NASA Contractor Report 191444

ICASE Report No. 93-13

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NASA Contract No. NAS1-19480
March 1993

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Operated by the Universities Space Research Association

National Aeronautics and
Space Administration

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ABSTRACT

In this paper, we discuss the use of a sensitivity equation method to compute derivatives for optimization based design algorithms. The problem of designing an optimal forebody simulator is used to motivate the algorithm and to illustrate the basic ideas. Finally, we indicate how an existing CFD code can be modified to compute sensitivities and a numerical example is presented.

[1]Supported in part by the Air Force Office of Scientific Research under Grant F-49620-92-J-0078.

[2]Supported in part by the Air Force Office of Scientific Research under Grant F-49620-92-J-0078, the National Science Foundation under Grant INT-89-22490 and by the National Aeronautics and Space Administration under Contract No. NAS1-19480 while the author was a visiting scientist at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA 23681-0001.

[3]Supported in part by the Air Force Office of Scientific Research under Grant F-49620-92-J-0078.

[4]Supported in part by the Air Force Office of Scientific Research under Grant AFOSR-90-0179.

1 Introduction

A large number of identification, control and design problems may be formulated as infinite dimensional optimization problems. These problems arise in almost all fields of science and engineering and range in scope from inverse problems in seismology, to LQR and H^∞ control, to shape optimization in fluid/structure dynamics. See [4,7] for typical applications. Although there are numerous approaches to solving these problems, each approach requires that some type of approximation be introduced at some point in the design process. Moreover, it is often the case that some iterative scheme is needed to solve the state equations (in black-box methods [3,8]) and the adjoint equations (in adjoint and "one-shot" methods [9]). Also, the optimization algorithm may itself be iterative. In any case, the development of computational methods for optimal design and control can produce several levels of approximation and the convergence properties of the overall algorithm are very much dependent on the approximations. In this paper we concentrate on the problem of computing accurate sensitivities for gradient based optimization algorithms. In order to keep the paper short and, at the same time illustrate the basic idea, we concentrate on a particular application. We give a brief description of the problem and use this problem to motivate the algorithm presented below.

2 Optimal Design of a Forebody Simulator

This problem is a 2D version of the problem described in [1,2,6]. The Arnold Engineering Development Center (AEDC) is developing a free-jet test facility for full-scale testing of engines in various free flight conditions. Although the test cells are large enough to house the jet engines, they are too small to contain the full airplane forebody and engine. Thus, the effect of the forward fuselage on the engine inlet flow conditions must be "simulated." One approach to solving this problem is to replace the actual forebody by a smaller object, called a "forebody simulator" (FBS), and determine the shape of the FBS that produces the best flow match at the engine inlet. The 2D version of this problem is illustrated in Figure 1 (see [1,2,5,6]).

The underlying mathematical model is based on conservation laws for mass, momentum and energy. For inviscid flow, we have that

$$\frac{\partial}{\partial t}\mathbf{Q} + \frac{\partial}{\partial x}\mathbf{F}_1 + \frac{\partial}{\partial y}\mathbf{F}_2 = 0 \tag{1}$$

where

$$\mathbf{Q} = \begin{pmatrix} \rho \\ m \\ n \\ E \end{pmatrix}, \qquad \mathbf{F}_1 = \begin{pmatrix} m \\ mu + P \\ mv \\ (E+P)u \end{pmatrix}, \qquad \text{and} \qquad \mathbf{F}_2 = \begin{pmatrix} n \\ nu \\ nv + P \\ (E+P)v \end{pmatrix}. \tag{2}$$

The velocity components u and v, the pressure P, the temperature T, and the Mach number M are related to the conservation variables, *i.e.*, the components of the vector $\mathbf{Q}$, by

$$\begin{aligned} u &= \frac{m}{\rho}, \qquad v = \frac{n}{\rho}, \qquad P = (\gamma - 1)\Big(E - \tfrac{1}{2}\rho(u^2 + v^2)\Big), \\ T &= \gamma(\gamma - 1)\left(\frac{E}{\rho} - \tfrac{1}{2}(u^2 + v^2)\right), \qquad \text{and} \qquad M^2 = \frac{u^2 + v^2}{T}. \end{aligned} \tag{3}$$

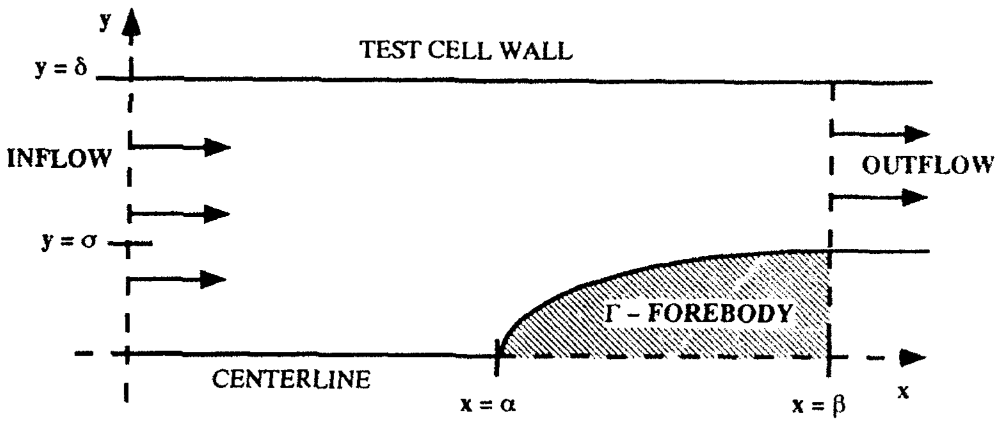

FIGURE 1.

At the inflow boundary, we want to simulate a free-jet, so that we specify the total pressure P_0, the total temperature T_0, and the Mach number M_0. We also set $v = 0$ at the inflow boundary. If u_I, P_I, and T_I denote the inflow values of the x-component of the velocity, the pressure, and the temperature, these may be recovered from T_0, P_0 and M_0 by

$$T_I = \frac{T_0}{(1+\frac{\gamma-1}{2}M_0^2)}\,, \quad P_I = \frac{P_0}{(1+\frac{\gamma-1}{2}M_0^2)^{\frac{\gamma}{\gamma-1}}}\,, \quad \text{and} \quad u_I^2 = M_0^2 T_I = \frac{M_0^2 T_0}{(1+\frac{\gamma-1}{2}M_0^2)}\,. \tag{4}$$

The components of $\mathbf{Q}$ at the inflow may then be determined from (4) through the relations

$$\rho_I = \frac{\gamma P_I}{T_I}\,, \qquad m_I = \rho_I u_I\,, \qquad n_I = 0\,, \qquad \text{and} \qquad E_I = \frac{P_I}{\gamma - 1} + \rho_I \frac{u_I^2}{2}\,. \tag{5}$$

The forebody is a solid surface, so that the normal component of the velocity vanishes, *i.e.*,

$$u n_1 + v n_2 = 0 \quad \text{on the forebody}\,. \tag{6}$$

where n_1 and n_2 are the components of the unit normal vector to the boundary. Note that we impose (6) on the velocity components u and v, and not on the momentum components m and n. Insofar as the state is concerned, it is clear that it does not make any difference whether (6) is imposed on m and n or on u and v, since $m = \rho u$ and $n = \rho v$ and $\rho \neq 0$. It can be shown that it does not make any difference to the sensitivities as well.

Assume that at $x = \beta$ the desired steady state flow $\hat{Q} = \hat{Q}(y)$ is given as data on the line (called the Inlet Reference Plane)

$$IRP = \{(x,y) | x = \beta, \sigma \leq y \leq \delta\}.$$

Also, we assume here that the inflow (total) Mach number M_0 can be used as a design (control) variable along with the shape of the forebody. Let the forebody be determined by the curve $\Gamma = \Gamma(x), \alpha \leq x \leq \beta$ and let $p = (M_0, \Gamma(\cdot))$. The problem can be stated as the following optimization problem:

Problem FBS. Given data $\hat{\mathbf{Q}} = \hat{\mathbf{Q}}(y)$ on the IRP, find the parameters $p^* = (M_0^*, \Gamma^*(\cdot))$ such that the functional

$$J(p) = \frac{1}{2}\int_\sigma^\delta \|\mathbf{Q}_\infty(\beta, y) - \hat{\mathbf{Q}}(y)\|^2 dy$$

is minimized, where $\mathbf{Q}_\sim(x,y) = \mathbf{Q}_\sim(x,y,p)$ is solution to the steady state Euler equation

$$\mathbf{G}(\mathbf{Q},p) = \frac{\partial}{\partial x}\mathbf{F}_1 + \frac{\partial}{\partial y}\mathbf{F}_2 = 0.$$

Clearly the statement of the problem is not complete. For example, one should carefully specify the set of admissible curves $\Gamma(\cdot)$ and questions remain about existence, uniqueness and integrability of "the" solution $\mathbf{Q}_\sim$. We will not address these issues in this short note.

Most optimization based design methods require the computat on of the derivatives $\frac{\partial}{\partial p}\mathbf{Q}_\sim(x,y,p)$. These derivatives are called sensitivities and various schemes have been developed to approximate the sensitivities numerically (see [3,5,10,11]). A common approach is to use finite differences. In particular, the steady state equation (8) is solved for p and again for $p+\Delta p$ and then $\frac{\partial}{\partial p}\mathbf{Q}_\sim(x,y,p)$ is approximated by $\frac{[\mathbf{Q}_\sim(x,y,p+\Delta p)-\mathbf{Q}_\sim(x,y,p)]}{\Delta p}$. This method is often costly and can introduce large errors. Another approach is to first derive an equation (the sensitivity equation) for $\mathbf{Q}' = \frac{\partial}{\partial p}\mathbf{Q}_\sim(x,y,p)$ and then numerically solve this equation. We shall illustrate this approach for the forebody design problem and present a comparison of the two methods.

3 Sensitivities with Respect to the Inflow Mach Number

First, we consider the design parameter M_0^2. Thus, we will derive equations for the sensitivity

$$\mathbf{Q}' \equiv \frac{\partial \mathbf{Q}}{\partial M_0^2} \equiv \begin{pmatrix} \rho' \\ m' \\ n' \\ E' \end{pmatrix}, \tag{7}$$

where

$$\rho' \equiv \frac{\partial \rho}{\partial M_0^2}, \qquad m' \equiv \frac{\partial m}{\partial M_0^2}, \qquad n' \equiv \frac{\partial n}{\partial M_0^2}, \qquad \text{and} \qquad E' \equiv \frac{\partial E}{\partial M_0^2}. \tag{8}$$

The differential equation system (1) has no explicit dependence on the design parameter M_0^2, so that equations for the components of $\mathbf{Q}'$ are easily determined by formally differentiating (1) with respect to M_0^2. The result is the system

$$\frac{\partial \mathbf{Q}'}{\partial t} + \frac{\partial \mathbf{F}_1'}{\partial x} + \frac{\partial \mathbf{F}_2'}{\partial y} = 0, \tag{9}$$

where

$$\mathbf{F}_1' = \begin{pmatrix} m' \\ mu' + m'u + P' \\ mv' + m'v \\ (E+P)u' + (E'+P')u \end{pmatrix} \qquad \text{and} \qquad \mathbf{F}_2' = \begin{pmatrix} n' \\ nu' + n'u \\ nv' + n'v + P' \\ (E+P)v' + (E'+P')v \end{pmatrix}, \tag{10}$$

and where,

$$u' = \frac{\partial u}{\partial M_0^2}, \qquad v' = \frac{\partial v}{\partial M_0^2}, \qquad P' = \frac{\partial P}{\partial M_0^2}, \qquad \text{and} \qquad T' = \frac{\partial T}{\partial M_0^2}, \tag{11}$$

and where, through (3), the sensitivities (8) and (11) are related by

$$\begin{aligned} u' &= \frac{1}{\rho}m' - \frac{m}{\rho^2}\rho', \qquad P' = (\gamma-1)\Big(E' - \tfrac{1}{2}\rho'(u^2+v^2) - \rho(uu'+vv')\Big), \\ v' &= \frac{1}{\rho}n' - \frac{n}{\rho^2}\rho', \qquad \text{and} \qquad T' = \gamma(\gamma-1)\left(\frac{1}{\rho}E' - \frac{E}{\rho^2}\rho' - (uu'+vv')\right) \end{aligned} \tag{12}$$

Note that (9) is of the same form as (1), with a different flux vector. In particular, (9) is in conservation form. As a result of the fact that (9) is *linear* in the primed variables, and that by (12) u', v', and P' are linear in the components of $\mathbf{Q}'$, (9) is a linear system in the sensitivity (7), *i.e.*, in the components of $\mathbf{Q}'$.

Now, we need to discuss the boundary conditions for $\mathbf{Q}'$. Except for the inflow conditions, all boundary conditions are independent of the design parameter M_0^2. Thus, the latter may be differentiated with respect to M_0^2 to obtain boundary conditions for the sensitivities. For example, at the forebody where (6) holds, we simply would have that

$$u'n_1 + v'n_2 = 0 \quad \text{on the forebody}. \tag{13}$$

Similar operations yield boundary conditions for the sensitivities along symmetry lines, other solid surfaces, and at the outflow boundary. Note that if instead of (6), one interprets the no penetration condition as one on the momentum, *i.e.*, $mn_1 + nn_2 = 0$ on the forebody, then instead of (13) we would have that

$$m'n_1 + n'n_2 = 0 \quad \text{on the forebody} \tag{14}$$

which is seemingly different from (13). However, (6) and (12) can be used to show that

$$m'n_1 + n'n_2 = \rho(u'n_1 + v'n_2) + \rho'(un_1 + vn_2) = \rho(u'n_1 + v'n_2) \tag{15}$$

so that, since $\rho \neq 0$, (13) and (14) are identical.

The inflow boundary conditions for the sensitivities may be determined by differentiating (4) and (5) with respect to the design parameter M_0^2. Note that this parameter appears explicitly in the right-hand-sides of the equations in (4) and (5). Without difficulty, one finds from (5) that

$$\begin{aligned} \rho_I' &= \frac{\gamma}{T_I}P_I' - \frac{\gamma P_I}{T_I^2}T_I', \qquad m_I' = \rho_I u_I' + u_I\rho_I' \\ n_I' &= 0, \qquad \text{and} \qquad E_I' = \frac{1}{\gamma-1}P_I' + \frac{1}{2}u_I^2\rho_I' + \rho_I u_I u_I', \end{aligned} \tag{16}$$

where, from (4),

$$\begin{aligned} T_I' &= -\left(\frac{\gamma-1}{2}\right)\frac{T_0}{\left(1+\frac{\gamma-1}{2}M_0^2\right)^2}, \qquad P_I' = -\left(\frac{\gamma}{2}\right)\frac{P_0}{\left(1+\frac{\gamma-1}{2}M_0^2\right)^{\frac{2\gamma-1}{\gamma-1}}}, \qquad \text{and} \\ u_I' &= \frac{\sqrt{T_I}}{2M_0} + \frac{M_0}{2\sqrt{T_I}}T_I' = \frac{\sqrt{T_0}}{2M_0\left(1+\frac{\gamma-1}{2}M_0^2\right)^{\frac{3}{2}}}\left(1+(\gamma-1)M_0^2\right). \end{aligned} \tag{17}$$

4 Sensitivities with Respect to the Forebody Design Parameters

We assume that the forebody is described in terms of a finite number of design parameters which we denote by P_k, $k = 1, \ldots, K$, and that the forebody may be described by the relation

$$y = \Phi(x; P_1, P_2, \ldots, P_K), \quad \alpha \le x \le \beta \tag{18}$$

We express the dependence of the state variable $\mathbf{Q}$ on the coordinates and the design parameters by $\mathbf{Q} = \mathbf{Q}(t, x, y; M_0^2, P_1, P_2, \ldots, P_K)$. We have already seen what equations can be used to determine the sensitivity of the state with respect to M_0^2, *i.e.*, for $\mathbf{Q}'$. We now discuss what equations can be used to determine the sensitivities with respect to the forebody design parameters P_k, $k = 1, \ldots, K$, *i.e.*, for

$$\mathbf{Q}_k \equiv \frac{\partial \mathbf{Q}}{\partial P_k} \equiv \begin{pmatrix} \rho_k \\ m_k \\ n_k \\ E_k \end{pmatrix} , \tag{19}$$

where

$$\rho_k \equiv \frac{\partial \rho}{\partial P_k}, \qquad m_k \equiv \frac{\partial m}{\partial P_k}, \qquad n_k \equiv \frac{\partial n}{\partial P_k}, \qquad \text{and} \qquad E_k \equiv \frac{\partial E}{\partial P_k}. \qquad k = 1, \ldots, K. \tag{20}$$

System (1) has no explicit dependence on the design parameters P_k, so that equations for the components of $\mathbf{Q}_k$ are easily determined by differentiating (1) with respect to P_k, $k = 1, \ldots, K$. This produces the systems, $k = 1, \ldots, K$, given by

$$\frac{\partial \mathbf{Q}_k}{\partial t} + \frac{\partial \mathbf{F}_{k1}}{\partial x} + \frac{\partial \mathbf{F}_{k2}}{\partial y} = 0, \tag{21}$$

where

$$\mathbf{F}_{k1} = \begin{pmatrix} m_k \\ m u_k + m_k u + P_k \\ m v_k + m_k v \\ (E+P)u_k + (E_k + P_k)u \end{pmatrix} \quad \text{and} \quad \mathbf{F}_{k2} = \begin{pmatrix} n_k \\ n u_k + n_k u \\ n v_k + n_k v + P_k \\ (E+P)v_k + (E_k + P_k)v \end{pmatrix}, \tag{22}$$

and where,

$$u_k = \frac{\partial u}{\partial P_k}, \qquad v_k = \frac{\partial v}{\partial P_k}, \qquad P_k = \frac{\partial P}{\partial P_k}, \qquad \text{and} \qquad T_k = \frac{\partial T}{\partial P_k}. \tag{23}$$

Moreover, by (3), the sensitivities (20) and (23) are related by

$$\begin{aligned} u_k &= \frac{1}{\rho} m_k - \frac{m}{\rho^2}\rho_k, \qquad & P_k &= (\gamma - 1)\Big(E_k - \tfrac{1}{2}\rho_k(u^2 + v^2) - \rho(u u_k + v v_k)\Big) \\ v_k &= \frac{1}{\rho} n_k - \frac{n}{\rho^2}\rho_k, \qquad \text{and} & T_k &= \gamma(\gamma - 1)\left(\frac{1}{\rho}E_k - \frac{E}{\rho^2}\rho_k - (u u_k + v v_k)\right), \end{aligned} \tag{24}$$

for $k = 1, \ldots, K$.

All boundary conditions except the one on the forebody also do not depend on the forebody design parameters P_k, $k = 1, \ldots, K$. For example, consider the inflow boundary conditions (4)-(5). Differentiating these with respect to P_k, $k = 1, \ldots, K$ yields that

$$\rho_{kI} = m_{kI} = n_{kI} = E_{kI} = T_{kI} = P_{kI} = u_{kI} = v_{kI} = 0, \tag{25}$$

at the inflow boundary. Now, consider the boundary condition (6) on the forebody. We have that on the forebody

$$\frac{n_1}{n_2} = -\frac{\partial \Phi}{\partial x}. \tag{26}$$

Combining (6) and (26) we have that

$$u\frac{\partial \Phi}{\partial x} - v = 0 \tag{27}$$

along the forebody or, displaying the full functional dependence on the coordinates and design parameters, we have at a point (x, y) on the forebody, and at any time t,

$$u\left(t, x, y = \Phi(x; P_1, P_2, \ldots, P_K); M_0^2, P_1, P_2, \ldots, P_K\right) \frac{\partial \Phi}{\partial x}(x; P_1, P_2, \ldots, P_K) \\ - v\left(t, x, y = \Phi(x; P_1, P_2, \ldots, P_K); M_0^2, P_1, P_2, \ldots, P_K\right) = 0 . \tag{28}$$

We can proceed to differentiate (28) with respect any of the forebody design parameters P_k, $k = 1, \ldots, K$. The result is that, along the forebody for $k = 1, \ldots, K$,

$$u_k \frac{\partial \Phi}{\partial x} - v_k = -\left(\frac{\partial u}{\partial y}\right)\left(\frac{\partial \Phi}{\partial P_k}\right)\left(\frac{\partial \Phi}{\partial x}\right) - u\frac{\partial}{\partial x}\left(\frac{\partial \Phi}{\partial P_k}\right) + \left(\frac{\partial v}{\partial y}\right)\left(\frac{\partial \Phi}{\partial P_k}\right) , \tag{29}$$

where u, v, and their derivatives are evaluated at the forebody $(x, y = \Phi(x))$.

If an iterative scheme is used to find a steady state solution of this system ((21), (25), (29)), then we assume that present guesses for the state variables u and v and their derivatives $\partial u/\partial y$ and $\partial v/\partial y$ and for the design parameters M_0^2 and P_k, $k = 1, \ldots, K$, are known. It follows that the right-hand-side of (29) is known as well and equation (29), the boundary conditions along the forebody for the sensitivities with respect to the forebody design parameters, is merely an inhomogeneous version of (27), the boundary condition along the forebody for the state.

Let us now specialize to the type of forebodies considered by Huddleston, [5,6], *i.e.*

$$\Phi(x; P_1, P_2, \ldots, P_K) = \sum_{k=1}^{K} P_k \phi_k(x) , \tag{30}$$

where $\phi_k(x)$, $k = 1, \ldots, K$, are prescribed functions, *e.g.*, Bezier curves. In this case,

$$\frac{\partial \Phi}{\partial P_k} = \phi_k(x) \qquad \text{and} \qquad \frac{\partial}{\partial x}\left(\frac{\partial \Phi}{\partial P_k}\right) = \frac{d\phi_k}{dx}(x) , \tag{31}$$

and

$$\frac{\partial \Phi}{\partial x} = \sum_{k=1}^{K} P_k \frac{d\phi_k}{dx}(x) . \tag{32}$$

Combining (29)-(32), one obtains that, at any point $(x, \Phi(x))$ on the forebody and for each $k = 1, \ldots, K$,

$$\left(\sum_{j=1}^{K} P_j \frac{d\phi_j}{dx}\right) u_k - v_k = -\left(\frac{\partial u}{\partial y}\right)\left(\sum_{j=1}^{K} P_j \frac{d\phi_j}{dx}\right)\phi_k - u\frac{d\phi_k}{dx} + \left(\frac{\partial v}{\partial y}\right)\phi_k . \tag{33}$$

For forebodies of the type (30), (33) gives the the boundary conditions along the forebody for the sensitivities with respect to the forebody design parameters P_k, $k = 1, \ldots, K$. It is now clear that, given guesses for the state variables u and v and their derivatives $\partial u/\partial y$ and $\partial v/\partial y$ and for the design parameters M_0^2 and P_k, $k = 1, \ldots, K$, then the right-hand-side of (33) is known.

5 Computing Sensitivities using an Existing Code for the State

Suppose one has available a code to compute the state variables, *i.e.*, to find approximate solutions of (1) along with boundary and initial conditions. In principle, it is an easy matter to amend such a code so that it can also compute sensitivities.

First, let us compare (1) with (9). If one wishes to amend the existing state code that can handle (1) so that it can treat (9) as well, one has to change the definitions of the flux functions from those given in (2) to those given in (10). Note that the solution for the state is needed in order to evaluate the flux functions of (10).

Next, note that (9) and (22) are identical differential equations. Thus, the changes made to the code in order to treat (9) can also be used to treat (22). In fact, as long as the differential equation and any other part of the problem specification do not explicitly depend on the design parameters, the analogous relations will be the same for all the sensitivities.

The only changes that vary from one sensitivity calculation to another are those that arise from conditions in which the design parameters appear explicitly. In our example, for the sensitivity with respect to M_0^2, one must change the portion of the code that treats the inflow conditions (4)-(5) so that it can instead treat (16)-(17). The only changes needed to accomplish this are to the data of the inflow conditions. In the problem considered here, the nature (*i.e.* what variables are specified) of the boundary conditions at the inflow, and everywhere else, is not affected. Note that for the sensitivity with respect to M_0^2 the boundary condition (13) on the forebody is the same as that for the state, given by (6).

For the sensitivities with respect to the forebody design parameters, the inflow boundary conditions simplify to (25), *i.e.*, they become homogeneous. The boundary condition at the forebody is now given by (29) or (33). Once again, the nature of the boundary conditions is unchanged from that for the state, and only the data that is specified is different. For the inflow boundary conditions, we may still specify the same conditions for the sensitivities, but now they would be homogeneous. The boundary conditions along the forebody change only in that they become inhomogeneous, (compare (27) and (33)).

In summary, to change a code for the state so that it also handles the sensitivities, one must redefine the flux functions in the differential equations, and the data in the boundary conditions. The changes necessary in the code to account for any particular relation that does not explicitly involve the design parameters are independent of which sensitivity one is presently considering.

The previous remarks are concerned only with the changes one must effect in a state code in order to handle the fact that one is discretizing a different problem when one considers the sensitivities. We have seen that these changes are not major in nature. However, there are additional changes that may be needed when one attempts to solve the discrete equations. In the numerical results presented below we use the finite difference code "PARC" (see [2,5]) to solve the state and sensitivity equations. However, the following comments apply equally well to other CFD codes of this type.

Since we are interested in the steady design problems, the time derivative in (1) is considered only to provide a means for marching to a steady state. Now, suppose that at any stage of a Gauss-Newton, or other iteration, we have used PARC to find an approximate steady state solution of (1) plus boundary conditions. In order to do this, one has to solve a sequence of linear algebraic systems of the type

$$\left(I + \Delta t\, \mathbf{A}(\mathbf{Q}_h^{(n)})\right)\mathbf{Q}_h^{(n+1)} = \left(\mathbf{Q}_h^{(n)} + \Delta t\, \mathbf{B}(\mathbf{Q}_h^{(n)})\right), \qquad n = 0, 1, 2, \ldots, \tag{34}$$

where the sequence is terminated when one is satisfied that a steady state has been reached and where $\mathbf{Q}_h^{(n)}$ denotes the discrete approximation to the state $\mathbf{Q}$ at the time $t = n\Delta t$. We denote this steady state solution for the approximation to the state by $\mathbf{Q}_h$. One problem of the type (34) is solved for every time step. In (34), the matrix $\mathbf{A}$ and vector $\mathbf{B}$ arise from the spatial discretization of the fluxes and the boundary conditions. Both of these depend on the state at the previous time level.

Having computed a steady state solution by (34), the task at hand is to now compute the sensitivities. We will focus on $\mathbf{Q}'$, the sensitivity with respect to the inflow Mach number. Analogous results hold for the sensitivities with respect to the forebody design parameters. Recall that given a state, the sensitivity equations are linear in the sensitivities. Therefore, if one is interested in the steady state sensitivities, instead of (9) one may directly treat its stationary version

$$\frac{\partial \mathbf{F}_1'}{\partial x} + \frac{\partial \mathbf{F}_2'}{\partial y} = 0\,. \tag{35}$$

Since (35) is linear in the components of $\mathbf{Q}'$, one does not need to consider marching algorithms in order to compute a steady sensitivity. One merely discretizes (35) and solves the resultant linear system, which has the form

$$A'(\mathbf{Q}_h)\mathbf{Q}_h' = \mathbf{B}'(\mathbf{Q}_h)\,, \tag{36}$$

where $\mathbf{Q}_h'$ denotes the discrete approximation to the steady sensitivity. The matrix A' and vector $\mathbf{B}'$ differ from the A and $\mathbf{B}$ of (34) because we have discretized different differential equations and boundary conditions. Note that A' and $\mathbf{B}'$ in (36) depend only on the steady state $\mathbf{Q}_h$ and thus (36) is a *linear system of algebraic equations* for the discrete sensitivity $\mathbf{Q}_h'$.

The cost of finding a solution of (36) is similar to that for finding the solution of (34) for a single value of n, *i.e.*, for a single time step. The differences in the assembly of the coefficient matrices and right-hand-sides of (34) and (36) are minor. Thus, in theory at least, *one can obtain a steady sensitivity in the same computer time it takes to perform one time step in a state calculation.* If one wants to obtain all the sensitivities, *e.g.*, $K+1$ in our example, one can do so at a cost similar to, *e.g.*, $K+1$ time steps of the state calculation. This is very cheap compared to the multiple state calculations necessary in order to compute sensitivities through the use of difference quotients.

In practice, these "optimal" estimates of speed up are rarely achieved. Moreover, it is important to note that finite difference (FD) and sensitivity equation (SE) methods do not necessarily produce the same results. Since the ultimate goal is to find useful and cheap gradients for optimization, the most important issue is whether or not the SE method combined with an optimization algorithm produces a convergent optimal design as fast as possible. We have tested this scheme on the forebody design problem with excellent results.

6 A Numerical Example

In order to illustrate the use of the SE method in computing sensitivities, we used the PARC code as described above to find approximate solutions of the sensitivity equations and compared the results to the finite difference method. In Figure 2 we show the approximations of $\frac{\partial}{\partial P_1} m(x, y, \hat{M}_0^2, \hat{P}_1, \hat{P}_2)$ for $\hat{M}_0 = 2, \hat{P}_1 = .1$ and $\hat{P}_2 = .15$ where the forebody is described by two Bezier parameters (P_1, P_2). Both pictures are "converged" estimates. Note that there are considerable differences between the FD method and the SE method. Moreover, in Figure 3 we see that not only do the FD and SE methods produce different sensitivities, the value of the step size ΔP_1 can greatly influence the FD approximations. Finally, we note that the SE method ran 4 to 5 times faster than the FD method. Also, although space prohibits a discussion of the optimization problem here, we have used the SE method in a trust region optimization scheme to produce an optimal forebody design for the 2D problem in [5,6]. These results will appear in a forthcoming paper.

7 Conclusions

The problem of computing accurate sensitivities in problems involving solutions to parameterized partial differential equations is an important part of optimal design. The goal is to find derivatives of solutions of partial differential equations with respect to various parameters (including domain shapes) and to use these derivatives in some type of optimization scheme. In almost all practical problems, solutions must be obtained by numerical approximations. This fact leads to "black box" methods for optimal design. In its most basic form, a black box method produces approximate solutions that are then differentiated (by finite differences, automatic differentiation, etc.). The sensitivity equation (SE) method presented here is based on first deriving partial differential equations for the derivatives and then approximating these equations numerically. Both approaches produce numerical approximations of the sensitivities. However, the (SE) method can often reduce computational effort, speed up the calculations and, provided that accurate computational schemes can be devised for the sensitivity equations, the derivatives can be computed with the same degree of accuracy as the state. The 2D optimal forebody simulator problem is an excellent problem for illustrating these points. The numerical results presented here show that the (SE) method is potentially applicable to real problems and, at the same time, raises many interesting theoretical and practical questions.

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Sensitivity of U-Momentum
with respect to First Bezier Parameter

Sensitivity Equation Method

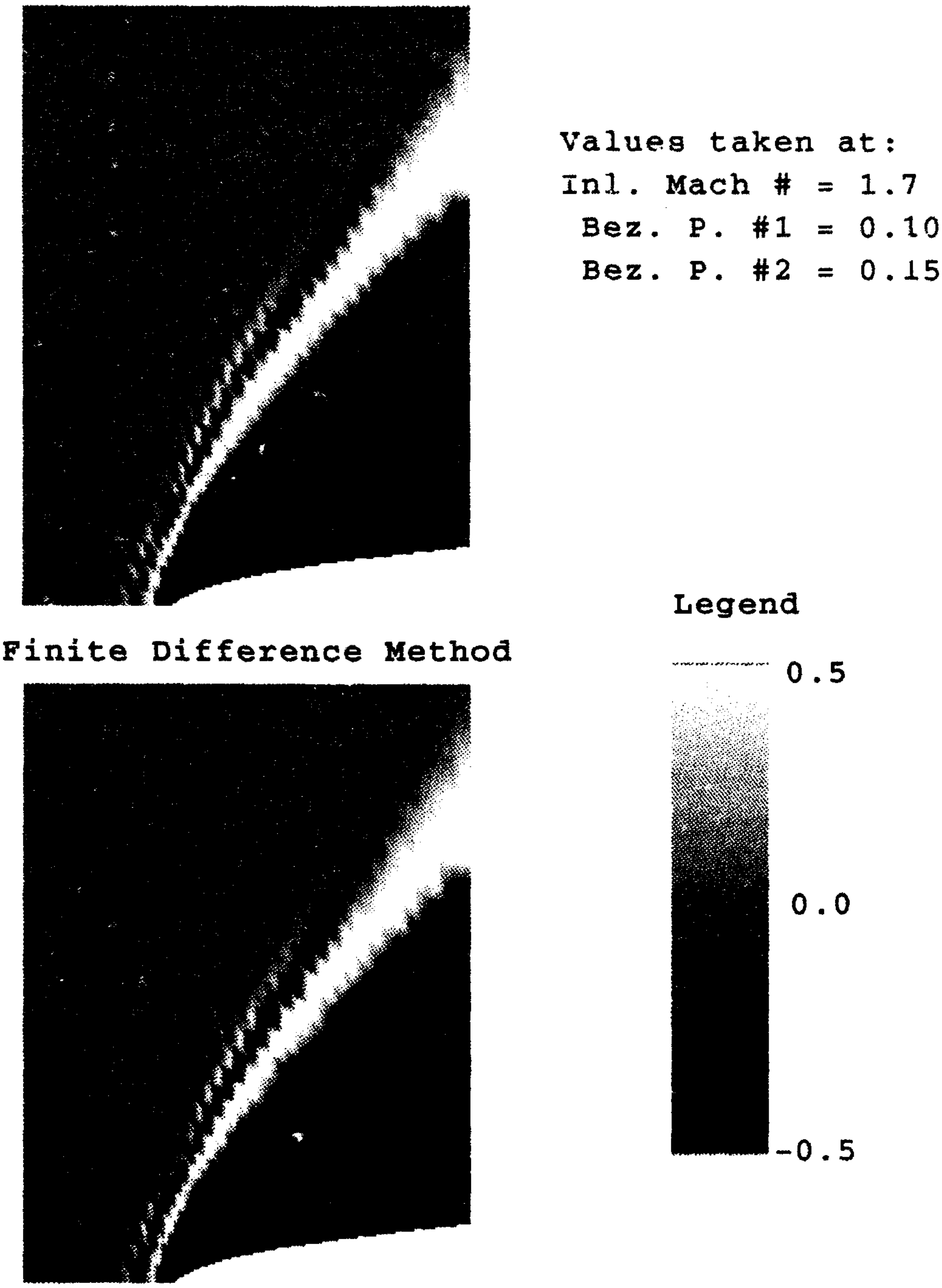

Figure 2

Absolute Difference of U-Mom. Sensitivities
with respect to First Bezier Parameter
obtained using F.D. and S.E. Methods

Values at: Inlet Mach # = 1.7
Bezier Parameter #1 = 0.10
Bezier Parameter #2 = 0.15

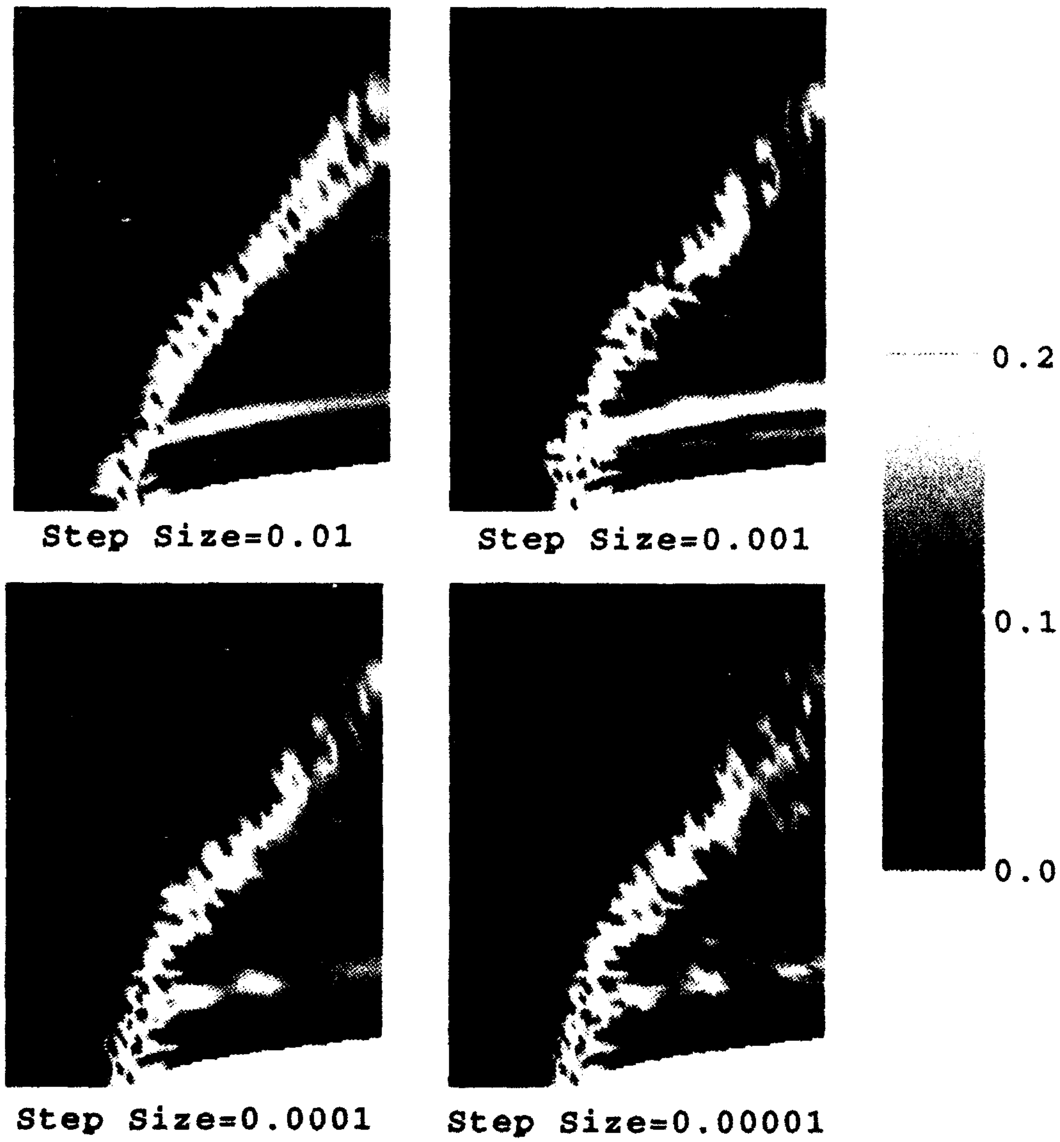

Figure 3

REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
March 1993

3. REPORT TYPE AND DATES COVERED
Contractor Report

4. TITLE AND SUBTITLE
SENSITIVITY CALCULATIONS FOR A 2D, INVISCID, SUPERSONIC FOREBODY PROBLEM

5. FUNDING NUMBERS
C NAS1-19480

WU 505-90-52-01

6. AUTHOR(S)
Jeff Borggaard, John A. Burns, Eugene Cliff, and Max Gunzburger

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Institute for Computer Applications in Science and Engineering
Mail Stop 132C, NASA Langley Research Center
Hampton, VA 23681-0001

8. PERFORMING ORGANIZATION REPORT NUMBER
ICASE Report No. 93-13

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
Langley Research Center
Hampton, VA 23681-0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
NASA CR-191444
ICASE Report No. 93-13

11. SUPPLEMENTARY NOTES
Langley Technical Monitor: Michael F. Card
Final Report

To appear in Proc. of AMS-IMS-SIAM Summer Research Conf. on Distributed Parameter Control, SIAM, 1993

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Unclassified - Unlimited

Subject Category 02, 64

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

In this paper, we discuss the use of a sensitivity equation method to computer derivatives for optimization based design algorithms. The problem of designing an optimal forebody simulator is used to motivate the algorithm and to illustrate the basic ideas. Finally, we indicate how an existing CFD code can be modified to compute sensitivities and a numerical example is presented.

14. SUBJECT TERMS
optimal design; sensitivities

15. NUMBER OF PAGES
13

16. PRICE CODE
A03

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified		

NSN 7540-01-280-5500

Standard Form 298 (Rev 2-89)
Prescribed by ANSI Std Z39-18
298-102

☆U.S. GOVERNMENT PRINTING OFFICE: 1993 - 728-064/66011