat{u}; u_h, \varphi_h) + (\mathscr{A}'(\hat{u})u_h - \lambda_h \mathscr{M} u_h, \mathscr{S}(\hat{u})\varphi_h)_{\delta}$$

Notice that this is not the derivative of the stabilized form  $a_{\delta}(\cdot; \cdot)$  used in the boundary value problem (3) but rather a consistent stabilization of  $a'(\hat{u}; \cdot, \cdot)$ . The discrete primal and dual eigenvalue problems seek  $u_h, u_h^* \in V_h$  and  $\lambda_h \in \mathbb{C}$ , such that

$$a_{\delta}'(\hat{u}_h; u_h, \varphi_h) = \lambda_h m(u_h, \varphi_h) \quad \forall \varphi_h \in V_h \tag{14}$$

$$a'_{\delta}(\hat{u}_h;\varphi_h,u_h^*) = \lambda_h m(\varphi_h,u_h^*) \quad \forall \varphi_h \in V_h$$
(15)

with  $m(u_h, u_h) = 1$  and  $m(u_h, u_h^*) = 1$ . Then, the blow-up

$$m(v_h^*, v_h^*) \to \infty \quad (h \to 0) \tag{16}$$

can be taken as an indicator for the limit eigenvalue  $\lambda$  to have non-trivial defect. In this case the *a posteriori* error analysis requires us to take into account the approximation of generalized eigenvectors (for a more detailed discussion of this point see Reference [4]).

# 3. GENERAL A POSTERIORI ERROR ESTIMATION

We present our theory of *a posteriori* error estimation in Galerkin methods within an abstract functional analytic setting. This approach incorporates ideas that were first introduced by C. Johnson and his collaborators (see Reference [13]) and have been further developed by the authors (see References [14, 15]); the following presentation is taken from Reference [8].

The abstract theory underlying this approach is based on elementary calculus. The crucial tool is the well-known error representation of the trapezoidal rule:

$$\int_0^1 f(t) \, \mathrm{d}t = \frac{1}{2} \left\{ f(0) + f(1) \right\} + \frac{1}{2} \int_0^1 f''(s) s(s-1) \, \mathrm{d}s \tag{17}$$

## 3.1. Approximation of stationary points

Let X be a function space and  $L(\cdot)$  a differentiable functional on X. Its derivatives at some  $x \in X$  are denoted by  $L'(x; \cdot)$ ,  $L''(x; \cdot, \cdot)$  and  $L'''(x; \cdot, \cdot, \cdot)$ . We seek a stationary point x of  $L(\cdot)$  on X,

$$L'(x; y) = 0 \quad \forall y \in X \tag{18}$$

This equation is approximated by a Galerkin method using finite-dimensional subspaces  $X_h \subset X$  parametrized by  $h \in \mathbb{R}_+$ . The discrete problems seek  $x_h \in X_h$  satisfying

$$L'(x_h; y_h) = 0 \quad \forall y_h \in X_h \tag{19}$$

For estimating the difference  $L(x) - L(x_h)$ , we start from the trivial identity

$$L(x) - L(x_h) = \int_0^1 L'(x_h + se_h; e_h) \,\mathrm{d}s + \frac{1}{2}L'(x_h; e_h) - \frac{1}{2}\{L'(x_h; e_h) + \frac{1}{2}L'(x; e_h)\}$$

Notice that the last two terms on the right are just the approximation of the integral term by the trapezoidal rule. Hence, recalling the corresponding error representation (17) and using (19), we obtain the following result:

#### **Proposition** 1

For any solutions of the problems (18) and (19), we have the *a posteriori* error representation

$$L(x) - L(x_h) = \frac{1}{2}L'(x_h; x - y_h) + R_h$$
(20)

for arbitrary  $y_h \in X_h$ . The remainder term  $R_h$  is cubic in the error  $e_h := x - x_h$ ,

$$R_h := \frac{1}{2} \int_0^1 L'''(x_h + se_h; e_h, e_h, e_h) \ s(s-1) \, \mathrm{d}s$$

Remark 1

In view of the possible non-uniqueness of the solutions x and  $x_h$ , the formulated goal of estimating the error quantity  $L(x) - L(x_h)$  needs some explanation. The error representation (20) does not explicitly require that the approximation  $x_h$  is close to x. However, since it contains a remainder term in which the difference  $x - x_h$  occurs, the result is useful only under the assumption that the convergence  $x_h \rightarrow x$ , as  $h \rightarrow 0$ , is known by *a priori* arguments. This constraint requires us to carefully formulate the concrete problem, for instance the discretization of an eigenvalue problem, for embedding it into the abstract framework.

## 3.2. Approximation of variational equations

Next, we consider the Galerkin approximation of variational equations. Let  $A(\cdot; \cdot)$  be a differentiable semi-linear form and  $F(\cdot)$  a linear functional defined on some function space V. We seek a solution  $u \in V$  to the variational equation

$$A(u;\varphi) = F(\varphi) \quad \forall \varphi \in V \tag{21}$$

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For a finite-dimensional subspace  $V_h \subset V$ , again parametrized by  $h \in \mathbb{R}_+$ , the corresponding Galerkin approximation  $u_h \in V_h$  is determined by

$$A(u_h; \varphi_h) = F(\varphi_h) \quad \forall \varphi_h \in V_h \tag{22}$$

We assume that Equations (21) and (22) possess solutions (not necessarily unique). Let the goal of the computation be the evaluation J(u), where  $J(\cdot)$  is a given differentiable functional. We want to embed this situation into the general setting of Proposition 1. To this end, we note that computing J(u) from the solution of (21) can be interpreted as computing a stationary point  $\{u, z\} \in V \times V$  of the Lagrangian

$$L(u;z) := J(u) - A(u;z) + F(z)$$

with the dual variable  $z \in V$ , that is solving

$$A(u;\psi) = F(\psi) \quad \forall \psi \in V \tag{23}$$

$$A'(u; \varphi, z) = J'(u; \varphi) \quad \forall \varphi \in V \tag{24}$$

In order to obtain a discretization of the system (23,24), in addition to (22), we solve the discrete adjoint equation

$$A'(u_h;\varphi_h,z_h) = J'(u_h;\varphi_h), \quad \varphi_h \in V_h$$

$$\tag{25}$$

We suppose that the dual problems also possess solutions  $z \in V$  and  $z_h \in V_h$ , respectively. Notice that at the solutions  $x = \{u, z\} \in X := V \times V$  and  $x_h = \{u_h, z_h\} \in X_h := V_h \times V_h$ ,

$$L(u;z) - L(u_h;z_h) = J(u) - J(u_h)$$

Hence, Proposition 1, applied to the Lagrangian  $L(\cdot; \cdot)$  on X yields a representation for the error  $J(u) - J(u_h)$  in terms of the residuals

$$\rho(u_h;\psi) := F(\psi) - A(u_h;\psi), \quad \rho^*(z_h;\varphi) := J'(u_h;\varphi) - A'(u_h;\varphi,z_h)$$

Since L(u;z) is linear in z, the remainder  $R_h$  contains only the following three terms:

$$J'''(u_h + se_h; e_h, e_h, e_h) - A'''(u_h + se_h; e_h, e_h, e_h, z_h + se_h^*) - 3A''(u_h + se_h; e_h, e_h, e_h^*)$$

This leads us to the following result:

#### **Proposition 2**

For any solutions of the Euler–Lagrange systems (23,24) and (22,25), we have the *a posteriori* error representation

$$J(u) - J(u_h) = \frac{1}{2}\rho(u_h; z - \psi_h) + \frac{1}{2}\rho^*(z_h; u - \varphi_h) + R_h$$
(26)

for arbitrary  $\psi_h$ ,  $\varphi_h \in V_h$ . The remainder term  $R_h$  is cubic in the errors  $e_h := u - u_h$  and  $e_h^* := z - z_h$ ,

$$R_h := \frac{1}{2} \int_0^1 \{ J'''(u_h + se_h; e_h, e_h, e_h) - A'''(u_h + se_h; e_h, e_h, e_h, z_h + se_h^*) - 3A''(u_h + se_h; e_h, e_h, e_h^*) \} s(s-1) \, \mathrm{d}s$$

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The remainder term  $R_h$  in (26) is usually neglected. The evaluation of the resulting error estimator

$$\eta_{\omega}(u_h, z_h) := \frac{1}{2}\rho(u_h; z - \psi_h) + \frac{1}{2}\rho^*(z_h; u - \varphi_h)$$
(27)

for arbitrary  $\psi$ ,  $\varphi \in V$ , requires us to determine approximations to the exact primal and dual solutions *u* and *z*. We note that the error representation (26) is the non-linear analogue of the (trivial) representation in the linear case,

$$J(e) = \rho(u_h, z - \psi_h) = \rho^*(z_h, u - \varphi_h) = F(e^*)$$
(28)

Integrating by parts in (26), we can derive a simpler error representation that does not contain the unknown primal solution u,

$$J(u) - J(u_h) = \rho(u_h, z - \psi_h) + \tilde{R}_h$$
<sup>(29)</sup>

for arbitrary  $\psi_h \in V_h$ , with the remainder term

$$\tilde{R}_h = \int_0^1 \{A''(u_h + se_h; e_h, e_h, z) - J''(u_h + se_h; e_h, e_h)\} s \, \mathrm{d}s$$

The evaluation of (29) only requires a guess for the dual solution z, but the remainder term  $\tilde{R}_h$  is only quadratic in the error.

# 3.3. Approximation of optimization problems

We continue to use the notation of the preceding sections. A differentiable 'cost-functional' J(u,q) is to be minimized under the equation constraint

$$A(u;\varphi) + B(q,\varphi) = F(\varphi) \quad \forall \varphi \in V$$
(30)

where q is the control from the 'control space' Q, and  $B(\cdot, \cdot)$  is a bilinear form on  $Q \times V$ . On the space  $X := V \times Q \times V$ , we introduce the Lagrangian

$$L(u,q,\lambda) := J(u,q) - A(u;\lambda) - B(q,\lambda) + F(\lambda)$$

with the adjoint variable  $\lambda \in V$ . We want to compute stationary points  $x = \{u, q, \lambda\} \in X$  of L, that is solutions of the variational equation

$$L'(x; y) = 0 \quad \forall y \in X \tag{31}$$

which is equivalent to the saddle-point system

$$A'(u; \varphi, \lambda) = J'_u(u, q; \varphi) \quad \forall \varphi \in V$$

$$A(u; \psi) + B(q, \psi) = F(\psi) \qquad \forall \psi \in V$$

$$B(\chi, \lambda) = J'_a(u, q; \chi) \quad \forall \chi \in Q$$
(32)

For discretizing equation (31), we introduce finite dimensional subspace  $V_h \subset V$  and  $Q_h \subset Q$ parametrized by  $h \in \mathbb{R}_+$ , and set  $X_h := V_h \times Q_h \times V_h \subset X$ . Then, approximations  $x_h = \{u_h, q_h, \lambda_h\} \in X_h$  are determined by

$$L'(x_h; y_h) = 0 \quad \forall y_h \in X_h \tag{33}$$

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what is equivalent to the discrete saddle-point problem

$$A'(u_h; \varphi_h, \lambda_h) = J'_u(u_h, q_h; \varphi_h) \quad \forall \varphi_h \in V$$

$$A(u_h; \psi_h) + B(q_h, \psi_h) = F(\psi_h) \qquad \forall \psi_h \in V_h$$

$$B(\chi_h, \lambda_h) = J'_q(u_h, q_h; \chi_h) \quad \forall \chi_h \in Q_h$$
(34)

The residuals of these equations are denoted by  $\rho^*(\lambda_h; \cdot)$ ,  $\rho(u_h; \cdot)$  and  $\rho^{**}(q_h; \cdot)$ . Again, since  $\{u, q\}$  and  $\{u_h, q_h\}$  satisfy the state equations, we have

$$L(u,q,\lambda) - L(u_h,q_h,\lambda_h) = J(u) - J(u_h)$$

Then, as in the preceding section, we obtain from Proposition 1 the following result:

#### **Proposition 3**

For any solutions of the saddle point problems (32) and (34), we have the *a posteriori* error representation

$$J(u) - J(u_h) = \frac{1}{2}\rho(u_h; \lambda - \psi_h) + \frac{1}{2}\rho^*(\lambda_h; u - \varphi_h) + \frac{1}{2}\rho^{**}(q_h; q - \chi_h) + R_h$$
(35)

for arbitrary  $\varphi_h$ ,  $\psi_h \in V_h$  and  $\chi_h \in Q_h$ . Again, the remainder term  $R_h$  is cubic in the errors  $e_h^u := u - u_h$ ,  $e_h^{\lambda} := \lambda - \lambda_h$  and  $e_h^q := q - q_h$ .

## 3.4. Approximation of eigenvalue problems

We continue to use the notation of the preceding sections. Let  $\hat{u}$  and  $\hat{u}_h$  be a base solution and its approximation given by Equations (21) and (22), respectively. We consider the eigenvalue problem associated with the linearization of the semi-linear form  $a(\cdot; \cdot)$  about  $\hat{u}$ ,

$$a'(\hat{u}; u, \varphi) = \lambda(u, \varphi) \quad \forall \varphi \in V \tag{36}$$

and its discrete analogues,

$$a'(\hat{u}_h; u_h, \varphi_h) = \lambda_h(u_h, \varphi_h) \quad \forall \varphi_h \in V_h \tag{37}$$

In order to derive an *a posteriori* estimate for the eigenvalue error  $\lambda - \lambda_h$ , we introduce the spaces  $\mathscr{V} := V \times V \times \mathbb{C}$  and  $\mathscr{V}_h := V_h \times V_h \times \mathbb{C}$ , and denote their elements by  $U := \{\hat{u}, u, \lambda\}$  and  $U_h := \{\hat{u}_h, u_h, \lambda_h\}$ , respectively. Further, for  $\Phi = \{\hat{\varphi}, \varphi, \mu\} \in \mathscr{V}$ , we introduce a semi-linear form  $A(\cdot; \cdot)$  by

$$A(U;\Phi) := f(\hat{\varphi}) - a_{\delta}(\hat{u};\hat{\varphi}) - \tilde{a}'_{\delta}(\hat{u};u,\varphi) + \lambda m(u,\varphi) + \bar{\mu}\{m(u,u) - 1\}$$

With this notation Equations (21), (36) and (22), (37) in compact form read:

$$A(U;\Phi) = 0 \quad \forall \Phi \in \mathscr{V}, \tag{38}$$

$$A(U_h; \Phi_h) = 0 \quad \forall \Phi_h \in \mathscr{V}_h \tag{39}$$

For controlling the error of this approximation, we choose the functional

$$J(\Phi) := \mu m(\varphi, \varphi)$$

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for  $\Phi = \{\hat{\phi}, \phi, \mu\} \in \mathcal{V}$ , what is motivated by the fact that  $J(U) = \lambda$ , since m(u, u) = 1. In order to apply the general result of Proposition 2 to this situation, we have to identify the dual problems corresponding to (38) and (39). The dual solutions  $Z = \{\hat{z}, z, \pi\} \in \mathcal{V}$  and  $Z_h = \{\hat{z}_h, z_h, \pi_h\} \in \mathcal{V}_h$  are determined by the equation

$$A'(U;\Phi,Z) = J'(U;\Phi) \quad \forall \Phi \in \mathscr{V}$$

$$\tag{40}$$

and its discrete analogue

$$A'(U_h; \Phi_h, z_h) = J'(U_h; \Phi_h) \quad \forall \Phi_h \in \mathscr{V}_h \tag{41}$$

respectively. By a lengthy calculation (for the details see Reference [4]), we find that the dual solution  $Z = \{\hat{z}, z, \pi\} \in \mathscr{V}$  is given by  $z = u^*$  and  $\pi = \lambda$ , while  $\hat{z} = \hat{u}^*$  is determined as solution of

$$a'(\hat{u};\psi,\hat{u}^*) = -a''(\hat{u};\psi,u,u^*) \quad \forall \psi \in V$$

$$\tag{42}$$

These results in the following proposition:

#### **Proposition 4**

For the eigenvalue approximation, we have the error representation

$$\lambda - \lambda_{h} = \frac{1}{2} \{ \rho(\hat{u}_{h}; \hat{u}^{*} - \hat{\psi}_{h}) + \rho^{*}(\hat{u}_{h}^{*}; \hat{u} - \hat{\varphi}_{h}) \}$$
  
+ 
$$\frac{1}{2} \{ \rho(\{u_{h}, \lambda_{h}\}; u^{*} - \psi_{h}) + \rho^{*}(\{u_{h}^{*}, \lambda_{h}\}; u - \varphi_{h}) \} - R_{h}$$
(43)

for arbitrary  $\hat{\psi}_h$ ,  $\psi_h$ ,  $\hat{\varphi}_h$ ,  $\varphi_h \in V_h$ , with the residuals

$$\rho(\hat{u}_h;\psi) := f(\psi) - a_\delta(\hat{u}_h;\psi) \tag{44}$$

$$\rho^*(\hat{u}_h^*;\psi) := -a_{\delta}''(\hat{u};\psi,u_h,u_h^*) - \tilde{a}_{\delta}'(\hat{u}_h;\psi,\hat{u}_h^*)$$
(45)

$$\rho(\{u_h,\lambda_h\};\psi) := \lambda_h m(u_h,\psi) - \tilde{a}'_{\delta}(\hat{u}_h;u_h,\psi)$$
(46)

$$\rho^*(\{u_h^*, \lambda_h\}; \psi) := \lambda_h m(\psi, u_h^*) - \tilde{a}'_{\delta}(\hat{u}_h; \psi, u_h^*)$$

$$\tag{47}$$

The remainder  $R_h$  is given by

$$R_{h} = \frac{1}{2}(\lambda - \lambda_{h})(e_{h}^{v}, e_{h}^{v*}) - \frac{1}{12}a_{\delta}^{\prime\prime}(\hat{u}; \hat{e}_{h}, \hat{e}_{h}^{*}) - \frac{1}{12}a_{\delta}^{\prime\prime}(\hat{u}; \hat{e}_{h}, e_{h}, e_{h}^{*})$$

where  $\hat{e}_h^v := \hat{v} - \hat{v}_h$ ,  $\hat{e}_h^{v*} := \hat{v}^* - \hat{v}_h^*$ ,  $e_h^v := v - v_h$ , and  $e_h^{v*} := v^* - v_h^*$ .

## 4. APPLICATION TO THE FLOW PROBLEMS

We report on some results for the model problem 'flow around a cylinder' obtained by mesh adaptation based on error indicators derived from the general *a posteriori* error representations developed above.

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Figure 2. Quadrilateral mesh patch with a 'hanging node'.

The first step in using an *a posteriori* error representation is the evaluating of the residuals of the discrete solutions. We illustrate this for the primal residual  $\rho(u_h; \psi)$  contained in (26) (for the details of the derivation see References [1, 5]):

$$\rho(u_h; z - \psi_h) := \sum_{T \in \mathbb{T}_h} \left\{ (R(u_h), z^v - \psi_h^v)_T + (r(u_h), z^v - \psi_h^v)_{\partial T} + (\nabla \cdot v_h, z^p - \psi_h^p)_T + \cdots \right\}$$

with the cell and edge residuals  $R^{v}(u_{h})_{|K} := -v\Delta v_{h} + v_{h} \cdot \nabla v_{h} + \nabla p_{h}$  and

$$r^{v}(u_{h})_{|\Gamma} := \begin{cases} -\frac{1}{2} [v\partial_{n}v_{h} - np_{h}], & \text{if } \Gamma \not\subset \partial\Omega \\ 0, & \text{if } \Gamma \subset \Gamma_{\text{rigid}} \cup \Gamma_{\text{in}} \\ -v\partial_{n}v_{h} + np_{h}, & \text{if } \Gamma \subset \Gamma_{\text{out}} \end{cases} \end{cases}$$

where  $[\cdot]$  indicates the jump across an interior edge  $\Gamma$ . The dots '...' stand for additional terms arising by the stabilization and the errors in approximating the inflow data and the curved cylinder boundary which are neglected. The dual solution z is approximated by the patchwise biquadratic interpolation  $i_h^2 z_h$  of its finite element solution  $z_h \in V_h$  computed on the current mesh  $\mathbb{T}_h$ . Accordingly we use the weight  $z - \psi_h \approx i_h^2 z_h - z_h$ , which avoids the use of any constants in the error estimate. The other residual terms are evaluated in an analogous manner. In this way, we obtain *a posteriori* error estimators  $\eta(u_h)$  of the form

$$|J(u) - J(u_h)| \approx \eta_{\omega}(u_h) := \sum_{T \in \mathbb{T}_h} \eta_T$$
(48)

Let TOL be a given error tolerance and  $N_{\text{max}}$  the maximum number of mesh cells that can be used. Grid refinement is realized by edge-bisection, that is by cutting a (two-dimensional) cell *T* into four regular subcells. This process may create cells with 'hanging nodes' such that the mesh is not compatible. The resulting non-conformity of the trial functions is avoided by eliminating the unknowns corresponding to any irregular node by linear interpolation of the values at the neighbouring regular nodes. Then, the resulting finite element space is again 'conforming', that is  $V_h \subset V$ .

On the basis of an *a posteriori* error estimator of the form (48) the adaptation of the mesh  $\mathbb{T}_h$  follows the strategy of equilibrating the error indicators  $\eta_T$  ('error-balancing' strategy) according to  $\eta_T \approx \frac{1}{2} \text{TOL}/N$ . However, this requires a delicate choice of several control parameters. Therefore, we prefer the somewhat cruder 'fixed rate' strategy. Here, in each refinement cycle, the goal is to increase the number of mesh cells N by a fixed rate or to reduce the error estimator  $\eta(u_h)$  by a fixed rate. First, the cells  $T \in \mathbb{T}_h$  are ordered according to the size of the indicator values:  $\eta_{T,1} \leq \cdots \leq \eta_{T,i} \leq \cdots \leq \eta_{T,N}$ . For prescribed rates X% and

	(	Computation of	of drag			Computation of lift						
L	Ν	$c_{\rm drag}$	$\eta_{ m drag}$	I <sub>eff</sub>	L	Ν	$c_{ m lift}$	$\eta_{ m lift}$	$I_{\rm eff}$			
4	984	5.66058	1.1e - 1	0.76								
5	2244	5.59431	3.1e - 2	0.47	4	2208	0.01318	1.3e - 2	0.19			
6	4368	5.58980	1.8e - 2	0.58	5	5088	0.01100	2.7e - 3	0.14			
6	7680	5.58507	8.0e - 3	0.69	7	14016	0.01071	7.8e - 4	0.12			
7	9444	5.58309	6.3e - 3	0.55	8	53040	0.01065	1.8e - 4	0.18			
8	22548	5.58151	2.5e - 3	0.77	9	142896	0.01064	6.4e - 5	0.25			
9	41952	5.58051	1.2e - 3	0.76	11	489648	0.01063	1.8e - 5	0.27			

Table I. Results for drag and lift on adaptively refined meshes (ref. values  $c_{\text{drag}} = 5.579535...$ and  $c_{\text{lift}} = 0.0106189...$ ); error level of 1% indicated by bold face.



Figure 3. Refined meshes generated by the 'energy error' estimator (left) and by the weighted error estimator (right).

Y% the cells are grouped, for instance, according to

$$\sum_{i=N^*}^N \eta_{T,i} \approx X \eta(u_h), \quad \sum_{i=1}^{N_*} \eta_{T,i} \approx Y \eta(u_h)$$

Then the cells  $T_i$   $(i = N^*, ..., N)$  are refined and the cells  $T_i$   $(i = 1, ..., N_*)$  are coarsened until  $N \approx N_{\text{max}}$ .

We note that the evaluation of the *a posteriori* error estimate (48) involves only the solution of *linearized* problems. Hence, the whole error estimation may amount to a relatively small fraction of the total cost for the solution process. This has to be compared to the usually much higher cost when working on non-optimized meshes.

## 4.1. Drag and lift computation

Table I shows the results of the computation of drag and lift coefficients using the weighted error estimator. The effectivity index is defined by  $I_{\text{eff}} := \eta_{\omega}(u_h)/|J(e_h)|$ . Figure 3 shows refined meshes generated by our 'weighted error estimator'  $\eta_{\text{weight}}(u_h)$  and by a (heuristic) 'energy norm' error indicator using only the cell residuals.

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Uniform	refinement	Adaptive refinement			
N	$J_{ m drag}$	N	$J_{ m drag}$		
10512 41504 164928	3.31321 3.21096 3.11800	1572 4264 11146	3.28625 3.16723 3.11972		

Table II. Uniform refinement (left) versus adaptive refinement (right).





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Figure 4. Velocity of the uncontrolled flow (top), the controlled flow (middle) and the corresponding adapted mesh (bottom).

# 4.2. Minimization of the drag

Next, we present some results obtained for the minimization of the drag coefficients by boundary control. The data is chosen such that  $Re = \overline{U}^2 D/\nu = 40$  for the uncontrolled flow. In Table II, we compare the values of the drag coefficient on optimized meshes as shown in Figure 4 with results obtained on globally refined meshes. It is clear from these numbers that a significant reduction in the dimension of the discrete model is possible by using appropriately refined meshes. Figure 4 shows streamline plots of the uncontrolled (q=0) and the controlled  $(q=q^{\text{opt}})$  solution and a corresponding 'optimal' mesh.

The locally refined mesh produced by the adaptive algorithm seems to contradict intuition since the recirculation behind the cylinder is not so well resolved. However, due to the particular structure of the optimal velocity field (most of the flow leaves the domain at

h	Ν	$ \lambda_h^1-\lambda $	$ \lambda_h-\lambda $	$\eta^\lambda_\omega$	$\ v_h^*\ $
$2^{-3}$	162	3.24e - 2	7.07e - 3	1.25e - 2	19.3
$2^{-4}$	578	1.79e - 2	1.80e - 3	2.77e - 3	38.8
$2^{-5}$	2178	9.42e - 3	4.55e - 4	6.54e - 4	77.9
$2^{-6}$	8450	4.82e - 3	1.16e - 4	1.39e - 4	155.9
$2^{-7}$	33282	2.43e - 3	3.11e - 5	3.47e - 5	311.9
$2^{-8}$	132098	1.21e - 3	8.02e - 6	8.58e - 6	623.9

Table III. Computation of the eigenvalue  $\lambda^{crit} = 2.1228...$  on uniform meshes (case  $\nu = 10^{-1}$ ).

the control boundary), it might be clear that this recirculation does not significantly influence the cost functional. Instead, a strong local refinement is produced near the cylinder, where the cost functional is evaluated, as well as near the control boundary.

#### 4.3. Computation of critical eigenvalues

Finally, we present a preliminary result for the computation of eigenvalues. The test case is the two-dimensional Burgers problem

$$-v\Delta\hat{v} + \hat{v}\cdot\nabla\hat{v} = 0 \quad \text{in } \Omega \tag{49}$$

on the rectangular domain  $\Omega := (0, 1)^2 \subset \mathbb{R}^2$ , with boundary conditions modelling plane shear flow  $\hat{v} \equiv \{x_2, 0\}$  ('Taylor-Couette flow'). Linearization about this base solution results in the non-selfadjoint eigenvalue problem

$$-v\Delta v_1 + x_2\partial_1 v_1 + v_2 = \lambda v_1$$
  
$$-v\Delta v_2 + x_2\partial_1 v_2 = \lambda v_2$$
 (50)

for  $v = \{v_1, v_2\}$ , with homogeneous boundary conditions. Due to the coupling of the second component  $v_2$  into the first equation, the most critical eigenvalue  $\lambda^{\text{crit}}$  turns out to be real and to have non-trivial defect. This results in an initial amplification of small perturbations, though all eigenvalues obviously have positive real part. The non-trivial defect persists under discretization because of the particular structure of the problem. In order to mimic the situation required for Proposition 4, we introduce an additional coupling term  $h^2v_1$  in the second equation which makes the discrete eigenvalue  $\lambda_h^{\text{crit}}$  split into two simple eigenvalues  $\lambda_h^1$  and  $\lambda_h^2$ . As suggested by *a priori* error analysis, we take  $\lambda_h := \frac{1}{2} \{\lambda_h^1 + \lambda_h^2\}$  as our primary approximation to the limit eigenvalue  $\lambda$ . Table III presents the corresponding results obtained on a sequence of uniformly refined meshes for  $v = 10^{-1}$ .

We observe the reduced order  $\mathcal{O}(h)$  for the error  $|\lambda_h^1 - \lambda|$  and  $\mathcal{O}(h^2)$  for  $|\lambda_h - \lambda|$ . The same order is obtained for the error estimator  $\eta_{\omega}^{\lambda}$  and, as predicted, the  $L^2$  norms of the dual eigenfunctions  $v_h^*$ , normalized by  $(v_h, v_h^*) = 1$  blow up with order  $\mathcal{O}(h^{-1})$ .

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