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Theoretical analysis and physical interpretation of temporal truncation errors in operator split algorithms

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Abstract

The temporal truncation error (TTE) associated with a noniterative operator split (OS) method for application to a system of m coupled transport partial differential equations (pdes) is analysed. The system incorporates arbitrary n-dimensional linear transport and arbitrary nonequilibrium coupling kinetics. An expression for the exact form of the $\mathcal{O}(\Delta t)$ TTE is derived for transport-reaction (TR) splitting as well as reaction-transport (RT) splitting. The analysis allows us to predict the characteristics of the TTE a priori from the structure of the governing equations. The TTE can be interpreted in the form of a pde. Some common examples of multicomponent reactive transport problems are solved to physically demonstrate the influence of the OS TTE and confirm the theoretical TTE expressions. The general expressions for the TR and RT TTE are equal and opposite implying that the $\mathcal{O}(\Delta t)$ TTE can always be removed with standard alternating OS schemes. This result differs from previous research which has shown that alternating OS schemes are not useful for other types of reactive transport pdes.

Keywords: Operator split; Reactive transport; Multicomponent transport; Multispecies transport; Numerical methods

1. Introduction

Operator split (OS) approaches are popular for developing numerical algorithms to solve nonlinear multicomponent coupled reactive transport partial differential equations (pdes) [4,2,3,7,10,11,15,19,20,23,25,34,35,32,36,41,42,47–49]. Noniterative OS methods are the most common approach in practical algorithm design [10,23,34,40]. These algorithms are constructed by separating each time integration step (of length Δt) into two substeps. First, the transport terms in the pdes are integrated over Δt to yield an intermediate solution. Second, the transport and reaction processes are approximately coupled by integrating the reaction terms over Δt using the intermediate result as the initial condition (TR) [4]. Alternatively an OS algorithm could be designed to integrate the reaction terms followed by the transport terms (RT) [18].

It is well-known that OS methods introduce a temporal truncation error (TTE) associated with splitting and that this error is innate and independent of numerical errors [4,3,7,14,15,19,39,38,46]. Until now, most existing analyses of the TTE have been limited to single species linear problems [4,17,39,46]. Hence there is an important gap in our

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knowledge regarding the characteristics of the TTE associated with OS methods for more complex problems, such as coupled nonlinear nonequilibrium multicomponent pdes.

The kind of TTE of interest in this analysis is strictly associated with temporal splitting and is different from the kind of spatial splitting considered in other analysis [24,44,47]. Formally, the spatial analysis presented by Strang [44], Yanenko [47] and Marchuk [24] is not applicable to reaction-transport splitting as the reaction terms involve temporal operators and not spatial operators [4].

Although OS methods are popular, the "rules" for their implementation are, at present, considered more of an art than science [32]. One way to improve our understanding of how to best implement OS methods is to analyze the TTE associated with splitting. From this analysis, we can anticipate how the TTE will affect the OS solution and whether or not the algorithm can be altered to remove or reduce the error [4,3,39,46].

Previous attempts at understanding the TTE associated with splitting have focused on single species transport with linear nonequilibrium reactions [4,17,39,46]. These analyses describe an error that is strictly associated with the domain boundary. Consequently, this error can be isolated and removed simply by considering homogeneous Dirichlet problems [4,39]. Various techniques have been used to analyse the OS TTE. For example Lanser and Verwer [19] use Lie operator formalism to derive expressions for splitting errors associated with pure initial value problems. Because Lanser and Verwer's work did not consider initial boundary value problems this analysis cannot predict the boundary error previously described. Other methods of analysis, such as multi-scale and perturbation techniques, have been used to investigate the splitting error for fast and stiff reaction problems [41,42].

The OS TTE associated with equilibrium type reactions involving linear or nonlinear isotherms has also been considered [4,3,14]. Unfortunately the equilibrium reaction analyses are not applicable for nonequilibrium reactions that are frequently encountered [10] and of primary concern in the current work. Recently, some progress towards understanding the OS TTE associated with a special case of a single species nonlinear nonequilibrium reactive transport pde has been made [38]. Therefore, it is of interest to extend this work by considering the OS TTE for a more general class of reactive transport pdes with nonequilibrium reactions.

The aim of this work is to derive expressions for the TTE associated with TR and RT splitting for a general system of m coupled n-dimensional multicomponent reactive transport pdes with arbitrary nonequilibrium coupling reactions. This procedure will enable the physical properties of the OS error to be deduced a priori according to the structure of the system of pdes. Theoretical results are confirmed with numerical experiments showing the OS error. This combined theoretical and experimental approach used to examine and describe the influence of the OS TTE is very important as many previous analyses have failed to relate theoretical results with practical and physically interpretable results. The characteristics of the RT and TR TTE expressions will be used to deduce how the $\mathcal{O}(\Delta t)$ TTE can be removed.

2. Analysis of temporal truncation errors

A system of n-dimensional pdes describing transport and reaction of m components is written

$$\frac{\partial u_i}{\partial t} = L_i(u_i) + F_i(u_1, u_2, \ldots, u_m), \tag{1}$$

for $i = 1, 2, \ldots, m$. Here L_i is the n-dimensional linear transport operator acting on the ith species and F_i is a kinetic process associated with the ith species. We will interpret F_i as a reaction and make no distinction between linear or nonlinear reaction kinetics. The m equations are coupled through the reaction terms F_i. The kinds of coupled transport phenomena represented by (1) are common and represent a challenging numerical problem especially when m is large and multidimensional transport is considered [10,32,48].

It is important to emphasize that the linear transport operator L_i in (1) is arbitrary so that the results derived in this work are applicable for a wide range of transport phenomena. The operator could be used to represent linear advection and/or standard second order linear diffusion transport processes. In addition the analysis is also applicable to other linear transport mechanisms such as higher order diffusion. Higher order diffusive transport mechanisms are important in several fields such as representing long-range diffusion effects in theoretical biology applications [30] as well as modelling surface-driven diffusion phenomena such as thermal grooving [28]. The fact that our analysis is applicable to any linear transport mechanism is important as this significantly extends previous works which have presented results for standard linear advection and/or linear diffusion transport mechanisms only [15,19].

A noniterative OS algorithm could be applied to (1) by either integrating the transport terms followed by the reaction terms (TR), or by integrating the reaction terms followed by the transport terms (RT). Both of these options are used in practice [10,18], and we will analyze the TTE for both options.

2.1. Transport reaction temporal truncation error

We consider first the case where the OS algorithm is designed to integrate the transport terms followed by the reaction terms. As in previous analyses [4,3], the discretized form of $L_i(u_i)$ is considered: $L_i(u_i) = \mathbf{A}_i\mathbf{u}_i + \mathbf{b}_i$. Here, $\mathbf{A}_i\mathbf{u}_i$ represents the discretized n-dimensional transport operator. The bold notation signifies that this term is a vector representation since the transport operator is spatially discretized on all internal nodes in the domain. The length of the vector corresponds to the number of nodes in the spatial mesh. This representation is appropriate for any common choice of spatial discretization including finite difference, finite volume and finite element techniques [2]. The $\mathbf{b}_i$ term represents the discretized boundary conditions in conjunction with the discretized transport operator. Note $\mathbf{b}_i = 0$ for homogeneous Dirichlet boundary conditions.

To determine the TTE for TR splitting, we consider integrating the system from t^k to t^{k+1} with $\Delta t = t^{k+1} - t^k$. The uncoupled transport equations are integrated from t^k over Δt to give the intermediate concentration, denoted as $\mathbf{u}_i^*$. This has the form

$$\frac{\mathbf{u}_i^* - \mathbf{u}_i^k}{\Delta t} = \frac{1}{2}(\mathbf{A}_i\mathbf{u}_i^* + \mathbf{A}_i\mathbf{u}_i^k + \mathbf{b}_i^* + \mathbf{b}_i^k), \quad \text{for } i = 1, \ldots, m. \tag{2}$$

Assuming Δt is small and taking Taylor series expansions around $t^{k+(1/2)}$ (where $t^{k+(1/2)} = t^k + \Delta t/2$), we express the intermediate solution $\mathbf{u}_i^*$ as a function of all terms evaluated at $t^{k+(1/2)}$ [4,3]. For simplicity the $k + (1/2)$ superscript is suppressed. This gives

$$\mathbf{u}_i^* = \mathbf{u}_i + \Delta t\left(\mathbf{A}_i\mathbf{u}_i + \mathbf{b}_i - \frac{1}{2}\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t}\right) + (\Delta t)^2\left(\frac{1}{8}\frac{\mathrm{d}^2\mathbf{u}_i}{\mathrm{d}t^2} + \frac{1}{2}\mathbf{A}_i^2\mathbf{u}_i - \frac{1}{2}\mathbf{A}_i\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t}\right) + \mathcal{O}[(\Delta t)^3], \quad \text{for } i = 1, \ldots, m. \tag{3}$$

Following the integration of the transport component, the reaction functions are also integrated over Δt using the intermediate solution as the initial condition

$$\frac{\mathbf{u}_i^{k+1} - \mathbf{u}_i^*}{\Delta t} = \frac{1}{2}(F_i^* + F_i^{k+1}), \quad \text{for } i = 1, \ldots, m. \tag{4}$$

All terms in (4) other than $\mathbf{u}_i^*$ are expanded in Taylor series about $t^{k+(1/2)}$ and the resulting expression is combined with (3) to give

$$\frac{\partial u_i}{\partial t} = L_i(u_i) + F_i(u_1, u_2, \ldots, u_m) + E_i^{\mathrm{TR}}, \quad \text{for } i = 1, \ldots, m, \tag{5}$$

where the last term represents an error associated with the ith species. This error contains an $\mathcal{O}(\Delta t)$ component that is the TTE arising from TR splitting. This error has the form

$$E_i^{\mathrm{TR}} = \frac{\Delta t}{2}\left[\sum_{j=1}^{m}\frac{\partial F_i}{\partial u_j}(\mathbf{A}_j\mathbf{u}_j + \mathbf{b}_j) - \mathbf{A}_i F_i\right] + \mathcal{O}[(\Delta t)^2], \quad \text{for } i = 1, \ldots, m \text{ and } j = 1, \ldots, m. \tag{6}$$

The $\mathcal{O}(\Delta t)$ term in this expression represents the TR TTE associated with any system of transport pdes incorporating n-dimensional linear transport and arbitrary nonequilibrium coupling reactions. By setting $m = 1$, (6) can be used to determine the TTE associated with a TR OS algorithm applied to single species reactive transport with arbitrary F_i. For example, choosing a simple constant or linear kinetic term recovers the TTE expressions previously derived by Barry et al. [4].

For multicomponent systems $m \geq 2$, (6) shows that the TTE associated with the ith species can be coupled to the discretization of the jth species so long as $(\partial F_i/\partial u_j) \neq 0$. This coupling will be crucial in determining the form of the net OS error.

2.2. Reaction transport temporal truncation error

To determine the TTE for RT splitting, a similar approach is taken except that the sequential order of integration is swapped so that the reaction terms are integrated first followed by the transport terms. The transport terms are integrated over Δt to the end of the time step t^{k+1} using the (as yet unknown) intermediate concentration $\mathbf{u}_i^{**}$ as the initial condition. This gives

$$\frac{\mathbf{u}_i^{k+1} - \mathbf{u}_i^{**}}{\Delta t} = \frac{1}{2}(\mathbf{A}_i\mathbf{u}_i^{k+1} + \mathbf{A}_i\mathbf{u}_i^{**} + \mathbf{b}_i^{k+1} + \mathbf{b}_i^{**}), \quad \text{for } i = 1, \ldots, m. \tag{7}$$

Assuming Δt is small and taking Taylor series expansions around $t^{k+(1/2)}$ (where $t^{k+(1/2)} = t^{k+1} - \Delta t/2$), $\mathbf{u}_i^{**}$ is expressed as a function of all terms evaluated at $t^{k+(1/2)}$. For simplicity the $k+(1/2)$ superscript is suppressed to give

$$\mathbf{u}_i^{**} = \mathbf{u}_i + \Delta t\left(-\mathbf{A}_i\mathbf{u}_i - \mathbf{b}_i + \frac{1}{2}\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t}\right) + (\Delta t)^2\left(\frac{1}{8}\frac{\mathrm{d}^2\mathbf{u}_i}{\mathrm{d}t^2} + \frac{1}{2}\mathbf{A}_i^2\mathbf{u}_i - \frac{1}{2}\mathbf{A}_i\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t}\right)$$
$$+\mathcal{O}[(\Delta t)^3], \quad \text{for } i = 1, \ldots, m. \tag{8}$$

Given $\mathbf{u}_i^{**}$, the reaction terms are integrated over Δt from t^k as

$$\frac{\mathbf{u}_i^{**} - \mathbf{u}_i^{k}}{\Delta t} = \frac{1}{2}(F_i^{**} + F_i^{k}), \quad \text{for } i = 1, \ldots, m. \tag{9}$$

All terms in (9) other than $\mathbf{u}_i^{**}$ are expanded in Taylor series about $t^{k+(1/2)}$ and the resulting expression is combined with (8) to give

$$\frac{\partial u_i}{\partial t} = L_i(u_i) + F_i(u_1, u_2, \ldots, u_m) + E_i^{\mathrm{RT}}, \quad \text{for } i = 1, \ldots, m, \tag{10}$$

where the last term represents an error associated with the ith species. This error contains an $\mathcal{O}(\Delta t)$ component that is the TTE arising from RT splitting. This error has the form

$$E_i^{\mathrm{RT}} = -\frac{\Delta t}{2}\left[\sum_{j=1}^{m}\frac{\partial F_i}{\partial u_j}(\mathbf{A}_j\mathbf{u}_j + \mathbf{b}_j) - \mathbf{A}_i F_i\right] + \mathcal{O}[(\Delta t)^2], \quad \text{for } i = 1, \ldots, m \text{ and } j = 1, \ldots, m. \tag{11}$$

Comparing (6) and (11) shows that the $\mathcal{O}(\Delta t)$ TTE associated with TR splitting is equal and opposite to the $\mathcal{O}(\Delta t)$ TTE for RT splitting. This has implications for how the $\mathcal{O}(\Delta t)$ TTE can be removed. Because the TR and RT TTE are equal and opposite, it follows that standard alternating OS methods will remove the $\mathcal{O}(\Delta t)$ TTE without difficulty.

Alternating OS methods involve swapping the sequential order of splitting in each subsequent step [4,38,46]. That is, the splitting is carried out as, (i) time step 1, reaction over Δt then transport over Δt (ii) time step 2, transport over Δt then reaction over Δt and so on. Alternatively the splitting can be carried out as, (i) time step 1, transport over Δt then reaction over Δt (ii) time step 2, reaction over Δt then transport over Δt and so on. Since the TTE associated with TR splitting is equal and opposite to the TTE associated with RT splitting, then for sufficiently small Δt, the $\mathcal{O}(\Delta t)$ TTE incurred in one time step will be removed by reversing the sequential order of splitting in the following step. This will lead to the $\mathcal{O}(\Delta t)$ TTE being removed after every second time step [46]. As noted by Valocchi and Malmstead [46] and Barry et al. [4] this kind of alternating approach is closely related to Strang splitting [44] used for spatial operators.

It is important to emphasize the effectiveness of alternating OS methods for nonequilibrium reactive transport pdes as previous analyses of equilibrium reactive transport [4,3] showed that alternating OS methods ought not be used as they can actually increase the TTE relative to a standard TR OS algorithm. The present analysis and numerical examples that follow in Section 3 shows that this caution is unnecessary for reactive transport with nonequilibrium

reactions. Our analysis and numerical examples will show that the TTE associated with a standard two step noniterative OS algorithm can always be removed for any arbitrary system of reactive transport pdes with nonequilibrium coupling reactions provided that Δt is sufficiently small.

Implementing alternating OS methods as described above can be problematic since the $\mathcal{O}(\Delta t)$ TTE is only removed after taking an even number of time steps. To avoid this, the time integration can be adjusted so that the $\mathcal{O}(\Delta t)$ TTE is removed after any number of steps. There are two ways to do this [4,27,38,49];

(1) Within each time step, a TRT alternating algorithm solves transport for $\Delta t/2$ then reaction for Δt and another transport for $\Delta t/2$.
(2) Within each time step, an RTR alternating algorithm solves reaction for $\Delta t/2$ then transport for Δt and another reaction for $\Delta t/2$.

3. Numerical investigation and physical interpretation of splitting errors

Three applications of reactive transport pdes will be presented. Clearly the analysis in Section 2 is applicable for arbitrary spatial dimensions, however for the sake of clarity we demonstrate the TTE for one-dimensional problems. The form of the $\mathcal{O}(\Delta t)$ TTE will be presented for these three applications as given by (6) for TR splitting. The equivalent expression for RT splitting is simply the negative of the TR expression. The $\mathcal{O}[(\Delta t)^2]$ component in (6) will be ignored since this term contains a contribution from the numerical truncation error.We first consider a single species nonlinear reactive transport problem relevant for a general class of invasion models. Following this, two coupled multicomponent problems will be analysed. These coupled problems will involve two species undergoing linear transport and either linear or nonlinear coupling reactions. The form of the TR or RT noniterative TTE associated with splitting has not been derived for any of these three cases previously. For notational simplicity we denote $u_1 = u$ and $u_2 = v$. Furthermore, we will focus on the OS TTE that acts independently of the boundary, that is we will explicitly analyze the internal OS TTE. The reason for focusing this analysis on the internal error is that many previous analyses have focused only on the boundary error [39,46] which can be easily removed by setting $\mathbf{b}_i = 0$, whereas there is no such short cut to remove the internal OS error. It should be noted that deriving the expression for the boundary error is simply a matter of retaining the $\mathbf{b}_i$ term in (6) and (11).

3.1. Single species nonlinear invasion phenomena

A continuum model for single species invasion can be written as [30]

$$\frac{\partial u}{\partial t} = L(u) + \lambda u^p(1 - u^q), \tag{12}$$

where p and q are the positive integers. Reactive transport pdes in this form are widely used in various applications such as population dispersals [30,31,43], tissue engineering [22], particle physics [6] and combustion phenomena [1]. In one dimension, this kind of invasion model generally supports travelling wave solutions that move with a constant speed and shape [30]. The expression (12) relaxes to some well-known cases for certain values of p, q and L, for example Fisher's equation is obtained by considering one-dimensional diffusive transport and $p = q = 1$ [12]. In writing (12) we have set the carrying capacity concentration to unity without loss of generality. We will consider, in detail, one-dimensional diffusive transport

$$L = D\frac{\partial^2}{\partial x^2}. \tag{13}$$

Evaluating (6) with (12) and (13) leads to

$$E_u^{\mathrm{TR}} = -\frac{D\,\Delta t}{2} f''(u)\left(\frac{\partial u}{\partial x}\right)^2, \tag{14}$$

where $f(u) = \lambda u^q(1 - u^p)$. If a one-dimensional transport operator including an advective component were considered ($L = D(\partial^2/\partial x^2) - v(\partial/\partial x)$), instead of (13), then the exact same error expression as (14) results. It is interesting that the TTE expression is proportional to $(\partial u/\partial x)^2$. We note that one of the two terms in the $\mathcal{O}(\Delta t)$ TR OS error deduced by Barry

et al. [3] for nonlinear equilibrium reactive transport is also proportional to $(\partial u/\partial x)^2$. However, the error expression in [3] arises from the advection component of $L(u)$ and is proportional to the square of the advective velocity v^2, whereas the error term (14) arises from the diffusion component in $L(u)$ and is proportional to the diffusivity D.

We will now consider results for Fisher's equation by setting $p = q = 1$. From (14), the TR TTE for Fisher's equation is

$$E_u^{\mathrm{TR}} = \left(D\lambda\, \Delta t\, \frac{\partial u}{\partial x} \right) \frac{\partial u}{\partial x}. \tag{15}$$

Written in this form, it is clear that the TTE can be interpreted as a nonlinear advection term. The error will only be present in regions of the solution where $(\partial u/\partial x) \neq 0$. Therefore, in a typical travelling wave solution the error will only be present at the wavefront. For a right-moving travelling wave $(\partial u/\partial x) < 0$ at the wavefront, so for TR splitting the error will advect the wavefront further to the right of the true solution. Conversely, for RT splitting, a right-moving travelling wave will be advected to the left of the true solution. The magnitude of the TTE increases with $|\partial u/\partial x|$, and so keeping $D\lambda\Delta t$ constant, a steep-fronted travelling wave will incur a larger TTE than a flatter wave regardless of the direction of propagation.

Travelling wave solutions of Fisher's equation will be used to demonstrate the TTE. Fixing $D = \lambda = 1$, we consider two travelling wave solutions that move with speed $c = 2$ (the minimum wave speed) and $c = 5$. Since analytical solutions for these problems do not exist [16,30], the shape of these waves are generated numerically. A Crank–Nicolson finite difference algorithm linearized with Newton–Raphson iteration is used to solve the fully coupled problem on a fine mesh yielding grid independent results. To generate the shape of the profiles, different initial conditions are chosen that will eventually form right-moving travelling waves with the desired wave speed [18,30]. Once obtained, the profiles are shifted to the left so that $u(0, t) = 0.5$ for both profiles. The shifted profiles are then used as an initial condition from which various OS solutions are computed.

Numerical computations are performed on $-l_1 < x < l_2$ and no flux boundary conditions are imposed with l_1 and l_2 chosen large enough so that the wave-front never interacts with the boundaries. The RT and TR OS algorithms are implemented over several time steps using a moderate Δt to show the influence of the TTE. The OS solutions are evaluated with the transport operator solved using a Crank–Nicolson finite difference method and the ordinary differential equations (odes) associated with the reaction kinetics at each point on the discretized domain, $(\mathrm{d}u/\mathrm{d}t) = \lambda u(1 - u)$, are solved analytically [38]. The TTE is detected by comparing the OS profiles with grid independent numerical solutions obtained using the fully coupled finite difference algorithm. Both the exact and OS profiles are shown in Fig. 1. The minimum speed travelling wave is steep-fronted and the influence of the TTE is clear. The TR OS solution is ahead of the exact solution and the RT OS solution lags behind. These kinds of errors are in accordance with the expression (15). The travelling wave profile for $c = 5$ is less steep than the minimum wave speed case [30], and for the same parameters, the difference between the grid independent fully coupled solution and the OS solutions is significantly reduced. Although the errors associated with the OS solutions are reduced, the same qualitative trends are observed with the TR solution slightly advanced relative to the exact solution and the RT solution lagging behind.

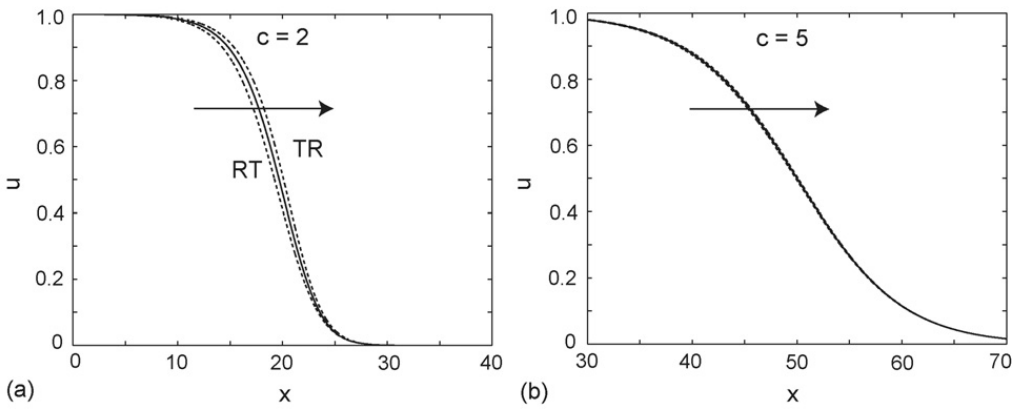

Fig. 1. Travelling wave solutions of Fisher's equation moving in the direction indicated by the arrow. Solutions are obtained for $D = \lambda = 1$ and are moving at speed $c = 2$ and $c = 5$ in (a) and (b), respectively. The grid independent fully coupled numerical solution obtained with $\Delta x = 0.01$ and $\Delta t = 0.01$ (solid line) is superimposed on the RT and TR OS solutions (dotted lines) evaluated with $\Delta x = 0.01$ and $\Delta t = 1$ until $t = 10$.

As the TR and RT TTE expressions are equal and opposite, we expect that standard alternating OS algorithms will remove the $\mathcal{O}(\Delta t)$ TTE for Fisher's equation. Both a TRT and an RTR OS algorithms were used to repeat the computations in Fig. 1. For the same discretizations, the TRT and RTR alternating solutions were indistinguishable from the fully coupled solutions. This confirms previous analysis [38] and heuristic evidence [1] that the $\mathcal{O}(\Delta t)$ OS TTE for Fisher's equation can be removed using alternating schemes.

Approximate perturbation solutions for the shape of right-moving travelling wave solutions of Fisher's equation show that the maximum gradient along the travelling wave profile is inversely proportional to the wave speed, $\max|\partial u/\partial x| \simeq 1/(4c)$ (for $D=\lambda=1$) [30]. Therefore, the OS TTE must scale with the inverse of the square of the wave speed $E_u^{\mathrm{TR}} \propto 1/(16c^2)$ (for $D=\lambda=1$). This result shows that the OS TTE decreases with the wave speed c, as was demonstrated in Fig. 1. This implies that the OS TTE will be greatest for the minimum wave speed solution. Usually, for practical purposes, the minimum wave speed solution is of interest as this solution evolves from initial conditions with compact support [22]. Therefore, analysts using OS methods should be mindful that the slowest travelling wave solution of Fisher's equation is more susceptible to the OS TTE than any other travelling wave solution of Fisher's equation.

The results presented in this section regarding the OS TTE associated with Fisher's equation are concordant with the results recently obtained using an exact analytical solution comparison method [38]. This previous analysis was carried out in the style of Valocchi and Malmstead's approach [46]. Although Fisher's equation has infinitely many travelling wave solutions for any wave speed $c \geq 2\sqrt{\lambda D}$ [12,30], there is only one known analytical travelling wave solution [16]. This analytical solution is relevant for one particular wave speed of $c = 5\sqrt{\lambda D}/\sqrt{6}$. The new expression derived here for the OS TTE associated with Fisher's Eq. (15), significantly extends the previous analysis which was only applicable to one of infinitely many travelling wave solutions. This previous analysis was unable to elucidate how the OS TTE varied with the invasion wave speed as has been shown in this work.

It is also interesting to note that the coefficient of the $(\partial u/\partial x)^2$ term in the general expression of the TTE error (14) can change sign along the invading profile for different choices of p and q. For example, with $p=2$ and $q=1$ (14) gives

$$E_u^{\mathrm{TR}} = D\lambda\,\Delta t(3u-1)\left(\frac{\partial u}{\partial x}\right)^2. \tag{16}$$

This expression shows that the sign of E_u^{TR} will be positive at the heel of the wave ($u \simeq 1$) and negative at the toe of the wave ($u \simeq 0$). Interpreting the TTE term as additional nonlinear advection means that the direction of this advection will change along the invasion profile. The point along the profile where the direction changes is $u=1/3$ in this case. The details of these errors have been numerically verified by repeating the kinds of numerical experiments shown in Fig. 1 with the appropriate value of p and q.

3.2. Coupled transport with distinct retardation factors

A two-species linear coupled transport problem will now be considered. According to single species analysis with a linear nonequilibrium reaction [4,39,46], the OS error is present at the boundary only and there is no internal error. Here we show that this is not true for multicomponent problems with nonequilibrium reactions. The reactive transport pdes considered here are related to the system proposed by Cho [8] to simulate the reactive transport of nitrogen compounds in soil:

$$R\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} - \kappa_1 u, \tag{17}$$

$$\frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2} - v\frac{\partial v}{\partial x} + \kappa_1 u - \kappa_2 v. \tag{18}$$

Here R is a constant known as the retardation coefficient. This coefficient is used to represent the presence of an instantaneous linear sorption reaction associated with the u species [8]. Typically $R \geq 1$ [48]. Dividing (17) by R allows the system to be recast in the form of (1) as

$$\frac{\partial u}{\partial t} = D_1\frac{\partial^2 u}{\partial x^2} - v_1\frac{\partial u}{\partial x} - k_1 u, \tag{19}$$

$$\frac{\partial v}{\partial t} = D_2 \frac{\partial^2 v}{\partial x^2} - \nu_2 \frac{\partial v}{\partial x} + k_2 u - k_3 v. \tag{20}$$

Evaluating the internal OS error for (19) and (20) gives

$$E_u^{\mathrm{TR}} = 0, \tag{21}$$

$$E_v^{\mathrm{TR}} = \frac{(\Delta t\, k_2)}{2}\left[(D_1 - D_2)\frac{\partial^2 u}{\partial x^2} - (\nu_1 - \nu_2)\frac{\partial u}{\partial x}\right]. \tag{22}$$

Clearly, there is no internal OS error for u. This is expected since u is uncoupled from v and so the single species analysis is relevant for u [4]. The OS error for v, however, is present whenever the transport terms for each species differ so long as $(\partial u/\partial x) \neq 0$ and $(\partial^2 u/\partial x^2) \neq 0$. In the case that $D_1 = D_2$ and $\nu_1 = \nu_2$ (or when $R = 1$ in (17)) the internal OS error vanishes. When the error is present it acts as either a source or sink depending on the shape of the u profile and values of the transport coefficients.

To numerically demonstrate the OS TTE we consider (19) and (20) with diffusive transport on $0 < x < 50$ and homogeneous Dirichlet boundary conditions for both species on both boundaries. The initial condition is $u(x, 0) = \mathrm{e}^{-(x-25)^2}$ and $v(x,0) = 0$. The fully coupled solutions are obtained using fine spatial and temporal discretizations with a centered in space finite difference approximation and an implicit Crank–Nicolson time integration. TR and RT OS solutions are evaluated by solving the transport component with a centered in space Crank–Nicolson finite difference method and the coupled reaction odes are solved analytically. Profiles are shown in Fig. 2 where parameters have been chosen to highlight the internal OS error. Numerical computations confirm that there is no internal error for u while the error in the v profile is clear.

For the particular shape of the u profile in Fig. 2(a), we see that $(D_1 - D_2)(\partial^2 u/\partial x^2) > 0$ at $x = 25$. Therefore, (22) predicts that the TR OS solution for v will include a TTE acting as an additional source term locally around $x = 25$. Conversely, the RT TTE is equal and opposite and we expect the RT OS error to act as a sink in the same region. Both of these theoretical predictions are confirmed by the numerical profiles in Fig. 2(b). Further numerical simulations show that the OS error is removed with either an RTR or TRT alternating OS algorithm as expected. Finally, when the computations in this section were repeated with identical discretizations and $R = 1$, both the u and v profiles in the TR and RT OS solutions were indistinguishable from the fully coupled solutions. Therefore, setting $R = 1$ in (17) removes the $\mathcal{O}(\Delta t)$ internal OS error as predicted by the analysis.

Similar results are also obtained when a combined advection and diffusion transport mechanism is used in (19) and (20) rather than pure diffusion as shown in Fig. 2. For combined advection and diffusion the TR and RT solutions are symmetric about the fully coupled solution and either the TRT or RTR alternating OS algorithms are able to remove the $\mathcal{O}(\Delta t)$ TTE. We chose to present results in Fig. 2 for diffusive transport only since this enables more freedom to select a Δt large enough to show the influence of the $\mathcal{O}(\Delta t)$ TTE without having to satisfy additional accuracy constraints imposed by the presence of advection, namely the Courant number constraint [48].

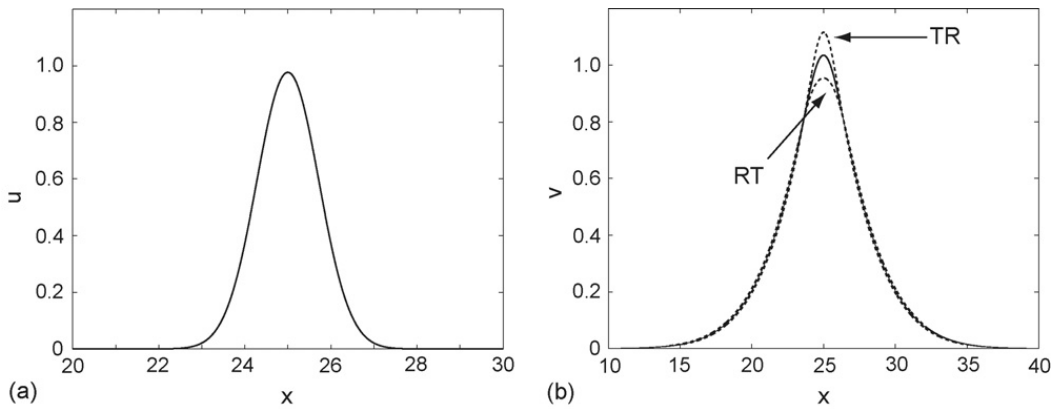

Fig. 2. Profiles of (a) $u(x, t)$ and (b) $v(x, t)$ at $t = 10$ for Cho's [8] linear multicomponent problem. Fully coupled fine mesh numerical solutions (solid lines) evaluated with $\Delta x = 0.01$ and $\Delta t = 0.01$ are superimposed on the TR and RT OS solutions (dotted lines). The OS solutions are evaluated with $\Delta x = 0.01$ and $\Delta t = 0.5$. The parameters for the problem are $D_1 = 0.001$, $D_2 = 1$, $\nu_1 = \nu_2 = 0$, $k_1 = 0.0004$, $k_2 = 0.4$ and $k_3 = 0.01$.

3.3. Pattern formation arising from a Turing instability

Pattern formation models generally involve coupled reaction diffusion equations with nonlinear coupled kinetics and linear diffusion [26,29–31]. This modelling paradigm emerged from Allan Turing's seminal work that hypothesized the existence of a chemical basis for embryonic morphogenesis [45]. Typically both an activator and inhibitor species are simulated with a variety of nonlinear nonequilibrium reactions, for example the Schnakenberg system [37] yields

$$\frac{\partial u}{\partial t} = D_1 \frac{\partial^2 u}{\partial x^2} + b - uv^2, \tag{23}$$

$$\frac{\partial v}{\partial t} = D_2 \frac{\partial^2 v}{\partial x^2} + a + uv^2 - v, \tag{24}$$

where a and b are parameters. This kind of system is known as a cross activator–inhibitor system with u acting as the self-inhibitor and v is the self-activator [33]. For cross activator-inhibitor systems the unstable (patterned) steady state consists of activator and inhibitor distributions that are 180° out of phase [33]. The expressions for the OS TTE are

$$E_u^{\mathrm{TR}} = \frac{\Delta t}{2}\left[2uv(D_1 - D_2)\frac{\partial^2 v}{\partial x^2} + 2uD_1\left(\frac{\partial v}{\partial x}\right)^2 + 4D_1 v\frac{\partial v}{\partial x}\frac{\partial u}{\partial x}\right], \tag{25}$$

$$E_v^{\mathrm{TR}} = \frac{\Delta t}{2}\left[v^2(D_1 - D_2)\frac{\partial^2 u}{\partial x^2} - 2uD_2\left(\frac{\partial v}{\partial x}\right)^2 - 4D_2 v\frac{\partial u}{\partial x}\frac{\partial v}{\partial x}\right]. \tag{26}$$

Clearly the TTE terms in (25) and (26) are more complicated than the other TTE terms presented in this work. The net TTE is a combination of nonlinear advection terms (as demonstrated for Fisher's equation) as well as multiple source/sink terms (as demonstrated with Cho's nitrogen transport problem).

The first terms in (25) and (26) act to couple the TTE of one species to the transport coefficient of the other species so long as $D_1 \neq D_2$ and $(\partial^2 u/\partial x^2) \neq 0$ and $(\partial^2 v/\partial x^2) \neq 0$. A necessary condition for the formation of Turing patterns is $D_1 \neq D_2$ [45]. Therefore, these coupling terms will play a role in determining the net OS error for this problem whenever $(\partial^2 u/\partial x^2) \neq 0$ and $(\partial^2 v/\partial x^2) \neq 0$.

To demonstrate the OS TTE for the Turing pattern problem, the system (23) and (24) is solved on $0 < x < 1$ using the Crank–Nicolson finite difference algorithm linearized with Newton–Raphson iteration. Fine spatial and temporal discretizations are used such that the results are grid independent. The initial condition represents the uniform unstable steady state profiles $v(x, 0) = a + b$ and $u(x, 0) = b/(a + b)^2$ [33]. A small perturbation $\epsilon(x) = \sin(\pi x)/100$ is added to the $u(x, 0)$ profile to enable the system to evolve towards the spatially nonuniform (patterned) state. No flux boundary conditions are imposed. The resulting patterned steady state solutions are given in Fig. 3 and clearly show the formation of six sharp peaks in the v profile. Each peak in v coincides with one of the six troughs in the u profile. This confirms that the patterned steady state for the cross activator–inhibitor system is 180° out of phase. To compute the OS solutions for this problem, the transport part of the pdes was solved with a Crank–Nicolson finite difference algorithm while the coupled nonlinear odes associated with the reaction terms were solved with a standard fourth order Runge–Kutta algorithm.

The spatial structure of the solutions in Fig. 3 is more complex than the problems considered previously in this work. Because of this complexity, some care must be exercised when interpreting the terms in (25) and (26). Certain trends in the solution profiles are important. The curvature of the v profile is very large locally in the vicinity of each peak in v. From this observation we expect some of the terms in (25) and (26) will dominate others. Numerical approximations show that $|\partial^2 v/\partial x^2|$ is several orders of magnitude larger than the other spatial gradients in (25) and (26). In particular $(\partial^2 v/\partial x^2) \simeq -2.1 \times 10^4$ at each location where there is a local maxima in v. Therefore, we expect that the TTE associated with this term in (25) will dominate the net TTE. Therefore, the TTE will be primarily associated with the u profile and will be most prominent at each location where there is a local minima in u (i.e. where there is a local maxima in v).

These theoretical predictions are confirmed with the numerical profiles shown in Fig. 3. The solutions for the u profile show a clear error in each location coinciding with a local minima in u. Because of the complicated nature of the u solution, we have shown a magnified region of the two central troughs in the u profile in Fig. 3(c). The magnified portion of the u profile shows the detail of the OS error in the vicinity of the troughs. In this region the TR OS profiles

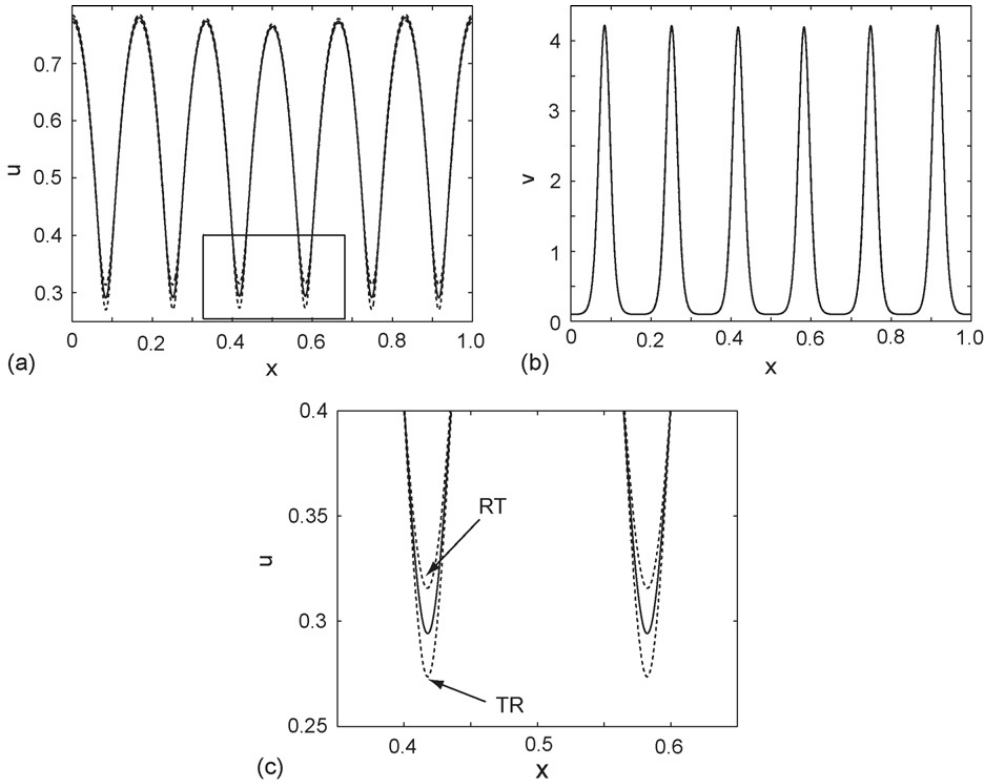

Fig. 3. Profiles showing (a) $u(x, t)$ and (b) $v(x, t)$ at $t = 100$ for the coupled nonlinear Turing instability pattern. Fully coupled fine mesh numerical solutions (solid lines) evaluated with $\Delta x = 0.0005$ and $\Delta t = 0.005$ are superimposed on the TR and RT OS solutions (dotted lines). The two middle troughs contained in the rectangle in subfigure (a) are magnified in subfigure (c) to highlight the details of the OS error. The OS solutions are evaluated with $\Delta x = 0.0005$ and $\Delta t = 0.01$. The parameters for the problem are $D_1 = 5 \times 10^{-3}$, $D_2 = 5 \times 10^{-5}$, $a = 0.09$ and $b = 0.9$.

for u are subject to an error in the form of a local sink while the RT OS profiles are subject to an error in the form of a local source. These observations are in agreement with the theoretical prediction and confirm the expression for the OS error (25) and (26). As expected, these errors are removed with either an RTR or TRT alternating algorithm applied with the same discretizations used in Fig. 3.

4. Discussion and conclusion

There are two important reasons why OS methodologies are adopted in practical algorithm design:

(1) For systems of nonlinear reactive transport pdes it can be computationally expensive to simultaneously solve all coupled terms implicitly. This method, known as the global implicit approach, becomes prohibitive for multidimensional problems with many species.
(2) For systems involving complicated reaction schemes, OS methods enable different approaches to be combined in a very straightforward manner. Therefore, well-tested and well-understood subalgorithms can be combined with ease to build a robust and modular code that can be easily modified to account for different reaction kinetics.

While these properties of OS algorithms are attractive, the benefits come at the cost of a TTE associated with splitting. Until recently, our knowledge of the types of error introduced by splitting has been limited to simple kinds of reactive transport pdes. Because of this, analysts using OS methods for more complex reactive transport pdes could only rely on simple physical reasoning to deduce how the TTE would influence the solution and how it could be reduced or removed. For example, Gazdag and Canosa [13] argued, without any supporting mathematical analysis, that the TR TTE associated with Fisher's equation [12,38] could be reduced by using small time steps. More recently, Bell and Binning [5] used a correction method to reduce the boundary TTE error for two species coupled reactive transport. While both these approaches were successful in reducing the OS TTE, the kind of physical reasoning used

to minimize the OS error does not offer any general insight as to the exact form or characteristics of the OS TTE. A mathematical analyses offers a more general and sophisticated way of determining the exact form of the TTE incurred by splitting.

Most existing analyses of the OS TTE have been focused on single species linear problems [4,14,17,39,46]. Although instructive, these analyses have had limited direct application since OS methods are usually implemented for coupled nonlinear multicomponent reactive transport [10,9,21,40]. Therefore, the error expressions derived in this work provide a more practical and comprehensive description of the OS TTE than previous single species linear analyses. The expressions for the TR and RT truncation error, associated with the arbitrary system of reactive transport pdes, is a useful tool. These expressions allow the TTE to be expressed in terms of a pde for any system of reactive transport pdes with nonequilibrium reactions. The three reactive transport pdes analysed in this work show that these newly derived OS error expressions reliably predict the OS TTE characteristics. This kind of mathematical analysis obviates the need for ad hoc physical reasoning in order to deduce the OS error characteristics for a particular problem.

A major strength of this work is that the theoretical analysis has been used to physically predict the characteristics of the splitting error. Practitioners using splitting algorithms are primarily interested in two questions: (i) does splitting introduce an error? (ii) If splitting introduces an error, what will the error look like and how can the error be detected? Previous analyses of splitting errors have failed to address both of these questions adequately. In fact most previous analyses have not considered the second question. In contrast, the current work thoroughly addresses both of these questions. By retaining the leading $\mathcal{O}(\Delta t)$ term in the Taylor series expansions, we can interpret the OS error as an additional mechanism introduced by splitting. Therefore, the OS TTE is physically interpretable and the characteristics of the TTE can be described and observed. For example, we show that the expression for the RT TTE is equal and opposite to the expression for the TR TTE. Accordingly, we expect that the TR and RT OS solutions will be symmetric about the fully coupled solution. The three examples given in this work confirm this theoretical prediction. We are not aware of any previous analysis which has practically illustrated the relationship between TR and RT splitting in this context. In addition we also theoretically describe the specific physical characteristics of the OS TTE. For example the OS TTE for Fisher's equation is shown theoretically to act as a nonlinear advection term while the TTE for Cho's linear multispecies equations acts as a source/sink term. These results are numerically confirmed.

The current analysis not only predicts the kind of TTE introduced by splitting, but also shows how the $\mathcal{O}(\Delta t)$ TTE can be removed. The results in Section 2 showed that the TTE for TR and RT splitting is equal and opposite for any arbitrary system of nonequilibrium reactive transport pdes. Therefore, alternating OS methods will remove the TTE without difficulty. Indeed, the numerical experiments in Section 3 confirm that the TTE was removed with alternating OS methods. This point needs to be emphasized since previous analyses of equilibrium reactions [4,3] have cautioned against using alternating OS methods. The present analysis shows that alternating OS methods are a simple and attractive way to remove the $\mathcal{O}(\Delta t)$ TTE for nonequilibrium coupled multicomponent reactive transport pdes provided that Δt is sufficiently small. In summary, alternating OS methods should always be used for reactive transport pdes involving nonequilibrium reactions, and never used for reactive transport pdes involving equilibrium reactions.

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