
Embedded pairs of Fractional Step Runge-Kutta methods and improved Domain Decomposition techniques for parabolic problems

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Abstract: In this paper we design and apply new embedded pairs of Fractional Step Runge-Kutta methods to the efficient resolution of multidimensional parabolic problems. These time integrators are combined with a suitable splitting of the elliptic operator subordinated to a decomposition of the spatial domain and a standard spatial discretization. With this technique we obtain parallel algorithms which have the main advantages of classical Domain Decomposition methods and, besides, avoid iterative processes like Schwarz iterations, typical of them. The use of these embedded methods permits to get a fast variable step time integration process.

1 Introduction

Let us consider a linear multidimensional parabolic problem with time dependent coefficients which we formulate in the following operational form: Find $u : [t_0, T] \rightarrow \mathcal{H}$ such that

$$\begin{cases} \frac{\partial u}{\partial t} = A(t)u + f(t) \quad \forall t \in (t_0, T], \\ u(t_0) = u_0 \in \mathcal{H}, \quad Bu(t) = g(t) \in \mathcal{H}^b, \end{cases} \quad (1)$$

where $(\mathcal{H}, \|\cdot\|)$ and $(\mathcal{H}^b, \|\cdot\|^b)$ are two Hilbert spaces of functions defined on a bounded open subset $\Omega \subseteq \mathbb{R}^d$ and on its boundary Γ , respectively. $A(t) : \mathcal{D} \subseteq \mathcal{H} \rightarrow \mathcal{H}$ is an unbounded elliptic differential operator which contains the derivatives of the unknown u with respect to the spatial variables and

** This research is partially supported by the MEC research project num. MTM2004-05221.

$B : \mathcal{D} \subseteq \mathcal{H} \rightarrow \mathcal{H}^b$ is an abstract trace operator which determines the type of boundary conditions considered. We assume that the source term f , the initial condition u_0 and the boundary data g are sufficiently smooth and compatible among them.

Numerical algorithms for the approximate resolution of (1) can be designed and analyzed as the result of combining a standard spatial discretization (using, for example, finite differences or finite elements) with an ODE solver as time integrator. It is well known that if we choose fine grids for the spatial discretization and classical ODE solvers like Runge-Kutta (RK) or multistep methods, a high computational effort must be assumed to obtain the numerical solution. Thus, the task of developing faster algorithms has been of great interest during the last decades and many different ideas have arisen in order to reduce somehow the computation time.

One alternative to obtain fast and robust algorithms is to discretize problem (1) firstly in time using an implicit Runge-Kutta scheme and then to use Domain Decomposition techniques (see [QV99]) to solve numerically the elliptic boundary value problems which arise on each internal stage. In this framework, where we consider the spatial domain Ω decomposed as the union of certain subdomains, the resolution of a large linear system per internal stage is reduced to the resolution of several sets of smaller linear systems. The main advantage of this technique is that the linear systems of every set can be solved in parallel. Nevertheless, the cost of an additional iterative process (f.e. Schwarz iterations) must be assumed due to the adjustment of the boundary conditions on the interior boundaries of the subdomains.

An interesting alternative to a classical ODE solver is to use a Fractional Step Runge-Kutta (FSRK) method as time integrator. The key of the efficiency of these schemes lies in splitting the original elliptic operator as the addition of certain “simpler” operators ($A = \sum_{i=1}^m A_i$). This decomposition combined with a FSRK method permits that only a piece A_i of the elliptic differential operator A acts implicitly at each internal stage of the method in such a way that the derived elliptic boundary value problems are easier to solve. In this work we propose to decompose operator A in pieces of the form $A_i = \psi_i A$, where $\{\psi_i\}_{i=1}^m$ is a smooth partition of unity subordinated to a decomposition of the spatial domain in m suitable overlapped subdomains. Similarly to what happens when classical Domain Decomposition techniques are used, in this case the numerical resolution of each fractionary step consists of solving a set of smaller linear systems whose resolution can be parallelized. Besides, these schemes have an advantage with respect to the classical Domain Decomposition schemes which is that they do not need any kind of Schwarz iterative processes to get the numerical solution. This technique was firstly introduced by Mathew et als. in [MPRW98], where they analyze this kind of splitting for certain low-order classical Fractional Step methods applied to solve parabolic equations with constant coefficients. The generalization of such technique to the class of FSRK schemes used to approximate the solution of parabolic equations with time dependent coefficients is developed in [PBJ04].

The aim of the current paper is to follow these ideas but to decrease the computational cost even more by means of performing a variable time step integration. This will permit us to adapt the step sizes to the local behaviour of the solution as long as we have an estimation of the local error. In order to obtain cheap estimations of such error we have developed some embedded pairs of FSRK methods of different orders. As it happens with other classical one-step methods, the use of embedded formulas provides estimations of the local errors with a lower computational cost than if we choose other classical options like extrapolation methods or the use of two methods with different orders which do not share the internal stages.

2 Time semidiscretization

Let us consider for A and f partitions of the form: $A(t) = \sum_{i=1}^m A_i(t)$, $f(t) = \sum_{i=1}^m f_i(t)$, with $A_i(t) = \psi_i A(t)$, $f_i(t) = \psi_i f(t)$, where $\psi_i(\bar{x})$ are sufficiently smooth functions such that $\sum_{i=1}^m \psi_i(\bar{x}) = 1$, $\forall \bar{x} \in \Omega$. To settle the definition of ψ_i , $i = 1, \dots, m$, we decompose Ω as the union of m overlapped subdomains $\Omega = \bigcup_{i=1}^m \Omega_i$, each one of them consisting of the union of a certain number of connected components $\Omega_i = \bigcup_{j=1}^{m_i} \Omega_{ij}$ such that $\Omega_{ij} \cap \Omega_{ik} = \emptyset$ for all $j, k \in \{1, \dots, m_i\}$ with $j \neq k$. Then the partition of unity $\{\psi_i\}_{i=1}^m$ subordinated to the previous domain decomposition is constructed in such a way that, for each $i = 1, \dots, m$, function ψ_i is identically null outside subdomain Ω_i , takes the value 1 in every point which belongs only to Ω_i and some values between 0 and 1 in the overlaps of Ω_i with the remaining subdomains. For domain decompositions which have internal boundaries with simple geometries, $\psi_i(x)$, $i = 1, \dots, m$, can be easily constructed as products of contractions, movements, ... of the following C^∞ function (see section 5)

$$h(x) = 1 \text{ if } x < 0, \quad h(x) = e^{\frac{1}{2}e^2 \log(2) \frac{-\frac{1}{x}}{x-1}} \text{ if } 0 \leq x \leq 1, \quad h(x) = 0 \text{ if } x > 1. \quad (2)$$

Let us establish now the formulation of a variable time step integration using an embedded pair of FSRK methods with m levels as follows

$$\begin{cases} \begin{cases} U^{n,j} = u_n + \tau_n \sum_{k=1}^j a_{jk}^{i_k} (A_{i_k}(t_{n,k})U^{n,k} + f_{i_k}(t_{n,k})), \\ B_{i_j} U^{n,j} = g_{i_j}(t_{n,j}), \quad \text{for } j = 1, \dots, s, \end{cases} \\ \tilde{u}_{n+1} = u_n + \tau_n \sum_{j=1}^s \tilde{b}_j^{i_j} (A_{i_j}(t_{n,j})U^{n,j} + f_{i_j}(t_{n,j})), \\ u_{n+1} = u_n + \tau_n \sum_{j=1}^s b_j^{i_j} (A_{i_j}(t_{n,j})U^{n,j} + f_{i_j}(t_{n,j})), \end{cases} \quad (3)$$

where $i_\bullet \in \{1, \dots, m\}$, τ_n is the variable time step, $t_n = t_{n-1} + \tau_n$ and $t_{n,j} = t_n + c_j \tau_{n+1}$. $B_i : \mathcal{D}_i \rightarrow \mathcal{H}_i^b$, $i = 1, \dots, m$, are the abstract trace operators

which establish the type of boundary conditions required to calculate each internal stage and g_i are the boundary data; in this case, $B_i = \psi_i B$, $g_i = \psi_i g$, $\forall i = 1, \dots, m$.

We assume that \tilde{u}_{n+1} approximates $u(t_{n+1})$ with order \tilde{p} and that u_{n+1} approximates the same semidiscrete solution also in t_{n+1} but with a higher order of approximation $p > \tilde{p}$. Consequently, $est_{n+1} = \|u_{n+1} - \tilde{u}_{n+1}\|$ estimates the local error for the lower order method at t_{n+1} . Notice that the most expensive calculations done to obtain \tilde{u}_{n+1} (i.e., the internal stages $U^{n,j}$, $j = 1, \dots, s$) are also used in the obtaining of u_{n+1} .

In order to come to a more compact notation for FSRK schemes, (3) can be formulated as an embedded pair of Additive RK schemes

$$\left\{ \begin{array}{l} U^{n,j} = u_n + \tau_n \sum_{i=1}^m \sum_{k=1}^s a_{jk}^i (A_i(t_{n,k})U^{n,k} + f_i(t_{n,k})), \\ B_{i_j} U^{n,j} = g_{i_j}(t_{n,j}), \quad \text{for } j = 1, \dots, s, \\ \tilde{u}_{n+1} = u_n + \tau_n \sum_{i=1}^m \sum_{j=1}^s \tilde{b}_j^i (A_i(t_{n,j})U^{n,j} + f_i(t_{n,j})), \\ u_{n+1} = u_n + \tau_n \sum_{i=1}^m \sum_{j=1}^s b_j^i (A_i(t_{n,j})U^{n,j} + f_i(t_{n,j})), \end{array} \right. \quad (4)$$

if we extend the summatories which appear in (3) by considering many additional null coefficients: $a_{jk}^i = 0$ for $k > j$ and $a_{jk}^i = b_k^i = \tilde{b}_k^i = 0$ for $i \neq i_k$.

Grouping the coefficients of the method into the following vectors and matrices $c = (c_i) \in \mathbb{R}^s$, $\tilde{b}_i = (\tilde{b}_j^i) \in \mathbb{R}^s$, $b_i = (b_j^i) \in \mathbb{R}^s$, $\mathcal{A}_i = (a_{jk}^i) \in \mathbb{R}^{s \times s}$ we can organize the coefficients of (4) in a table

$$\begin{array}{c|c|c|c|c} c & \mathcal{A}_1 & \mathcal{A}_2 & \dots & \mathcal{A}_m \\ \hline \text{order } \tilde{p} & \tilde{b}_1^T & \tilde{b}_2^T & \dots & \tilde{b}_m^T \\ \hline \text{order } p & b_1^T & b_2^T & \dots & b_m^T \end{array},$$

which is an extension of the Butcher's notations for a classical RK scheme. From now on, we will denote with $(c, (\mathcal{A}_i)_{i=1}^m, (\tilde{b}_i)_{i=1}^m)$ and $(c, (\mathcal{A}_i)_{i=1}^m, (b_i)_{i=1}^m)$ the FSRK schemes involved in the embedded pair (3).

3 Spatial discretization and convergence results

We have to complete the previous time semidiscretization with a suitable spatial discretization to obtain a totally discrete scheme. Thus, we introduce a spatial discretization parameter h which tends to zero and we consider Ω_h meshes of $\bar{\Omega}$ which have been constructed taking into account the interior boundaries of the m subdomains. Next we denote with $(\mathcal{H}_h, \|\cdot\|_h)$ and $(\mathcal{H}_{i,h}^b, \|\cdot\|_{i,h}^b)$ some finite dimensional Hilbert spaces of functions whose dimensions grow to infinity as h tends to zero; f.e. \mathcal{H}_h consists of discrete functions

on Ω_h if we use finite differences or piecewise polynomial functions associated to the mesh Ω_h if we use finite elements. In this framework we define operators $A_{i,h} : \mathcal{H}_h \rightarrow \mathcal{H}_h$ and $B_{i,h} : \mathcal{H}_h \rightarrow \mathcal{H}_{i,h}^b$ as certain consistent approximations of operators A_i and B_i and we define $r_{i,h}(t) : \mathcal{D}_i \subseteq \mathcal{H} \rightarrow \mathcal{H}_h$, $\pi_h : \mathcal{H} \rightarrow \mathcal{H}_h$ and $\pi_{i,h}^b : \mathcal{H} \rightarrow \mathcal{H}_{i,h}^b$ as certain restriction or projection operators depending on whether we consider a spatial discretization using finite differences or finite elements, respectively. Under the previous notations, the totally discrete scheme can be expressed as follows

$$\left\{ \begin{array}{l} U_h^{n,j} = u_{n,h} + \tau_n \sum_{k=1}^j a_{jk}^{i_k} \left(A_{i_k,h}(t_{n,k}) U_h^{n,k} + \pi_h f_{i_k}(t_{n,k}) \right), \\ B_{i_j,h} U_h^{n,j} = \pi_{i_j,h}^b g_{i_j}(t_{n,j}), \quad \text{for } j = 1, \dots, s, \\ \tilde{u}_{n+1,h} = u_{n,h} + \tau_n \sum_{j=1}^s \tilde{b}_j^{i_j} \left(A_{i_j,h}(t_{n,j}) U_h^{n,j} + \pi_h f_{i_j}(t_{n,j}) \right), \\ u_{n+1,h} = u_{n,h} + \tau_n \sum_{j=1}^s b_j^{i_j} \left(A_{i_j,h}(t_{n,j}) U_h^{n,j} + \pi_h f_{i_j}(t_{n,j}) \right). \end{array} \right. \quad (5)$$

We can now take $est_{n,h} = \|u_{n,h} - \tilde{u}_{n,h}\|_h$ as an approximation of est_n and use the same ideas of time step adaptation of classical variable step ODE solver codes in order to keep $est_{n,h}$ under the value of a tolerance but close to it.

The resolution of each internal stage in (5) consists of solving a linear system of the form $(\mathcal{I}_h - \tau_n a_{jj}^k A_{kh}(t_{n,j}) U_h^{n,j}) = F_h^{n,j}$, ($k = i_j$), which can be decomposed into m_k independent linear subsystems that can be solved in parallel. Each one of those subsystems has a number of unknowns related to the number of mesh points on each component Ω_{ki} of Ω_k . It is also important to notice that no Schwarz iterations are required to obtain $u_{h,n+1}$.

Let us now give a brief review of the hypotheses assumed in order to guarantee an unconditional convergence result for the totally discrete scheme (5). The local errors of the time semidiscretization are $\rho_{n+1} = \|u(t_{n+1}) - u_{n+1}[t_n, u(t_n)]\|$ and $\tilde{\rho}_{n+1} = \|u(t_{n+1}) - \tilde{u}_{n+1}[t_n, u(t_n)]\|$, where $u_{n+1}[t_n, u(t_n)]$ and $\tilde{u}_{n+1}[t_n, u(t_n)]$ are the approximations to $u(t_{n+1})$ obtained after one step of scheme (3) starting from $u_n = u(t_n)$. We assume that the embedded pair of FSRK methods (3) has orders $\tilde{p}(p)$, i.e., $\tilde{\rho}_{n+1} \leq C\tau^{\tilde{p}+1}$, $\rho_{n+1} \leq C\tau^{p+1}$, where $\tau \equiv \max_n \tau_n$ and C is a constant independent of τ . With the aim of obtaining a convergence result for the semidiscrete scheme (3), we combine the consistency with a suitable stability property. We say that the FSRK method $(c, (\mathcal{A}_i)_{i=1}^m, (b_i)_{i=1}^m)$ is A-stable iff $|R(z_1, \dots, z_m)| \leq 1$, $\forall z_1, \dots, z_m \in \mathbb{C}^- \equiv \{z \in \mathbb{C} : \text{Re}(z) \leq 0\}$, where $R(z_1, \dots, z_m) = 1 + \sum_{i=1}^m z_i b_i^T (\mathcal{I} - \sum_{j=1}^m z_j \mathcal{A}_j)^{-1} e$ is the amplification function associated to the FSRK method. In [BJ01] it is proven that, under suitable hypotheses on operators $A_i(t)$ the use of an FSRK scheme which is consistent and A-stable guarantees the convergence of the time discretization process. Regarding the spatial discretization, we must assume typical order r properties of consistency as well as suitable stability properties.

Combining all these properties, the following unconditional convergence results are obtained for the totally discrete scheme (5) $\|r_h(t_n)u(t_n) - \tilde{u}_{h,n}\|_h \leq C(h^r + \tau^{\tilde{p}})$, $\|r_h(t_n)u(t_n) - u_{h,n}\|_h \leq C(h^r + \tau^p)$, where C is a constant independent of τ and h (see [PBJ04]).

4 Design of two embedded pairs of FSRK methods

We start with the design of a simple pair of orders 1(2). Let us consider the Fractionary Implicit Euler scheme with two levels

$$\begin{array}{c|cc|cc} 1 & 1 & & & 0 & & & \\ 1 & 1 & 0 & & 0 & 1 & & \\ \hline & 1 & 0 & & 0 & 1 & & \end{array} \quad (6)$$

as the lower order method of the pair; it is first order consistent and A-stable. Now we want to construct a second order scheme whose two first stages coincide with the two first stages of (6). The sufficient and necessary conditions which a FSRK scheme should satisfy to have order p are shown in [BJ03]; in this case ($p = m = 2$) such order conditions are $b_i^T e = 1$, $b_i^T c = \frac{1}{2}$, $b_i^T \mathcal{A}_j e = \frac{1}{2} \forall i, j \in \{1, 2\}$, where $e = (1, \dots, 1) \in \mathbb{R}^s$.

We need to add two implicit stages to (6) in order to obtain a second order method; in such a case we come to a system of 8 non linear equations which depend on 13 unknowns. After solving it we obtain a family of embedded pairs of FSRK methods of orders 1(2) with 5 free parameters ($b_3^1, b_4^2, a_{33}^1, a_{43}^1, a_{44}^2$).

Next we impose the property of A-stability. To simplify the study, we assume that $a_{33}^1 = a_{44}^2 = a$ and then we impose that $a_{43}^1 = \frac{2ab_3^1}{b_4^2}$ to permit a nearly L-stable behaviour (i.e., $R(\infty, \infty) \simeq 0$). By means of a numerical swept we obtain that $a \geq 2.35$ is a necessary requirement in order to have an A-stable FSRK scheme of order 2. We still have three parameters: a, b_3^1, b_4^2 , which we fix in such a way that the method has simple rational coefficients and also that the main term of the local error of the second order FSRK method is almost minimized. Using these ideas we have chosen the values $b_4 = \frac{3}{4}$, $b_3 = \frac{9}{10}$, $a = \frac{12}{5}$ and the resulting pair is

1	1				0			
1	1	0			0	1		
$\frac{4}{9}$	$-\frac{88}{45}$	0	$\frac{12}{5}$		0	$\frac{5}{9}$	0	
$\frac{1}{3}$	$-\frac{407}{75}$	0	$\frac{144}{25}$	0	0	$-\frac{31}{15}$	0	$\frac{12}{5}$
order 1	1	0	0	0	0	1	0	0
order 2	$\frac{1}{10}$	0	$\frac{9}{10}$	0	0	$\frac{1}{4}$	0	$\frac{3}{4}$

Following a similar technique, we have designed an embedded pair of FSRK schemes of orders 2(3). In this case we have chosen as second order method

the time integrator involved in the classical Peaceman & Rachford scheme and, by adding 4 suitable implicit stages, we have obtained the following pair

0	0						0						
$\frac{1}{2}$	0	$\frac{1}{2}$					$\frac{1}{2}$	0					
1	0	1	0				$\frac{1}{2}$	0	$\frac{1}{2}$				
$\frac{7}{17}$	0	$-\frac{3}{34}$	0	$\frac{1}{2}$			$\frac{7}{17}$	0	0	0			
$\frac{1}{2}$	0	$-\frac{11}{12}$	0	$\frac{17}{12}$	0		$\frac{1}{8}$	0	$-\frac{1}{8}$	0	$\frac{1}{2}$		
$\frac{13}{17}$	0	$-\frac{27}{34}$	0	$\frac{18}{17}$	0	$\frac{1}{2}$	$\frac{113}{289}$	0	0	0	$\frac{108}{289}$	0	
1	0	$-\frac{208}{81}$	0	$\frac{289}{108}$	0	$\frac{289}{324}$	$\frac{1}{6}$	0	$-\frac{1}{3}$	0	$\frac{2}{3}$	0	$\frac{1}{2}$
order 2	0	1	0	0	0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	0	0
order 3	0	$-\frac{208}{81}$	0	$\frac{289}{108}$	0	$\frac{289}{324}$	$\frac{1}{6}$	0	$-\frac{1}{3}$	0	$\frac{2}{3}$	0	$\frac{1}{2}$

5 Numerical examples

We consider the following diffusion-reaction problem

$$\begin{cases} \frac{\partial u}{\partial t} = (1 + e^{-t})xy\Delta u - u + f(t, x, y), & (t, x, y) \in (0, 500] \times \Omega, \\ u(0, x, y) = u_0(x, y), & (x, y) \in \bar{\Omega}, \\ u(t, x, y) = 0, & (t, x, y) \in (0, 500] \times \Gamma, \end{cases}$$

where $\Omega = (0, 1) \times (0, 1)$ and data f and u_0 are chosen in such a way that $u(t, \bar{x}) = 3te^{-3t+1} \sin(\pi x) \sin(\pi y)$ is its exact solution.

We have decomposed domain Ω as the union of two overlapped subdomains $\Omega_1 = ((0, \frac{5}{16}) \cup (\frac{7}{16}, \frac{13}{16})) \times (0, 1)$, $\Omega_2 = ((\frac{3}{16}, \frac{9}{16}) \cup (\frac{11}{16}, 1)) \times (0, 1)$; each subdomain has two disjoint components. The partition of unity chosen subordinated to this decomposition is: $\psi_1(x, y) = h(8x - \frac{3}{2})$, if $x \in (0, \frac{3}{8})$, $\psi_1(x, y) = h(8x - \frac{7}{2})$, if $x \in [\frac{3}{8}, \frac{5}{8})$, $\psi_1(x, y) = h(8x - \frac{11}{2})$, if $x \in [\frac{5}{8}, 1)$, where $h(x)$ is given in (2), and $\psi_2(x, y) = 1 - \psi_1(x, y)$. Finally, we decompose the elliptic operator and the source term in two pieces as follows: $A_i(t, x, y) \equiv \psi_i(x, y)((1 + e^{-t})xy\Delta - \mathcal{I})$, $f_i(t, x, y) = \psi_i(x, y)f(t, x, y)$, $i = 1, 2$.

We show in the following table the results obtained with the designed embedded pairs of orders 1(2) and 2(3), respectively. The spatial discretization chosen in both cases is central differences on a uniform rectangular mesh of $N \times N$ points which is convergent of second order; that is the reason why we have chosen a tolerance equal to $\frac{1}{N^2}$ to control the sizes of the time steps with the aim of having errors of the same size in space and time.

For different values of N , we show in such table the total number of steps (including the accepted and rejected ones), the efficacy, which is the percentage of accepted steps with respect to the total number of steps, the average

1(2)	2(3)	n_{tot}		efficacy %		$\bar{\tau}$		global error	
$N = 16$		71	34	91.55	88.24	7.6923	16.6667	3.4636E-2	3.8192E-2
$N = 32$		234	52	95.30	90.38	2.2422	10.6383	1.3269E-2	1.3289E-2
$N = 64$		630	81	97.46	93.83	0.8143	6.5789	4.5409E-3	4.5367E-3
$N = 128$		1532	128	98.63	96.09	0.3309	4.0650	1.4294E-3	1.4173E-3
$N = 256$		2017	211	99.90	95.73	0.2481	2.4752	4.3804E-4	4.7210E-4

sizes of the accepted time steps and the maximum global errors committed along the whole integration interval. Note that the efficacy is very high and it improves for smaller tolerances and that the global errors obtained show a reduction according to the reduction of the tolerance ($\frac{1}{4}$) chosen when N doubles. As the exact solutions of these problems use to decay exponentially (in t) to the stationary state (0 in this case), the sizes of the time steps τ_n tend to grow along the integration in time from a certain point which provides a time integration which requires much less steps than using constant time step integrators. Notice also that the same tolerance ($\frac{1}{N^2}$) has been used in both pairs for every value of N and that for these tolerances the embedded pair 1(2) needs much more time steps than the pair 2(3) to realize the integration. This implies that, although the pair 2(3) has two internal implicit stages more than the pair 1(2), the total computational cost of the integration for the same tolerance is much lower for the embedded pair of orders 2(3), as it was expected. On the basis of this comparison, we think that the design of embedded pairs of FSRK schemes of higher orders is a very interesting task which we plan to do in the near future.

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