Lecture Note
Laplace Transform for Solving Linear Diffusion Equations
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Abstract
A ‘mesh free’ and ‘time free’ numerical method, based on the method of fundamental solutions, the particular solution for the modified Helmholtz operator and the Laplace transform, is introduced to solve diffusion-type and diffusion-reaction problems.

1 Laplace Transform for Diffusion Equations
Let $\Omega$ be a bounded domain in $\mathbb{R}^d$, where $d$ is the dimension of the domain, with boundary $S = S_1 \cup S_2, S_1 \cap S_2 = \emptyset$. We consider the following diffusion equation

$$
\frac{1}{k} \frac{\partial u(x,t)}{\partial t} = \Delta u(x,t), \quad x \in \Omega, \quad t > 0,
$$

with boundary conditions

$$
u(x,t) = f_1(x,t), \quad x \in S_1, \quad t > 0, \quad (2)$$
$$
\frac{\partial u(x,t)}{\partial n} = f_2(x,t), \quad x \in S_2, \quad t > 0, \quad (3)
$$

and initial condition

$$
u(x,0) = u_0(x), \quad x \in \Omega, \quad (4)
$$

where $n$ is the unit outward vector normal to $S$. The diffusion coefficient $k$ is assumed to be constant with respect to space and time. $u_0(x), f_1(x,t)$ and $f_2(x,t)$ are given functions.

To employ the Laplace transform (LT) to temporarily remove the time variable, we first define the Laplace transform of a given function $u(x,t)$, when it exists, by

$$
L[u(x,t)] = U(x; s) = \int_0^\infty u(x,t)e^{-st}dt
$$

where the transform parameter $s$ is real and positive. By integration by parts, we have

$$
L \left[ \frac{\partial u(x,t)}{\partial t} \right] = sU(x; s) - u_0(x).
$$

Harmonic initial condition

If the initial condition $u_0(x)$ is harmonic, then by a change of variable

$$
v(x,t) = u(x,t) - u_0(x),
$$

we have

$$
\frac{1}{k} \frac{\partial v(x,t)}{\partial t} = \Delta v(x,t), \quad x \in \Omega, \quad t > 0, \quad (8)
$$
$$
v(x,t) = f_1(x,t) - u_0(x), \quad x \in S_1, \quad t > 0, \quad (9)
$$
$$
\frac{\partial v(x,t)}{\partial n} = f_2(x,t) - \frac{\partial u_0(x)}{\partial n}, \quad x \in S_2, \quad t > 0, \quad (10)
$$
$$
v(x,0) = 0, \quad x \in \Omega. \quad (11)
$$
Applying the Laplace transformation to Eqs. (8)-(11), we obtain the following modified Helmholtz equation

\[ \left( \Delta - \frac{s}{k} \right) V(x; s) = 0, \quad x \in \Omega, \]  
\[ V(x; s) = F_1(x; s) - \frac{u_0(x)}{s}, \quad x \in S_1, \]  
\[ \frac{\partial V(x; s)}{\partial n} = F_2(x; s) - \frac{1}{s} \frac{\partial u_0(x)}{\partial n}, \quad x \in S_2, \]

where \( V(x; s) = \mathcal{L}[v(x, t)] \). The modified Helmholtz equation in Eq. (12) is homogeneous in LT space and the standard MFS can be applied directly. Once the solution \( V \) is determined in the LT space, using \( v = \mathcal{L}^{-1}[V(x; s)] \), the final solution \( u \) in the time domain can be obtained from Eq. (7) by \( u = v + u_0 \).

### Non-harmonic initial condition

In general, the initial condition \( u_0(x) \) in Eq. (4) is a non-harmonic function. By direct substitution of Eqs. (5) and (6) into Eqs. (1)-(3), we obtain

\[ \left( \Delta - \frac{s}{k} \right) U(x; s) = -\frac{u_0(x)}{k}, \quad x \in \Omega, \]  
\[ U(x; s) = F_1(x; s), \quad x \in S_1, \]  
\[ \frac{\partial U(x; s)}{\partial n} = F_2(x; s), \quad x \in S_2, \]

where \( F_i(x; s) = \mathcal{L}[f_i(x, t)], i = 1, 2 \). The modified Helmholtz equation in (15) is inhomogeneous and a domain integration is necessary in the BEM reformulation. In the next section we apply the MPS to evaluate the particular solution without domain integration.

### 2 The Method of Particular Solutions (MPS)

To solve Eqs. (15)-(17) we apply the method of particular solutions which is an extension of the well-known technique for solving ordinary differential equations by subtracting off a particular solution of Eq. (15). We define

\[ U_h = U - U_p \]

where \( U_p \) is a particular solution which satisfies the modified Helmholtz equation

\[ \left( \Delta - \frac{s}{k} \right) U_p(x; s) = -\frac{u_0(x)}{k}, \quad x \in \Omega, \]  

but does not necessarily satisfy the boundary conditions Eqs. (16)-(17). By linearity,

\[ \left( \Delta - \frac{s}{k} \right) U_h = \left( \Delta - \frac{s}{k} \right) (U - U_p) = -\frac{u_0(x)}{k} + \frac{u_0(x)}{k} = 0. \]

Thus \( U_h \) satisfies the homogeneous equation

\[ \left( \Delta - \frac{s}{k} \right) U_h(x; s) = 0, \quad x \in \Omega, \]  

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with boundary conditions determined by $U_p$ and the original boundary conditions in Eqs. (16)-(17)

$$U_h(x; s) = F_1(x; s) - U_p(x; s), \quad x \in S_1,$$

$$\frac{\partial U_h(x; s)}{\partial n} = F_2(x; s) - \frac{\partial U_p(x; s)}{\partial n}, \quad x \in S_2.$$

Here we split the original modified Helmholtz equation Eqs. (15)-(17) into two parts; i.e., $U_h$ and $U_p$. Solving the homogeneous equation for $U_h$ is a routine matter in the context of the MFS provided that the particular solution $U_p$ is known. Hence, the major task in solving Eqs. (15)-(17) is to evaluate particular solutions accurately and efficiently.

### 3 The Particular Solution for Modified Helmholtz Equation

The key idea of the MPS is to expand the forcing term in terms of a series of radial basis functions so that an approximate particular solution of the governing equation can be obtained. To be able to do this effectively is a major step in the MPS. In general, a less complicated forcing term is more desirable so that it can be easily approximated. Traditionally, due to the difficulty of obtaining particular solutions, the Laplace operator has been largely used as the main differential operator while other terms of the original differential operator were moved to the right hand side of the equation and treated as part of the forcing term. For instance, Eq. (19) can be rewritten as

$$\Delta U_p(x; s) = \frac{1}{k} (sU_p(x; s) - u_0(x)).$$

By using only the Laplace operator in Eq. (23) instead of the modified Helmholtz operator in Eq. (19) as a whole in the MPS, some information in the governing equation may be lost and the forcing terms $(sU_p(x; s) - u_0(x))/k$ in Eq. (23) become more difficult to approximate by RBFs. Hence, for more complicated differential equations, such as convection-diffusion equations, the MPS becomes less effective.

In general, the problem of using more sophisticated differential operators in the MPS, as we shall see, is the difficulty of finding the approximate particular solution analytically. Generally this is not possible.

To illustrate how to construct a closed form approximate particular solution, we will give a brief review of the MPS using rbfs. Let $L = \Delta - s/k$ and $g = -u_0(x)/k$. Then, Eq. (19) can be written as

$$LU_p = g(x), x \in \Omega \subset \mathbb{R}^d.$$  

To approximate $g(x)$ in Eq. (24) accurately by RBFs is crucial using the MPS. Let $\varphi(||x - x_i||) : \mathbb{R}^n \rightarrow \mathbb{R}$, where $||\cdot||$ is the Euclidean norm, be a globally defined basis function. In the DRM, $g$ is approximated by a linear combination of basis function $\{\varphi_i\}_1^N$

$$g(x) \approx \hat{g}(x) = \sum_{i=1}^N a_i \varphi_i(||x - x_i||) + \sum_{k=1}^t b_k p_k(x)$$

with the further constraints

$$\sum_{i=1}^N a_i p_k(x_i) = 0, \quad 1 \leq k \leq t,$$
where
\[ t = \left(\frac{m + d - 1}{d}\right) \]
and \( \{p_k\}_{k=1}^t \) is a basis for \( P_{m-1} \), the set of polynomials of degree \( \leq m - 1 \).

The polynomial terms of Eq. (25) and constraints in Eq. (26) are added to ensure that
\[ g(x_j) = \hat{g}(x_j), \quad 1 \leq j \leq N, \quad x_j \in \hat{\Omega}, \quad (27) \]
where \( \Omega \subseteq \hat{\Omega} \), is uniquely defined. Then from Eqs. (24) and (25) the approximate particular solution \( \hat{U}_p \approx U_p \) can be obtained by solving
\[ L\hat{U}_p(x) = \sum_{i=1}^{N} a_i \varphi(||x - x_i||) + \sum_{k=1}^{t} b_k p_k(x). \quad (28) \]

By the principle of superposition, \( \hat{U}_p \) can be written in the form
\[ \hat{U}_p = \sum_{i=1}^{N} a_i \Phi(||x - x_i||), \quad 1 \leq i \leq N, \quad \Phi \]
\[ L\varphi_i(x) = \varphi(||x - x_i||), \quad 1 \leq i \leq t, \quad \Phi \]
\[ L\chi_i(x) = p_i(x), \quad 1 \leq i \leq t. \quad \Phi \]

As we have indicated earlier in this section, the major challenge of the MPS is the solving Eq. (30) analytically for the chosen basis function \( \varphi \). Among all the rbfs, the MQ function \( \varphi(r) = \sqrt{r^2 + c^2} \), Gaussian \( \varphi(r) = \exp(-c^2r^2) \) (c is a parameter in both cases) and TPS \( \varphi(r) = r^2 \log r \) are known to be particularly useful in many applications. It is natural for us to consider the TPS as basis function. It turn out that the analytical solution of Eq. (30) can be obtained by choosing \( \varphi \) as TPS. The closed form of \( \Phi \) [3] is as follows: (i) two dimensional case \( \varphi = r^2 \log r, \{p_i\}_{i=1}^3 = \{1, x, y\} \)
\[ \Phi = \begin{cases} \frac{-4}{\lambda^3} - \frac{4 \log r}{\lambda^4} - \frac{r^2 \log r}{\lambda^4} - \frac{4K_0(\lambda r)}{\lambda^4}, & r \neq 0, \\ \frac{-4}{\lambda^3} - \frac{4\gamma}{\lambda^4} + \frac{4}{\lambda^4} \log \left(\frac{\lambda}{2}\right), & r = 0, \end{cases} \quad (32) \]
\[ \chi_1 = -\frac{1}{\lambda^2}, \quad \chi_2 = -\frac{x}{\lambda^2}, \quad \chi_3 = -\frac{y}{\lambda^2}, \quad (33) \]

where \( \lambda = \sqrt{s/k}, K_0 \) and \( K_0 \) are the Bessel function of third kind with order zero and one respectively.

(ii) three dimensional case \( \varphi = r, \{p_i\}_{i=1}^4 = \{1, x, y, z\} \)
\[ \Phi = \begin{cases} \frac{-r}{\lambda^2} - \frac{2}{\lambda^4} + \frac{2e^{-\lambda r}}{\lambda^4}, & r \neq 0, \\ \frac{-2}{\lambda^3}, & r = 0, \end{cases} \quad (34) \]
\[ \chi_1 = -\frac{1}{\lambda^2}, \quad \chi_2 = -\frac{x}{\lambda^2}, \quad \chi_3 = -\frac{y}{\lambda^2}, \quad \chi_4 = -\frac{z}{\lambda^2}. \quad (35) \]
The MFS for Modified Helmholtz Equation

The MFS can be considered as a modified Trefftz method for approximating the solution by fundamental solutions and boundary data. In the MFS we place the source points outside the physical domain $\Omega$ in order to avoid the singularities of the fundamental solution. Another attractive feature of the MFS is its spectral convergence.

In analogy to the Laplace equation, let $\Gamma$ be a fictitious boundary containing $\Omega$ and assume that the solution $U_h(x; s)$ of Eqs. (20)-(22) has an analytic continuation defined at every point within the region enclosed by $\Gamma$ and let $n$ be the number of collocation points on the boundary. Figure 1 shows the source points on a spherical fictitious boundary in 3D.

![Figure 1: Source Points on the fictitious boundary.](image)

An approximate solution $\hat{U}_h(x; s)$ to $U_h$ can be represented by

$$
\hat{U}_h(x; s) = \sum_{i=1}^{n} a_i G(x, \xi_i; s), \quad x \in S_1 \cup S_2, \xi_i \in \Gamma,
$$

where the fundamental solution $G(x, \xi; s)$ is given by

$$
G(x, \xi; s) = \begin{cases} 
\frac{1}{2\pi} K_0 \left( r \sqrt{\frac{s}{k}} \right), & \text{for 2D,} \\
\frac{1}{4\pi r} \exp \left( -r \sqrt{\frac{s}{k}} \right), & \text{for 3D.}
\end{cases}
$$

$K_0$ is the modified Bessel function of the second kind and of order zero and $r = ||\xi - x||$ is the Euclidean distance between $\xi$ and $x$. By collocation, we choose $\{x_j\}_{j=1}^{m}$ on $S_1$ and $\{x_j\}_{j=m+1}^{n}$ on $S_2$ such that

$$
\sum_{i=1}^{n} a_i G(x_j, \xi_i; s) = F_1(x_j; s) - \hat{U}_p(x_j; s), \quad \{x_j\}_{j=1}^{m} \in S_1,
$$
\[
\sum_{i=1}^{n} a_i \frac{\partial G(x_j, \xi; s)}{\partial n} = F_2(x_j; s) - \frac{\partial \hat{U}_p(x_j; s)}{\partial n}, \quad \{x_j\}_{j=m+1}^{n} \in S_2,
\]

Eqs. (38)-(39) are a system of \(n\) equations and can be solved by Gaussian elimination. Once \(\{a_i\}_{i=1}^{n}\) is found, \(\hat{U}_h(x; s)\) can be evaluated by equation Eq. (36) at any point \(x \in \Omega \cup S\).

After \(\hat{U}_h\) and \(\hat{U}_p\) are computed, an approximation \(\hat{U}(x; s)\) to \(U(x; s)\) can be given by

\[
\hat{U}(x; s) = \sum_{i=1}^{n} a_i G(x, \xi; s) + \hat{U}_p(x; s).
\]

5 Inverse Laplace Transform

Notice that the computation of \(\hat{U}_h\) in Eq. (36) and \(\hat{U}_p\) in Eq. (29) involves a parameter \(s\) in the LT space. Among all the numerical Laplace transform inverse schemes, Stehfest’s algorithm [4] has been successfully implemented in science and engineering. Based on this algorithm, we numerically inverted the solution in the LT space to the time domain. For the first part of Stehfest’s algorithm, we need to use \(n_s\) distinct parameters \(s\) for a given observation time \(t\); i.e.,

\[
s_\nu = \frac{\ln 2}{t} \nu, \quad \nu = 1, 2, \ldots, n_s,
\]

where \(n_s\) is the number of terms in Stehfest’s algorithm and must be an even number. For each \(s_\nu\), we need to obtain a solution \(\hat{U}(x; s_\nu)\) from Eq. (40) at any given point \(x \in \Omega \cup S\).

The second part of Stehfest’s algorithm is to invert the solution from the LT space to time domain at any given time. Let \(\hat{u}\) be an approximation of \(u\). The inversion procedure is the following:

\[
\hat{u}(x, t) = \ln 2 \frac{n_s}{t} \sum_{\nu=1}^{n_s} W_\nu \cdot \hat{U}(x; s_\nu)
\]

where

\[
W_\nu = (-1)^{\frac{n_s}{2} + \nu} \sum_{k=\frac{1}{2}(\nu+1)}^{\min\{\nu, \frac{n_s}{2}\}} \frac{k^{n_s/2} (2k)!}{(n_s/2 - k)! k! (\nu - k)! (2k - \nu)!}.
\]

The accuracy of Stehfest’s algorithm depends on the correct choice of \(n_s\), the number of terms in equation (42). As \(n_s\) increases, the accuracy improves and then round-off error becomes a factor and eventually the accuracy declines. The optimal \(n_s\) has a significant impact on the final solution of our proposed method. According to Stehfest’s test of his algorithm on 50 test functions with known inverse Laplace transform, he concluded that the optimal value of \(n_s\) is 10 for single precision variables and 18 for double precision variables.

6 Numerical Results

In the following examples, we use the notation LTMPS-H to differentiate it from LTDRM in [2]. We also denote by LTMFS as the method used to solve diffusion equations with harmonic initial condition mentioned in Section 1.

Example 1 In this example we investigate the flow of heat in the finite rectangle \(-a \leq x \leq a, -b \leq y \leq b\), where \(a = b = 0.2\) m with a unit initial temperature and boundaries kept at zero
temperature. The analytical solution for the temperature distribution was given by Carslaw and Jaeger [5]:

\[ u(x, y, t) = \frac{16}{\pi^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} L_{n,m} \cos \left( \frac{(2n+1)\pi x}{2a} \right) \cos \left( \frac{(2m+1)\pi y}{2b} \right) \exp(-D_{n,m}t) \] (44)

where

\[ L_{n,m} = \frac{(-1)^{n+m}}{(2n+1)(2m+1)} \quad \text{and} \quad D_{n,m} = \frac{k\pi^2}{4} \left[ \frac{(2n+1)^2}{a^2} + \frac{(2m+1)^2}{b^2} \right]. \] (45)

Here \( k \) is the thermal diffusibility of the substance with units of \([L^2][T^{-1}]\). To compare our result with theirs, we choose the same thermal diffusibility of \( k = 5.8 \times 10^{-7} \text{ m}^2/\text{sec}\) and observation time \( t_{\text{obs}} = 9000 \text{ second}\). The solution profile is shown in Figure 2.

![Figure 2: The profile of temperature distribution on the whole domain.](image)

To approximate the forcing term in Eq. (19) by TPS, we choose 20 collocation points as shown in Figure 3. To obtain the approximate homogeneous solution \( \hat{U}_h \) by the MFS, we choose 16 equally distributed collocation points on the boundary in Figure 3 and the same number of source points uniformly distributed on a circle with center at \((0,0)\) and radius \( r = 3.0 \text{ m}\).

In Figure 4 we denote \( n_s = n_s \) and • stands for the relative error of the LTPMPS-H and the solid line the relative error of LTMFS. The relative errors were calculated on \((x,0.025), 0 \leq x \leq 0.2\). As shown in Figure 4, both the relative errors of the LTPMPS and LTMFS are bounded within 0.16% for \( n_s \geq 10\). With increasing \( n_s \) the relative error becomes stable.

The overall profile of the absolute error for \( n_s = 12\) is shown in Figure 5. The accuracy of the LTPMPS method is far superior than the LTDRM in [2] and the LTBEM in [1]. In order to make the comparison for LTMFS and LTPMPS-H, we choose the same collocation and source points in computing homogeneous solution \( \hat{U}_h \) in Eq. (36) and \( V \) in Eq. (12). We also notice that solutions obtained by the LTPMPS-H and LTMFS are basically identical. This implies that interpolation errors in finding particular solutions in the LT space are practically not existent and the primary computational errors came from the MFS and inversion of the Laplace transform. In the LT space the forcing term of the modified Helmholtz equation is \( 1/k \), a constant, and the TPS with the augmented linear term approximates \( 1/k \) exactly. Furthermore, \( \Psi(r) \) in Eq. (30) can be evaluated analytically. In contrast to the LTDRM, the interpolation error of the forcing term in Eq. (23) which involves an unknown term is quite uncertain.
Figure 3. Interpolation points on a square for the MPS.

Figure 3: Relative errors for the LTDRM-H and LTMFS for various $n_s$.

Figure 4: Absolute errors of the LTDRM-H for $n_s = 12$.

**Example 2** To further demonstrate the effectiveness of LTMPS-H, we extend Example 1 to a 3D problem as given in [1]. We consider the flow of heat in the box $-a \leq x \leq a, -b \leq y \leq b, -c \leq z \leq c$ where $a = b = c = 0.2 \text{ m}$ with a unit initial temperature and boundaries kept at zero temperature. The analytical solution for the temperature distribution was given by Carslaw
and Jaeger [5]:

\[
    u(x, y, z, t) = \frac{64}{\pi^3} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{\ell=0}^{\infty} \frac{(-1)^{n+m+\ell}}{(2n+1)(2m+1)(2\ell+1)} \exp(-D_{n,m,\ell} \cdot t) \\
    \times \cos \left(\frac{(2n+1)\pi x}{2a}\right) \cos \left(\frac{(2m+1)\pi y}{2b}\right) \cos \left(\frac{(2\ell+1)\pi z}{2c}\right)
\]

where

\[
    D_{n,m} = \frac{k\pi^2}{4} \left[ \frac{(2n+1)^2}{a^2} + \frac{(2m+1)^2}{b^2} + \frac{(2\ell+1)^2}{c^2} \right].
\]

The thermal diffusibility \(k\) and observation time \(t_{obs}\) were chosen the same as in Example 1. The temperature distribution was calculated on \(\{(x, 0.025, 0.08) \mid 0 \leq x \leq 0.2\}\). The exact solution along this line is shown in Figure 6.

![Figure 5: Temperature distribution in the direction of x-axis with y = 0.025, z = 0.08.](image)

Figure 5: Temperature distribution in the direction of x-axis with \(y = 0.025, z = 0.08\).

We choose 30 evenly distributed points inside the domain to interpolate the forcing term of Eq. (19) by the TPS. To evaluate the approximate homogeneous solution \(\hat{U}_h\) by the MFS, we choose 62 evenly distributed collocation points on the boundary surface. The collocation points on each surface are shown in Figure 7. The same number of source points were chosen on the fictitious boundary of a box with \(a = b = c = 2m\). The source points on the fictitious boundary are distributed in the same manner as boundary collocation points as in Figure 7.

The results in this example presented similar behavior as that in Example 1. The notation in Figure 8 is defined in the same way as in Figure 4. Again, there is practically no difference between LTMFS and LTMPS-H as shown in Figure 8. The relative errors are bounded within 2.5% for \(n_s \geq 10\). The analytic solution close to the boundary is tending to zero and this leads to the relative error becoming magnified near the boundary. The argument for the interpolation error is similar to Example 1.
Figure 7. Collocation points on each surface of the cube.

Figure 6: Relative errors of the LTDRM-H and LTMFS for various $n_s$.

References


