MULTIDISCIPLINARY INVERSE DESIGN

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Abstract. *A limited survey of multidisciplinary applications and various techniques for the solution of several classes of inverse problems as developed and practiced by our research team has been performed. Sketches of solution methods for inverse shape determination, boundary conditions determination, sources determination, and physical properties determination are presented from the fields of aerodynamics, heat transfer, elasticity, and electrostatics. Needs for development of new numerical algorithms have been outlined.*

Keywords: *Inverse Problems, Boundary Conditions, Thermoelasticity, Fluid Mechanics, Non-Destructive Evaluation, Physical Properties*

1. INTRODUCTION

If it is possible to provide governing equation(s), shape(s) and size(s) of the domain(s), boundary and initial conditions, material properties of the media contained in the field, and internal sources and external forces or inputs, then such a mathematically well-posed analysis problem is considered solvable. If any piece of this information is unknown or unavailable, the field problem becomes incompletely defined (ill-posed) and is of an indirect (or inverse) type (Kubo, 1993). The inverse problems can therefore be classified as determination of unknown shapes, boundary/initial values, sources and forces, material properties, or governing equation(s). If sufficient amount and type of additional information is provided, the inverse problems can become sufficiently specified so that with the use of appropriate algorithms they can be solved. The algorithmic methods for the solution of inverse problems could be grouped in two basic approaches: pure inverse methods and optimization-based methods. Following is a very brief survey of the solution methods for multidisciplinary inverse problems that have been researched in our Multidisciplinary Analysis, Inverse Design and Optimization (MAIDO)

Laboratory (Dulikravich et al., 1999).

2. SHAPE DETERMINATION INVERSE PROBLEMS

The problem of determining sizes, shapes, and locations of objects or cavities inside a given object can be solved only if certain quantity (pressure, heat flux, stress, magnetic field, etc.) can be specified on these unknown boundaries in addition to their complementary field quantities (velocity, temperature, deformation, electric field, etc.) on the same boundaries (Dulikravich, 1984; 1987; 1991; 1992; 1995; 1997; Fujii & Dulikravich, 1999; Tanaka and Dulikravich, 1998). .

2.1 Aerodynamic Shape Inverse Design

Two basic classes of tools for inverse aerodynamic shape design are: a) methods with coupled shape modification and flow-field analysis, and b) methods with uncoupled shape modification and flow-field analysis. Industry is interested only in such shape design methods that are equally applicable to both two-dimensional and three-dimensional arbitrary configurations and that can utilize existing proven flow-field analysis codes with minimum alterations needed. This means that any flow-field analysis code (a panel code, an Euler code, a Navier-Stokes code, or even surface pressures obtained from a wind tunnel testing) could be used in certain aerodynamic shape inverse design methods without a need for alterations of such an analysis tool. One such heuristic method treats the surface of a body as an elastic membrane that deforms under aerodynamic loads until it achieves a desired (target) distribution of surface pressure coefficient, Cp. This simple non-physical shape evolution model named MGM after its initiators (Malone et al., 1987) can be formulated as

$$\pm \beta_{ss} \frac{d^2 \Delta y}{ds^2} + \beta_s \frac{d\Delta y}{ds} \mp \beta_0 \Delta y = \Delta C_p \,, \tag{1}$$

where the upper signs correspond to the upper body contour, lower signs correspond to the lower body contour, s is the airfoil contour-following coordinate, Δy is the local shape correction, ΔCp is the local difference between the specified and actual coefficient of surface pressure, while βo, βs, and βss are the user supplied constants. Traditionally, the derivatives of Eq. (1) are evaluated using a finite differencing. Numerically integrating such discretized equation for shape corrections, Δy, is an extremely slow converging process when using non-linear flow-field analysis codes. This can be eliminated with a new formulation that allows a Fourier series analytical solution to the shape evolution equation (Dulikravich & Baker, 1999a, 1999b). The arbitrary surface distribution of ΔCp (the forcing function of Eq. (1)) can be represented via the Fourier series expansion as (in a 2-D example)

$$\Delta C_p(s) = a_0 + \sum_{n=1}^{n_{max}} \left[a_n \cos(N_n s) + b_n \sin(N_n s) \right] \tag{2}$$

where $N_n = \frac{2n\pi}{L}$ and L is the total length of the object's contour. The particular solution of Eq. (1) can be represented using Fourier series as

$$\Delta y_p = A_0 + \sum_{n=1}^{n_{max}} [A_n \cos(N_n s) + B_n \sin(N_n s)] \tag{3}$$

Substitution of Eq. (2) and analytical derivatives of Eq. (3) into the airfoil contour evolution equation (1) yields the analytic relationship among various coefficients

$$A_n = \frac{\pm a_n(\beta_0 + N_n{}^2\beta_{ss}) - b_n(\beta_s N_n)}{(\beta_0 + N_n^2\beta_{ss})^2 + (\beta_s N_n)^2}, n = 0,1,2,\cdots \tag{4}$$

$$B_n = \frac{\pm b_n(\beta_0 + N_n^2\beta_{ss}) + a_n(\beta_s N_n)}{(\beta_0 + N_n^2\beta_{ss})^2 + (\beta_s N_n)^2}, n = 1,2,3,\cdots \tag{5}$$

Then, the analytic solution for the correction of the airfoil contour is given by

$$\Delta y = Fe^{\pm\lambda_1 s} + Ge^{\pm\lambda_2 s} + \sum_{n=0}^{n_{max}} \left[A_n \cos(N_n s) + B_n \sin(N_n s)\right] \tag{6}$$

where the upper signs correspond to the upper contour and the eigenvalues are

$$\lambda_{1,2} = \frac{\beta_s \pm \sqrt{\beta_s{}^2 + 4\beta_0\beta_{ss}}}{2\beta_{ss}} \tag{7}$$

The unknown constants F and G can now be determined for the upper and lower airfoil contours such that zero trailing edge displacement, trailing edge closure, leading edge closure, and smooth leading edge deformation are satisfied. This shape inverse design method requires typically 10-20 calls to any unmodified three-dimensional flow-field analysis code to match the target pressures. This inverse shape design technique can be further improved by researching the ways to make the β coefficients as functions of the local surface pressure variations thus further accelerating its convergence.

Notice that this general formulation should be conceptually applicable to shape inverse design in other fields like elasticity, heat transfer, magnetism, electrostatics, etc.

2.2 Determination of Number, Sizes, Locations, and Shapes of Internal Coolant Flow Passages

During the past 17 years, our research team has been developing a unique inverse shape design methodology and accompanying software which allows a thermal system designer to determine the minimum number and correct sizes, shapes, and locations of coolant passages in arbitrarily-shaped internally-cooled configurations (Dulikravich, 1988; Dulikravich & Martin, 1996). The designer needs to specify both the desired temperatures and heat fluxes on the hot surface, and either temperatures or convective heat coefficients on the guessed internal coolant passage walls. The designer must also provide an initial guess of the total number, sizes, shapes, and locations of the coolant flow passages. Afterwards, the design process uses a constrained optimization algorithm to minimize the difference between the specified and computed hot surface heat fluxes by automatically relocating, resizing, reshaping and reorienting the initially-guessed coolant passages. All unnecessary coolant flow passages are reduced to a very small size and eliminated while honoring the specified minimum distances between the neighboring passages and between any passage and the thermal barrier coating if such exists. This type of computer code is highly economical, reliable, and geometrically flexible, if it utilizes the boundary element method (BEM) instead of finite element or finite difference method for the thermal field analysis. The BEM does not require generation of the interior grid and it is non-iterative. Thus, the method is computationally efficient and robust. The resulting shapes of coolant passages are smooth, and easily manufacturable. The methodology has been successfully demonstrated on coated and non-coated turbine blade airfoils, scramjet combustor struts, and three-dimensional coolant passages in the walls of rocket engine combustion chambers and axial gas turbine blades (Dulikravich & Martin, 1997).

2.3 Interior Void and Crack Shape Determination

The inverse determination of locations, sizes, and shapes of unknown interior voids subject to over-specified stress-strain outer surface field is a common inverse design problem in elasticity (Bezera & Saigal, 1993). Utilizing surface thermal boundary conditions (Dulikravich & Martin, 1993)) can also solve the void detection problem. The typical approach is to formulate a sum of least squares differences in the surface values of given and computed stresses or deformations (or temperatures or fluxes) for a guessed configuration of voids. This cost function is then minimized using any of the standard optimization algorithms by perturbing the number, sizes, shapes, and locations of the guessed voids. The process is identical to the already described inverse design of coolant flow passages subject to over-specified surface thermal conditions.

It should be pointed out that this approach to inverse detection of interior cavities and cracks could generate interior configurations that are non-unique.

3. BOUNDARY CONDITIONS DETERMINATION

A very common practical problem in any field theory is determination of the unknown boundary and initial conditions. Here, we will focus only on boundary conditions determination.

3.1 Determination of Steady Thermal Boundary Conditions

Determination of unknown steady thermal boundary conditions when neither temperature nor heat flux data are available on certain boundaries, is another common class of inverse problem. These unknown boundary conditions can be found if both temperature and heat flux are available on some other, more accessible boundaries or at a finite number of points within the domain. When using a BEM algorithm, let four vertices of a quadrilateral computational grid cell be designated with subscripts 1, 2, 3, and 4. Now assume that heat sources are known at all four vertices, at two vertices both temperature and heat flux are known, while at the remaining two vertices neither temperature or heat flux is known. The boundary integral equation then results in the following (Martin & Dulikravich, 1997).

$$
\begin{bmatrix} \tilde{h}_{11} & \tilde{h}_{12} & \tilde{h}_{13} & \tilde{h}_{14} \\ \tilde{h}_{21} & \tilde{h}_{22} & \tilde{h}_{23} & \tilde{h}_{24} \\ \tilde{h}_{31} & \tilde{h}_{32} & \tilde{h}_{33} & \tilde{h}_{34} \\ \tilde{h}_{41} & \tilde{h}_{42} & \tilde{h}_{43} & \tilde{h}_{44} \end{bmatrix} \begin{Bmatrix} \overline{\Theta}_1 \\ \Theta_2 \\ \overline{\Theta}_3 \\ \Theta_4 \end{Bmatrix} = \begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} \\ g_{21} & g_{22} & g_{23} & g_{24} \\ g_{31} & g_{32} & g_{33} & g_{34} \\ g_{41} & g_{42} & g_{43} & g_{44} \end{bmatrix} \begin{Bmatrix} \bar{q}_1 \\ q_2 \\ \bar{q}_3 \\ q_4 \end{Bmatrix} + \begin{Bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{Bmatrix} \tag{8}
$$

Coefficients of matrices [h] and [g] are easy to evaluate since they depend on geometric relations and the configuration is known. Then, moving all of the unknowns to the right-hand side and all of the known thermal quantities to the left-hand side results in

$$
\begin{bmatrix} \tilde{h}_{12} & -g_{12} & \tilde{h}_{14} & -g_{14} \\ \tilde{h}_{22} & -g_{22} & \tilde{h}_{24} & -g_{24} \\ \tilde{h}_{32} & -g_{32} & \tilde{h}_{34} & -g_{34} \\ \tilde{h}_{42} & -g_{42} & \tilde{h}_{44} & -g_{44} \end{bmatrix} \begin{Bmatrix} \Theta_2 \\ q_2 \\ \Theta_4 \\ q_4 \end{Bmatrix} = \begin{bmatrix} -\tilde{h}_{11} & g_{11} & -\tilde{h}_{13} & g_{13} \\ -\tilde{h}_{21} & g_{21} & -\tilde{h}_{23} & g_{23} \\ -\tilde{h}_{31} & g_{31} & -\tilde{h}_{33} & g_{33} \\ -\tilde{h}_{41} & g_{41} & -\tilde{h}_{43} & g_{43} \end{bmatrix} \begin{Bmatrix} \overline{\Theta}_1 \\ \bar{q}_1 \\ \overline{\Theta}_3 \\ \bar{q}_3 \end{Bmatrix} + \begin{Bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{Bmatrix} \tag{9}
$$

The entire right-hand side is known and it is rewritten as a vector of known quantities, {F}. The left-hand side remains in the form [A]{X}. Additional equations may be added if, for example, temperature measurements are known at certain locations within the domain.

In general, the geometric coefficient matrix [A] will be non-square and highly ill conditioned. Most matrix solvers will not work well enough to produce a correct solution. Singular Value Decomposition (SVD) methods (Press et al., 1992), are widely used in solving most linear least squares problems of this type. Thus, by using an SVD type algorithm, it is possible to solve for the unknown surface temperatures and heat fluxes simultaneously, very accurately, and non-iteratively.

A very useful by-product of inversely determining surface temperatures and heat fluxes is that these values can readily be used to accurately predict values of the convective heat transfer coefficients. Thus, rather than trying to evaluate the surface variation of the convective heat transfer coefficient using flow-field analysis, it is possible to treat the heat convection coefficient determination problem as an ill-posed boundary value problem of pure heat conduction in the solid that in contact with the moving fluid. Here, no thermal data is assumed available on parts of the boundary exposed to a moving fluid, while temperatures and heat fluxes are available on other boundaries or inside the solid. Once the thermal boundary values are determined on the boundary in contact with the moving fluid, the convective heat transfer coefficients can be determined from

$$
h_{conv} = -k \frac{\partial T}{\partial n}\bigg|_{\Gamma_{conv}} \Bigg/ \left(T\big|_{\Gamma_{conv}} - T_{amb} \right) \tag{10}
$$

Here, T_{amb} is considered as known (Martin & Dulikravich, 1998). When repeated for a variety of practical Biot numbers ($B_i = h_{conv}\, b/k$), this method was found to be reliable, and very fast, allowing realistic values of h_{conv} to be predicted in a few seconds on a standard PC.

The BEM was also used to solve the energy equation in a fluid flow where the velocity field is decoupled from the energy equation. It is sufficient to make an initial guess to the exit temperature and solve the Navier-Stokes equations for the velocity field (Dulikravich & Martin, 1996). Then, the steady BEM for the energy equation uses this velocity to non-iteratively solve for the temperature field in the fluid with the exit boundary partially or entirely unspecified. In order to compensate for the missing information, additional boundary conditions of heat flux can be over-specified at the inlet. The BEM will compute new temperatures on the exit boundary which can be iteratively applied to the flow-field analysis.

3.2 Determination of Steady Elasticity Boundary Conditions

An elastostatic problem is well-posed when the geometry of the general multiply-connected object is known and either displacement vectors, {u}, or surface traction vectors, {p}, are specified everywhere on the surface of the object. The elastostatic problem becomes ill posed when either a part of the object' s geometry is not known or when both {u} and {p} are unknown on certain parts of the surface. Both types of inverse problems can be solved only if both {u} and {p} are simultaneously provided at least on certain surfaces of the body.

Using the BEM, a system of algebraic equation can be formed for such inverse problems in elasticity that is similar to Eq. (8). Notice that each of the entries in the [h] and [g] matrices will be a 3x3 sub-matrix in the case of a three-dimensional elasticity. Additional equations may be added to the equation set if u measurements are known at locations within the solid in order to enhance the accuracy of the inverse steady boundary condition determination algorithm. The equation system can be rearranged similar to Eq. (9) and solved non-iteratively using an SVD type algorithm (Martin et al., 1994).

4. INTERNAL SOURCES DETERMINATION

Many field quantities can be generated by either continuously spatially varying or discretely distributed sources of those field quantities. Determination of these continuously distributed or discretely distributed quantities is often of significant practical interest.

4.1 Determination of Continuous Heat Source Distribution

A standard test case for any such inverse algorithm is finding the internal heat generation function distribution when provided with over-specified thermal boundary conditions. We used (Martin & Dulikravich, 1996) an annular disk geometry with axisymmetric boundary conditions, $T_{outer} = T_{inner} = 0$ and a constant value of the heat source function. This well-posed problem has an analytic solution. These analytical values of heat fluxes were then used as the over-specified boundary conditions on the outer and inner circular boundaries in order to predict the value of the heat generation field. When the annular domain was discretized with quadrilateral cells circumferentially, having only one cell between the outer and inner circular boundaries, the heat generation field was predicted with an average error less than 0.01%. Similar results were found when the heat generation field was linearly varying with radius.

But, when the domain was discretized with two or more radial rows of quadrilateral cells, the results produced errors that were, at worst, in error by about 30%. This is because the assembled BEM matrix had at least twice as many unknowns as it had equations. The results were significantly improved whenever internal temperature measurements were included in the analysis. For example, when the domain was discretized with two rows of quadrilateral cells, an addition of a single row of nine known internal temperatures produced results which averaged an error of less than 0.1%.

Further results have shown that whenever the temperature field is entirely known everywhere in the domain, the resulting solution matrix is both square and well conditioned. After inversion of this matrix, the unknown heat source vector can be found with an accuracy comparable to the well-posed (forward) problem, where this vector is known and temperature field is the objective of the computation (Martin & Dulikravich, 1996).

4.2 Determination of Electric Dipoles in Electro-Cardiography

It is important to recognize that inverse BEM formulation is especially suitable for the detection of point-wise, isolated sources like in the ill-conditioned inverse problem of electro-cardiography (Bates, 1997). The accuracy of a variety of the existing techniques for inverse electro-cardiography is still very low since these problems result in highly ill conditioned systems of equations. Concentric spheres with centrally located multiple electric dipoles were used to simulate a heart and a torso and to evaluate the accuracy of the inverse BEM algorithm. The objective was to determine the strength of each of the dipoles that generates the measured electric potential on the surface of the torso. Results indicate that the inverse BEM technique provides solutions of comparable or higher accuracy with less computational time than other techniques (Bates, 1997). But, they also show that equivalent cardiac source models with large numbers of dipoles are still unreliable for computation of the inverse problems of this type due to uniqueness considerations. That is, more than one possible combination of numbers, strengths, and orientations of the electric dipoles in the heart can create practically the same distribution of the electric potential on the torso surface.

5. PHYSICAL PROPERTY DETERMINATION

An increasingly important application of inverse methodology is determination of physical properties (thermal conductivity, electric conductivity, specific heat, thermal diffusivity, viscosity, magnetic permitivity, etc.) of the media. These properties could depend on certain field variables (temperature, pressure, density, frequency, etc.). Moreover, standards and regulations require that certain physical properties can be evaluated experimentally only by testing a specifically shaped, sized, and otherwise prepared material sample. Obviously, many applications do not allow the destruction of an object in order to extract such a sample. Thus, inverse determination of the physical properties is very popular in the non-destructive evaluation (NDE) community.

5.1 Determination of Temperature-Dependent Thermal Conductivity

This represents an inverse numerical procedure that differs substantially from the typical iterative approaches. It will be assumed that measured values of heat fluxes (or convection heat transfer coefficients) are available everywhere on the surface of an arbitrarily shaped solid. Kirchhoff's transformation is then used to convert the governing steady heat conduction equation into a linear boundary value problem that can be solved for the unknown Kirchhoff's heat functions on the boundary using the BEM. Given several boundary temperature measurements, these heat functions are then inverted to obtain thermal conductivity at the points where the over-specified temperature measurements were taken (Martin & Dulikravich, 1997).

The experimental part of this inverse method requires thermocouples and heat flux probes placed only on the surface of an arbitrarily shaped and sized specimen. Thus, this method is non-intrusive and directly applicable to field testing since special test specimens do not need to be manufactured. For steady-state problems, only one of each measurement device is needed for this methodology to work. This method could still use temperature measurements at isolated interior points if additional accuracy is desired. The method is inherently multi-dimensional and allows for temperature gradients in the test specimen.

The present method does not require that experimentally measured surface temperatures must be in equal temperature intervals. The present method also allows that convective heat transfer coefficients can be used instead of heat flux boundary conditions. This algorithm also accepts experimentally measured temperatures having same value, but measured at different boundary points.

Several different inversion procedures were attempted, including regularization, finite differencing, and least squares fitting with a variet of basis functions. The program was very accurate when the data was without error, and it did not excessively amplify input temperature measurement errors when those errors were less than 1-5% standard deviation. The program was found to be less sensitive to measurement errors in heat fluxes than to errors in temperatures. The accuracy of the algorithm was greatly increased with the use of *a priori* knowledge about the thermal conductivity basis functions.

It should be pointed out that in all applications and formulations that are briefly outlined in this paper, the inverse application of the BEM results in errors that are of the same order of magnitude as the errors in the over-specified boundary conditions (Martin & Dulikravich, 1996; 1997; 1999).

6. SIMULTANEOUS SOLUTION OF THERMO-ELASTICITY INVERSE PROBLEMS

The inverse problems of linear thermo-elasticity are created when both thermal and elasticity boundry conditions are unknown on some boundaries, while they are over-specified on some other boundaries, and regularly specified on the remaining boundaries. After similar algebraic manipulations like in the inverse BEM, it is possible to transform the original system of algebraic equations resulting from Finite Elements Method (FEM) into a system that enforces the over-specified boundary conditions and includes the unknown boundary conditions as a part of the unknown solution vector (Dennis & Dulikravich, 1999).

Three regularization methods and three solution strategies were applied separately to the solution of this system of equations in attempts to increase the method' s tolerance for the anticipated measurement errors in the over-specified boundary conditions.

The first method of regularization uses a constant damping parameter over the entire domain. This method can be considered the traditional Tikhonov method where the penalty term being minimized is the square of the L_2 norm of the solution vector. This will ultimately drive each component of the solution vector to zero, thus completely destroying the real solution. The second method of regularization uses a constant damping parameter only for equations corresponding to the unknown boundary values since the largest errors occur at the boundaries where the temperatures, fluxes, stresses, and deformations are unknown. The third method uses Laplacian smoothing only on the boundaries where the boundary conditions are unknown.

The efficient solution of the resulting linear system of algebraic equations is very challenging. The systems are sparse and often rectangular. The first solution strategy is to normalize the equations by multiplying both sides by the matrix transpose and solve the resulting square system with common sparse solvers. The resulting normalized system is less sparse than the original system, but it is square, symmetric, and positive definite. It is typically solved with a direct method (Cholesky or LU factorization) or with an iterative method (preconditioned conjugate gradient). Disadvantages are computation expense of matrix multiplication, the large in-core memory requirements, and the round-off error incurred during the matrix-matrix multiplication.

A second strategy is to use iterative methods suitable for unsymmetrical and least squares problems. One such method is the LSQR method, which is an extension of the well-known conjugate gradient (CG) method. The LSQR method and other similar methods such as the conjugate gradient for least squares (CGLS) solve the normalized system, but without explicit matrix-matrix multiplication. However, convergence rates of these methods depend strongly on the condition number of the normalized system, which is roughly equivalent to the square of the condition number of the original system.

The third strategy is to use a direct method for non-symmetrical and least square problems such as QR factorization or SVD. However, sparse implementations of QR or SVD solvers are needed to reduce the in-core memory requirements for the inverse FEM problems.

7. SUMMARY AND RECOMMENDATIONS

A number of different concepts and applications have been briefly exposed for formulating and solving a variety of seemingly unsolvable (ill-posed) problems. A common result of most of these analytical formulations and their discretized versions are highly ill-conditioned matrix problems. Boundary element methods typically result in dense ill-conditioned matrices and finite element methods typically result in sparse ill-conditioned matrices. Existing algorithms for solution of both types of ill-conditioned matrix problems are not sufficiently fast and accurate when applied to arbitrary multiply connected three-dimensional domains, unsteady problems, and especially multidisciplinary problems. Another persisting issue in the numerical solution of inverse problems is the control of numerical errors in the iterative solution methods. Thus, further innovative research is needed in the development of appropriate regularization concepts that do not deteriorate the accuracy of the solution and that are applicable to large initial and boundary data errors.

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