45th Aerospace Sciences Meeting and Exhibit, January 8–11, 2007, Reno, Nevada

Adjoint Formulations for Topology, Shape and Discrete Optimization

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I. Introduction

The use of adjoints for PDE constrained optimization problems has become a common design tool in many areas of applied engineering. The use of adjoint methods for shape optimization has received much attention as it exploits the inherent advantage of computing the Frechet derivative of a single or small number of objectives with minimal computational effort.[1] Topology optimization primarily for problems in structural mechanics has also used adjoints to efficiently compute sensitivities of the weight of the structure.[4] Inverse design to recover the shape that results in a particular scattering pattern have used adjoints to quickly morph topologies.[3] Eulerian network models[5] of transportation (personal and commercial) fleets have also been controlled using adjoints to determine the control authority that maximizes throughput of hubs and transportation corridors.

The objective of this paper is to formulate and solve the adjoint problem for a variety of PDE constrained optimization problems. The PDEs we will address include Euler equations, linear elasticity, helmholtz and wave equations. For the Euler equations, building on experience of the second author, we plan to tackle new objective functions that include derivatives of the state variables. For the problems in linear elasticity we compare continuous and discrete formulations for minimum weight structures. For the Hemlhotz problem, we study objective functions that contain a mix of polynomial and derivatives in the state-variable. For the wave propagation problem, we use the linear wave equation and its adjoint formulation to determine time dependent optimal controls that enable the identification of the scattering object. Finally, we look at problems in which the PDEs constraining the optimization problem discontinuously change in time and space.

II. The general formulation of the Adjoint Approach to Optimal Design

The cost function are functions of the state variables, w, and the control variables, which may be represented by the function, $\mathcal{F}$, say. Then

$$I = I(w, \mathcal{F}),$$

and a change in $\mathcal{F}$ results in a change

$$\delta I = \frac{\partial I^T}{\partial w}\delta w + \frac{\partial I^T}{\partial \mathcal{F}}\delta \mathcal{F}, \tag{1}$$

in the cost function. Using control theory, the governing equations for the state variables are introduced as a constraint in such a way that the final expression for the gradient does not require re-evaluation of the state. In order to achieve this, δw must be eliminated from equation 1. Suppose that the governing equation R which expresses the dependence of w and $\mathcal{F}$ within the domain D can be written as

$$R(w, \mathcal{F}) = 0 \tag{2}$$

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Then δw is determined from the equation

$$\delta R = \left[\frac{\partial R}{\partial w}\right] \delta w + \left[\frac{\partial R}{\partial \mathcal{F}}\right] \delta \mathcal{F} = 0 \tag{3}$$

Next, introducing a Lagrange Multiplier ψ, we have

$$\delta I = \frac{\partial I^T}{\partial w} \delta w + \frac{\partial I^T}{\partial \mathcal{F}} \delta \mathcal{F} - \psi^T \left(\left[\frac{\partial R}{\partial w}\right] \delta w + \left[\frac{\partial R}{\partial \mathcal{F}}\right] \delta \mathcal{F} \right)$$

$$\delta I = \left(\frac{\partial I^T}{\partial w} - \psi^T \left[\frac{\partial R}{\partial w}\right] \right) \delta w + \left(\frac{\partial I^T}{\partial \mathcal{F}} - \psi^T \left[\frac{\partial R}{\partial \mathcal{F}}\right] \right) \delta \mathcal{F}$$

Choosing ψ to satisfy the adjoint equation

$$\left[\frac{\partial R}{\partial w}\right]^T \psi = \frac{\partial I}{\partial w} \tag{4}$$

the first term is eliminated and we find that

$$\delta I = \mathcal{G} \delta \mathcal{F} \tag{5}$$

where

$$\mathcal{G} = \frac{\partial I^T}{\partial \mathcal{F}} - \psi^T \left[\frac{\partial R}{\partial \mathcal{F}}\right] \tag{6}$$

This process allows for elimination of the terms that depend on the flow solution with the result that the gradient with respect with an arbitrary number of design variables can be determined without the need for additional flow field evaluations.

After taking a step in the negative gradient direction, the gradient is recalculated and the process repeated to follow the path of steepest descent until a minimum is reached. In order to avoid violating constraints, such as the minimum acceptable wing thickness, the gradient can be projected into an allowable subspace within which the constraints are satisfied. In this way one can devise procedures which must necessarily converge at least to a local minimum and which can be accelerated by the use of more sophisticated descent methods such as conjugate gradient or quasi-Newton algorithms. There is a possibility of more than one local minimum, but in any case this method will lead to an improvement over the original design.

III. Design using the Euler Equations

In this section, we discuss the use of the adjoint-based approach for optimal design for a problem that was formulated by the second author and since altered our view of gradient-based shape optimization.

The application of control theory to aerodynamic design problems is illustrated in this section for the case of three-dimensional wing design using the compressible Euler equations as the mathematical model. It proves convenient to denote the Cartesian coordinates and velocity components by x_1, x_2, x_3 and u_1, u_2, u_3, and to use the convention that summation over $i = 1$ to 3 is implied by a repeated index i. Then, the three-dimensional Euler equations may be written as

$$\frac{\partial w}{\partial t} + \frac{\partial f_i}{\partial x_i} = 0 \quad \text{in } D, \tag{7}$$

where

$$w = \left\{ \begin{array}{c} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{array} \right\}, \quad f_i = \left\{ \begin{array}{c} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} \\ \rho u_i u_2 + p\delta_{i2} \\ \rho u_i u_3 + p\delta_{i3} \\ \rho u_i H \end{array} \right\} \tag{8}$$

and δ_{ij} is the Kronecker delta function. Also,

$$p = (\gamma - 1)\,\rho \left\{ E - \frac{1}{2}\left(u_i^2\right) \right\}, \tag{9}$$

and

$$\rho H = \rho E + p \tag{10}$$

where γ is the ratio of the specific heats.

Consider a transformation to coordinates ξ_1, ξ_2, ξ_3 where

$$K_{ij} = \left[\frac{\partial x_i}{\partial \xi_j} \right], \quad J = \det\left(K\right), \quad K_{ij}^{-1} = \left[\frac{\partial \xi_i}{\partial x_j} \right],$$

and

$$S = JK^{-1}.$$

The elements of S are the cofactors of K, and in a finite volume discretization they are just the face areas of the computational cells projected in the x_1, x_2, and x_3 directions. Using the permutation tensor ϵ_{ijk} we can express the elements of S as

$$S_{ij} = \frac{1}{2}\epsilon_{jpq}\epsilon_{irs}\frac{\partial x_p}{\partial \xi_r}\frac{\partial x_q}{\partial \xi_s}. \tag{11}$$

Then

$$\begin{aligned} \frac{\partial}{\partial \xi_i} S_{ij} &= \frac{1}{2}\epsilon_{jpq}\epsilon_{irs}\left(\frac{\partial^2 x_p}{\partial \xi_r \partial \xi_i}\frac{\partial x_q}{\partial \xi_s} + \frac{\partial x_p}{\partial \xi_r}\frac{\partial^2 x_q}{\partial \xi_s \partial \xi_i} \right) \\ &= 0. \end{aligned} \tag{12}$$

Now, multiplying equation(7) by J and applying the chain rule,

$$J\frac{\partial w}{\partial t} + R\left(w\right) = 0 \tag{13}$$

where

$$R\left(w\right) = S_{ij}\frac{\partial f_j}{\partial \xi_i} = \frac{\partial}{\partial \xi_i}\left(S_{ij} f_j\right), \tag{14}$$

using (12). We can write the transformed fluxes in terms of the scaled contravariant velocity components

$$U_i = S_{ij} u_j$$

as

$$F_i = S_{ij} f_j = \begin{bmatrix} \rho U_i \\ \rho U_i u_1 + S_{i1} p \\ \rho U_i u_2 + S_{i2} p \\ \rho U_i u_3 + S_{i3} p \\ \rho U_i H \end{bmatrix}.$$

Assume now that the new computational coordinate system conforms to the wing in such a way that the wing surface B_W is represented by $\xi_2 = 0$. Then the flow is determined as the steady state solution of equation (13) subject to the flow tangency condition

$$U_2 = 0 \quad \text{on } B_W. \tag{15}$$

At the far field boundary B_F, conditions are specified for incoming waves, as in the two-dimensional case, while outgoing waves are determined by the solution.

The weak form of the Euler equations for steady flow can be written as

$$\int_{\mathcal{D}} \frac{\partial \phi^T}{\partial \xi_i} F_i d\mathcal{D} = \int_{\mathcal{B}} n_i \phi^T F_i d\mathcal{B}, \tag{16}$$

where the test vector ϕ is an arbitrary differentiable function and n_i is the outward normal at the boundary. If a differentiable solution w is obtained to this equation, it can be integrated by parts to give

$$\int_{\mathcal{D}} \phi^T \frac{\partial F_i}{\partial \xi_i} d\mathcal{D} = 0$$

and since this is true for any ϕ, the differential form can be recovered. If the solution is discontinuous (16) may be integrated by parts separately on either side of the discontinuity to recover the shock jump conditions.

Suppose now that it is desired to control the surface pressure by varying the wing shape. For this purpose, it is convenient to retain a fixed computational domain. Then variations in the shape result in corresponding variations in the mapping derivatives defined by K. As an example, consider the case of an inverse problem, where we introduce the cost function

$$I = \frac{1}{2} \int\int_{B_W} (p - p_d)^2 \, d\xi_1 d\xi_3,$$

where p_d is the desired pressure. The design problem is now treated as a control problem where the control function is the wing shape, which is to be chosen to minimize I subject to the constraints defined by the flow equations (13). A variation in the shape will cause a variation δp in the pressure and consequently a variation in the cost function

$$\delta I = \int\int_{B_W} (p - p_d)\, \delta p \;\; d\xi_1 d\xi_3 + \frac{1}{2} \int_{\mathcal{B}} (p - p_t)^2 d\delta S \tag{17}$$

where typically the second term is negligible and can be dropped.

Since p depends on w through the equation of state (9–10), the variation δp can be determined from the variation δw. Define the Jacobian matrices

$$A_i = \frac{\partial f_i}{\partial w}, \quad C_i = S_{ij} A_j. \tag{18}$$

The weak form of the equation for δw in the steady state becomes

$$\int_{\mathcal{D}} \frac{\partial \phi^T}{\partial \xi_i} \delta F_i d\mathcal{D} = \int_{\mathcal{B}} (n_i \phi^T \delta F_i) d\mathcal{B},$$

where

$$\delta F_i = C_i \delta w + \delta S_{ij} f_j,$$

which should hold for any differential test function ϕ. This equation may be added to the variation in the cost function, which may now be written as

$$\begin{aligned} \delta I = & \int\int_{B_W} (p - p_d)\, \delta p \;\; d\xi_1 d\xi_3 \\ & - \int_{\mathcal{D}} \left(\frac{\partial \phi^T}{\partial \xi_i} \delta F_i \right) d\mathcal{D} \\ & + \int_{\mathcal{B}} \left(n_i \phi^T \delta F_i \right) d\mathcal{B}. \end{aligned} \tag{19}$$

On the wing surface B_W, $n_1 = n_3 = 0$. Thus, it follows from equation (15) that

$$\delta F_2 = \begin{bmatrix} 0 \\ S_{21} \delta p \\ S_{22} \delta p \\ S_{23} \delta p \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \delta S_{21} p \\ \delta S_{22} p \\ \delta S_{23} p \\ 0 \end{bmatrix}. \tag{20}$$

Since the weak equation for δw should hold for an arbitrary choice of the test vector ϕ, we are free to choose ϕ to simplify the resulting expressions. Therefore we set $\phi = \psi$, where the co-state vector ψ is the solution of the adjoint equation

$$\frac{\partial \psi}{\partial t} - C_i^T \frac{\partial \psi}{\partial \xi_i} = 0 \quad \text{in } D. \tag{21}$$

At the outer boundary incoming characteristics for ψ correspond to outgoing characteristics for δw. Consequently one can choose boundary conditions for ψ such that

$$n_i \psi^T C_i \delta w = 0.$$

Then, if the coordinate transformation is such that δS is negligible in the far field, the only remaining boundary term is

$$-\int\int_{B_W} \psi^T \delta F_2 \, d\xi_1 d\xi_3.$$

Thus, by letting ψ satisfy the boundary condition,

$$S_{21}\psi_2 + S_{22}\psi_3 + S_{23}\psi_4 = (p - p_d) \quad \text{on } B_W, \tag{22}$$

we find finally that

$$\begin{aligned} \delta I \quad &= -\int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i} \delta S_{ij} f_j d\mathcal{D} \\ &- \int\int_{B_W} (\delta S_{21}\psi_2 + \delta S_{22}\psi_3 + \delta S_{23}\psi_4) \, p \, d\xi_1 d\xi_3. \end{aligned} \tag{23}$$

Here the expression for the cost variation depends on the mesh variations throughout the domain which appear in the field integral. However, the true gradient for a shape variation should not depend on the way in which the mesh is deformed, but only on the true flow solution. In the final version of the paper, we show how the field integral can be eliminated to produce a reduced gradient formula which depends only on the boundary movement.

A. The need for a Sobolev inner product in the definition of the gradient

Another key issue for successful implementation of the continuous adjoint method is the choice of an appropriate inner product for the definition of the gradient. It turns out that there is an enormous benefit from the use of a modified Sobolev gradient, which enables the generation of a sequence of smooth shapes. This can be illustrated by considering the simplest case of a problem in calculus of variations.

Choose $y(x)$ to minimize

$$I = \int_a^b F(y, y') dx$$

with fixed end points $y(a)$ and $y(b)$. Under a variation $\delta y(x)$,

$$\begin{aligned} \delta I &= \int_a^b \left(\frac{\partial F}{\partial y} \delta y + \frac{\partial F}{\partial y'} \delta y' \right) dx \\ &= \int_a^b \left(\frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'} \right) \delta y dx \end{aligned}$$

Thus defining the gradient as

$$g = \frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'}$$

and the inner product as

$$(u, v) = \int_a^b uv dx$$

we find that

$$\delta I = (g, \delta y)$$

Then if we set

$$\delta y = -\lambda g, \qquad \lambda > 0$$

we obtain a improvement

$$\delta I = -\lambda (g, g) \leq 0$$

unless $g = 0$, the necessary condition for a minimum. Note that g is a function of $y, y^{'}, y^{''}$,

$$g = g(y, y^{'}, y^{''})$$

In the case of the Brachistrone problem, for example

$$g = -\frac{1 + y^{'2} + 2yy^{''}}{2\left(y(1 + y^{'2})\right)^{3/2}}$$

Now each step

$$y^{n+1} = y^n - \lambda^n g^n$$

reduces the smoothness of y by two classes. Thus the computed trajectory becomes less and less smooth, leading to instability.

In order to prevent this we can introduce a modified Sobolev inner product

$$\langle u, v \rangle = \int (uv + \epsilon u^{'} v^{'}) dx$$

where ϵ is a parameter that controls the weight of the derivatives. If we define a gradient $\overline{g}$ such that

$$\delta I = \langle \overline{g}, \delta y \rangle$$

Then we have

$$\begin{aligned} \delta I &= \int (\overline{g} \delta y + \epsilon \overline{g}^{'} \delta y^{'}) dx \\ &= \int (\overline{g} - \frac{\partial}{\partial x} \epsilon \frac{\partial \overline{g}}{\partial x}) \delta y dx \\ &= (g, \delta y) \end{aligned}$$

where

$$\overline{g} - \frac{\partial}{\partial x} \epsilon \frac{\partial \overline{g}}{\partial x} = g$$

and $\overline{g} = 0$at the end points. Thus $\overline{g}$ is obtained from g by a smoothing equation.

Now the step

$$y^{n+1} = y^n - \lambda^n \overline{g}^n$$

gives an improvement

$$\delta I = -\lambda^n \langle \overline{g}^n, \overline{g}^n \rangle$$

but y^{n+1} has the same smoothness as y^n, resulting in a stable process.

In applying control theory for aerodynamic shape optimization, the use of a Sobolev gradient is equally important for the preservation of the smoothness class of the redesigned surface and we have employed it to obtain all the results in this study. We refer the reader to numerous studies performed by the second author in the area of shape optimization for transonic and supersonic flows for a complete mathematical formulation and a wide variety of practical results.

IV. Design using the Equations of Linear Elasticity

Topological optimization is an important aspect in the design of engineering structures. Typically, an engineer is interested in the design of a structure with minimum weight while satisfying the compliance conditions with respect to the external loads, while satisfying the constraints on maximum allowable stress. This problem has been widely studied using a discrete adjoint formulation in conjunction with the use of a regularizing method that transforms the originally ill-conditioned integer optimization problem to one of continuous optimization. Thus the optimization problem can be written using a penalty function approach as

$$I(\sigma, \rho) = \int_D \rho dV + \alpha \int_D (\sigma(x^s) - \sigma_{max})\delta(x^s - x)dV$$

where ρ is the density at each point in the structural domain (D), α is the penalty parameter on the violation of the stress constraints, σ is the stress field in the domain, σ_{max} is the maximum allowable stress, δ is the kronecker delta function that enables the inclusion of a domain integral in the objective function for the pointwise stress constraints.

The constraint equations are the governing equations for linear elasticity

$$\frac{\partial \sigma_{ij}(u)}{\partial x_j} + f_j = 0$$

where f_j are the combined external and internal loads on the structure and u is the displacement field. The optimization problem can now be posed as follows,

$$\begin{aligned} &\min_{\rho} I(\sigma, \rho) \\ s.t. \quad &\sigma_{ij,j} + f_j = 0 \\ and \quad &0 \leq \rho \leq 1 \end{aligned} \tag{24}$$

Note that constraint equation is similar in form to the viscous operator for the Navier-Stokes equation. Proceeding in a manner similar to shape optimization for flow problems, we write the variation in the cost function as,

$$\delta I = \frac{\partial I}{\partial \sigma}\delta\sigma(u) + \frac{\partial I}{\partial \rho}\delta\rho$$

The variational form the constraint equations, $R(\sigma, \rho) = 0$, for an arbitrary test function ϕ, can be written as,

$$\int_D \phi \delta R(\sigma, \rho) = 0$$

where,

$$\delta R = \frac{\partial R}{\partial \sigma}\delta\sigma + \frac{\partial R}{\partial \rho}\delta\rho$$

. Here the dependence of the constraint equation on the control variable, ρ, is through the definition of the Young's modulus,

$$E(\rho) = \left(\frac{\rho}{\rho_0}\right)^{\beta} E(\rho_0)$$

This regularization enables ρ to vary smoothly between 0 and 1. Integration of the terms in the variational form of the constraint that contain terms corresponding to the variation in the stresses by parts can be written as

$$\int_B \phi \delta\sigma dB - \int_D \frac{\partial \phi}{\partial x_i}\sigma_{ij} dV$$

The first term represents an integral over the boundary of the domain and the test function on the boundary can be chosen to cancel the term in the variation of the cost function that depends on the variation in the stresses. The second term can be integrated by parts again after noting that

$$\sigma_{ij} = E(\rho)\frac{\partial u_i}{\partial x_j}$$

$$\int_B \frac{\partial \phi}{\partial x} E \delta u_i - \int_D \frac{\partial}{\partial x_i} E \frac{\partial \phi}{\partial x_j}$$

where the first term is identically equal to zero as the displacements are either prescribed as boundary conditions or as a compliance condition. The second term along with the boundary conditions on the test function along the boundary is the adjoint equation. It has a form similar to the constraint equation (as is well-known that equations of linear elasticity are self-adjoint) and can be solved using the FE procedure used to obtain the displacement field. The gradient can now be written as,

$$\int_D \left(1 - \phi^T \frac{\partial}{\partial x_i} \frac{\partial E}{\partial \rho} \frac{\partial u_i}{\partial x_j}\right) dV$$

Compared to the discrete adjoint formulation that starts with $Ku = f$, it appears that the adjoint equations, its boundary conditions and the gradient term are exactly similar.

Using this formulation, we use a freely available software, FEAP, from Robert Taylor at University of California at Berkeley and optimize the structural layout of a plate with different boundry conditions and loads. Figure 1 shows the optimized structural layout of aplte with pin-jointed ends and point load at the center. The red portions in the figure shows regions of high material density. It can be seen that the optimal topology that is similar to a truss-like structure. Figure 2 shows the optimal layout for a plate with clamped ends and point load in the middle. Again a truss like-layout is recovered by the optimization process.

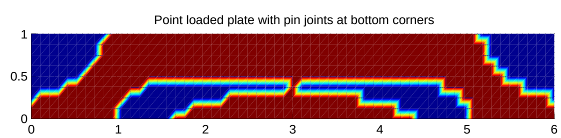

Figure 1. Optimal Topological layout of a plate with pin-jointed ends

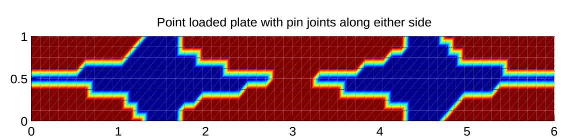

Figure 2. Optimal Topological layout of a plate with clamped ends

V. PDEs with Discontinuous State Transitions

There exists many areas of engineering where the constrained equation changes behavior and form in state and time. Eulerian models for transportation fleets and biological systems are common examples. As the state variables discontinuously change value when the PDE changes behavior, additional mathematical difficulties arise in the adjoint formulations due to the non-differentiable nature of the resulting weak form of the constraint equation and the gradients for the optimization problem. While similar problems exist for transonic shape optimization problems when shocks are present, the computational strategy that employs adjoints recovers meaningful designs.

Figure 3 shows the evolution of the state equation that has the form

$$\frac{\partial \rho}{\partial t} + c_i(t)\frac{\partial \rho}{\partial x} = 0$$

where ρ represents the density of cars over the interval in space, $c_i(t)$ is a constant that controls the speed of traffic at different instants in time. The numerical solution of this PDE has been obtqained using a SLIP construction to accurately capture the discontinuous nature in the evolution of the density of vehicles. The objective is to determine when to switch the speed of traffic so that the flux of cars is maximized. Figure 5 shows the flux of cars as a function of time illustrating the discontinuous nature of the functional to be maximized.

$$maxJ = max \sum_{i=1}^{2} \int_{t_{1_i}}^{t_{2_i}} \int_0^l \rho \, u \, dx \, dt$$

It is easy to see that the co-state equation has a similar form as the state equation, linear wave-equation like PDE. Figure 4 shows the evolution of the co-state equation for a given initial condition and the state equation that evolves according to figure 3.

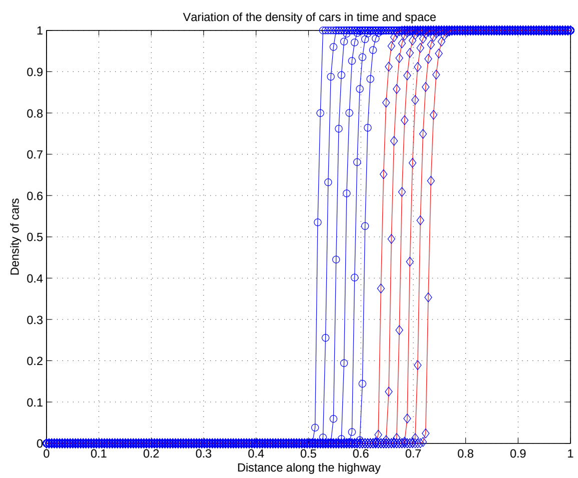

Figure 3. Evolution of the density of vehicles along the highway, $c_1(x) = \mathbf{1}$ $0 < x < 0.5$, $c_2(x) = \mathbf{1.5}$ $0.5 < x < 1.0$

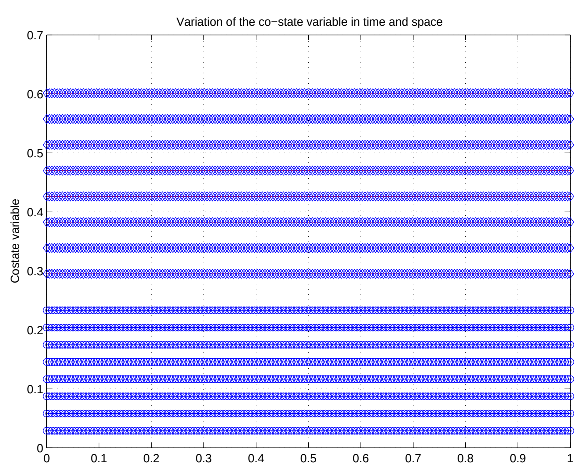

Figure 4. Evolution of the adjoint variable in time and space

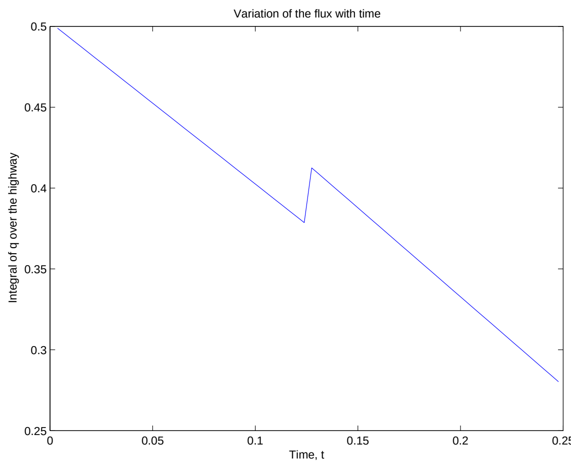

Figure 5. Discontinuous flux of vehicles

It is straight-forward to follow the procedure outlined for aerodynamic shape optimization to derive the gradient of the cost function with respect to the instant in time when the traffic flow switches from one speed to another. This is a simple problem where it is easy to see that to maximize the traffic flow through the interval in space, one would want to allow all traffic to pass through in the mode with maximum speed. Figure 6 shows that this is captured by the numerical procedure. The switching time gradually moves towards the final time as the first mode allows vehicles to travel at twice the speed.

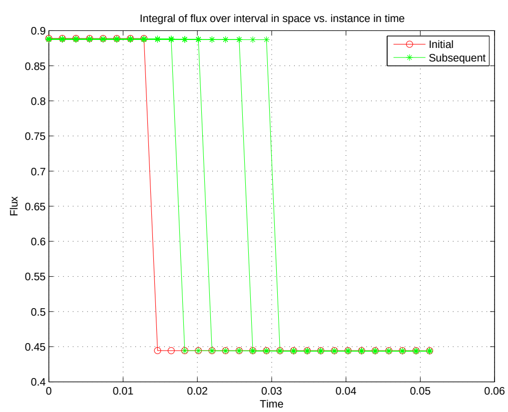

Figure 6. Evolution of flux during optimization

VI. Conclusions

The aim of this study was to take a closer look at the adjoint formulations for problems other than shape optimization for flow problems. We show that using the same frame-work, one can easily extend the adjoint technique to other PDEs. Towards this end, we have looked at other PDEs common in engineering systems and formulated adjoints and the corresponding gradients for them. This has been demonstarted for model problems in linear elasticity and traffic flow problems.

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