New graphical user interface for an application to assist solution analysis with optimization of the 1D inverse heat conduction problem

Nueva interfaz gráfica de usuario para una aplicación de asistencia del análisis de solución con optimización del problema inverso de conducción de calor 1D

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Abstract

Computer applications facilitate the analysis of large amounts of information. Currently, its development is a frequent activity for various fields of knowledge. Especially for those systems under study that require optimization processes to obtain precise answers to the solution of some approach. The answers must be reliable and offered at an increasingly higher speed since decisionmaking may depend on them. In particular, inverse analyzes are into these concepts. These approaches are illconditioned, so the control efforts are robust and complex to guarantee a unique solution. Some techniques are known, but new proposals will develop. In analyzing phenomena in materials, the solution to heat transfer problems helps improve the performance of the components manufactured with them. Therefore, to understand thermal phenomena, proposals for controlled experiments are developed. Where complicated working conditions can be implemented to the extent of mastery of the solution scope of mathematical formulations, in this work, an example is presented a whose analysis of results is successfully accepted. Likewise, a platform is established to evolve to more demanding systems.

Inverse problems, Optimization, Heat conduction, Computer application

Las aplicaciones computacionales facilitan el análisis de grandes cantidades de información. Actualmente, su desarrollo es una actividad frecuente para aquellos sistemas bajo estudio que requieren de procesos de optimización para obtener respuestas precisas a la solución de algún planteamiento. Las respuestas deben ser confiables y ofrecerse a una velocidad cada más más alta puesto que de ello puede depender la toma de decisiones. Los análisis inversos se integran en estos conceptos. Estos planteamientos se definen como mal condicionados y por lo tanto los esfuerzos de control son robustos y complejos para garantizar la aproximación a una solución única. Algunas técnicas son ya populares, pero continúan desarrollándose nuevas propuestas. En el ámbito de análisis de fenómenos en materiales, la solución de problemas de transferencia de calor ayuda a mejorar el desempeño de los componentes manufacturados con ellos. Por lo tanto, para comprender fenómenos térmicos se desarrollan experimentos controlados, donde pueden implementarse diversas condiciones en la medida del dominio del alcance de solución de formulaciones matemáticas correspondientes. En este trabajo se presenta un ejemplo cuyo análisis de resultados se acepta exitosamente y se establece una plataforma para evolucionar a sistemas más demandantes.

Problemas inversos, Optimización, Conducción de calor, Aplicación computacional

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Introduction

The formulation of inverse problems is defined as ill-conditioned mathematical problems. Therefore, they generally require applying specific mathematical techniques that ensure the stability of the solution method and its uniqueness.

The previously disclosed work Apud (Téllez-Martínez, Hernández Morales, Rodríguez Ortíz, & Barraza Fierro, 2018) that the methods for solving the inverse heat conduction problem (IHCP) are classified into classic and recent. Within the classical methods, the sequential function specification method (SFS) stands out for its efficiency (Beck, Litkouhi, & St. Clair, 1982). The latest methods Apud (Gadala & Vakili, 2011) are called: 1) Genetic Algorithm (GA), 2) Particle Swarm Optimization (PSO), and 3) Artificial Neural Networks (ANN). The applicability analysis in materials characterization establishes that for conditions where the dependence of physical properties on temperature tends to be nullified, even with noise in the source data, great precision is obtained with contemporary techniques. Notwithstanding, the computation time is relatively much longer.

Since temperature dependence is inherent for thermal analysis in materials of interest in manufacturing processes (nonlinearity of the governing equations), the SFS technique continues to offer high efficiency. In this way, reliable answers can be obtained by controlling the solution optimization parameters of the mathematical formulations and applying appropriate data mining. The SFS technique was Op. Cit Beck and evaluated in multiple works to date Apud (Beck, Blackwell, & Haji-Sheikh, 1996) (Blanc, Raynaud, & Chau, 1998) (Krzysztof, 2011). Several computer applications have been developed, such as the one presented Apud (Meekisho, Hernandez-Morales, Tellez-Martinez, & Chen, 2005) named *WinProbe*.

A graphical user interface was available on the Microsoft Windows 98 platform in the original version. It was possible only to analyze cooling curves obtained from measurements inside metal alloy specimens. Subsequently, the Visual Basic 6.0 environment was used to create a composite application between Visual Basic and Fortran 77 applications. The analysis with this IHCP solution was incorporated with limited conditions for the specification of parameters and the ability to visualize data. The update of the operating system of the current computers involved the renewal of the IHCP solution code, eliminating some data processing features that are optimally mastered with office tools. Likewise, the design of a clean interface with crucial functions for analyzing a large amount of data began; that could even be adapted to the operating systems of mobile or portable devices such as tablets or smartphones. Such availability could evolve to real-time analysis systems during some physical processes (Hernández-Morales, Cruces-Reséndez, & Téllez-Martínez, 2018).

Development

Through the Visual Studio Express 2017 tool, the IHCP 1D radial solution algorithm for the cylinder problems: 1) hollow and 2) solid was coded entirely in the Visual Basic language. The structure of the computational work is summarized as follows:

- a) Revision of the solution algorithm of the IHCP 1D radial for problems posed in a transitory state.
- b) Approach the optimization of the solution by implementing a selection criterion for the stabilization parameter of the solution using the sequential function estimation method (SFS) for each calculation step.
- c) Programming and debugging the IHCP solution code, designing a friendly graphical user interface to introduce essential data for each case study.
- d) Verification of the code carrying out several executions with data of cooling processes derived from solutions to problems raised directly.

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e) Use the computer application with recorded data of a physical test using the previous and updated version.

In Fig. 1, the optimization circuit is expressed within the calculation circuit of the temperature field variable as a result of the estimation of the thermal boundary condition function C.F.2. on the outer surface at parent time. In this regard, the problem of temperature distribution in the proposed systems is defined in Figs. 2(a) and 2(b). Each scheme represents a differential portion of the solid of radius $r = R$ in which the symmetry condition coincides with the axial axis z . In the case of the hollow cylinder, the interior boundary condition $q_1(t)$ at $r = r_i$ is specified in the pre-processing.

According to the procedure of Fig. 1, a virtual value of q_2 is defined at each time step t and the Direct Heat Conduction Problem (DHCP). The problem is solved to obtain the temperature value Y_j , which, together with the source value Y_j , is evaluated in the IHCP optimization problem to estimate a new value of the boundary condition \hat{q}_2 that satisfies the heat balance. The DHCP approach is solved in this last datum, and the calculated temperature \hat{Y}_j is compared with the source value Y_j . Finally, if optionally specified by the user, the value of the stabilization parameter l is increased by one unit, and the difference in the result of this new solution is analyzed against an error magnitude criterion. If the error decreases, the calculation procedure is performed again, increasing the value of l ; otherwise, the previous result is kept.

Figure 1 Schematic procedure for the development of data generation and its analysis

Source: Own elaboration [MS Word LTSC Pro Plus 2021]

Figure 2 Schematic representation of the axisymmetric systems of a) solid cylinder and b) hollow cylinder for the IHCP 1D radial approach *Source: Self-Made [MS Word LTSC Pro Plus 2021]*

As already mentioned, the thermophysical properties: thermal conductivity and thermal capacity of the material, k and C_p , respectively, are temperature dependent. The mathematical formula that governs the heat transfer for the approach of the direct problem for the case of Fig. 2(a) can be defined as:

$$
\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) = \rho C_p \frac{\partial T}{\partial t}, \qquad 0 \le r \le R, \qquad t > 0 \tag{1}
$$
\n
$$
\frac{\partial T}{\partial T} \Big|_{t=0} \qquad 0 \le r \le R, \qquad t > 0 \tag{2}
$$

$$
\left. \frac{\partial^2 F}{\partial r} \right|_{r=0} = 0, \qquad -kr \left. \frac{\partial^2 F}{\partial r} \right|_{r=R} = q(t) \tag{2}
$$

$$
T(r,T) = T_0, \qquad 0 \le r \le R, \qquad t > 0 \quad (3)
$$

Where the Greek letter ρ represents the density of the material that is defined as constant, on the other hand, the IHCP approach is formulated similarly to DHCP with changes in equations (2) and (3), such that:

$$
\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0, -kr \frac{\partial T}{\partial r} \Big|_{r=R} = q(t) = \lambda
$$
 (4)

$$
T_j = (r_j, t_i) = \hat{Y}_j, \qquad j = 1, 2, ..., n,
$$

$$
i = 1, 2, ..., M
$$
 (5)

Where i represents the number of elapsed time steps or time index until the current calculation step M in the temporal analysis interval of the thermal phenomenon.

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The only difference with the formulation of the system problem statement in Fig. 2(b) is the definition of the boundary condition C.F.1. Equation (6) establishes this change.

$$
-kr\frac{\partial T}{\partial r}\Big|_{r=r_i} = q(t) \tag{6}
$$

The IHCP optimization problem is formulated as:

$$
q_M = q_{M-1} + \frac{1}{\Delta M} \left[\sum_{l=1}^{L} \sum_{j=1}^{n} (Y_{j,M+l-1} - \widehat{Y}_{j,M+l-1})^2 \right] (\widehat{Y}_{j,M+l-1;q}) \tag{7}
$$

With:

$$
\Delta M = \sum_{l=1}^{L} \sum_{j=1}^{n} (\hat{Y}_{j,M+l-1;q})^2, \hat{Y}_{j,M+l-1;q} = \frac{\hat{Y}_{j,M+l-1}}{\partial q_M}
$$
(8)

 l is the index that defines the number of discrete temperature data at time instants after calculating instant M . This datum allows for the solution's stabilization to estimate the thermal boundary condition.

The term $\hat{Y}'_{(j,M+l-1;q)}$ represents the values of the variable called sensitivity coefficient, which is obtained by deriving equations (1) to (3) concerning the variable q calculated.

About the characteristics of the graphical user interface, the application will be based on the stages of the computational simulation process and the verification of results.

Pre-processing. Creation of a friendly interface for a compendium of necessary data through the groups with a logical sequence of information definition assisted by a tabular control according to the following items:

- *Dimension:* Set the magnitude of the radius of a cylindrical structure as the analysis dimension.
- *Material:* Selection of material for the specification of thermophysical properties for the IHCP solution, implementing the functionality of generating new databases and eventually deleting them.
- *Discretization*: Establish information related to the partition of the model according to the approach of the numerical solution of the mathematical formulation of the one-dimensional IHCP in cylindrical coordinates.
- *Thermal history*: Establish the reference to thermal history data recorded by physical means in a specific position inside the cylindrical specimen.
- *Boundary condition*: Define the function that establishes heat source or extraction on a hollow cylinder's internal surface.
- *Processing parameters*: Establish the conditions of the stabilization parameter of the IHCP solution (number of future time steps), defined by the optimization characteristics of the SFS technique.

Processing. The 1D IHCP solution algorithm in cylindrical coordinates was coded and optimized by defining the number of discrete temperature data l as:

- A constant value throughout the calculation process.
- A self-adjusting value based on the residual errors obtained throughout the calculation process.

Post-processing. Create spreadsheet analysis databases by writing to files with text format delimited by space.

Results

The graphical user interface development work is shown in Figs. 3 to 9. According to the data specification items defined for pre-processing, the access structure by tabulation to each information group is determined.

Figure 3 Section of the form for the selection of the system a) cylinder and b) concentrically bored cylinder *Source: Own elaboration [Formatted screenshot in MS Paint]*

Figs. 3 (a) and (b) show screenshots of the form for entering information related to the dimensional characteristics of the system to be evaluated.

Figure 4 Section of the form specifies the analyzed material, a) from an existing list or b) defining data *Source: Own elaboration [Formatted screenshot in MS Paint]*

The following section, from left to right, corresponds to the designation of the material. It can be selected from a list, as evidenced in Fig. 4(a), if it is already defined. Otherwise, it can be specified to create a custom database.

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The position specification fields for the known thermal history are defined for discretization. The generation of control volumes, before and after this virtual border, for the solution of the system of equations by applying the finite difference method concerning the corresponding formulation of the differential equations that govern the thermal phenomenon. Figs. 5(a) to 5(c) show that focusing on each text box; an image is displayed that supports the definition of the requested data.

Likewise, at least one thermal history necessary for the solution of the IHCP can be specified through the following tabulation. The file can be created in MS Excel or structured as a comma delimited text file (.csv format). Fig. 6 shows a screenshot of the interface that establishes the source file search procedure through the standard Windows wizard.

Figure 5 Section of the form to define the discretization structure from a virtual frontier that establishes: a) the position where the thermal history in the material is known, b) the number of control volumes from the outer surface, and c) the number of volumes controlled to the inner surface

Source: Own elaboration [Formatted screenshot in MS Paint]

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Figure 6 Data loading procedure of at least one thermal history for the IHCP solution using the standard tools for searching and opening files in MS Windows

Source: Own elaboration [Formatted screenshot in MS Paint]

As already defined in the problem statement with hollow cylinders, the specification of the thermal boundary condition on the inner surface is required. Currently, the application is limited to the constant heat flux value specification. The data can be uploaded in the corresponding form section (refer to figure 7).

Figure 7 Data loading procedure of at least one thermal history for the IHCP solution using the standard tools for searching and opening files in MS Windows

Source: Own elaboration [Formatted screenshot in MS Paint]

Finally, to conclude the pre-processing process and establish the characteristics of the execution of the stabilization parameter of the solution, the number of discrete temperature data is captured in instants of time after the instant of calculation, or the number of time steps future, through the last tab in the form. Establish a maximum limit value up to which it will be increased sequentially according to the tolerance of the estimated error. As shown in the image in Fig. 8, the value can be fixed or allow an autoadjustment during the calculation.

Source: Own elaboration [Formatted screenshot in MS Paint]

Once the information has been entered, the coded solution algorithm is executed through the *Process* button. As a result, plain text files with a defined format are obtained for analysis using spreadsheets. Result files are stored in the folder where the run file is located. The files: CTI.txt, CXI.txt, IHCP.txt, and PerfHist.txt, contain the information corresponding to the calculations of the thermal fields and sensitivity coefficients, the thermal boundary condition, and the temperature distribution by each control volume for each instant.

The solution algorithm was verified by posing the solution of a direct problem with known thermal boundary conditions for a solid cylinder. Subsequently, following the procedure expressed in Fig. 1, the boundary condition was estimated and compared against the known one. The acceptable results allowed the application to be used to process the thermal history of an experimental system with the same geometric characteristics. Graphic 1 shows the plot of the thermal history (continuous blue line), as well as those obtained by solving the IHCP using the old code (continuous red line) and the updated code (continuous black line). It can be seen in the plot of the curves that there are no significant differences that object to calculation errors with the new code.

Graphic 1 Thermal history of: a) the experimental source (blue line) and calculated using the IHCP solution by: b) with the old code (red line) and c) with the new code (black line)

Source: Own elaboration [MS Excel LTSC Pro Plus 2021]

In the Graphic 2, the percentages of deviation of the thermal history are calculated in the IHCP solution using a value $l = 2$ and an auto-adjustable value with a maximum of 10. It can be noted that with the implementation of the self-adjustable value for the number of future time steps, the deviation from the target temperature is reduced, especially in the critical cooling stage, which occurs between 20 and 30 seconds. Adjustments of the value of the number of future time steps are shown together with the magnitude of the estimated residual error in Graphic 3. It can be noted that the estimated error curves (residual) are a picture of the percentage deviation. The same results are obtained for the calculation with the old code and the new code for $l = 2$. While for a selfadjustable calculation process, a difference is presented concerning the previous ones in which the residual curve always has minor values.

Graphic 2 Percent deviation of the thermal histories calculated by solving the IHCP with the experimental thermal history for the number of future time steps: a) fixed and equal to 2 (dashed line), and b) self-adjusting to a maximum of 10 (continuous line)

Source: Own elaboration [MS Excel LTSC Pro Plus 2021]

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Graphic 3 Magnitude of the error (residual) for the IHCP solution calculations considering a value of 2 for the number of future time steps (l) . The old code (dotted line) and the new code (dashed line), compared to the result of a self-adjusting value (continuous line). Note the autoadjusted value of l during the calculation process (solid red line)

Source: Own elaboration [MS Excel LTSC Pro Plus 2021]

Finally, Graphic 4 shows the shape of the function of the estimated thermal boundary condition $q_2(t)$.

The differences between the calculations of the heat flux density for the IHCP solution are insignificant for the cases of $l = 2$ with respect to the self-adjusting l . However, the global minimum value of the function represents a critical fact since, around that moment, the maximum cooling rate is established in the solid cooling process. For some physical systems, this condition is critical and should be known as possible. In this sense, the self-adjustable curve represents the best $q_2(t)$ estimate.

Graphic 4 Function of the estimated boundary condition with a value of 2 for the number of future time steps (l) . The old code (dotted line) and the new code (dashed line), compared with the result of a self-adjusting value (continuous line)

Source: Own elaboration [MS Excel LTSC Pro Plus 2021]

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Conclusions

In updating the *WinProbe* application, the algorithm encoded in the Visual Basic language for the solution of the radial 1D inverse heat conduction problem (IHCP) performs calculations correctly and efficiently according to the nature of the sequential specification technique of the function (SFS). In the creative process of the graphical user interface, the requirements of the pre-processing stage and organization of the information are calculated for post-processing, corresponding to the systems of interest for research purposes on controlled experimentation and impact on teaching.

The incorporation of the stability criterion of the solution through the selfadjusting number of future time steps allows the estimation error to be reduced and establishes a criterion of low uncertainty in the uniqueness of the IHCP solution for the estimation of a single function of the thermal boundary condition.

Several mathematical formulations of physical cases can be proposed for solutions to the IHCP. Future work in this regard will consist of implementing them and continuing to modify the algorithm with variants in the optimization criteria.

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