# A FRACTIONAL-ORDER ALTERNATIVE FOR PHASE-LAGGING EQUATION 

CUI-CUI JI, WEIZHONG DAI*, AND RONALD E. MICKENS


#### Abstract

Phase-lagging equation (PLE) is an equation describing micro/nano scale heat conduction, where the lagging response must be included, particularly under low temperature or high heat-flux conditions. However, finding the analytical or numerical solutions of the PLE is tedious in general. This article aims at seeking a fractional-order heat equation that is a good alternative for the PLE. To this end, we consider the PLE with simple initial and boundary conditions and obtain a fractional-order heat equation and an associated numerical method for approximating the solution of the PLE. In order to better approximate the PLE, the Levenberg-Marquardt iterative method is employed to estimate the optimal parameters in the fractional-order heat equation. This fractional-order alternative is then tested and compared with the PLE. Results show that the fractional method is promising.


Key words. Phase-lagging equation, fractional-order heat equation, numerical scheme, parameter estimation.

## 1. Introduction

Phase-lagging equation (PLE) is an equation describing micro/nano scale heat conduction, where the lagging response must be included, particularly under low temperature or high heat-flux conditions [1, 2]. The PLE can be expressed as follows [3, 4]:

$$
\begin{equation*}
\frac{\partial \theta\left(\vec{r}, \tau+\tau_{0}\right)}{\partial \tau}=D \nabla^{2} \theta(\vec{r}, \tau) \tag{1}
\end{equation*}
$$

where $\theta$ is the temperature, $\vec{r}$ is the position vector, $t$ is the time, $D$ is the thermal diffusivity, $\tau_{0}$ represents the time lag required to establish steady thermal conduction in a volume element once a temperature gradient has been imposed across it. Based on the Taylor series expression, the zeroth-order approximation of (1) or $\tau_{0}=0$ leads to the common diffusion equation as

$$
\begin{equation*}
\frac{\partial \theta(\vec{r}, \tau)}{\partial \tau}=D \nabla^{2} \theta(\vec{r}, \tau) \tag{2}
\end{equation*}
$$

On the other hand, the first-order approximation of (1) yields a damped wave equation as

$$
\begin{equation*}
\frac{\partial \theta(\vec{r}, \tau)}{\partial \tau}+\tau_{0} \frac{\partial^{2} \theta(\vec{r}, \tau)}{\partial \tau^{2}}=D \nabla^{2} \theta(\vec{r}, \tau) \tag{3}
\end{equation*}
$$

By introducing some non-dimensional quantities $u=\theta / \theta_{0}, \vec{x}=\vec{r} / l, t=\tau D / l^{2}$, where $\theta_{0}>0$ is taken as a constant and $l$ is the length of the space domain, the damped wave equation (3) can be transformed in dimensionless form as

$$
\begin{equation*}
\frac{\partial u(\vec{x}, t)}{\partial t}+\kappa_{0} \frac{\partial^{2} u(\vec{x}, t)}{\partial t^{2}}=\nabla^{2} u(\vec{x}, t), \tag{4}
\end{equation*}
$$

where the dimensionless lag time is given by $\kappa_{0}=\tau_{0} D / l^{2}$. Dai and his co-workers $[5,6]$ compared the difference of the solutions between the PLE and the damped wave equation and showed the damped wave equation is a good approximation for the PLE when the dimensionless time lag $\kappa_{0}$ is small.

It should be pointed out that finding the analytical or numerical solutions of the PLE is tedious in general. Notably, fractional calculus is an emerging field in mathematics with deep applications in all related fields of science and engineering, such as in physics, biology, material science, etc; for example, see $[7,8,9,10,11$, $12,13,14,15,16,17]$. Recently, some fractional models have been successfully applied to simulate the heat and thermal transfer in non-uniform porous medium, viscoelastic materials, dynamic electro-magnetic fields [18, 19, 20, 21, 22, 23, 24, 25]. This article aims at seeking a fractional-order heat equation that can be a good alternative for the PLE, where the dimensionless time lag $\kappa_{0}$ takes any suitable value, in order to avoid the violation of the second law of thermodynamics $[18,19$, $26,27,28,29]$.

As we know, the fractional calculus possesses the convolution structure, which is similar to the hereditary property of the analytic solution of the PLE (see [5, 6]). This gives us a hint to develop an innovative and accurate fractional-order heat equation to replace the PLE. As such, one could use the solution of the fractionalorder heat equation to approximate the solution of the PLE and hence simplify the computation. For this purpose, we propose the fractional-order heat equation

$$
\begin{equation*}
\kappa_{1} \cdot \frac{\partial u(\vec{x}, t)}{\partial t}+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{\alpha} u(\vec{x}, t)=\nabla^{2} u(\vec{x}, t), \tag{5}
\end{equation*}
$$

where ${ }_{0}^{C} D_{t}^{\alpha}$ is the Caputo fractional derivative of order $\alpha \in(1,2)$, and $\kappa_{1}$ and $\kappa_{2}$ are two constants to be determined, which is a good alternative of (1).

The rest of this paper is organized as follows. In Sect. 2, we consider the fractional-order heat equation and estimate its energy. In Sect. 3, we construct a compact difference scheme for solving the fractional-order heat equation. In Sect. 4 , we analyze the unconditional stability and convergence of the scheme rigorously by the discrete energy method. In Sect. 5, we employ the Levenberg-Marquardt iterative method to estimate the parameters of the fractional-order heat equation. In Sect. 6, we compare the solutions between the fractional-order heat equation and the PLE by investigating a testing problem. We summarize the major results of this work in Sect. 7.

## 2. Fractional-order heat equation

Consider a dimensionless fractional-order heat equation with initial and boundary conditions as follows:

$$
\begin{align*}
& \kappa_{1} \cdot u_{t}(x, t)+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{1+\beta} u(x, t)=\frac{\partial^{2} u(x, t)}{\partial x^{2}},(x, t) \in(0,1) \times(0, \infty),  \tag{6}\\
& u(0, t)=0, \quad u(1, t)=0, \quad t>0,  \tag{7}\\
& u(x, 0)=\psi(x), \quad \partial u(x, 0) / \partial t=\phi(x), \quad x \in(0,1),
\end{align*}
$$

where $0<\beta<1(\alpha=1+\beta)$, and the Caputo fractional derivative is defined by [8]

$$
\begin{equation*}
{ }_{0}^{C} D_{t}^{1+\beta} u(x, t)=\frac{1}{\Gamma(1-\beta)} \int_{0}^{t} \frac{u_{s s}(x, s)}{(t-s)^{\beta}} d s, \quad t>0 . \tag{9}
\end{equation*}
$$

Here, we analyze the energy estimation of the model (6)-(8). To this end, we present two useful lemmas with respect to the Caputo factional derivative operator, which will be used for estimating the energy of the governing model (6)-(8).

Lemma 2.1. [30] For any function $y(t) \in C^{1}([0, T])$, if $0<\mu<1$, it holds that

$$
\begin{equation*}
y(t) \cdot{ }_{0}^{C} D_{t}^{\mu} y(t) \geq \frac{1}{2}{ }_{0}^{C} D_{t}^{\mu} y^{2}(t) . \tag{10}
\end{equation*}
$$

Lemma 2.2. [19] Let the function $y(t) \in C^{1}([0, T])$. If $0<\mu<1$, then it holds that

$$
\begin{equation*}
\int_{0}^{t}{ }_{0}^{C} D_{\eta}^{\mu} y(\eta) d \eta={ }_{0}^{R L} D_{t}^{\mu-1} y(t)-\frac{t^{1-\mu}}{\Gamma(2-\mu)} y(0), \tag{11}
\end{equation*}
$$

where the operator ${ }_{0}^{R L} D_{t}^{-\mu}$ denotes the Riemann-Liouville (RL) fractional integral of order $\mu$, i.e.,

$$
\begin{equation*}
{ }_{0}^{R L} D_{t}^{-\mu} y(t)=\frac{1}{\Gamma(\mu)} \int_{0}^{t} \frac{y(s) d s}{(t-s)^{1-\mu}}, \quad t>0 . \tag{12}
\end{equation*}
$$

Theorem 2.1. Let $u(x, t)$ be the solution of the problem (6)-(8). And we assume that $u(x, t) \in C^{2,2}([0,1] \times[0, T])$. We define an energy function
$E(t)=\kappa_{1} \cdot \int_{0}^{t} \int_{0}^{1} u_{s}^{2}(x, s) d x d s+\kappa_{2} \cdot{ }_{0}^{R L} D_{t}^{\alpha-1}\left(\int_{0}^{1} u_{t}^{2}(x, t) d x\right)+\int_{0}^{1} u_{x}^{2}(x, t) d x$.
Then, it holds that,

$$
\begin{equation*}
E(t) \leq E(0), \quad t>0 \tag{13}
\end{equation*}
$$

Proof. Taking an inner product of (6) with $u_{t}(x, t)$, we have

$$
\begin{equation*}
\kappa_{1} \cdot \int_{0}^{1} u_{t}^{2}(x, t) d x+\kappa_{2} \cdot \int_{0}^{1}{ }_{0}^{C} D_{t}^{1+\beta} u(x, t) \cdot u_{t}(x, t) d x=\int_{0}^{1} u_{x x}(x, t) \cdot u_{t}(x, t) d x \tag{14}
\end{equation*}
$$

By virtue of Lemma 2.1, we obtain the following estimate as:

$$
\begin{equation*}
\int_{0}^{1}{ }_{0}^{C} D_{t}^{1+\beta} u(x, t) \cdot u_{t}(x, t) d x \geq \frac{1}{2}{ }_{0}^{C} D_{t}^{\beta}\left(\int_{0}^{1} u_{t}^{2}(x, t) d x\right) . \tag{15}
\end{equation*}
$$

Applying the integration by parts and noticing the boundary condition (7), it holds that

$$
\begin{equation*}
\int_{0}^{1} u_{x x}(x, t) \cdot u_{t}(x, t) d x=-\frac{1}{2} \frac{d}{d t} \int_{0}^{1} u_{x}^{2}(x, t) d x \tag{16}
\end{equation*}
$$

Inserting (15)-(16) into (14) and multiplying the result by 2 lead to

$$
2 \kappa_{1} \cdot \int_{0}^{1} u_{t}^{2}(x, t) d x+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{\beta}\left(\int_{0}^{1} u_{t}^{2}(x, t) d x\right)+\frac{d}{d t} \int_{0}^{1} u_{x}^{2}(x, t) d x \leq 0 .
$$

We use Lemma 2.2 for the second term on the left-hand-side of the above inequality. This gives

$$
\begin{equation*}
\frac{d}{d t} E(t) \leq 0 \tag{17}
\end{equation*}
$$

Replacing the variable $t$ with $s$ on both sides of (17), and integrating the result with respect to the variable $s$ from 0 to $t$, we arrive at the energy estimation conclusion.

Remark 2.1. Recent discussions have showed that the solutions of the time fractional partial differential equations may have a weak singularity near the initial time $t=0$ under certain circumstances. Based on the analysis in [31], the weak
singularity may occur when the solution of the fractional-order heat equation (6) satisfies

$$
\begin{equation*}
\left|\frac{\partial^{l} u}{\partial t^{l}}(x, t)\right| \leq C_{u}\left(1+t^{1+\beta-l}\right), \quad l=0,1,2,3 . \tag{18}
\end{equation*}
$$

In our proof for Theorem 2.1, we obtained an energy estimate based on Lemmas 2.1 and 2.2 by assuming $u(x, t) \in C^{2,2}([0,1] \times[0, T])$. However, in the case of weak singularity at $t=0$, Lemmas 2.1 and 2.2 may not work for the energy estimate. Thus, how to estimate the energy of (6) under the required regularity (18) needs to further analyze. We would like to point out that our focus in this study is to see if the phase-lagging equation (1.1) can be replaced with a fractional-order heat equation since finding the analytical or numerical solution of PLE is tedious in general.

## 3. Compact finite difference for fractional-order heat equation

Since the exact solution of the fractional-order heat equation is difficult to obtain in general, we solve the fractional-order model (6)-(8) by using a finite difference scheme. To this end, we first divide the interval $[0, T]$ into $N$-subintervals with the temporal step size $\Delta t=\frac{T}{N}$, and denote $t_{k}=k \Delta t, 0 \leq k \leq N$, and $t_{k-\frac{1}{2}}=$ $\frac{1}{2}\left(t_{k-1}+t_{k}\right), 1 \leq k \leq N$. Let $v(t)=u^{\prime}(t)$ and $v^{k}=v\left(t_{k}\right)$ for $k \geq 1$. Denote the difference quotient $\delta_{t} v^{k-\frac{1}{2}}=\left(v^{k}-v^{k-1}\right) / \Delta t_{k}$. For $n=1, \cdots, N$, we have the following $L 1$ formula for the Caputo derivative ${ }_{0}^{C} D_{t}^{\beta} v(t)$ of order $\beta \in(0,1)$ at $t=t_{n}$ :

$$
\begin{align*}
{ }_{0}^{C} D_{t}^{\beta} v\left(t_{n}\right) & =\frac{1}{\Gamma(1-\beta)} \sum_{k=1}^{n} \int_{t_{k-1}}^{t_{k}} \frac{v^{\prime}(s)}{\left(t_{n}-s\right)^{\beta}} d s \\
& =\sum_{k=1}^{n} a_{n-k}^{(\beta)}\left(v^{k}-v^{k-1}\right)+O\left(\Delta t^{2-\beta}\right), \quad 1 \leq n \leq N, \tag{19}
\end{align*}
$$

where the coefficient $\left\{a_{n-k}^{(\beta)}\right\}$ is given by

$$
\begin{align*}
a_{n-k}^{(\beta)} & =\frac{(\Delta t)^{-1}}{\Gamma(1-\beta)} \int_{t_{k-1}}^{t_{k}} \frac{d s}{\left(t_{n}-s\right)^{\beta}}  \tag{20}\\
& =\frac{(\Delta t)^{-\beta}}{\Gamma(2-\beta)}\left[(n-k+1)^{1-\beta}-(n-k)^{1-\beta}\right], \quad 1 \leq k \leq n
\end{align*}
$$

By using the relation ${ }_{0}^{C} D_{t}^{1+\beta} u(t)={ }_{0}^{C} D_{t}^{\beta} v(t)$, we can readily obtain

$$
\begin{equation*}
{ }_{0}^{C} D_{t}^{1+\beta} u\left(t_{n}\right)=\sum_{k=1}^{n} a_{n-k}^{(\beta)}\left(v\left(t_{k}\right)-v\left(t_{k-1}\right)\right)+O\left(\Delta t^{2-\beta}\right), \quad 1 \leq n \leq N . \tag{21}
\end{equation*}
$$

Averaging ${ }_{0}^{C} D_{t}^{1+\beta} u\left(t_{n}\right)$ and ${ }_{0}^{C} D_{t}^{1+\beta} u\left(t_{n-1}\right)$, and also using the approximation

$$
\begin{equation*}
\frac{u^{\prime}\left(t_{k}\right)+u^{\prime}\left(t_{k-1}\right)}{2}=\delta_{t} u^{k-\frac{1}{2}}+O\left(\Delta t^{2}\right), \quad 1 \leq k \leq N \tag{22}
\end{equation*}
$$

we have

$$
\begin{align*}
\frac{{ }_{0}^{C} D_{t}^{1+\beta} u\left(t_{n}\right)+{ }_{0}^{C} D_{t}^{1+\beta} u\left(t_{n-1}\right)}{2} & =\sum_{k=1}^{n} a_{n-k}^{(\beta)}\left(\delta_{t} u^{k-\frac{1}{2}}-\delta_{t} u^{k-\frac{3}{2}}\right)+O\left(\Delta t^{2-\beta}\right)  \tag{23}\\
& \stackrel{\text { def }}{=} \delta_{t}^{\beta}\left(\delta_{t} u^{n-\frac{1}{2}}, u^{\prime}\left(t_{0}\right)\right)+O\left(\Delta t^{2-\beta}\right),
\end{align*}
$$

where $\delta_{t} u^{-\frac{1}{2}}=u^{\prime}\left(t_{0}\right)$.

For the space domain, we divide the interval $[0,1]$ into $M$-subintervals with a step size $\Delta x=\frac{1}{M}$ and denote $x_{i}=i \Delta x, 0 \leq i \leq M$. Let $\mathcal{U}_{h}=\{u \mid u=$ $\left.\left(u_{0}, u_{1}, \cdots, u_{M}\right)\right\}$ be the grid function space defined on $\Omega_{h}=\left\{x_{i} \mid 0 \leq i \leq M\right\}$. For any $u, v \in \mathcal{U}_{h}$, we denote $\delta_{x} u_{i-\frac{1}{2}}=\left(u_{i}-u_{i-1}\right) / \Delta x, 1 \leq i \leq M ; \delta_{x}^{2} u_{i}=$ $\left(\delta_{x} u_{i+\frac{1}{2}}-\delta_{x} u_{i-\frac{1}{2}}\right) / \Delta x, 1 \leq i \leq M-1$ and an averaging operator

$$
\mathcal{A} u_{i}=\left\{\begin{array}{l}
u_{i}, \quad i=0, M  \tag{24}\\
\frac{1}{12} u_{i-1}+\frac{10}{12} u_{i}+\frac{1}{12} u_{i+1}, \quad 1 \leq i \leq M-1 .
\end{array}\right.
$$

Define the grid function space $\stackrel{\mathcal{U}}{h}^{h}=\left\{u \mid u=\left(u_{0}, u_{1}, \cdots, u_{M}\right), u_{0}=0, u_{M}=\right.$ $0\}$. For any $u, v \in \stackrel{\circ}{\mathcal{U}}_{h}$, we denote the inner products as $(u, v)=\Delta x \sum_{i=1}^{M-1} u_{i} v_{i}$, $\langle u, v\rangle=(\mathcal{A} u, v),\left(\delta_{x} u, \delta_{x} v\right)=\Delta x \sum_{i=1}^{M}\left(\delta_{x} u_{i-\frac{1}{2}}\right) \delta_{x} v_{i-\frac{1}{2}}$ and the corresponding norms as $\|u\|=\sqrt{(u, u)},\left\|\delta_{x} u\right\|=\sqrt{\left(\delta_{x} u, \delta_{x} u\right)},\|u\|_{\mathcal{A}}=\sqrt{\langle u, u\rangle}$. It is easy to verify that, for any grid function $u \in \dot{\mathcal{U}}_{h}$, there exist two constants $C_{1}$ and $C_{2}$ satisfying $C_{1}\|u\| \leq\|u\|_{\mathcal{A}} \leq C_{2}\|u\|$ (see [32]).

We now derive a difference scheme for the model (6)-(8). Assume that $u(x, t)$ is the solution (6)-(8). We define $U_{i}(t)=u\left(x_{i}, t\right)$ on $\Omega_{h}$ and $U_{i}^{k}=u\left(x_{i}, t_{k}\right)$ on grid points $\left(x_{i}, t_{n}\right), 0 \leq i \leq M, 0 \leq n \leq N$. For the space discretization, considering (6) at the grid point $\left(x_{i}, t\right)$, we have

$$
\begin{equation*}
\kappa_{1} \cdot u_{t}\left(x_{i}, t\right)+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{1+\beta} u\left(x_{i}, t\right)=u_{x x}\left(x_{i}, t\right), \quad 0 \leq i \leq M, t \in(0, T] . \tag{25}
\end{equation*}
$$

Performing the average operator $\mathcal{A}$ on both sides of (25) yields

$$
\begin{align*}
\mathcal{A}\left(\kappa_{1} \frac{d}{d t} U_{i}(t)+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{1+\beta} U_{i}(t)\right)= & \delta_{x}^{2} U_{i}(t)+(\Delta x)^{4} \cdot r_{i}(t)  \tag{26}\\
& 1 \leq i \leq M-1, t \in(0, T] .
\end{align*}
$$

Here, we have used the compact finite difference scheme [33]

$$
\mathcal{A} u_{x x}\left(x_{i}, t\right)=\delta_{x}^{2} u\left(x_{i}, t\right)+(\Delta x)^{4} \cdot r_{i}(t)
$$

For the time discretization, averaging (26) at $t=t_{n-1}$ and $t=t_{n}$, we have

$$
\begin{align*}
\mathcal{A}\left(\kappa_{1} \cdot \delta_{t} U_{i}^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} U_{i}^{n-\frac{1}{2}}, \phi_{i}\right)\right)= & \delta_{x}^{2} U_{i}^{n-\frac{1}{2}}+\left(R^{x}\right)_{i}^{n-\frac{1}{2}}+\left(R^{t}\right)_{i}^{n-\frac{1}{2}}  \tag{27}\\
& 0 \leq i \leq M, \quad 1 \leq n \leq N
\end{align*}
$$

where $\delta_{t}^{\beta}\left(\delta_{t} U_{i}^{n-\frac{1}{2}}, \phi_{i}\right)=\sum_{k=1}^{n} a_{n-k}^{(\beta)}\left(\delta_{t} U_{i}^{k-\frac{1}{2}}-\delta_{t} U_{i}^{k-\frac{3}{2}}\right)$ defined in (23), and the truncation errors satisfy

$$
\begin{align*}
& \left|\left(R^{x}\right)_{i}^{n-\frac{1}{2}}\right|=(\Delta x)^{4}\left|\frac{r_{i}\left(t_{n}\right)+r_{i}\left(t_{n-1}\right)}{2}\right| \lesssim(\Delta x)^{4}, \quad 0 \leq i \leq M  \tag{28}\\
& \left|\left(R^{t}\right)_{i}^{n-\frac{1}{2}}\right| \lesssim(\Delta t)^{2-\beta}, \quad 0 \leq i \leq M \tag{29}
\end{align*}
$$

for $n=1, \cdots, N$. Noticing the boundary conditions (7) and the initial condition

$$
\begin{align*}
& U_{0}^{n}=0, \quad U_{M}^{n}=0, \quad 1 \leq n \leq N,  \tag{30}\\
& U_{i}^{0}=\psi\left(x_{i}\right), \quad 0 \leq i \leq M,
\end{align*}
$$

and dropping small terms in (27), and replacing $U_{i}^{n}$ with its numerical approximation $u_{i}^{n}$, we obtain a compact finite difference scheme for the problem (6)-(8) as follows

$$
\begin{array}{ll}
\mathcal{A}\left(\kappa_{1} \cdot \delta_{t} u_{i}^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} u_{i}^{n-\frac{1}{2}}, \phi_{i}\right)\right)= & \delta_{x}^{2} u_{i}^{n-\frac{1}{2}}, \\
& 1 \leq i \leq M-1,1 \leq n \leq N, \\
u_{0}^{n}=0, \quad u_{M}^{n}=0, \quad 1 \leq n \leq N, & \\
u_{i}^{0}=\psi\left(x_{i}\right), \quad 0 \leq i \leq M . & \tag{34}
\end{array}
$$

It can be seen that the truncation error of the above scheme is $O\left((\Delta t)^{2-\beta}+(\Delta x)^{4}\right)$ for $i=1,2, \cdots, M-1$.

## 4. Stability and convergence

In this section, we analyze the stability of the present scheme in (32)-(34). Suppose that $\left\{v_{i}^{n} \mid 0 \leq i \leq M, 0 \leq n \leq N\right\}$ is the solution of

$$
\begin{align*}
& \mathcal{A}\left(\kappa_{1} \cdot \delta_{t} v_{i}^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} v_{i}^{n-\frac{1}{2}}, \phi_{i}+\tilde{\varphi}_{2, i}\right)\right)=\delta_{x}^{2} v_{i}^{n-\frac{1}{2}}+G_{i}^{n-\frac{1}{2}},  \tag{35}\\
& \\
& \quad 1 \leq i \leq M-1,1 \leq n \leq N,  \tag{36}\\
& v_{0}^{n}=0, \quad v_{M}^{n}=0, \quad 1 \leq n \leq N,  \tag{37}\\
& v_{i}^{0}=\psi\left(x_{i}\right)+\tilde{\varphi}_{1, i}, \quad 0 \leq i \leq M,
\end{align*}
$$

where $\tilde{\varphi}_{1, i}, \tilde{\varphi}_{2, i}$ and $G_{i}^{n-\frac{1}{2}}$ are small perturbation functions. Denote the perturbation term $\eta_{i}^{n}=v_{i}^{n}-u_{i}^{n}, 0 \leq i \leq M, 0 \leq n \leq N$. Then, we have the perturbation system

$$
\begin{align*}
& \mathcal{A}\left(\kappa_{1} \cdot \delta_{t} \eta_{i}^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} \eta_{i}^{n-\frac{1}{2}}, \tilde{\varphi}_{2, i}\right)\right)=\delta_{x}^{2} \eta_{i}^{n-\frac{1}{2}}+G_{i}^{n-\frac{1}{2}},  \tag{38}\\
& \quad 1 \leq i \leq M-1, \quad 1 \leq n \leq N, \\
& \eta_{0}^{n}=0, \quad \eta_{M}^{n}=0, \quad 1 \leq n \leq N,  \tag{39}\\
& \eta_{i}^{0}=\tilde{\varphi}_{1, i}, \quad 0 \leq i \leq M . \tag{40}
\end{align*}
$$

Theorem 4.1 (Stability). Let $\left\{\eta_{i}^{n} \mid 0 \leq i \leq M, 0 \leq n \leq N\right\}$ be the solution of the perturbation system. It holds that the difference scheme (32)-(34) is stable with respect to the perturbations $\left\{G_{i}^{n-\frac{1}{2}}, \tilde{\varphi}_{1, i}, \tilde{\varphi}_{2, i}\right\}$, i.e.,

$$
\begin{equation*}
\left\|\delta_{x} \eta^{n}\right\|^{2} \leq\left\|\delta_{x} \tilde{\varphi}_{1}\right\|^{2}+\frac{\kappa_{2} t_{n}^{1-\beta}}{\Gamma(2-\beta)}\left\|\tilde{\varphi}_{2}\right\|_{\mathcal{A}}^{2}+\frac{\Delta t}{2 \kappa_{1} \cdot C_{1}^{2}} \sum_{s=1}^{n}\left\|G^{s-\frac{1}{2}}\right\|^{2}, \quad 1 \leq n \leq N . \tag{41}
\end{equation*}
$$

Proof. We take an inner product of (38) with $\delta_{t} \eta^{n-\frac{1}{2}}$ and obtain

$$
\begin{align*}
& \left\langle\left(\kappa_{1} \cdot \delta_{t} \eta^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} \eta^{n-\frac{1}{2}}, \tilde{\varphi}_{2}\right)\right), \delta_{t} \eta^{n-\frac{1}{2}}\right\rangle  \tag{42}\\
& \quad=\left(\delta_{x}^{2} \eta^{n-\frac{1}{2}}, \delta_{t} \eta^{n-\frac{1}{2}}\right)+\left(G^{n-\frac{1}{2}}, \delta_{t} \eta^{n-\frac{1}{2}}\right), \quad 1 \leq k \leq N .
\end{align*}
$$

For simplicity, we denote

$$
Q^{n}:=\Delta t \sum_{l=1}^{n} a_{n-l}^{(\beta)}\left\|\delta_{t} \eta^{l-\frac{1}{2}}\right\|_{\mathcal{A}}^{2}, \quad 1 \leq k \leq N
$$

We use Lemma 6 in [19] ( $\epsilon=\frac{1}{2}$ ) to estimate the term on the left-hand-side of (42). This gives

$$
\begin{align*}
& \left\langle\left(\kappa_{1} \cdot \delta_{t} \eta^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} \eta^{n-\frac{1}{2}}, \tilde{\varphi}_{2}\right)\right), \delta_{t} \eta^{n-\frac{1}{2}}\right\rangle  \tag{43}\\
& \quad \geq \kappa_{1} \cdot\left\|\delta_{t} \eta^{n-\frac{1}{2}}\right\|_{\mathcal{A}}^{2}+\frac{\kappa_{2}}{2 \Delta t}\left(Q^{n}-Q^{n-1}\right)-\frac{\kappa_{2}}{2} a_{n-1}^{(\beta)}\left\|\tilde{\varphi}_{2}\right\|_{\mathcal{A}}^{2} .
\end{align*}
$$

Using the summation by parts for the first term on the right-hand-side of (42), we obtain

$$
\begin{equation*}
\left(\delta_{x}^{2} \eta^{n-\frac{1}{2}}, \delta_{t} \eta^{n-\frac{1}{2}}\right)=-\frac{1}{2 \Delta t}\left(\left\|\delta_{x} \eta^{n}\right\|^{2}-\left\|\delta_{x} \eta^{n-1}\right\|^{2}\right) . \tag{44}
\end{equation*}
$$

Using the Cauchy-Schwarz inequality for the second term on the right-hand-side of (42), we have

$$
\begin{align*}
\left(G^{n-\frac{1}{2}}, \delta_{t} \eta^{n-\frac{1}{2}}\right) & \leq\left\|\delta_{t} \eta^{n-\frac{1}{2}}\right\| \cdot\left\|G^{n-\frac{1}{2}}\right\| \\
& \leq \frac{1}{C_{1}}\left\|\delta_{t} \eta^{n-\frac{1}{2}}\right\|_{\mathcal{A}} \cdot\left\|G^{n-\frac{1}{2}}\right\|  \tag{45}\\
& \leq \kappa_{1} \cdot\left\|\delta_{t} \eta^{n-\frac{1}{2}}\right\|_{\mathcal{A}}^{2}+\frac{1}{4 \kappa_{1} \cdot C_{1}^{2}}\left\|G^{k-\frac{1}{2}}\right\|^{2} .
\end{align*}
$$

Inserting (43)-(45) into (42) yields

$$
\begin{align*}
& \left(\kappa_{2} Q^{n}+\left\|\delta_{x} \eta^{n}\right\|^{2}\right)-\left(\kappa_{2} Q^{n-1}+\left\|\delta_{x} \eta^{n-1}\right\|^{2}\right) \\
\leq & \kappa_{2} a_{k-1}^{(\beta)} \Delta t\left\|\tilde{\varphi}_{2}\right\|_{\mathcal{A}}^{2}+\frac{\Delta t}{2 \kappa_{1} \cdot C_{1}^{2}}\left\|G^{n-\frac{1}{2}}\right\|^{2} . \tag{46}
\end{align*}
$$

Replacing the superscript $n$ with $s$ and summing up $s$ from 1 to $n$ on both sides of (46), we have

$$
\begin{equation*}
\left(\kappa_{2} Q^{n}+\left\|\delta_{x} \eta^{n}\right\|^{2}\right) \leq\left\|\delta_{x} \eta^{0}\right\|^{2}+\frac{\kappa_{2} t_{n}^{1-\beta}}{\Gamma(2-\beta)}\left\|\tilde{\varphi}_{2}\right\|_{\mathcal{A}}^{2}+\frac{\Delta t}{2 \kappa_{1} \cdot C_{1}^{2}} \sum_{s=1}^{n}\left\|G^{s-\frac{1}{2}}\right\|^{2} \tag{47}
\end{equation*}
$$

which gives (41) and hence the theorem holds.
Theorem 4.2 (Convergence). Suppose that the solution $u(x, t)$ of the problem (6)(8) is sufficiently smooth. Let $\left\{u_{i}^{n} \mid 0 \leq i \leq M, 0 \leq n \leq N\right\}$ be the solution of the difference scheme (32)-(34). Then, the following optimal error estimate holds

$$
\begin{equation*}
\left\|U^{n}-u^{n}\right\|_{\infty} \leq C_{3}\left((\Delta t)^{2-\beta}+(\Delta x)^{4}\right), \quad 1 \leq n \leq N \tag{48}
\end{equation*}
$$

Here, $C_{3}$ is a positive constant independent of $\Delta t$ and $\Delta x$.
Proof. Denote the error $e^{n}=U^{n}-u^{n}$. We subtract (32)-(34) from (27), (30)-(31), respectively, and take an inner product of the resulting error equation with $\delta_{t} e^{n-\frac{1}{2}}$. This gives

$$
\begin{align*}
& \left\langle\left(\kappa_{1} \cdot \delta_{t} e^{n-\frac{1}{2}}+\kappa_{2} \cdot \delta_{t}^{\beta}\left(\delta_{t} e^{n-\frac{1}{2}}, 0\right)\right), \delta_{t} e^{n-\frac{1}{2}}\right\rangle  \tag{49}\\
& \quad=\left(\delta_{x}^{2} e^{n-\frac{1}{2}}, \delta_{t} e^{n-\frac{1}{2}}\right)+\left(R^{n-\frac{1}{2}}, \delta_{t} e^{n-\frac{1}{2}}\right), \quad 1 \leq n \leq N,
\end{align*}
$$

where $R_{i}^{n-\frac{1}{2}}=\left(R^{x}\right)_{i}^{n-\frac{1}{2}}+\left(R^{t}\right)_{i}^{n-\frac{1}{2}}$. Adopting the analysis strategy of (42) in the stability theorem, we have

$$
\begin{equation*}
\left\|\delta_{x} e^{n}\right\|^{2} \leq \frac{\Delta t}{2 \kappa_{1} \cdot C_{1}^{2}} \sum_{s=1}^{n}\left\|R^{s-\frac{1}{2}}\right\|^{2}, \quad 1 \leq n \leq N . \tag{50}
\end{equation*}
$$

Noticing the truncation errors (28)-(29) and the estimate $\left\|e^{n}\right\|_{\infty} \leq \frac{1}{2}\left\|\delta_{x} e^{n}\right\|$, we obtain the convergence conclusion.

## 5. Parameter estimation for the fractional-order heat equation using the Levenberg-Marquardt algorithm

In this section, we regard the parameter estimation as an optimization problem and use the Levenberg-Marquardt algorithm to estimate the parameters $\beta, \kappa_{1}, \kappa_{2}$. Let $\mathbf{P}$ be a vector of the unknown parameters $\beta, \kappa_{1}$ and $\kappa_{2}$, i.e., $\mathbf{P}=\left[\beta, \kappa_{1}, \kappa_{2}\right]$. Then we need find $\mathbf{P}$ to minimize the objective function $S(\mathbf{P})$, i.e.

$$
\begin{equation*}
S(\mathbf{P})=[\mathbf{Y}-\mathbf{U}(\mathbf{P})]^{\mathrm{T}}[\mathbf{Y}-\mathbf{U}(\mathbf{P})], \tag{51}
\end{equation*}
$$

where $\mathbf{Y}=\left[y_{1}, y_{2}, \cdots, y_{\Omega}\right]^{\mathrm{T}}$ is a measured heat flux vector obtained from the solution of the direct problem at the measurement location, $\mathbf{U}(\mathbf{P})=\left[U_{1}(\mathbf{P}), \cdots, U_{\Omega}(\mathbf{P})\right]^{\mathrm{T}}$ is an estimated heat flux vector calculated from the direct problem by the compact difference method (32)-(34).

The Levenberg-Marquardt algorithm is an optimization method for solving nonlinear least-squares problem of parameter estimation by iteration. This iterative algorithm is given by [34]

$$
\begin{equation*}
\mathbf{P}^{(k+1)}=\mathbf{P}^{(k)}+\left[\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}} \mathbf{J}^{(k)}+\mu_{k} \mathbf{D}^{(k)}\right]^{-1}\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}}\left[\mathbf{Y}-\mathbf{U}\left(\mathbf{P}^{(k)}\right)\right], \tag{52}
\end{equation*}
$$

where the superscript $(k)$ is the number of iterations, $\mu_{k}$ is a damping parameter, and the Jacobian matrix $\mathbf{J}$ is the sensitivity coefficient matrix defined by $\mathbf{J} \equiv$ $\partial \mathbf{U} / \partial \mathbf{P}$. The matrix $\mathbf{D}^{(k)}=\operatorname{diag}\left(\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}} \mathbf{J}^{(k)}\right)$, which is a diagonal matrix. In each iteration, the matrix term $\mu_{k} \mathbf{D}^{(k)}$ can be viewed as a regulator to make the matrix $\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}} \mathbf{J}^{(k)}$ reversible if necessary.

The Levenberg-Marquardt algorithm is summarized as follows. Suppose that the measurement value $\mathbf{Y}$ is available, and the initial guess $\mathbf{P}^{(0)}$ is given for the unknown parameter $\mathbf{P}$, we choose $\nu=2, \eta=1, \mu_{0}=\epsilon \cdot \max \left\{\operatorname{diag}\left(\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}} \mathbf{J}^{(k)}\right)\right\}$, where $\epsilon$ is chosen by the user, for example, $\epsilon=10^{-3}$, and set $k=0$.
Step 1. Solve the direct problem with the compact difference scheme (32)-(34) by using the estimated value $\mathbf{P}^{(k)}=\left\{\beta, \kappa_{1}, \kappa_{2}\right\}^{\mathrm{T}}$ at the $k$-th iteration and compute $\mathbf{U}\left(\mathbf{P}^{(k)}\right)$;
Step 2. Compute $S\left(\mathbf{P}^{(k)}\right)$;
Step 3. Solve the direct problem with the compact difference scheme (32)-(34) three more times with each time perturbing only one of the parameters by a small amount and compute

$$
\begin{aligned}
& \mathbf{U}^{(k)}\left(\beta+\Delta \beta, \kappa_{1}, \kappa_{2} ; t\right) \\
& \mathbf{U}^{(k)}\left(\beta, \kappa_{1}+\Delta \kappa_{1}, \kappa_{2} ; t\right) \\
& \mathbf{U}^{(k)}\left(\beta, \kappa_{1}, \kappa_{2}+\Delta \kappa_{2} ; t\right)
\end{aligned}
$$

For each case $U_{i}^{(k)} \equiv T\left(t_{i}\right), i=1, \cdots, \Omega$ are readily available.
Step 4. Compute the sensitivity coefficients in the Jacobian matrix $\mathbf{J}$ for each parameter $\beta, \kappa_{1}, \kappa_{2}$. For example, with respect to $\beta$, we compute

$$
\begin{equation*}
\frac{\partial U_{i}^{(k)}}{\partial \beta}=\frac{\mathbf{U}^{(k)}\left(\beta+\Delta \beta, \kappa_{1}, \kappa_{2} ; t_{i}\right)-\mathbf{U}^{(k)}\left(\beta, \kappa_{1}, \kappa_{2} ; t_{i}\right)}{\Delta \beta} \tag{53}
\end{equation*}
$$

for $i=1, \cdots, \Omega$, then determine the Jacobian matrix $\mathbf{J}^{(k)}$;
Step 5. Compute $\mathbf{g}^{(k)}=\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}}\left[\mathbf{Y}-\mathbf{U}\left(\mathbf{P}^{(k)}\right)\right]$ and $\mathbf{d}^{(k)}=\left[\left(\mathbf{J}^{(k)}\right)^{\mathrm{T}} \mathbf{J}^{(k)}+\mu_{k} \mathbf{D}^{(k)}\right]^{-1} \mathbf{g}^{(k)}$;
Step 6. Compute step size $\eta$ by linear search method, and compute $\mathbf{h}^{(k)}=\eta \mathbf{d}^{(k)}$ and $\mathbf{P}^{(k+1)}=\mathbf{P}^{(k)}+\mathbf{d}^{(k)}$;

Step 7. Solve the direct problem with the compact difference scheme (32)-(34) by using the new estimated value $\mathbf{P}^{(k+1)}$ and compute $\mathbf{U}\left(\mathbf{P}^{(k+1)}\right), S\left(\mathbf{P}^{(k+1)}\right)$, and compute

$$
\begin{equation*}
\rho=\frac{S\left(\mathbf{P}^{(k)}\right)-S\left(\mathbf{P}^{(k+1)}\right)}{\left(\mathbf{h}^{(k)}\right)^{\mathrm{T}}\left(\mu_{k} \mathbf{h}^{(k)}-\mathbf{g}^{(k)}\right)} ; \tag{54}
\end{equation*}
$$

Step 8. If $\rho>0$, replace $\mu_{k}$ with $\mu_{k} \max \left\{\frac{1}{3}, 1-(2 \rho-1)^{3}\right\}$, and $\nu=2$;
Step 9. If $\rho \leq 0$, replace $\mu_{k}$ with $\nu * \mu_{k}$, and $\nu=2 * \mu$;
Step 10. Check the stopping criteria. If satisfied, stop the iteration; otherwise, replace $k$ with $k+1$, and return to Step 3.

## 6. Numerical results and testing

In this section, we compare the difference of the solutions between the dimensionless fractional-order heat equation and the dimensionless PLE in one dimensional case. On the other hand, we will show the advantage of the fractional-order heat equation for approximating the PLE over the damped wave equation and the diffusion equation.

The PLE with simple initial and boundary conditions is considered as follows:

$$
\begin{align*}
& \frac{\partial u\left(x, t+\kappa_{0}\right)}{\partial t}=\frac{\partial^{2} u(x, t)}{\partial x^{2}}, \quad(x, t) \in(0,1) \times(0, \infty)  \tag{55}\\
& u(0, t)=0, \quad u(1, t)=0, \quad t>0  \tag{56}\\
& u(x, t)=\sin (\pi x), \quad(x, t) \in(0,1) \times\left[-\kappa_{0}, 0\right] \tag{57}
\end{align*}
$$

Using the Laplace transform coupled with the separation of variables method, the exact solution to the governing equations (55)-(57) can be found to be

$$
\begin{equation*}
u(x, t)=H(t)\left\{\sum_{m=0}^{\left\lfloor t / \kappa_{0}\right\rfloor+1}\left(-\kappa_{0} \pi^{2}\right)^{m} \frac{\left(t / \kappa_{0}-(m-1)\right)^{m}}{m!}\right\} \sin (\pi x) \tag{58}
\end{equation*}
$$

where $H(\cdot)$ denotes the Heaviside unit step function, and $\lfloor\cdot\rfloor$ denotes the greatest integer (or floor) function, i.e., $\lfloor p\rfloor$ denotes the greatest integer smaller than the real number $p$.

The fractional-order approximation for (55)-(57) can be written as

$$
\begin{align*}
& \kappa_{1} \cdot u_{t}(x, t)+\kappa_{2} \cdot{ }_{0}^{C} D_{t}^{1+\beta} u(x, t)=\frac{\partial^{2} u(x, t)}{\partial x^{2}},  \tag{59}\\
& (x, t) \in(0,1) \times(0, \infty), \\
& u(0, t)=0, \quad u(1, t)=0, \quad t>0,  \tag{60}\\
& u(x, 0)=\sin (\pi x), \quad \partial u(x, 0) / \partial t=0, \quad x \in(0,1) . \tag{61}
\end{align*}
$$

The solution of the fractional-order heat equation (59)-(61) is approximated by using the compact finite difference scheme (32)-(34).

The damped wave equation is presented as follows [5]:

$$
\begin{align*}
& \frac{\partial u(x, t)}{\partial t}+\kappa_{0} \frac{\partial^{2} u(x, t)}{\partial t^{2}}=\frac{\partial^{2} u(x, t)}{\partial x^{2}}, \quad(x, t) \in(0,1) \times(0, \infty),  \tag{62}\\
& u(0, t)=0, \quad u(1, t)=0, \quad t>0  \tag{63}\\
& u(x, 0)=\sin (\pi x), \quad \partial u(x, 0) / \partial t=0, \quad x \in(0,1) \tag{64}
\end{align*}
$$

The exact solution to the above initial-boundary condition problem can be obtained using the separation of variables method and is given by [35]:

$$
u(x, t)= \begin{cases}\exp \left[-t /\left(2 \kappa_{0}\right)\right] \sin [\pi x]\left\{\cosh [w t]+\frac{\sinh [w t]}{\sqrt{|\Delta|}}\right\}, & \kappa_{0}<\kappa_{c}  \tag{65}\\ \exp \left[-t /\left(2 \kappa_{0}\right)\right] \sin [\pi x]\left(1+\frac{t}{2 \kappa_{0}}\right), \quad \kappa_{0}=\kappa_{c} \\ \exp \left[-t /\left(2 \kappa_{0}\right)\right] \sin [\pi x]\left\{\cos [w t]+\frac{\sin [w t]}{\sqrt{|\Delta|}\}}\right\}, & \kappa_{0}>\kappa_{c}\end{cases}
$$

where $\kappa_{c}=(2 \pi)^{-2}$ is a critical value of the thermal lag time, $w=\left(2 \kappa_{0}\right)^{-1} \sqrt{|\Delta|}$, and $\Delta=1-4 \pi^{2} \kappa_{0}$. However, we must reject the case $\kappa_{0}>\kappa_{c}$ as it allows $u$ to assume negative values, in opposition to the fact that $u$ denotes an absolute quantity [35]. Furthermore, by letting $\kappa_{0} \rightarrow 0$ in (65), the solution of the classical diffusion equation is recovered, i.e.,

$$
\begin{equation*}
u(x, t)=e^{-\pi^{2} t} \sin [\pi x] . \tag{66}
\end{equation*}
$$

6.1. Convergence test of the compact scheme. We first check the efficiency and convergence orders of the scheme (32)-(34). In numerical simulations, we computed the time domain $t \in(0,1)$, and chose the parameters $\kappa_{1}=1, \kappa_{2}=1$ and the fractional order $\beta=0.1,0.5,0.9$, respectively, in (59)-(61). Without loss of generality, we assume that $N=2^{J}$, where $J$ is a positive integer. Since the exact solution is not available in general, we use

$$
\begin{aligned}
& \operatorname{Error}_{1}(\Delta t)=\max _{0 \leq i \leq M}\left|u_{i}^{N}(\Delta x, \Delta t)-u_{i}^{2 N}\left(\Delta x, \frac{\Delta t}{2}\right)\right| \\
& \operatorname{Error}_{2}(\Delta x)=\max _{0 \leq i \leq M}\left|u_{i}^{N}(\Delta x, \Delta t)-u_{2 i}^{N}\left(\frac{\Delta x}{2}, \Delta t\right)\right|
\end{aligned}
$$

to measure the numerical errors in time and in space, respectively, where $u_{i}^{N}(\Delta x, \Delta t)$ denotes the numerical solution at grids $\left(x_{i}, t_{N}\right)$. The corresponding temporal and spatial convergence orders are defined by

$$
\operatorname{Order}_{t}=\log _{2} \frac{\operatorname{Error}_{1}(2 \Delta t)}{\operatorname{Error}_{1}(\Delta t)}, \quad \operatorname{Order}_{x}=\log _{2} \frac{\operatorname{Error}_{2}(2 \Delta x)}{\operatorname{Error}_{2}(\Delta x)}
$$

Due to the convolution structure of the Caputo derivative, the linear system from the difference scheme (32)-(34) of the fractional-order heat equation (59)-(61) generates a coefficient matrix in the form of the block lower triangular Toeplitzlike with tri-diagonal block (BL3TB-like). Recently, the divide-and-conquer (DAC) strategy [36] has been developed to efficiently compute this type of the linear system in a recursive fashion. It should be noted that the workload of the DAC method is the magnitude of $O\left(N M \log ^{2} N\right)$ superior to the operation of $O\left(N^{2} M\right)$ in the direct block forward substitution (BFS) method, where $N$ is the number of the blocks in the system and $M+1$ is the size of each block.

Next, we reported the maximum norm errors of numerical solution, the convergence orders and the CPU times took by the difference scheme (32)-(34), which was solved via the DAC fast method and the direct BFS method, respectively. From Table 1 and Table 2, one may see that the scheme (32)-(34) provides the fourthorder accuracy in space and $(2-\beta)$-order accuracy in time with both the DAC fast solver and the direct BFS solver. Numerical results show the convergence rate of the compact difference scheme (32)-(34) coincides with the theoretical analysis. And, it can be seen that the difference scheme (32)-(34) with the DAC method took less CPU time than the same scheme with the BFS method.

Table 1. Maximum errors and temporal convergence orders $(M=500)$.

|  |  | DAC method $^{c}$ |  |  |  | BFS method $^{$$\beta}$ |  |  | $N$ | Error $_{1}(\Delta t)$ | Order $_{t}$ | CPUtime(s) | Error $_{1}(\Delta t)$ | Order $_{t}$ | CPUtime(s) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.1 | $2^{10}$ | $9.242 \mathrm{e}-08$ | - | 0.502 | $9.242 \mathrm{e}-08$ | - | 5.999 |  |  |  |  |  |  |  |  |
|  | $2^{11}$ | $2.399 \mathrm{e}-08$ | 1.946 | 1.047 | $2.399 \mathrm{e}-08$ | 1.946 | 24.860 |  |  |  |  |  |  |  |  |
|  | $2^{12}$ | $6.234 \mathrm{e}-09$ | 1.944 | 2.371 | $6.234 \mathrm{e}-09$ | 1.944 | 102.958 |  |  |  |  |  |  |  |  |
|  | $2^{13}$ | $1.622 \mathrm{e}-09$ | 1.942 | 5.346 | $1.622 \mathrm{e}-09$ | 1.942 | 406.862 |  |  |  |  |  |  |  |  |
|  | $2^{14}$ | $4.224 \mathrm{e}-10$ | 1.941 | 11.985 | $4.224 \mathrm{e}-10$ | 1.941 | 1601.262 |  |  |  |  |  |  |  |  |
|  | $2^{15}$ | $1.102 \mathrm{e}-10$ | 1.939 | 26.521 | $1.102 \mathrm{e}-10$ | 1.939 | 6355.748 |  |  |  |  |  |  |  |  |
| 0.5 | $2^{10}$ | $3.002 \mathrm{e}-06$ | - | 0.505 | $3.002 \mathrm{e}-06$ | - | 6.066 |  |  |  |  |  |  |  |  |
|  | $2^{11}$ | $1.051 \mathrm{e}-06$ | 1.514 | 1.046 | $1.051 \mathrm{e}-06$ | 1.514 | 25.476 |  |  |  |  |  |  |  |  |
|  | $2^{12}$ | $3.689 \mathrm{e}-07$ | 1.510 | 2.371 | $3.689 \mathrm{e}-07$ | 1.510 | 104.752 |  |  |  |  |  |  |  |  |
|  | $2^{13}$ | $1.297 \mathrm{e}-07$ | 1.507 | 5.371 | $1.297 \mathrm{e}-07$ | 1.507 | 423.661 |  |  |  |  |  |  |  |  |
|  | $2^{14}$ | $4.570 \mathrm{e}-08$ | 1.505 | 12.053 | $4.570 \mathrm{e}-08$ | 1.505 | 1723.243 |  |  |  |  |  |  |  |  |
|  | $2^{15}$ | $1.612 \mathrm{e}-08$ | 1.504 | 26.403 | $1.612 \mathrm{e}-08$ | 1.504 | 6567.524 |  |  |  |  |  |  |  |  |
| 0.9 | $2^{10}$ | $2.863 \mathrm{e}-04$ | - | 0.508 | $2.863 \mathrm{e}-04$ | - | 6.339 |  |  |  |  |  |  |  |  |
|  | $2^{11}$ | $1.338 \mathrm{e}-04$ | 1.098 | 1.050 | $1.338 \mathrm{e}-04$ | 1.098 | 26.019 |  |  |  |  |  |  |  |  |
|  | $2^{12}$ | $6.244 \mathrm{e}-05$ | 1.099 | 2.373 | $6.244 \mathrm{e}-05$ | 1.099 | 103.926 |  |  |  |  |  |  |  |  |
|  | $2^{13}$ | $2.914 \mathrm{e}-05$ | 1.099 | 5.375 | $2.914 \mathrm{e}-05$ | 1.099 | 419.073 |  |  |  |  |  |  |  |  |
|  | $2^{14}$ | $1.360 \mathrm{e}-05$ | 1.100 | 12.021 | $1.360 \mathrm{e}-05$ | 1.100 | 1714.831 |  |  |  |  |  |  |  |  |
|  | $2^{15}$ | $6.344 \mathrm{e}-06$ | 1.100 | 26.482 | $6.344 \mathrm{e}-06$ | 1.100 | 6563.333 |  |  |  |  |  |  |  |  |

Table 2. Maximum errors and spatial convergence orders $\left(N=2^{13}\right)$.

|  | DAC method $^{c}$ |  |  |  | BFS method |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\beta$ | $M$ | $\operatorname{Error}_{2}(\Delta t)$ | Order $_{x}$ | CPUtimes $(\mathrm{s})$ | $\operatorname{Error}_{2}(\Delta t)$ | Order $_{x}$ | CPUtime(s) |
| 0.1 | 6 | $6.084 \mathrm{e}-06$ | - | 0.228 | $6.084 \mathrm{e}-06$ | - | 60.699 |
|  | 12 | $3.766 \mathrm{e}-07$ | 4.014 | 0.321 | $3.766 \mathrm{e}-07$ | 4.014 | 62.900 |
|  | 24 | $2.349 \mathrm{e}-08$ | 4.003 | 0.364 | $2.349 \mathrm{e}-08$ | 4.003 | 66.349 |
|  | 48 | $1.467 \mathrm{e}-09$ | 4.001 | 0.567 | $1.467 \mathrm{e}-09$ | 4.001 | 69.995 |
| 0.5 | 6 | $2.885 \mathrm{e}-05$ | - | 0.279 | $2.885 \mathrm{e}-05$ | - | 61.910 |
|  | 12 | $1.789 \mathrm{e}-06$ | 4.011 | 0.349 | $1.789 \mathrm{e}-06$ | 4.011 | 65.399 |
|  | 24 | $1.116 \mathrm{e}-07$ | 4.003 | 0.411 | $1.116 \mathrm{e}-07$ | 4.003 | 67.972 |
|  | 48 | $6.971 \mathrm{e}-09$ | 4.001 | 0.569 | $6.971 \mathrm{e}-09$ | 4.001 | 70.848 |
| 0.9 | 6 | $2.565 \mathrm{e}-06$ | - | 0.205 | $2.565 \mathrm{e}-06$ | - | 61.594 |
|  | 12 | $1.543 \mathrm{e}-07$ | 4.055 | 0.339 | $1.543 \mathrm{e}-07$ | 4.055 | 65.421 |
|  | 24 | $9.616 \mathrm{e}-09$ | 4.004 | 0.436 | $9.616 \mathrm{e}-09$ | 4.004 | 66.824 |
|  | 48 | $6.257 \mathrm{e}-10$ | 3.942 | 0.579 | $6.257 \mathrm{e}-10$ | 3.942 | 69.900 |

6.2. Comparison between fractional-order heat equation and PLE. Next, we estimate the optimal parameters $\beta, \kappa_{1}$ and $\kappa_{2}$ in the fractional-order heat equation (59)-(61) with various values of $\kappa_{0}$. In our simulation, we set the time domain $t \in[0,0.8]$, and chose the time step (denoted by $\Delta t$ ), and the space step (denoted by $\Delta x$ ), to be $\frac{0.8}{2^{10}}$ and 0.01 , respectively. We chose different initial guess $\mathbf{P}^{0}=\left[\beta^{0}, \kappa_{1}^{0}, \kappa_{2}^{0}\right]$, the tolerance $\epsilon=10^{-10}$, the measurement value $u_{\text {measurement }}=u_{\text {exact }}=u(x, t=10(\Delta t), 100(\Delta t), 1024(\Delta t))$ from the solution (58) of the direct problem (55)-(57). It should be noted that we applied the divide-and-conquer fast solver to reduce the computational work in the simulation. Table 3 lists the estimated values of the parameter $\mathbf{P}^{\mathrm{inv}}=\left[\beta, \kappa_{1}, \kappa_{2}\right]^{\text {inv }}$ and the number
of iterations for different initial guess with various values of $\kappa_{0}=0.25 \kappa_{c}, 0.5 \kappa_{c}, \kappa_{c}$. From the numerical results in Tables 3, one can see that, after several iterations, the optimal parameter $\mathbf{P}^{\text {inv }}=\left[\beta, \kappa_{1}, \kappa_{2}\right]^{\text {inv }}$ can be obtained, and the different initial guesses have no effect on the final estimation. This indicates that the present compact difference scheme with the Levenberg-Marquardt algorithm is effective to obtain the estimation of the parameters $\beta, \kappa_{1}, \kappa_{2}$.

Table 3. Optimal estimation of the parameter $\mathbf{P}=\left[\beta, \kappa_{1}, \kappa_{2}\right]$.

| Value $\kappa_{0}$ | Initial guess $\mathbf{P}^{0}$ | Number of iterations | Estimated value $\mathbf{P}^{\text {inv }}$ |
| :---: | :---: | :---: | :---: |
| $0.25 \kappa_{c}$ | $\left(0.9,1.0, \kappa_{0} / 10\right)$ | 44 | $(0.999263,0.937547,0.000203)$ |
|  | $\left(0.9,1.0, \kappa_{0} / 20\right)$ | 44 | $(0.999263,0.937547,0.000203)$ |
|  | $\left(0.8,0.9, \kappa_{0} / 10\right)$ | 51 | $(0.999263,0.937547,0.000203)$ |
| $0.5 \kappa_{c}$ | $\left(0.9,1.0, \kappa_{0} / 10\right)$ | 38 | $(0.987517,0.875621,0.000683)$ |
|  | $\left(0.9,1.0, \kappa_{0} / 20\right)$ | 38 | $(0.987517,0.875621,0.000683)$ |
|  | $\left(0.8,0.9, \kappa_{0} / 10\right)$ | 39 | $(0.987517,0.875621,0.000683)$ |
| $\kappa_{c}$ | $\left(0.9,1.0, \kappa_{0} / 10\right)$ | 37 | $(0.976879,0.756798,0.001504)$ |
|  | $\left(0.9,1.0, \kappa_{0} / 20\right)$ | 34 | $(0.976879,0.756798,0.001504)$ |
|  | $\left(0.8,0.9, \kappa_{0} / 10\right)$ | 30 | $(0.976879,0.756798,0.001504)$ |



Case 3. $\kappa_{0}=\kappa_{c}$
Fig. 1. $u$ vs. $x$ for $\kappa_{0}=0.25 \kappa_{c}, 0.5 \kappa_{c}, \kappa_{c}$ at the time $t=$ $10(\Delta t), 100(\Delta t), 1024(\Delta t)$, respectively.


Case 3. $\kappa_{0}=\kappa_{c}$
Fig. 2. The numerical solution (left) of the fractional-order heat equation (6)-(8) and the exact solution (right) of the PLE (55)(57) at $\kappa_{0}=0.25 \kappa_{c}, 0.5 \kappa_{c}, \kappa_{c}$, respectively.

Finally, we computed and plotted the approximate solution of the fractionalorder heat equation (59)-(61) based on the compact difference scheme (32)-(34), the exact solution (58) of the PLE (55)-(57), the exact solution (65) of the damped wave equation (62)-(64), and the exact solution (66) of the diffusion equation. The values of the parameters $\beta, \kappa_{1}, \kappa_{2}$ in the fractional-order heat equation (59)-(61) were chosen based on the corresponding estimated values in Table 3. In Fig. 1, we plotted the temporal evolution of the temperature vs. $x$ profile for $\kappa_{0}=0.25 \kappa_{c}, 0.5 \kappa_{c}, \kappa_{c}$ at the time $t=10(\Delta t), 100(\Delta t), 1024(\Delta t)$, respectively. From Fig. 1, one may see that the solution of the fractional-order heat equation (59)-(61) agrees very well with the solution of the PLE (55)-(57). Fig. 2 shows 3D comparison between the numerical solution of the compact difference scheme (32)-(34) and the exact solution of the PLE (55)-(57) at three different values of $\kappa_{0}$. These further confirm that the present compact difference scheme with the Levenberg-Marquardt algorithm is effective to
obtain the estimation of the parameters $\beta, \kappa_{1}, \kappa_{2}$. It indicates that the fractionalorder heat equation (59)-(61) is a good alternative of the PLE (55)-(57).

## 7. Conclusion

In this paper, we have provided a fractional-order alternative for the phaselagging equation(PLE). The well-posedness of the obtained fractional-order heat equation is proved. To obtain the solution of the fractional-order heat equation, we have developed an unconditionally stable compact difference scheme. By optimizing the parameters $\beta, \kappa_{1}, \kappa_{2}$ in the fractional-order heat equation, we have obtained an optimal fractional-order heat equation and an associated numerical scheme whose solutions we take as approximations to the corresponding solutions of the PLE.

It should be noted that the phase-lagging equation (1), the damped wave equation (3), and the fractional-order heat equation (5) are independent models of the same underlying physical phenomena. However, they are not mathematical equivalent. Consequently, in a fundamental sense neither is an approximation of the others. The particular equation selected for a given application depends on the ease of obtaining numerical solutions.

## Acknowledgements

The authors are deeply grateful to the anonymous reviewers for their valuable comments and suggestions which greatly enhance the quality of this manuscript. Cui-cui Ji was partially supported by National Natural Science Foundation of China (Grant No. 12001307) and Natural Science Foundation of Shandong Province (Grant No. ZR2020QA033).

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School of Mathematics and Statistics, Qingdao University, Qingdao, 266071, China E-mail: cuicuiahuan@163.com

Mathematics and Statistics, Louisiana Tech University, Ruston, LA 71272, USA
E-mail: dai@coes.latech.edu
Department of Physics, Clark Atlanta University, Atlanta, GA 30314, USA
E-mail: RMickens@cau.edu

