Space–Time Parallel Methods for Evolutionary Reaction–Diffusion Problems

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1 Introduction and problem setting

In recent years, the gradual saturation of parallelization in space has been a strong motivation for the design and analysis of new parallel-in-time algorithms. Among these methods, the parareal algorithm, first introduced by Lions, Maday and Turinici [9], has received significant attention. This scheme has been formulated in the literature as a multiple shooting method [7], a predictor-corrector scheme [13], and a two-level multigrid method in time (see [3, 5] in the linear setting, and [7] for nonlinear problems using the full approximation storage (FAS) multigrid solver).

The key idea of the parareal method is to decompose the time interval into a certain number of subintervals, and solve the original problem concurrently over each one of them. In doing so, it defines two propagation operators which provide fine and coarse approximations to the exact solution. Since the coarse propagator usually considers large stepsizes, implicit time integrators are often used in this case to ensure stability. Choosing the implicit Euler method as the coarse propagator, different fine propagators have been analyzed in the literature: implicit Euler [7, 11, 18],

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trapezoidal rule [7, 11, 18], Radau IIA [7], diagonally implicit Runge–Kutta (DIRK) [18] and Gauss Runge–Kutta [18], among others. Several combinations of A- and L-stable singly diagonally Runge–Kutta (SDIRK) fine and coarse propagators have been further studied in [6].

The main contribution of this work is to consider domain decomposition splitting time integrators as the fine and coarse propagators of the parareal algorithm. Since these methods are related to an overlapping decomposition of the spatial domain, spatial parallelization can also be exploited. Consequently, the resulting algorithms allow for parallelization in both time and space. This class of splitting methods was introduced in [15] in the context of regionally-additive schemes, and has been subsequently extended for solving linear parabolic problems [1, 2, 10, 12, 16] (see [4] for a recent work on nonlinear degenerate parabolic equations). The advantage of the new algorithms with respect to related existing methods (as parareal Schwarz waveform relaxation methods) is that they do not require any iteration to adjust the boundary conditions of the subdomains. As shown later, they are robust with respect to the discretization parameters, the number of disjoint components in each subdomain, the overlapping size and the coarsening factor under consideration.

In the rest of this section, we introduce the time-dependent reaction–diffusion problem to be solved, and derive the stiff system of ordinary differential equations resulting from the spatial discretization. More precisely, let us consider an initial-boundary value problem of the form

$$\begin{cases} u_t + Lu = f, & \text{in } \Omega \times (0,T], \\ u = g, & \text{on } \Gamma \times (0,T], \\ u = u_0, & \text{in } \overline{\Omega} \times \{0\}, \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^2$ is a bounded connected Lipschitz domain with boundary $\Gamma = \partial\Omega$, and $L = L(\mathbf{x})$ is an elliptic operator such that $Lu = -\nabla \cdot (K\nabla u) + cu$. Herein, $K = K(\mathbf{x}) \in \mathbb{R}^{2\times 2}$ is a symmetric tensor with coefficients $K_{i,j} \in L^\infty(\Omega)$, for $i, j \in \{1, 2\}$, that satisfies

$$\kappa_* \xi^T \xi \le \xi^T K \xi \le \kappa^* \xi^T \xi \qquad \forall\, \xi \in \mathbb{R}^2 \text{ and for almost all } \mathbf{x} \in \Omega,$$

for some $0 < \kappa_* \le \kappa^* < \infty$. In addition, the functions $u = u(\mathbf{x}, t)$, $f = f(\mathbf{x}, t)$, $g = g(\mathbf{x}, t)$, $u_0 = u_0(\mathbf{x})$ and $c = c(\mathbf{x})$, with $c \ge 0$, are assumed to be sufficiently smooth, and g and u_0 further satisfy suitable compatibility conditions, so that problem (1) admits a unique weak solution (see [14] for details).

Following the method of lines, we first define a suitable mesh Ω_h covering the spatial domain Ω, where h refers to the maximal grid spacing. Then, using a suitable discretization of the spatial variables (by means of finite difference, finite element or finite volume schemes), we obtain the initial value problem[1]

[1] If we consider a standard finite element method for discretizing (1), we initially obtain a system of ordinary differential equations of the form $M_h U_h'(t) + L_h U_h(t) = F_h(t)$, which is similar to the first equation in (2), but involves two symmetric and positive definite matrices, usually referred to as the mass (M_h) and stiffness (L_h) matrices. Now, considering the Cholesky decomposition

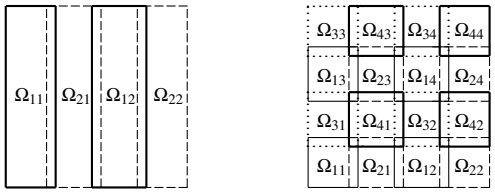

Fig. 1: Overlapping decompositions $\{\Omega_k\}_{k=1}^{s}$ of the unit square Ω into $s = 2$ (left) and $s = 4$ (right) subdomains. Each subdomain Ω_k is further decomposed into $\{\Omega_{kl}\}_{l=1}^{s_k}$ disjoint connected components, with $s_k = 2$ (left) and $s_k = 4$ (right).

$$\begin{cases} U_h'(t) + L_h U_h(t) = F_h(t), \quad t \in (0, T], \\ U_h(0) = \mathcal{R}_h u_0, \end{cases} \tag{2}$$

where $\mathcal{R}_h$ stands for an appropriate restriction or projection operator acting on the initial condition. If we denote by M the number of degrees of freedom in Ω_h for any $t \in [0, T]$, $U_h(t) \in \mathbb{R}^M$ and $L_h \in \mathbb{R}^{M \times M}$ denote the corresponding approximations to $u(\mathbf{x}, t)$ and $L(\mathbf{x})$, respectively. Finally, $F_h(t) \in \mathbb{R}^M$ includes the approximation to $f(\mathbf{x}, t)$ and the contribution of the boundary data $g(\mathbf{x}, t)$.

2 Domain decomposition splitting methods

In this section, we describe how to construct a smooth partition of unity subordinate to an overlapping decomposition of the spatial domain Ω. In addition, we define suitable splittings for the discrete operator L_h and the right-hand side F_h, and further use them in a time integrator with a multiterm partitioning structure.

Let $\{\Omega_k\}_{k=1}^{s}$ be an overlapping decomposition of Ω into s subdomains, i.e., $\Omega = \bigcup_{k=1}^{s} \Omega_k$. Each subdomain $\Omega_k \subset \Omega$ is further defined as an open set involving s_k connected components $\Omega_k = \bigcup_{l=1}^{s_k} \Omega_{kl}$, for $k = 1, 2, \ldots, s$, that are considered to be pairwise disjoint ($\Omega_{ki} \cap \Omega_{kj} = \emptyset$, for $i \neq j$). The overlapping size is denoted by ε. Figure 1 shows two different decompositions of the unit square into $s = 2$ and $s = 4$ subdomains, each consisting of $s_k = 2$ and $s_k = 4$ disjoint connected components, respectively.

Subordinate to this descomposition, we define a smooth partition of unity consisting of a family of s non-negative and $C^\infty(\overline{\Omega})$ functions $\{\rho_k(\mathbf{x})\}_{k=1}^{s}$. Each function $\rho_k : \overline{\Omega} \to [0, 1]$ is chosen to be

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$M_h = N_h N_h^T$, where N_h is a lower triangular matrix with positive diagonal entries, we can define the new unknown $V_h(t) = N_h^T U_h(t)$. It is immediate to see that $V_h(t)$ satisfies a system like (2); in particular, $V_h'(t) + \hat{L}_h V_h(t) = \hat{F}_h(t)$, where $\hat{L}_h = N_h^{-1} L_h N_h^{-T}$ is symmetric and positive definite and $\hat{F}_h(t) = N_h^{-1} F_h(t)$ (cf. [8]).

$$\rho_k(\mathbf{x}) = \begin{cases} 0, & \text{if } \mathbf{x} \in \overline{\Omega} \setminus \overline{\Omega}_k, \\ h_k(\mathbf{x}), & \text{if } \mathbf{x} \in \bigcup_{l=1;\, l\neq k}^{s} (\overline{\Omega}_k \cap \overline{\Omega}_l), \\ 1, & \text{if } \mathbf{x} \in \overline{\Omega}_k \setminus \bigcup_{l=1;\, l\neq k}^{s} (\overline{\Omega}_k \cap \overline{\Omega}_l), \end{cases}$$

where $h_k(\mathbf{x})$ is $C^\infty(\Omega)$ and such that $0 \leq h_k(\mathbf{x}) \leq 1$ and $\sum_{k=1}^{s} h_k(\mathbf{x}) = 1$, for any $\mathbf{x} \in \bigcup_{l=1;\, l\neq k}^{s} (\overline{\Omega}_k \cap \overline{\Omega}_l)$. By construction, the family of functions $\{\rho_k(\mathbf{x})\}_{k=1}^{s}$ satisfies

$$\text{supp}(\rho_k(\mathbf{x})) \subset \overline{\Omega}_k, \qquad 0 \leq \rho_k(\mathbf{x}) \leq 1, \qquad \sum_{k=1}^{s} \rho_k(\mathbf{x}) = 1, \tag{3}$$

for any $\mathbf{x} \in \overline{\Omega}$. In practice, $h_k(\mathbf{x})$ may not necessarily be $C^\infty(\Omega)$, but only a continuous and piecewise smooth function [10].

In this framework, given the parabolic problem (1), we can define a domain decomposition operator splitting $L = L_1 + L_2 + \ldots + L_s$ and $f = f_1 + f_2 + \ldots + f_s$ such that each split term is given by

$$L_k u = -\nabla \cdot (\rho_k K \nabla u) + \rho_k c u, \qquad f_k = \rho_k f, \qquad \text{for } k = 1, 2, \ldots, s. \tag{4}$$

Accordingly, in the discrete setting (2), we may introduce the domain decomposition matrix splitting $L_h = L_{1h} + L_{2h} + \ldots + L_{sh}$ and $F_h = F_{1h} + F_{2h} + \ldots + F_{sh}$, where each term L_{kh} and F_{kh} is defined to be a suitable spatial discretization of its continuous counterpart (4), for $k = 1, 2, \ldots, s$. Typically, the discrete split terms L_{kh} have a simpler structure than L_h, but they do not commute pairwise. This lack of commutativity demands the use of suitable time integrators which preserve the unconditional stability even in the non-commuting case. The simplest of such methods is given by the so-called fractional implicit Euler scheme, first proposed by Yanenko in [19] and described in the sequel.

Let us divide the time interval $[0, T]$ into N_t subintervals $[t_n, t_{n+1}]$, with stepsize $\Delta t = t_{n+1} - t_n = T/N_t$, for $n = 0, 1, \ldots, N_t - 1$. We further define the fully discrete solution $U_h^n \approx U_h(t_n)$ at times $t_n = n\Delta t$, for $n = 0, 1, \ldots, N_t$. Then, given $U_h^0 = \mathcal{R}_h u_0$, the fractional implicit Euler method can be written recursively, for $n = 0, 1, \ldots, N_t - 1$, as

$$(I + \Delta t\, L_{kh})\, U_h^{n+k/s} = U_h^{n+(k-1)/s} + \Delta t\, F_{kh}(t_{n+1}), \quad \text{for } k = 1, 2, \ldots, s. \tag{5}$$

Note that one integration step with (5) can be seen as s consecutive steps with the implicit Euler method, each with a different right-hand side function. In consequence, this time integrator is first-order convergent [17]. Eliminating the internal stages $U_h^{n+k/s}$, for $k = 1, 2, \ldots, s-1$, (5) can be expressed as

$$U_h^{n+1} = \left(\prod_{k=1}^{s} (I + \Delta t\, L_{kh}) \right)^{-1} U_h^n + \sum_{j=1}^{s} \left(\prod_{k=j}^{s} (I + \Delta t\, L_{kh}) \right)^{-1} \Delta t\, F_{jh}(t_{n+1}). \tag{6}$$

For later use, we will denote the right-hand side of this expression by $\mathcal{S}_{\Delta t}(U_h^n)$. The linear system to be solved at the k-th internal stage of (5) involves just the split

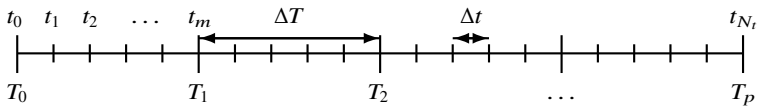

Fig. 2: Fine and coarse time grids considered in the parareal method.

term L_{kh} in the system matrix. As stated in (3), the function $\rho_k(\mathbf{x})$ has compact support on $\overline{\Omega}_k$. Hence, by construction, the entries of L_{kh} corresponding to the nodes that lie outside of this subdomain are zero. Moreover, since Ω_k involves s_k disjoint connected components Ω_{kl}, the previous linear system is indeed a collection of s_k uncoupled subsystems, which can be solved in parallel.

3 The parareal method

In this section, we briefly review the basis for the parareal algorithm, and further establish the connection with domain decomposition splitting schemes in order to derive our new proposal.

Let us first divide the time interval $[0, T]$ into p large time subintervals $[T_n, T_{n+1}]$, for $n = 0, 1, \ldots, p-1$, with stepsize $\Delta T = T_{n+1} - T_n = T/p$. Thus, $T_n = n\Delta T$, for $n = 0, 1, \ldots, p$. Subsequently, we further divide each $[T_n, T_{n+1}]$ into $m \geq 2$ smaller time subintervals $[t_n, t_{n+1}]$, for $n = 0, 1, \ldots, N_t - 1$, with stepsize $\Delta t = \Delta T/m = T/N_t$, where $N_t = pm$. In this case, $t_n = n\Delta t$, for $n = 0, 1, \ldots, N_t$. The parameter m is sometimes referred to as coarsening factor. A representation of these fine and coarse grids is shown in Figure 2.

In this setting, the parareal method makes use of two propagation operators which provide fine and coarse approximations to the solution of (2). We will denote by $\mathcal{F}_{\Delta t}$ the fine propagator, with stepsize Δt, and by $\mathcal{G}_{\Delta T}$ the coarse propagator, with stepsize ΔT. Essentially, the algorithm generates a sequence of iterations $U_h^{n,\ell}$, for $\ell = 0, 1, \ldots$, which converges to the solution of (2). To this end, we sequentially obtain an initial approximation to the numerical solution at the coarse time levels by using the coarse propagator $\mathcal{G}_{\Delta T}$ on the interval $[0, T]$: given $U_h^{0,0} = \mathcal{R}_h u_0$,

$$U_h^{n+1,0} = \mathcal{G}_{\Delta T}(U_h^{n,0}), \quad \text{for } n = 0, 1, \ldots, p-1. \tag{7}$$

Then, for $\ell = 0, 1, \ldots$, until convergence, we do:

1. On each subinterval $[T_n, T_{n+1}]$, we solve on the fine grid using the fine propagator $\mathcal{F}_{\Delta t}$: given $\tilde{U}_h^{nm} = U_h^{n,\ell}$, for $n = 0, 1, \ldots, p-1$,

$$\tilde{U}_h^{nm+j+1} = \mathcal{F}_{\Delta t}(\tilde{U}_h^{nm+j}), \quad \text{for } j = 0, 1, \ldots, m-1. \tag{8}$$

2. On the interval $[0,T]$, we solve on the coarse grid using the coarse propagator $\mathcal{G}_{\Delta T}$: given $U_h^{0,\ell+1} = \mathcal{R}_h u_0$,

$$U_h^{n+1,\ell+1} = \mathcal{G}_{\Delta T}(U_h^{n,\ell+1}) + \tilde{U}_h^{nm} - \mathcal{G}_{\Delta T}(U_h^{n,\ell}), \quad \text{for } n = 0, 1, \ldots, p-1. \quad (9)$$

As suggested in [18], if we denote $\tilde{U}_h^{nm} = \mathcal{F}_{\Delta t}^m(U_h^{n,\ell})$, indicating that we are taking m steps of the fine propagator with initial value $U_h^{n,\ell}$ and a stepsize Δt, the previous algorithm can be compactly written as

$$U_h^{n+1,\ell+1} = \mathcal{G}_{\Delta T}(U_h^{n,\ell+1}) + \mathcal{F}_{\Delta t}^m(U_h^{n,\ell}) - \mathcal{G}_{\Delta T}(U_h^{n,\ell}), \quad \text{for } n = 0, 1, \ldots, p-1.$$

Based on this expression, the parareal method can be interpreted as a predictor-corrector scheme in which $\mathcal{G}_{\Delta T}(U_h^{n,\ell+1})$ plays the role of the predictor, while $\mathcal{F}_{\Delta t}^m(U_h^{n,\ell}) - \mathcal{G}_{\Delta T}(U_h^{n,\ell})$ is the correction term. Note that, at the $(\ell+1)$-th iteration, we can use p processors to compute both $\{\mathcal{F}_{\Delta t}^m(U_h^{n,\ell})\}_{n=1}^p$ and $\{\mathcal{G}_{\Delta T}(U_h^{n,\ell})\}_{n=1}^p$ in parallel.

Now, we are in position to introduce the new family of parareal domain decomposition splitting methods by suitably combining the fractional implicit Euler method (5) with the parareal algorithm (7)-(9). More precisely, we propose using (5) for solving the fine- and coarse-grid problems in the parareal method. Recalling the definition of $\mathcal{S}_{\Delta t}(U_h^n)$ as the right-hand side of (6), we shall consider $\mathcal{F}_{\Delta t}(\cdot) = \mathcal{S}_{\Delta t}(\cdot)$ in (8), and $\mathcal{G}_{\Delta T}(\cdot) = \mathcal{S}_{\Delta T}(\cdot)$ in (7) and (9). In consequence, the resulting method allows for parallelization in both space and time. Remarkably, unlike related existing schemes (e.g., parareal Schwarz waveform relaxation methods), our proposal does not require Schwarz iterations, since the internal stages in (5) are solved sequentially (i.e., interface conditions need not be imposed on subdomains during the solution process). In the next section, we illustrate the performance of the new algorithm as compared to the classical parareal method using implicit Euler propagators $\mathcal{F}_{\Delta t}$ and $\mathcal{G}_{\Delta T}$.

4 Numerical experiments

Let us consider the two-dimensional heat equation with a simple reaction term (i.e., $K = I$ and $c = 1$) on $\overline{\Omega} \times [0,T] = [0,1]^3$, with homogeneous initial and Dirichlet boundary conditions, whose right-hand side is chosen such that the exact solution is $u(x,y,t) = te^{-t}x(1-x)y(1-y)$. We consider a five-point finite difference spatial discretization with $N = N_x = N_y$ spatial nodes on each direction (so that the total number of degrees of freedom for the spatial discretization is $M = N^2$), and the parareal time integrator with p coarse intervals, each containing m fine subintervals. Both the fine and coarse propagators, $\mathcal{F}_{\Delta t}$ and $\mathcal{G}_{\Delta T}$, are chosen to be either the implicit Euler method or the fractional implicit Euler method. In the sequel, we will refer to these methods as Euler and DD-Euler, respectively. In the latter case, Ω is further

Table 1: Number of iterations, varying the number k of disjoint components (left) and the overlapping size ε (right), for a fixed value of $\Delta t = T/(pm)$ and increasing values of N.

Parameters: $p = 16$, $m = 20$, $\varepsilon = 2^{-6}$						
	N	10	20	40	80	160
Euler		8	8	8	8	8
DD-Euler	$k = 2$	11	13	14	14	14
	$k = 4$	12	13	15	14	15
	$k = 8$	9	14	15	14	15

Parameters: $p = 16$, $m = 20$, $k = 4$						
	N	10	20	40	80	160
Euler		8	8	8	8	8
DD-Euler	$\varepsilon = 2^{-4}$	12	12	13	14	13
	$\varepsilon = 2^{-5}$	12	13	12	14	15
	$\varepsilon = 2^{-6}$	12	13	15	14	15

Table 2: Number of iterations, varying the number k of disjoint components (left) and the overlapping size ε (right), for a fixed value of N and decreasing values of $\Delta t = T/(pm)$.

Parameters: $p = 16$, $N = 160$, $\varepsilon = 2^{-6}$						
	m	20	40	80	160	320
Euler		8	8	8	8	8
DD-Euler	$k = 2$	14	15	15	15	15
	$k = 4$	15	15	15	15	15
	$k = 8$	15	16	16	16	16

Parameters: $p = 16$, $N = 160$, $k = 4$						
	m	20	40	80	160	320
Euler		8	8	8	8	8
DD-Euler	$\varepsilon = 2^{-4}$	13	13	14	14	14
	$\varepsilon = 2^{-5}$	15	15	16	16	16
	$\varepsilon = 2^{-6}$	15	15	15	15	15

decomposed into $s = 2$ subdomains, each consisting of k disjoint components, with overlapping size ε. Figure 1 (left) illustrates the case $s = 2$ and $k = 2$.

Tables 1 and 2 show the asymptotic dependence of the two parareal algorithms on the parameters N and m. In addition, for the DD-Euler method, we also show the asymptotic dependence on the values k and ε. In all the cases, we stop the iteration process when the difference between the iterate and the target solution[2] is less than 10^{-8}. Notice that the number of iterations for the DD-Euler method does not increase when considering either a larger number k of disjoint connected components or a smaller overlapping size ε. Although not reported here, a similar number of iterations is obtained for larger values of p. In conclusion, the newly proposed algorithms are robust with respect to the discretization parameters, the number of disjoint components k, the overlapping size ε, and the coarsening factor m.

Finally, for the implicit Euler method, if we have a time grid with pm nodes, we need to solve sequentially pm linear systems with N^2 unknowns. If we perform it_E iterations of the parareal Euler method to satisfy the stopping criterion, we need to solve sequentially $it_E\ (m + p + 1)$ linear systems with N^2 unknowns. Thus, for large values of m with respect to p, the parallelization of computations make the effective cost of the parareal Euler method smaller than that of the classical Euler scheme. In turn, if we perform it_{DD} iterations of the parareal DD-Euler method, considering s

[2] The target solution is the solution obtained at the coarse time levels using the fine propagator $\mathcal{F}_{\Delta t}$ on the whole time interval in a sequential way.

subdomains and k disjoint connected components, and assuming $\varepsilon \approx 0$, we need to solve sequentially $it_{DD}\,(m+p+1)\,s$ linear systems with $N^2/(sk)$ unknowns. Thus, for large values of m with respect to p and large values of k, the effective cost of the parareal DD-Euler method will be even smaller than that of the parareal Euler method.

Acknowledgements. The work of Andrés Arrarás and Carmen Rodrigo was supported by the Spanish State Research Agency under project PGC2018-099536-A-I00 (MCIU/AEI/FEDER, UE). The work of Francisco J. Gaspar and Laura Portero was supported by the Spanish State Research Agency under project PID2019-105574GB-I00 (AEI/10.13039/501100011033).

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