Design of free-surface interfaces using RANS equations

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In this paper, the continuous adjoint methodology to compute shape sensitivities in free-surface hydrodynamic design problems (RANS governing systems) has been developed. This technique will allow the specific design of the free-surface interface (typically air/water), which has a great potential in problems where the target is to reduce the wave energy, e.g. ship hull design. A detailed description of the methodology as well as numerical experiments to demonstrate the ability of this new technique to reduce the wave energy will be shown.

I. Introduction

In the past, lot of work has been done in shape optimization for ship hydrodynamics using Computational Fluid Dynamics. However, in most of the cases, the total resistance of the ship has been selected as the objective function to minimize (subject to geometrical constraints). In this particular paper, a new point of view is presented, and a different objective function has been defined to minimize the energy of the waves generated by an object submerged in the water. The complete adjoint methodology to evaluate the gradients will be presented in this article as well as some examples that demonstrate the ability of this technique to reduce the total resistance by minimizing the size of the waves.

Hydrodynamic applications of optimal shape design in systems governed by partial differential equations are formulated on a fluid domain Ω , delimited by disconnected boundaries divided into an inlet, outlet, and solid wall boundaries S . From now on we will restrict ourselves to the analysis of optimization problems involving a functional J defined on the solid wall S , and in the entire domain Ω , whose value depends on the flow variables U obtained from the solution of the fluid flow equations. In this context, the generic optimization problem can be succinctly stated as follows: find $S^{min} \in \mathcal{S}_{ad}$ such that

$$J(S^{min}) = \min_{S^{min} \in \mathcal{S}_{ad}} J(S) \quad (1)$$

where S is the geometry to be designed (hydrofoil profile, bottom of a channel, the surface of a ship hull, etc.) and $\mathcal{S}_{ad}$ is the set of admissible boundary geometries and

$$J(S) = \int_S j_S(U, \vec{n}) ds + \int_{\Omega} j_{\Omega}(U) d\Omega \quad (2)$$

is the objective function (total resistance, waves height and amplitude, etc.), where $j_S(U, \vec{n})$, and $j_{\Omega}(U)$ are smooth functions which depends on $\vec{n}$ (inward-pointing unit vector normal to S) and the flow variables.

Gradients of this objective function can be computed in a variety of ways, some of the most popular are the adjoint methods^{13,24,1,5,17} due, among other factors, to their ability of computing these derivatives at a cost comparable to solving the state equations. Adjoint methods are conventionally divided into continuous and discrete.^{16,21,4,5} In this work, the continuous adjoint approach will be used, so the adjoint system has a unique form independent of the scheme used to solve the flow-field system, and hence offers flexibility in choosing the discretization scheme for the adjoint system.

With respect to the numerical method, the artificial compressibility^{7,25} method has been chosen to solve this fluid problem. And a level set technique^{31,30,6,27} will be used to identify the free-surface interface. This technique can handle nonlinear steep waves, near-breaking waves and complex geometries.

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Optimal shape design using free-surface problems has been an important area of research,^{3,10,20,11,8,9} and several successful methodologies have been developed to minimize a pressure based functional using high and low fidelity models. However, the introduction of the free-surface shape on the optimization process is not common,²² and to the best of our knowledge this is one of the first papers in which this methodology is described for RANS equations.

The organization of the paper is be as follows: In Sec. II the hydrodynamic model is described; In Sec. III the optimization problem and the continuous adjoint method to compute the surface sensitivity is stated; Some numerical experiments illustrating the relevance of the developments described in this work are presented in Sec. IV; Major conclusions will be shown in Sec. V.

II. Description of the model

A. Free-surface model using level set and artificial compressibility equations

The incompressible Navier-Stokes equations express the conservation of mass and momentum of an incompressible viscous fluid. In this paper we will assume that two fluids of different densities and viscosities (typically water and air) are governed by these equations on a domain $\Omega \subset \mathbb{R}^3$, delimited by disconnected boundaries divided into an inlet Γ_{in} , outlet Γ_{out} and a solid wall denoted by S . In this particular two phase problem, the density and the laminar viscosity are prescribed via an auxiliary variable $\phi = \phi(\vec{v}, \vec{x})$ described below. The non-dimensional artificial compressibility formulation (only valid for steady-state) can be written in the following form:

$$\begin{cases} R_U(U, \hat{\nu}, \phi) \equiv \vec{\nabla} \cdot \vec{F}^c - \vec{\nabla} \cdot \vec{F}^v - S = -\partial_t U & \text{in } \Omega, t > 0, \\ U(t) = U_0 & \text{in } \Omega, t = 0, \\ \vec{v} = 0 & \text{on } S, \\ (W)_{\vec{v}} = W_{in} & \text{on } \Gamma_{in}, t > 0, \\ (W)_P = W_{out} & \text{on } \Gamma_{out}, t > 0, \end{cases} \quad (3)$$

where $U = (P, \rho u, \rho v, \rho w)^T$ stands for the vector of conservative variables, $\rho = \rho(\phi)$ is the fluid density, P is the pressure, $\vec{v} = (u, v, w) \in \mathbb{R}^3$ is the flow speed in a Cartesian system of reference, $\vec{n}$ is the inward-pointing unit vector normal to the surface S . The last two equations in (3) are the inlet/outlet boundary conditions. The convective fluxes $\vec{F}^c = (F_x^c, F_y^c, F_z^c)$, and the source term S are

$$F_x^c = \begin{pmatrix} \beta^2 u \\ \rho u^2 + P \\ \rho uv \\ \rho uw \end{pmatrix}, \quad F_y^c = \begin{pmatrix} \beta^2 v \\ \rho vu \\ \rho v^2 + P \\ \rho vw \end{pmatrix}, \quad F_z^c = \begin{pmatrix} \beta^2 w \\ \rho wu \\ \rho wv \\ \rho w^2 + P \end{pmatrix}, \quad S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\frac{\rho}{Fr^2} \end{pmatrix}, \quad (4)$$

where Fr stands for the Froude number and β^2 is the artificial compressibility parameter. Finally, the viscous fluxes are

$$F_x^v = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \end{pmatrix}, \quad F_y^v = \begin{pmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \end{pmatrix}, \quad F_z^v = \begin{pmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \end{pmatrix}. \quad (5)$$

where $\bar{\tau} = \mu (\nabla \vec{v} + (\nabla \vec{v})^T)$ is the viscous stress tensor for incompressible flows, and μ is the total viscosity (laminar and eddy viscosity). Note that, thanks to the mass conservation equation, the viscous contribution can be written in differential form as $\mu \vec{\nabla}^2 \vec{v}$ (this simplification is critical from the numerical point of view).

As usual in turbulent modeling based upon the Boussinesq hypothesis, the viscosity is divided into a laminar μ_{lam} and a turbulent μ_{tur} component. The laminar viscosity is taken constant at each fluid, whereas μ_{tur} is obtained from a suitable turbulence model involving the flow and a set of new variables.

To identify the free-surface, a level set method is used. The main idea consists in using a level set function ϕ to track the interface between the gas and the liquid.^{31,30,29} In particular, the interface will be the zero level set of ϕ , and the level set function will be positive in the gas and negative in the liquid. The

values of the density and laminar viscosity are defined using an approximation of the Heaviside step function $H = H(\phi, \epsilon)$:

$$H(\phi) = \begin{cases} 1 & \text{if } \phi < -\epsilon, \\ 1 - \frac{1}{2} \left[1 + \frac{\phi}{\epsilon} + \frac{1}{\pi} \sin(\pi\phi/\epsilon) \right] & \text{if } |\phi| \leq \epsilon, \\ 0 & \text{if } \phi > \epsilon, \end{cases} \quad (6)$$

where ϵ is a measure of the interface thickness. It is also useful to define a numerical version of the Dirac's delta function based on the discrete Heaviside step function:

$$\delta(\phi) = \begin{cases} \frac{1}{2} [1 + \cos(\pi\phi/\epsilon)] / \epsilon & \text{if } |\phi| \leq \epsilon, \\ 0 & \text{otherwise.} \end{cases} \quad (7)$$

Finally, density and laminar viscosity are computed as:

$$\begin{cases} \rho(\phi) = & H(\phi) + \left(\frac{\rho_g}{\rho_l} \right) (1 - H(\phi)), \\ \mu_{lam}(\phi) = & H(\phi) + \left(\frac{\mu_g}{\mu_l} \right) (1 - H(\phi)), \end{cases} \quad (8)$$

where g stands for gas, and l for liquid. The level set variable ϕ should satisfy the following basic transport equation:

$$\begin{cases} R_\phi(\vec{v}, \phi) \equiv \vec{\nabla} \cdot (\phi \vec{v}) = -\partial_t \phi & \text{in } \Omega, t > 0, \\ \phi(t) = \phi_0 & \text{in } \Omega, t = 0, \\ (W)_\phi = W & \text{on } S, \Gamma_{in}, \Gamma_{out}, t > 0, \end{cases} \quad (9)$$

which simply states that the interface moves with the fluid, $\phi_0 = \phi_0(\vec{x})$ is the initial distance from the free-surface to the boundaries, and W represents the incoming characteristic on the boundaries.

III. Optimal shape design problem using the continuous adjoint methodology

A. Objective function definition

In this paper we will consider the following general choice of objective function:

$$J = \int_S j(\vec{f}, \vec{n}) ds + \int_\Omega \frac{1}{2} (\phi - \phi^d)^2 d\Omega, \quad (10)$$

where $\vec{f} = P\vec{n} + \bar{\tau}\vec{n}$ is the force on the surface, $\vec{n}$ is the inward-pointing unit vector normal to the surface S , and the variable ϕ^d is a target level set value used for wave minimization.

B. Variation of the objective function

The cost function varies due to the changes in the solution induced by the infinitesimal deformation δS of the control surface along the normal direction,

$$\delta J(S) = \int_{\delta S} j(\vec{f}, \vec{n}) ds + \int_S \delta j(\vec{f}, \vec{n}) ds + \int_S \frac{1}{2} (\phi - \phi^d)^2 \delta S ds + \int_\Omega (\phi - \phi^d) \delta \phi d\Omega. \quad (11)$$

Using the convention of summation repeated indexes, the two first terms in the previous equation read

$$\int_{\delta S} j(\vec{f}, \vec{n}) ds = \int_S \left(\frac{\partial j}{\partial f_i} \partial_n f_i - 2H_m j \right) \delta S ds. \quad (12)$$

$$\begin{aligned} \int_S \delta j(\vec{f}, \vec{n}) ds &= \int_S \frac{\partial j}{\partial f_i} \delta f_i - \frac{\partial j}{\partial \vec{n}} \cdot \nabla_S(\delta S) ds \\ &= \int_S \frac{\partial j}{\partial \vec{f}} \cdot (\delta P\vec{n} - \delta \bar{\tau} \cdot \vec{n}) - \left(\frac{\partial j}{\partial \vec{n}} + \frac{\partial j}{\partial \vec{f}} P - \frac{\partial j}{\partial \vec{f}} \cdot \bar{\tau} \right) \cdot \nabla_S(\delta S) ds \end{aligned} \quad (13)$$

We have used $\delta \vec{n} = -\nabla_S(\delta S)$, which holds for small deformations, and H_m is the mean curvature of S computed as $(\kappa_1 + \kappa_2)/2$, where (κ_1, κ_2) are curvatures in two orthogonal directions on the surface. Here ∇_S represents the tangential gradient operators on S .

An important simplification is obtained if we assume that the objective function depends only on $\vec{f}$ in the following way

$$j(\vec{f}) = \vec{f} \cdot \vec{d} \quad (14)$$

where $\vec{d}$ is a constant vector (this is the case in drag or lift optimization problems). The variation of J is given by

$$\begin{aligned} \delta J &= \int_S \vec{d}(\delta P \vec{n} - \delta \vec{\tau} \cdot \vec{n}) ds + \int_S \vec{d} \cdot \partial_n f_i \delta S ds - \int_S (P \vec{d} - \vec{d} \cdot \vec{\tau}) \cdot \nabla_S (\delta S) ds \\ &\quad - \int_S 2H_m j \delta S ds + \int_S \frac{1}{2}(\phi - \phi^d)^2 \delta S ds + \int_\Omega (\phi - \phi^d) \delta \phi d\Omega. \end{aligned} \quad (15)$$

Integrating now by parts, and assuming that either S is smooth or $\delta S = 0$ at its singular points, yields

$$\begin{aligned} \delta J &= \int_S \vec{d}(\delta P \vec{n} - \delta \vec{\tau} \cdot \vec{n}) ds + \int_S \partial_n (P \vec{d} \cdot \vec{n} - \vec{d} \cdot \vec{\tau} \cdot \vec{n}) \delta S ds + \int_S \nabla_S \cdot (P \vec{d} - \vec{d} \cdot \vec{\tau}) \delta S ds \\ &\quad - \int_S 2H_m j \delta S ds + \int_S \frac{1}{2}(\phi - \phi^d)^2 \delta S ds + \int_\Omega (\phi - \phi^d) \delta \phi d\Omega \\ &= \int_S \vec{d}(\delta P \vec{n} - \delta \vec{\tau} \cdot \vec{n}) ds + \int_S \nabla \cdot (P \vec{d} - \vec{d} \cdot \vec{\tau}) \delta S ds + \int_S \frac{1}{2}(\phi - \phi^d)^2 \delta S ds \\ &\quad + \int_\Omega (\phi - \phi^d) \delta \phi d\Omega, \end{aligned}$$

where we have used the fact that the divergence operator, on local coordinates of S , is given by

$$\nabla \cdot \vec{q} = \partial_n (\vec{q} \cdot \vec{n}) + \nabla_S \cdot \vec{q} - 2H_m \vec{q} \cdot \vec{n} \quad (16)$$

for a general vector field $\vec{q}$. A further simplification is possible noticing that following identity holds

$$\nabla \cdot (P \vec{d} - \vec{d} \cdot \vec{\tau}) = (\nabla P - \nabla \cdot \vec{\tau}) \cdot \vec{d} = 0 \quad \text{on } S, \quad (17)$$

which is obtained assuming that the momentum equations in the Navier-Stokes system are satisfied on the boundary, i.e. $\nabla P = \nabla \cdot \vec{\tau}$ on S .

Finally, the variation of the objective function is computed as

$$\delta J = \int_S \vec{d}(\delta P \vec{n} - \delta \vec{\tau} \cdot \vec{n}) ds + \int_S \frac{1}{2}(\phi - \phi^d)^2 \delta S ds + \int_\Omega (\phi - \phi^d) \delta \phi d\Omega. \quad (18)$$

As usual in the adjoint approach, flow equations are incorporated into the cost functional as constraints by means of Lagrange multipliers $\Psi_U^\top = (\psi_1, \psi_2, \psi_3, \psi_4)$ for the Navier-Stokes equations, and ψ_ϕ for the level set transport equation. The Lagrangian reads:

$$\mathcal{J}(S) = J(S) - \int_\Omega (\Psi_U^\top R_U(U, \phi) + \psi_\phi R_\phi(\vec{v}, \phi)) d\Omega, \quad (19)$$

where we have placed a special emphasis on the boundary surface dependence S . Let us consider an arbitrary (but small) perturbation δS of the boundary. Assuming a regular flow solution U and a smooth boundary S , the variation of the augmented functional $\mathcal{J}(S)$ under the deformation of the geometry can be evaluated as

$$\delta \mathcal{J} = \delta J(S) - \int_\Omega (\Psi_U^\top \delta R_U(U, \phi) + \psi_\phi \delta R_\phi(\vec{v}, \phi)) d\Omega, \quad (20)$$

where $\delta J(S)$ has been computed in Eq. (18), and δR_U and δR_ϕ represent the variations of R_U and R_ϕ , respectively. Supposing a steady-state solution, the linearized system of equations is:

$$\begin{cases} \delta R_U(U, \phi) = \frac{\partial R_U}{\partial U} \delta U + \frac{\partial R_U}{\partial (\vec{\nabla} U)} \delta (\vec{\nabla} U) + \frac{\partial R_U}{\partial \phi} \delta \phi = 0 & \text{in } \Omega, \\ \delta \vec{v} = -\partial_n \vec{v} \delta S & \text{on } S, \\ (\delta W_{in})_{\vec{v}} = 0 & \text{on } \Gamma_{in}, \\ (\delta W_{out})_P = 0 & \text{on } \Gamma_{out}. \end{cases} \quad (21)$$

$$\begin{cases} \delta R_\phi(\vec{v}, \phi) = \frac{\partial R_\phi}{\partial U} \delta U + \frac{\partial R_\phi}{\partial \phi} \delta \phi = 0 & \text{in } \Omega, \\ \delta \phi = 0 & \text{on } S, \Gamma_{in}, \Gamma_{out}. \end{cases} \quad (22)$$

where $(\delta W)_{\vec{v}}$, and $(\delta W)_P$ represent the incoming characteristics on the boundaries.

As usual, the domain integrals in Eq. (20) are eliminated using integration by parts and introducing the associated adjoint operators. The integration by parts also provides some boundary terms. These boundary terms are combined with the boundary terms in Eq. (18) resulting the boundary conditions for the adjoint operators.

Next, the entire procedure is detailed. Starting with the linearized form of the incompressible Navier-Stokes and level set equations, taking the inner product with the adjoint variables, supposing that the functions are smooth, and then integrating over the domain one gets:

$$\begin{aligned} 0 &= \int_{\Omega} \Psi_U^T \vec{\nabla}(\delta \vec{F}^c) d\Omega - \int_{\Omega} \Psi_U^T \vec{\nabla}(\delta \vec{F}^v) d\Omega - \int_{\Omega} \Psi_U^T \delta S d\Omega + \int_{\Omega} \psi_{\phi} \vec{\nabla}(\phi \delta \vec{v} + \vec{v} \delta \phi) d\Omega \\ &= \int_{\Omega} \Psi_U^T \vec{\nabla}(\vec{A}_U \delta U) d\Omega + \int_{\Omega} \Psi_U^T \vec{\nabla}(\vec{A}_{\phi} \delta \phi) d\Omega - \int_{\Omega} \Psi_U^T \vec{\nabla}(\mathbf{D}_U \vec{\nabla} \delta U) d\Omega - \int_{\Omega} \Psi_U^T \vec{\nabla}(\vec{D}_{\phi} \delta \phi) d\Omega \\ &\quad - \int_{\Omega} \Psi_U^T B_U \delta U d\Omega - \int_{\Omega} \Psi_U^T B_{\phi} \delta \phi d\Omega + \int_{\Omega} \psi_{\phi} \vec{\nabla}(\phi \delta \vec{v}) d\Omega + \int_{\Omega} \psi_{\phi} \vec{\nabla}(\vec{v} \delta \phi) d\Omega \end{aligned} \quad (23)$$

where

$$\left. \begin{aligned} \vec{A}_U &= (A_x^c, A_y^c, A_z^c), & A_i^c &= \left. \frac{\partial F_i^c}{\partial U} \right|_{U(x,y,z)} \\ \mathbf{D}_U &= \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix}, & D_{ij} &= \left. \frac{\partial F_i^v}{\partial (\partial_j U)} \right|_{U(x,y,z)} \end{aligned} \right\} \quad i, j = 1 \dots 3$$

and $\vec{A}_{\phi} = \partial_{\phi} \vec{F}^c$, $\vec{D}_{\phi} = \partial_{\phi} \vec{F}^v$, $B_U = \partial_U S$, and $B_{\phi} = \partial_{\phi} S$. Finally, integrating by parts (twice in the case of the viscous terms) the following expression is obtained:

$$\begin{aligned} 0 &= - \int_{\Omega} (\vec{\nabla} \Psi_U^T) \vec{A}_U \delta U d\Omega - \int_{\Omega} \vec{\nabla}((\vec{\nabla} \Psi_U^T) \mathbf{D}_U) \delta U d\Omega - \int_{\Omega} \vec{\nabla} \psi_{\phi}(\phi \delta \vec{v}) d\Omega \\ &\quad - \int_{\Omega} \vec{\nabla} \psi_{\phi}(\vec{v} \delta \phi) d\Omega - \int_{\Omega} (\vec{\nabla} \Psi_U^T) \vec{A}_{\phi} \delta \phi d\Omega + \int_{\Omega} (\vec{\nabla} \Psi_U^T) \vec{D}_{\phi} \delta \phi d\Omega - \int_{\Omega} \Psi_U^T B_{\phi} \delta \phi d\Omega \\ &\quad + \int_S (\vec{n} \cdot \delta \vec{v}) \left(\frac{\beta^2}{\rho} \psi_1 + \psi_{\phi} \phi \right) ds - \int_S \vec{\varphi} \cdot (\delta P \vec{n} - \delta \vec{\tau} \cdot \vec{n}) + \int_S \vec{n} \cdot \vec{\tau}^{\varphi} \cdot \partial_n \vec{v} \delta S \end{aligned} \quad (24)$$

where $\vec{\tau}^{\varphi} = \mu (\nabla \vec{\varphi} + \nabla \vec{\varphi}^T)$. Note that the boundary condition of the linearized level set problem has been used, and the integral over the inlet/outlet boundary can be forced to vanish with the appropriate choice of boundary conditions. The final step to obtain the adjoint equations is collecting the terms that depend on δU and $\delta \phi$.

The variation of the velocity should be written in terms of the conservative variables:

$$\int_{\Omega} \vec{\nabla} \psi_{\phi}(\phi \delta \vec{v}) d\Omega = \int_{\Omega} \frac{\phi}{\rho} \vec{\nabla} \psi_{\phi}(\delta(\rho \vec{v}) - \vec{v} \delta \rho) d\Omega = \int_{\Omega} \frac{\phi}{\rho} \vec{\nabla} \psi_{\phi} \delta(\rho \vec{v}) d\Omega - \int_{\Omega} \frac{\phi}{\rho} \vec{\nabla} \psi_{\phi} \vec{v} \frac{\partial \rho}{\partial \phi} \delta \phi d\Omega \quad (25)$$

Combining the previous result with the variation of the objective function, the adjoint equations are:

$$\left\{ \begin{aligned} -\vec{A}_U^T \cdot \vec{\nabla} \Psi_U - \vec{\nabla}((\vec{\nabla} \Psi_U^T) \mathbf{D}_U) &= \frac{\phi}{\rho} (0 \quad \partial_x \psi_{\phi} \quad \partial_y \psi_{\phi} \quad \partial_z \psi_{\phi})^T && \text{in } \Omega, \\ -\vec{v} \cdot \vec{\nabla} \psi_{\phi} &= \left(\vec{\nabla} \Psi_U^T \frac{\partial \vec{F}^c}{\partial \rho} - \frac{\phi \vec{\nabla} \Psi_{\phi} \vec{v}}{\rho} - \frac{\Psi_4}{F r^2} \right) \frac{\partial \rho}{\partial \phi} - \vec{\nabla} \Psi_U^T \frac{\partial \vec{F}^v}{\partial \mu} \frac{\partial \mu}{\partial \phi} + (\phi - \phi^d) && \text{in } \Omega, \\ \vec{\varphi} &= \vec{d} && \text{on } S, \end{aligned} \right. \quad (26)$$

where we have chosen the appropriate boundary conditions on the external boundaries. As in the direct problem, from the numerical point of view it is important to use the adjoint mass conservation equation to simplify the viscous adjoint terms. Those terms can be written, in differential form, as $\mu \vec{\nabla}^2 \vec{\varphi}$.

Finally, the variation of the functional, or shape sensitivity, is written as

$$\delta J = \int_S \left(\frac{1}{2} (\phi - \phi^d)^2 - (\vec{n} \cdot \partial_n \vec{v}) \left(\frac{\beta^2}{\rho} \psi_1 + \psi_{\phi} \phi \right) + \vec{n} \cdot \vec{\tau}^{\varphi} \cdot \partial_n \vec{v} \right) \delta S ds \quad (27)$$

where there is no dependence on the variation of the flow variables, and the linearized boundary condition on the surface S has been used to eliminate the dependence on $\delta \vec{v}$.

C. Numerical implementation

The incompressible RANS (direct and adjoint) equations are solved using the artificial compressibility method first proposed by Chorin.⁷ The equations have been discretized using an standard edge-based finite volume formulation on the dual grid, obtained by applying the integral formulation of the equations to a dual grid control volume surrounding any given node of the grid and performing an exact integration around the outer boundary of this control volume.^{2,14,15}

In this paper an upwind scheme and a central scheme with Jameson-Schmidt-Turkel (JST)-type¹⁸ scalar artificial dissipation are used for the discretization of the convective flux. Additionally, an agglomeration multigrid method is used to speed up the simulation. The time integration is implicit, and a dual time stepping artificial compressibility method has been also implemented to perform non-steady simulations.

A Spalart-Allmaras turbulence model²⁸ has been used in this particular paper to introduce the effect of the turbulence in the simulations. It is important to note that the model has not being differentiated in the adjoint methodology (frozen viscosity assumption).

Finally, the convection of the direct and adjoint level set variable is discretized using an upwind scheme; second order accuracy is achieved via reconstruction of variables on the cell interfaces. A discretized version of the Diracs delta and Heaviside step function has been used to introduce the terms that depend on the density and viscosity derivatives with respect to the level set variable.

The entire implementation has been made with the Stanford University Unstructured (SU²) flow solver.^{23,22} SU² is a suite of C++ analysis tools (including an iterative PDE solver, mesh perturbation and adaptation tools, among others) linked through python-based driver scripts, specifically architected to perform analysis and design of multi-physics problems on unstructured grid topologies.

The gradient based optimization uses the SciPy library,¹⁹ a well-established open-source software for mathematics, science and engineering. The SciPy library provides many user-friendly and efficient numerical routines for the solution of non-linear constrained optimization problems, such as conjugate gradient, Quasi-Newton or sequential least-squares programming algorithms. At each design iteration, the SciPy routines require as inputs the values and gradients of the objective functions as well as the chosen constraints, but not necessarily in a sequential order. Thus the shape optimization wrapper must also keep track of what simulations have been run to avoid unnecessarily repeating an analysis.

IV. Numerical results

In this section, a detailed description of the numerical experiments will be presented to illustrate the capabilities of the developed methodology. First a validation of the free-surface RANS solver will be shown including some canonical problems to verify the applicability of the artificial compressibility method in this framework (free-surface RANS). Then, an elaborate study of some selected adjoint simulations will illustrate the accuracy of the computed shape sensitivity. Finally, two free-surface optimizations problem (Euler and RANS) will be used to explain the flexibility and potential of the developed technique.

A. Validation of the RANS artificial compressibility solver

Three Verification and Validation problems will be described in this subsection: First, a laminar cylinder case will be used to illustrate the important roll of the artificial compressibility factor β^2 in the overall convergence and accuracy of the simulations. Secondly, a NACA 0012 airfoil validation case will be used to demonstrate the accuracy of the implemented Spalart-Allmaras turbulence model. Finally a 2D sub-critical steady-state flow over a submerged bump without wave breaking (baseline test problem of this article) will be used to analyze the free-surface simulation using Euler and RANS governing equations.

As test case to understand the key roll of the artificial compressible factor in the simulations, a subsonic cylinder at low Reynolds number has been selected ($Re = 40$). The steady-state simulation has been obtained using a second order upwind scheme, and a multigrid convergence strategy. The convergence history is presented in Fig. 1 (second order in space). Between 100 and 300 multigrid iterations are needed to drop 5 orders of magnitude the pressure residual, it is important to note that there is an optimal value of the artificial compressibility factor. In Fig. 2 it is possible to appreciate that the pressure distribution does not depend on the compressibility factor if it is higher than 10 but, the code convergence degrades when increasing the artificial compressibility value.

Figure 1. Convergence of the pressure residual using a second order upwind scheme.

Figure 2. Pressure distribution on a cylinder, second order upwind scheme. The steady-state solution does not depend on the artificial compressibility factor.

Looking at the non-dimensional values, the C_D coefficients are 1.52 ($\beta^2 = 1$), 1.56 ($\beta^2 = 10$) and 1.57 ($\beta^2 = 20$), being 1.52 the value in better agreement with the existing literature.

Next, the implemented Spalart-Allmaras turbulence model will be validated (incompressible conditions, NACA0012, free-stream Mach number = 0.15 and $Re = 6 \cdot 10^6$). A structured 897x257 mesh has been used, the far-field boundary has been located at 500 chords, and simulations at angle-of-attack 0° and 10° have been performed to study the accuracy of the JST centered scheme and the upwind second order scheme (Venkatakrishnan's limiter). The value of the artificial compressibility factor has been fixed at $\beta^2 = 5$.

In Fig. 3 and Fig. 4, the C_p and C_f coefficients are shown for a zero angle-of-attack, a very good agreement with the experimental data is obtained. On the other hand, the same results are presented for angle-of-attack 10° in Fig. 5, and Fig. 6, again, very good agreement between experiments and simulations.

Once the artificial dissipation method and the Spalart-Allmaras turbulence model have been validated in canonical problems, the next step is the application of these techniques to the free-surface channel simulation. In particular, as a final RANS validation case, a 2D sub-critical steady-state flow over a submerged bump without wave breaking is presented. The selected 2D bump has the following shape.¹²

$$z = 0.675 x(x - 1)^2, \quad 0 \leq x \leq 1 \quad (28)$$

The bump is placed on the bottom of a channel, and a final steady-state solution is achieved using $Fr_L = 0.304$, with $H = 0.500$ (undisturbed depth water). The Froude number is based on the bump length, $L = 1.0$. The computation domain extends from $-1 < x < 7$, $-H < z < H$. Appropriate absorbing boundary conditions for free-surface waves has been also implemented.²⁶ The air/water density ratio is 0.00129, being the viscosity ratio 0.02322, and the air/water transition thickness was nominally set to 0.1.

This sub-critical simulation admits steady-state solutions and has been investigated by Cahouet.¹² In Fig. 7 the time evolution of the simulation is presented. It is very important to note that, despite this is a steady state simulation, the solution is obtained via a real unsteady numerical algorithm (dual-time stepping), otherwise the solver is not able to locate the free-surface in the right position and the entire simulation diverges. However, as the objective is the steady state solution, very large physical time steps (of the order of 0.1s) are allowed, and a first order time integration produces satisfactory results.

Cahouets experiment has been chosen as the cornerstone simulation of this paper and many simulations have been performed to understand all the key ingredients of the developed methodology. First of all, the solution of the RANS flow is presented in Fig. 8. In this particular simulation, the size of the numerical grid is 250x400 with an a priori adaptation on the solid walls to capture the viscous effects. The steady state solution has been obtained via an unsteady procedure where only the zero level set is physically relevant.

Figure 3. Pressure coefficient, NACA 0012 (SA), Mach 0.15, $Re = 6 \cdot 10^6$, angle-of-attack 0° .

Figure 4. Friction coefficient, NACA 0012 (SA), Mach 0.15, $Re = 6 \cdot 10^6$, angle-of-attack 0° .

Figure 5. Pressure coefficient, NACA 0012 (SA), Mach 0.15, $Re = 6 \cdot 10^6$, angle-of-attack 10° .

Figure 6. Friction coefficient, NACA 0012 (SA), Mach 0.15, $Re = 6 \cdot 10^6$, angle-of-attack 10° .

Figure 7. Sub-critical free-surface channel simulation (Cahouets experiment). Iterations, 10, 20, 30, and 590 (steady state).

Figure 8. Sub-critical free-surface channel flow solution (Cahouets experiment).

The grid resolution on the free-surface and the size of the interface play a fundamental roll in the free-surface simulations. For that reason some numerical experiments have been performed to understand those variables. Starting with Euler simulations, in Fig. 9 the effect of grid refinement is presented, it is important to highlight that even a very coarse grid is able to capture the free-surface location over the bump, however the downstream waves are clearly dissipated in the coarse grids. A similar problem is presented in Fig. 10 using RANS equations, in this particular problem, the same expected behavior is shown.

On the other hand, the size of the air/water interface affects the final solution. Fig. 11 shows the effect of changing the value of the interface thickness (RANS simulation). In particular, a reduction of ϵ increases the frequency of the waves just after the obstacle improving the agreement with the experimental data. A further reduction in ϵ , without increasing the grid density in the y direction, produces the code divergence.

Finally, as main result of this subsection, a comparison between experiments and the numerical simulation is presented in Fig. 12. It is important to highlight the very good agreement from $x = 0$ to $x = 1.5$ then, despite the simulation predicts a peak in the pressure, that overpressure is not as big as expected. The same results are compared with Euler simulations (using a coarser grid in the y direction).

B. Validation of the adjoint RANS artificial compressibility solver

In this subsection, the implemented adjoint solver will be analyzed, and the adjoint-based gradients will be compared with the finite-difference ones. A basic laminar Navier-Stokes validation will be performed using a low-Reynolds cylinder configuration, then the Euler bump in a channel (without free-surface) will be used to evaluate the inflow-outflow boundary conditions. Finally, lift and free-surface objective functions sensitivities will be computed in systems governed by the RANS equations.

As starting point, the flow around a cylinder ($Re = 40$) is used to validate the surface sensitivity computed with the developed adjoint methodology. In Fig. 13 the solution of the direct and adjoint problem is shown. Using the adjoint formulation described in this article it is possible to compute the sensitivity of the functional with respect to perturbations in the normal direction. In Fig. 14 the shape sensitivity is computed and compared with the pressure distribution over the cylinder.

Figure 9. Effect of grid refinement using Euler simulations.

Figure 10. Effect of grid refinement using RANS simulations.

Figure 11. Effect of the air/water interface thickness (RANS simulation).

Figure 12. Comparison between experiments and simulations (sub-critical free-surface channel flow).

Figure 13. Direct and adjoint solution, flow around a cylinder ($Re = 40$).

Figure 14. Surface shape sensitivity and pressure, flow around a cylinder ($Re = 40$).

Figure 15. Gradient (continuous adjoint and finite-differences, flow around a cylinder ($Re = 40$).

In Fig. 15 finite-difference and continuous adjoint based gradients are compared (using bump function design variables). It is important to highlight the very good agreement between both methodologies. This final test demonstrates that the developed surface formulation works correctly in Navier-Stokes laminar cases with far-field boundary conditions.

Once the adjoint methodology for laminar Navier-Stokes problems has been validated. We focus again our attention in the bump in a channel case (without free-surface). The objective of this particular simulation is to determine the effect of the inflow boundary in the proximity of the the bump geometry. For that reason, an Euler simulation has been used, the selected objective function is the lift computed over the bump.

Figure 16. Effect of grid adaptation in the pressure distribution.

Figure 17. Effect of grid adaptation in the adjoint pressure distribution (lift objective function).

A grid adaptation strategy has been also performed to determine the effect of increasing the number of points in the sensitivity computation. In Fig. 16 the pressure distribution is shown for different grid resolution (from 75 to 250 points in the x direction). On the other hand, in Fig. 17 the adjoint pressure solution is shown. At this point it is important to note that the adjoint variables have a greater variability than direct variables when adapting the computational grid.

A step forward in the methodology consists in computing the shape sensitivity (lift objective function). In Fig. 18 the shape sensitivity is plotted for different grid resolution. Despite the general trend is correct for coarse grids, only the sensitivity computed in the finest grid is smooth over the obstacle (as we expect). However, projecting that sensitivity into a set of particular bump functions (see Fig. 19) the agreement between the adjoint and the finite-differences methodology is acceptable for shape optimization purposes. As we expect, due to the proximity of the inflow boundary condition, the most important differences are in the front of the obstacle.

The same channel analysis is performed for RANS simulations with free-surface. In this case, two objective functions have been studied: lift over the bump, and free-surface wave minimization. The adjoint solution for the lift objective function is plotted in Fig. 20, and the adjoint solution for the free-surface objective function is plotted in Fig. 21. It is important to highlight the impact of the thickness of the interface in the adjoint solution via the derivative of the density and viscosity with respect to the level set function (which introduces a discrete version of the Dirac's delta).

Finally, as conclusion of the developed adjoint methodology, the shape sensitivities with respect to free-surface design and lift design are shown in Fig. 23, it is fundamental to note that the order of magnitude of both shape sensitivities is completely different. In fact, the shape of the free-surface is very insensitive to changes in the bottom of the channel.

Figure 18. Pressure distribution, and lift shape sensitivity for different numerical grid resolution.

Figure 19. Comparison between continuous adjoint and finite-differences for different numerical grid resolution.

Figure 20. RANS adjoint solution (lift objective function).

Figure 21. RANS adjoint solution (free-surface objective function).

Figure 22. Diagram of the free-surface sensitivity problem.

Figure 23. Shape sensitivity for free-surface, and lift design problems.

C. Shape optimization using a free-surface objective function

Once the adjoint methodology is in place, the next step is to use the resulting gradients in a shape optimization process. In this subsection we will show Euler and RANS results for free-surface wave minimization. At this point, it is important to stress that the absolute value of the free-surface gradients are small and the sensitivity of the wave shape with respect to changes in the geometry of the channel after the main bump will also be small.

Figure 24. Example of design variables: Fourier based decomposition (left), cosine bumps (right).

In this particular application, the objective of the problem is the reduction of the free-surface waves by controlling the shape of a small region of the surface just behind the main bump. Specifically, the functional is defined from $x = 1.0$ to $x = 4.0$ (see Fig. 22) and the region of the surface that can be modified is defined from $x = 1.0$ to $x = 3.0$, note that the main bump is located between $x = 0$ and $x = 1$. As design variables two different method have been selected: cosine bumps (see Eq. 29), and Fourier like decomposition of the

surface (see Eq. 30). In Fig 24 an example of the design variables is presented, and the particular equations are presented below:

$$f(x, x_m, \epsilon) = \begin{cases} \frac{1}{2} [1 + \cos(\pi(x - x_m)/\epsilon)] & \text{if } |x - x_m| \leq \epsilon, \\ 0 & \text{otherwise.} \end{cases} \quad (29)$$

$$f(x, n, m) = \begin{cases} \cos\left(\frac{2n\pi}{T}x\right) & \text{if } m = 0, \\ \sin\left(\frac{2n\pi}{T}x\right) & \text{if } m = 1, \\ 0 & \text{otherwise.} \end{cases} \quad (30)$$

where $n \in \mathbb{N}$, $m = 0, 1$, the variable T stands for the period (size of the region to be designed), and x_m is the location of the bump maximum thickness.

Starting with the Euler formulation, the final geometry is presented in Fig. 25. In this particular problem, 20 Fourier like design variables have been used, and the objective function has been reduced a 15%. The final free-surface geometry is presented in Fig. 26. The design area ($1 < x < 3$) is smaller than the area where the objective function has been defined ($1 < x < 4$) and, as we expected, relatively strong deformations on the bottom of the channel have a minor impact in the shape free-surface waves.

Finally, an optimization problem using free-surface and RANS equations is presented in Fig. 27. In this particular problem, the design variables are 20 cosine bump functions. As in the Euler case, it is important to highlight that oscillations produced by the main bump can not be removed (see Fig. 28), but a relevant reduction of the objective function (10%) has been obtained.

As a general conclusion of these preliminary optimization tests, it is important to note that, due to the small value of the sensitivity, a high level of convergence of the direct problem is required to correctly drive the optimization problem (keeping in mind the unsteady nature of the problem and methodology). On the other hand, small changes in the original surface produce an adjustment in the main frequency of the free-surface (or shape sensitivity). For that reason, the Fourier like design variables are more appropriated than bump design variables to track the new surfaces. In other words, the design variables should be able to express a change in the frequency of the channel shape.

V. Conclusions

The objective of this paper is the application of the continuous adjoint approach to the design of free-surface interfaces in problems governed by the RANS equations. This new methodology allows the specific design of the free-surface, which has a great potential in problems where the target is to reduce the wave energy (ship design), or increase the size of the wave (surfing wave pools).

In this paper, the complete formulation has been presented, as well as a detailed numerical experiment section to illustrate the accuracy of the developed technique. It is important to remark that, to the best of our knowledge this is the first application of the continuous adjoint methodology to the design of free-surface interfaces in problems governed by the RANS equations.

The shape design of air/water free-surface interfaces is a promising technique. However, during the development of this paper we have found the following challenges:

- These simulations are very expensive (unsteady), and difficult to converge to machine precision. A high level of convergence is required to compute finite-difference gradients, but also to drive an optimization problem where the sensitivity of the functional is very small.
- The sensitivity of the functional with respect to perturbations in the geometry is very small, making more difficult the work of the optimizer which doesn't count on an exact value of the gradient.
- The selection of the design variables and the region to be designed is critical to obtain satisfactory results. Bump design variables are not optimal in this particular application, where changes in the main frequency of the free-surface are expected.
- The convection of the level set function using the flow velocity in the entire domain degrades very quickly the shape of the air/water transition computed by an approximated Heaviside step function.
- The effect of the eddy turbulence should be introduced in the adjoint methodology.

Figure 25. Pressure contours and final designed geometry (Eulers solution using Fourier like design variables).

Figure 26. Baseline and final shape of the free-surface (Eulers solution).

Figure 27. Pressure contours and final designed geometry (RANS solution using cosine bump functions as design variables).

Figure 28. Baseline and final shape of the free-surface (RANS solution).

Once the continuous adjoint theory of this promising technique has been developed, we next natural step will be the optimization of some of the numerical techniques to face real engineering problems.

References

- ¹W.K. Anderson and V. Venkatakrishnan. Aerodynamic design optimization on unstructured grids with a continuous adjoint formulation. *AIAA Paper*, 97-0643, 1997.
- ²T. Barth and M. Ohlberger. *Finite Volume Methods: Foundation and Analysis*. Encyclopedia of Computational Mechanics, 2004.
- ³E. H. Brummelen and A. Segal. Adjoint shape optimization for steady free-surface flows. *Int. J. Numer. Meth. Fluids*, 40:605614, 2002.
- ⁴A. Bueno-Orovio, C. Castro, F. Palacios, and E. Zuazua. Continuous adjoint approach for the spalart-allmaras model in aerodynamic optimization. *AIAA Journal*, 50(3), 2012.
- ⁵C. Castro, C. Lozano, F. Palacios, and E. Zuazua. A systematic continuous adjoint approach to viscous aerodynamic design on unstructured grids. *AIAA Journal*, 45(9):2125–2139, 2007.
- ⁶Y. C. Chang, T. Y. Hou, B. Merriman, and S. Osher. A level set formulation of Eulerian interface capturing methods for incompressible fluid flows. *J. Comput. Phys.*, 124:449–464, 1996.
- ⁷A. J. Chorin. A numerical method for solving incompressible viscous flow problems. *J. Comput. Phys.*, 137:118–125, 1997.
- ⁸J. Farmer, L. Martinelli, and A. Jameson. Multigrid solution of the euler and navier-stokes equations for a serie 60 cb = 0.6 ship hull for froude numbers 0.160, 0.220 and 0.316. *CFD Workshop Tokyo*, 1994.
- ⁹J. Farmer, L. Martinelli, and A. Jameson. Yacht97: A fully viscous nonlinear free-surface analysis tool for iacc yacht design. *12th Chesapeake Sailing Yacht Symposium*, 1995.
- ¹⁰I. Y. Gejadze and G. J. M. Copeland. Adjoint sensitivity analysis for fluid flow with free surface. *Int. J. Numer. Meth. Fluids*, 47:1027–1034, 2005.
- ¹¹T. Hino, L. Martinelli, and A. Jameson. A finite-volume method with unstructured grid for free surface flow simulations. *Sixth International conference on numerical ship hydrodynamics*, 1993.
- ¹²Cahouet J. Etude numerique et experimentale du probleme bidimensionnel de la resistance de vagues non-lineaire. Technical report, Technical report 185, Ecole Nationale Supérieure de Techniques Avancées, 1984.
- ¹³A. Jameson. Aerodynamic design via control theory. *J. Sci. Comput.*, 3:233–260, 1988.
- ¹⁴A. Jameson. Analysis and design of numerical schemes for gas dynamics 1 artificial diffusion, upwind biasing, limiters and their effect on accuracy and multigrid convergence. *RIACS Technical Report 94.15, International Journal of Computational Fluid Dynamics*, 4:171–218, 1995.
- ¹⁵A. Jameson. Analysis and design of numerical schemes for gas dynamics 2 artificial diffusion and discrete shock structure. *RIACS Report No. 94.16, International Journal of Computational Fluid Dynamics*, 5:1–38, 1995.
- ¹⁶A. Jameson. Aerodynamic shape optimization using the adjoint method. In *Lecture Notes Presented at the VKI Lecture Series*, Rhode Saint Genese Begium, 2 2003. Von karman Institute for fluid dynamics.
- ¹⁷A. Jameson and K. Ou. *Optimization Methods in Computational Fluid Dynamics*. Encyclopedia of Aerospace Engineering, 2010.
- ¹⁸A. Jameson, W. Schmidt, and E. Turkel. Numerical solution of the euler equations by finite volume methods using runge-kutta time stepping schemes. *AIAA Paper*, 81-1259, 1981.
- ¹⁹E. Jones, T. Oliphant, P. Peterson, et al. SciPy: Open source scientific tools for Python, 2001.
- ²⁰L. Martinelli and A. Jameson. An adjoint method for design optimization of ship hulls. *9th International conference on numerical ship hydrodynamics*, 2007.
- ²¹S.K. Nadarajah and A. Jameson. A comparison of the continuous and discrete adjoint approach to automatic aerodynamic optimization. *AIAA Paper*, 2000-0667, 2000.
- ²²F. Palacios, J. J. Alonso, and A. Jameson. Shape sensitivity of free-surface interfaces using a level set methodology. *AIAA Paper*, 2012-3341, 2012.
- ²³F. Palacios, M. R. Colonno, A. C. Aranake, A. Campos, S. R. Copeland, T. D. Economon, A. K. Lonkar, T. W. Lukaczyk, T. W. R. Taylor, and J. J. Alonso. Stanford University Unstructured (SU2): An open-source integrated computational environment for multi-physics simulation and design. *AIAA Paper*, 2013-0287, 2013.
- ²⁴O. Pironneau. On optimum design in fluid mechanics. *J. Fluid Mech.*, 64:97–110, 1974.
- ²⁵A. Rizzi and L-E. Eriksson. Computation of inviscid incompressible flow with rotation. *J. Fluid Mech.*, 153:275–312, 1985.
- ²⁶J. E. Romate. Absorbing boundary conditions for free surface waves. *J. Comput. Phys.*, 99:135–145, 1992.
- ²⁷E. Shirani, A. Jafari, and N. Ashgriz. Turbulence models for flows with free surfaces and interfaces. *AIAA Journal*, 44(7):1454–1462, 2006.
- ²⁸P. Spalart and S. Allmaras. A one-equation turbulence model for aerodynamic flows. *AIAA Paper*, 92-0439, 1992.
- ²⁹M. Sussman, A.S. Almgren, J.B. Bell, P. Colella, L.H. Howell, and M.L. Welcome. An adaptive level set approach for incompressible two-phase flows. *J. Comput. Phys.*, 148(1):81–124, 1999.
- ³⁰M. Sussman, E. Fatemi, P. Smereka, and S. Osher. An improved level set method for incompressible two-phase flows. *Computers and Fluids*, 27:663–680, 1997.
- ³¹M. Sussman, P. Smereka, and S. Osher. A level set approach for computing solutions to incompressible two-phase flow. *J. Comput. Phys.*, 114(1):146–159, 1997.