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Characterizing and minimizing the operator split error for Fisher's equation

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Abstract

Operator splitting (OS) is a popular and convenient technique used to numerically solve reactive transport problems such as Fisher's equation. Although OS has been widely used to solve Fisher's equation, no characterization of the innate OS error has been presented. Here the exact characteristics of the OS error for travelling wave solutions of Fisher's equation are revealed and explored. The analysis shows that the OS error behaves differently to previously studied linear problems by smoothing or steepening the wave front depending on the sequential order of splitting. Further analysis confirms that the OS error is reduced by implementing an alternating OS scheme.

Keywords: Operator split; Fisher's equation; Alternating operator split

1. Introduction

Constructing accurate and efficient algorithms to obtain numerical solutions of nonlinear reaction–diffusion systems is important because of the ubiquitous nature of these problems and limited availability of analytical solutions. Fisher's equation [1–3] is a nonlinear reaction–diffusion equation of broad interest in various applications including tissue engineering [4], combustion [5], and gene propagation [3]. Fisher's equation describes the evolution of a one-dimensional mass density field

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undergoing transport by linear diffusion, and proliferation by a logistic process:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + \lambda c\left(1 - \frac{c}{c_{\max}}\right). \tag{1}$$

Introducing length, time and concentration scales (L, T and $c_{\max}$), the variables are nondimensionalized: $x^* = x/L$, $t^* = t/T$ and $c^* = c/c_{\max}$. Choosing $T = 1/\lambda$, $L = \sqrt{D/\lambda}$ and dropping the asterisk notation gives the nondimensional Fisher's equation:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + c(1 - c). \tag{2}$$

Obtaining accurate numerical solutions of (2) is critical, since there are infinitely many travelling wave solutions on $-\infty < x < \infty$, but only one known analytical case [1,6]. A common strategy used to numerically solve (2) is operator splitting (OS) [5,7–13]. OS involves applying a combination of techniques, either sequentially or iteratively [14], to temporally integrate a spatially discrete form of (2). OS has been used within several frameworks to solve Fisher's equation including Eulerian finite element [8] and finite difference methods [5,9], Lagrangian random walk methods [10,12] and pseudospectral methods [7,13]. OS offers several advantages; the most obvious is that splitting the nonlinear partial differential equation (PDE) (2) into the sequence

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2}, \qquad -\infty < x < \infty,\ t > 0, \tag{3}$$

$$\frac{\mathrm{d}c}{\mathrm{d}t} = c(1 - c), \qquad x = x_i,\ i = 1, 2, 3 \ldots M,\ t > 0, \tag{4}$$

conveniently converts the single nonlinear PDE (2) into a linear PDE and a system of nonlinear ordinary differential equations (ODEs) [14–21]. Although we have presented the splitting (3) and (4) in the sequential order of transport then reaction (T–R), it is also possible to split in the reverse direction (4) and (3), reaction then transport (R–T). Both these options have been used to solve Fisher's equation; for example, Tompson and Dougherty [12] use a T–R OS scheme, while Landman et al. [8] use an R–T OS scheme. Here, we investigate the characteristics of both options as well as two alternating OS schemes.

One possible method for implementing OS for the noniterative two-step procedure (3) and (4), would be to solve the linear PDE (3) with a standard implicit finite difference method over the time interval Δt yielding a vector of discrete intermediate concentrations $c^*_{\text{T–R}}(x_i, \Delta t)$, for $i = 1, 2, 3 \ldots M$. For the second step, the ODE system (4) can be integrated over Δt with a Runge–Kutta algorithm using $c^*_{\text{T–R}}(x_i, \Delta t)$ as the initial condition. Completing these two steps approximately advances the whole system through the time interval Δt.

In comparison with an implicit Eulerian algorithm applied to the full nonlinear problem (2), the computational overhead per time increment is typically reduced using an OS approach. For a spatial discretization with M nodes, an implicit Eulerian method applied to (2) requires the solution of an $M \times M$ system of nonlinear equations per time step; this is typically achieved by linearizing and iteratively solving an $M \times M$ linear system several times. Alternatively, a standard two-step noniterative OS algorithm requires the solution of an $M \times M$ linear system once only, together with the solution of M ODEs. Improvements in efficiency offered by OS techniques are particularly attractive for multi-dimensional [19] and/or multi-species [8,21] problems. Other advantages of invoking OS include the opportunity for parallel computation [12], increasing algorithm modularity [17,19], and coupling different algorithms [21].

The benefits of invoking OS are not without penalty. In general, separating reaction and transport introduces an $\mathcal{O}(\Delta t)$ error [15,18]. The OS error is innate and independent of numerical errors [15,18,21]. Since the OS error is $\mathcal{O}(\Delta t)$, any improved accuracy offered by higher order temporal integration methods is negated by splitting, and the algorithm must be executed with very small time steps to maintain sufficient accuracy. Understanding the nature of the error introduced by OS is essential for using the technique appropriately. The characteristics of the OS error for certain linear reactive transport problems are well known [14,15,18,21] and will be discussed subsequently. In contrast, the form of the OS error for Fisher's equation has not been determined and the characteristics of the error are unknown.

Without any knowledge of the form of the OS error for Fisher's equation, it is impossible to visually detect the error as it is unclear exactly how it will manifest in the overall solution. Therefore, analysts implementing an OS algorithm must accept the introduction of an unknown $\mathcal{O}(\Delta t)$ error, and use very small time increments to prevent the OS error compromising the numerical solution. The present study improves our understanding of the nature of the OS error by explicitly examining the OS error in isolation from other errors. The analysis shows that the form of the OS error is different to that in previously analyzed cases. Further analysis confirms that the OS error is reduced by using an alternating scheme [15,18,20,22]. This result is important as alternating OS schemes can, in certain cases, increase the OS error [18,23].

2. Characterizing and minimizing the operator split error

To examine the OS error, an exact analytical solution was used [6] to measure the accuracy of various OS solutions. For the analytical solution, travelling waves with speed $\mathrm{WS} = 5/\sqrt{6}$ occur on $-\infty < x < \infty$ for initial conditions

$$c(x, 0) = \left(1 + \mathrm{e}^{x/\sqrt{6}}\right)^{-2}. \tag{5}$$

The analytical solution evolving from (5) after time Δt is $c_{\mathrm{exact}}(x, \Delta t) = c(x - 5\Delta t/\sqrt{6}, 0)$. To compute the OS solution for T–R splitting over the interval Δt, (3) is solved exactly with the initial condition (5) to yield the intermediate solution $c^*_{\mathrm{T-R}}(x, \Delta t)$. The intermediate solution is evaluated on a truncated and uniformly discretized domain. The discretized profile, $c^*_{\mathrm{T-R}}(x_i, \Delta t)$, is then used as the initial condition for analytically integrating (4) at each node yielding the exact T–R OS solution. A similar approach is used to evaluate the OS profiles for R–T splitting. This method of examining the exact OS profile over one time step has been used to analyze linear cases [15,20,21] and is convenient for isolating the OS error from other possible sources of error, such as numerical truncation error. Alternative methods of analysis, such as Taylor series expansions of numerical schemes, are popular [14,18]; however, this approach has not been applied to nonlinear nonequilibrium reaction problems, such as Fisher's equation, and is not pursued here.

To evaluate $c^*_{\mathrm{T-R}}(x, \Delta t)$, a Fourier transform is used to solve (3) with the initial condition (5). The solution can be written as

$$c^*_{\mathrm{T-R}}(x, \Delta t) = \frac{1}{\sqrt{4\pi\,\Delta t}} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\frac{-(x-s)^2}{4\Delta t}}}{(1 + \mathrm{e}^{s/\sqrt{6}})^2}\,\mathrm{d}s. \tag{6}$$

Unfortunately, the integral in (6) is analytically intractable; however the integral can be accurately evaluated using standard numerical techniques [24]. To complete the T–R OS solution, the reaction

ODEs (4) are solved at each location x_i on the discretized domain:

$$c(x_i, t) = \frac{c(x_i, 0)\mathrm{e}^t}{1 + c(x_i, 0)(\mathrm{e}^t - 1)}. \tag{7}$$

The solution of the reaction stage for the T–R OS algorithm is (7) with $t = \Delta t$ and $c(x_i, 0) = c^*_{\mathrm{T\text{–}R}}(x_i, \Delta t)$ for $i = 1, 2, 3 \ldots M$. Evaluating these two steps yields the T–R OS solution.

For the R–T OS case, we evaluate (7) at $t = \Delta t$ with (5) as the initial condition. This intermediate solution is used as the initial condition to solve (3), for which the solution is

$$c_{\mathrm{R\text{–}T}}(x, \Delta t) = \frac{1}{\sqrt{4\pi \Delta t}} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\Delta t}\, \mathrm{e}^{\frac{-(x-s)^2}{4\Delta t}}}{\left(1 + \mathrm{e}^{s/\sqrt{6}}\right)^2 + \mathrm{e}^{\Delta t} - 1}\, \mathrm{d}s. \tag{8}$$

The expression (8) can be evaluated with a numerical procedure analogous to that used for (6). Evaluating the T–R and R–T OS solutions in this way ensures that the OS error has been preserved and isolated from other sources of error that would normally be present in a standard numerically generated OS solution [5, 7–13].

Two alternating OS schemes are also evaluated. Within each time step for the R–T–R scheme, three intermediate steps are taken [18,22,23]:

(1) Integrate (4) over $\Delta t/2$ with the initial condition (5) to give the first intermediate solution $c^*_{\mathrm{R\text{–}T\text{–}R}}(x, \Delta t/2)$.
(2) Integrate (3) over Δt using $c^*_{\mathrm{R\text{–}T\text{–}R}}(x, \Delta t/2)$ as the initial condition to give the second intermediate solution $c^{**}_{\mathrm{R\text{–}T\text{–}R}}(x, \Delta t)$.
(3) Integrate (4) over $\Delta t/2$ using $c^{**}_{\mathrm{R\text{–}T\text{–}R}}(x_i, \Delta t)$ as the initial condition to give the final solution $c_{\mathrm{R\text{–}T\text{–}R}}(x_i, \Delta t)$.

The expression for the second step in the R–T–R scheme is

$$c^{**}_{\mathrm{R\text{–}T\text{–}R}}(x, \Delta t) = \frac{1}{\sqrt{4\pi \Delta t}} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\Delta t/2}\, \mathrm{e}^{\frac{-(x-s)^2}{4\Delta t}}}{\left(1 + \mathrm{e}^{s/\sqrt{6}}\right)^2 + \mathrm{e}^{\Delta t/2} - 1}\, \mathrm{d}s. \tag{9}$$

Equation (9) is evaluated numerically using the same procedure applied to (6). The solution of the third step in the R–T–R OS scheme is (7) with $t = \Delta t/2$ and $c(x_i, 0) = c^{**}_{\mathrm{R\text{–}T\text{–}R}}(x_i, \Delta t)$ for $i = 1, 2, 3 \ldots M$. A second alternating scheme with sequential ordering T–R–T is also evaluated. The expression for the T–R–T OS profile is significantly more complicated than in the previous OS cases and is not detailed here. The derivation of the expression for the T–R–T profile follows naturally from the previous cases. Prior analyses indicate that alternating OS schemes can reduce the OS error [15,20]; however, Barry et al. [18] show that an alternating OS scheme applied to linear equilibrium reactive transport can increase the OS error. Bell and Binning [23] also provide evidence that a T–R–T alternating scheme performs poorly for reactive transport with nonlinear nonequilibrium Monod reactions. Therefore, alternating schemes are not a general panacea against OS error and should be invoked with care.

To demonstrate the form of the OS error, the exact solution, T–R, R–T, R–T–R and T–R–T OS solutions were computed on $-20 < x < 30$, discretized with $\Delta x = 0.1$. The solutions are computed for various Δt. In each case the exact solution translates a distance $5\Delta t/\sqrt{6}$ to the right; therefore, to compare solutions over a range of Δt each solution is evaluated and then translated to the left a distance of $5\Delta t/\sqrt{6}$. In the absence of any OS error, the OS solutions would superimpose exactly onto

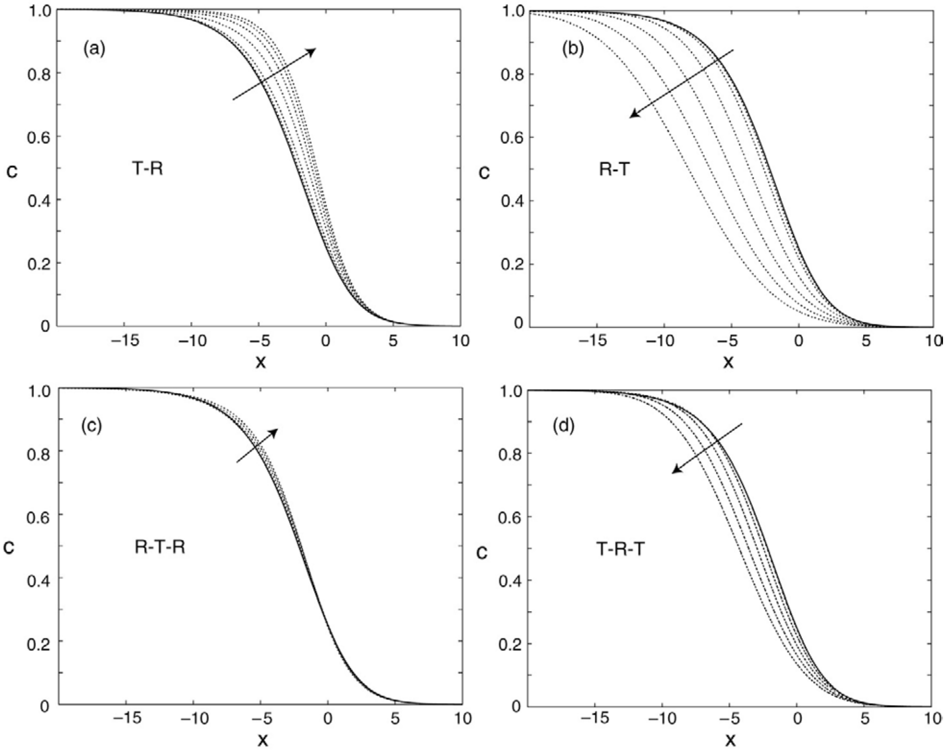

Fig. 1. Analytical travelling wave solution of Fisher's equation (solid line) compared to several exact OS solutions (dotted line) for various Δt. (a) T–R OS, (b) R–T OS, (c) R–T–R OS, and (d) T–R–T OS. In each case six OS profiles are shown with $\Delta t = 1, 2, 4, 6, 8$ and 10; the arrows indicate the direction of increasing Δt.

the initial condition profile (5). Results are shown in Fig. 1. For all OS algorithms, the OS error is only present at the wave front as the exact and OS solutions converge away from the wave front. The forms of the OS error are strikingly different depending on the sequential order of splitting. For T–R splitting (Fig. 1(a)), the OS profiles are further advanced and steepened relative to the exact profile. The steepening of the profile is most severe at the heel of the wave. For R–T splitting (Fig. 1(b)), the OS profiles are retarded and smoothed relative to the exact profile. For the R–T–R alternating case (Fig. 1(c)), the OS error is significantly reduced and good results are obtained for all Δt. The T–R–T profiles (Fig. 1(d)) also demonstrate a reduced error for $\Delta t \leq 4$. For larger time steps, $\Delta t > 4$, the T–R–T algorithm does not perform as well as the R–T–R algorithm.

For all profiles in Fig. 1, the OS error increases with Δt; the relationship between the error and Δt will be examined in detail in Section 3. The profiles in Fig. 1 suggest that one way the OS error would manifest in a typical numerical simulation would be through errors in the wave speed. These results suggest that T–R splitting would overestimate the wave speed while R–T splitting would underestimate the wave speed. In comparison, we expect that the R–T–R or T–R–T alternating schemes would give improved wave speed predictions for small to moderate values of Δt, ($\Delta t \leq 4$). These hypotheses will be explored in Section 3.

It is interesting that the characteristics of the OS error for Fisher's equation are remarkably different to those of the OS errors encountered in previously analyzed cases. The OS error for Fisher's equation is

Table 1
Deducing the order of accuracy p, for T–R, R–T, T–R–T and R–T–R OS algorithms

Δt_1	Δt_2	p(T–R)	p(R–T)	p(T–R–T)	p(R–T–R)
0.5	1.0	1.00	1.02	2.00	1.98
1.0	2.0	1.03	1.05	1.99	1.95

confined to the location of the wave front only, and is therefore not strictly associated with the boundary as in the case of the advection–diffusion–reaction (ADR) equation with linear nonequilibrium decay [15,18,21]. Unlike for the ADR equation with a linear equilibrium reaction, the OS error for Fisher's equation does not result in additional artificial diffusion [14,18] as the OS error can act to steepen the wave front instead of smoothing it. Fortunately, our results suggest that the alternating OS schemes will minimize the OS error for small to moderate Δt.

3. Numerical analysis of the operator split error

Although the exact analysis of the OS error over one time step is useful for characterizing the OS error [15,20,21], this approach cannot be applied in a standard algorithm where several time steps are taken. Here we analyze the order of the temporal error by computing numerical solutions and examining the error dependence on Δt. We consider (2) with the initial condition (5); various numerical OS solutions are computed over several time steps until $t = 10$. The solution of (3) in the OS algorithms is obtained with a Crank–Nicolson finite difference approximation [21,24]. Numerical computations are performed on $-100 < x < 100$, with $c(-100, t) = 1$ and $c(100, t) = 0$. For the reaction component of the OS procedure, the ODEs are solved analytically (7). In order to focus on the OS temporal error, a fine spatial discretization is used with $\Delta x = 0.02$. Knowing the exact travelling wave solution, the total error associated with a particular OS solution can be measured:

$$E = \frac{1}{M} \sum_{i=1}^{M} |c_{\text{exact}}(x_i, t) - c_{\text{OS}}(x_i, t)|, \tag{10}$$

where i is the node index, $c_{\text{exact}}(x_i, t)$ is the exact analytical travelling wave solution and $c_{\text{OS}}(x_i, t)$ is an approximate OS numerical solution.

All four OS schemes are evaluated. Three numerical solutions for each OS scheme are computed with $\Delta t = 0.5$, 1 and 2 until $t = 10$. Using a sequence of two time steps Δt_1 and Δt_2, the errors, E_1 and E_2, are used to extract the order of accuracy, p:

$$\frac{E_1}{E_2} = \left(\frac{\Delta t_1}{\Delta t_2}\right)^p. \tag{11}$$

Results in Table 1 confirm that the errors for the R–T and T–R OS schemes have the same linear dependence on Δt. Therefore, this low order of accuracy demands that small time steps must be used to minimize the OS error. The R–T–R and T–R–T alternating schemes provide an $\mathcal{O}(\Delta t)^2$ solution where the error is proportional to $(\Delta t)^2$. Therefore, either of the alternating schemes will enhance the performance of an OS algorithm for Fisher's equation.

To practically demonstrate the relative performances of the four OS schemes, profiles of $c(x, 10)$ are given in Fig. 2(a) after a small number of time steps (five steps). Comparing the OS solutions shows that

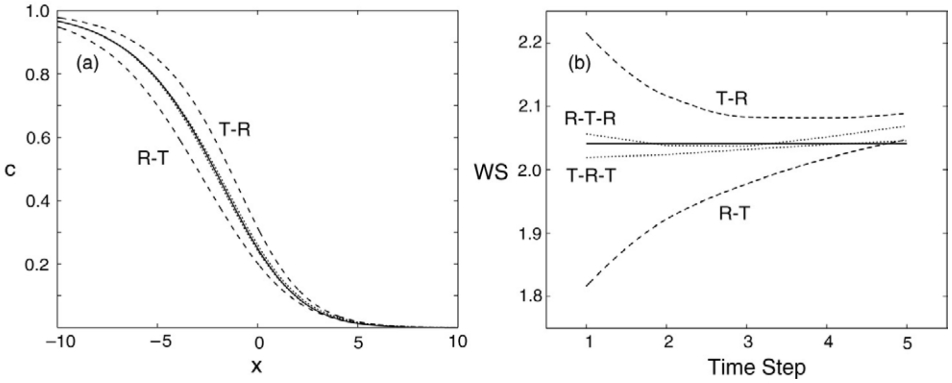

Fig. 2. Numerical OS solutions of Fisher's equation with initial condition (5), $\Delta t = 2$ and $\Delta x = 0.02$. (a) Profiles of $c(x, 10)$. (b) Numerical wave speed as a function of the number of time steps. Solutions shown include the exact case (solid line), T–R OS (dashed), R–T OS scheme (dashed), alternating T–R–T OS (dotted) and the alternating R–T–R OS (dotted).

both alternating schemes outperform the T–R and R–T algorithms. The characteristics of the errors in the T–R and R–T profiles correspond to those demonstrated in Fig. 1. The T–R profile is steepened and advanced relative to the exact case. Conversely, the R–T solution is smoothed and retarded. Note that, for these results, the overall difference between the OS and analytical profiles cannot be attributed to OS error alone as numerical truncation error is also present.

The numerical solutions were also used to compute the wave speed [8]. Discrete values of WS were computed by tracking the position of the $c(x, t) = 0.5$ contour over successive time steps. Results for the first five time steps are shown in Fig. 2(b). We focus on profiles after only a few time steps since we wish to establish whether the trends in the exact analysis over one time step (Fig. 1) are observed in a standard algorithm. The results confirm that T–R OS overestimates the wave speed while the R–T OS underestimates the wave speed. These observations corroborate our conjecture in Section 2 where the analysis implied that the OS error would be detectable through measurements of the wave speed. The performances of the alternating schemes are superior to those of both the T–R and R–T methods as the alternating OS wave speeds closely approximate the exact value $\mathrm{WS}_{\mathrm{exact}} = 5/\sqrt{6} \simeq 2.04$.

Further numerical solutions of the results in Fig. 2 after many time steps show that the asymptotic numerical wave speeds for R–T, T–R and R–T–R OS algorithms all converge to WS $= 2.16$ at $t = 100$ (50 steps), while the corresponding speed for the T–R–T alternating scheme is WS $= 2.07$. In this case, the T–R–T alternating scheme gives the best results; however, the analysis conducted here does not explain why the T–R–T OS outperforms the R–T–R method. For simulations with many time steps, the increased wave speed means that all OS solutions eventually overtake the exact solution. Therefore, the similarity between the exact single time step profiles (Fig. 1) and the numerical profiles after a small number of time steps (Fig. 2) is no longer observed. Under these conditions the net error is a combination of accumulated truncation and OS errors and so the single time step analysis is not directly applicable. Finally, it is worthwhile to comment that repeating the simulations in Fig. 2 for sufficiently small Δt yields results where all OS solutions converge to the analytical result.

All analysis presented in this study corresponds to the particular case where WS $= 5/\sqrt{6}$. This is convenient as the shape of the advancing profile is known exactly and the OS error can be isolated and characterized in detail. To check the generality of these results, the numerical analysis in Section 3 was repeated for the minimum wave speed WS $= 2$, and also for WS $= 10/\sqrt{6}$. This was possible by numerically generating "fine mesh" solutions to the full problem (2). A particular initial condition is chosen which gives rise to the required wave speed [1]. Using these fine mesh profiles, the simulations in Section 3 were repeated. These additional simulations confirmed that the characteristics of all OS errors examined with $\mathrm{WS} = 5/\sqrt{6}$ are also relevant for other wave speeds.

4. Discussion and conclusion

OS is a convenient and widespread technique used to numerically solve reactive transport problems. OS techniques are particularly advantageous for problems involving nonlinear reactions, such as Fisher's equation. While OS algorithms offer several advantages compared to solving the full conservation equation, these benefits come at the cost of an innate OS error. Although this error is incurred in every standard two-step OS solution for Fisher's equation [5,7–13], the nature of this error has not been explicitly examined nor characterized. Without any knowledge of the form of the OS error, it is impossible to detect the presence of this error since its characteristics are unknown.

The characteristics of the OS error for Fisher's equation have been explored here by applying four different OS techniques in the absence of other sources of error. The OS error is only present at the wave front and the error depends on the sequential order of splitting. For R–T splitting, the OS error smooths and retards the travelling wave. For T–R OS, the error acts to steepen and advance the travelling wave profile. Therefore, the OS error can change both the shape and speed of the travelling wave. The characteristics of the OS error for Fisher's equation are different to those of other reactive transport problems previously explored. Profiles show that R–T–R or T–R–T alternating OS schemes are effective in minimizing the OS error for small to moderate Δt.

To gain a further understanding of the implementation of OS for Fisher's equation, the order of the temporal error was deduced in a numerical simulation for all four OS schemes investigated. This analysis showed that the standard two-step $\mathcal{O}(\Delta t)$ error is removed by using an alternating scheme. The R–T–R and T–R–T alternating schemes both incur an $\mathcal{O}(\Delta t)^2$ error and either should be used in preference to the standard two-step schemes.

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