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Adjoint shape optimization for steady free-surface flows

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SUMMARY

Numerical solution of flows that are partially bounded by a freely moving boundary is of great importance in practical applications such as ship hydrodynamics. Free boundary problems can be reformulated into optimal shape design problems, which can in principle be solved efficiently by the adjoint method. This work examines the suitability of the adjoint shape optimization method for solving steady free-surface flows. It is shown that preconditioning is imperative to avoid mesh-width dependence of the convergence behaviour. Numerical results are presented for 2D flow over an obstacle in a channel. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: numerical solution methods; steady free-surface flows; optimal shape design; adjoint methods

1. INTRODUCTION

The numerical solution of flows which are partially bounded by a freely moving boundary is of great practical importance, e.g. in ship hydrodynamics [1–3]. A practically relevant class of free-surface flow problems are *steady* free-surface flows. An example of such a steady free-surface flow is the wave pattern carried by a ship at forward speed in still water. Numerical methods for free-surface potential flow are mature (for an overview, see Reference [4]) and dedicated techniques have been developed for solving the steady free-surface potential-flow equations, e.g. Reference [5]. In contrast, methods for the steady free-surface Navier–Stokes equations typically continue a transient process until a steady state is reached. This time integration method is often computationally inefficient, due to the specific transient behaviour of free-surface flows; see References [6, 7]. Alternative solution methods for the steady free-surface Navier–Stokes equations exist. However, the performance of these methods usually depends sensitively on the parameters in the problem, or their applicability is too restricted; see, for instance, References [8, 9]. In Reference [6], an efficient iterative algorithm was presented. However, the implementation of the quasi-free-surface condition that underlies the

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efficiency of this method can be involved. Hence, the investigation of numerical methods for the steady free-surface Navier–Stokes equations is warranted.

A general characteristic of free-boundary problems is that the number of free-boundary conditions is one more than the number of boundary conditions required by the governing boundary value problem. A free-boundary problem can therefore be reformulated into the equivalent shape optimization problem of finding the boundary that minimizes a norm of the residual of one of the free-surface conditions, subject to the boundary value problem with the remaining free-surface conditions imposed.

Optimal shape design problems can in principle be solved efficiently by means of the adjoint method. In recent years, much progress has been made in the development of adjoint techniques for problems from fluid dynamics. Applications to the Navier–Stokes equations include flow control (see Reference [10] and the references therein), *a posteriori* error-estimation and adaptivity (for instance, Reference [11]) optimal design (e.g., Reference [12, 13]) and domain decomposition (cf. Reference [14]). The techniques that are required to solve the optimal shape design problem associated with steady free-surface flow are readily available.

The present work investigates the suitability of the adjoint shape optimization method for solving steady free-surface flow problems. Our primary interest is in the steady free-surface Navier–Stokes equations. However, because inviscid, irrotational flow adequately describes the features of free-surface flow and to avoid the complexity of the Navier–Stokes equations, our investigation is based on the free-surface potential flow equations. The adjoint shape optimization method is equally applicable to the free-surface Navier–Stokes equations, although the specifics of the method are much more involved in that case. Our investigation serves as an indication of the properties of the adjoint shape optimization method for steady free-surface flow problems.

The contents of the paper are organized as follows: In Section 2 the equations governing steady free-surface potential flow and the associated design problem are stated. Section 3 describes the adjoint optimization method. Section 4 examines the convergence behaviour of the adjoint method and discusses preconditioning. Numerical experiments and results are presented in Section 5. Section 6 contains concluding remarks.

2. PROBLEM STATEMENT

We consider an incompressible, inviscid fluid flow, subject to a constant gravitational force, acting in the negative vertical direction. The fluid occupies a domain $\mathscr{V}\subset\mathbb{R}^d$ $(d=2,3)$ which is bounded by a free boundary, $\mathscr{S}$, and a fixed boundary $\partial\mathscr{V}\backslash\mathscr{S}$. The fixed boundary can be subdivided in an inflow boundary, an outflow boundary and a rigid, impermeable boundary.

The (non-dimensionalized) fluid velocity and pressure are identified by $\mathbf{v}(\mathbf{x})$ and $p(\mathbf{x})$, respectively. Assuming that the velocity-field is irrotational, a velocity-potential $\phi(\mathbf{x})$ exists such that $\mathbf{v}=\nabla\phi$. Incompressibility implies that the velocity-potential satisfies. The Laplace equation:

$$\Delta\phi=0, \quad \mathbf{x}\in\mathscr{V} \tag{1}$$

Assuming that $|\nabla\phi|=1$ at the inflow boundary, Bernoulli's equation relates the pressure to the velocity-potential as

$$p(\mathbf{x})=\tfrac{1}{2}-(\tfrac{1}{2}|\nabla\phi|^2+\mathrm{Fr}^{-2}x_d) \tag{2}$$

with x_d the vertical co-ordinate and Fr the Froude number, defined by $\mathrm{Fr} \equiv V/\sqrt{gL}$ with V an appropriate reference velocity, g the gravitational acceleration and L an assigned reference length.

The free-surface conditions prescribe that the free-surface is impermeable and that the pressure vanishes at the free-surface:

$$\mathbf{n}\cdot\nabla\phi = 0, \quad \mathbf{x}\in\mathscr{S} \tag{3a}$$

$$p = 0, \quad \mathbf{x}\in\mathscr{S} \tag{3b}$$

with $\mathbf{n}(\mathbf{x})$ the unit normal vector to $\mathscr{S}$. Conditions (3a) and (3b) are referred to as the kinematic condition and the dynamic condition, respectively. A single appropriate boundary condition must be specified at the fixed boundary. We assume that this condition is of the form:

$$a\mathbf{n}\cdot\nabla\phi + b\phi = c, \quad \mathbf{x}\in\partial\mathscr{V}\backslash\mathscr{S} \tag{4}$$

for certain functions $a, b, c : \partial\mathscr{V}\backslash\mathscr{S} \mapsto \mathbb{R}$.

The steady free-surface flow problem under consideration is the problem of finding $\mathscr{S}$ and ϕ such that ϕ satisfies (1)–(4). Several issues relate to well-posedness of this problem. Firstly, arbitrary non-physical upstream can impair uniqueness. These waves must be removed by a radiation condition; cf. for instance, References [15, 16]. In numerical computations, this radiation condition can be conveniently enforced by introducing artificial damping (see Section 5) or by selecting a suitable discretization (see Reference [5]). Secondly, a physically meaningful solution can be non-existent, as the transient problem underlying (1)–(4) does not necessarily approach a steady state as time progresses ad infinitum; see Reference [7].

To obtain an optimal-shape design formulation of the steady free-surface flow problem, the *cost functional* E is defined by

$$E(\mathscr{S}, \phi) = \int_{\mathscr{S}} \tfrac{1}{2} p(\mathbf{x})^2 \,\mathrm{d}\mathbf{x} \tag{5}$$

and the *constraint* C is defined by the boundary value problem (1), (3a) and (4):

$$C(\mathscr{S}, \phi) = \begin{cases} \Delta\phi = 0, & \mathbf{x}\in\mathscr{V} \\ \mathbf{n}\cdot\nabla\phi = 0, & \mathbf{x}\in\mathscr{S} \\ a\mathbf{n}\cdot\nabla\phi + b\phi = c, & \mathbf{x}\in\partial\mathscr{V}\backslash\mathscr{S} \end{cases} \tag{6}$$

The free-surface flow problem is equivalent to the optimal shape design problem

$$\min_{\mathscr{S}} \{E(\mathscr{S}, \phi) : C(\mathscr{S}, \phi)\} \tag{7}$$

i.e. minimize (5) over all $\mathscr{S}$, subject to the constraint that ϕ satisfies (6). Because the boundary value problem (6) associates a unique ϕ with each free boundary $\mathscr{S}$, it is convenient to use the notation $E(\mathscr{S})$ for $E(\mathscr{S}, \phi)$ with ϕ from (6).

3. ADJOINT OPTIMIZATION METHOD

To describe the adjoint optimization method for (7), we consider a domain $\mathscr{V}$ with free boundary $\mathscr{S}$ and a perturbed domain $\mathscr{V}_{\varepsilon\alpha}$ with free boundary

$$\mathscr{S}_{\varepsilon\alpha} = \{\mathbf{x} + \varepsilon\alpha(\mathbf{x})\,\mathbf{n}(\mathbf{x}) : \mathbf{x} \in \mathscr{S}\} \tag{8}$$

where α is a smooth function on $\mathscr{S}$, independent of ε. Following Reference [17], $\mathscr{V}$ and $\mathscr{V}_{\varepsilon\alpha}$ are embedded in a bounded set $\mathscr{E}$ and it is assumed that a solution of the constraint can be extended smoothly beyond the boundary, so that it is well defined in $\mathscr{E}$. A function $\operatorname{grad} E(\mathscr{S}) : \mathscr{S} \mapsto \mathbb{R}$ then exists, with the property that the value of the cost functional corresponding to the modified free boundary can be expanded as

$$E(\mathscr{S}_{\varepsilon\alpha}) = E(\mathscr{S}) + \varepsilon \int_{\mathscr{S}} \alpha(\mathbf{x}) \operatorname{grad} E(\mathscr{S})(\mathbf{x})\,\mathrm{d}\mathbf{x} + O(\varepsilon^2) \tag{9}$$

for all suitable functions α. This function $\operatorname{grad} E(\mathscr{S})$ is called the *gradient* of the cost functional with respect to the free boundary. If the gradient is available, improvement of the free boundary is straightforward. The adjoint optimization method explicitly determines the gradient of the cost functional by means of the solution of a dual problem. Omitting details for succinctness, we state that the gradient associated with (7) is given by

$$\operatorname{grad} E(\mathscr{S}) = -\lambda\,\mathbf{nn} : \nabla\nabla\phi - \sum_{j=1}^{d-1} \mathbf{t}_j \cdot \nabla(\lambda\,\mathbf{t}_j \cdot \nabla\phi) - \frac{p^2}{2R} - p\,\mathrm{Fr}^{-2}\mathbf{n}\cdot\mathbf{e}_d \tag{10}$$

with $\lambda(\mathbf{x})$ the solution of the dual problem

$$\Delta\lambda = 0, \quad \mathbf{x} \in \mathscr{V} \tag{11a}$$

$$\mathbf{n}\cdot\nabla\lambda = \sum_{j=1}^{d-1} \mathbf{t}_j \cdot \nabla(p\mathbf{t}_j \cdot \nabla\phi), \quad \mathbf{x} \in \mathscr{S} \tag{11b}$$

$$a\mathbf{n}\cdot\nabla\lambda + b\lambda = 0, \quad \mathbf{x} \in \partial\mathscr{V}\backslash\mathscr{S} \tag{11c}$$

In (10) and (11), $\mathbf{t}_j$ are orthogonal unit tangent vectors to $\mathscr{S}$, $\mathbf{e}_d$ is the vertical unit vector and $R(\mathbf{x})$ is the radius of curvature ($d=2$) or mean radius of curvature ($d=3$).

If ε in (9) is set to a small positive number, then $\alpha = -\operatorname{grad} E(\mathscr{S})$ reduces the cost functional and thus improves the free-boundary position. The steady free-surface-flow problem (7) can therefore be solved by repeating the following operations:

(A1) For given $\mathscr{S}$, solve ϕ from (6).
(A2) Solve λ from (11).
(A3) Determine $\alpha = -\operatorname{grad} E(\mathscr{S})$ from (10).
(A4) Choose a step size $\gamma > 0$ and adjust $\mathscr{S}$ to $\mathscr{S}_{\gamma\alpha}$.

The iterative process (A1)–(A4) is called the *adjoint optimization method*.

The actual free-boundary $\mathscr{S}^*$ yields $\operatorname{grad} E(\mathscr{S}^*) = 0$. However, $\operatorname{grad} E(\mathscr{S}^*) = 0$ only ensures that a *local* minimum is attained. If the cost functional is non-convex, then multiple local minima can occur. The actual solution to the steady free-surface flow problem is the *global* minimum. Because the dynamic condition (3b) implies that the cost functional vanishes for the actual solution, the correct minimum is identifiable. If the cost functional is indeed non-convex, the adjoint optimization method must be provided with a sufficiently accurate initial approximation to the solution, for instance, a prolongated coarse-grid approximation.

4. CONVERGENCE AND PRECONDITIONING

The convergence behaviour of the adjoint method can be conveniently examined by means of Fourier analysis; see Reference [18]. We consider the typical case of a two-dimensional uniform horizontal flow in a channel $\mathscr{V}^* = \{(x, y) \in \mathbb{R} \times [-1, 0]\}$. The boundary $\mathscr{S}^* = \{y = 0\}$ is the free boundary and $\{y = -1\}$ is a rigid, impermeable boundary. The potential $\phi^* = x$ then satisfies (7) and $\operatorname{grad} E(\mathscr{S}^*) = 0$, i.e. $\mathscr{S}^*$ is the optimal free boundary.

Next, we consider the perturbed boundary $\mathscr{S}^*_{\varepsilon\alpha}$, with $\alpha(x) = \hat{\alpha}(k)\exp(\mathrm{i}kx)$ a Fourier mode. The gradient at $\mathscr{S}^*_{\varepsilon\alpha}$ reads $\operatorname{grad} E(\mathscr{S}^*_{\varepsilon\alpha})(x) = \varepsilon \hat{H}(k)\,\hat{\alpha}(k)\exp(\mathrm{i}kx)$, with

$$\hat{H}(k) = (\mathrm{Fr}^{-2} - |k|/\tanh|k|)^2 \tag{12}$$

An important property of (12) is that for subcritical flows ($\mathrm{Fr} < 1$), there is a wave number k_* such that $\hat{H}(k_*) = 0$. This mode corresponds to a steady surface gravity wave (see, e.g. References [15, 16]). For supercritical flows ($\mathrm{Fr} > 1$), such a gravity wave does not occur.

One iteration of the adjoint method replaces $\varepsilon\alpha$ by $\varepsilon\alpha - \gamma \operatorname{grad} E(\mathscr{S}^*_{\varepsilon\alpha})$. Fourier analysis yields that to ensure stability, γ must satisfy $|1 - \gamma\hat{H}(k)| \leqslant 1$ for all k. If the optimization problem is solved numerically on a grid with mesh width h, only wave numbers $k \in [-\pi/h, \pi/h]$ appear. As $h \to 0$, $\hat{H}$ attains its maximum in $[-\pi/h, \pi/h]$ for $|k| = \pi/h$. The asymptotic behaviour of $\hat{H}(\pi/h) = O(h^{-2})$ as $h \to 0$. Therefore, γ must be $O(h^2)$ to maintain stability. However, the modes for which $\hat{H} = O(1)$ then converge as $|1 - O(h^2)|$, so that the convergence behaviour of the adjoint method deteriorates with decreasing mesh width.

This mesh-width dependence of γ can be removed through preconditioning; see also Reference [19]. The mesh-width dependence is caused by the $O(k^2)$ behaviour of (12) for large k. This implies that oscillatory errors in the boundary position contribute disproportionally to the gradient. The aim of preconditioning is to restore the relation between the boundary adjustment and the error in the boundary position.

An accurate approximation to the error in the free-boundary can be recovered from the gradient by solving

$$P\beta = \operatorname{grad} E(\mathscr{S}^*_{\varepsilon\alpha}) \tag{13}$$

where P is any convenient operator of which the Fourier symbol resembles $\hat{H}$. If the adjoint method uses β instead of the gradient to displace the boundary, then the corresponding stability condition reads $|1 - \gamma\hat{H}(k)/\hat{P}(k)| \leqslant 1$. Therefore, if $\hat{P}$ satisfies $\hat{P} \geqslant \hat{H}$ for all k, then γ can be set to 1 and the mesh-width dependence is avoided. It is important that the numerical methods for solving (13) do not reintroduce the mesh-width dependence. In general, preconditioners can be constructed for which efficient solution methods, e.g. multigrid methods [20, 21], are available.

An operator of which the Fourier symbol resembles $\hat{H}$ for large k is

$$P_H\beta = (\mathrm{Fr}^{-2} - 1)^2\beta - \frac{\partial^2\beta}{\partial t^2} \tag{14}$$

where $\partial/\partial t$ denotes the tangential derivative along the free boundary. The Fourier symbol of P_H is $\hat{P}_H(k) = (\mathrm{Fr}^{-2} - 1)^2 + k^2$. For small k a suitable operator is

$$P_L\beta = (\mathrm{Fr}^{-2} - 1)^2 \left(\beta + \frac{2 - 2\mu}{k_*^2} \frac{\partial^2 \beta}{\partial t^2} + \frac{1 - \mu}{k_*^4} \frac{\partial^4 \beta}{\partial t^4} \right) \tag{15}$$

with μ a small positive constant, which ensures stability of the operator P_L. The Fourier symbol of P_L is given by $\hat{P}_L(k) = (\mathrm{Fr}^{-2} - 1)^2 (1 - (2 - 2\mu)(k/k_*)^2 + (1 - \mu)(k/k_*)^4)$. For supercritical flows, $\hat{P}_H$ is an accurate approximation to $\hat{H}$ for all k and the adjustment of the free-boundary can be obtained from (13) and (14). For subcritical flows, $\hat{P}_H$ fails for small k and (13)–(15) should be used.

5. NUMERICAL EXPERIMENTS

The preconditioned adjoint optimization method is tested for 2D sub- and super-critical flow over and obstacle in a channel at $\mathrm{Fr} = 0.43$ and 2.05. The fluid depth is assigned as reference length. The geometry of the obstacle is

$$y(x) = -1 + \frac{27}{4} \frac{H}{L^3} x(x - L)^2, \quad 0 \leqslant x \leqslant L \tag{16}$$

with H and L the (non-dimensionalized) height and length of the obstacle, respectively. We choose $H = 0.2$, $L = 2$ for the subcritical test case and $H = 0.44$ and $L = 4.4$ for the supercritical test case, in accordance with the experimental set-up from Reference [22].

The boundary value problems (7) and (11) are discretized with bilinear finite elements. The differential operators in the gradient (10) are discretized with central differences. The resulting discrete optimization problem is unstable and displays odd/even oscillations. These are simply removed by smoothing the gradient with the biharmonic operator. For subcritical flows ($\mathrm{Fr} < 1$), a radiation condition must be imposed to avoid non-physical upstream waves. The radiation condition is enforced by smoothing the gradient upstream of the obstacle with the Laplace operator, and by applying the low wave number preconditioner P_L only downstream.

The numerical experiments are performed on grids with horizontal mesh width $h \in \{L/72, L/144\}$ and vertical mesh width $\frac{1}{24}$. For the supercritical test case, the correction β is computed using (13) and (14). For the subcritical test case, the upstream correction is determined in the same manner and the downstream correction is taken as $(\beta_L + \beta_H)/2$, with β_H from (13) and (14), and β_L from (13) and (15). The constant μ in (15) is set to 0.025. In all cases the step size is set to $\gamma = 1$.

For the supercritical test case, Figure 1 plots the norm of the correction after n iterations, $\|\beta_n\|$, versus the iteration counter. The correction in the adjoint method converges exponentially, i.e. $\|\beta_n\| = O(\zeta^n)$, for some constant $0 < \zeta < 1$. The norm of the *error* after n iterations, $\mathsf{E}_n(\mathbf{x})$, can be bounded by

$$\|\mathsf{E}_n\| \leqslant \sum_{j=n}^{\infty} \|\beta_j\| \tag{17}$$

This implies that the error converges exponentially as well. From Figure 1 we obtain $\zeta \approx 0.5$. Observe that ζ is indeed independent of the mesh width. Figure 2 compares the computed

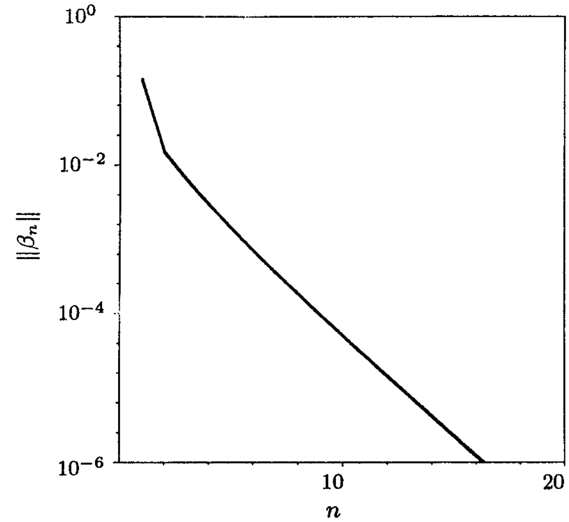

Figure 1. Supercritical test case: convergence with $H = 0.44$ ($L/144$ and $L/72$ coincide).

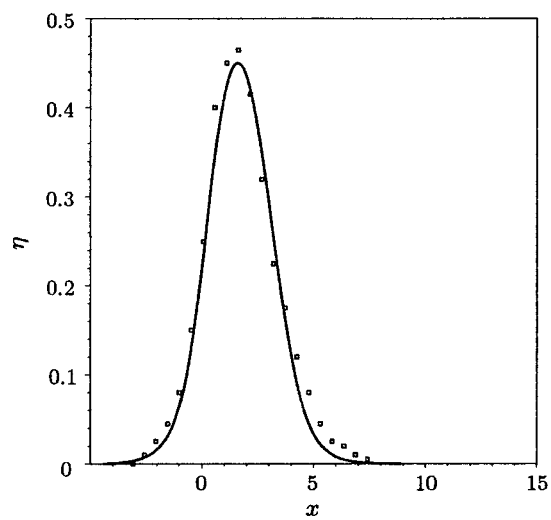

Figure 2. Supercritical test case: computed surface elevation with $H = 0.44$, $h = L/144$ (solid line) and measurements from Reference [22] (markers only).

surface elevation with measurements from Reference [22] for the supercritical test case. The computed result agrees well with the measurements.

For the subcritical test case, $\|\beta_n\|$ is plotted versus n in Figure 3. Note that Figure 3 is a log–log plot. In this case, the convergence behaviour of the correction is just algebraic, i.e.

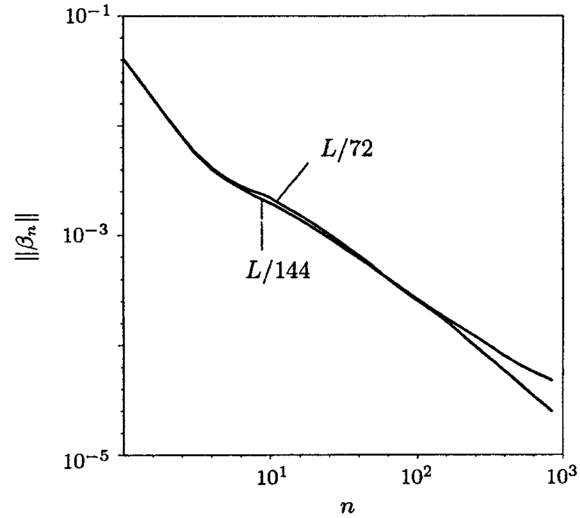

Figure 3. Subcritical test case: convergence with $H=0.20$.

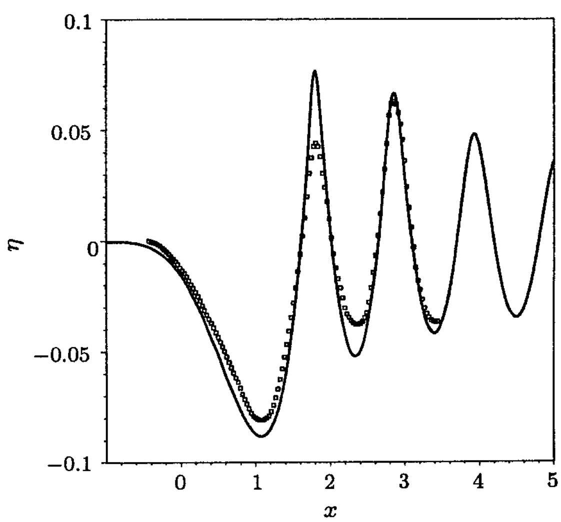

Figure 4. Subcritical test case: computed surface elevation with $H=0.20$, $h=L/144$ (solid line) and measurements from Reference [22] (markers only).

$\|\beta_n\|=O(n^{-\sigma})$. From Figure 3 we obtain $\sigma\approx 1.2$, virtually independent of the mesh width. Equation (17) then yields that the convergence behaviour of the error is $O(n^{-0.2})$. The computed surface elevation is compared with measurements from Reference [22] in Figure 4. The amplitude of the trailing wave is overestimated, but the overestimation is not unusual; see, for instance, References [6, 23, 24]. The wavelength of the computed result agrees well with the measurements.

6. DISCUSSION AND CONCLUSIONS

We examined the suitability of the adjoint shape-optimization method for solving steady free-surface flows. The free-surface potential flow problem was rephrased as an equivalent optimal-shape-design problem. We then presented the adjoint optimization method for solving the design problem. We showed that preconditioning is imperative to avoid mesh-width dependence of the convergence behaviour of the adjoint method and we presented a suitable preconditioning for the free-surface-flow problem.

Numerical results were presented for two-dimensional flow over an obstacle in a channel. For the supercritical test case, the error in the boundary position converges exponentially. For the subcritical test case, the convergence behaviour is just algebraic. The numerical results confirm that the convergence behaviour of the preconditioned adjoint method is independent of the mesh width. For both test cases the computed results agree well with measurements.

For the considered test cases, the convergence behaviour of the adjoint method is similar to that of time-integration methods (see also Reference [6]): the error converges exponentially for supercritical flows and algebraically for subcritical flows. However, the convergence behaviour of the preconditioned adjoint method is independent of the mesh width, whereas the convergence behaviour of the usual time-integration method for free-surface flows deteriorates with decreasing mesh width, due to a CFL-restriction on the allowable time step. Therefore, the preconditioned adjoint method is more efficient than the usual time-integration method. On the other hand, the algebraic convergence behaviour of the adjoint method for subcritical problems is less efficient than the exponential convergence behaviour of the method proposed in Reference [6].

We conjecture that the poor convergence behaviour of the adjoint method for subcritical flows is caused by Fourier modes in the neighbourhood of k_*: Because $\hat{H}(k) \ll 1$ for such modes, their contribution to the gradient is negligible, although their contribution to the error in the free-boundary position can be significant. It is therefore anticipated that exponential convergence behaviour can be recovered if the adjoint method is combined with a solution method that eliminates the Fourier modes in the error in the neighbourhood of k_*.

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