Numerical simulation of a nonlinear problem modeling the cooling of a metal

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Abstract. In this work, the finite difference method was used to calculate the heat distribution during cooling by the boundary part of a cylindrical material subjected to high temperature. A mathematical model of the process was formulated using cylindrical coordinates. The heat transfer coefficient occurring in the Robin condition at the cooled boundary is nonlinear. We use quasi-Newton techniques combined with gradient-like methods to solve the discrete nonlinear problem.

1. Introduction

To understand a material it is essential to characterize it, that is to say to analyze its properties. The thermal characterization of material has been the subject of numerous studies [7, 10, 11, 12, 19, 20]. The methods for obtaining these characteristics are multiple and various, and each method has its advantages and disadvantages. These materials characterization techniques are based on various basic physical principles: radiation-matter interactions, thermodynamics and mechanics.

Most characterization techniques are said to be destructive because the material is damaged at the end of the test. There are also so-called non-destructive testing techniques, which do not degrade the material. Thanks to these methods, it is possible, for example, to test the mechanical quality (absence of cracking and corrosion) of each part after the production of aeronautical parts or during their maintenance check.

There are many gaps in the characterization of the properties of metals at high temperatures, since although the evils of thermal distortion are well known, they are probably not fully appreciated.

This work is part of a project aiming to characterize a certain number of metals used in industry, in the field of high temperatures using non-destructive active measurement methods which consist in heating the sample by a heat source of electromagnetic radiation and in studying its temperature drop during the cooling phase. We therefore place ourselves in an iterative precess of identifying the heat transfer coefficient. The objective of this work is to solve the direct problem which appears in this inversion precess, that is to say the determination of the two-dimensional and unsteady temperature field, inside a finite cylinder, subjected to given thermal conditions. The model is approached by a finite difference method. The problem
obtained after discretization, is a non-linear system to which one cannot apply the methods requiring the computation of the Jacobian matrix.

We discuss the application of some quasi-Newton methods. To validate our approach, we compare the obtained solutions with those given by some constructed solutions.

1.1. Sample presentation
The modeling is done on a full cylindrical sample, subjected to a high temperature. Our objective is to study the radial temperature distribution within a cylinder as it is cooled by a surrounding medium.

The dimensions of this sample are as follows:
- \( T_0 \): is the initial temperature (K) assumed to be uniform throughout the whole domain;
- \( T_{er}, T_{ez} \): denote the ambient temperature (K), \( T_{er} = T_{ez} = T_\infty \);
- \( \lambda \): is the thermal conductivity of the material (W/m/K);
- \( C_p \): is the specific heat (J/kg.K);
- \( \rho \): is the volumic mass (kg/m\(^3\)).

The transfer with the outside environment is represented by heat transfer coefficients:
- \( h_r \): the exchange coefficient in the direction \( r \) (W/m\(^2\)K\(^{-1}\));
- \( h_z \): the exchange coefficient in the direction \( z \) (W/m\(^2\)K\(^{-1}\)).

The body is supposed to be limited by the same ambient medium in both directions, \( h_r = h_z = h \). This coefficient includes convective and radiative exchanges with the surrounding environment.

In the present study, the computed interfacial heat transfer coefficients are the result of the total heat transfer resistance at the interface.

2. Mathematical formulation
Inside the cylinder the thermal energy is transported by diffusion. Thanks to the symmetry of the problem, temperature distribution is the same for each half of the cylinder, and so just one half can be considered.

![Figure 1. Schematic of cylinder](image)
2.1. Thermal model

To describe the temperature field in the sample the heat conduction equation in cylindrical variables can be written

\[
\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}, \quad \text{for } 0 < r < R, 0 < z < Z, \tag{2.1}
\]

where \( \alpha = \frac{\lambda}{\rho C_p} \).

The cylinder cools by exchanging thermal energy with the surrounding medium by convection and this energy exchange is proportional to the difference between the cylinder’s surface temperature and the temperature of the surrounding medium.

The heat transfer coefficient depends nonlinearly on the temperature.

Thus equation (2.1) is supplemented by Robin boundary conditions:

\[
\lambda \frac{\partial T}{\partial r} = h(T)(T_{\infty} - T) \quad \text{for } r = R, 0 < z < Z, \tag{2.2}
\]

\[
\lambda \frac{\partial T}{\partial z} = h(T)(T_{\infty} - T) \quad \text{for } z = Z, 0 < r < R. \tag{2.3}
\]

Insulating of the cylinder on the two other surfaces results in zero flux through these interfaces and we then have the following two boundary conditions:

\[
\lambda \frac{\partial T}{\partial r} = 0 \quad \text{for } r = 0, 0 < z < Z, \tag{2.4}
\]

and

\[
\lambda \frac{\partial T}{\partial z} = 0 \quad \text{for } z = 0 \text{ and } 0 < r < R. \tag{2.5}
\]

2.2. Discretization of the equations

The cylinder is broken into shells and the temperature of each shell is computed using an implicit finite difference approximation to the radial heat equation in cylindrical coordinates.

So the discretized heat equation is written in the following form:

\[
\gamma_1 T_{i-1,j}^{n+1} - \gamma_2 T_{i,j-1}^{n+1} + \gamma_3 T_{i,j}^{n+1} - \gamma_4 T_{i+1,j}^{n+1} - \gamma_5 T_{i,j+1}^{n+1} - \gamma_6 T_{i,j}^{n} = 0 \tag{2.6}
\]

where

\[
\gamma_1 = \frac{1}{2\delta r^2} - \frac{1}{\alpha \delta t^2},
\]

\[
\gamma_2 = \frac{1}{\delta z^2},
\]

\[
\gamma_3 = \left( \frac{2}{\alpha \delta t} + \frac{2}{\delta r^2} + \frac{2}{\delta z^2} \right),
\]

\[
\gamma_4 = \left( \frac{1}{\delta r^2} + \frac{1}{2i \delta r^2} \right),
\]

\[
\gamma_5 = \frac{1}{\delta z^2},
\]

\[
\gamma_6 = \frac{1}{\alpha \delta t},
\]

for

\[
2 < i < N_r - 1, 2 < j < N_z - 1, n > 1
\]
and

\[
\frac{T_{i+1,j}^{n+1} - T_{i-1,j}^{n+1}}{2\delta r} = h(T_{i,j}^{n+1})(T_{\infty} - T_{i,j}^{n+1}) \text{ for } i = N_r, 1 < j < N_z, \quad (2.7)
\]

\[
\frac{T_{i,j+1}^{n+1} - T_{i,j-1}^{n+1}}{2\delta z} = h(T_{i,j}^{n+1})(T_{\infty} - T_{i,j}^{n+1}) \text{ for } j = N_z, 1 < i < N_r - 1. \quad (2.8)
\]

This gives rise to a system of non-linear algebraic equations of the following form:

\[F(u) = 0,\quad (2.11)\]

where \( u = T^{n+1} \), temperature at the step \( n + 1 \), is a vector of order \( N = N_r \times N_z \).

3. Numerical methods

A common strategy for solving the system of nonlinear algebraic equations (2.11) is Newtons method. This method requires the computation of the Jacobian matrix \( F'(u^k) \) and the inversion of a linear system at each step.

However for our problem the non-linearity is due to the function \( h(t) \), the convective and radiative exchange with the ambient medium, for which we do not have an analytical expression as in [7], and therefore impossibility of calculating \( F'(u^k) \).

We consider different quasi-Newton methods to solve the non-linear system (2.11). These methods are generally given by

\[u^{n+1} = u^n - \alpha_n^{-1}F(u^n),\quad (3.1)\]

\( \alpha_n \) is a square matrix of order \( N \), and the different approaches in the construction of this matrix have given rise to different quasi-Newton methods.

A classical technique for choosing \( \alpha_n \), called "Broyden’s actualisation" [4], is written in Algorithm 1.

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**Algorithm 1: Broyden**

1. Take initial \( \alpha_0, u^0 \).
2. Compute \( u^{n+1} \) using :

\[u^{n+1} = u^n - \alpha_n^{-1}F(u^n)\]

3. If \( \frac{||u^{n+1} - u^n||}{||u^n||} < \varepsilon \) then stop.
4. Else, compute \( \alpha_{n+1} \) using

\[\alpha_{n+1} = \alpha_n + \frac{F(u^{n+1})(u^{n+1} - u^n)^T}{(u^{n+1} - u^n, u^{n+1} - u^n)}\]

5. \( n \leftarrow n + 1 \) and go to step 2.
For the sake of simplicity the matrix $\alpha_0$ can be chosen diagonal, however the matrices generated by this procedure are full matrices. The inversion of these kind of matrices is very expensive.

As the very sparse structure of the Jacobian matrix is known, we can use the sparse Broydens method proposed by Shubert [18, 15] that is, the Schuberts method which preserves this structure.

Kim and Tewarson [13] proposed a method based on a convex combination of the formula used in Algorithm 1 and another updating formula proposed in [8].

We have implemented this method using Schubert’s approximation which gives rise to the following algorithm:

**Algorithm 2: Schubert-Kim**

1. Take initial $\alpha_0, u^0$.
2. compute $u^{n+1}$ using
   \[
   u^{n+1} = u^n - \alpha_n^{-1} F(u^n)
   \]
3. If $\frac{|u^{n+1} - u^n|}{||u^{n+1}||} < \varepsilon$ then stop.
4. Else, compute $v_n, s_n, \mu$ and $\alpha_{n+1}$ using
   \[
   v_n = -\alpha_n^T F(u^n),
   s_n = u^{n+1} - u^n,
   \mu = \frac{(v_n, s_n)^2}{(s_n, s_n)(v_n, v_n)},
   \alpha_{n+1} = \alpha_n + (1 - \mu) \frac{F(u^n)s_n^T}{(s_n, s_n)} + \mu \frac{F(u^n)v_n^T}{(v_n, s_n)}.
   \]
5. $n \leftarrow n + 1$ and go to step 2.

The drawback of the methods described above is that there is no guarantee that the generated matrices will be non-singular. A method which takes this eventuality into account is the Powell method [16] which is a modification of the Broyden method, written in Algorithm 3.
Algorithm 3: Schubert-Powell

1: Take initial $\alpha_0, u^0$.
2: Compute $u^{n+1}$ using

$$u^{n+1} = u^n - \alpha_n^{-1} F(u^n)$$

3: If $\|u^{n+1} - u^n\| < \varepsilon$ then stop.
4: Else, compute $s_n, \gamma_n$ and $\alpha_{n+1}$ using

$$s_n = u^{n+1} - u^n$$

$$\gamma_n = \frac{\langle s_n, \alpha_n^{-1}[F(u^{n+1}) - F(u^n)] \rangle}{\langle s_n, s_n \rangle}$$

$$\alpha_{n+1} = \alpha_n + \theta_n \frac{F(u^{n+1}) s_n^T}{\langle s_n, s_n \rangle}$$

where

$$\theta_n = \begin{cases} 
1 & \|\gamma_n\| \geq \eta \\
\frac{1 - \text{sign}(\gamma_n) \eta}{1 - \gamma_n} & \|\gamma_n\| < \eta, \text{ for some } \eta \in (0, 1).
\end{cases}$$

5: $n \leftarrow n + 1$ and go to step 2.

In this algorithm (or its simplification-generalization), a non-trivial update of $\alpha_n$ is necessary as well as solving a linear system at each iteration. We present in the following algorithm, an approach whose implementation does not require much effort.

Algorithm 4:

1: Take initial $\alpha_0, u^0$.
2: Compute $u^{n+1}$ using

$$u^{n+1} = u^n - \alpha_n^{-1} F(u^n)$$

3: If $\|u^{n+1} - u^n\| < \varepsilon$ then stop.
4: Else, compute $\alpha_{n+1}$ using

$$\alpha_{n+1} = \frac{\|F(u^{n+1}) - F(u^n)\|}{\|F(u^n)\|} \alpha_n.$$

5: $n \leftarrow n + 1$ and go to step 2.

This algorithm is a generalization of the one used in [14] for an interface problem in dimension 1. It was introduced for the computation of the potential electrostatics of a semiconductor [9].
An advantage of this algorithm is that if the matrix \( \alpha_0 \) is a diagonal matrix then no inversion of the system is necessary.

4. Solving linear systems

Algorithm 1, Algorithm 2 and Algorithm 3 give rise to linear systems where the matrices are not symmetrics. To solve these systems we used a conjugate gradient-like iterative method introduced in [21]. Let the system to be solved is such that \( Ax = b \). Then the the algorithme for solving this linear system is as follows:

**Algorithm 5:**

1: For given \( x_0 \) take \( r_0 = b - Ax_0 \);
   Choice \( \tilde{r} \) arbitrary, such that \( (\tilde{r}, r_0) \neq 0 \);
   Take \( \omega_0 = \rho_0 = \alpha = 1 \); \( v_0 = 0 \); \( i = 1 \);
2: Compute
   \[ \rho = \langle \tilde{r}, r_i \rangle \beta = \left( \frac{\rho}{\rho - 1} \right) \left( \frac{\alpha}{\omega_{i-1}} \right) ; \]
   solve \( K \hat{p} = p \);
   \( v_i = \hat{A} \hat{p} \)
   \( \alpha = \rho_i / \langle \tilde{r}, v_i \rangle \)
   \( s = r_{i-1} - \alpha v_i \)
   solve \( K \hat{s} = s \);
   \( t = A \hat{s} \)
   \( \omega_i = \langle K^{-1} t, K^{-1} s \rangle / \langle K^{-1} t, K^{-1} t \rangle \)
   \( x_i = x_{i-1} + \alpha \hat{p} + \omega_i \hat{s} \)
   \( r_i = s - \omega_i \hat{s} \)
3: If \( || r_i || < \varepsilon \) then stop.
4: Else \( i \leftarrow i + 1 \) and go to step 2.

The matrix \( K = K_L K_R \) in Algorithm 5 represents the preconditioning matrix.

One of the strong points of the BI-CGSTAB method is that it avoids the irregular behavior of convergence observed in the use of certain methods for solving linear system. This behavior induces a damaged solution which can prevent the non-linear solver from converging.

The conditioning we have applied, for our numerical experiments, is based on an incomplete factorization of the matrix \( A \). We chose as initial vector \( \tilde{r} = r_0 \), for all algorithms.

5. Numerical results

In order to observe the numerical behavior of the different methods used to solve the non-linear systems, we have treated as an example the cooling of the cylindrical sample with the following considerations.

As we have assumed that the coefficient \( h \) is only available in a discrete way, we used a linear interpolation to estimate the coefficient \( h \) for any temperature value between the ambient temperature and the initial temperature of the material.

The studied properties of material, assumed to be constant, are as follows:
Table 1. Material properties

| Parameter | Value |
|-----------|-------|
| $\rho$ (Kg/m$^3$) | 4450 |
| $C_P$ (J/Kg$^o$C) | 915 |
| $\lambda$ (W/m$^2$K) | 17 |

Table 2. Initial and boundary given data

| Data | Value |
|------|-------|
| $T_0$ (K) | 1000 |
| $T_{cr}$ (K) | 300 |
| $T_{ez}$ (K) | 300 |

The duration of the numerical simulation is taken equal to 1200 s, as is often the case for the physical experiment [11].

We noticed that the BI-CGSTAB method does not work with several of the quasi Newton methods (see Table 4), so we implemented the QMRCGSTAB method [6], a quasi-minimal residual variant of the biconjugate gradient stabilized (Bi-CGSTAB). Algorithm 1, Algorithm 2 and Algorithm 3

| Quasi-Newton iterations | total iterations |
|-------------------------|------------------|
| Algorithm 1 | 48 | 285 |
| Algorithm 2 | 126 | 676 |
| Algorithm 3 | 271 | 690 |
| Algorithm 4 | 52 | 366 |

Table 3. Iterations required for QMRCGSTAB

We compare, in Table 4, the various methods of quasi-Newton, for the same step of discretization $s = 0.1$, the same tolerance $Tol = 10^{-6}$ and the same solver of the linear system QMRCGSTAB [6]. We observe from this table that the total number of iterations necessary to reach the convergence is very important for the different variants of the Schubert algorithm while the Broyden algorithm and Algorithm 4 have a small number of iterations. But this information can be misleading if it is not taken in its context, namely that the structure of the matrices is not the same which requires a different time for the resolution of the resulting linear systems.

| Algorithm | QMRCGSTAB | BI-CGSTAB | PREC_BI-CGSTAB |
|----------|-----------|-----------|----------------|
| Algorithm 1 | 21.69 | - | - |
| Algorithm 2 | 5.41 | 5.11 | 3.01 |
| Algorithm 3 | 23.45 | - | - |
| Algorithm 4 | 3.39 | 1.63 | 0.68 |

Table 4. Time (second) required for convergence
We therefore compare the efficiency of the different quasi-Newton methods, combined with the different solvers for the linear system, showing the time necessary for convergence. We observe that in fact the method of Broyden, despite the fact that it requires the smallest number of iterations is very slow, this is explained by the fact that the matrices generated by this method are full and very ill-conditioned. We also observe that preconditioning improves convergence. The fastest of all these algorithms is our Algorithm 4.

The fact that this algorithm preserves the structure of the initial matrix makes it expressly fast in the case where we start with a diagonal matrix (only 0.68 second is needed to reach convergence).

This is due to the generated matrices which, in this case, all remain diagonals and no inversion of these matrices is necessary.

![Temperature evolution](image)

**Figure 2.** Temperature evolution

Figures 2 shows the temporal evolution of the temperature in the cooling phase of the cylinder, plotted for a chosen point inside the domain of study. We observe that the curve obtained by the simulation follows exactly the curve of the cooling of the cylinder. The difference between the two curves is really small in particular in the last time steps of the simulation.

In Figure 3 we plotted the number of iteration required by Algorithm 4 at each step of time. We observe from this figure that a few iterations are sufficient for the convergence of Algorithm 4. When the temperature approaches that of the surrounding medium 2 to 3 iterations are enough to reach convergence, which explains the speed of the algorithm.

6. Conclusion

The results presented here are part of an ongoing research project that aims a comprehensive analysis of heat source in diffusive processes through the solution of inverse heat transfer problems.

The set of the obtained results shows the quality of the solution of the non linear problems via the use of the quasi-Newton methods, and constitutes an important step in the simulation of
the nonlinear inverse problems where the objective is to predict the convective heat transfer coefficient that would be necessary for the study of cooling of metals subjected to high temperature.

The idea is to determine materials with the desired characteristics in order to optimize certain processes.

As in [1], we have shown that Quasi Newton techniques allow to efficiently solve the discrete nonlinear problem where the nonlinearity is not expressed analytically. The algorithm will be integrated into a nonlinear inverse problem solving process using new iterative methods [5, 3, 17]. We plan also to use this technique to solve nonlinear boundary value problems in unbounded domain, for example the one described in [2].

7. Acknowledgement
This work was initiated during the visit of Fatima Aboud, at the "Laboratoire de Mathmatiques Jean Leray, Universit de Nantes (France), CNRS UMR 6629". This scientific stay was funded by the International Center for Pure and Applied Mathematics (CIMPA) and the "Fderation de Recherche Mathmatiques des Pays de Loire-FR CNRS 2962".

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