A novel parametric spectral technique to solve inverse heat problems for the estimation of wall thermophysical properties

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Résumé - Cette étude propose de réduire le coût de calcul des méthodes de descente pour résoudre les problèmes inverses de transfert de chaleur liés à l'estimation de la diffusivité thermique. L'approche repose sur un modèle d'ordre réduit spectral paramétrique pour construire une solution dépendant des coordonnées spatio-temporelles et d'un paramètre extra, dans ce cas, la diffusivité thermique. La solution paramétrique du problème direct et de sa fonction de sensibilité est construite off-line, réduisant ainsi le coût de la procédure itérative. Des données synthétiques sont utilisées pour évaluer la méthode, avec des résultats prometteurs pour caractériser les propriétés thermiques des parois de bâtiments.

Abstract - This study proposes reducing the computational cost of gradient-based method for solving inverse heat conduction problem of the thermal diffusivity estimation. It relies on using a spectral parametric reduced order model to build a solution dependent on spatial and temporal coordinates, as well as on an extra-parameter of the problem, such as the thermal diffusivity. This parametric solution of the direct problem and its sensitivity function is computed off-line significantly lowering the computational cost of the iterative inverse problem algorithm. Synthetic data are used to assess the reliability of the method. Results show its potential for building diagnostics and energy efficiency, offering a reliable tool for characterizing building wall thermal properties.

Nomenclature

temperature, K time coordinate, s surface heat transfer coeff., W.m⁻².K⁻¹ h ∞ wall length, m space coordinate, m parameter to be estimated Greek symbols thermal diffusivity, $\mathrm{m}^2.\mathrm{s}^{-1}$ thermal conductivity, $W.m^{-1}.K^{-1}$ Bi Biot number λ *Index and exponent*

right initial ambient air **Abbreviations** Tol tolerance ODE ordinary differential equation Dimensionless parameters Fo Fourier number

1. Introduction

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Accurately determining the thermophysical properties of building walls is essential for assessing the energy performance and design retrofitting scenarios. Those properties are determined by solving an inverse heat conduction problem. A so-called cost function measuring the discrepancy between the insitu experimental measurement in building walls and the direct problem simulation, is minimized to retrieve the unknown parameters [1]. Among all the techniques implemented to solve inverse problems in building walls, the gradient-based methods have been used in several works of the literature, as for instance in [2, 3]. Starting from an initial guess, those techniques iterates to estimate the unknown parameters that minimize the cost function. At each iteration, the new candidate parameters are computed

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using the direct problem solution and its sensitivity functions. These computations require the solution of partial differential equations and are directly related to the global computational cost of the gradient-based methods. It is worth investigation to reduce such computational burden.

Recently, in [4], a spectral method was developed as a reduced-order model for the solution of parametric problems of moisture transfer in building walls. This method enables to build a solution that depends on space, time coordinates and an extra parameter of the problem, such as the thermal diffusivity. By doing so, the computations of the solution and its sensitivity according to the thermal diffusivity are very fast and straightforward.

This work proposes to explore the use of such a spectral parametric solution in the framework of a gradient-based method to solve the inverse heat conduction problem. The main idea is to compute the parametric solution for a given range of thermal diffusivity before the estimation procedure. Then, during the online estimation process, the new candidate parameters are computed very quickly since no partial differential equations are solved. The reliability of the proposed approach is evaluated as follows: First, the error of the spectral parametric solution in computing the direct problem and its sensitivity function is evaluated against a given reference solution. Then, a benchmark is defined using synthetic data, ensuring a controlled environment. The accuracy and computational time of the proposed approach are assessed to prove its reliability.

The paper is organized as follows: Section 2 presents the mathematical problem in dimensionless form. Section 3 details the spectral reduced-order model technique, and Section 4 presents the inverse heat conduction problem. Section 5 covers the results of the case studies. The paper concludes with a summary of findings and potential future directions.

2. Mathematical problem

The one-dimensional heat diffusion equation is assumed in the domain $\Omega = [0, \ell]$ over the simulation horizon $[0, t_f]$:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}, \quad \forall x \in \Omega, \quad \forall t \in \left] 0, t_f \right], \tag{1}$$

where α is the thermal diffusivity. Convective heat transfer occurs at the boundaries, so that a ROBIN-type boundary condition is considered:

$$\lambda \frac{\partial T}{\partial x} = h^L \left(T - T_{\infty}^L(t) \right), \qquad x = 0, \quad \forall t \in \left[0, t_f \right], \tag{2a}$$

$$\lambda \frac{\partial T}{\partial x} = -h^R \left(T - T_{\infty}^R(t) \right), \qquad x = \ell, \quad \forall t \in \left[0, t_f \right], \tag{2b}$$

where λ is the thermal conductivity of the slab, h^L and h^R are the surface transfer coefficients and, T_{∞}^L and T_{∞}^R are the time dependent ambient air temperature. Initially, the slab is at constant temperature T_0 :

$$T(x, t = 0) = T_0, \quad \forall x \in \Omega.$$
 (3)

For numerical motivations, a dimensionless formulation of the problem (1),(2),(3) is obtained:

$$\frac{\partial u}{\partial t^{\star}} = \operatorname{Fo} \frac{\partial^{2} u}{\partial x^{\star 2}}, \quad \forall x^{\star} \in \left[0, 1\right], \qquad t^{\star} > 0$$
(4)

with boundary conditions:

$$\frac{\partial u}{\partial x^*} = \operatorname{Bi}^L \left(u - u_{\infty}^L \right), \quad \text{for } x^* = 0, \quad t^* > 0,$$

$$\frac{\partial u}{\partial x^*} = -\operatorname{Bi}^R \left(u - u_{\infty}^R \right), \quad \text{for } x^* = 1, \quad t^* > 0,$$

and initial condition:

$$u(x^{\star}, t^{\star} = 0) = 0, \quad \forall x^{\star} \in [0, 1].$$

To obtained such formulation, the following dimensionless quantities are defined:

$$u = \frac{T - T_0}{T_{\text{ref}} - T_0}, \ x^* = \frac{x}{\ell}, \ t^* = \frac{t}{t_{\text{ref}}}, \ \text{Bi}^L = \frac{h^L L}{\lambda}, \ \text{Bi}^R = \frac{h^R L}{\lambda}, \ \text{Fo} = \frac{\alpha t_{\text{ref}}}{\ell^2}.$$

3. Spectral parametric solution

In order to estimate the thermal diffusivity, it is necessary to compute both the direct problem and the sensitivity coefficient. The spectral parametric solution is used to solve both problems simultaneously. We will use the notation p to refer to the parameter to be estimated, in our case, p = Fo. Its description follows.

3.1. Solution of the direct problem

Before applying the spectral method, the range of the domains of the parameter p and x must be transformed to the canonical one [-1, 1] since we will be working with orthogonal polynomials. Thus, \bar{p} and \bar{x} represents the transformation to the desired interval.

The Spectral method assumes that the unknown u, which depends on (t^*, \bar{x}, \bar{p}) , can be accurately represented as a finite sum:

$$u(t^{\star}, \bar{x}, \bar{p}) \approx u_{nm}(t^{\star}, \bar{x}, \bar{p}) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij}(t^{\star}) \mathsf{T}_{i-1}(\bar{x}) \mathsf{P}_{j-1}(\bar{p}).$$
 (5)

Here, $\{\mathsf{T}_{i-1}\left(\bar{x}\right)\}_{i=1}^n$ and $\{\mathsf{P}_{j-1}\left(\bar{p}\right)\}_{j=1}^m$ are the sets of basis functions; $\{a_{ij}\left(t\right)\}_{i,j=1}^{n,m}$ are the corresponding time-dependent spectral coefficients, and $n\cdot m$ represents the number of degrees of freedom of the solution. Equation (5) can be seen as a series truncation after n and m modes. The CHEBYSHEV polynomials are chosen for the spatial and parametric basis functions [5].

Therefore, the residual R is written by substituting the approximation (5) into the governing equation (1), which leads to:

$$R(t^{\star}, \bar{x}, \bar{p}) = \sum_{i=1}^{n} \sum_{j=1}^{m} \left[\dot{a}_{ij}(t^{\star}) - \operatorname{Fo} \tilde{\tilde{a}}_{ij}(t^{\star}) \right] \mathsf{T}_{i-1}(\bar{x}) \mathsf{P}_{j-1}(\bar{p}), \tag{6}$$

where \dot{a} is defined as $\dot{a} \stackrel{\text{def}}{:=} \frac{\partial a}{\partial t^{\star}}$ according to NEWTON's notation. Spectral coefficients $\{\tilde{a}_{ij}(t^{\star})\}_{i,j=1}^{n,m}$ and $\{\tilde{\tilde{a}}_{ij}(t^{\star})\}_{i,j=1}^{n,m}$ are re-expressed in terms of $\{a_{ij}(t^{\star})\}_{i,j=1}^{n,m}$ according to the recursive expression of the derivatives.

The purpose is to minimize the residual $\|R(\bar{x}, t^*, \bar{p})\|_2 \longrightarrow \min$, which is performed via two methods: the TAU-GALERKIN and the Pseudospectral methods [4]. For this, the residual (6), is required to be orthogonal to the CHEBYSHEV basis functions $\langle R, \mathsf{T}_k \rangle = 0$ at the collocation points \bar{p}_p :

$$\langle R, \mathsf{T}_k \rangle = \int_{-1}^1 \frac{R(\bar{x}, t^*, \bar{p}_p) \mathsf{T}_k(\bar{x})}{\sqrt{1 - \bar{x}^2}} \, \mathrm{d}\bar{x} = 0,$$

The collocation points used here are the extrema points of the CHEBYSHEV polynomials. As a result, the projected residual can be written as:

$$\sum_{i=1}^{n} \sum_{j=1}^{m} \underbrace{\dot{a}_{ij}(t^{*})}_{\dot{A}} \underbrace{\mathsf{P}_{j-1}(\bar{p}_{p}) \int_{-1}^{1} \frac{\mathsf{T}_{i-1}(\bar{x})\mathsf{T}_{k}(\bar{x})}{\sqrt{1-\bar{x}^{2}}} d\bar{x}}_{\mathcal{M}} = \underbrace{\sum_{i=1}^{n} \sum_{j=1}^{m} \mathsf{Fo}_{p} \tilde{a}_{ij}(t^{*}) \mathsf{P}_{j-1}(\bar{p}_{p}) \int_{-1}^{1} \frac{\mathsf{T}_{i-1}(\bar{x})\mathsf{T}_{k}(\bar{x})}{\sqrt{1-\bar{x}^{2}}} d\bar{x}}_{\mathbf{G}}.$$
(7)

Equation (7) gives $(n-2) \cdot m$ equations. The extra coefficients are obtained by substituting the decomposed solution into the boundary conditions.

Thus, by using the Spectral approach to build the reduced-order model, the time-dependent coefficients $\{a_i(t^*)\}_{i,j=1}^{n,m}$ are computed by solving the following system:

$$\begin{cases}
M \dot{A}_{ij}(t^*) &= G(t^*, A_{ij}) + b(t^*, A_{ij}), \\
A_{ij}(0) &= A_0.
\end{cases}$$
(8)

Initial values of the coefficients $\{a_{ij}(t^*=0)\}$ are calculated by the projection of the initial condition $u_0(\bar{x})$.

Different approaches can be used to solve the system of Ordinary Differential Equations (ODE) presented in Equation (8). In this work, we shall employ ODE solvers, such as the ones based on numerical integration schemes. After solving the *reduced* system regarding a, it is possible to compose the solution of Equation (5) along with the CHEBYSHEV polynomial.

3.2. Computation of the sensitivity function

The sensitivity function of the temperature related to the parameter p is defined as:

$$X = \frac{\partial u}{\partial p}, \quad \forall x^* \in [0, 1], \quad \forall t^* \in [0, t_f^*]. \tag{9}$$

Given the spectral approximation of the solution, it is possible to compute the sensitivity function directly from Eq. (5):

$$X = \frac{\partial u_{nm}}{\partial \bar{p}} = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij}(t^{\star}) \mathsf{T}_{i-1}(\bar{x}) \frac{\partial \mathsf{P}_{j-1}}{\partial \bar{p}}(\bar{p}). \tag{10}$$

The derivative of the CHEBYSHEV polynomials is known analytically and can be presented in the recursive form:

$$\mathsf{P}_0'(\bar{p}) = 0\,, \qquad \mathsf{P}_1'(\bar{p}) = 1\,, \qquad \mathsf{P}_k'(\bar{p}) = 2\,\mathsf{P}_{k-1}(\bar{p}) + 2\,\bar{p}\,\mathsf{P}_{k-1}'(\bar{p}) - \mathsf{P}_{k-2}'(\bar{p})\,. \tag{11}$$

Therefore, once the spectral coefficients $\{a_{ij}(t^*)\}_{i,j=1}^{n,m}$ are known, one access directly, with a low computational cost, the solution of the direct problem and its sensitivity.

4. Inverse heat conduction problem

4.1. General consideration

The inverse heat conduction problem aims at computing the parameter $\hat{p} \in \Omega_p$ verifying:

$$\widehat{p} = \arg\min_{\Omega_p} J(p), \qquad (12)$$

where J is the least squares estimator:

$$J(p) = (\boldsymbol{Y} - \boldsymbol{T}(p))^{\top} (\boldsymbol{Y} - \boldsymbol{T}(p)), \qquad (13)$$

where T(p) is the solution of mathematical formulation (1),(2),(3) of the direct problem computed with the parameter p and set as described in [6], Y is the vector of temperature measurement.

4.2. GAUSS method for minimization with Spectral parametric solution

The minimization of the cost function (12) is realized using the GAUSS algorithm [6, 7]. The methodology is first recalled. It is an iterative process over iterations k, where the candidate $p^{(k+1)}$ is computed with the following equation:

$$p^{(k+1)} = p^{(k)} + (\mathbf{X}^{\top} \mathbf{X})^{-1} (\mathbf{X}^{\top} (\mathbf{Y} - \mathbf{T}(p^{(k)}))),$$
 (14)

where X is the sensitivity matrix computed at the M sensor positions and at time t^i , $i \in \{1, \ldots, I\}$. The iterative procedure of the GAUSS algorithm is implemented starting from the initial guess $p^{(0)}$. Two stopping criteria γ_1 and γ_2 are defined as a given tolerance (ToI) based on the magnitude of relative changes of the cost function and of the estimated parameter. The computation of the candidate $p^{(k+1)}$ in Eq. (14) requires the knowledge of the sensitivity matrix, defined by:

$$\boldsymbol{X} = \begin{bmatrix} \frac{\partial u}{\partial p}(x_1, t^1, p) & \dots & \frac{\partial u}{\partial p}(x_1, t^I, p) & \frac{\partial u}{\partial p}(x_2, t^1, p) & \dots & \frac{\partial u}{\partial p}(x_M, t^1, p) & \dots & \frac{\partial u}{\partial p}(x_M, t^I, p) \end{bmatrix}^{\top}.$$
 (15)

where I is the number of observation time and M is the number of sensor positioned in the wall.

In classical approaches, the sensitivity function $\frac{\partial u}{\partial p}$ is computed *on-line* with three typical approaches: finite differences approximation, solution of the sensitivity equations or complex-step differentiation. Here, the originality is to compute *off-line* (i.e. before solving the inverse problem) the spectral parametric solutions (5) and (10) so that during the on-line phase, Eq. (14) is computed very fast by just evaluating spectral solution at parameter $p^{(k)}$. Thus, with this approach, no numerical solution of partial differential equation is required through the iterations of the GAUSS algorithm. Algorithm 1 synthesized the main steps of the modified algorithm using Spectral parametric solution. In the classical version, there is no *off-line* phase. Furthermore, at step 8 as indicated in the algorithm, the temperature and sensitivity function needs to be assessed through numerical computations.

Algorithm 1 Modified GAUSS algorithm using Spectral parametric solution.

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1: — off-line phase — 2: Solve Eqs. (4) using spectral model reduction techniques 3: Save the spectral coefficients \left\{a_{ij}\right\} 4: — on-line phase — 5: Set p^{(0)} 6: k=0 7: while \gamma_1\geqslant Tol and \gamma_2\geqslant Tol do 8: Evaluate T(p^{(k)}) and \frac{\partial u}{\partial p}(p^{(k)}) using Eqs (5) and (10), respectively 9: Compute p^{(k+1)} using Eq. (14) 10: Compute J(p^{(k+1)}) 11: Compute convergence criteria \gamma_1 and \gamma_2 12: k\leftarrow k+1 13: end while
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5. Results

5.1. Description of the case study

Simulations are performed for a time period of $t_{\rm f}=24$ h, in a slab of length $\ell=0.2$ m . The surface transfer coefficients are $h^L=50$ W . m $^{-2}$. K $^{-1}$ and $h^R=5$ W . m $^{-2}$. K $^{-1}$, respectively. The boundary conditions are expressed as sinusoidal variations of 12 and 24 h periods:

$$T_{\infty}^{L}\left(t\right) = 20 \; + \; 10 \; \sin\left(\frac{2 \, \pi \, t}{12 \cdot 3600}\right) \; + \; 8 \; \sin\left(\frac{2 \, \pi \, t}{24 \cdot 3600}\right) \; , \qquad \qquad T_{\infty}^{R}\left(t\right) = 20 \; + \; 16 \cdot \sin\left(\frac{2 \, \pi \, t}{24 \cdot 3600}\right) \; . \label{eq:T_initial_transformation}$$

The initial condition is $T_0=20~{\rm ^{\circ}C}$. The domain of variation of the thermal diffusivity is $[0.1,5.5]~{\rm mm^2}$. s $^{-1}$.

5.2. Verification of the Spectral parametric solution

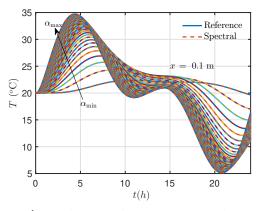
To verify the numerical solution provided by the parametric spectral approach, it is compared with a reference solution provided by the MatlabTM open-source toolbox Chebfun. Therefore, the error between the simulated solution and the reference solution is determined using the EUCLIDEAN norm and its maximal and mean values, which are defined as in [4].

The parametric problem considers 50 different values of diffusivity α between $0.1 \, \mathrm{mm}^2 \cdot \mathrm{s}^{-1}$ and $5.5 \, \mathrm{mm}^2 \cdot \mathrm{s}^{-1}$. The reference solution used in the verification is built with the Chebfun toolbox. The

reference solution of the sensitivity function was computed using the whole definition of the problem, while the spectral approach computed the solution using equation (10).

To perform this case study, the Spectral-Parametric approach used n=10 modes for the spatial basis and m=20 modes for the parametric basis, with the tolerance of the solver ode15s set to Tol = 10^{-4} . The solution is projected on a grid composed by $dx^* = 2 \cdot 10^{-2}$ and $dt^* = 10^{-2}$. The time step of solver ode15s is adaptive, but we can choose to have the output in the time step we want. The solver will integrate the solution with its time step and then give the solution on the time step asked.

Figure 1 presents the evolution of the temperature in the middle of the material, at $x=0.1\,\mathrm{m}$. The solution of the proposed method agrees with the reference one on the order of $\mathcal{O}(10^{-4})$. Figure 2 shows the evolution of the scaled sensitivity function also in the middle of the spatial domain. The Spectral-parametric approach is in good agreement with the reference solution, with the error on the order of $\mathcal{O}(10^{-2})$. We lose two orders of accuracy in the computation of the sensitivity problem because we are dealing directly with the derivative definition. Even if it is computed analytically, it is still an approximation.



 $\begin{array}{c} 6 \\ 4 \\ 2 \\ 2 \\ 3 \\ 4 \\ 4 \\ 6 \\ -8 \\ 0 \end{array}$

Figure 1 : Evolution of the temperature at the center of the material.

Figure 2: Evolution of the scaled sensitivity function at the center of the spatial domain.

The error ε_{∞} is shown as a function of α in Figure 3. As the value of the diffusivity coefficient α increases, the error decreases because the diffusion process becomes less stiff, making it easier to solve. The convergence of the solution \boldsymbol{X} with respect to the number of spectral modes m is presented in Figure 4 for different numbers of parameters N_{α} . As observed, the error decreases as the number of modes increases. To maintain good accuracy of the solution \boldsymbol{X} , a minimum of 20 modes is required. For more than 30 parameters, increasing the number of modes is not worthwhile because the computational effort will also increase. The same analysis is performed for the convergence of the solution of u and the error is two orders of magnitude $O(10^{-2})$ more precise.

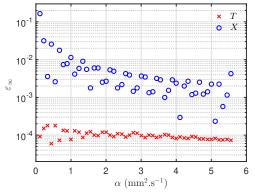


Figure 3: Maximum error of the temperature field and the sensitivity coefficient as a function of the diffusivity value.

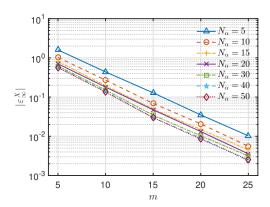


Figure 4: Convergence of the spectral modes m for the sensitivity coefficient X for different quantities of the diffusivity parameter N_{α} .

5.3. Parameter estimation problem

The procedure to evaluate the reliability of the proposed methodology for inverse heat conduction problem is divided into two steps. First, synthetic experimental observations are generated using a numerical model based on finite-differences and the Du Fort-Frankel numerical method [8]. The *real* parameter used for these computations is denoted $\alpha^{\rm r}=0.55$ mm² . s⁻¹. The sensor position is located in the middle of the slab and the time step between two measurements is 30 min. To simulate experimental data, a noise of 0.5 °C is added to the numerical results. A total of $N_s=10^4$ samples of synthetic observations are generated *in silico*. The second steps consists in solving the parameter estimation problem using the GAUSS method with Spectral parametric solution or with the classical approach. For the former, the solution is computed *off-line* for n=10 and m=20 modes, which guarantees a satisfying accuracy according to the results in previous section. For the latter, the sensitivity function is computed using the sensitivity equation, combined with a Du Fort-Frankel numerical scheme. The initial parameter is sampled uniformly in the interval of thermal diffusivity [0.1, 5.5] mm² . s⁻¹. For the stopping criteria, the tolerance in the GAUSS algorithm are set to Tol $=10^{-6}$.

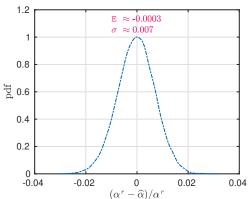


Figure 5 : The probability density function (pdf) of the relative error on the estimated parameter.

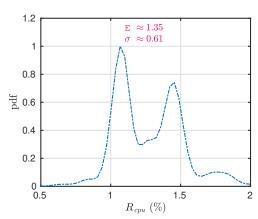


Figure 6: The probability density function (pdf) of the computational time ratio to estimate the parameter.

To evaluate the reliability of the estimation procedure, the expectation E and the standard deviation σ are computed using the N_s samples of a random variable. Figure 5 presents the probability density function of the relative error on the estimated parameter using the Spectral parametric approach. For all the N_s tests, the method estimates the unknown diffusivity with a very satisfying accuracy. The expectation of the relative error is 0.03% with a standard deviation of 0.7%. Figure 6 shows the probability of the computational time ratio reported to the classical approach (The computational time is measured in the Matlab™ environment, on a computer equipped with Intel Xeon(R) Gold, 2.2GHz and 125.6 GB of RAM). The proposed method is faster than the classical approach, with a computation time of only 0.0155 (1.55%) of that of the classical approach. In other words, the parametric solution approach enables to cut by 74 the computational cost of the classical approach to estimate the unknown parameter. As presented in Figure 7, the classical and Spectral parametric solution requires the same number of iterations to estimate the parameters. Thus, the computational gain are due to the off-line computations of the parametric solution and its sensitivity function. Last, Figure 8 compares the synthetic data sample of temperature with the Spectral solution computed with the parameter at iteration k=0 and with the estimated parameter. A satisfying agreement is observed between the calibrated model and the measurement.

6. Conclusion

This article investigates the use of a Spectral parametric solution to reduce the computational cost of inverse heat conduction problem using the GAUSS algorithm. The parametric solution is computed *offline*, *i.e.* before the GAUSS iterative process. It enables direct access to the solution of the direct problem

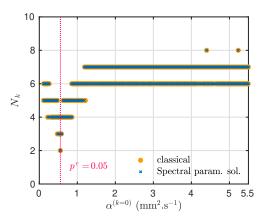


Figure 7: Number of iterations to estimate the parameter according to the N_s sampled initial parameter

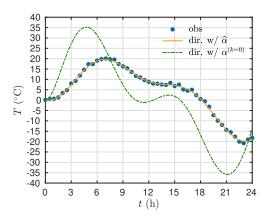


Figure 8: Evolution of one synthetic data sample (obs) and the spectral parametric solution of the direct problem, for initial guess and the estimated parameter.

and its sensitivity. In this way, during the *on-line* process of the algorithm, there is no need to solve the direct problem nor the sensitivity equations to compute the new candidate of the estimated parameter. The reliability and efficiency of the proposed approach is evaluated on a case study where the thermal diffusivity of a mono-layer wall is unknown. A total of 10^4 different samples of synthetic observations are generated to test this methodology. Then, for each set of synthetic observations, the inverse problem is solved using the Spectral parametric solution. The method demonstrates good accuracy and efficiency, with a computational run time corresponding to only 1.55% of the standard approach. Future works should focus on extending the methodology for more complex heat transfer problem with measured experimental data.

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