

SCHWARZ WAVEFORM RELAXATION ALGORITHM FOR HEAT EQUATIONS WITH DISTRIBUTED DELAY

by

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Heat equations with distributed delay are a class of mathematic models that has wide applications in many fields. Numerical computation plays an important role in the investigation of these equations, because the analytic solutions of partial differential equations with time delay are usually unavailable. On the other hand, due to the delay property, numerical computation of these equations is time-consuming. To reduce the computation time, we analyze in this paper the Schwarz waveform relaxation algorithm with Robin transmission conditions. The Robin transmission conditions contain a free parameter, which has a significant effect on the convergence rate of the Schwarz waveform relaxation algorithm. Determining the Robin parameter is therefore one of the top-priority matters for the study of the Schwarz waveform relaxation algorithm. We provide new formula to fix the Robin parameter and we show numerically that the new Robin parameter is more efficient than the one proposed previously in the literature.

Key words: *Schwarz waveform relaxation, heat equation, distributed delay, parameter optimization, convergence analysis*

Introduction

Differential equations with time delay model physical systems for which the evolution not only depend on the present state of the system but also on the past history. These models are found, for example, in population dynamics and epidemiology [1, 2], where the delay is due to a gestation or maturation period arising from the processing in the loop of controller feedback. Unlike the regular differential equations, the analytic solution of the delay differential equation is usually unavailable. Therefore, numerical computation plays an important role for studying these equations. A good starting point to study the analysis and numerical computation of delay differential equations is the monograph by Bellen and Zennaro [3], and the references therein. Very recently, delay models are also found useful in fractional calculus [1, 2, 4-10].

There is little experience with numerical methods for solving delay partial differential equations (PDE). Zubik-Kowal and Vandewalle [11] analyze the convergence of a waveform relaxation scheme of Gauss-Seidel and Jacobi type, for solving the discretized problems. Waveform relaxation schemes using domain decomposition in space, which is for parabolic equations without delay were introduced by Gander and Stuart [12] and independently by Gi-ladi and Keller [13]. In these papers, it was shown that domain decomposition leads to a fun-

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damentally faster convergence rate than the classical waveform relaxation methods. The algorithms are characterized by firstly partitioning the whole spatial domain into several sub-domains and then solving all the sub-problems simultaneously by exchanging the value of the solution between sub-domains through iterations.

The way that one chooses to exchange the value of solution between sub-domains is terminologically called transmission conditions (TC), and the Dirichlet and Robin TC are two popular choices. The Dirichlet TC lead to the so-called classical Schwarz waveform relaxation (SWR) algorithm, which got considerable attention in the literature [11-15]. The performance of the SWR algorithm can be drastically improved by using better more efficient TC, *e. g.*, the Robin TC, between sub-domains. The Robin TC contain a free parameter, which has a significant effect on the convergence rate of the algorithm. Therefore, optimizing the Robin parameter is one of the top-priority matters. For PDE without delay, this issue is deeply studied by Gander and his colleagues (see, *e. g.*, [16-19] and references therein).

However, for PDE with time delay much less results for the SWR algorithm are known in the literature. Vandewalle and Gander [20] studied the SWR algorithm with Robin TC for a class of representative delay problems, the heat equation with a distributed delay:

$$\begin{cases} \partial_t u - \partial_{xx} u + a \int_{t-\tau}^t u(x, s) ds = f(x, t), & (x, t) \in \mathbb{R} \times (0, T) \\ u(x, t) = u_0(x, t), & (x, t) \in \mathbb{R} \times [-\tau, 0] \end{cases} \quad (1)$$

where $a > 0$ and $\tau > 0$. It was shown that the existing techniques for optimizing the Robin parameters cannot be generalized to PDE with time delay. The main difficult arises from the complexity of the curve along which one needs to solve the min-max problem for determining an ideal Robin parameter. The main idea in [20] lies in selecting a regular box containing the complex curve and then solving the related min-max problem over the box. Based on this idea, the authors in [20] proposed a formula to compute the Robin parameter, which results in satisfactory convergence rate for the SWR algorithm.

The goal of this paper is to provide a new formula to compute the Robin parameter for the SWR algorithm applied to *eq. (1)*. We present details for the parameter optimization and numerical comparison shows that the new Robin parameter is more efficient than the old one given in [20].

The SWR algorithm with Robin TC

Following the work in [20], we decompose the spatial domain $\Omega = \mathbb{R}$ into two sub-domains $\Omega_1 = (-\infty, 0]$ and $\Omega_2 = [0, +\infty)$. Then, the SWR algorithm consist of solving iteratively subproblems on space-time domains $\Omega_j \times (0, T)$ ($j = 1, 2$), as:

$$\begin{cases} \partial_t u_j^k - \partial_{xx} u_j^k + a \int_{t-\tau}^t u_j^k(x, s) ds = f(x, t), & (x, t) \in \Omega_j \times (0, T), \\ [\partial_x + (-1)^{j+1} p] u_j^k(0, t) = [\partial_x + (-1)^{j+1} p] u_{3-j}^{k-1}(0, t), & t \in (0, T), \\ u_j^k(x, t) = u_0(x, t), & (x, t) \in \Omega_j \times [-\tau, 0], \end{cases} \quad (2)$$

where $j = 1, 2$ and $k \geq 1$ denotes the iteration index. For $k = 0$, the initial guesses $u_j^0(x, t)$ are arbitrarily chosen. If $p = \infty$, the Robin TC are reduced to the Dirichlet TC. Let e_j^k be the errors on sub-domain Ω_j at iteration $k \geq 0$, *i. e.*, $e_j^k = u|_{\Omega_j} - u_j^k$. Then, following the analysis in [20]:

$$\|e_j^k\|_{L^2[(\Omega_j \times (0,T))]} \leq \rho(p) \|e_j^{k-2}\|_{L^2[\Omega_j \times (0,T)]}, \quad j=1,2 \quad (3)$$

where $\rho(p, L)$ is the convergence factor of the SWR algorithms and is defined by:

$$\rho(p) = \max_{\omega \in [-\omega_{\max}, \omega_{\max}]} \left| \frac{\lambda(\omega) - p}{\lambda(\omega) + p} \right|^2, \text{ with } \lambda(\omega) = \sqrt{i \left(\omega - \frac{a}{\omega} (1 - e^{-i\omega\tau}) \right)}$$

Here and hereafter, the real part of the square root of any complex number is non-negative. The convergence factor $\rho(p)$ can be represented as:

$$\rho(p) = \max_{z \in \Gamma} \left| \frac{(z-p)^2}{(z+p)^2} \right|, \text{ with } \Gamma := \left\{ z : z = \sqrt{i \left(\omega - \frac{a}{\omega} (1 - e^{-i\omega\tau}) \right)}, \quad \omega \in [-\omega_{\max}, \omega_{\max}] \right\} \quad (4)$$

Naturally, we want $\rho(p) \ll 1$ and this leads to the min-max problem:

$$\min_{p \in \mathbb{R}} \max_{z \in \Gamma} \left| \frac{z-p}{z+p} \right|^2 \quad (5)$$

For the case $\tau = 0$, i. e., the regular heat equation, we have $\Gamma = \{z : z = (i\omega)^{1/2}, \omega \in [-\omega_{\max}, \omega_{\max}]\}$, which is obviously a simple curve in the complex plane and therefore solving the min-max problem (5) is easy. However, for $\tau > 0$ the curve Γ is very complicated as shown in fig. 1 on the left. The idea proposed by Vandewalle and Gander [20] lies in choosing a regular box (denote by \mathbb{B}) that covers the curve Γ and then solving the min-max problem over this box instead of along the complicated Γ . (An illustration of the box is shown in fig. 1 on the right.) This idea leads to the following min-max problem:

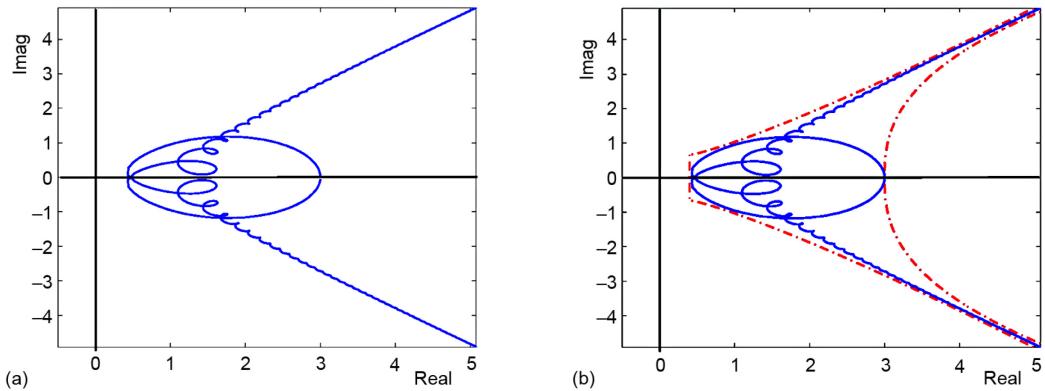


Figure 1. (a) The curve Γ defined by (4) with $a = 1.48$ and $\tau = 5$; (b) illustration of the box \mathbb{B} that covers Γ

$$\min_p \max_{z \in \mathbb{B}} \left| \frac{z-p}{z+p} \right|^2 \quad (6)$$

Since \mathbb{B} covers Γ , it is easy to see:

$$\min_p \max_{z \in \Gamma} \left| \frac{z-p}{z+p} \right|^2 \leq \min_p \max_{z \in \mathbb{B}} \left| \frac{z-p}{z+p} \right|^2$$

This implies that the Robin parameter obtained by solving (6) is an approximate solution of (5). The solution of the min-max problem (6) is given in the following theorem.

Theorem 1 (Theorem 6, [20])

Let

$$\tau = 0 \quad \text{and} \quad b = \Re\left(\sqrt{i\left(\omega_{\max} + \frac{2\pi}{\tau}\right) + ae^{-i\omega_{\max}\tau}}\right), \text{ then}$$

1. the SWR algorithm (2) is convergent for any $p > 0$, provided $0 < a\tau^2 \leq \pi^2/2$ and
2. if $0 < a\tau \leq 1$, the solution of the min-max problem (6) is given by:

$$p_{\text{old}}^* = \begin{cases} \sqrt{2\cos(a\tau)b - a}, & \text{if } b \geq a\cos(a\tau) + \frac{1}{\cos(a\tau)}, \\ \sqrt{2a^2\cos^2(a\tau) + a}, & \text{if } b < a\cos(a\tau) + \frac{1}{\cos(a\tau)}. \end{cases} \quad (7)$$

The formula (7) for computing the Robin parameter requires $0 < a\tau \leq 1$ and we do not know whether the parameter p_{old}^* given by (7) is still efficient or not when $a\tau > 1$.

A new formula to compute the Robin parameter

In this section, we give a new formula to get the Robin parameter. We rewrite $\rho(p)$ as:

$$\rho(p) = \max_{z \in \Gamma} \left| \frac{(z-p)^2}{(z+p)^2} \right| = \max_{\omega \in [-\omega_{\max}, \omega_{\max}]} \frac{[\zeta(\omega) - p]^2 + \psi^2(\omega)}{[\zeta(\omega) + p]^2 + \psi^2(\omega)} \quad (8)$$

where

$$\zeta(\omega) = \sqrt{\frac{\left[a \frac{\sin(\omega\tau)}{\omega}\right]^2 + \left[\omega - a \frac{1 - \cos(\omega\tau)}{\omega}\right]^2 + a \frac{\sin(\omega\tau)}{\omega}}{2}}$$

and

$$\psi(\omega) = \sqrt{\frac{\left[a \frac{\sin(\omega\tau)}{\omega}\right]^2 + \left[\omega - a \frac{1 - \cos(\omega\tau)}{\omega}\right]^2 - a \frac{\sin(\omega\tau)}{\omega}}{2}}$$

From Theorem 1, we shall restrict our analysis to the case $p > 0$, since otherwise $\rho(p) \geq 1$.

Define

$$\begin{aligned} \eta_0 &= \min_{\omega \in [-\omega_{\max}, \omega_{\max}]} \zeta(\omega), \quad \eta_1 = \max_{\omega \in [-\omega_{\max}, \omega_{\max}]} \zeta(\omega), \quad s_0 = -0.21723236496763, \\ \alpha &= \begin{cases} a\tau, & \text{if } a < 0, \\ a\tau s_0, & \text{if } a > 0, \end{cases} \quad Y(p, \eta, s) = \frac{(\eta - p)^2 + \eta^2 - a\tau s}{(\eta + p)^2 + \eta^2 - a\tau s}, \quad \mathcal{R}(\eta, p) = \frac{(\eta - p)^2 + \eta^2 - \alpha}{(\eta + p)^2 + \eta^2 - \alpha} \end{aligned} \quad (9)$$

The quantities α and η_0 satisfy;

$$\eta_0^2 \geq \alpha \quad (10)$$

To see this, we note that $\min_{\omega \in \mathbb{R}} [a\tau \sin(\omega\tau)/\omega\tau] = a\tau$ for $a < 0$ and $a\tau s_0$ for $a < 0$. It thus holds that:

$$-2\alpha + a \frac{\sin(\omega\tau)}{\omega} \geq -a \frac{\sin(\omega\tau)}{\omega}$$

which implies $\zeta^2(\omega) - \alpha \geq 0$ for all $\omega \in \mathbb{R}$.

Lemma 1. With the function $\mathcal{R}(\eta, p)$ defined by (9), it holds that $\rho(p) \leq \max_{\eta \in [\eta_0, \eta_1]} \mathcal{R}(p, \eta)$.

Proof. Let $s = \sin(\omega\tau)/(\omega\tau)$. Then, it is easy to know $s \in [s_0, 1]$ for $\omega\tau \in \mathbb{R}$. It holds that:

$$\rho(p) = \max_{\omega \in [-\omega_{\max}, \omega_{\max}]} \frac{[\zeta(\omega) - p]^2 + \zeta^2(\omega) - \frac{a\tau \sin(\omega\tau)}{(\omega\tau)}}{[\zeta(\omega) + p]^2 + \zeta^2(\omega) - \frac{a\tau \sin(\omega\tau)}{(\omega\tau)}} \leq \max_{\eta \in [\eta_0, \eta_1], s \in [s_0, 1]} Y(p, \eta, s)$$

We have:

$$\partial_s Y(p, \eta, s) = -4a\tau p \eta [(\eta + p)^2 + \eta^2 + a\tau s]^{-2}$$

and

$$\max_{s \in [s_0, 1]} Y(p, \eta, s) = \mathcal{R}(p, \eta)$$

since Y is increasing (resp. decreasing) function of s when $a < 0$ (resp. $a > 0$).

This lemma implies that we can get a reliable Robin parameter by solving:

$$\min_{p > 0} \max_{\eta \in [\eta_0, \eta_1]} = \mathcal{R}(p, \eta) \quad (11)$$

Theorem 2

Let $\tau > 0$ and $\eta_0 > 0$. Then Robin parameter can be chosen as $p = p_{\text{new}}^*$, where p_{new}^* is the solution of the min-max problem (11), is given by:

$$p_{\text{new}}^* = \sqrt{2\eta_0\eta_1 + \alpha} \quad (12)$$

if $\eta_0^2 - \eta_0\eta_1 - \alpha \leq 0$ and $\eta_1^2 - \eta_0\eta_1 - \alpha \geq 0$, otherwise:

$$p_{\text{new}}^* = \begin{cases} p_0, & \text{if } \mathcal{R}(p_0, \eta_0) \geq \mathcal{R}(p_0, \eta_1), \\ p_1, & \text{if } \mathcal{R}(p_0, \eta_0) < \mathcal{R}(p_0, \eta_1), \end{cases} \quad \text{with } p_0 = \sqrt{2\eta_0^2 - \alpha} \text{ and } p_1 = \sqrt{2\eta_1^2 - \alpha} \quad (13)$$

The quantities η_0 , η_1 , α , and the function $\mathcal{R}(p, \eta)$ are given by eq. (9).

Proof. For any $p > 0$ and $\eta \in [\eta_0, \eta_1]$, routine calculation yields:

$$\frac{\partial \mathcal{R}(p, \eta)}{\partial p} = 4\eta \frac{p^2 - 2\eta^2 + \alpha}{[(\eta + p) + \eta^2 - \alpha]^2} \Rightarrow \text{sign} \left[\frac{\partial \mathcal{R}(p, \eta)}{\partial p} \right] = \text{sign} \left(p - \sqrt{2\eta^2 - \alpha} \right) \quad (14)$$

The square root $(2\eta^2 - \alpha)^{1/2}$ is a negative real quantity, since from (10) it holds $2\eta^2 - \alpha \geq 2\eta_0^2 - \alpha \geq \eta_0^2$. Hence, the solution p_{new}^* of (11) should satisfy $p_0 \leq p_{\text{new}}^* \leq p_1$,

since otherwise we can uniformly reduce $\mathcal{R}(p_{\text{new}}^*, \eta)$ by increasing or decreasing p_{new}^* . We next claim that the function $\mathcal{R}(p, \eta)$ does not have a local maximum for $\eta \in [\eta_0, \eta_1]$. A derivative of $\mathcal{R}(p, \eta)$ with respect to η gives:

$$\partial_\eta \mathcal{R}(p, \eta) = 4p(2\eta^2 - p^2 + \alpha)[(\eta + p) + \eta^2 - \alpha]^{-2} \quad (15)$$

This implies that the $\mathcal{R}(p, \eta)$ has a unique local extremum located at $\eta = \eta^* = [(p^2 - \alpha)/2]^{1/2}$. It holds that $\partial_\eta^2 \mathcal{R}(p, \eta^*) = 16p\eta^*[(\eta + p) + \eta^2 - \alpha]^{-2} > 0$. Hence, p^* must be a local minimum of $\mathcal{R}(p, \eta)$. For any $p > 0$, the previous analysis implies that:

$$\max_{\eta \in [\eta_0, \eta_1]} \mathcal{R}(p, \eta) = \max \{\mathcal{R}(p, \eta_0), \mathcal{R}(p, \eta_1)\} \quad (16)$$

From (14) we know that $\mathcal{R}(p, \eta_0)$ [resp. $\mathcal{R}(p, \eta_1)$] is increasing (resp. decreasing) function for $p \in [p_0, p_1]$. This relation together with (15)-(16) gives p_{new}^* in (12)-(13).

Numerical comparisons

In this section, we compare the parameters p_{old}^* (Theorem 1) and p_{new}^* (Theorem 2). Since both p_{old}^* and p_{new}^* only depended on a and τ , the convergence factor $\rho(p)$ defined by (3) by using $p = p_{\text{old}}^*$ and $p = p_{\text{new}}^*$ also only depends on a and τ . In fig. 2, we show $\rho(p_{\text{old}}^*)$ and $\rho(p_{\text{new}}^*)$ on the (a, τ) plane. We see that the advantage of using $p = p_{\text{new}}^*$ is very apparent, since with this parameter the region $\rho(p) \leq r$ (with some $r \in (0, 1)$) on the (a, τ) plane is obviously larger than the region with $p = p_{\text{old}}^*$. Moreover, we find numerically that $\rho(p_{\text{new}}^*) < 1$ holds on a region with boundary $a\tau^2 = \pi^2/2$, while $\rho(p_{\text{old}}^*) < 1$ only holds on a region with boundary $a\tau = \pi^2/2$. We next fix one of the two problem parameters a or τ and show in fig. 3 the convergence factor as a function of the other parameter. The results shown in figs. 2 and 3 imply that the Robin parameter, p_{new}^* , proposed in this paper results in smaller convergence factor than the one p_{old}^* given in [20].

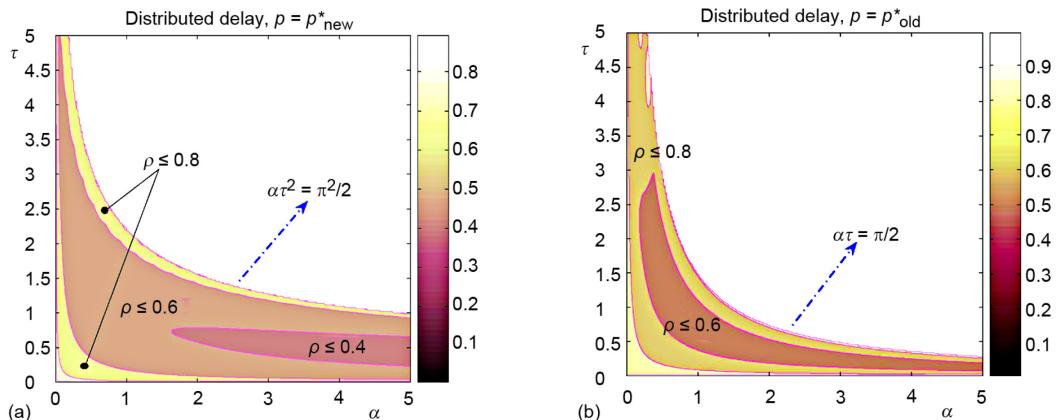


Figure 2. (a) The convergence factor $\rho(p)$ with $p = p_{\text{new}}^*$ and (b) $p = p_{\text{old}}^*$ on the (a, τ) plane

At the end of this section, we do numerical experiments to compare the convergence rates of the SWR algorithm using two Robin parameters, $p = p_{\text{new}}^*$ proposed in this paper and $p = p_{\text{old}}^*$ given in [20]. We consider the initial and source functions:

$$u_0(x, t) = \sin(\pi x) \cos(t), \quad f(x, t) = (x-1)(x-3) \sin(t), \quad \text{with } (x, t) \in [0, 3] \times [0, 10] \quad (17)$$

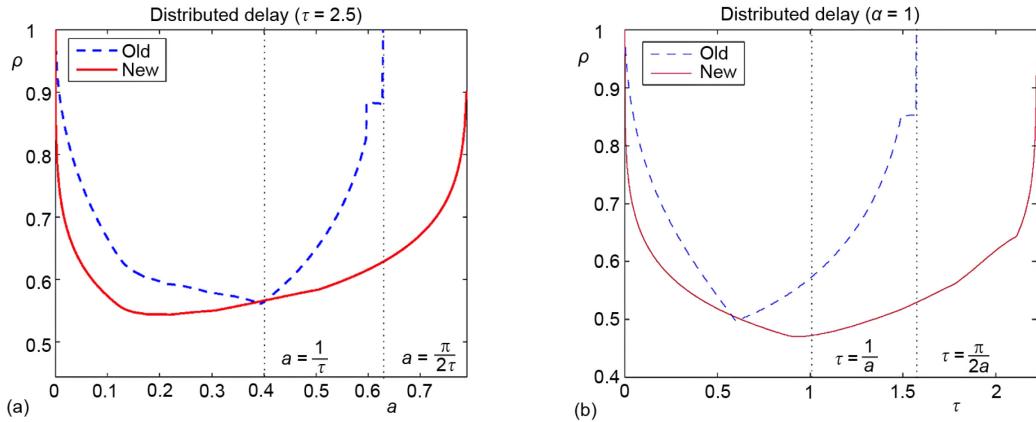


Figure 3. (a) For $\tau = 2.5$ the convergence factor by using $p = p_{\text{new}}^*$ and $p = p_{\text{old}}^*$ as a function of a and (b) for $a = 1$ the convergence factor using the two Robin parameters as a function of τ

Then, we discretize the continuous SWR algorithm (2) using a centered finite difference scheme in space with mesh parameter $\Delta x = 0.025$ and a backward Euler method in time $\Delta t x = 0.02$. Let $a = 0.25$ and $\tau = 3.5$. Then, we get from Theorems 1 and 2 that the two Robin parameters, $p_{\text{new}}^* = 2.3191$ and $p_{\text{old}}^* = 3.3417$, respectively. In fig. 4(a), we show the measured error of the SWR algorithm using these two Robin parameters, where we can see that, compared to the Robin parameter $p = p_{\text{old}}^*$ given in [20], the new parameter results in much faster convergence rate. It would be interesting to verify to what degree the choices $p = p_{\text{new}}^*$ and $p = p_{\text{old}}^*$ correspond to the best choice as one can make in the fully discretized situation. In fig. 4(b) we show the error obtained after five iterations of the algorithm using various values for the Robin parameter, p , in the transmission conditions. The choices $p = p_{\text{new}}^*$ and $p = p_{\text{old}}^*$ are indicated by a circle and a star, respectively. One can find in fig. 4(b) that the parameter $p = p_{\text{new}}^*$ analyzed in this paper is very close to the best one, while $p = p_{\text{old}}^*$ is far away from the best one.

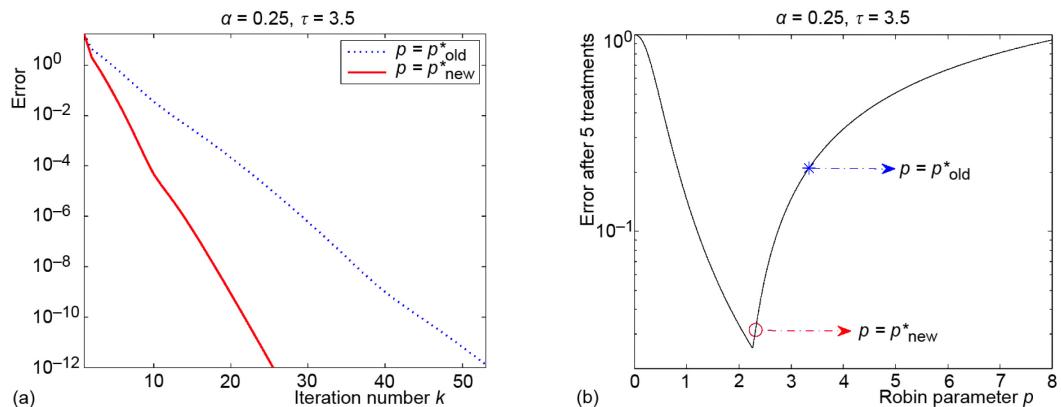


Figure 4. (a) Convergence rates of the SWR algorithm using $p = p_{\text{new}}^*$ (solid line) and $p = p_{\text{old}}^*$ (dash line) as the Robin parameter and (b) the errors after five iterations of the algorithm by using various values of the Robin parameters p ; the choice $p = p_{\text{new}}^*$ proposed in this paper and $p = p_{\text{old}}^*$ given in [20] are respectively indicated by a circle and a star

Conclusion

We have analyzed the SWR algorithm with Robin TC for a class of representative heat equations with distributed delay. We provided a new formula to determine the free parameter contained in the TC and numerical results show that the new Robin parameter is more efficient than the one proposed in the literature.

Nomenclature

a	- reaction rate, [molcm ⁻³]
f	- source term, [molcm ⁻³]
p	- Robin parameter, [-]
T, t	- time, [s]
u	- concentration, [molcm ⁻³]
x	- displacement, [cm]

Greek symbols

Γ	- a curve in the complex plane, [-]
Ω	- spatial domain, [cm]
τ	- delay quantity, [s]

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