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THERMAL CONTACT CONDUCTANCE ESTIMATION USING OPTIMIZATION ALGORITHMS

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Abstract. *This paper aims to solve an inverse problem (IP) in the heat transfer context in order to estimate thermal contact conductances (TCC), a property that represents the adherence between two or more bodies subjected to a heat exchange phenomenon. This property is evaluated on the internal interface of a bi-composite material by using temperature measurements on the external surface of the object of study. In this paper, the measured temperatures, used in the IP, are synthetically obtained by solving a direct problem (DP) via the Finite Difference Method (FDM). A steady-state regime was considered, as well as the nonexistence of internal heat sources, for a bi-dimensional and homogeneous body. In the DP framework, from the prior knowledge of the thermal physical properties (in which TCC is included), as well as the geometry and boundary conditions, it is possible to calculate the temperature distribution on the external surface.*
The IP approach, then, intends to indirectly estimate TCCs when one is able to measure the temperature distribution in a certain region of the body, such as in a laboratory environment. This can be performed, for instance, using optimization techniques based on gradient evaluations, such as the Levenberg-Marquardt (LM) and the Gauss-Newton (GN) methods. Test cases with different noise levels added to the synthetically measured temperatures were analyzed, with good results. Six types of functions, chosen to represent the TCC distribution, were analysed. A Zeroth-Order Tikhonov regularization was applied to the GN method during the minimization process, where the regularization parameter was chosen automatically.

Keywords: *Inverse Problems, Tikhonov, Levenberg-Marquardt, Gauss-Newton. Thermal Contact Conductance.*

1. INTRODUCTION

The evaluation of interface properties in science and engineering applications are considered relevant when one aims to have a holistic understanding of the energy flow phenomena when two materials are in contact. Such interfaces might be solid, fluid or a mix of them, as in live organisms, for example (Padilha *et al.*, 2016). Regarding thermal sciences, when a heat flux is applied to two bodies in a non-perfect contact, it is experimentally possible to observe temperature variations on the interface between them (Polozine, 2009).

The physical property that describes this phenomenon is the thermal contact conductance (TCC), which may be understood as the parameter or function that represents the ease in which the heat crosses one surface to the other (Padilha, 2016; Gonçalves, 2018). The application of this matter is relevant in different areas of knowledge in order to increase productivity, efficiency and precision in engineering projects (Frekers *et al.*, 2017), as in aerospacial and biomedics (Sunil Kumar and Ramamurthi, 2004; McWaid and Marschall, 1992; Tang *et al.*, 2015), electronics (Cui *et al.* (2014); Sartre and Lallemand (2001)), machinery (Liu *et al.*, 2020), cooling systems (Sharafian *et al.*, 2014), manufacturing processes (Polozine, 2009; Hamasaiid *et al.*, 2010), and heat exchangers (Taler and Oclon, 2014), to name a few.

The present work intends to estimate TCCs by solving an inverse heat conduction problem (IHCP), using temperature measurements taken on an external boundary of a two-layer material. The inverse problem was solved by a gradient-based method, together with a Tikhonov regularization scheme when applicable, where the regularization parameter was chosen automatically, following the development in Pacheco *et al.* (2022). The direct problem was solved by the Finite Differences Method (FDM), where two different grid sizes were used for the direct and for the inverse problem, avoiding the so-called inverse crime (Kaipio and Somersalo, 2005).

2. DIRECT PROBLEM (PD)

The problem in this work follows the model considered by Colaço and Alves (2013); Abreu *et al.* (2016); Padilha (2016), in which a double-layered specimen (Ω) constituted by two media (Ω_1 e Ω_2) is considered, as shown in Fig. 1.

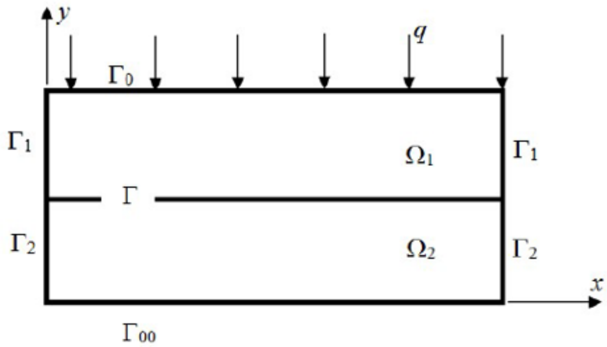


Figure 1: Illustration of the problem (Padilha (2016)).

Between the two bodies there is an interface Γ, which may be mathematically described by the TCC, h_c. The materials have thermal conductivities κ_1 and κ_2, and side surfaces Γ_1 and Γ_2, which are kept thermally insulated. The bottom boundary, Γ_∞, from the specimen Ω_2, is subjected to a first-type boundary condition, i.e., constant temperature. Finally, on the superior boundary of Ω_1, Γ_0, there is an imposed heat flux (q).

A steady-state case was considered, for a two-dimensional geometry in (x, y) with constant physical properties, space-varying TCC ($h_c = h_c\,(x)$), and a constant applied heat flux, evenly distributed within Γ_0. On the interface Γ it was considered a third-type boundary condition, such as:

$$-\kappa_1 \frac{\partial T_1}{\partial \mathbf{n_1}} = h_c\,(T_1 - T_2). \tag{1}$$

in which $\mathbf{n_1}$ is the unitary normal vector, pointing outwards to the boundary considered. Temperatures T_1 e T_2 are located on the interface Γ, at the Ω_1 and Ω_2 sides, respectively.

Mathematically, the DP is then modelled as (Colaço and Alves, 2013; Özisik, 1980):

$$\nabla^2 T_1 = 0 \quad \text{in} \quad \Omega_1 \tag{2a}$$

$$-\kappa_1 \frac{\partial T_1}{\partial n_1} = q \quad \text{on} \quad \Gamma_0 \tag{2b}$$

$$\frac{\partial T_1}{\partial n_1} = 0 \quad \text{on} \quad \Gamma_1 \tag{2c}$$

$$-\kappa_1 \frac{\partial T_1}{\partial n_1} = h_c\,(T_1 - T_2) \quad \text{on} \quad \Gamma \tag{2d}$$

$$\nabla^2 T_2 = 0 \quad \text{in} \quad \Omega_2 \tag{2e}$$

$$\frac{\partial T_2}{\partial n_2} = 0 \quad \text{on} \quad \Gamma_2 \tag{2f}$$

$$T_2 = 0 \quad \text{on} \quad \Gamma_\infty \tag{2g}$$

$$-\kappa_1 \frac{\partial T_1}{\partial n_1} = \kappa_2 \frac{\partial T_2}{\partial n_2} \quad \text{on} \quad \Gamma \tag{2h}$$

The DP can be iteractively solved by applying the FD method (Patankar, 1980), which showed good adherence when results were compared to those available in the literature (Padilha, 2016). By solving it, it is possible to compute the temperature distribution within the domain of the observed object.

3. INVERSE PROBLEM (IP)

In this paper, the inverse problem is solved by the application of gradient-based optimization algorithms, namely the Levenberg-Marquardt (LM) and the Gauss-Newton (GN) methods. For the former, since in the presence of noisy data the resulting system of equations is ill-posed (Kaipio and Somersalo, 2005), it was also necessary to include a regularization procedure, such as a Tikhonov regularization technique (Hansen, 1998). As for the Levenberg-Marquardt, the algorithm itself provides a regularization strategy.

Therefore, the purpose of the inverse problem here is to estimate the TCC by using temperature measurements, taken on Γ_0. Since no experiments were build as part of this research, these measurements were obtained synthetically from the solution of the PD, in which a Gaussian noise was added. Then, from this experimental data, the inverse problem consists of finding the TCC via an optimization technique that minimizes the following objective function:

$$S(\mathbf{x}) = ||\mathbf{A}\mathbf{x} - \mathbf{y}||_2^2 + \lambda^2||\mathbf{x}||_2^2 \tag{3}$$

where $\mathbf{A}$ is the matrix that contains the coefficients of the system of equation, $\mathbf{x}$ is the vector that represents what needs to be estimated by the optimization process and $\mathbf{y}$ stores the experimental data. The parameter λ^2 is a constant to mathematically stabilize the solution, called in this paper as damping factor for the LM method, and regularization parameter for the Gauss-Newton approach.

The problem consists of finding an increment to be added to the initial estimate of h, obtained from a Taylor expansion around h_0 (Pacheco *et al.*, 2022):

$$(\mathbf{J}^T\mathbf{W}\,\mathbf{J} + \lambda^2\mathbf{I})\Delta\mathbf{h}_p = \mathbf{J}^T\,\mathbf{W}(\mathbf{y}\text{ - }\mathbf{f}_p) \tag{4}$$

where $\mathbf{y}$ is the noisy data. In this equation, $\mathbf{I}$ is the identity matrix, $\mathbf{J}$ is the jacobian matrix, $\mathbf{W}$ is the inverse of the error covariance matrix and $\mathbf{f}_p$ is the solution of the DP for the TCC calculated at the iteration p.

The jacobian matrix may be calculated using finite differences, considering a small value for Δx_j, such as $\Delta x_j = 10^{-5}$ (Padilha *et al.*, 2016):

$$J_{ij} \approx \frac{\mathbf{f}(\mathbf{x}_p^*) - (\mathbf{x}_p)}{\Delta x_j} \tag{5a}$$

$$\mathbf{f}(\mathbf{x}_p^*) = \mathbf{f}([x_1 \quad x_2 \quad \dots \quad x_{j-1} \quad x_{j+\Delta x_j} \quad x_{j+1} \quad \dots \quad x_n]^T) \tag{5b}$$

$$\mathbf{f}(\mathbf{x}_p) = \mathbf{f}([x_1 \quad x_2 \quad \dots \quad x_{j-1} \quad x_j \quad x_{j+1} \quad \dots \quad x_n]^T) \tag{5c}$$

Therefore:

$$\Delta\mathbf{h}_p = (\mathbf{J}^T\mathbf{W}\mathbf{J} + \lambda^2\mathbf{I})^{-1}\mathbf{J}^T\,\mathbf{W}(\mathbf{y}\text{ - }\mathbf{f}_p) \tag{6}$$

and the new estimate can be found as:

$$\mathbf{h}_{p+1} = \mathbf{h}_p + \Delta\mathbf{h}_p \tag{7}$$

In this case, the solution of the system (6) requires a matrix inversion, which besides being computationally expensive, relies on the condition that the matrix must be invertible.

The accuracy of the solution may be expressed as the RMSE (root mean square error), that is calculated as (Padilha, 2016):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}\left[y(x=n) - f_p(x=n)\right]}{n}} \tag{8}$$

3.1 Levenberg-Marquardt

For the Levenberg-Marquardt technique (Levenberg, 1944; Marquardt, 1963), one aims to solve Eq. (4),in which λ^2 is called *damping factor* and is iteratively updated according to the estimates, what results in the Gauss-Newton method for small values of it and in the Steepest-Descent for large ones (Madsen *et al.*, 2004).

Here, the damping factor is calculated by the jacobian matrix (Umar *et al.*, 2020), as:

$$\lambda_k^2 = ||\mathbf{J}_k^T\mathbf{J}_k|| \tag{9}$$

The procedure then consists of applying the following pseudo-algorithm to find a new estimate, similarly to Eq. (6). Considering an initial estimation for λ, a maximum number of iterations (p_{max}) or a stop criterion ϵ, as in:

Algorithm 1 Pseudo-algorithm to solve IHTP via LM

```
Require: λ², ϵ:
1: S(h_{p=0}) = initial large value
2: p ← p + 1
3: Set an initial guest for h_p; solve the DP to find y and calculate J_p according to Eq. (5)
4: Calculate the damping factor given by Eq. (9)
5: Find Δh_p according to Eq. (6)
6: Find h_{p+1} as stated in Eq. (7)
7: Calculate the objective function with Eq. (3)
8: if S(h_{p+1}) < ϵ then
9:     Accept h_{p+1} as solution
10: else
11:     Return to step 3 until convergence.
12: end if
```

3.2 Gauss-Newton with Automatic Tikhonov Regularization

When solving the optimization problem by applying the Gauss-Newton algorithm, the Eq. (6) must be modified to include zeroth-order Tikhonov regularization (Hansen, 2010), the updates in the estimated is also applied by Eq. 4, in which λ^2, is the so-called regularization parameter. It is worth saying that the equation is basically the same as the one used for the LM method, but , in this case, the regularization parameter will be choosen differently.

The problem, then, consists of finding a right estimation for TCC that minimizes Eq. (3), while λ^2 is also a part of the estimation process. The importance of this term is to stabilize and smooth the solution, so a special treatment must be proposed.

The regularization parameter can be found, for example, via the L-curve technique, which is computationally expensive since it requires the solution of the inverse problem for multiple values of λ^2 (Hansen, 1998).

In this work, a methodology based on the technique described in Pacheco *et al.* (2022) was applied, where the regularization parameter is calculated automatically by a Generalized Cross Validation (GCV) procedure, and the system of equations is solved by the Singular Value Decomposition (SVD) technique. Here, it is aimed to solve the system by inverting the matrix, as proposed in Eq. (6), but automatically adding a parameter selection as described below.

Thereby, the methodology to seek for the regularization parameter consists of finding a value for λ that minimizes the functional $G(\lambda)$ (Hansen, 2010; Golub *et al.*, 1979; Pacheco *et al.*, 2022):

$$G(\lambda) = \frac{||\mathbf{A}\mathbf{x}_\lambda - \mathbf{b}||_2^2}{\left(n - \sum\limits_{i=1}^{n} \phi_i^{[\lambda]}\right)^2} \tag{10}$$

for n parameters , as a function of the filter factor vector $\phi_i^{[\lambda]}$.

To compute the filter factor, the coefficient matrix must be expanded as SVD (Hansen, 2010):

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \sum_{i=1}^{n} \mathbf{u}_i \boldsymbol{\sigma}_i \mathbf{v}_i^T \tag{11}$$

being $\mathbf{U}$ and $\mathbf{V}$ matrices that consists of the left and right singular vectors, whose columns are respectively $\mathbf{u}_i$ and $\mathbf{v}_i$. Additionally, the main diagonal of $\boldsymbol{\sigma}$ includes the singular vectors, being

$$\boldsymbol{\Sigma} = \text{diag}(\sigma_1, \ldots, \sigma_n) \tag{12}$$

where, necessarily, $\sigma_1 \geq \sigma_2 \geq \sigma_1 \geq \cdots \geq \sigma_n \geq 0$.

Therefore, the filter factor is written as:

$$\phi_i^{[\lambda]} = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \tag{13}$$

To calculate the norm in the numerator of Eq. (10), treating Eq. (6) as a system of equations in the type **A x = b**, it is possible to implement the following expression (Pacheco *et al.*, 2022):

$$||\mathbf{A}\mathbf{x}_\lambda - \mathbf{b}||_2^2 = \sum_{i=1}^{n} b_i^2 - \sum_{i=1}^{n} \frac{\sigma_i^2(\sigma_i^2 + 2\lambda^2)}{(\sigma_i^2 + \lambda^2)^2} \left(\mathbf{u}_i^T \mathbf{b}\right)^2 \tag{14}$$

In this case, by simplifying **A** = $\mathbf{J}_p$, $\boldsymbol{\Delta x}_\lambda$ = $\mathbf{h}_p$ and **b** = (**y** - $\mathbf{f}_p$), then, it becomes possible to include a sub-routine to calculate and select the best functional $G(\lambda)$ as stated in Eq. (10), viz. (Padilha *et al.*, 2016):

$$\gamma_k = ln(\lambda_k) \tag{15a}$$

$$\gamma_{k+1} = \gamma_k - \frac{\mathrm{d}lnG(\lambda_k)}{\mathrm{d}\gamma} = \gamma_p - \frac{1}{G(\lambda)}\frac{\mathrm{d}G}{\mathrm{d}\lambda}\lambda_k \tag{15b}$$

$$\frac{\mathrm{d}G}{\mathrm{d}\lambda} = \frac{G[\lambda(1+\epsilon)] - G(\lambda)}{\epsilon} \tag{15c}$$

in which a forwarded FD scheme was chosen to estimate $dG/d\lambda$.

The computational implementation can be represented by the following pseudo-algorithm :

Algorithm 2 Pseudo-algorithm to solve the IHTP via GN method and matrix inversion.

```
Require: λ², ε₁, ε₂
1: S(h_{p=0}) = 10^100
2: p ← p + 1
3: Set an initial guest for h_p; solve the DP to find y and calculate J_p by Eq. (5)
4: Evaluate the SVD of J_p
5: k ← 0
6: k ← k + 1
7: Find G(λ_{k+1}) by Eq. (10), using Eq. (14) where A ← J_p
8: Calculate the new estimates of λ_{k+1} and γ_{k+1} with the help of Eq. (15)
9: if |γ_{k+1} - γ_{k+1}| < ε₂ then
10:     Accept γ_{k+1} and λ_{k+1} = e^{γ_{k+1}} as solution for the regularization parameter
11: else
12:     Return to step 6 until convergence
13: end if
14: Find Δh_p as stated in Eq. (6) using the regularization parameter obtained from step 8 for λ²
15: Find h_{p+1} as stated in Eq. (7)
16: Calculate the objective function with Eq. (3)
17: if S(h_{p+1}) < ε₁ then
18:     Accept h_{p+1} as solution
19: else
20:     Return to step 2 until convergence.
21: end if
```

4. RESULTS

The computational procedure described in subsections 3.1 and 3.2 were computationally implemented with an integrated approach. The DP was written in C while the IP in Mathematica, the former calling the latter. This strategy was useful to speed up the computational simulations (Paul, 1998). For instance, six thermal contact conductance functions were considered in this work (Padilha, 2016), as follows in Tab.1, which consider a certain maximum value for the TCC (h_{max}) and their respective spatial distribution:

The values for the geometric and thermophysical properties can be seen in Tab. 2, as suggested by (Padilha, 2016), regards the specimen illustrated in Fig. 1.

To demonstrate the effectiveness of the proposed methodology, for the first TCC profile (h_1), different noise levels (ω_{exp}) were added to the problem in order to verify the impact on the quality of the results. It was considered the range $0.0°$C, 10^{-3} °C, $0.5°$C, and $2.0°$C. For the IP, a mesh with 30 points in x-direction and 10 in y-direction was considered. To avoid inverse crime, a finer mesh, with 150 by 40 points in the x and y directions respectively, was applied. Then, the experimental data was obtained by adding noise to the solution obtained by the DP (**T**) when the aforementioned CTC was added (Padilha, 2016):

$$\mathbf{Y} = \mathbf{T} + \epsilon\, \sigma_{exp} \tag{16}$$

where

$$\epsilon = cos(2\pi v)\sqrt{-2ln(u)} \tag{17}$$

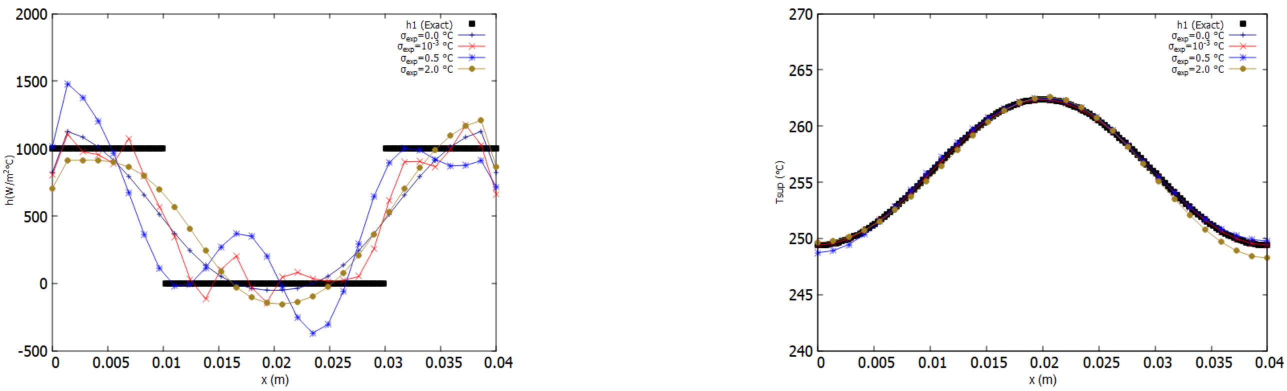
Table 1: Thermal contact conductance profiles

Profile	$\mathbf{h}_c$ $[W/m^2\ {}^\circ C]$
1	$h_1 = \begin{cases} h_{max}, & x < a/4 \text{ and } x > 3a/4 \\ 0, & a/4 < x < 3a/4 \end{cases}$
2	$h_2 = \begin{cases} h_{max}, & x < a/4 \text{ and } a/2 < x < 3a/4 \\ 0, & a/4 < x < a/2 \text{ and } x > 3a/4 \end{cases}$
3	$h_3 = h_{max}\ \ sin(\pi x/a)$
4	$h_4 = h_{max}\ \ \lvert sin(2\pi x/a)\rvert$
5	$h_5 = h_{max}$
6	$h_6 = \begin{cases} h_{max}, & x < a/4 \text{ and } a/2 < x < 3a/4 \\ h_{max}/2, & a/4 < x < a/2 \\ 0, & x > 3a/4 \end{cases}$

Table 2: Simulation parameters

Parameter	Value
b_1 (m)	0.01
b_2 (m)	0.01
a (m)	0.04
q (W/m^2)	0.04
k_1 $(W/m^\circ C)$	54.0
k_2 $(W/m^\circ C)$	54.0
T $(^\circ C)$ at Γ_∞	0
h_{max} $(W/m^{2\circ}C)$	1000

being u and v two random numbers, $u \in [0, 1]$ and $v \in [0, 1]$. The results may be seen in Fig. 2 and 3.

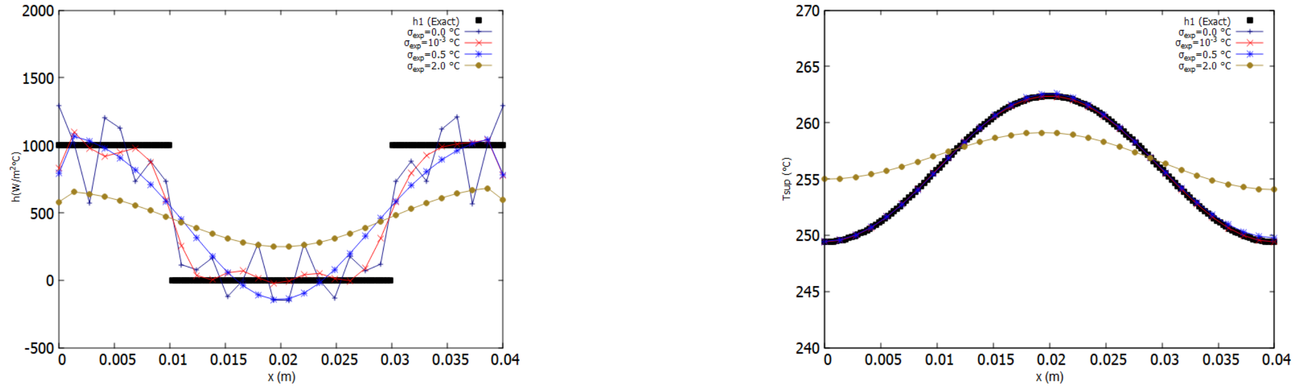


(a) h_c (b) T at Γ_0

Figure 2: IP solution with multiple noise levels obtained by the GN algorithm.

In general, the two techniques (LM and GN) led to good temperature estimations, except for LM with $\sigma_{exp} = 2.0^\circ C$. In this case, the large magnitude of the errors might be tackled by implementing a different scheme for the damping factor calculation , as suggested by Umar *et al.* (2020).

While the LM method solved the IP during 100 iterations within 6800s of CPU time in average, the use of the GN method with automatic Tikhonov regularization demanded approximately 10600s of CPU time. Naturally, this is due to the fact that for the latter, it is necessary to calculate the regularization parameter multiple times to achieve the best

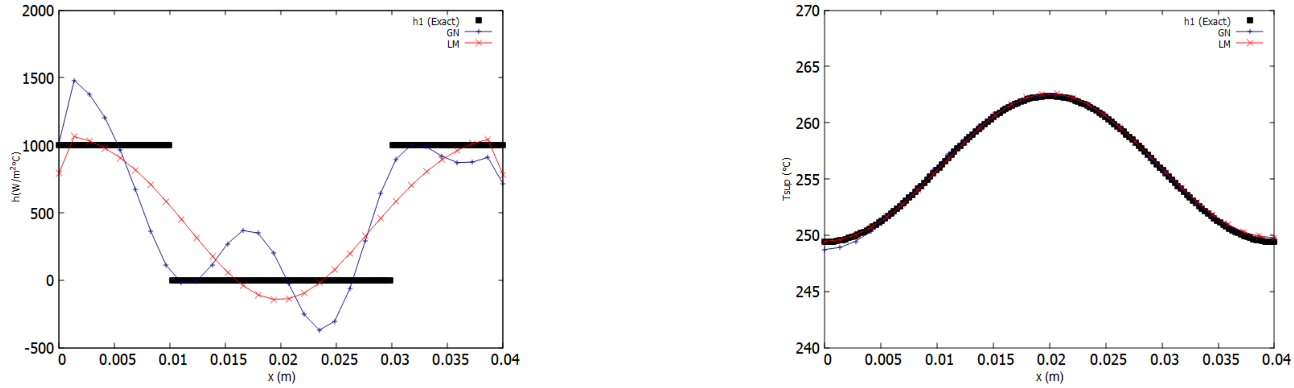


(a) h_c (b) T at Γ_0

Figure 3: IP solution with multiple noise levels obtained by the LM algorithm.

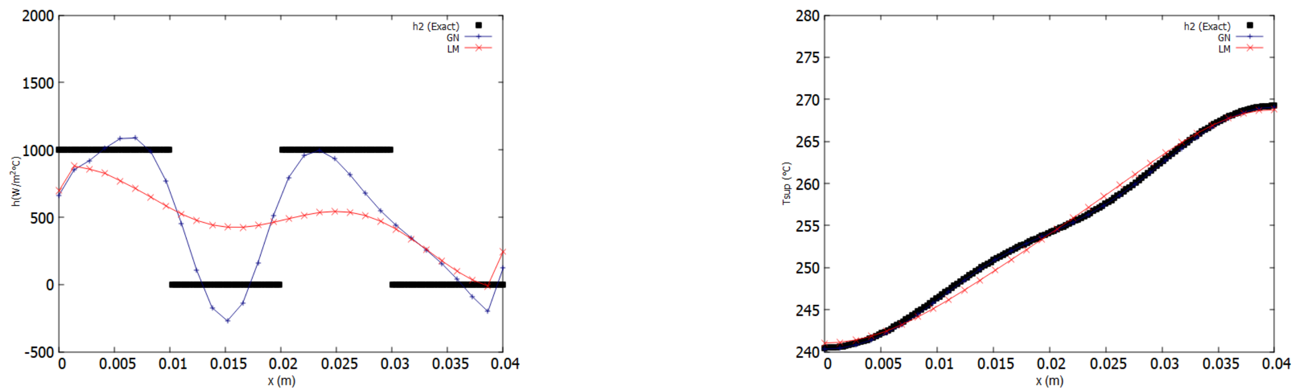
candidate as proposed in sec.3.2

The comparison between the two algorithms may also be seen in Figs. 4 and 9, considering the six TCC profiles as seen in Tab. 1, for a fixed uncertainty of $\sigma_{exp} = 0.5°C$:



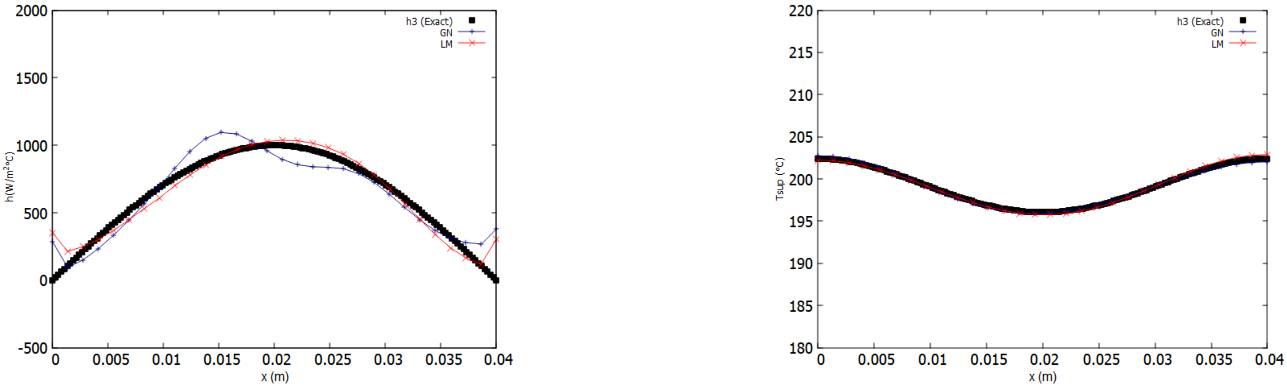
(a) h_c (b) T at Γ_0

Figure 4: h_1



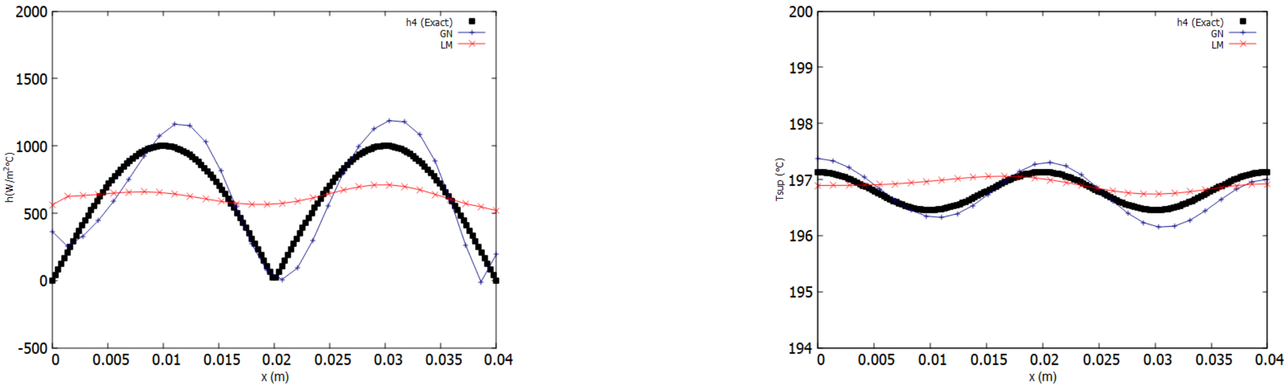
(a) h_c (b) T at Γ_0

Figure 5: h_2



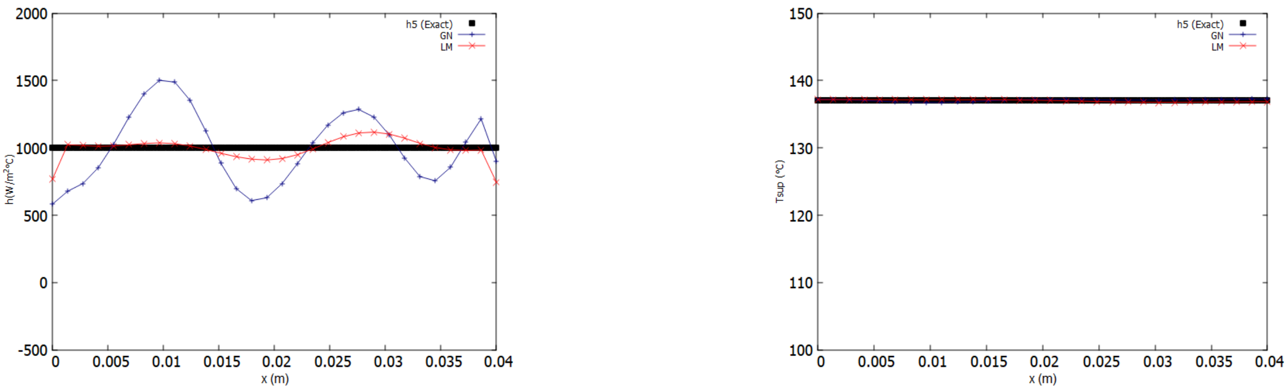
(a) h_c (b) T at Γ_0

Figure 6: h_3



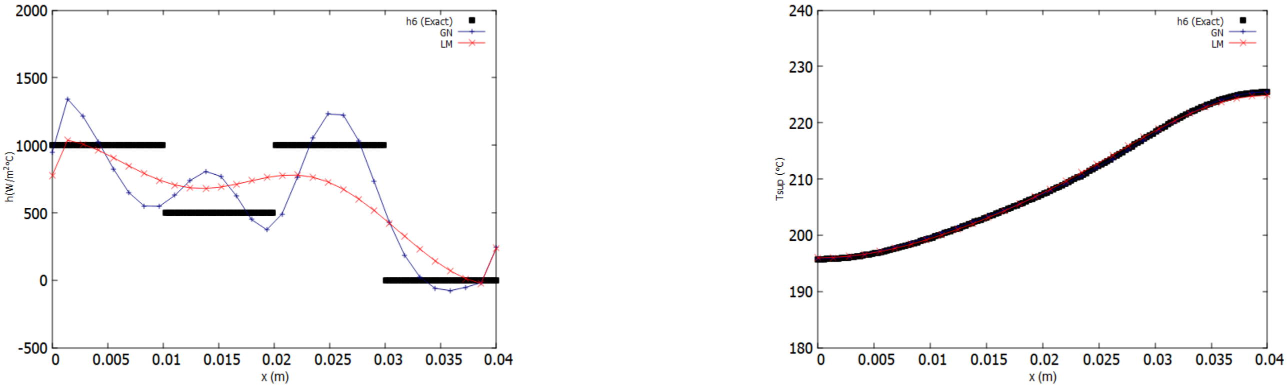
(a) h_c (b) T at Γ_0

Figure 7: h_4



(a) h_c (b) T at Γ_0

Figure 8: h_5



(a) h_c (b) T at Γ_0

Figure 9: h_6

It is also possible to calculate RMSE (root mean square error) to evaluate the discrepancies between the exact solution and the estimated temperature profiles, as seen in Eq. (8). The results are presented in Tab. 3.

Table 3: RMS for all CTC profiles, considering the GN and LM algorithms.

Profile	GN $(°C)$	LM $(°C)$
h_1	0.269791	0.166018
h_2	0.018759	0.018759
h_3	0.216944	0.247212
h_4	0.182649	0.247547
h_5	0.167462	0.169777
h_6	0.156614	0.317389

Therefore, in general the GN technique (except for the h_1 case), was able to achieve better results than the LM method, but with more computational effort (almost 60% slower). However, as seen in 3, the proposed method to calculate the damping parameter in the LM method does not seem to work well for larger noise levels, which was not observed in the regularized GN approach. Besides that, the LM technique presented difficulties when estimating functions with period $a/2$, as seen in h_4 and h_2. In those cases, the damping parameter did not regularize properly the algorithm.

The main advantage of using the automatic regularization procedure in the GN method relies on the fact that it allows the solution of ill-posed problems without having to solve the IP multiple times to obtain a L-curve, as for example in (Hansen, 1998). Therefore, the solution, besides becoming more efficient, does not require that the user determine the best regularization parameter by observing the L-curve graph. Nevertheless, both methods (GN and LM) were useful to provide good estimates and smooth the solutions, considering that there is not abrupt variations within two adjacent points.

5. CONCLUSIONS

This work suggests that the Levenberg-Marquardt algorithm, with iterative updates on the damping parameter by the jacobian matrix, as well as Gauss-Newton, with automatic Tikhonov regularization, were able to estimate TCCs in the presence of experimental noise. Both methodologies did not require a lot of computational effort, since they not need the L-curve to be drawn so a best parameter value is chosen. The results = here presented suggest that GN with Zeroth-Order Tikhonov regularization led to better RMSE results, being more efficient when solving the IP for higher levels of noise.

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