Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2026 (44) 18** : 1–13.
ISSN-0037-8712
doi:10.5269/bspm.82855

Comparative Study of MFS with Tikhonov and RSVD for the Backward Heat Conduction Problem

Mohammed Baati, Mohamed Louzar and Abdellah Lamnii

ABSTRACT: This paper investigated an application designed to identify the most effective regularization technique by employing a meshless method of fundamental solutions to address the backward heat conduction problem (BHCP), which is characterized by its ill-posed nature. To enable a comparative analysis, this study applies both the Tikhonov and Randomized Singular Value Decomposition regularization methods to improve solution accuracy and stability. The numerical results from two benchmark examples are presented in this paper.

Keywords: Inverse problem, heat conduction, method of fundamental solutions, tikhonov, randomized singular value decomposition.

Contents

1. Introduction and preliminaries

Partial differential equations (PDEs) model many physical processes that involve variations in space and time. Because exact solutions are often unavailable, numerical methods are essential for approximating them [1,2]. Therefore, PDEs play a central role in applied mathematics, simulations, and scientific computing [3,4,5,6].

The backward heat conduction problem (BHCP) is a classic example of an ill-posed inverse problem under the heat equation. The goal is to determine the initial temperature distribution from known data on temperatures at a later time [7]. Small errors in the final data measurements may not only lead to large variations in the reconstructed solutions but also indicate high sensitivity; this is indeed a highly sensitive problem. Therefore, regularization techniques are necessary rather than optional when seeking meaningful and dependable results from such inherently unstable problems. Some numerical methods that have been successfully formulated to address this particular problem include the Method of Fundamental Solutions (MFS) and Tikhonov regularization.

The MFS is a stable meshless numerical scheme for solving boundary value problems governed by linear partial differential equations (PDE) [8,9,10]. Thus, there is no need for domain meshing or numerical integration; hence, simplicity, accuracy, and very low computational cost can be considered its main advantages. The boundary conditions are imposed at some collocation points, and the solution is assumed to be in the form of a linear combination of fundamental solutions satisfying the governing PDE [11].

2020 *Mathematics Subject Classification:* 78A46, 80A23.
Submitted March 20, 2026. Published June 22, 2026.

The MFS has been successfully used for time-dependent heat transfer and various elliptic and parabolic problems [12]. The MFS has also been extended for layered materials [13], free-surface and inverse Stefan problems [14], and even the inverse Cauchy–Stefan problem [15], where the approach showed exceptional adaptability when paired with appropriate regularization methode.

Randomized singular value decomposition is an effective technique for estimating the dominant singular components of large matrices. Random projections are used to reduce the dimensionality and capture the most important features. Compared to the traditional Singular Value Decomposition, the computational costs are significantly reduced. The RSVD efficiently reduces the impact of noise and ill-conditioning by truncating smaller singular values. As such, it provides a reliable and precise solution to several inverse problems [16].

The primary contribution of this paper is to compare, in detail, the usefulness of combining the Method of Fundamental Solutions (MFS) with two methods of regularization, Tikhonov regularization and Randomized Singular Value Decomposition, to successfully solve the Backward Heat Conduction Problem. The implemented computational framework enables the performance evaluation of each method's ability to produce accurate and numerically stable solutions when applied to ill-posed inverse problems. We conducted systematic numerical experiments to evaluate the effect of each technique on the quality of the reconstructed initial temperature distributions. We also examined the extent to which the reconstructed solutions exhibited sensitivity to noise and the selection of parameters. We also compared the computational efficiency and convergence rate of each technique to illustrate the benefits of using the RSVD-based approach to reconstruct the BHCP. Together, our comparisons provide valuable guidance on which method is likely to yield stable and precise results for reconstructing the BHCP.

The remainder of this paper is structured as follows: The mathematical formulation of The BHCP is described in Section 2. Section 3 describes the MFS from the perspective of linear combinations of fundamental solutions; Section 4 describes how the MFS is implemented for Tikhonov and regularized singular value decomposition; and Section 5 presents two numerical examples showing how accurate and stable approximations can be achieved efficiently.

2. Mathematical formulation

Let x be in R, and let $T > 0$ be a real number. A one-dimensional bounded domain in R with a smooth boundary surface $\Gamma = \partial D$, where C^2 smoothness is sufficient, is called conduction domain D. $\overline{D} = D \cup \Gamma$ represents the closure of the domain D. We define

$$D_T = D \times (0, T], \quad \Gamma_T = \Gamma \times (0, T],$$

and their closures are given by

$$\overline{D_T} = \overline{D} \times [0, T], \quad \overline{\Gamma_T} = \Gamma \times [0, T],$$

respectively.

Our goal is to find the function u that solves the heat equation in the region D_T with the prescribed time and boundary values. Therefore, u is the solution to the following problem:

$$\frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) = 0, (x,t) \in D_T \tag{2.1}$$

$$u(x,t) = h(x,t), (x,t) \in \Gamma_T \tag{2.2}$$

$$u(x,T) = u_T(x), x \in D \tag{2.3}$$

where $u_T(x)$ and $h(x,t)$ are assumed to be sufficiently smooth functions.

It is important to note that with only slight modifications to the MFS implementation, the Neumann boundary condition can be used in place of the Dirichlet boundary condition.

Moreover, while the solution to the BHCP, as delineated by equations (2.1)–(2.3), is unique, it does not demonstrate a continuous dependence on boundary condition (2.2) and the final data (2.3), as observed in [17]. Several studies have proposed restrictive classes of smooth or analytic functions to ensure the well-posedness of the BHCP. However, these ideal conditions are rarely encountered in practice. Consequently, regularization techniques are frequently employed to derive approximate solutions with satisfactory accuracy and convergence properties.

3. Method of fundamental solutions

We refer to the fundamental solutions found in [18] for the one-dimensional heat Equation (2.1).

$$E(x,t,y,\mu) = \frac{H(t-\mu)}{(4\pi(t-\mu))^{\frac{1}{2}}} e^{\frac{-(x-y)^2}{4(t-\mu)}}$$

The Heaviside function is denoted by H.
We aim to develop a solution u that resides in this domain

$$D_T = [0, 0.5] \times [0, T],$$

where $D = (0, 0.5)$, $\Gamma = \{0, 0.25\}$ represents the boundary of D_T, $\Gamma_E = \{-h, 0.5 + h\}$ denotes an external boundary with $d(\Gamma, \Gamma_E) = h > 0$, and $T > 0$ signifies the final time point, which resolves

$$\frac{\partial u(x,t)}{\partial t} - \frac{\partial^2 u(x,t)}{\partial x^2} = 0, (x,t) \in D_T \tag{3.1}$$

$$u(0,t) = h_1(t), t \in (0,T] \tag{3.2}$$

$$u(0.5,t) = h_2(t), t \in (0,T] \tag{3.3}$$

$$u(x,T) = u_T(x), x \in D_T \tag{3.4}$$

We propose a new version of the method of fundamental solutions to approximate the Eqs. (3.1)–(3.4). The approach represents the solution as a linear combination of the fundamental solutions presented in [18]. This formulation enables an accurate and efficient numerical approximation.

$$u_\infty(x,t) = \sum_{j=1}^{2} \sum_{n=1}^{\infty} c_n^{(j)} E\big(x,t,y_j(\mu_n),\mu_n\big), (x,t) \in D_T \tag{3.5}$$

Using the MFS to approximate the BHCP states keeps a finite set of terms in (3.5) and truncates after that point, so it can be feasible to compute while still maintaining accuracy in the solution. The finite set of terms selected adequately describes the main features of the solution.

$$u_N(x,t) = \sum_{j=1}^{2} \sum_{n=1}^{2N} c_n^{(j)} E\big(x,t,y_j(\mu_n),\mu_n\big), (x,t) \in D_T \tag{3.6}$$

The following time points were used to create collocation points:

$$t_i = \frac{i}{M_1} T, \quad i = 1, \ldots, M_1$$

and on D_T let

$$x_T^{(l)} = \frac{l}{K+1}, \quad \ell = 1, \ldots, K$$

Boundary conditions (3.2)–(3.4) are applied to estimate the coefficients $c_n^{(j)}$ using relation (3.6) through collocation at predetermined collocation points. By applying these boundary conditions, the unknown coefficients can be evaluated. Using this method, a linear system of the main equations was created, and an approximate solution to the BHCP was obtained by solving this linear system.

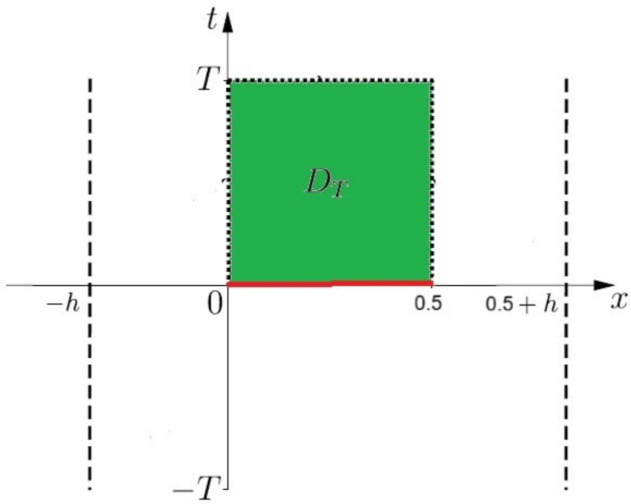

Figure 1: The domain is represented over time with collocation, source points, and boundary distribution.

$$u_N\left(x_T^{(l)},0\right)=u_T\left(x_T^{(l)}\right),\ell=1,\ldots,K \tag{3.7}$$

$$u_N(0,t_i)=h_1(t_i),i=1,\ldots,M \tag{3.8}$$

$$u_N(1,t_i)=h_2(t_i),i=1,\ldots,M \tag{3.9}$$

In this case, we develop a system for A, which represents a linear system of equations (3.7)–(3.9). Because A is ill-conditioned, small variations in our inputs may yield large variations in our output. To guard against instability in such systems, we utilize Tikhonov regularization, which adds a penalty imbalance between the goodness of fit for our data and the smoothness of our predicted curve. In contrast, the RSVD method allows for an approximation of A with a low rank, so that we can perform our calculations at a lower cost without sacrificing accuracy. Both methods provide improved numerical stability to the solution. For these reasons, we can confidently compute the coefficients of $c_n^{(j)}$, even in the presence of noise or missing data.

4. Regularization methods

The system of equations, as presented in (3.7)–(3.9) for a one-dimensional context, can be expressed in the following general form:

$$Ac=g \tag{4.1}$$

The BHCP is intrinsically ill-posed, although the matrix A generated by the MFS is typically ill-conditioned. A stable solution was obtained using Tikhonov regularization. When a square or overdetermined system is represented by $M\geq N$, we solve the problem by

$$\left(A^TA+\lambda I\right)c=A^Tg \tag{4.2}$$

where I is the identity matrix, and λ is a regularization parameter that controls the quality of the approximate solution. The L-curve criterion is used to determine the regularization parameter $\lambda\geq 0$; see [19,20].

Principal information is extracted from the convolution using random singular value decomposition (SVD). The main goal of this method is to calculate a q-rank approximation of matrix A, where q≪n.

$$\tilde{A}_q = \tilde{U}\tilde{\sum}\tilde{V}^{t_f}$$

In this context, the matrices U and V are orthogonal unitary matrices of size $n \times q$, which means that their columns form orthonormal bases in $\mathbb{R}^n$. The reduced matrices $\tilde{U} = (\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_q)$ and $\tilde{V} = (\tilde{v}_1, \tilde{v}_2, \dots, \tilde{v}_q)$ preserve this orthonormality and represent the main singular directions of the original matrix A. The diagonal matrix $\tilde{\Sigma}$ holds the nonzero approximate singular values $\tilde{\sigma}_1, \tilde{\sigma}_2, \dots, \tilde{\sigma}_q$, each of which is sorted in descending order, such that $\tilde{\sigma}_1 > \tilde{\sigma}_2 > \cdots > \tilde{\sigma}_q > 0$.This arrangement establishes a clear hierarchy of the contributions of each singular component to the approximation of A. In practical terms, the largest singular values capture the most significant energy of the system, whereas the smaller ones correspond to less important components. Consequently, the triplet $(\tilde{U}, \tilde{V}, \tilde{\Sigma})$ provides a compact and numerically stable approximation of the SVD of A.

Below is a detailed exposition of the procedure for the randomized SVD (RSVD) algorithm [21]:

Algorithm 1: Randomized Singular Value Decomposition (RSVD)

Data: Matrix $A \in \mathbb{R}^{m\times n}$, target rank k, oversampling parameter p
Result: Rank-k approximation $A \approx U_k \Sigma_k V_k^T$
Step 1: Random Sampling
Generate a Gaussian random matrix $\Omega \in \mathbb{R}^{n\times(k+p)}$.
Form the sample matrix: $Y = A\Omega$.
Step 2: Orthogonalization
Compute the QR factorization of Y: $Y = QR$, where $Q \in \mathbb{R}^{m\times(k+p)}$ has orthonormal columns.
Step 3: Projection
Project A onto the subspace spanned by Q: $B = Q^T A$.
Step 4: Reduced SVD
Compute the singular value decomposition of the reduced matrix: $B = \widetilde{U}\Sigma V^T$.
Construct the approximate left singular vectors: $U = Q\widetilde{U}$.
Truncation
Retain the k dominant singular values and corresponding singular vectors.
Return: $A \approx U_k \Sigma_k V_k^T$.

Because the obtained linear system is well conditioned, it can be effectively handled using traditional numerical methods. Among these, the Gaussian elimination method provides a straightforward and reliable procedure for solving these systems. Its computational simplicity and stability make it suitable for this type of problem. Therefore, any classical approach, such as Gaussian elimination, can be successfully applied [22].

5. Numerical results

The numerical experiments conducted to evaluate the effectiveness of the Method of Fundamental Solutions in combination with Tikhonov [23] and rSVD regularization are described in this section. Two illustrative examples were used to evaluate the proposed method, successfully demonstrating its accuracy and stability.

5.1. Example 1

We applied the numerical scheme to verify the accuracy and stability of a one-dimensional test case using meshless techniques. In this context, the exact analytical solution is provided as a standard by which to evaluate the effectiveness of the proposed meshless approach.

$$u(x,t) = \sin(\pi x)\,\exp(-\pi^2 t), (x,t) \in [0, 0.5] \times [0, T] \tag{5.1}$$

The following final and boundary conditions result from the use (5.1) to produce the required data.

$$u(0,t) = 0, t \in (0,T] \tag{5.2}$$

$$u(0.5,t) = \exp(-\pi^2 t), t \in (0,T] \tag{5.3}$$

$$u(x,T) = \sin(\pi x)\ \exp(-\pi^2 T), x \in (0, 0.5) \tag{5.4}$$

The final data (5.4) were supplemented with random additive noise as follows:

$$u_T^\delta(x) = \sin(\pi x)\ \exp(-\pi^2 T) + N(0, \sigma^2) \tag{5.5}$$

A normal distribution with a mean of zero and a standard deviation of σ is represented by the notation $N(0, \sigma^2)$. This probabilistic model represents the random noise or uncertainty that affects the system.

$$\sigma = \delta \max_{x \in D} |u_T| = \delta\ \exp(-\pi^2 T)$$

where the relative noise level is represented by δ. This example aims to numerically recover the initial data at time t = 0, which is provided by

$$u(x,0) = \sin(\pi x), x \in (0, 0.5) \tag{5.6}$$

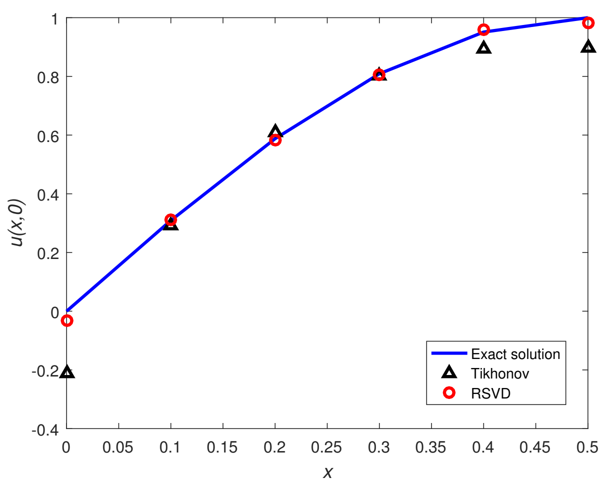

Figure 2: Comparison between the exact solution and the MFS approximation obtained using two regularization methods for $h = 1$, $\lambda = 10^{-2}$, $T = 0.25$, $N = 128$ and $\delta = 5\%$.

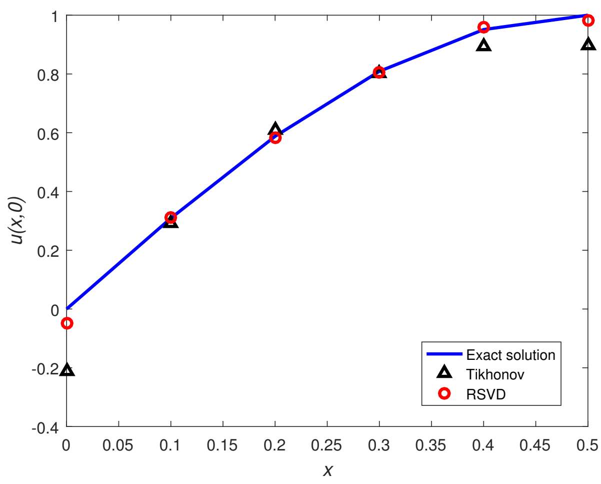

Figure 3: Comparison between the exact solution and the MFS approximation obtained using two regularization methods for $h = 1$, $\lambda = 10^{-2}$, $T = 0.25$, $N = 128$ and $\delta = 10\%$.

In this numerical example, the objective was to reconstruct the initial condition $u(x,0)$. Figure 2 and 3 present a comparison of the Method of Fundamental Solutions outcomes obtained using the two regularization techniques: Tikhonov and randomized singular value decomposition. The parameters considered included $\lambda = 10^{-2}, h = 0.5, T = 0.25, N = 128$, and noise levels of $\delta = 5\%$ and $\delta = 10\%$. The approximation confirmed the effectiveness of the MFS by demonstrating that both approaches closely resembled the exact solution. However, the results from the rSVD approach are smoother and more stable, particularly in the vicinity of the boundary regions, where the classical Tikhonov method tends to oscillate. This finding implies that rSVD provides improved numerical stability and robustness against noise. Overall, the accuracy and computational efficiency of the backward heat conduction problem were enhanced by the rSVD-based regularization.

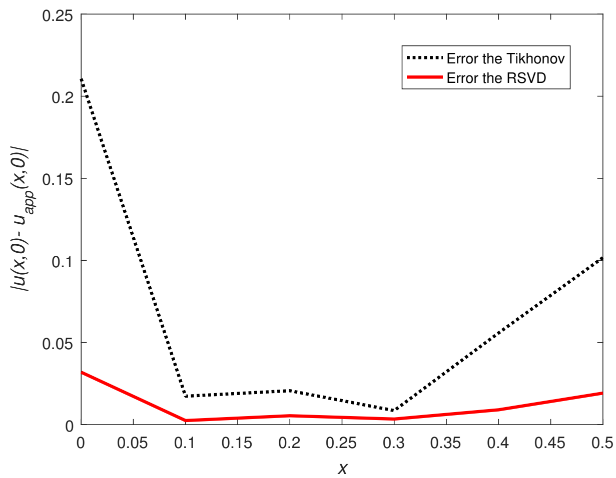

Figure 4: Evaluation of reconstruction errors using two regularization methods, with parameters specified as $h = 1$, $\lambda = 10^{-2}$, $T = 0.25$, $N = 128$, and $\delta = 5\%$.

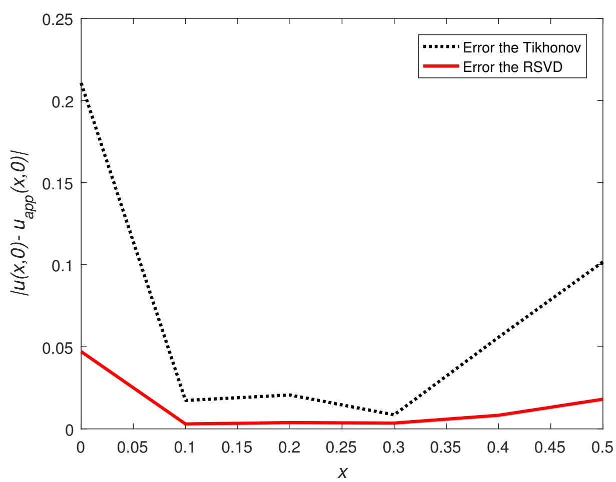

Figure 5: Evaluation of reconstruction errors using two regularization methods, with parameters specified as $h = 1$, $\lambda = 10^{-2}$, $T = 0.25$, $N = 128$, and $\delta = 10\%$.

The MFS error comparison between the RSVD and Tikhonov regularization methods is shown in Figure 4 and 5 for noise levels $\delta = 5\%$ and $\delta = 10\%$, as well as the exact analytical solution. The results show that the MFS with RSVD regularization is numerically more stable throughout the entire computational domain than the Tikhonov regularization methods. In addition, RSVD had consistently fewer error magnitudes than Tikhonov regularization, particularly at the boundary and at later times of computation, indicating that it better reduces the effects of ill-conditioning associated with the BHCP. The MFS-RSVD scheme produced a more accurate and reliable approximation of the actual temperature distribution. In summary, RSVD regularization has been demonstrated to be as stable and precise as the traditional Tikhonov method for solving the BHCP.

Table 1: Error in noise levels on Tikhonov and RSVD methods using MFS

N	Noise levels	Tikhonov	RSVD
128	1%	2.106×10^{-1}	7.56×10^{-2}
128	3%	2.106×10^{-1}	4.79×10^{-2}
128	5%	2.106×10^{-1}	2.50×10^{-2}
128	7%	2.109×10^{-1}	6.05×10^{-2}
128	10%	2.107×10^{-1}	3.56×10^{-2}

Table 1 presents the impact of increasing noise levels on the performance of the Tikhonov and RSVD regularization methods in the MFS framework. For a fixed number of boundary points $N = 128$, the Tikhonov method demonstrates nearly constant error values, indicating low sensitivity to noise perturbations. Conversely, the RSVD approach achieved significantly lower errors across all noise levels, indicating enhanced numerical accuracy. Although minor fluctuations were observed as the noise level increased, the RSVD consistently maintained greater accuracy than that of Tikhonov. These findings confirm the robustness and efficacy of the RSVD in addressing noisy inverse problems.

5.2. Example 2

Our goal in this example is to determine an approximation for the inverse problem in one dimension as follows:

The precise solution provided by

$$u(x,t) = \sin(\pi x/2)e^{(-\pi^2 t/4)} \tag{5.7}$$

At the fixed boundary x=0, the Dirichlet and Neumann boundary conditions are provided by

$$u(0,t) = 0, t \in [0, 0.25] \tag{5.8}$$

$$u(0.5,t) = \sin(\pi/4)e^{(-\pi^2 t/4)}, t \in [0, 0.25] \tag{5.9}$$

$$u(x,T) = \sin(\pi x/2)e^{(-\pi^2 T/4)} \tag{5.10}$$

The final data (5.10) were supplemented with random additive noise that simulated measurement errors as follows:

$$u_T^\delta(x) = \sin(\pi x/2)e^{(-\pi^2 T/4)} + N(0,\sigma^2), x \in [0, 0.5] \tag{5.11}$$

Where σ is the relative noise level.

The objective of this example is to recover the data numerically at the initial condition specified by

$$u(x,0) = \sin(\pi x/2), x \in [0, 0.5] \tag{5.12}$$

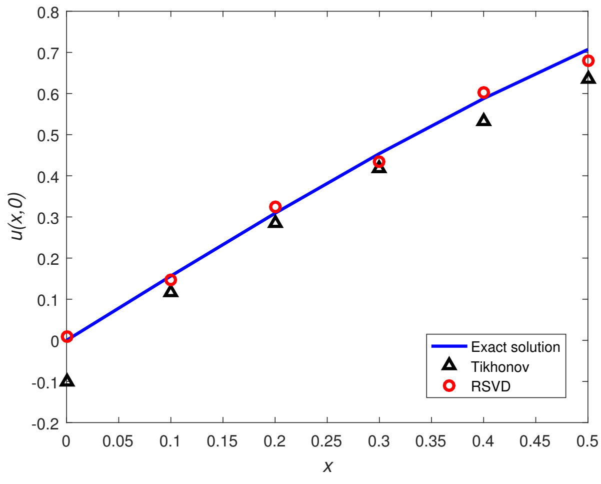

Figure 6: Comparison between the exact solution and the MFS approximation obtained using two regularization methods for $h = 1.7$, $\lambda = 10^{-2}$, $T = 1$, $N = 128$ and $\delta = 5\%$.

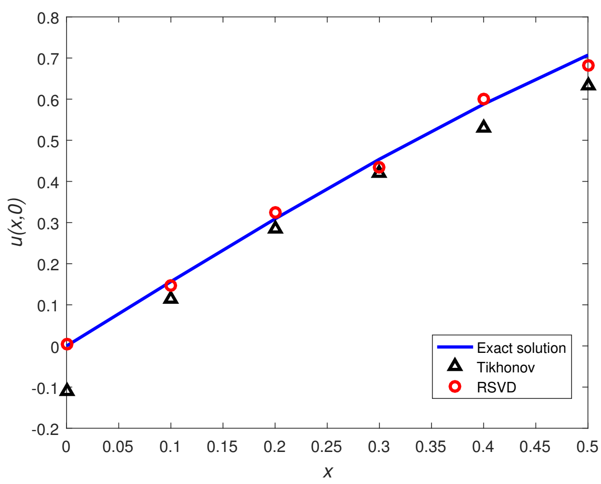

Figure 7: Comparison between the exact solution and the MFS approximation obtained using two regularization methods for $h = 1.7$, $\lambda = 10^{-2}$, $T = 1$, $N = 128$ and $\delta = 10\%$.

In this numerical test, the aim was to reconstruct the initial condition $u(x, 0)$ for the Backward Heat Conduction Problem. Figure 6 and 7 show a comparison between the MFS results obtained using the Tikhonov and randomized SVD regularization methods. The parameters adopted in this simulation were $h = 1.7, \lambda = 10^{-2}, T = 1, N = 128$, and noise levels of $\delta = 5\%$ and $\delta = 10\%$. The numerical results revealed that both regularization approaches successfully approximated the exact solution, thereby validating the effectiveness of the MFS formulation. However, the rSVD-based regularization yielded smoother and more stable results, particularly near the domain boundaries, where the Tikhonov method exhibited oscillatory behavior. This confirms that the rSVD method provides better noise resistance and improved numerical stability for the BHCP than the Tikhonov regularization.

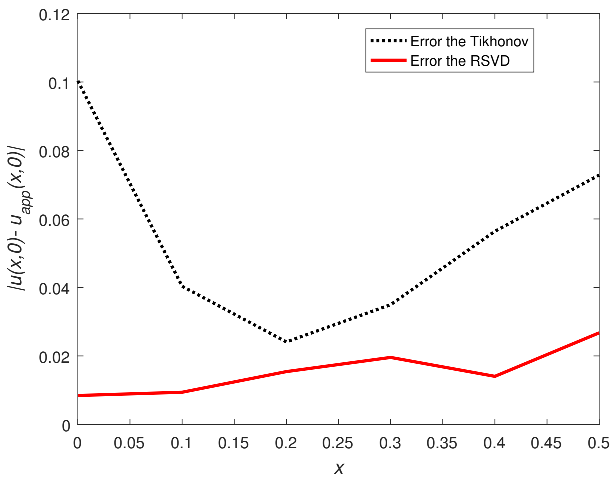

Figure 8: Evaluation of reconstruction errors using two regularization methods, with parameters specified as $h = 1.7$, $\lambda = 10^{-2}$, $T = 1$, $N = 128$ and $\delta = 5\%$.

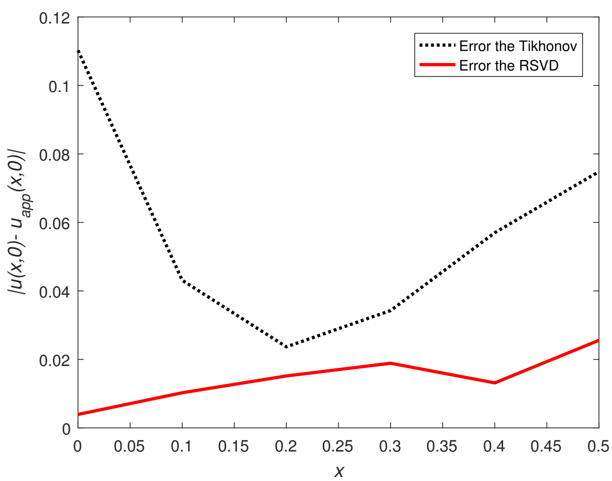

Figure 9: Evaluation of reconstruction errors using two regularization methods, with parameters specified as $h = 1.7$, $\lambda = 10^{-2}$, $T = 1$, $N = 128$ and $\delta = 10\%$.

Figures 8 and 9 show a comparison of the error distributions when working with the MFS while using two types of regularization: Tikhonov and randomized SVD with noise levels of $\delta = 5\%$ and $\delta = 10\%$. We also include an analytical solution for reference to see how closely the numerical results compare with it. From this information, it is clear that using MFS with RSVD regularization produces more stable numerical results across all areas within the computational domain than using MFS with Tikhonov regularization. Additionally, the RSVD produced lower error levels than the Tikhonov results. Therefore, the RSVD successfully mitigated the negative impact of the ill-conditioned behavior associated with the BHCP, resulting in a more accurate and stable estimation of the temperature field using the MFS and RSVD. Overall, the findings demonstrate the greater robustness and computational efficiency of the RSVD regularization technique compared with the standard Tikhonov regularization technique for resolving BHCP.

Table 2 reports the reconstruction errors obtained by the Tikhonov and RSVD regularization methods using MFS for different noise levels with a fixed number of boundary points $N = 128$. The Tikhonov

Table 2: Error in noise levels on Tikhonov and RSVD methods using MFS

N	Noise levels	Tikhonov	RSVD
128	1%	1.001×10^{-1}	2.66×10^{-2}
128	3%	1.028×10^{-1}	2.62×10^{-2}
128	5%	1.003×10^{-1}	2.67×10^{-2}
128	7%	1.007×10^{-1}	2.64×10^{-2}
128	10%	1.102×10^{-1}	2.56×10^{-2}

method showed relatively stable but higher error values as the noise level increased. In contrast, the RSVD approach consistently achieved significantly lower errors, demonstrating superior robustness to noise.

6. Conclusion

We investigated how the Method of Fundamental Solutions can be used to reconstruct the initial condition of the one-dimensional Backward Heat Conduction Problem. To stabilize the ill-posed nature of this inverse problem, two different regularization methods were employed: Tikhonov and randomized Singular Value Decomposition. Numerical implementation was performed using a noisy dataset to assess the robustness and reliability of each regularization technique. The results of our analysis suggest that both the Tikhonov and RSVD regularization techniques produce results that replicate the exact solutions of the BHCP; however, the MFS combined with the RSVD regularization is smoother and more stable than the Tikhonov regularization technique in areas where the Tikhonov regularization oscillates. The enhancement of the RSVD regularization results is primarily due to the selective truncation of smaller singular values through randomization, which filters out both the noise and the numerical instability associated with these values. Therefore, RSVD regularization provides a more accurate and computationally efficient method for reconstructing initial conditions than the classical Tikhonov regularization method. Overall, the results of our study demonstrate that the combination of MFS and RSVD provides a viable and credible route for solving the BHCP.

The results of the numerical experiments presented in this research demonstrate that the Method of Fundamental Solutions (MFS) is both extremely effective and stable when applied to reconstruct the initial condition for the solution to the Backward Heat Conduction Problem. Moreover, our results show that this method provides highly accurate results when the input data are contaminated with noise, indicating that MFS is also a robust method for solving ill-posed problems. This indicates the potential of the MFS framework as a reliable numerical tool for inverse heat transfer analyses. Further research will focus on extending the proposed method to more complex system configurations. This will include investigations of both direct heat conduction problems and the two-dimensional Inverse Stefan Problem. Extensions of this methodology will allow researchers to explore the versatility and efficiency of the MFS for a broader array of thermal problems. Fuzzy theory applications and stochastic decision-making processes proposed by [24,25] can be useful building blocks for improving the robustness of regularization methods in inverse problem settings.

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Mohammed BAATI,

Department of Mathematics and Computer Science,

Hassan First University of Settat, FST, MISI Lab, Settat,

Morocco.

E-mail address: `m.baati@uhp.ac.ma`

and

Mohamed LOUZAR,

Department of Mathematics and Computer Science,

Hassan First University of Settat, FST, MISI Lab, Settat,

Morocco.

E-mail address: `mohamed.louzar@uhp.ac.ma`

and

Abdellah LAMNII,
Department of Mathematics and Computer Science,
Abdelmalek Essaadi University, ISI, ENSATé, 93030 Tetouan,
Morocco.
E-mail address: a.lamnii@uae.ac.ma