AN INVERSE METHOD FOR NON LINEAR ABLATIVE THERMICS WITH EXPERIMENTATION OF AUTOMATIC DIFFERENTIATION

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Abstract : Thermal Protection System is a key element for atmospheric re-entry missions of aerospace vehicles. The high level of heat fluxes encountered in such missions has a direct effect on mass balance of the heat shield. Consequently, the identification of heat fluxes is of great industrial interest but is in flight only available by indirect methods based on temperature measurements. This paper is concerned with inverse analyses of highly evolutive heat fluxes. An inverse problem is used to estimate transient surface heat fluxes (convection coefficient), for degradable thermal material (ablation and pyrolysis), by using time domain temperature measurements on thermal protection. The inverse problem is formulated as a minimization problem involving an objective functional, through an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient steepest descent method combined with quasi-Newton method computations) is then developed and applied, using Monopyro, a transient one-dimensional thermal model with one moving boundary (ablative surface) that has been developed since many years by ASTRIUM-ST. To compute numerically the adjoint and gradient quantities, for the inverse problem in heat convection coefficient, we have used both an analytical manual differentiation and an Automatic Differentiation (AD) engine tool, Tapenade, developed at INRIA Sophia-Antipolis by the TROPICS team. Several validation test cases, using synthetic temperature measurements are carried out, by applying the results of the inverse method with minimization algorithm. Accurate results of identification on high fluxes test cases, and good agreement for temperatures restitutions, are obtained, without and with ablation and pyrolysis, using bad fluxes initial guesses. First encouraging results with an automatic differentiation procedure are also presented in this paper.

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1. Introduction

The success of atmospheric re-entry missions is bound to the design of the Thermal Protection System (TPS) of the aerospace vehicles involved. The high level of heat fluxes encountered in such missions has a direct effect on mass balance of the heat shield. Consequently, the identification of heat fluxes is of great industrial interest but is in flight only available by indirect methods based on temperature measurements. A more detailed description of the problem can be found for instance in some publications on the Atmospheric Reentry Demonstrator (ARD) [1], [2]. The difficulty with flight data is that the uncertainty on the heat flux is coupled with an uncertainty coming also from the material (thermal properties for instance). In this contribution, we restrict ourselves to a supposed well known complex degradable material (with ablation and pyrolysis) and study in details the modeling and identification of thermal fluxes. A lot of studies on degradable materials can be found for pyrolysis and ablation processes and the corresponding applications, like on-ground validations with arc plasma torch, or various work on Thermal Protection Systems and reentry vehicles design. Many authors have already adressed the so-called Inverse Heat Conduction problem, and the estimation of fluxes from temperature measurements [3],[4],[5].

The inverse problem in this paper is concerned with the estimation of time domain surface heat fluxes convection coefficient, for thermally degradable material (ablation and pyrolysis processes), on a one-dimensional slab of thickness e, by using time domain temperature measurements on thermal protection, taken below the boundary surface, at thermocouple position x_0, during the time interval $0 \leq t \leq t_f$, where t_f denotes the final time. This inverse problem is formulated as a minimization problem involving a least square problem through an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient computations, [6]) is then applied and implemented for the optimal control theory on some industrial applications of inverse problems at EADS (European Aeronautics Defense and Space Company) [7].

2. Direct problem

For the direct problem, the Monopyro direct and inverse code, which was developed at EADS Astrium-ST Les Mureaux, is used. It is a transient one-dimensional thermal software with one moving boundary (ablative surface) to model complex chemical processes of simultaneous heating, ablation, pyrolysis, thermal degradation of materials [8][9][10]. The internal energy balance is a transient conduction equation with additional pyrolysis terms :

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \left[F_V + h_g - \int_{T0}^{T} A_1 dT\right]\frac{\partial \rho}{\partial t} + \frac{\partial(\dot{m}_g h_g)}{\partial x} \qquad (1)$$

with x the abscissa, t the time, T (x,t) the temperature, ρ (x,t) the specific mass, C_p the heat capacity, λ the thermal conductivity, F_v the pyrolysis gas formation heat, $\dot{m}_g$ the pyrolysis gas mass flow rate, h_g the pyrolysis gas enthalpy, A_1 a function of temperature T. The rate of storage of sensible energy is balanced by the net rate of thermal conductive heat flux, the pyrolysis energy-consumption rate and the net rate of energy convected by pyrolysis gas. The evolution of specific mass is given by a first-order rate process based on the Arrhenius equation :

$$\frac{1}{\rho_v} \cdot \frac{\partial \rho}{\partial t} = -\left(\frac{\rho - \rho_c}{\rho_v}\right)^{np} \cdot A \cdot e^{-\frac{B}{T}} \qquad (2)$$

ρ_c and ρ_v are the charred and virgin material densities, *A* the frequency factor in pyrolysis, *B* the fictitious temperature in pyrolysis, *np* the order of the reaction. The pyrolysis gas mass flow rate is related to the decomposition by the simple mass balance:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \dot{m}_g}{\partial x} \qquad (3)$$

Let *s* be the abscissa of the moving interface (ablation value), then $\dot{s}$ is the recession rate. The physical process can be splitted in three kinds of ablation: $\dot{s}_{meca}$ the mechanical recession rate, $\dot{s}_{chem}$ the chemical recession rate (most of the time a tabulated function), and $\dot{s}_{hy}$ the hydroerosion recession rate. The surface energy balance on the moving boundary takes the following form:

$$\alpha_0(h_r - h_w) - \varepsilon\sigma(T_w^4 - T_r^4) + \dot{m}_g\left[H_c - \eta_1(h_r - h_w)\right] + \dot{m}_c\left[H_v - \eta_2(h_r - h_w)\right] = \lambda\frac{\partial T}{\partial x} \qquad (4)$$

with α_0(t) the convection coefficient (unknown for the inverse problem), h_r the athermanous enthalpy, h_w the surface enthalpy, ε the total emissivity, σ the Stefan-Boltzmann constant, T_w the surface temperature, T_r the equivalent temperature, η_1 the pyrolysis gas blocking factor, H_c the pyrolysis gas heat combustion, $\dot{m}_c$ the ablation mass flow rate, η_2 the ablation gas blocking factor, H_v the ablation heat. The first term of equation (4) is the convective heat flux, the second one represents the heat loss by re-radiation of the surface. The third and fourth terms are the contributions of pyrolysis and ablation gas respectively. The right hand of (4) represents the rate of conduction into the TPS. Let $U = \begin{pmatrix} T \\ s \end{pmatrix}$ be the vector of temperatures *T* and ablation *s*, functions of time *t* and position *x*. The direct problem can be represented in condensed vector form by the following system of coupled nonlinear time domain evolution differential equations:

$$\frac{dU}{dt} = F(U) \quad T(x,0) = T_0 \quad s(x,0) = 0 \quad t \in \left[0, t_f\right], x \in \left[s(t), e\right] \qquad (5)$$

where $F(U)$ is a non linear operator and T_0 the reference initial temperature. The other physical quantities and variables described above are hidden in the formulation of F. Space partial derivatives are computed with a centered finite difference type scheme. The abscissa x belongs to the interval $[s(t), e]$. It is parameterized by a reduced scaled space variable $\xi \in [0,1]$ $x = (1-\xi)s(t) + \xi e$

The system (5) is rewritten relatively to the variables (t, ξ) with implicit Euler scheme and a constant time step Δt. Let *K* denote the number of one-dimensional grid points, *k* the space index, *N* the number of time iterations, *n* the time index in the numerical scheme, $u = (u^1, ..., u^N)$ the discrete direct state variables with the discrete vector $u^n = (T_1^n, T_2^n, \cdots, T_K^n, s^n)$ of dimension (*K+1*), T_m^n the discrete computed temperature at time *n*, at grid point m, s^n the discrete computed ablation, at time n. The equation (5) is written at time *(n+1) :*

$$\frac{u^{n+1} - u^n}{\Delta t} = f\left(u^{n+1}\right) \qquad u^0 = 0 \qquad 0 \le n \le N \qquad (6)$$

We make a linearization of the equation (6) at time *n* and after some calculations, we finally obtain a forward time discrete linearized Euler scheme, with initial vanishing condition. To solve the discrete matrix problem, we use an adapted sparse solver.

3. Inverse problem

The aim of the inverse problem in this paper is to estimate time domain surface heat fluxes (convection coefficient), for degradable material (ablation and pyrolysis), on a one-dimensional slab of thickness e, by using time domain temperature measurements $\theta(t)$ on thermal protection, taken below the boundary surface, at thermocouple position x_0, during the time interval $0 \leq t \leq t_f$, with t_f the final time. The inverse problem is formulated as a minimization problem involving a cost objective functional, through an optimization loop, requiring the computation of derivatives or gradients quantities and adjoint variables (optimal control formulation).

For a good accurate approximation of the gradient, the key strategy is to compute the exact gradient of the discretized problem, instead of applying a discretization scheme to the above systems of PDE-s. Let us consider that the time domain heat flux convection coefficient is represented by a vector $p = \left(p^1,..., p^N\right)$, where the subscripts refer to the sampled time. These sampled values are the *control parameter variables* for the optimization process. The quadratic error or cost function j(p), which measures the difference between model predictions T_m^n of temperature, given a heat flux parameter *p* value, and measurements temperatures θ_m^n, depending on the source parameters (p), is defined by :

$$J(p) = J\underbrace{\left(u^1(p),..., u^N(p)\right)}_{\text{var}\,iables\,U} = \frac{1}{2}\sum_{n=1}^{N}\left(T_m^n - \theta_m^n\right)^2 \Delta t \qquad (7)$$

To minimize this quantity, by optimization algorithm, we need to compute the derivatives of this least squares objective function J(p), with respect to the parameters p.

We introduce the adjoint state matrix $u^* = \left(u^{*1/2} \cdots ; u^{*N+1/2}\right)$ adjoint of the direct state u, $u^{*n+1/2}$ being a vector (K+1)*1, for all n=0,N. A Lagrangian formalism is used in the minimization of the functional *J(p)* because the estimated dependent variable $u(p)$ appearing in such functional *J(p)* needs to satisfy a constraint, which is the solution of the discrete direct problem. The governing equation of the direct problem, is therefore multiplied by the Lagrange multiplier, integrated in the space and time domains and added to the original cost functional *J(p)*. The Lagrangian *L* is :

$$\begin{aligned} L(p,u,u^*) &= L\left(\underbrace{p^1,..., p^N}_{parameter\ p}, \underbrace{u^1,..., u^N}_{\text{var}\,iables\,u}, \underbrace{u^{*1/2},..., u^{*N+1/2}}_{adjo\text{int var}\,iables\,u^*}\right) \\ &= \sum_{n=1}^{N}\left(T_m^n - \theta^n\right)^2 \Delta t + \sum_{n=0}^{N-1}\left\langle u^{*n+1/2}, \frac{u^{n+1} - u^n}{\Delta t} - f\left(u^n\right) - (df)\left(u^n\right)\left(u^{n+1} - u^n\right)\right\rangle \end{aligned} \qquad (8)$$

Differentiating the Lagrangian *L* with first order variations $\delta p, \delta u, \delta u^*$, the variations of δL with respect to δu are cancelled with an adequate choice of the adjoint state u^* (saddle point condition). It leads to the discrete adjoint system in $u^{*n-1/2}$ unknown, *n* going backward from N to 0,

$$\begin{aligned} &\frac{u^{*n-1/2} - u^{*n+1/2}}{\Delta t} = df^t\left(u^{n-1}\right)u^{*n-1/2} + \left[\left(d^2 f\right)\left(u^n\right)\left(u^{n+1} - u^n\right)\right]u^{*n+1/2} + \left(T_m^n - \theta_m^n\right)\Delta t \\ &u^{N+1/2} = 0 \qquad N \geq n \geq 0 \end{aligned} \qquad (9)$$

With this particular choice of u^*, the gradient of the cost function is simply obtained by :

$$\nabla J = \frac{\partial J}{\partial p} = \frac{\partial L}{\partial p} = \sum_{n=0}^{N-1} \left\langle u^{*n+1/2}, -\frac{\partial f}{\partial p}\left(u^n\right) - \frac{\partial df}{\partial p}\left(u^n\right)\left(u^{n+1} - u^n\right) \right\rangle \qquad (10)$$

Gradient expression is a combination of direct and adjoint discrete quantities. Once the gradient of cost function is computed, we can apply an iterative inverse minimizing procedure to *J(p)* to obtain an estimation of the optimal parameter p_{opt}. We use a combination of a gradient steepest descent method at the beginning of minimization and a Quasi Newton method [11] at the end.

4. Inverse problem computation using automatic differentiation

To compute numerically the adjoint and gradient discrete quantities for the inverse problem in heat convection coefficient, we have also used the Automatic Differentiation (AD) engine tool, Tapenade, developed at INRIA Sophia-Antipolis by the Tropics team [12]. Automatic differentiation is a family of techniques for computing the derivatives of a function defined by a computer program, for sensitivity and gradient analysis applications [13]. The derivatives of the instructions of a program are combined with chain rules of differential calculus, leading to major modes of computing derivatives with AD, the forward (tangent-linear) mode and reverse (cotangent-linear or adjoint) mode.

- The forward mode uses derivatives on a given vector in the input space (tangent approach. It is appropriate to derive functions with small numbers of independent variables (input).
- The reverse mode uses derivatives starting with the dependent variables (output) and proceeding toward the independent variables (input), and it is computed in the reverse of the original program's order. It is appropriate for functions with small numbers of dependent variables (output) and lots of input independent variables. The reverse mode of automatic differentiation is functionally equivalent to hand written discrete adjoint codes.

The implementation of robust automatic differentiation tools offers advantages to be accurate and to reduce software costs: automatic differentiation eliminates the time spent developing and debugging derivative code by hand, or with experimenting step sizes for finite difference approximations.

These techniques have been applied to our inverse thermal problem, considering the flow of instructions in the direct program (Monopyro direct code). The final output of the program is the discrete cost function $J(p) = J(u(p)) = J((u^1,...,u^N)(p))$. The adjoint code in u^* variables is built by automatic backward differentiation of the output J versus u direct state variables, following and analyzing the flow of instructions in the direct program, and the dependences in u. The gradient computation of $J(p)$ versus p parameter is built by automatic backward differentiation of the output $J(p)$ versus p parameter, also following the flow of instructions in the direct and adjoint programs.

5. Numerical results

We now present some applications of this inverse problem of estimation of time domain surface heat convection coefficient for a thermally degradable material, on a one-dimensional slab of thickness *e*, by using time domain temperature measurements taken below the boundary surface, at a given thermocouple position, during a time interval $[0, t_f]$. The final time is denoted by t_f.Theses tests have been carried out for the problem of fluxes identification on a carbon/resin material. We first tried to examine the effects of pyrolysis (test 1), ablation (test 2) separately, then we applied the new method to operationnal cases, such as the ARD (Atmospheric Reentry Demonstrator, test 3 with a different material: alestrasil). For test 1 and test 2, we used synthetic data (errorless measurements).

Test 1 : Identification of Virgin material flux : without ablation , pyrolysis,, x0=1.3 mm

We start (INI) with a bad initial guess, half the value of the convection coefficient used to generate the synthetic data, with sharp discontinuity. Figure 1 shows a good agreement for the reconstruction (NUM) of the convection coefficient, compared to the reference convection coefficient (OBS). This good result (except near the final time) is obtained with the inverse code developed in section 4 (Automatic Differentiation tool was used). The RMS error on the flux is 0.04. Near final time, the value of the estimated flux has very little influence on the temperature in the material, at x0 and is all the more difficult to compute accurately.

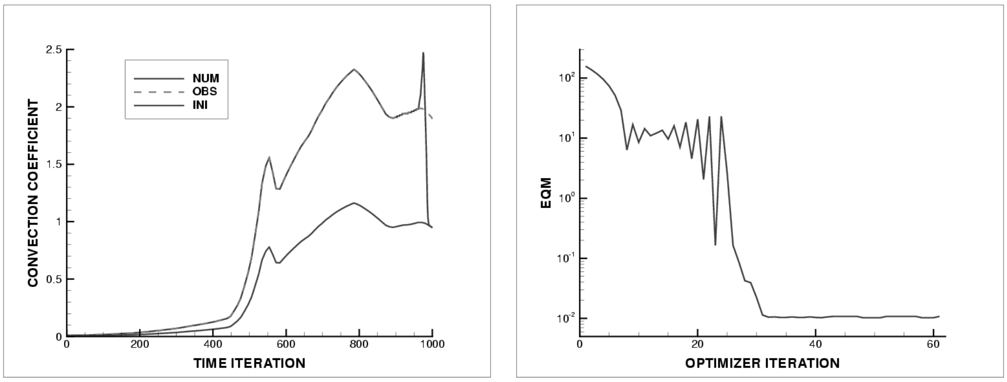

Figure 1.Flux Identification ; Temperature RMS error Automatic Differentiation tool
Test1 : Virgin material : without ablation , pyrolysis, x0=1.3 mm

Figure 1 shows also that the RMS error on temperature obtained at the end of optimization process is very low (0.01), and we can observe the change in optimizer (iteration 25), switching from gradient steepest descent at the beginning, to Quasi Newton after. The gain in convergence is promising, after 60 optimizer iterations.

Test 2 : Identification of High Flux with ablation, Carbon/Resin material , x0=2.6 mm

It is a quite difficult test case, with high fluxes. In figure 2, a good agreement in the reconstructed convection coefficient value is observed, except at final time, with an initial guess of half the expected value and using synthetic data (errorless measurements). The RMS error on the flux is 0.06 and RMS error on measured temperature obtained at the end of optimization process is very low (0.7), after 70 optimizer iterations.

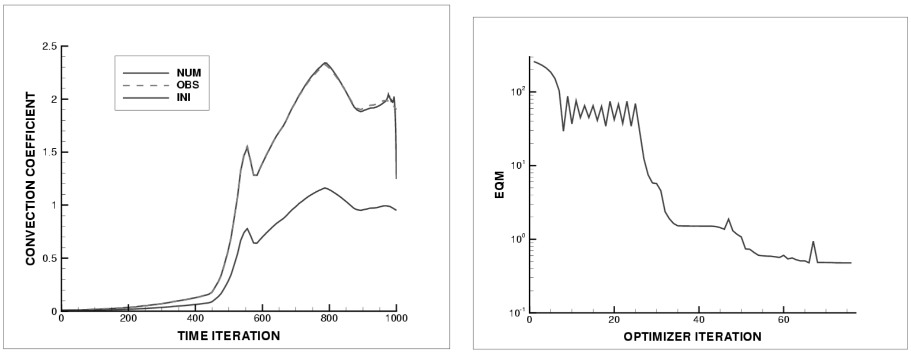

Figure 2. Flux Identification ; Temperature RMS error
Test 2 : Identification of High Flux with ablation, x0=2.6 mm

Test 3 : ARD Test case

We examine the inverse analysis approach for the ARD flight test case. The Atmospheric Reentry Demonstrator (ARD) was a suborbital reentry test flown on the third Ariane 5 flight. ARD was launched in october 1998 from Kourou, French Guyana, by an Ariane 5. It was recovered and transported in EADS Astrium Aquitaine plant for expertise (Figure 3). More than 200 different parameters were recorded during flight. After ARD recovery, a preliminary analysis of recorded data was performed. Successful results are obtained in the reconstructed flux (Figure 4), which are very similar to those obtained before.

Figure 3. ARD heat shield

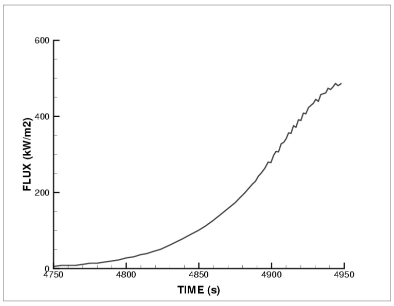

Figure 4. ARD heat flux restitution

6. Conclusion

Motivated by atmospheric re-entry of aerospace vehicles and Thermal Protection System dimensioning problems, this article is concerned with inverse analyses of highly dynamical heat fluxes. It addresses the inverse problem of using temperature measurements to estimate the heat flux (convection coefficient), at the surface of ablating materials. Several validation test cases, using synthetic, noisy on-ground and in-flight data temperature measurements are carried out, by applying the results of the minimization algorithm. Main results are:

- Validity of the inverse formulation for the temperature and ablation variables evolution
- Improvement by using a combined gradient steepest descent method at the beginning of minimization process and Quasi Newton method to finish the minimization,
- Convection coefficient restitution has been improved for hard cases (with great ablation) for fluxes functions containing sharp corners and discontinuities,
- Successful test case on carbon/resin material with high heat fluxes and large magnitudes, ablation and pyrolysis effects, and on operational data,
- Encouraging results with an automatic differentiation tool are also obtained, without ablation

Future works have to be done on the:

- Robustness to initial guess, sensitivity to measurements, number and position of sensors, and application of regularization methods to stabilize noise errors on measurements,
- Validation of the automatic differentiation tool used to generate the inverse code, especially for ablation test cases,
- Thermal model uncertainties influences on the accuracy of identified flight heat flux, athermanous enthalpy identification,
- Validations on aerothermal flight measurements.

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