

# A Combined Fractional Step Domain Decomposition Method for the Numerical Integration of Parabolic Problems

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**Abstract.** In this paper we develop parallel numerical algorithms to solve linear time dependent coefficient parabolic problems. Such methods are obtained by means of two consecutive discretization procedures. Firstly, we realize a time integration of the original problem using a Fractional Step Runge Kutta method which provides a family of elliptic boundary value problems on certain subdomains of the original domain. Next, we discretize those elliptic problems by means of standard techniques. Using this framework, the numerical solution is obtained by solving, at each stage, a set of uncoupled linear systems of low dimension. Comparing these algorithms with the classical domain decomposition methods for parabolic problems, we obtain a reduction of computational cost because of, in this case, no Schwarz iterations are required. We give an unconditional convergence result for the totally discrete scheme and we include two numerical examples that show the behaviour of the proposed method.

## 1 Introduction

It is well known that the numerical resolution of multidimensional parabolic problems by using standard methods requires a strong computational effort, specially if very accurate solutions are wanted. The development and analysis of such methods can be done by means of the combination of two discretization stages: a time integration procedure (f.e. via Runge-Kutta or multistep methods) and a spatial discretization method like finite differences or finite elements. For the time integration it is usually chosen between the two following possibilities: an explicit method that provides totally discrete schemes which are cheap per time step in terms of computational cost, but have the disadvantage of being conditionally convergent (that is to say, there is a strong restriction between the time step and the spatial grid sizes to obtain convergence) or an implicit method. In the last case we obtain totally discrete algorithms that are unconditionally

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convergent but have the drawback of involving one or several large linear systems per time step, whose resolution implies a high computational cost.

In order to accelerate the resolution of such systems, specially if we use parallel computer devices, one of the most successful techniques is the domain decomposition (see [7]). Such technique permits to reduce the original system to a set of systems of lower dimensions, as well as to parallelize the resolution of them. When classical implicit methods are used to discretize the time variable, the user must assume the cost of a Schwarz iterative process if overlapped subdomains are taken; in order to get a fast convergence for these iterative processes, it is essential to choose carefully the dimensions of the overlapping zones (see [7]). In the case of non-overlapped subdomains, another kind of iterations are needed; these ones are related to the transmission conditions that must be imposed between the boundaries of the subdomains.

In this paper we propose to use a Fractional Step Runge-Kutta (shortly FSRK, see [3]) method for the time discretization process, in which the operator splitting is subordinated to the decomposition of the domain considered. After that, the numerical algorithm will be easily obtained if we consider a standard discretization method for the spatial variables (for example finite difference or finite element methods). Following this technique, we only have to solve several linear systems per stage of low dimensions that can be computed in parallel without the need of doing any kind of iteration. In [5], the authors develop a similar idea for the case of combining classical (low-order) FSRK methods with finite differences to integrate linear parabolic problems with constant coefficients.

In section 3, we prove that a numerical method of this kind preserve the property of unconditional convergence, which is typical for suitable implicit methods. The last section contains two numerical experiments for one-dimensional and two-dimensional problems integrated both with this kind of methods.

## 2 Obtaining the Totally Discrete Scheme

Let us consider the linear parabolic initial boundary value problem that consists in finding  $u : \Omega \times [t_0, T] \rightarrow \mathcal{H}$  such that

$$\begin{cases} \frac{du}{dt} = A(\bar{x}, t)u + f(\bar{x}, t), & (\bar{x}, t) \in \text{Int}(\Omega) \times (t_0, T], \\ u(\bar{x}, t_0) = u_0(\bar{x}) \in \mathcal{H}, & \bar{x} \in \Omega, \\ Bu(\bar{x}, t) = g(\bar{x}, t) \in \mathcal{H}^b, & (\bar{x}, t) \in \partial\Omega \times (t_0, T], \end{cases} \quad (1)$$

where  $\mathcal{H}$  and  $\mathcal{H}^b$  are Hilbert spaces and, for each  $t \in [t_0, T]$ ,  $A(\bar{x}, t) : \mathcal{D} \subseteq \mathcal{H} \rightarrow \mathcal{H}$  is an unbounded elliptic differential operator that involves the partial derivatives of the unknown  $u$  with respect to the spatial variables.

In order to discretize in time problem (1) using an FSRK method, we introduce a partition for the elliptic operator in the form  $A(\bar{x}, t) = \sum_{i=1}^m A_i(\bar{x}, t)$  and for the source term  $f(\bar{x}, t) = \sum_{i=1}^m f_i(\bar{x}, t)$  that will be specified later. Classically, when the elliptic operator does not contain any crossed derivative, the splitting is

taken by grouping in each addend the derivatives with respect to each coordinate (obtaining a method of type Alternating Directions).

An FSRK method, considering  $\tau$  as (constant) time step, provides a numerical approximation of the solution of the semidiscrete problem at each time  $t_n$ ,  $u_n(\bar{x}) \approx u(\bar{x}, t_n)$ , by solving

$$\begin{cases} \begin{cases} U^{n,j} = u_n + \tau \sum_{k=1}^j a_{jk}^{i_k} (A_{i_k}(\bar{x}, t_{n,k})U^{n,k} + f_{i_k}(\bar{x}, t_{n,k})), \\ B_{i_j}U^{n,j} = g(\bar{x}, t_{n,j}), \quad \text{for } j = 1, \dots, s, \end{cases} \\ u_{n+1} = u_n + \tau \sum_{j=1}^s b_j^{i_j} (A_{i_j}(\bar{x}, t_{n,j})U^{n,j} + f_{i_j}(\bar{x}, t_{n,j})), \end{cases} \quad (2)$$

where  $t_n = t_0 + n\tau$  and  $t_{n,j} = t_n + c_j\tau$ . With the aim of using a more comfortable matrix notation, we can consider an FSRK method as an Additive Runge-Kutta method (see [4]) with many null columns (in particular, we consider  $a_{jk}^i = b_j^i = 0$  for  $i \neq i_k$ ) and, using a notation similar to Butcher's table for classical Runge-Kutta methods, we can express it in the following compacted form

$$\frac{c}{b_1^T} \left| \begin{array}{c|c|c|c} \mathcal{A}_1 & \mathcal{A}_2 & \dots & \mathcal{A}_m \\ \hline b_1^T & b_2^T & \dots & b_m^T \end{array} \right|,$$

where  $\mathcal{A}_i = (a_{jk}^i) \in \mathbb{R}^{s \times s}$  and  $b_i = (b_j^i)$ ,  $c = (c_1, \dots, c_s)^T \in \mathbb{R}^s$  for  $i = 1, \dots, m$ .

The advantage that these methods may provide, in comparison with classical implicit methods, comes from the fact that the calculus of each stage  $U^{n,j}$  is done by solving linear elliptic boundary value problems of the form

$$\begin{cases} (\mathcal{I} - \tau a_{jj}^{i_j} A_{i_j}(\bar{x}, t_{n,j}))U^{n,j} = F^{n,j}, \\ B_{i_j}U^{n,j} = g(\bar{x}, t_{n,j}), \end{cases} \quad (3)$$

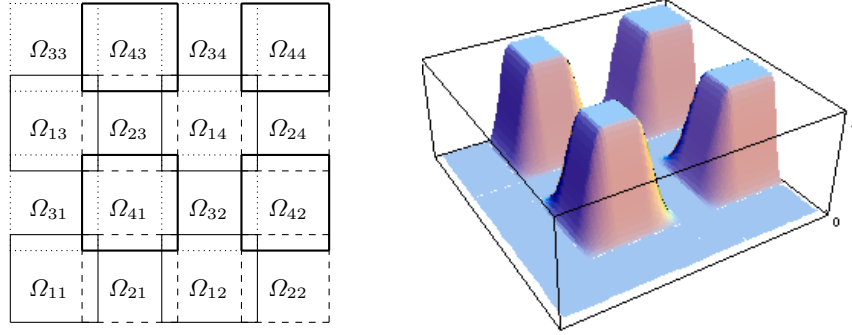
where  $F^{n,j}$  is computed from the data of the problem and the results of previous stages. If operators  $A_i(\bar{x}, t)$  are simpler than the global operator  $A(\bar{x}, t)$ , then a suitable spatial discretization of these problems permits the obtaining of numerical algorithms which are much cheaper than classical implicit methods.

In this work we propose a smooth splitting of  $A(\bar{x}, t)$  related to a decomposition of domain  $\Omega$  in the form  $\Omega = \bigcup_{i=1}^m \Omega_i$ , where each subdomain  $\Omega_i$  consists of a set of  $m_i$  disjoint components  $\Omega_{ij}$  satisfying  $\Omega_i = \bigcup_{j=1}^{m_i} \Omega_{ij}$ . Concretely, we consider  $A_i(\bar{x}, t) = \psi_i(\bar{x})A(\bar{x}, t)$ ,  $f_i(\bar{x}, t) = \psi_i(\bar{x})f(\bar{x}, t)$ , where  $\psi_i(\bar{x})$  is a sufficiently smooth function which satisfies

$$\begin{aligned} \psi_i(\bar{x}) &= 0 \quad \text{if } \bar{x} \in \Omega \setminus \Omega_i, \quad \psi_i(\bar{x}) = 1 \quad \text{if } \bar{x} \in \Omega_i \setminus \bigcup_{\substack{j=1 \\ j \neq i}}^m (\Omega_i \cap \Omega_j), \\ \text{and } \psi_i(\bar{x}) &= h_i(\bar{x}) \quad \text{if } \bar{x} \in \bigcup_{\substack{j=1 \\ j \neq i}}^m (\Omega_i \cap \Omega_j), \\ \text{with } 0 \leq h_i(\bar{x}) &\leq 1 \quad \text{and } \sum_{\substack{i=1 \\ j \neq i}}^m h_i(\bar{x}) = 1 \quad \forall \bar{x} \in \bigcup_{\substack{j=1 \\ j \neq i}}^m (\Omega_i \cap \Omega_j). \end{aligned} \quad (4)$$

We include below, in Figure 1, an example of a two-dimensional domain which is decomposed in four subdomains and each one of them consists of four components, i.e.  $m = 4$ ,  $m_i = 4 \forall i = 1, \dots, 4$ . We have also included, in the same figure,

a graphic representing a possible function  $\psi_4(x, y)$  that would be associated to the subdomain  $\Omega_4$ .



**Fig. 1.** Domain decomposition in four subdomains

After the time integration, we proceed to discretize in space the resultant family of elliptic boundary value problems (2) by means of classical methods. Let us consider a spatial discretization parameter  $h$  which is going to tend to zero. For each value of  $h$ , we consider a mesh  $\Omega_h$  (of the original domain  $\Omega$ ) which has been constructed taking into account the boundaries of every subdomain  $\Omega_i$  and we denote with  $\mathcal{H}_h$  a finite dimensional space made up of discrete functions in  $\Omega_h$ , if we use finite differences, or piecewise polynomial functions associated to the meshing  $\Omega_h$ , if we use finite elements. We denote with  $A_{ih} : \mathcal{H}_h \rightarrow \mathcal{H}_h$  the operators that discretize  $A_i$  and with  $f_{ih} = \pi_h f_i$ ,  $g_h = \pi_h g$  the restrictions or projections of the continuous functions  $f_i$ ,  $g$ , depending on the spatial discretization method used.

In this context, the totally discrete scheme can be expressed as follows

$$\begin{cases} U_h^{n,j} = u_{h,n} + \tau \sum_{k=1}^j a_{jk}^{i_k} (A_{i_k h}(t_{n,k}) U_h^{n,k} + f_{i_k h}(t_{n,k})), \\ B_{i_j h} U_h^{n,j} = g_h(t_{n,j}), \quad \text{for } j = 1, \dots, m, \\ u_{h,n+1} = u_{h,n} + \tau \sum_{j=1}^m b_j^{i_j} (A_{i_j h}(t_{n,j}) U_h^{n,j} + f_{i_j h}(t_{n,j})). \end{cases} \quad (5)$$

Looking at (5) it is clear that the calculus of each stage involves a linear system of the form

$$(\mathcal{I}_h - a_{jj}^k A_{kh}(t_{n,j})) U_h^{n,j} = F_h^{n,j}, \quad (k = i_j)$$

which, in practice, implies the resolution of  $m_k$  uncoupled linear systems whose sizes depend of the number of mesh points that belong to the components  $\Omega_{ki}$  of subdomain  $\Omega_k$ ; this permits a straightforward parallelization for their resolution. On the other hand, it is important to notice that the main advantage of our method is that no Schwarz iterations are required to obtain  $u_{h,n+1}$ .

### 3 Global Convergence of the Totally Discrete Scheme

To study the convergence of the totally discrete scheme, we suppose that the elliptic operators  $-A(\bar{x}, t)$  are maximal, monotone and satisfy the following bound

$$\|A(\bar{x}, t)u - A(\bar{x}, s)u\| \leq |t - s| M \|A(\bar{x}, t)u\|, \quad \forall t, s \in [t_0, T]. \quad (6)$$

Operators  $-A_i(\bar{x}, t)$ , due to their construction, are also maximal and monotone and verify bounds similar to (6). Henceforth, we denote with  $r_h(t), r_{i,h}(t) : \mathcal{D} \rightarrow \mathcal{H}_h$  certain restrictions or projections, depending on the spatial discretization used, and with  $C$  any constant independent of  $\tau$  and  $h$ .

Moreover, we suppose that the spatial discretization is stable, i.e., the discrete operators  $-A_{ih}(t)$  are monotone, and that such discretization is consistent of order  $r$ , that is to say, for sufficiently smooth functions  $u(\bar{x}, t)$ , we have

$$\begin{aligned} \|A_{ih}(t)r_{i,h}(t)u(\bar{x}, t) - \pi_h A_i(\bar{x}, t)u(\bar{x}, t)\|_h &\leq C h^r, \\ \|B_{ih}r_{i,h}(t)u(\bar{x}, t) - \pi_h B_i u(\bar{x}, t)\|_h &\leq C h^r, \end{aligned} \quad (7)$$

where  $\|\cdot\|_h$  denotes a suitable norm in  $\mathcal{H}_h$ .

We define the global error associated to the total discretization in the moment  $t_n$  in the usual form  $E_{h,n} = \|r_h(t_n)u(\bar{x}, t_n) - u_{h,n}\|_h$  and it is said that the totally discrete scheme (5) is convergent, of order  $p$  in time and order  $r$  in space, if  $E_{h,n} \leq C(\tau^p + h^r)$ . If the spatial discretization is stable, the totally discrete scheme possesses unique solution which can be expressed in the form (see [3])

$$u_{h,n+1} = \tilde{R}(\tau \hat{A}_{1h}^n, \dots, \tau \hat{A}_{sh}^n) u_{h,n} + \tilde{S}(-\tau \hat{A}_{1h}^n, \dots, -\tau \hat{A}_{sh}^n, \tau \hat{F}_{1h}^n, \dots, \tau \hat{F}_{sh}^n),$$

where we group the evaluations of the partitioned source terms and operators as follows  $\hat{F}_{ih}^n = (f_{ih}(t_{n,1}), \dots, f_{ih}(t_{n,s}))^T \in \mathcal{H}_h^s$  and  $\hat{A}_{ih}^n = \text{diag}(A_{ih}(t_{n,1}), \dots, A_{ih}(t_{n,s})) \in \mathcal{H}_h^{s \times s}$ , for  $i = 1, \dots, s$  and  $n = 1, 2, \dots$ .

When operators  $A_{ih}(t)$  preserve bounds of type (6) and we choose FSRK methods satisfying certain linear absolute stability properties, the following bound for the linear transition operator can be obtained (see [1])

$$\|\tilde{R}(\tau \hat{A}_{1h}^n, \dots, \tau \hat{A}_{sh}^n)\|_h \leq e^{\gamma\tau}. \quad (8)$$

In [3] it is proven that, if the time discretization is accomplished with an FSRK method of order  $p$  and the problem data in (1) are sufficiently regular and compatible, the scheme (2) is uniformly consistent of order  $p$ , that is to say,

$$\|u(t_n) - \check{u}_n\| \leq C \tau^{p+1}, \quad (9)$$

where  $\check{u}_n$  is obtained after a step of the semidiscrete scheme (2) starting from  $\check{u}_{n-1} = u(t_{n-1})$ .

To deduce the convergence of (5) we decompose the global error as  $E_{h,n} \leq \|r_h(t_n)(u(t_n) - \check{u}_n)\|_h + \|r_h(t_n)\check{u}_n - \check{u}_{h,n}\|_h + \|\check{u}_{h,n} - u_{h,n}\|_h$ , where  $\check{u}_{h,n}$  is obtained after a step of the totally discrete method (5) taking  $\check{u}_{h,n-1} = r_h(t_{n-1})u(t_{n-1})$  as starting point.

The first addend is bounded using (9) together with certain compatibility properties for the continuous and discrete norms (see [3]). The bound for the second addend is deduced combining the consistency and stability of the spatial discretization (see [3]). Finally, using (8), we can write

$$E_{h,n} \leq C \tau^{p+1} + C \tau h^r + e^{\beta\tau} \|E_{h,n-1}\|_h \leq C \tau \sum_{k=0}^{n-1} e^{\beta k\tau} (\tau^p + h^r) \leq C (\tau^p + h^r).$$

## 4 Numerical Examples

*Example a)* We consider the parabolic problem

$$\begin{cases} \frac{\partial u}{\partial t} = A(x,t)u + f(x,t), \quad \forall (x,t) \in (0,1) \times (0,2], \\ u(x,0) = u_0(x), \quad \forall x \in (0,1), \quad u(0,t) = u(1,t) = 0, \quad \forall t \in [0,2], \end{cases}$$

with  $A(x,t) = (1+x)(1+t)e^{-t}\frac{\partial^2}{\partial x^2} - (1+2x)(1+e^{-t})\frac{\partial}{\partial x} - (1+x^2)\mathcal{I}$  and where  $f(x,t)$  and  $u_0(x)$  are data functions chosen so that  $u(x,t) = e^{-t}x^2(1-x)^2$  is the exact solution. In this experiment we consider the spatial domain made up of two overlapped subdomains  $([0,1] = \Omega_1 \cup \Omega_2)$ , where  $\Omega_1 = [0, \frac{1}{2} + d]$ ,  $\Omega_2 = [\frac{1}{2} - d, 1]$ , being  $d = \frac{1}{8}$ .

We integrate this problem following two different ways. On one hand, we use standard SDIRK methods of order 2, 3 and 4 (with 1, 2 and 3 internal stages, respectively) for the time integration together with a central difference discretization of the spatial variables on a uniform grid and we apply the Schwarz iterative method. On the other hand, we combine a time integration by means of FSRK methods of order 2, 3 and 4 (with 2, 6 and 8 implicit stages, respectively, see [2]) with a central difference spatial discretization. Following the ideas presented in the previous sections, we choose a partition for the original elliptic operator  $A(x,t)$  in two addends  $A_i(x,t) = \psi_i(x)A(x,t)$ ,  $i = 1, 2$  with  $\{\psi_i(x)\}_{i=1,2}$  a partition of unity (4) associated to the domain decomposition  $\{\Omega_i\}_{i=1,2}$ , where we have chosen  $h_1(x) = \frac{1}{2} - \frac{3}{4d}(x - \frac{1}{2}) + \frac{1}{4d^3}(x - \frac{1}{2})^3$  and  $h_2(x) = 1 - h_1(x)$ .

In both options we will take the following relations between  $N = \frac{1}{h}$  and the time step size:  $N^2\tau^2 = 0.16$ ,  $N^2\tau^3 = 8E - 3$  or  $N^2\tau^4 = 4E - 4$ , depending on whether the consistency order of the time integrator used is 2, 3 or 4, respectively.

The maximum global errors obtained for these six totally discrete methods have been computed as

$$E_{h,n} = \max_{\substack{x_i \in \Omega_h \\ t_n = n\tau, n=1,2,\dots,\frac{2}{\tau}}} |u_{h,n}^i - u(x_i, t_n)|,$$

where  $u(x_i, t_n)$  is the exact solution evaluated in the grid node  $x_i = ih$  at time  $t_n = n\tau$  and  $u_{h,n}^i$  is the numerical solution obtained in the same grid point and at the same time moment. All of them have shown almost the same propagation of global errors and, consequently, the same numerical orders of convergence, so we only include in Table 1 the corresponding errors for the methods with second

order in time and in space (FSRK2 refers to the classical Peaceman & Rachford method and RK2 to the Crank-Nicolson method) .

Finally, in order to show the reduction of computational cost achieved with our proposal, we show in Table 2 the average number of linear systems of size  $\frac{N}{2} + Nd$  involved, per time step, for each method. This average has been computed in the time interval  $[0, 0.2]$  which is the most relevant zone attending to the variation of the solution and the time steps considered. In a variable time step integration procedure this average should be watched in the whole interval  $[0, 2]$  to compare suitably the efficiencies. Concretely, when we use an FSRK method for the time integration, we have to solve a linear system of  $\frac{N}{2} + Nd$  unknowns per stage (and we don't need any kind of iterations), whereas when we use classical domain decomposition techniques we have to solve  $2k$  linear systems of size  $\frac{N}{2} + Nd$  per stage, where  $k$  is the number of Schwarz iterations required (the tolerance imposed for this iterative method has been  $10^{-1}\tau h^2$ ).

*Example b)* We consider now a two-dimensional problem associated to the equation  $\frac{\partial u}{\partial t} = (1 + e^{-t}) \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - (1 + 2xy)e^{-2t}u + f(x, y, t)$  in the domain  $\Omega = (0, 1) \times (0, 1)$  for  $t \in (0, 2]$  with homogeneous Dirichlet boundary conditions, where the source term  $f$  and the initial condition  $u_0$  are chosen in order to have  $u(x, y, t) = e^{-t+7.5} \left( \frac{1+e}{e} - e^{-x} - e^{-1+x} \right)^2 \left( \frac{1+e}{e} - e^{-y} - e^{-1+y} \right)^2$  as exact solution.

Now we have considered the spatial domain  $\Omega$  decomposed as the union of 4 overlapped subdomains (an example of a decomposition of this type can be observed in Figure 1). In this numerical experiment we use a first and a second order FSRK method (with 4 and 6 implicit stages, respectively) both combined with a second order spatial discretization using central differences. We compare their results with the ones obtained with standard RK methods of order 1 and 2 (both with 1 internal stage) combined with a central difference spatial discretization, using the Schwarz iterative method with tolerance  $10^{-1}\tau h^2$ .

Let us define the following functions of one variable

$$i_1(x) = \begin{cases} 1 & \text{if } x \in [0, \frac{1}{4} - d] \cup [\frac{1}{2} + d, \frac{3}{4} - d], \\ 0 & \text{if } x \in [\frac{1}{4} + d, \frac{1}{2} - d] \cup [\frac{3}{4} + d, 1], \\ \frac{1}{2} - \frac{3}{4d}(x - \alpha) + \frac{1}{4d^3}(x - \alpha)^3 & \text{if } x \in [\alpha - d, \alpha + d], \text{ with } \alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{4} \end{cases}$$

and  $i_2(x) = 1 - i_1(x)$ . The splitting operators used in this example are  $A_1(x, y) = i_1(x)i_1(y)A$ ,  $A_2(x, y) = i_2(x)i_1(y)A$ ,  $A_3(x, y) = i_1(x)i_2(y)A$  and  $A_4(x, y) = i_2(x)i_2(y)A$  and the overlapping zones are again determined by  $d = \frac{1}{8}$ . In this experiment we consider the relations  $N^2\tau = 5.12$  and  $N^2\tau^2 = 0.1024$  for the time integrators of first and second order, respectively. Due, again, to the fact that the four totally discrete methods provide very similar maximum global errors, we only include in Table 1 the global errors for the methods with second order in time and in space. At last, in Table 2, we show the difference between the number of linear systems that we have to solve in each case. This number will again depend on the number of internal implicit stages of the time integrator used and on the average number of Schwarz iterations per stage (only for the case of classical domain decomposition techniques).

**Table 1.** Global errors

	N=16	N=32	N=64	N=128	N=256	N=512	N=1024
Example a)							
FSRK2	8.4121E-4	2.0942E-4	5.2304E-5	1.3072E-5	3.2678E-6	8.1695E-7	2.0424E-7
RK2	8.3353E-4	2.1018E-4	5.2758E-5	1.3213E-5	3.3063E-6	8.2692E-7	2.0678E-7
Example b)							
FSRK2	1.6364E-2	4.6055E-3	1.2801E-3	3.3917E-4	8.6694E-5	2.1794E-5	5.4278E-6
RK2	1.2747E-2	3.1979E-3	8.0116E-4	2.0049E-4	5.0130E-5	1.2501E-5	3.1254E-6

**Table 2.** Number of systems to solve

FSRK	RK	N=16	N=32	N=64	N=128	N=256	N=512	N=1024
Example a)								
order 2		2 6	2 6	2 6	2 6.1	2 6	2 6	2 4
order 3		6 30.9	6 34.5	6 31.8	6 32.6	6 28.5	6 24.4	6 24.1
order 4		8 76.4	8 81	8 82.2	8 77.6	8 77.7	8 72	8 73.2
Example b)								
order 1		16 96	16 80	16 48	16 48	16 32	16 32	16 32
order 2		24 80	24 88	24 64	24 64	24 48	24 64	24 64

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