On Computation of Coupled Advection-Diffusion-Reaction Problems by Schwarz Waveform Relaxation Methods

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ABSTRACT  A study is presented on the computation of coupled advection-diffusion-reaction equations by Schwarz waveform relaxation methods. Unlike in most earlier work, which primarily focuses on linear, homogeneous scenarios at the continuous/semi-continuous levels, we deal with the equations that may not be identical in different subdomains and analyze their computation at the full discretization level, plus a discussion on nonlinear equations. The analysis starts with the linear systems resulting from the discretization of the equations by explicit schemes. Conditions for convergence are derived, and its speedup and the effects of difference in the equations are discussed. Then, it proceeds to discretization by an implicit scheme, and a recursive expression for convergence speed is derived. An optimal interface condition for Schwarz waveform relaxation is also obtained, which leads to "perfect convergence", that is, convergence within two times of iteration. Furthermore, the methods and analyses are extended to the coupling of the viscous Burgers equations. Numerical experiments indicate that the conclusions, such as the "perfect convergence", drawn in the linear situations may remain mostly in the computation of the Burgers equations.

Keywords: Domain decomposition, advection-diffusion-reaction equation, the viscous Burgers equation, Scarborough criterion, optimized Schwarz waveform relaxation

1. Introduction

Advection, diffusion, and reaction are fundamental physical phenomena, and they and their interactions take place in various real-world problems. These phenomena and interactions are described by coupled advection-diffusion-reaction equations, which have been solved numerically to understand the underlying physical processes such as migration of pollutants in a porous medium, chemical reaction in a nuclear reactor, and propagation of tsunamis in the ocean [1, 2, 3]. Additionally, it has become a trend to couple more complicated partial differential equations (PDEs), such as the Navier-Stokes equations and their hydrostatic versions [4, 5, 3], for simulation of realistic multiscale/multiphysics problems. Since advection-diffusion-reaction equations exhibit behaviors of parabolic, hyperbolic, and elliptic equations, they are commonly used as models to study these complicated PDEs [6, 7, 8]. Naturally, the coupling of the former serves as a simplification of the coupling of the latter. As a result, a study on the computation of coupled advection-diffusion-reaction equations promotes simulations of actual physical problems and development in numerical methods for PDEs.

Domain decomposition (DD) has emerged as an indispensable avenue to the scientific computation of various problems, and its development in methods and analysis for equations of advection, diffusion, and reaction can trace back over 30 years ago, e.g., [9]. In order to deal with evolution in time, an approach is to discretize the time terms at each time step and then handle the resulting equations with methods for elliptic equations (e.g., [10, 11]). Another approach is to discretize in space first and then deal with the resulting ordinary differential equations (ODEs) with waveform relaxation algorithms. In past years, the second approach has become popular in DD computation,

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as seen in most literature discussed here, and even in application, e.g., simulation of flow problems [12]. Investigations have covered diffusion equations [10, 13, 14, 15], advection equations [11, 16], advection-diffusion equations [17, 18, 19], and the particular forms (e.g., the Darcy law, a fractional equation, and the Schrödinger equation) [20, 21, 22], all with or without reaction. The research topics include convergence analysis [16, 23, 21, 24], optimal transmission conditions [19, 18], and algorithm study [14, 25, 24]. Additionally, interface conditions in heterogeneous problems, e.g., between an advection-diffusion equation and an advection equation, have been investigated [9, 26, 20]. A thorough survey for DD for these types of equations is available in [27]. As an extension of regular advection-diffusion-reaction equations, hyperbolic systems of conservation laws have also been investigated intensively [28, 29], especially in the context of fluid flow simulation [30]. In the computation of the systems, explicit discretization is commonly used, and, therefore, no iteration between subdomains is needed. Interface algorithms and stability issues have become the main research topics for the systems [29, 31, 32].

Progress has been made in understanding DD computation of advection-diffusion-reaction equations. It is concluded that, when waveform relaxation is in use for an ODE, which may result from the spatial discretization of a PDE, the convergence rate is linear when an unbounded time interval is considered, and it may become super-linear when the interval is bounded [13]. It is shown that computation of the standard advection-diffusion-reaction equation by waveform relaxation and Dirichlet conditions at interfaces is well-posed, and the convergence rate increases with the size of the overlapping region but decreases with diffusion coefficients [19]. It is agreed that convergence is slow when a regular Dirichlet transmission condition is adopted, and its speed up is possible by adopting an optimal condition [18, 21]. The convergence rate can be greatly accelerated by methods such as precondition in iteration matrices and optimization for interface conditions, and such speedup can be over an order of magnitude [18, 27]. For systems of conservation laws, it is proven that, when conservative interface algorithms are adopted at grid interfaces, numerical solutions converge to weak solutions of the systems if they converge [29]. Then, it is shown that, under certain conditions that can be verified, even when non-conservative interface algorithms are used, still convergent solutions will become weak solutions, and the conservation errors are bounded [32]. Later, it is further proved that the conservation error tends to zero at the speed of $O(\Delta t)$, regardless of the smoothness of solutions at the interfaces [33]. In the computation of the systems, discretization is necessary to avoid numerical oscillations, nonphysical solutions, and multiple solutions [31, 34, 35].

Despite the substantial study, more topics deserve investigation. As fundamental research, heterogeneous DD problems of advection-diffusion-reaction equations is such a topic. In the past, research has been focused on homogeneous problems, e.g., identical equations in subdomains, and investigations on inhomogeneous problems are sparse, although a few relevant efforts have been made previously [9, 26]. Additionally, previous analysis investigations are primarily conducted at the continuous level and semi-discretizations levels [36, 23]. While studies at such levels are successful and have revealed many important patterns of the problems, their results may not be conveniently or directly applied to practical computation. For instance, mostly, the analysis of optimal interface conditions is made based on the Laplace transform, and the corresponding obtained optimal parameters are expressed in a spectral space and thus need to be approximated for actual computation [37]. Moreover, most studies are about linear problems in the past, with sparse discussion on nonlinear equations. This paper presents a systematic analysis of the computation of coupled advection-diffusion-reaction equations, and it intends to fill the gaps listed above and also deals with situations beyond those in existing work. Notably, such equations, with different
coefficients in subdomains in general, are fully discretized using either explicit or implicit schemes. The analysis starts with explicit schemes for the computation of the resulting algebraic systems. Conditions for the convergence are derived, and its speedup and behaviors are examined, together with a discussion on the effects of difference in PDEs in subdomains. Then, the analysis proceeds to an implicit scheme and derivation of convergence speed. Following these, optimized Schwarz wave relaxation is presented, together with an optimal interface condition. Finally, the study is extended to the coupling of the viscous Burgers equations, and analysis based on linearization is made on their computation.

2. The problem of study

This paper considers computation of the following initial value problem of coupled advection-diffusion-reaction equations in two subdomains:

\[
\begin{align*}
\frac{u_1}{t} + f_1^k(u_1) &= b_1 u_1 x - c_1 u_1, & x < x_2 \\
u_1 &= u_2, & x = x_2 \\
u_1 &= g(x), & t = 0
\end{align*}
\]

\[
\begin{align*}
\frac{u_2}{t} + f_2^k(u_2) &= b_2 u_2 x - c_2 u_2, & x > x_1 \\
u_2 &= u_1, & x = x_1 \\
u_2 &= g(x), & t = 0
\end{align*}
\]

in which \( t \) is the time, and \( x \) is the space coordinate. Subdomain 1 is on the left, \( x \leq x_2 \), and subdomain 2 is on the right, \( x \geq x_1 \). The two subdomains overlap with each other, i.e., \( x_1 < x_2 \), and \( x = x_1 \) and \( x = x_2 \) are the interface of subdomain 2 and 1, respectively. In this study, \( f^k(u_k) = a_k u_k, u_k^2 / 2 \) will be considered. \( a_k, b_k, \) and \( c_k \) are constant coefficients, and their values may be different in the two subdomains. As a result, problem (1) includes a number of coupling scenarios, such as coupling between two advection-diffusion-reaction equations with different coefficient, between an advection-diffusion equation \((a_1, b_1, c_1 \neq 0)\) and an advection equation \((b_2, c_2 = 0)\), and an advection equation \((b_1, c_1 = 0)\) and a diffusion-reaction equation \((a_2 = 0)\). As seen in (1), Dirichlet conditions are used at the interfaces. Moreover, boundary conditions at the left and right ends of subdomain 1 and 2, respectively, may be added. Without loss of generality, it is assume that \( g(x) \) has a finite support.

Consider computation of problem (1) on two grids as shown in Fig. 1, with the left and right grid covering subdomain 1 and 2, respectively. Node \( I \) of the left grid and node 1 of the right grid are the interfaces of the two grids, and they correspond to the interfaces of the two subdomains. On the two grids, the advection-diffusion-reaction equations are discretized with backward difference and central difference in time and space, respectively, and this leads to an implicit scheme for problem \((k = 1, 2)\):

\[
\frac{u_{k_1}^{n+1} - u_{k_1}^n}{\Delta t} + f_{u_1}^k + \frac{u_{k_1+1}^{n+1} - u_{k_1-1}^{n+1}}{2\Delta x} = b_k \frac{u_{k_1+1}^{n+1} - 2u_{k_1}^{n+1} + u_{k_1-1}^{n+1}}{\Delta x^2} - c_k u_{k_1}^{n+1}
\]

where \( \Delta t \) and \( \Delta x \) are the time step and the grid spacing, respectively, superscript \( n \) and subscript \( i \) indicate time level and grid node, respectively, and \( f_{u_1}^k = \partial f^k(u_k)/\partial u_k \). Note that, instead of (2), the equations may be discretized using an explicit scheme, but this study focuses on an implicit scheme given its advantages such as better numerical stability and wide use in practical computation. Moreover, it is readily checked that the discretization accuracy of (2) is \( O(\Delta t + \Delta x^2) \). If needed, \( O(\Delta t^2 + \Delta x^2) \) can be achieved, for instance, by discretizing the time derivative with a second-order accurate, three-time-level backward difference \((\text{e.g., [12]}\)\), or, discretizing the whole equation with the Crank–Nicholson scheme \((\text{e.g., [33]}\)\). However, the analysis of (2) in this paper remains same.
This paper aims to analyze the computation of discretization (2) via explicit and implicit schemes, together with Schwarz waveform relaxation methods. Particularly, when marching from time level $n$ to $n + 1$ via an explicit scheme, the problem will be solved as ($m = 1, 2, ...$):

$$\begin{align*}
F(..., u_1^m, ..., u_1^{m-1}, ..., u_1^n) &= 0, \quad i \leq I - 1; \quad u_1^m = u_2^m \\
F(..., u_2^m, ..., u_2^{m-1}, ..., u_2^n) &= 0, \quad i \geq 2; \quad u_2^m = u_1^m_{I-1}
\end{align*}$$

Here, $F$ represents an iterative scheme to compute discretization (2) in subdomains. As $m \rightarrow \infty$, if convergent, the iterated solution converges to the solution at time level $n + 1$: $u_1^m \rightarrow u_1^{n+1}$, $u_2^m \rightarrow u_2^{n+1}$. In above, the two grids exchange solutions at a same level of iteration, i.e. $m$, at their interfaces, and this is possible when an explicit iterative scheme is adopted in subdomains. When an implicit scheme is used, the exchange will be made between different levels of iteration: $u_1^m = u_1^{m-1}$, and $u_2^m = u_2^{m-1}$. Such interface conditions, with solution exchange either at a same or at a different level, are Dirichlet conditions, and they are referred to as classic interface conditions hereafter.

3. Explicit scheme

3.1 Convergence criterion

Consider a linear system

$$AU = b$$

in which $A = (a_{ij})$, $U = (u_i)$, and $b = (b_i)$, with $i, j = 1, 2, ... I$. When the system is solved by the Jacobi iteration, one has ($m = 1, 2, ...$)

$$U^m = (I - D^{-1}A)U^{m-1} + D^{-1}b$$

in which $I$ is the identity matrix, and $D$ is a diagonal matrix with the diagonal elements of $A$ as its diagonal elements. The following condition is frequently used as a sufficient condition for convergence of (5):

$$\sum_{j=1, \neq i}^{n} |a_{ij}|/|a_{ii}| \leq 1, \quad i = 1, ..., I$$

$$< 1, \text{ at least one } i$$

which is proposed by Scarborough [38, 39]. This condition is referred to as the Scarborough criterion,
and it is widely used in practical computation, e.g., heat and mass transfer [40, 41]. On the basis of the the Scarborough criterion, it is readily derived that the following is also a sufficient condition for the Jacobi iteration to converge (because the transpose of \((I - D^{-1}A)\) in the following iteration will satisfy the Scarborough criterion and therefore its spectral radius must be less than 1):

\[
\sum_{i=1, \neq j}^{l} \frac{|a_{ij}|}{|a_{ii}|} \leq 1, \ j = 1, ..., I < 1, \ at\ least\ one\ j
\]

Note that, instead of over columns, the summation in above is over rows. In the following, we present a trivial case for a more general conclusion.

**Proposition 3.1** Given an iteration

\[ U^m = CU^{m-1} + d \]

where \(C = (c_{ij})\), and \(d = (d_i)\), with \(i, j = 1, 2, ..., I\). A sufficient condition for the iteration to converge is

\[
\sum_{j=1}^{I} |c_{ij}| < 1
\]

for every \(i\).

**Proof:** It suffices to consider the associated homogeneous iteration

\[ U^m = CU^{m-1} \]

Let

\[
K = \max_i \left\{ \sum_{j=1}^{I} |c_{ij}| \right\} = ||C||_{\infty}
\]

By (9), one has \(K < 1\). Therefore

\[ ||U^m||_{\infty} \leq K||U^{m-1}||_{\infty} \]

which concludes the proof.

**Remark 3.1** In the work of Scarborough [39], criterion (6) is proposed but not actually proved, and in fact condition (7) is proved instead, all without "=". Application of above proposition to (5) provides a proof for the Scarborough criterion, without "=".

**3.2 Condition for convergence**

Consider computation of (3) by iterative, explicit schemes in the two subdomains. Two common explicit schemes will be considered, and the first one reads as \((k = 1, 2)\)

\[
\frac{u_{k+1}^m - u_k^n}{\Delta t} + a_k \frac{u_{k+1}^{m-1} - u_{k-1}^{m-1}}{2\Delta x} = \theta_k \frac{u_{k+1}^{m-1} - 2u_k^m + u_{k-1}^{m-1}}{\Delta x^2} - c_k u_k^{m-1}, \quad (11)
\]
which is iterative and actually the Jacobi iteration [42]. This scheme is simple and slow in convergence, but it permits parallel computation and is in frequent use for practical problems [40, 41]. With this scheme, Schwarz iteration (3) reads as

$$
\begin{cases}
(1 + 2\epsilon_1 + \gamma_1)u_{1i}^m = (\eta_1 + \epsilon_1)u_{1i-1}^{m-1} + (\epsilon_1 - \eta_1)u_{1i+1}^{m-1} + u_{1i}^{n}, & i \leq I - 1; \\
(1 + 2\epsilon_2 + \gamma_2)u_{2i}^m = (\eta_2 + \epsilon_2)u_{2i-1}^{m-1} + (\epsilon_2 - \eta_2)u_{2i+1}^{m-1} + u_{2i}^{n}, & i \geq 2;
\end{cases}
$$

(12)

in which \( \eta_k = a_k \Delta t/(2\Delta x), \epsilon_k = b_k \Delta t/\Delta x^2, \) and \( \gamma_k = \Delta t c_k \) \((k = 1, 2)\). By rearranging terms, iteration (12) can be expressed as (5), in which

\[
A = \begin{bmatrix}
\cdots & \cdots & \cdots \\
1 & s_1 & t_1 \\
1 & s_1 & t_1 \\
| & | & |
\end{bmatrix}, \quad U = \begin{bmatrix}
\cdots \\
\vdots \\
\vdots \\
\cdots \\
\end{bmatrix}, \quad b = \begin{bmatrix}
\cdots \\
\vdots \\
\vdots \\
\cdots \\
\end{bmatrix}
\]

in which \( r_k = -\epsilon_k - \eta_k, s_k = 1 + 2\epsilon_k + \gamma_k, t_k = \eta_k - \epsilon_k \). By Scarborough principle (6), the following is concluded.

**Proposition 3.2** A sufficient condition for iteration (12) to converge is

\[
\max_k \left\{ \frac{|\epsilon_k + \eta_k| + |\eta_k - \epsilon_k|}{|1 + 2\epsilon_k + \gamma_k|} \right\} < 1
\]

(13)

Now, let us discuss if (13) is, or, how to make it satisfied. In view that \( \eta_k = a_k \Delta t/(2\Delta x), \epsilon_k = b_k \Delta t/\Delta x^2, \) and \( \gamma_k = \Delta t c_k, \) it is readily seen that, the LHS of (13) decreases with \( \Delta t, \) and, as \( \Delta t \) becomes sufficiently small, (13) will be guaranteed. Additionally, it is seen that the LHS also decreases with \( \gamma_k. \) Note that the LHS is \( K, \) or, \( ||C||_\infty, \) see (10). In view that \( \rho(C) \leq ||C||_\infty, \) a small value of \( \Delta t \) and a large value of \( \gamma_i \) lead to a smaller \( K \) and thus are helpful to assure the convergence.

The coefficients of the PDEs may be different in the two subdomains. For instance, when \( \epsilon_1, \gamma_1, \gamma_2 = 0, \) the coupling becomes one between an advection equation and an advection-diffusion equation. In this scenario, the LHS becomes

\[
K = \max_k \left\{ \frac{2|\eta_1|}{1 + 2\epsilon_1}, \frac{|\epsilon_2 + \eta_2| + |\eta_2 - \epsilon_2|}{|1 + 2\epsilon_2|} \right\}
\]

which will be less than 1 as along as \( \Delta t \) is sufficiently small, as discussed above. Another scenario is \( \eta_k = 0, \) that is, the problem becomes coupling between two diffusion equations. Because \( \epsilon_k, \gamma_k > 0, \) one has

\[
K = \max_k \left| \frac{2\epsilon_k}{1 + 2\epsilon_k + \gamma_k} \right| < 1
\]

or, (13) holds automatically. Discussion for more scenarios can be made.
Another iterative, explicit algorithm is the so-called artificial compressibility method, which is a main approach used in computation of incompressible flow problems [43, 33]. By this approach, an artificial term is added, and the discretization reads as

\[
\frac{u_{ki}^m - u_{ki}^{m-1}}{\Delta \tau} + \frac{u_{ki}^m - u_{ki}^n}{\Delta t} + a_k \frac{u_{ki+1}^{m-1} - u_{ki-1}^{m-1}}{2\Delta x} = b_k \frac{u_{ki+1}^{m-1} - 2u_{ki}^{m-1} + u_{ki-1}^{m-1}}{\Delta x^2} - \kappa_k u_{ki}^{m-1}
\] (14)

in which \(\Delta \tau\) is a pseudo-time step. At the convergence, the artificial term disappears. While the artificial compressibility method is adopted, the Schwarz iteration becomes

\[
\begin{align*}
&\text{if } i \leq I - 1; \quad \text{then } u_{i}^m = u_{i}^{m-1}, \\
&\text{else } \kappa \eta_{i} \leq \Delta t / \Delta \tau \Rightarrow \text{then } u_{i}^m = (\kappa - 2\epsilon_t - \gamma_1) u_{i}^{m-1} + (\epsilon_t - \eta_1) u_{i+1}^{m-1} + u_{i}^{n}, \\
&\text{else } \kappa \eta_{i} > \Delta t / \Delta \tau \Rightarrow \text{then } u_{i}^m = (\kappa - 2\epsilon_t - \gamma_2) u_{i}^{m-1} + (\epsilon_t - \eta_2) u_{i+1}^{m-1} + u_{i}^{n},
\end{align*}
\] (15)

where \(\kappa = \Delta t / \Delta \tau\). Above can be formulated into form of iteration (8). In this situation, \(C\) is a tri-diagonal matrix, and, from the left to the right in a row, its non-zero elements are \(r_k = (\epsilon_t + \eta_k) / (1 + \kappa), s_k = (\kappa - 2\epsilon_t + \gamma_k)(1 + \kappa), t_k = (\epsilon_t - \eta_k)(1 + \kappa)\), together with \(d = (u_{1}^{n+1}/(1 + \kappa), u_{2}^{n+1}/(1 + \kappa), \ldots, u_{I-1}^{n+1}/(1 + \kappa))\). According to (9), we have the following conclusion.

**PROPOSITION 3.3** A sufficient condition for (15) to converge is

\[
\max_k \left\{ \frac{\epsilon_k + \eta_k}{1 + \kappa} + \frac{\kappa - (2\epsilon_k + \gamma_k)}{1 + \kappa} + \frac{\epsilon_k - \eta_k}{1 + \kappa} \right\} < 1
\] (16)

Now, let us also examine if (16) can be satisfied. Actually, (16) will hold as long as \(\Delta \tau\) is sufficiently small. This is because in this situation, when \(\epsilon_k \geq \eta_k\), its LHS becomes

\[
K = \max_k \left| \frac{\kappa - \gamma_k}{1 + \kappa} \right| < 1
\]

When \(\epsilon_k < \eta_k\), it is easy to check that

\[
K = \max_k \left| \frac{\kappa - (2\epsilon_k - \eta_k) + \gamma_k}{1 + \kappa} \right| < 1
\]

Discussions can be made for more possible scenarios.

### 3.3 Analysis of convergence speed

Convergence speed Introducing relaxation into the interface condition in (12), one has

\[
\begin{align*}
&u_{1i}^m = u_{2i}^{m-1} + \omega_1 (u_{2i}^{m-1} - u_{2i}^{m-1}) \\
u_{2i}^m = u_{1i}^{m-1} + \omega_2 (u_{1i}^{m-1} - u_{1i}^{m-1})
\end{align*}
\]

where \(\omega_1, \omega_2 = \text{consts}\), being the relaxation coefficients. With such an interface condition, the
Jacobi iteration (5) is formulated as (8), in which

\[
C = \begin{bmatrix}
... & ... & ... \\
\cdot & \cdot & \cdot \\
r_1 & 0 & t_1 \\
0 & 0 & 0 \\
\omega_2 r_1 & (1 - \omega_2) & \omega_2 t_3 \\
\end{bmatrix}, \quad U = \begin{bmatrix}
... & ... & ... \\
u_1 & ... & u_I \\
\cdot & ... & \cdot \\
\omega_1 r_2 & (1 - \omega_1) & \omega_1 t_2 \\
0 & 0 & 0 \\
r_2 & 0 & t_2 \\
\omega_2 r_1 & (1 - \omega_2) & \omega_2 t_3 \\
\cdot & ... & \cdot \\
\end{bmatrix}
\]

and \( r_k = (\epsilon_k + \eta_k)/(1 + 2\epsilon_k + \gamma_k), \quad t_k = (\epsilon_k - \eta_k)/(1 + 2\epsilon_k + \gamma_k). \) According to Proposition 3.1, a sufficient condition for convergence is

\[
\max_{k, k'} \left\{ |\omega_k| \left( \frac{\epsilon_{k'} + \eta_{k'}}{1 + 2\epsilon_{k'} + \gamma_{k'}} \right) + \frac{\epsilon_{k'} - \eta_{k'}}{1 + 2\epsilon_{k'} + \gamma_{k'}} + |1 - \omega_k| \right\} < 1
\]

where \( k, k' = 1, 2, \) and \( k \neq k'. \) Note that the LHS becomes the summation of the other rows without \( \omega_k, \omega_{k'} \) in \( C \) when \( \omega_k, \omega_{k'} = 1. \) As discussed above, it is anticipated that the convergence of the iteration may become faster as \( K \) becomes smaller. It is readily checked that \( \partial K/\partial \omega_k < -1, > -1, \) and > 1 when \( \omega_k \leq 0, 0 < \omega_k \leq 1, \) and \( \omega_k > 1, \) respectively. It is expected that \( K \) will have a minimum within \( 0 \leq \omega_k \leq 1, \) and, particularly, at either \( \omega_k = 0, \) or, = 1, which correspond to interface condition \( u_{1m} = u_{2m-1}, \) \( u_{2m} = u_{1m-1} \) and that in (12), respectively.

An a numerical experiment, three cases as shown in Table 1 are computed. The three cases represent typical situations of problem (1). Particularly, Case 1, 2, and 3 involve coupling between two diffusion-dominant equations, between two advection-dominant equations, and between a diffusion-dominant and an advection-dominant equation, respectively. The result is given in Table 2, which shows that spectral radius, \( \rho, \) for \( \omega_k = 1 \) is lower than that for \( \omega_k = 0, \) exhibiting a faster convergence.

| Case | \( a_1 \) | \( b_1 \) | \( c_1 \) | \( a_2 \) | \( b_2 \) | \( c_2 \) |
|------|------|------|------|------|------|------|
| 1    | 0.01 | 0.5  | 0.0  | 0.01 | 0.5  | 0.0  |
| 2    | 0.5  | 0.002| 0.0  | 0.25 | 0.001| 0.0  |
| 3    | 0.25 | 0.01 | 0.25 | -0.25| 0.01 | 0.5  |

Table 2: Spectral radii of the Jacobi iteration associated with the relaxation interface condition. (I,J)=(40,80).

| Case | \( \omega_1, \omega_2 = 0 \) | \( \omega_1, \omega_2 = 1 \) |
|------|-----------------|-----------------|
| 1    | 0.967363        | 0.966594        |
| 2    | 0.267145        | 0.197162        |
| 3    | 0.431927        | 0.359324        |

Now, let us consider the convergence of artificial compressibility method (15) in association with different values for \( \kappa. \) For above three cases, \( K, \) together with \( \rho, \) at different values of \( \kappa \) are plotted.
in Fig. 2. It is seen that in all of the three cases, $K$ takes a smallest value at $\omega_k = 1$. Additionally, $K$ is a good indicator for the value of $\rho$, and both of them take lowest values at about a same $\kappa$. Therefore, in practical computation, choosing a value of $\kappa$ at the smallest $K$ tends to lead to a smallest $\rho$, which corresponds to the fast convergence speed.

![Figure 2: Correlation of $K$ and $\rho$ in the artificial compressible method. a) Case 1. b) Case 2. c) Case 3.](image)

Dependence of convergence speed on grid spacing and time step Earlier studies at the continuous or semi-continuous levels conclude that, for waveform relaxation methods, convergence rates deteriorate as grid spacing decrease, e.g., [13]. Let us look into the convergence speed and start with two identical equations in subdomains. It is seen in above that the iteration matrices for the Jacobi method and the artificial compressibility method are tridiagonal. For an $N \times N$ tridiagonal matrix with elements $p_{-1}$, $p_0$, $p_1$, its eigenvalues read as [44]

$$\lambda_i = p_0 - 2 \cos \left( \frac{i \pi}{N+1} \right) \sqrt{p_{-1} p_1}, \quad i = 1, 2, ..., N$$  (17)
by which, the spectral radius of the Jacobi method becomes

$$\rho = 2\cos\left(\frac{N\pi}{N+1}\right) \frac{\sqrt{\epsilon_k^2 - \eta_k^2}}{1 + 2\epsilon_k + \gamma_k}$$

Let $\epsilon_k = \text{const}$ and $\epsilon_k \geq \eta_k$, the latter of which is always true when grid spacing is sufficiently small. Then, as $\Delta t, \Delta x$ decrease, the term of “cos” increases, and $\eta_k$ and $\gamma_k$ decreases, leading to increase in the term of fraction. As a result, $\rho$ increases monotonically as $\Delta t, \Delta x$ decrease, and this is what concluded in the literature [9], also shown in Case 1 and 3 in Fig. 3a. However, this is not the situation in some scenarios. For instance, if $\eta_k = \text{const}$ and $\epsilon_k < \eta_k$, as the mesh gets finer, the term of fraction does not increase or even decreases, and this may lead to no increase on even a decrease in the spectral radius. A numerical example is Case 2 in the figure. This indicates that in this situation, the spectral radius, or, the convergence speed, is scalable with mesh resolution. Note that the radius may increase again at much finer grids. Similar discussion may be made for the artificial compressibility method, for which the spectral radius becomes

$$\rho = \frac{\kappa - (2\epsilon_k + \gamma_k)}{1 + \kappa} + \frac{2}{1 + \kappa} \cos\left(\frac{N\pi}{N+1}\right) \sqrt{\frac{\epsilon_k^2 - \eta_k^2}{\kappa^2}}$$

Again, the spectral radius may be scalable in terms of grid spacing when $\kappa$ takes certain values, and numerical examples are shown in Fig. 3b.

Figure 3: Spectral radius at different mesh resolution. Subscripts for $K$ and $\rho$ indicate the case numbers. $N = I + J - 4$, $I$ and $J$ are the number of grid nodes in subdomain 1 and 2, respectively. \( (I, J) = (10, 10), (10, 20), (20, 20), (20, 40), (40, 40), (40, 80), (80, 80), (80, 160), (160, 160). \) $\Delta t/\Delta x = 0.5$. a) The Jacobi method. b) The compressibility method. $\kappa = 59.25, 0.19,$ and 1.19 for Case 1, 2, and 3, respectively.

**Outer and inner iteration** If an iterative scheme is adopted in the subdomains, two types of iteration are involved when marching from time level $n$ to $n + 1$: one is the iteration within subdomains, referred to as the inner iteration, and the other is the Schwarz iteration between them, called the outer iteration. Such a situation is commonly encountered in computation of
Table 3: Computational load with different combinations of the inner and outer iteration. ‘1:1’, means after one outer iteration, one inner iteration is made, and ‘conver.’ indicates that after one outer iteration, inner iteration keeps going until convergence. The computational load is defined as the times of computation in each subdomain, or, the total number of times of inner iteration in each subdomain, together with convergence tolerance of $10^{-12}$.

| Case | 1:1 | 1:5 | 1:15 | conver. |
|------|-----|-----|------|---------|
| 1    | 8   | 43  | 102  | 131     |
| 2    | 8   | 43  | 111  | 147     |
| 3    | 8   | 43  | 115  | 152     |

realistic problems, e.g., [12]. To illustrate the computation, Jacobi iteration (12) is modified as

\[
\begin{aligned}
(1 + 2\epsilon_1 + \gamma_1)u_{1i}^l &= (\eta_1 + \epsilon_1)u_{1i}^{l-1} + (\epsilon_1 - \eta_1)u_{1i+1}^{l-1} + u_{1i}^n, \quad l = 1, 2, \ldots L; \quad i \leq I - 1; \\
(1 + 2\epsilon_2 + \gamma_2)u_{2i}^l &= (\eta_2 + \epsilon_2)u_{2i}^{l-1} + (\epsilon_2 - \eta_2)u_{2i+1}^{l-1} + u_{2i}^n, \quad l = 1, 2, \ldots L; \quad i \geq 2;
\end{aligned}
\]

in which $l$ is the inner iteration index, and $m$ is the outer iteration index. After inner iteration fully converges, $u_{1i}^1 \to u_{1i}^m$, $u_{2i}^1 \to u_{2i}^m$. Similar formulation can also be made for the artificial compressibility method. A natural question in computation of (18) will be how to arrange the inner and outer iteration to achieve fast convergence, or, after how many times of inner iteration an outer iteration should be started to achieve a minimal count of computational load.

It is not straightforward to theoretically answer the above question, and a numerical experiment is made to achieve a preliminary understanding. Particularly, computation is made for the three cases in Table 1 in association with the following initial and boundary conditions

\[
g(x) = -\sin(\pi x), \quad t = 0; \quad u_1 = 0, \quad x = -1, \quad u_2 = 0, \quad x = 1
\]

In the experiment, the corresponding conditions for convergence, i.e., (13) and (16), are satisfied. Also, the computation starts the outer iteration after every 1, 5, and 15 times of the inner iteration, and also after complete convergence of the inner iteration. The results are presented in Table 3. Note that in the computation, for each case, the difference in computational load mainly comes from the numbers of inner iteration, while its number of outer iteration remains about the same. The table shows that the earlier to start the outer iteration, the smaller the amount of computational load. More particularly, the 1:1 strategy is the best; the computation that starts an outer iteration after every inner iteration spends the least amount of computational load.

4. Implicit scheme

4.1 Convergence speed

An implicit scheme to compute (2) in the subdomains reads as

\[
\frac{u_{ki}^m - u_{ki}^n}{\Delta t} + a_k \frac{u_{ki+1}^m - u_{ki-1}^m}{2\Delta x} = b_k \frac{u_{ki+1}^m - 2u_{ki}^m + u_{ki-1}^m}{\Delta x^2} - c_k u_{ki}^m
\]
Together with the interface condition, the computation can be formulated as

\[
\begin{align*}
(\eta_1 + \epsilon_1)u_{1i}^m &+ (1 + 2\epsilon_1 + \gamma_1)u_{1i}^{m+1} + (\epsilon_1 - \eta_1)u_{1i}^{m+1} + u_{i}^m, & i \leq I - 1; \\
(\eta_2 + \epsilon_2)u_{2i}^m &+ (1 + 2\epsilon_2 + \gamma_2)u_{2i}^{m+1} + (\epsilon_2 - \eta_2)u_{2i}^{m+1} + u_{2i}^m, & i \geq 2;
\end{align*}
\]

(21)

The computation in each subdomain needs to solve a linear system. At convergence, \(u_1^m\) and \(u_2^m\) become \(u_1^{n+1}\) and \(u_2^{n+1}\), respectively. In terms of residual, i.e., \(e_1^m = u_1^m - u_1^{n+1}\) and \(e_2^m = u_2^m - u_2^{n+1}\), above computation becomes

\[
\begin{align*}
-(\eta_1 + \epsilon_1)e_{1i}^m &+ (1 + 2\epsilon_1 + \gamma_1)e_{1i}^{m+1} - (\eta_1 - \epsilon_1)e_{1i}^{m+1} = 0, & i \leq I - 1; \\
-(\eta_2 + \epsilon_2)e_{2i}^m &+ (1 + 2\epsilon_2 + \gamma_2)e_{2i}^{m+1} - (\eta_2 - \epsilon_2)e_{2i}^{m+1} = 0, & i \geq 2;
\end{align*}
\]

(22)

Let us derive the convergence speed by the induction method. We start from the situation in which the both subdomains have only three grid nodes and overlap at two grids, that is, a subdomain has one boundary node, an internal node, and an interface node:

\[
\begin{align*}
(1 + 2\epsilon_1 + \gamma_1)e_{12}^m &+ (\eta_1 - \epsilon_1)e_{13}^{m+1} = 0, & e_{13}^m = e_{22}^{m-1}, \\
-(\eta_2 + \epsilon_2)e_{21}^m &+ (1 + 2\epsilon_2 + \gamma_2)e_{22}^{m+1} = 0, & e_{21}^m = e_{12}^{m-1}
\end{align*}
\]

In above, without loss of generality (e.g., \(g(x)\) in (1) has a finite support), \(e_{11}^m, e_{23}^m = 0\) are used. By substitution of the interface conditions and change of index \(m\), above two equations become

\[
\begin{align*}
(1 + 2\epsilon_1 + \gamma_1)e_{12}^m &+ (\eta_1 - \epsilon_1)e_{22}^{m-1} = 0, \\
-(\eta_2 + \epsilon_2)e_{21}^m &+ (1 + 2\epsilon_2 + \gamma_2)e_{22}^{m-1} = 0
\end{align*}
\]

which lead to

\[
\tilde{\rho} = \frac{(\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{(1 + 2\epsilon_1 + \gamma_1)(1 + 2\epsilon_2 + \gamma_2)}
\]

where \(\tilde{\rho} = e_{12}^m / e_{12}^{m-2}\), being a convergence speed, or, precisely, the contraction factor, of the iteration. Similarly, one obtains the above convergence speed when \(\tilde{\rho} = e_{22}^m / e_{22}^{m-2}\).

Now let us consider the situation in which subdomain 1 and 2 have four and three nodes, respectively. In this situation, one has

\[
\begin{align*}
(1 + 2\epsilon_1 + \gamma_1)e_{12}^m &+ (\eta_1 - \epsilon_1)e_{13}^m = 0, \\
-(\eta_1 + \epsilon_1)e_{13}^m &+ (1 + 2\epsilon_1 + \gamma_1)e_{13}^m + (\eta_1 - \epsilon_1)e_{14}^m = 0, & e_{14}^m = e_{22}^{m-1}, \\
-(\eta_2 + \epsilon_2)e_{21}^m &+ (1 + 2\epsilon_2 + \gamma_2)e_{22}^m = 0, & e_{21}^m = e_{13}^{m-1}
\end{align*}
\]

Again, by substitution of interface conditions, elimination of \(e_{12}^m\), and change of index \(m\), the last two equations become

\[
\begin{align*}
(1 + 2\epsilon_1 + \gamma_1 + \frac{\eta_1 - \epsilon_1}{1 + 2\epsilon_1 + \gamma_1})e_{13}^m + (\eta_1 - \epsilon_1)e_{22}^{m-1} = 0, \\
-(\eta_2 + \epsilon_2)e_{13}^{m-2} + (1 + 2\epsilon_2 + \gamma_2)e_{22}^{m-1} = 0
\end{align*}
\]
which lead to
\[ \tilde{\rho} = \frac{(\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{(1 + 2\epsilon_1 + \gamma_1 + \frac{\eta_1^2 - \epsilon_1^2}{1 + 2\epsilon_1 + \gamma_1})(1 + 2\epsilon_2 + \gamma_2)} \]

where \( \tilde{\rho} = \frac{\eta_1 m}{\epsilon_1 m - 2}. \) Similarly, in above derivation, instead of \( \frac{\eta_1 m}{\epsilon_1 m - 2}, \) elimination of \( \frac{\eta_2 m}{\epsilon_2 m - 2} \) yields

\[ (1 + 2\epsilon_1 + \gamma_1 + \frac{\eta_1^2 - \epsilon_1^2}{1 + 2\epsilon_1 + \gamma_1})(1 + 2\epsilon_1 + \gamma_1) = 0 \]

which lead to above expression for \( \tilde{\rho}, \) too, but in association with \( \tilde{\rho} = \frac{\eta_1 m}{\epsilon_1 m - 2}. \) Additionally, the same can be derived when \( \tilde{\rho} = \frac{\eta_2 m}{\epsilon_2 m - 2}. \) Continuation of above derivation to larger numbers of nodes in the two grids, the following is concluded by induction.

**Proposition 4.1** The contraction factor of computation (22) is a recursive expression:

\[ \tilde{\rho} = \frac{(\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{R_1(I - 2)R_2(2)} \] (23)

where \( \tilde{\rho} = \frac{\eta_1 m}{\epsilon_1 m - 2}, \frac{\eta_2 m}{\epsilon_2 m - 2} \) and

\[
R_1(i) = 1 + 2\epsilon_1 + \gamma_1 + \frac{\eta_1^2 - \epsilon_1^2}{R_1(i - 1)}; \quad i = 3, \ldots, I - 1; \quad R_1(2) = 1 + 2\epsilon_1 + \gamma_1 \\
R_2(j) = 1 + 2\epsilon_2 + \gamma_2 + \frac{\eta_2^2 - \epsilon_2^2}{R_2(j + 1)}; \quad j = J - 2, \ldots, 2; \quad R_2(J - 1) = 1 + 2\epsilon_2 + \gamma_2 
\] (24)

in which \( I, J \geq 3. \)

In order to validate the derived convergence rate (23), a numerical experiment is made in computation of the three cases in Table 1 in conjunction with initial and boundary conditions (19). The theoretical contraction factor from (23) and numerical one computed directly from the solutions of the experiment are listed in Table 4, which shows that the two factors are basically identical, validating the derived one.

**Table 4:** Theoretical and numerical convergence speeds. \((I, J) = (40, 80), \Delta t, \Delta x = 0.0171.\)

| Cases | \( \rho_{\text{theo}} \) | \( \rho_{\text{num}} \) |
|-------|----------------|----------------|
| 1     | 0.691235       | 0.691197       |
| 2     | -0.017007      | -0.017007      |
| 3     | 0.082962       | 0.082962       |

**Remark 4.1** Contraction factor in (23) is defined at a grid node, and it is the same at all nodes. On this basis, it is readily seen that such factor is actually the global convergence speed, e.g., \( \tilde{\rho} = \| e_{1i}^m \|_2 / \| e_{1i}^{m-2} \|_2. \)
4.2 Optimal interface condition

In order to speed up convergence in computation of (21), the following optimal interface condition is adopted:

\[
\begin{align*}
(\bar{u}_1^m - u_{1 I-1}^m) + \alpha u_1^m &= (\bar{u}_2^m - u_{2 I-1}^m) + \alpha u_2^m \\
(\bar{u}_2^m - u_{1 I-1}^m) + \beta u_2^m &= (\bar{u}_1^m - u_{1 I-1}^m) + \beta u_1^m
\end{align*}
\]

(25)

in which \(\alpha, \beta = c o n s t s.\) Such optimal interface condition was first proposed for waveform relaxation of circuit problems by Gander et al., and it was effective in speeding up the convergence [45]. They show that, if \((\alpha + 1)(\beta - 1) + 1 \neq 0,\) the optimal interface condition recovers to the classic condition, i.e., the interface condition in (21), at convergence as \(m \rightarrow \infty.\) Also, obviously, the optimal condition returns to the classic condition as \(\alpha, \beta \rightarrow \infty.\)

With the optimal interface condition, (22) is modified as

\[
\begin{align*}
&\begin{cases}
-(\eta_1 + \epsilon_1)e_{1 I-1}^m + (1 + 2\epsilon_1 + \gamma_1)e_{1 I}^m - (\eta_1 - \epsilon_1)e_{1 I+1}^m = 0, &i \leq I - 1 \\
(\epsilon_1^m - \epsilon_{I-1}^m) + \alpha e_1^m = (\epsilon_{2 I-1}^m - \epsilon_{2 I}^m) + \alpha e_{2 I-1}^m \\
(\eta_2 + \epsilon_2)e_{2 I-1}^m + (1 + 2\epsilon_2 + \gamma_2)e_{2 I}^m - (\eta_2 - \epsilon_2)e_{2 I+1}^m = 0, &i \geq 2 \\
(\epsilon_2^m - \epsilon_{2 I}^m) + \beta e_2^m = (\epsilon_{1 I-1}^m - \epsilon_{1 I}^m) + \beta e_{1 I-1}^m
\end{cases}
\end{align*}
\]

(26)

The convergence speed for computation of (26) can be derived by following the same method and steps adopted to those in computation of (22), and this is based on a fact that the grid nodes involved in the former are exactly same as those in the latter. The derived results are summarized as follows.

**Proposition 4.2** The contraction factor in computation of (26) is

\[
\bar{\rho} = - \frac{(\alpha + 1)(\eta_2 + \epsilon_2) - R_2(2)}{(\alpha + 1)R_1(I-1) + \eta_1 - \epsilon_1} \cdot \frac{(\beta - 1)(\eta_1 - \epsilon_1) - R_1(I-1)}{(\beta - 1)R_2(2) + \eta_2 + \epsilon_2}
\]

(27)

in which \(I, J \geq 3.\)

In expression (27), letting the numerators be zero while keeping denominators be non-zero leads to zero contraction factor, i.e., \(\bar{\rho} = 0,\) and the following optimal \(\alpha\) and \(\beta:\n
\[
\alpha = \frac{R_2(2)}{\eta_2 + \epsilon_2} - 1, \quad \beta = \frac{R_1(I-1)}{\eta_1 - \epsilon_1} + 1
\]

(28)

together with condition \(R_1(I-1)R_2(2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2) \neq 0.\) From (27) and (28), it is derived that

\[
\begin{align*}
\frac{\partial \bar{\rho}}{\partial \alpha} &= - \frac{R_1(I-1)R_2(2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{(\alpha + 1)(\eta_2 + \epsilon_2) - R_2(2)} \cdot \frac{(\beta - 1)(\eta_1 - \epsilon_1) - R_1(I-1)}{[(\beta - 1)R_2(2) + (\eta_2 + \epsilon_2)]^2} \\
\frac{\partial \bar{\rho}}{\partial \beta} &= - \frac{R_1(I-1)R_2(2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{(\alpha + 1)R_1(I-1) + (\eta_1 - \epsilon_1)} \cdot \frac{R_1(I-1)R_2(2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}{[(\beta - 1)R_2(2) + (\eta_2 + \epsilon_2)]^2}
\end{align*}
\]
additionally,
\[ \frac{\partial^2 \bar{\rho}}{\partial \alpha^2} = \frac{2 R_1 (I-1) [R_1 (I-1) R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)]}{(\beta - 1)(\eta_1 - \epsilon_1) - R_1 (I-1)}, \]
\[ \frac{\partial^2 \bar{\rho}}{\partial \beta^2} = \frac{(\alpha + 1) (\eta_2 + \epsilon_2) - R_2 (2)}{(\alpha + 1) R_1 (I-1) + (\eta_1 - \epsilon_1)} \cdot \frac{2 R_2 (2) [R_1 (I-1) R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)]}{[\beta - 1] R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)}, \]
\[ \frac{\partial^2 \bar{\rho}}{\partial \alpha \partial \beta} = \frac{(\alpha + 1) R_1 (I-1) + (\eta_1 - \epsilon_1)}{[\beta - 1] R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)} \cdot \frac{[(\beta - 1) R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)]^2}{[(\beta - 1) R_2 (2) + (\eta_1 - \epsilon_1)(\eta_2 + \epsilon_2)]^2}. \]

Under conditions (28), it is readily verified that
\[ \frac{\partial \bar{\rho}}{\partial \alpha} = 0, \quad \frac{\partial \bar{\rho}}{\partial \beta} = 0, \]
\[ \frac{\partial^2 \bar{\rho}}{\partial \alpha^2} = 0, \quad \frac{\partial^2 \bar{\rho}}{\partial \beta^2} = 0, \quad \frac{\partial^2 \bar{\rho}}{\partial \alpha \partial \beta} \neq 0. \]

As a result, one has
\[ \frac{\partial^2 \bar{\rho}}{\partial \alpha^2} \frac{\partial^2 \bar{\rho}}{\partial \beta^2} - \left( \frac{\partial^2 \bar{\rho}}{\partial \alpha \partial \beta} \right)^2 < 0. \]

With above, it is known that \((\alpha, \beta)\) given by (28) is a saddle point of \(\bar{\rho}\) [46]. All above proves the following theorem.

**THEOREM 4.1** At the optimal value of \((\alpha, \beta)\) given in (28), the contraction factor (27) is zero. Moreover, the optimal value of \((\alpha, \beta)\) is a saddle point of \(\bar{\rho}\).

**Remark 4.2** Actually, contraction factor (27) becomes zero when either \(\alpha\) takes the value in (28), regardless that of \(\beta\), or, \(\beta\) takes the value in (28), regardless that of \(\alpha\). Also, the zero contraction factor occurs only when \((\alpha, \beta)\) are given as (28).

**Remark 4.3** The past work is at the continuous or semi-continuous level, and its optimal values for \((\alpha, \beta)\) can only be derived in a transformed space. As a result, search and approximation for them at the algebraic level have to be made in actual computation, e.g., [37]. As a distinct feature in this study, the optimal \((\alpha, \beta)\) can be directly computed by (28), without any approximation. Therefore, the derived theoretical convergence speed exactly matches that in practical computation, as shown in the following numerical examples.

Again, a numerical experiment is made on the three cases in Table 1 with initial and boundary conditions (19), and the results are shown in Table 5. The table shows that, at the optimal values for \((\alpha, \beta)\), the numerical contraction factors in the numerical solutions are very small or almost zeros. The result that these factors are not zeros exactly, as the theoretical values, is contributed to the lack of enough accuracy in the computer. Calculations indicate that the value of \(\bar{\rho}\) is subtle to the values of \(\alpha\) and \(\beta\), or, enough digits should be kept in calculation of (28) to achieve zero for a contraction factor. In order to directly illustrate the effectiveness of the optimal interface condition, the convergence residuals in the experiment are shown in Fig. 4a. The figure shows that, in comparison to the classic condition, the optimal condition greatly speeds up the convergence. In view that the contraction factor is the ratio of residual between two subsequent times of iteration, a zero convergence factor implies that convergence will be achieved with no more than two times of convergence. The figure shows that indeed the convergence is achieved in about two times of
iteration. Moreover, Fig. 4b illustrates a distribution of the contraction factor on the \(\alpha-\beta\) plane, and it clearly shows that the values of \(\alpha\) and \(\beta\) given by (28) is a saddle point.

Table 5: Optimal \((\alpha, \beta)\) and convergence speed. \((I,J)=(40,80), \Delta t, \Delta x = 0.017.\)

| Cases | \(\alpha\) | \(\beta\) | \(\rho_{num}\) |
|-------|-----------|-----------|---------------|
| 1     | 2.02577\times 10^{-1}, -2.02988\times 10^{-1} | 1.31\times 10^{-14} |
| 2     | 5.14615\times 10^{0}, 1.05666\times 10^{1} | -6.12\times 10^{-15} |
| 3     | 1.74955\times 10^{0}, -3.38389\times 10^{0} | 0 |

Figure 4: Computation with optimal interface condition. a) Convergence processes. b) Contraction factor. Case 1, \((I,J)=(40,80).\)

5. Extension to Burgers’ equation

5.1 Explicit scheme

Consider the coupling between two viscous Burgers’ equations with reaction terms. Now the discretization (2) becomes

\[
\frac{u_{ki,n+1} - u_{ki,n}}{\Delta t} + u_{ki,n+1} \frac{u_{ki,n+1} - u_{ki,n+1}}{2\Delta x} = b_k \frac{u_{k+1,n+1} - 2u_{ki,n+1} + u_{ki,n+1}}{\Delta x^2} - c_k u_{ki,n+1},
\]

which can be computed with an extension of (11), i.e., the Jacobi method for the linear advection-diffusion-reaction equation, particularly, by letting its \(a_k\) be replaced by \(u_{ki,m-1}\). With such an extension, computation of above discretization in association with the classic interface condition leads to an explicit algorithm

\[
\begin{align*}
(1 + 2\epsilon_1 + \gamma_1)u_{1m} &= (\eta_1 m - 1 + \epsilon_1)u_{1m-1} + (\epsilon_1 - \eta_1 m - 1)u_{1m+1} + u_{1m}, \quad i \leq I - 1; \\
\end{align*}
\]

\[
\begin{align*}
(1 + 2\epsilon_2 + \gamma_2)u_{2m} &= (\eta_2 m - 1 + \epsilon_2)u_{2m-1} + (\epsilon_2 - \eta_2 m - 1)u_{2m+1} + u_{2m}, \quad i \geq 2;
\end{align*}
\]
A difference of above iteration from the previous iteration is that now the value of \( \eta \) becomes solution dependent. In order to analyze above iteration, linearization is made by replacing its \( \eta_{k_i}^{m-1} \) with \( \eta_{k_i}^n = \Delta t u_{k_i}^n/(2\Delta x) \) \((k = 1, 2)\). As a result, the iteration between the two time levels can be formulated in form of (12) with \( \eta_k \) be replaced by \( \eta_{k_i}^n \), and the associated coefficient matrix \( A \) remains constant during the iteration while marching from time level \( n \) to \( n + 1 \). According to the Scarborough criterion, the following conclusion is achieved (Note that LHS is not a constant but changes with \( i, n \)).

**Proposition 5.1** A sufficient condition for the linearized version of (30) to converge is

\[
\max_{i,k} \left\{ \frac{|\epsilon_k + \eta_{k_i}^n| + |\eta_{k_i}^n - \epsilon_k|}{|1 + 2\epsilon_k + \gamma_k|} \right\} < 1
\]

(31)

Discretization (29) can also be computed using the artificial compressibility method, and this is realized by replacing \( a_k \) with \( u_{k_i}^{m-1} \) in (14). Consequently, method (15) is extended as

\[
\begin{align*}
(1 + \gamma)u_{1i}^m &= (\eta_{i}^{m-1} + \epsilon_1)u_{1i}^{m-1} + (\kappa - 2\epsilon_1 - \gamma_1)u_{1i}^{m-1} + (\epsilon_1 - \eta_{i}^{m-1})u_{1i}^{m-1} + u_{1i}^n, \\
& \quad i \leq I - 1; \ u_{1i}^m = u_{2i}^m \\
(1 + \gamma)u_{2i}^m &= (\eta_{i}^{m-1} + \epsilon_2)u_{2i}^{m-1} + (\kappa - 2\epsilon_2 - \gamma_2)u_{2i}^{m-1} + (\epsilon_2 - \eta_{i}^{m-1})u_{2i}^{m-1} + u_{2i}^n, \\
& \quad i \geq 2; \ u_{2i}^m = u_{2i}^{m-1}
\end{align*}
\]

(32)

By linearization to replace \( \eta_{k_i}^{m-1} \) with \( \eta_{k_i}^n \) \((k = 1, 2)\) and with a similar discussion, the following is obtained.

**Proposition 5.2** A sufficient condition for the linearized version of (32) to converge is

\[
\max_{i,k} \left\{ \frac{|\epsilon_k + \eta_{k_i}^n|}{1 + \kappa} + \left| \frac{\kappa - (2\epsilon_k + \gamma_k)}{1 + \kappa} \right| + \left| \frac{\epsilon_k - \eta_{k_i}^n}{1 + \kappa} \right| \right\} < 1
\]

(33)

The analysis for computation of (30) and (32) can be made similarly as in Section 3.3 for the linear advection-diffusion-reaction equations. As an illustration of the analysis, numerical experiments are made on four cases in Table 6. Case 4 and 5 are respectively diffusion and advection dominated, respectively, and Case 6 and 7 are a combination of them. Initial and boundary conditions in (19) are used in Case 4 and 7. For case 5 and 6, the initial condition becomes piecewise: \( g(x) = 1, x \in [-0.5, 0.5], \ g(x) = 0, x \in [-1, -0.5), (0.5, 1] \).

| Cases | \( b_1 \) | \( c_1 \) | \( b_2 \) | \( c_2 \) |
|-------|-----------|-----------|-----------|-----------|
| 4     | 0.5       | 0.0       | 0.5       | 0.0       |
| 5     | 0.02      | 2.0       | 0.02      | 3.0       |
| 6     | 0.1       | 0.2       | 0.2       | 0.1       |
| 7     | 0.5       | 0.0       | 0.51      | 0.0       |

Table 7 presents the values for LHS of (31) and (33), together with those for the spectral radii. It is seen that when these two conditions are satisfied, all radii are less than 1, and thus convergence in these linearized versions of (30) and (32) is guaranteed. Noted that since the equations become nonlinear, particularly, in general, \( \eta_{k_i}^n \) changes with solutions, and its values are distinct at different
time steps. To illustrate this, results at three moments in time are presented in the table. In computation of (32), effects of $\kappa$ on $K$ and $\rho$ are plotted in Fig. 5. Again, it is seen that the value of $\kappa$ corresponding to the lowest $K$ is a good approximation of its value for the lowest $\rho$, which results in the fastest convergence.

Table 7: LHS of (31) and (33), and corresponding spectral radius. $(I,J) = (10,20)$, $\Delta t, \Delta x = 0.0741$. For the artificial compressibility method, $\kappa = 1.350, 0.069, 0.542$, and $1.378$ are used in Case 4, 5, 6, and 7, respectively. These values of $\kappa$ correspond to the lowest values of $K$, as shown in Fig. 5.

| Time     | Method, Case | 0.074 | 0.222 | 0.370 |
|----------|--------------|-------|-------|-------|
|          |              | $K$   | $\rho$| $K$   | $\rho$|
| Jacobi, 4| 0.574468     | 0.558299| 0.574468| 0.566377| 0.574468| 0.568848|
| Jacobi, 5| 0.080057     | 0.055298| 0.057561| 0.041587| 0.050176| 0.044854|
| Jacobi, 6| 0.350481     | 0.340231| 0.350481| 0.342112| 0.350481| 0.343251|
| Jacobi, 7| 0.574468     | 0.572429| 0.574468| 0.573695| 0.574468| 0.574239|
| Artificial, 4 | 0.574468 | 0.568429| 0.574468| 0.569622| 0.574468| 0.570135|
| Artificial, 5 | 0.081437 | 0.054665| 0.058767| 0.047987| 0.051325| 0.041229|
| Artificial, 6 | 0.635802 | 0.623317| 0.635802| 0.625591| 0.635802| 0.626952|
| Artificial, 7 | 0.597447 | 0.589117| 0.597447| 0.590465| 0.597447| 0.591051|

Lastly, let us look into the issue of inner and outer iteration, and extend Jacobi iteration (18) by replacing $\eta_k$ with $\eta_{k-1}$. The results of computation for the cases in Table 6 are presented in Table 8, and they show a same trend observed in the linear advection-diffusion-reaction equations. Particularly, the earlier to start the outer iteration, the smaller the computational load, or, the quicker the overall convergence. The smallest computational load occurs at the 1:1 strategy. Therefore, an understanding is that the 1:1 strategy leads to the fastest convergence in the examples of this paper, regardless the equations are linear or nonlinear. Such a strategy has been used in practical problems [12].

Table 8: Computational load associated with different combinations of the inner and outer iteration, for the Burgers equations, together with convergence tolerance of $10^{-12}$, at $t = 0.170$.

| Case No. | 1:1 | 1:5 | 1:15 | conver. |
|----------|-----|-----|------|---------|
| 4        | 7   | 63  | 72   | 120     |
| 5        | 9   | 70  | 86   | 132     |
| 6        | 8   | 66  | 78   | 125     |
| 7        | 7   | 62  | 72   | 120     |

5.2 Implicit scheme

Now consider computation of discretization (29) by an implicit scheme, and this is realized by replacing its $a_k$ with $u_{k-1}^m$ in scheme (20). With such modification, the computational problem
Figure 5: Correlation of $K$ and $\rho$ in the artificial compressible method for the Burgers equations. Subscript 1, 2, and 3 indicate $t=0.074$, 0.222, and 0.370, respectively. 
a) Case 4. b) Case 5. c) Case 6. d) Case 7.

becomes

$$
\begin{align*}
&\begin{cases}
\eta_1^{m-1} + \epsilon_1)u_1^{m-1} + (1 + 2\epsilon_1 + \gamma_1)u_1^m + (\epsilon_1 - \eta_1^{m-1})u_1^{m+1} + u_1^n, \quad i \leq I - 1; \\
\eta_2^{m-1} + \epsilon_2)u_2^{m-1} + (1 + 2\epsilon_2 + \gamma_2)u_2^m + (\epsilon_2 - \eta_2^{m-1})u_2^{m+1} + u_2^n, \quad i \geq 2;
\end{cases}
\end{align*}
$$

which requires to solve linear systems in subdomains at each iteration over $m$.

Let us analyze computation of (34) by linearization with $\eta_1^{m-1}$ and $\eta_2^{m-1}$ being replaced by $\eta_1^n$ and $\eta_2^n$, respectively. As a result, (34) becomes similar to (21), and the difference is that in the former that $\eta_k$ is not a constant but dependent on solution at grid nodes. Luckily, following the methods for derivation of (23), still a contraction factor can be derived with discretion on terms with $\eta_1^n$ and $\eta_2^n$. For the purpose of illustration, consider the situation in which subdomain 1 and
2 have four and three nodes, respectively. In this situation, one has

\[(1 + 2\epsilon_1 + \gamma_1)\epsilon_{12}^m + (\eta_{12}^n - \epsilon_1)\epsilon_{13}^m = 0,
- (\eta_{13}^n + \epsilon_1)\epsilon_{12}^m + (1 + 2\epsilon_1 + \gamma_1)\epsilon_{13}^m + (\eta_{13}^n - \epsilon_1)\epsilon_{14}^m = 0,
- (\eta_{22}^n + \epsilon_2)\epsilon_{21}^m + (1 + 2\epsilon_2 + \gamma_2)\epsilon_{22}^m = 0\]

Then, it is derived that

\[\epsilon_{14}^m = \epsilon_{22}^{m-1}, \quad \epsilon_{21}^m = \epsilon_{13}^{m-1}\]

By substitution of the interface condition, elimination of \(\epsilon_{12}^m\), and change of index \(m\), the last two equations become

\[
(1 + 2\epsilon_1 + \gamma_1 + (\eta_{12}^n - \epsilon_1)(\eta_{13}^n + \epsilon_1))(\eta_{13}^n - \epsilon_1)\epsilon_{22}^{m-1} = 0
- (\eta_{22}^n + \epsilon_2)\epsilon_{13}^{m-2} + (1 + 2\epsilon_2 + \gamma_2)\epsilon_{22}^{m-1} = 0
\]

Then, it is derived that

\[
\bar{\rho} = \frac{(\eta_{13}^n - \epsilon_1)(\eta_{22}^n + \epsilon_2)}{(1 + 2\epsilon_1 + \gamma_1 + (\eta_{13}^n - \epsilon_1)(\eta_{13}^n + \epsilon_1))(1 + 2\epsilon_2 + \gamma_2)}
\]

where \(\bar{\rho}^n = \epsilon_{13}^m/\epsilon_{13}^{m-2}\). By mathematical induction, the following recursive formula is concluded for a general situation:

**Proposition 5.3** The contraction factor for computing the linearized Burgers equations, (34), is

\[
\bar{\rho} = \frac{(\eta_{13}^n - \epsilon_1)(\eta_{22}^n + \epsilon_2)}{R_1(I - 1)R_2(2)}
\]

where \(\bar{\rho} = \epsilon_{ki}^m/\epsilon_{ki}^{m-2}\) \((k = 1, 2)\), and

\[
R_1(i) = 1 + 2\epsilon_1 + \gamma_1 + \frac{(\eta_{13}^n - \epsilon_1)(\eta_{13}^n + \epsilon_1)}{R_1(i - 1)}; \quad i = 3, ..., I - 1, \quad R_1(2) = 1 + 2\epsilon_1 + \gamma_1
R_2(j) = 1 + 2\epsilon_2 + \gamma_2 + \frac{(\eta_{22}^n - \epsilon_2)(\eta_{22}^n + \epsilon_2)}{R_2(j + 1)}; \quad j = J - 2, ..., 2, \quad R_2(J - 1) = 1 + 2\epsilon_2 + \gamma_2
\]

in which \(I, J \geq 3\).

From (35), it is seen that the contraction factor is the same in the two subdomains and at all grid nodes. However, the factor is related to \(\eta_{13}^n\) and \(\eta_{22}^n\), or solutions of the problem, and this is distinct from that of the linear advection-diffusion-reaction equations. Computation of (34) is made in association with the previous four cases. The contraction factor calculated from the numerical solutions and the theoretical one obtained from (35) are presented in Table 9, from which it is seen that they are close. The difference is attributed to the linearization adopted in the derivation of the theoretical contraction factor.

Now consider the computation of (34) but in association with optimal interface condition (25). Following the derivation in Sec. 4.2, the following is concluded:

**Proposition 5.4** When interface condition (25) is adopted, the contraction factor for compu
Table 9: Theoretical and numerical contraction factors. \((I,J)=(40,80), \Delta t, \Delta x = 0.017\).

| Time | \(\rho_{\text{theo}}\) | \(\rho_{\text{num}}\) | \(\rho_{\text{theo}}\) | \(\rho_{\text{num}}\) | \(\rho_{\text{theo}}\) | \(\rho_{\text{num}}\) |
|------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0.085 | 0.679514 | 0.689539 | 0.690238 | 0.690248 | 0.690612 | 0.690608 |
| 0.170 | 0.295124 | 0.295112 | 0.299041 | 0.299082 | 0.302137 | 0.302190 |
| 0.255 | 0.457115 | 0.473308 | 0.462127 | 0.478952 | 0.466882 | 0.483229 |

The linearized Burgers equations are

\[
\bar{\rho} = \frac{-(1 + \alpha)(\eta_{22}^2 + \epsilon_2) - R_2(2)}{(1 + \alpha)R_1(I - 1) + (\eta_{11}^I - \epsilon_1)} - \frac{(\beta - 1)(\eta_{11}^I - \epsilon_1) - R_1(I - 1)}{(\beta - 1)R_2(2) + (\eta_{22}^2 + \epsilon_2)},
\]

where \(I, J \geq 3\).

**Theorem 5.1** The contraction factor (37) becomes zero when

\[
\alpha = \frac{R_2(2)}{\eta_{22}^2 + \epsilon_2} - 1, \quad \beta = \frac{R_1(I - 1)}{\eta_{11}^I - \epsilon_1} + 1
\]

in association with \(R_1(I - 1)R_2(2) + (\eta_{11}^I - \epsilon_1)(\eta_{22}^2 + \epsilon_2) \neq 0\). In addition, above values of \((\alpha, \beta)\) is a saddle point of the contraction factor.

**Proof:** The proof can be made by following the steps for Theorem 4.1.

Numerical results for the four cases in Table 6 are presented in Table 10. It is seen that, when the optimal values for \((\alpha, \beta)\) in (38) are adopted, the actual contraction factors in the computation of the first two cases are almost zero, or the theoretical values, while they are somewhat away from zero in the rest two cases. The convergence residual is plotted in Fig. 6. The figure shows that, again, computation of the first two cases exhibits the “perfect convergence”, that is, it converges within about two times of iteration. In the rest two cases, the speed of convergence slows down, and the computation with the optimal interface condition needs many more times of iteration. However, it is still much faster than that associated with the classic interface condition. In the numerical experiment, it noticed that the slowdown in convergence, as in the last two cases, happens once the diffusion coefficients \(b_1\) and \(b_2\) become different, even slightly. The reason for the slow down needs further investigation.

6. Concluding remarks

A study is presented on the computation of two coupled advection-diffusion-reaction equations. The research starts with the computation of the equations by explicit schemes. Then, it proceeds to an implicit scheme and speedup of convergence by an optimal interface condition. Further, the study is extended to coupled Burgers equations. This study achieves the following main results.

1. Conditions are presented for convergence of the computation by explicit schemes, and they are easy to use and check in practical problems. Also, such conditions bear clues to speed up convergence.

2. When an implicit scheme is adopted, an expression for convergence speed is derived. Addi-
Table 10: Convergence speed in computation of the Burgers equations, together with the optimized interface condition (25). (I, J)=(40,80), \( \Delta t, \Delta x = 0.017 \).

| Case | Time | \( \alpha \), \( \beta \) | \( \hat{\rho}_{\text{num}} \) |
|------|------|----------------|----------------|
| 4    | 0.085 | \( 1.90740 \times 10^{-1}, -2.17642 \times 10^{-1} \) | \( -1.25 \times 10^{-14} \) |
|      | 0.170 | \( 1.94634 \times 10^{-1}, -2.12571 \times 10^{-1} \) | \( 8.63 \times 10^{-15} \) |
|      | 0.255 | \( 1.97387 \times 10^{-1}, -2.09199 \times 10^{-1} \) | \( 6.46 \times 10^{-15} \) |
| 5    | 0.085 | \( 6.09587 \times 10^{-1}, -0.99418 \times 10^{-1} \) | \( 0.00 \times 10^{+0} \) |
|      | 0.170 | \( 6.37715 \times 10^{-1}, -0.70900 \times 10^{-1} \) | \( -1.69 \times 10^{-14} \) |
|      | 0.255 | \( 6.66389 \times 10^{-1}, -9.82950 \times 10^{-1} \) | \( 0.00 \times 10^{+0} \) |
| 6    | 0.085 | \( 7.58689 \times 10^{-1}, -4.29258 \times 10^{-1} \) | \( 9.44 \times 10^{-2} \) |
|      | 0.170 | \( 7.62619 \times 10^{-1}, -1.64360 \times 10^{-1} \) | \( 7.72 \times 10^{-2} \) |
|      | 0.255 | \( 7.67611 \times 10^{-1}, -9.94238 \times 10^{-1} \) | \( 6.31 \times 10^{-2} \) |
| 7    | 0.085 | \( 2.39686 \times 10^{-1}, -1.47483 \times 10^{-1} \) | \( -1.64 \times 10^{-2} \) |
|      | 0.170 | \( 2.44286 \times 10^{-1}, -1.41768 \times 10^{-1} \) | \( -1.67 \times 10^{-2} \) |
|      | 0.255 | \( 2.46275 \times 10^{-1}, -1.39353 \times 10^{-1} \) | \( -1.68 \times 10^{-2} \) |

Additionally, an optimal interface condition is presented, which leads to “perfect convergence”, that is, convergence after two times of iteration.

3. Conclusions drawn in the above linear situations remain mostly true in the situations of the Burgers equations, such as the speedup by the optimal interface condition.

This study focuses on issues that lack investigations and achieves understating beyond that in literature. For instance, this study confirms that convergence becomes slower as grid spacing gets fine, e.g., Fig. 3, as concluded in the literature. However, it observes that, in a wide range of parameters, the convergence speed may not increase or even decrease with grid spacing. Additionally, numerical evidence indicates that the overall convergence speed becomes the fastest if an outer iteration is made after every inner iteration, e.g., Table 3 and 8. Moreover, unlike those obtained in the transformed spaces in most earlier investigations, the convergence speeds’ expressions are explicit, and they directly predict those in actual computation. Actually, the method to derive these convergence speeds is extendable to other situations; we have derived the speeds for Poisson equations, which will be reported in a separate paper.

Some topics deserve further study, and one of them is to find out an exact reason why the convergence rate with an optimal interface condition slows down in some scenarios of the Burgers equations. Another topic will be theoretical analysis on the relation between inner and outer iteration, and why and under what conditions the 1:1 strategy leads to the fastest convergence. Moreover, it will be interesting to explore methods to derive convergence speed and their optimal conditions in problems with higher dimensions. We shall keep all of these as our future topics of study.

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Figure 6: Computation with optimal interface conditions for the Burgers equations. a) Case 4. b) Case 5. c) Case 6. d) Case 7.

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