A New Quasi-Boundary Scheme for Three-Dimensional Backward Heat Conduction Problems

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Abstract: In this study, we employ a semi-analytical scheme to resolve the three-dimensional backward heat conduction problem (BHCP) by utilizing a quasi-boundary concept. First, the Fourier series expansion method is used to estimate the temperature field $u(x, y, z, t)$ at any time $t < T$. Second, we ponder a direct regularization by adding an extra term $\alpha(x, y, z, 0)$ to transform a second-kind Fredholm integral equation for $u(x, y, z, 0)$. The termwise separable property of the kernel function allows us to acquire a closed-form regularized solution. In addition, a tactic to determine the regularization parameter is recommended. We find that the proposed method is robust and applicable to the three-dimensional BHCP when several numerical experiments are examined.

Keywords: Backward heat conduction problem, Ill-posed problem, Regularized solution, Fourier series, Fredholm integral equation

1 Introduction

General speaking, the direct problem means an effect from a cause. On the contrary, the inverse problem denotes a cause from an effect. In many engineering application domains such as archeology and heat destruction of materials, it requires to reveal the temperature history from the given final data. This is the commonly named backward heat conduction problem (BHCP), which is a seriously ill-posed problem because the solution is unstable for the known final data. For the two-dimensional (2-D) and three-dimensional (3-D) homogeneous BHCPs, many schemes have been studied. Liu (2002) proposed the regularized successive over-relaxation (SOR) inversion approach and the direct SOR inversion method to solve the ill-posed BHCPs. He remarked that the regularized SOR approach is stable even under the influence of high noise level, but its retrieved time is merely $5 \times 10^{-3}$. On
the contrary, the direct SOR inversion approach is unstable for small disturbances. Iijima (2004) constructed a high order lattice-free finite difference approach by employing the Taylor expansion and the Fourier transform; however, this study did not discuss its robustness when the final time data were disturbed with noises. Apart from this, Mera (2005) commented that the method of fundamental solutions is an accurate and efficient approach for tackling the BHCP in one-dimensional and 2-D domains; however, the standard Tikhonov regularization technique with the L-curve method are still needed for the numerical stability problem. Later, Liu (2004) and Liu, Chang and Chang (2006) have employed the group preserving scheme (GPS) and the backward group preserving scheme to resolve the BHCP, respectively. Without a priori regularization in use makes these two schemes more appealing for ill-posed problems with a final value problem. Another useful algorithm, on the basis of the GPS [Liu (2001)], so-called the Lie-group shooting method (LGSM), was further proposed to deal with boundary-value problems (BVPs). Because adding a quasi-boundary regularization at the final time condition, the BHCP, originally a final value problem, can be converted into a BVP; therefore, the LGSM [Chang, Liu and Chang (2007, 2008)] is utilized to solve the BHCP and acquires a good result. Recently, Tsai, Young and Kolibal proposed the time evolution method of fundamental solutions to resolve 3-D BHCPs with good results; however, their recovery time is small.

Through this article, a direct regularization technique is adopted to transform the 3-D BHCP into a second-kind Fredholm integral equation by utilizing the quasi-boundary method. By using the separating kernel function and eigenfunctions expansion tactics, we can derive a closed-form solution of the second-kind Fredholm integral equation, which is a major contribution of this paper. Another one is the application of the Fredholm integral equation to develop an effective numerical algorithm, whose accuracy is much better than that of other numerical schemes.

This sort approach of second-kind Fredholm integral equation regularization was first employed by Liu (2007a) to tackle a direct problem of elastic torsion in an arbitrary plane domain, where it was called a meshless regularized integral equation method. Then, Liu (2007b, 2007c) extended it to resolve the Laplace direct problem in arbitrary plane domains. A similar second-kind Fredholm integral equation regularization method was utilized to address the inverse problems; Liu, Chang and Chiang (2008) have applied the new scheme to select the geometrical shape of a constant temperature curve, Liu (2009a) has used this new algorithm to resolve the Robin problem in the Laplace equation, and Liu (2009b) has employed it to tackle the backward heat conduction problem. Furthermore, we have utilized this approach to solve the backward in time advection-dispersion equation [Liu, Chang and Chang (2009)]. Especially, the proposed method is easy to implement and time
saving.

In the following, Section 2 delineates the BHCP with a quasi-boundary regularization of its final time condition, and then we derive the second-kind Fredholm integral equation by a direct regularization in Section 3. In Section 4, we derive a closed-form solution of the second-kind Fredholm integral equation. Section 5 offers a choice principle of the regularization parameter. Numerical experiments are also utilized to validate the new scheme. A summary with some conclusions is presented in Section 6.

2 Backward heat conduction problems

We contemplate a homogeneous body of length $a$, width $b$ and height $c$. In many practical engineering applications we would like to recover all the past temperature distribution $u(x, y, z, t)$, for $t < T$, when the temperature is presumed to be known at a given final time $T$. Here, we set the following problem:

$$
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}, \quad 0 < x < a, \quad 0 < y < b, \quad 0 < z < c, \quad 0 < t < T, \quad (1)
$$

$$
u(0, y, z, t) = u(a, y, z, t) = u(x, 0, z, t) = u(x, b, z, t) = u(x, y, z, 0) = u(x, y, c, t) = 0, \quad 0 \leq t \leq T, \quad (2)
$$

$$u(x, y, z, T) = f(x, y, z), \quad 0 \leq x \leq a, \quad 0 \leq y \leq b, \quad 0 \leq z \leq c. \quad (3)
$$

This is the so-called a three-dimensional BHCP, which is known to be highly ill-posed, that is, the solution does not count continuously on the input data $u(x, y, z, T)$. In fact, the rapid decay of temperature with time results in fast fading memory of initial conditions. Hence, the numerical recovery of initial temperature from the data measured at time $T$ is a rather difficult issue owing to the influence of the noise and computational error.

One way to tackle an ill-posed problem is by a disturbance of it into a well-posed one. Many perturbing techniques have been proposed, including a biharmonic regularization developed by Lattés and Lions (1969), a pseudo-parabolic regularization proposed by Showalter and Ting (1970), a stabilized quasi-reversibility proposed by Miller (1973), the method of quasi-reversibility proposed by Mel’nikova (1997), a hyperbolic regularization proposed by Ames and Cobb (1997), the Gajewski and Zacharias quasi-reversibility proposed by Huang and Zheng (2005), a quasi-boundary value method by Denche and Bessila (2005), and an optimal regularization proposed by Boussetila and Rebbani (2006). We extend the regularization of
the one-dimensional BHCP of Showalter (1983) by pondering a quasi-boundary-value approximation to the final value problem, that is, to supplant Eq. (3) by

\[ \alpha u(x, y, z, 0) + u(x, y, z, T) = f(x, y, z). \]  

(4)

The problems (1), (2) and (4) can be tendered to be well-posed for each \( \alpha > 0 \).

3 The Fredholm integral equation

By employing the technique for separation of variables, we can easily write a series expansion of \( u(x, y, z, t) \) satisfying Eqs. (1) and (2):

\[ u(x, y, z, t) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk} \exp \left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2) \pi^2 t \right] \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \]  

(5)

where \( d_{ijk} \) are coefficients to be chosen. By imposing the two-point boundary condition (4) on the above equation, we acquire

\[ u(x, y, z, T) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk} \exp \left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2) \pi^2 T \right] \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c} = f(x, y, z) - \alpha u(x, y, z, 0). \]  

(6)

Fixing any \( t < T \) and applying the eigenfunctions expansion to Eq. (5), we have

\[ d_{ijk} = \frac{8 \exp \left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2) \pi^2 t \right]}{abc} \int_0^c \int_0^b \int_0^a \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \phi}{b} \sin \frac{k\pi \rho}{c} u(\xi, \phi, \rho, t) d\xi d\phi d\rho. \]  

(7)

Substituting Eq. (7) for \( d_{ijk} \) into Eq. (6) and assuming that the order of summation and integral can be interchanged, it follows that

\[ \left( K_{xyz}^{T-t} u(\cdot, \cdot, \cdot, t) \right)(x, y, z) := \int_0^c \int_0^b \int_0^a K(x, \xi; y, \phi; z, \rho; T-t) u(\xi, \phi, \rho, t) d\xi d\phi d\rho = f(x, y, z) - \alpha u(x, y, z, 0), \]  

(8)
where

\[ K(x, \xi; y, \phi; z, \rho; t) = \frac{8}{abc} \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} \exp\left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 t \right] \times \sin \frac{i\pi x}{a} \sin \frac{i\pi \xi}{a} \sin \frac{j\pi y}{b} \sin \frac{j\pi \phi}{b} \sin \frac{k\pi z}{c} \sin \frac{k\pi \rho}{c} \]  

is a kernel function, \( \alpha \) is a regularization parameter, and \( K_{xyz}^T \) is an integral operator generated from \( K(x, \xi; y, \phi; z, \rho; T-t) \). Corresponding to the kernel \( K(x, \xi; y, \phi; z, \rho; t) \), the operator is indicated by \( K'_{xyz} \).

To recover the initial temperature \( u(x, y, z, 0) \), we have to resolve the three-dimensional second-kind Fredholm integral equation:

\[ \alpha u(x, y, z, 0) + \int_0^c \int_0^b \int_0^a K(x, \xi; y, \phi; z, \rho; T)u(\xi, \phi, \rho, 0)d\xi d\phi d\rho = f(x, y, z), \]  

which is obtained from Eq. (8) by taking \( t = 0 \). Taking \( x = \eta, y = \omega \) and \( z = \tau \) in Eq. (10), we can acquire

\[ \alpha u(\eta, \omega, \tau, 0) + \int_0^c \int_0^b \int_0^a K(\eta, \xi; \omega, \phi; \tau, \rho; T)u(\xi, \phi, \rho, 0)d\xi d\phi d\rho = f(\eta, \omega, \tau), \]  

and applying the operator \( K'_{xyz} \) on the above equation and noting that

\[ K'_{xyz}u(\cdot, \cdot, \cdot, 0)(x, y, z) = \int_0^c \int_0^b \int_0^a K(x, \eta; y, \omega, z, \rho; \tau)u(\eta, \omega, \tau, 0)d\eta d\omega d\tau = u(x, y, z, t), \]

\[ (K_{xyz}^T K_{\eta\omega\tau}^T u(\cdot, \cdot, \cdot, 0))(x, y, z) = (K_{xyz}^T K_{\eta\omega\tau}^T u(\cdot, \cdot, \cdot, 0))(x, y, z), \]

we have

\[ \alpha u(x, y, z, t) + \int_0^c \int_0^b \int_0^a K(\xi, \eta; y, \phi; z, \rho; T)u(\xi, \phi, \rho, t)d\xi d\phi d\rho = F(x, y, z, t) \]

\[ = \int_0^c \int_0^b \int_0^a K(x, \xi; y, \phi; z, \rho; t)f(\xi, \phi, \rho)d\xi d\phi d\rho. \]  

This equation was extended from Ames, Clark, Epperson and Oppenheimer (1998) to the three-dimensional case, and the numerical implementation has been carried out merely for the one-dimensional case.
4 A closed-form solution

However, we start from Eq. (10) by a different approach, rather than Eq. (12), because Eq. (10) is simpler than Eq. (12). We presume that the kernel function in Eq. (10) can be approximated by \( q, n \) and \( m \) terms with

\[
K(x, \xi; y, \varphi; z, \rho; T) = \frac{8}{a b c} \sum_{k=1}^{m} \sum_{j=1}^{n} \sum_{i=1}^{q} \exp\left[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T\right]
\times \sin\left(\frac{i\pi x}{a}\right) \sin\left(\frac{i\pi \xi}{a}\right) \sin\left(\frac{j\pi y}{b}\right) \sin\left(\frac{j\pi \varphi}{b}\right) \sin\left(\frac{k\pi z}{c}\right) \sin\left(\frac{k\pi \rho}{c}\right)
\]

(13)

owing to \( T > 0 \). The above kernel is termwise separable, which is also called the degenerate kernel or the Pincherle-Goursat kernel [Tricomi (1985)]. By inspection of Eq. (13), we can get

\[
K(x, \xi; y, \varphi; z, \rho; T) = P(x, y, z; T) \cdot Q(\xi, \varphi, \rho),
\]

(14)
where \( \mathbf{P} \) and \( \mathbf{Q} \) are \( mnq \)-vectors given by

\[
\mathbf{P} := \frac{8}{abc} \begin{bmatrix}
\exp(-\rho_{111}^2 \pi^2 T) \sin \frac{\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{211}^2 \pi^2 T) \sin \frac{2\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\
\vdots \\
\exp(-\rho_{q11}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{112}^2 \pi^2 T) \sin \frac{\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{212}^2 \pi^2 T) \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\
\vdots \\
\exp(-\rho_{q12}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{121}^2 \pi^2 T) \sin \frac{\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\
\exp(-\rho_{221}^2 \pi^2 T) \sin \frac{2\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\
\vdots \\
\exp(-\rho_{q21}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\
\exp(-\rho_{122}^2 \pi^2 T) \sin \frac{\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\
\exp(-\rho_{222}^2 \pi^2 T) \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\
\vdots \\
\exp(-\rho_{q22}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\
\exp(-\rho_{12m}^2 \pi^2 T) \sin \frac{\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{22m}^2 \pi^2 T) \sin \frac{2\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{q2m}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{\pi z}{c} \\
\exp(-\rho_{qnm}^2 \pi^2 T) \sin \frac{q\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{n\pi z}{c}
\end{bmatrix},
\tag{15}
\]
\[
Q := \begin{bmatrix}
\sin \frac{\pi \xi}{a} \sin \frac{\pi \phi}{b} \sin \frac{\pi \rho}{c} \\
\sin \frac{2 \pi \xi}{a} \sin \frac{2 \pi \phi}{b} \sin \frac{\pi \rho}{c} \\
\vdots \\
\sin \frac{q \pi \xi}{a} \sin \frac{q \pi \phi}{b} \sin \frac{\pi \rho}{c} \\
\sin \frac{2 \pi \xi}{a} \sin \frac{2 \pi \phi}{b} \sin \frac{\pi \rho}{c} \\
\vdots \\
\sin \frac{2 \pi \xi}{a} \sin \frac{2 \pi \phi}{b} \sin \frac{\pi \rho}{c}
\end{bmatrix},
\]

where

\[
\rho_{ijk}^2 = i^2/a^2 + j^2/b^2 + k^2/c^2, \quad i = 1, 2, \ldots, q, \quad j = 1, 2, \ldots, n, \quad k = 1, 2, \ldots, m
\]

and the dot between \( P \) and \( Q \) denotes the inner product, which is sometimes written as \( P^T Q \), where the superscript \( T \) denotes the transpose. With the aid of Eq. (14),
Eq. (10) can be written as

\[ \alpha u(x, y, z, 0) + \int_c^b \int_a^b \int_0^a P^T(x, y, z)Q(\xi, \varphi, \rho)u(\xi, \varphi, \rho, 0)d\xi d\varphi d\rho = f(x, y, z), \]  

(16)

where we abridge the parameter \( T \) in \( P \) for clarity. Let us define

\[ c := \int_c^b \int_a^b \int_0^a Q(\xi, \varphi, \rho)u(\xi, \varphi, \rho, 0)d\xi d\varphi d\rho \]  

(17)

to be an unknown vector with dimensions \( qnm \).

Multiplying Eq. (16) by \( Q(x, y, z) \), and integrating it, we can acquire

\[
\alpha \int_c^b \int_a^b \int_0^a Q(x, y, z)u(x, y, z, 0)dxdydz \\
+ \int_c^b \int_a^b \int_0^a Q(x, y, z)P^T(x, y, z)dxdydz \\
\times \int_c^b \int_a^b \int_0^a Q(\xi, \varphi, \rho)u(\xi, \varphi, \rho, 0)d\xi d\varphi d\rho \\
= \int_c^b \int_a^b f(x, y, z)Q(x, y, z)dxdydz. 
\]

(18)

By definition (17) we therefore have

\[
\left( \alpha I_{nmq} + \int_0^a \int_0^a \int_0^a Q(\xi, \varphi, \rho)P^T(\xi, \varphi, \rho)d\xi d\varphi d\rho \right) c := \int_0^a \int_0^a \int_0^a f(\xi, \varphi, \rho)Q(\xi, \varphi, \rho)d\xi d\varphi d\rho , 
\]

(19)

where \( I_{nmq} \) denotes an identity matrix of order \( qnm \). Solving Eq. (19) one has

\[
c = \left( \alpha I_{nmq} + \int_0^a \int_0^a \int_0^a Q(\xi, \varphi, \rho)P^T(\xi, \varphi, \rho)d\xi d\varphi d\rho \right)^{-1} \int_0^a \int_0^a \int_0^a f(\xi, \varphi, \rho)Q(\xi, \varphi, \rho)d\xi d\varphi d\rho .
\]

(20)

On the other hand, from Eq. (16) we get

\[
\alpha u(x, y, z, 0) = f(x, y, z) - P(x, y, z) \cdot c.
\]

(21)
Inserting Eq. (20) into the above equation, we obtain

\[
\alpha u(x, y, z, 0) = f(x, y, z) - P(x, y, z) \cdot \left( \alpha I_{mnq} + \int_0^c \int_0^b \int_0^a Q(\xi, \varphi, \rho)P^T(\xi, \varphi, \rho)d\xi d\varphi d\rho \right)^{-1} \\
\times \int_0^c \int_0^b \int_0^a f(\xi, \varphi, \rho)Q(\xi, \varphi, \rho)d\xi d\varphi d\rho.
\]

(22)

Owing to the orthogonality of

\[
\int_0^c \int_0^b \int_0^a \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \xi}{a} \sin \frac{k\pi \xi}{a} \sin \frac{q\pi \varphi}{b} \sin \frac{m\pi \varphi}{b} \sin \frac{n\pi \varphi}{b} \\
\times \sin \frac{r\pi \rho}{c} \sin \frac{s\pi \rho}{c} \sin \frac{w\pi \rho}{c} d\xi d\varphi d\rho \\
= \frac{abc}{8} \delta_{ijk} \delta_{rsw},
\]

(23)

where \( \delta_{ijk} \), \( \delta_{qmn} \) and \( \delta_{rsw} \) are the Kronecker delta, the \( qnm \times qnm \) matrix can be written as

\[
\int_0^c \int_0^b \int_0^a Q(\xi, \varphi, \rho)P^T(\xi, \varphi, \rho)d\xi d\varphi d\rho = \\
\text{diag}[\exp(-\rho_{111}^2 \pi^2 T), \exp(-\rho_{211}^2 \pi^2 T), \ldots, \exp(-\rho_{q11}^2 \pi^2 T), \\
\exp(-\rho_{121}^2 \pi^2 T), \exp(-\rho_{221}^2 \pi^2 T), \ldots, \exp(-\rho_{q21}^2 \pi^2 T), \\
\exp(-\rho_{112}^2 \pi^2 T), \exp(-\rho_{212}^2 \pi^2 T), \ldots, \exp(-\rho_{q12}^2 \pi^2 T), \\
\exp(-\rho_{122}^2 \pi^2 T), \exp(-\rho_{222}^2 \pi^2 T), \ldots, \exp(-\rho_{q22}^2 \pi^2 T), \\
\exp(-\rho_{12m}^2 \pi^2 T), \exp(-\rho_{22m}^2 \pi^2 T), \ldots, \exp(-\rho_{q2m}^2 \pi^2 T),],
\]

(24)

where \( \text{diag} \) means that the matrix is a diagonal matrix. Inserting Eq. (24) into Eq. (22), we thus acquire

\[
u(x, y, z, 0) = \frac{1}{\alpha} f(x, y, z) - \frac{1}{\alpha} P^F(x, y, z) \\
\text{diag} \left[ \frac{1}{\alpha + \exp(-\rho_{111}^2 \pi^2 T)}, \frac{1}{\alpha + \exp(-\rho_{211}^2 \pi^2 T)}, \ldots \right],
\]
\[
\frac{1}{\alpha + \exp(-\rho_{q11}^2 \pi^2 T)} \cdot \frac{1}{\alpha + \exp(-\rho_{121}^2 \pi^2 T)} \cdot \frac{1}{\alpha + \exp(-\rho_{221}^2 \pi^2 T)} \cdots ,
\]
\[
\frac{1}{\alpha + \exp(-\rho_{q12}^2 \pi^2 T)} \cdots , \frac{1}{\alpha + \exp(-\rho_{122}^2 \pi^2 T)} \cdot \frac{1}{\alpha + \exp(-\rho_{222}^2 \pi^2 T)} \cdots ,
\]
\[
\frac{1}{\alpha + \exp(-\rho_{q22}^2 \pi^2 T)} \cdots , \frac{1}{\alpha + \exp(-\rho_{12m}^2 \pi^2 T)} \cdot \frac{1}{\alpha + \exp(-\rho_{22m}^2 \pi^2 T)}
\]
\[
\frac{1}{\alpha + \exp(-\rho_{qm2}^2 \pi^2 T)} \int_{0}^{a} \int_{0}^{b} \int_{0}^{c} f(\xi, \phi, \rho) Q(\xi, \phi, \rho) \, d\xi \, d\phi \, d\rho.
\]

Using Eq. (15) for \( P \) and \( Q \), we can attain
\[
u(x, y, z, 0) =
\frac{1}{\alpha} f(x, y, z) - \frac{8}{\alpha abc} \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2) \pi^2 T] \]
\[
\times \int_{0}^{c} \int_{0}^{b} \int_{0}^{a} \sin \frac{i\pi x}{a} \sin \frac{i\pi y}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c} \sin \frac{k\pi \rho}{c} f(\xi, \phi, \rho) \, d\xi \, d\phi \, d\rho,
\]

where the summation upper bound \( q, n \) and \( m \) can be superseded by \( \infty \) because our argument is independent of \( q, n \) and \( m \). For a given \( f(x, y, z) \), through some integrals one may use the above equation to calculate \( u(x, y, z, 0) \).

If \( u(x, y, z, 0) \) is given, we can calculate \( u(x, y, z, t) \) at any time \( t < T \) by
\[
u^\alpha(x, y, z, t) =
\sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk} \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2) \pi^2 T] \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c},
\]
where

\[ d_{ijk}^\alpha = \frac{8}{abc} \int_0^a \int_0^b \int_0^c \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \phi}{b} \sin \frac{k\pi \rho}{c} u(\xi, \phi, \rho, 0) d\xi d\phi d\rho. \] (28)

Inserting Eq. (26) into the above equation and using the orthogonality equation (23), one obtains

\[ d_{ijk}^\alpha = \frac{8}{abc} \left\{ \alpha + \exp \left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right] \right\} \int_0^a \int_0^b \int_0^c \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \phi}{b} \sin \frac{k\pi \rho}{c} \times f(\xi, \phi, \rho) d\xi d\phi d\rho. \] (29)

Eqs. (27) and (29) compose an analytical solution of the three-dimensional BHCP. To discriminate it from the exact solution \( u(x, y, z, t) \), we have utilized the symbol \( u^\alpha(x, y, z, t) \) to denote that it is a regularization solution.

5 Selection of the regularization parameter \( \alpha \) and numerical examples

Up to this point, we have not yet specified how to determine the regularization parameter \( \alpha \). Presume that \( f \) has the following Fourier sine series expansion:

\[ f(x, y, z) = \sum_{k=1}^\infty \sum_{j=1}^\infty \sum_{i=1}^\infty d_{ijk}^* \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \] (30)

where

\[ d_{ijk}^* = \frac{8}{abc} \int_0^a \int_0^b \int_0^c \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \phi}{b} \sin \frac{k\pi \rho}{c} f(\xi, \phi, \rho) d\xi d\phi d\rho. \] (31)

Substituting Eq. (30) into Eq. (26), we attain

\[ u^\alpha(x, y, z, 0) = \sum_{k=1}^\infty \sum_{j=1}^\infty \sum_{i=1}^\infty \exp \left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right] d_{ijk}^* \exp\left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right] \] (32)

\[ \times \sin \frac{k\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \]

where we indicate that

\[ \frac{\exp\left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right]}{\alpha + \exp\left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right]} = \frac{1}{1 + \alpha \exp\left[ -(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T \right]}. \]
For a better numerical solution, we require to set
\[ \alpha \exp[(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2T] = \alpha_0 << 1. \]

On the other hand, the term \( \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2T] / (\alpha + \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2T]) \) in Eq. (32) will be very small when \( i, j, k, \) and/or \( T \) are large, which may result in a large numerical error. Therefore, we obtain an approximation
\[ \frac{\exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2T]}{\alpha + \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2T]} = \frac{1}{1 + \alpha_0} = 1 - \alpha_0 + \alpha_0^2 - \alpha_0^3 + \ldots. \]

When the terms with order higher than one are truncated, we acquire a good approximation of \( u(x, y, z, 0) \) by
\[ u^{a_0}(x, y, z, 0) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} (1 - \alpha_0)d_{ijk}^* \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}. \tag{33} \]

The regularization parameter \( \alpha_0 \) is a small number, and \( i, j \) and \( k \) represent a number of the finite terms in the numerical experiments. In doing so, we can filter out the noise induced by the higher-modes in Eq. (32).

We will apply the quasi-boundary approach on the calculations of BHCP through numerical examples. We are interested in the stability of our approach when the input final measured data are contaminated by random noise. We can evaluate the stability by increasing the different levels of random noise on the terminal data:
\[ \hat{f}(x_i, y_j, z_k) = f(x_i, y_j, z_k) + sR(i, j, k), \tag{34} \]

where \( f(x_i, y_j, z_k) \) is the exact data. We employ the function RANDOM_NUMBER given in Fortran to generate the noisy data \( R(i, j, k) \), which are random numbers in \([-1, 1]\), and \( s \) denotes the level of noise. Then, the noisy data \( \hat{f}(x_i, y_j, z_k) \) are used in the calculations.

### 5.1 Example 1

Let us deliberate the first numerical experiment of three-dimensional BHCP:
\[ u_t = u_{xx} + u_{yy} + u_{zz}, \quad 0 < x < 1, \quad 0 < y < 1, \quad 0 < z < 1, \quad 0 < t < T, \tag{35} \]

with the boundary conditions
\[ u(0, y, z, t) = u(1, y, z, t) = u(x, 0, z, t) = u(x, 1, z, t) = u(x, y, 0, t) = u(x, y, 1, t) = 0, \tag{36} \]
and the final time condition
\[ u(x, y, z, T) = e^{-3\pi^2 T} \sin(\pi x) \sin(\pi y) \sin(\pi z). \] (37)

The exact solution is given by
\[ u(x, y, z, t) = e^{-3\pi^2 t} \sin(\pi x) \sin(\pi y) \sin(\pi z). \] (38)

In Fig. 1, we display the errors of numerical solutions acquired from the quasi-boundary semi-analytical scheme for the case of \( T = 25 \) in this comparison and the final data are very small in the order of \( O(10^{-322}) \), where the grid lengths \( \Delta x = \Delta y = \Delta z = 1/40 \) are used. At the point \( x = 0.1 \) the error is drawn with respect to \( y \) and \( z \) by a solid line, at the point \( y = 0.8 \) the error is plotted with respect to \( x \) and \( z \) by a circle symbol, and at the point \( z = 0.9 \) the error is plotted with respect to \( x \) and \( y \) by a cross symbol. This example is a very hard problem of BHCP to examine the numerical performance of novel numerical approaches. Nevertheless, the errors are much smaller than that calculated by Chang, Liu and Chang (2009) as displayed in Figure 9, Chang and Liu (2010) as shown in Figure 22(b) and Tsai, Young and Kolibal (2011) as illustrated in Figures 3 and 4 therein.

The numerical results were calculated by Tsai, Young and Kolibal (2011), of which the final time was 0.01 and the maximum error was about 0.1, under a noise of \( s = 0.1 \). In Fig. 2, we compare the numerical errors with \( T = 25 \) for two cases: one without the random noise and another one with two different levels of random noise \( s = 0.01 \) and 0.1. In Figs. 3(a)-(c), we represent the exact solution and numerical solutions sequentially. Even under the large noise \( s = 0.1 \), the numerical solution shown in Fig. 3(c) is a good estimation to the exact initial data as displayed in Fig. 3(a). Besides, we should emphasize that in all the calculations, we can use \( \alpha_0 = 0 \) without any difficulty because Eq. (33) is still applicable. To the author’s best knowledge, there has been no open report that the numerical methods can calculate this ill-posed BHCP very well as the quasi-boundary semi-analytical approach.

5.2 Example 2

Let us contemplate another instance of three-dimensional BHCP:
\[ u_t = u_{xx} + u_{yy} + u_{zz}, \quad 0 < x < 1, \ 0 < y < 1, \ 0 < z < 1, \ 0 < t < T, \] (39)

with the boundary conditions
\[ u(0,y,z,t) = u(1,y,z,t) = u(x,0,z,t) = u(x,1,z,t) = u(x,y,0,t) = u(x,y,1,t) = 0, \] (40)
and the initial condition
\[
 u(x, y, z, 0) = \begin{cases} 
 8xyz, & \text{for } 0 \leq x \leq 0.5, 0 \leq y \leq 0.5, 0 \leq z \leq 0.5, \\
 8y(1-x), & \text{for } 0.5 \leq x \leq 1, 0 \leq y \leq 0.5, 0 \leq z \leq 0.5, \\
 8x(1-y)(1-z), & \text{for } 0 \leq x \leq 0.5, 0.5 \leq y \leq 1, 0.5 \leq z \leq 1, \\
 8xz(1-y), & \text{for } 0 \leq x \leq 0.5, 0.5 \leq y \leq 1, 0 \leq z \leq 0.5, \\
 8z(1-x)(1-y), & \text{for } 0.5 \leq x \leq 1, 0.5 \leq y \leq 1, 0 \leq z \leq 0.5, \\
 8xy(1-z), & \text{for } 0 \leq x \leq 0.5, 0 \leq y \leq 0.5, 0.5 \leq z \leq 1, \\
 8y(1-x)(1-z), & \text{for } 0.5 \leq x \leq 1, 0 \leq y \leq 0.5, 0.5 \leq z \leq 1, \\
 8(1-x)(1-y)(1-z), & \text{for } 0.5 \leq x \leq 1, 0.5 \leq y \leq 1, 0.5 \leq z \leq 1. 
\end{cases} \tag{41}
\]

The exact solution is given by
\[
 u(x, y, z,t) = 
\]
Figure 2: The numerical errors of semi-analytical solutions with and without random noise effect for Example 1 are plotted in (a) with respect to $x$ at fixed $y = 0.8$ and $z = 0.9$, in (b) with respect to $y$ at fixed $x = 0.1$ and $z = 0.9$, and in (c) with respect to $z$ at fixed $x = 0.1$ and $y = 0.8$. 
Figure 3: The exact solution for Example 1 of three-dimensional BHCP are shown in (a), in (b) the semi-analytical solution without random noise effect, and in (c) the semi-analytical solution with random noise.
Inserting it into Eq. (27), we have

\[\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \frac{512(-1)^i(-1)^j(-1)^k}{abc\pi^6(2i+1)^2(2j+1)^2(2k+1)^2} \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 t] \times \sin \left(\frac{(2i+1)\pi x}{a}\right) \sin \left(\frac{(2j+1)\pi y}{b}\right) \sin \left(\frac{(2k+1)\pi z}{c}\right). \quad (42)\]

The backward numerical solution is subjected to the final condition at time \(T\):

\[f(x, y, z) = u(x, y, z, T) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \frac{512(-1)^i(-1)^j(-1)^k}{abc\pi^6(2i+1)^2(2j+1)^2(2k+1)^2} \exp[-(i^2/a^2 + j^2/b^2 + k^2/c^2)\pi^2 T] \times \sin \left(\frac{(2i+1)\pi x}{a}\right) \sin \left(\frac{(2j+1)\pi y}{b}\right) \sin \left(\frac{(2k+1)\pi z}{c}\right). \quad (43)\]

The difficulty of this problem is emanated from that we utilize a smooth final data to recover a non-smooth initial data.

Let \(a = b = c = 1\) and insert Eq. (42) for \(f(x, y, z)\) into Eq. (29) to attain

\[d_{ijk}^\alpha = \frac{1}{\{\alpha + \exp[-(i^2 + j^2 + k^2)\pi^2 T]\}} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} \frac{512(-1)^q(-1)^n(-1)^m}{\pi^6(2q+1)^2(2n+1)^2(2m+1)^2} \delta_{i,(2q+1)}(2q+1) \delta_{j,(2n+1)} \delta_{k,(2m+1)} \times \exp\{-[(2q+1)^2 + (2n+1)^2 + (2m+1)^2]\pi^2 T\}. \quad (44)\]

Inserting it into Eq. (27), we have

\[u^\alpha(x,y,z,t) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \frac{1}{\{\alpha + \exp[-(i^2 + j^2 + k^2)\pi^2 T]\}} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} \frac{512(-1)^q(-1)^n(-1)^m}{\pi^6(2q+1)^2(2n+1)^2(2m+1)^2} \delta_{i,(2q+1)}(2q+1) \delta_{j,(2n+1)} \delta_{k,(2m+1)} \times \exp\{-[(2q+1)^2 + (2n+1)^2 + (2m+1)^2]\pi^2 T\} \times \exp[-(i^2 + j^2 + k^2)\pi^2 t] \sin(i\pi x) \sin(j\pi y) \sin(k\pi z). \quad (45)\]
Interchanging the order of summation and employing the $\delta$ property, we acquire

$$u^\alpha(x, y, z, t) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} \frac{512(-1)^q(-1)^n(-1)^m}{\pi^6(2q + 1)^2(2n + 1)^2(2m + 1)^2}$$

$$\exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}$$

$$\{\alpha + \exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}\}$$

$$\times \exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 t\}$$

$$\sin[(2q + 1)\pi x] \sin[(2n + 1)\pi y] \sin[(2m + 1)\pi z].$$

(46)

It gives

$$u^\alpha(x, y, z, 0) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} \frac{512(-1)^q(-1)^n(-1)^m}{\pi^6(2q + 1)^2(2n + 1)^2(2m + 1)^2}$$

$$\exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}$$

$$\{\alpha + \exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}\}$$

$$\times \sin[(2q + 1)\pi x] \sin[(2n + 1)\pi y] \sin[(2m + 1)\pi z].$$

(47)

The term

$$\exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}$$

$$\{\alpha + \exp\{-[(2q + 1)^2 + (2m + 1)^2 + (2n + 1)^2]\pi^2 T\}\} = 1 - \alpha_0$$

is already derived at the first of this section. Therefore, we obtain

$$u^\alpha_0(x, y, z, 0) = (1 - \alpha_0) \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} \frac{512(-1)^q(-1)^n(-1)^m}{\pi^6(2q + 1)^2(2n + 1)^2(2m + 1)^2}$$

$$\sin[(2q + 1)\pi x] \sin[(2n + 1)\pi y]$$

$$\times \sin[(2m + 1)\pi z].$$

(48)

Therefore, we employ this solution to compare that in Eq. (41). In practice, the data are attained by taking the sum of the first one hundred terms, which guarantees the convergence of the series.

Tsai, Young and Kolibal (2011) calculated the initial data with a terminal time $T = 0.01$ and the maximum error was about 0.125. In Fig. 4(a), we show the errors of numerical solutions obtained from the quasi-boundary semi-analytical method for the case. $T = 10$ is used in this comparison, where the grid lengths $\Delta x = \Delta y = \Delta z = 0.02$ are employed. At the point $x = 0.1$ the error is plotted with respect to $y$ and $z$ by a solid line, at the point $y = 0.7$ the error is drawn with respect to $x$
and \( z \) by a dashed line, and at the point \( z = 0.9 \) the error is plotted with respect to \( x \) and \( y \) by a dotted line. Furthermore, the maximum error occurring at \( x = 0.5 \) is only \( 3 \times 10^{-4} \). Then, we offer a more ill-posed instance than the above one by employing the current scheme at \( T = 30 \). The errors of numerical solutions were displayed in Fig. 4(b).

Figure 4: The errors of semi-analytical solutions for Example 2 are shown in (a) with \( T = 10 \), and in (b) with \( T = 30 \).

The numerical results were calculated by Tsai, Young and Kolibal (2011), of which the final time was 0.01 and the maximum error was about 0.09, under a noise of \( s \).
Figure 5: The numerical errors of semi-analytical solutions with and without random noise effect for Example 2 are drawn in (a) with respect to $x$ at fixed $y = 0.7$ and $z = 0.9$, in (b) with respect to $y$ at fixed $x = 0.1$ and $z = 0.9$, and in (c) with respect to $z$ at fixed $x = 0.1$ and $y = 0.7$. 
Figure 6: The exact solution for Example 2 of three-dimensional BHCP are shown in (a), in (b) the semi-analytical solution without random noise effect, and in (c) the semi-analytical solution with random noise.
= 0.05. In Fig. 5, we compare the numerical errors with $T = 30$ for two cases: one without the relative random noise and another one with the relative random noise in the level of $s = 0.05$. In Figs. 6(a)-(c), we show the exact solution and numerical solutions sequentially. Even under the noise the numerical solution shown in Fig. 6(c) is a good estimation to the exact initial data as represented in Fig. 6(a).

5.3 Example 3

Let us ponder the third example of three-dimensional BHCP:

$$u_t = u_{xx} + u_{yy} + u_{zz}, \quad -\pi < x < \pi, \quad -\pi < y < \pi, \quad -\pi < z < \pi, \quad 0 < t < T,$$

(49)

with the boundary conditions

$$u(-\pi, y, z, t) = u(\pi, y, z, t) = u(x, -\pi, z, t) = u(x, \pi, z, t) = u(x, y, -\pi, t) = u(x, y, \pi, t) = 0,$$

(50)

and the final time condition

$$u(x, y, z, T) = e^{-3\beta^2 t} \sin(\beta x) \sin(\beta y) \sin(\beta z).$$

(51)

The exact solution is given by

$$u(x, y, z, t) = e^{-3\beta^2 t} \sin(\beta x) \sin(\beta y) \sin(\beta z),$$

(52)

where $\beta \in \mathbb{N}$ is a positive integer.

In Fig. 7(a), we exhibit the errors of numerical solutions attained from the quasi-boundary semi-analytical scheme for the case of $\beta = 1$. $T = 100$ is employed in this comparison and the final data are very small in the order of $O(10^{-87})$, where the grid lengths $\Delta x = \Delta y = \Delta z = 2\pi/40$ are employed. At the point $x = -\pi + 60\pi/40$ the error is plotted with respect to $y$ and $z$ by a solid line, at the point $y = -\pi + 66\pi/40$ the error is drawn with respect to $x$ and $z$ by a circle symbol, and at the point $z = -\pi + 72\pi/40$ the error is plotted with respect to $x$ and $y$ by a cross symbol. However, the errors are much smaller than that calculated by Tsai, Young and Kolibal (2011) as presented in Figure 9 therein.

We will give a more ill-posed example than the above one by utilizing the quasi-boundary semi-analytical scheme. Let $\beta = 3$, $T = 40$, and the final data are very small in the order of $O(10^{-313})$. Nevertheless, we can use this approach to recover the desired initial data $\sin(\beta x) \sin(\beta y) \sin(\beta z)$, which is in the order of $O(1)$. In Fig. 7(b), the errors of numerical solutions calculated by the proposed approach with
Figure 7: The errors of semi-analytical solutions for Example 3 are shown in (a) with $T = 100$ and $\beta = 1$, and in (b) with $T = 40$ and $\beta = 3$. 
Figure 8: The numerical errors of semi-analytical solutions with and without random noise effect for Example 3 are plotted in (a) with respect to $x$ at fixed $y = 2\pi/3$ and $z = 4\pi/5$, in (b) with respect to $y$ at fixed $x = \pi/2$ and $z = 4\pi/5$, and in (b) with respect to $z$ at fixed $x = \pi/2$ and $y = 2\pi/3$. 

(a) 

(b) 

(c)
Figure 9: The exact solution for Example 3 of three-dimensional BHCP are shown in (a), in (b) the semi-analytical solution without random noise effect, and in (c) the semi-analytical solution with random noise.
\[ \Delta x = \Delta y = \Delta z = \frac{2\pi}{40}, \text{ and the result was much better than calculated by Tsai, Young and Kolibal (2011), where they employed } T = 0.5. \]

The numerical results were calculated by Tsai, Young and Kolibal (2011), of which \( \beta = 1 \), the final time was 0.75 and the maximum error was about 0.09, under a noise of \( s = 0.1 \). In Fig. 8, we compare the numerical errors with \( T = 100 \) and \( \beta = 1 \) for two cases: one without the random noise and another one with two different levels of random noise \( s = 0.01 \) and 0.1. In Figs. 9(a)-(c), we represent the exact solution and numerical solutions sequentially. Even under the large noise \( s = 0.1 \), the numerical solution presented in Fig. 9(c) is a good estimation to the exact initial data as displayed in Fig. 9(a). In addition, we should emphasize that in all the calculations, we can employ \( \alpha_0 = 0 \) without any difficulty since Eq. (33) is still applicable. To the author’s best knowledge, there has been no open literature that the numerical approaches can calculate this ill-posed BHCP very well as the quasi-boundary semi-analytical scheme.

6 Conclusions

In this article, we have transformed the three-dimensional BHCP into a second-kind three-dimensional Fredholm integral equation through a direct regularization tactic and a quasi-boundary idea. By employing the Fourier series expansion technique and a termwise separable property of kernel function, an analytical solution of the regularized type for estimating the exact solution is displayed. Besides, we explain that the effect of regularization parameter on the disturbed solution. Three numerical examples have illustrated that the proposed algorism can recover all initial data very well, even though the final data are very small or noised by a large perturbation, and the initial data to be retrieved are not smooth. Thus, the current scheme is recommended to cope with the three-dimensional BHCPs.

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References


