Operator Splitting for stiff nonlinear reaction-diffusion systems : order reduction and application to spiral waves

Stéphane Descombes, Thierry Dumont, and Marc Massot

Abstract. This paper is concerned with the numerical analysis of nonlinear reaction-diffusion systems in the presence of fast scales in the reaction term. We analyse two different classes of schemes : implicit-explicit multistep methods and operator splitting. We then compare numerically these two classes on stiff and very stiff reaction-diffusion systems coming from nonlinear chemical kinetics (the Belousov-Zhabotinski reaction).

1. Introduction

Let d be an integer and ε a small parameter, we consider the following nonlinear reaction-diffusion system

$$\begin{cases} \dfrac{\partial u^\varepsilon}{\partial t} - \Delta u^\varepsilon = f(u^\varepsilon, v^\varepsilon), & x \in \mathbb{R}^d,\ t > 0, \\ \dfrac{\partial v^\varepsilon}{\partial t} - \Delta v^\varepsilon = \dfrac{g(u^\varepsilon, v^\varepsilon)}{\varepsilon}, & x \in \mathbb{R}^d,\ t > 0, \\ u^\varepsilon(0,x) = u_0(x), & x \in \mathbb{R}^d, \\ v^\varepsilon(0,x) = v_0(x), & x \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where f, g, u_0 and v_0 are smooth functions. We denote by $T_\varepsilon^t(u_0, v_0)$ the semiflow associated to (1.1). To solve numerically this system, there are several strategies in order to treat the induced stiffness. The most

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natural idea is to solve the complete system where diffusion and reaction are coupled together. Two main directions exists, the first one is to use fully implicit or semi-implicit methods. The second one is based on error estimates and local time adaptation; one can think of the method of lines in conjunction with a dedicated stiff ODE solver like LSODE [**9**] so that the time discretization and the spatial discretization are disconnected. The fully implicit method yields to the resolution of strongly coupled nonlinear systems, it is most of the time too costly, even with the use of adaptative time steps. The second type of method can only be used in some simplified situations with a few unknowns and in low dimensional situations, since the CPU cost becomes most of the time highly expensive. Thus the only way is then to use implicit-explicit multistep methods : the diffusive part of the equation is discretized implicitly and the reaction part explicitly. When $\varepsilon = O(1)$, it has been shown by Akrivis, Crouzeix and Makridakis in [**1**] that the resulting schemes are stable, consistent and very efficient, since their implementation requires at each time step the solution of linear systems with the same matrices for all time levels. But an interesting question is the capability of such schemes to handle a stiff reaction part, in other words, when assuming stability of the implicit scheme for the diffuse part might not be that enough to ensure stability of the implict-explicit scheme.

It is also natural to consider the possibility to use reduced models where the fastest chemical scales have been already relaxed [**8**]. These simplified models provide reasonable predictions when the fastest characteristic chemical times are small in comparison with the flow time, and the associated computational costs are significantly reduced in comparison with comprehensive chemical models. The derivation of the reduced model is usually accessible once the fast scales have been isolated and if the system is well-partitioned [**12**] and one can conduct rigourous singular perturbation analysis even in the context of nonlinear source terms [**11**]. The identification of these fast scales in terms of reaction rates or species, which can change with time, relies on sensitivity analysis, it is most of the time difficult to conduct and justify. It reveals the need for other strategies which do not rely on the knowledge of the fast scales.

Another idea is to use splitting methods [**10**] also called fractional step methods [**15**], these methods have been well known for a long time and there exists a large litterature showing the efficiency of such methods for evolutionary problems when $\varepsilon = O(1)$. However, the classical analysis of such methods fails in the presence of fast scales and an order reduction of these methods appears due to the stiffness of the reaction

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term [**3**]. We will prove in Section 2 that, in our case, one splitting method, the Strang formula, does not suffer from order reduction and is a good candidate for solving our problem when ε is very small.

As a conclusion, without requiring the knowledge of the fast scales and to limit the cost of computations, we have two possibilites : implicit-explicit methods and splitting methods. This paper is a comparison between these two methods on stiff problems.

An outline of the paper is as follows: In Section 2, we recall the definition of implicit-explicit multistep methods and splitting methods, specially the Strang formula, we analyse the local order of some splitting methods. In Section 3, we give some numerical results on the Oregonator problem. We show a good behaviour of the Strang splitting method and we show that to ensure the stability of implicit-explicit methods, we need a drastic condition on the step size.

2. Implicit-explicit multistep methods and splitting methods for reaction-diffusion system

2.1. Implicit-explicit multistep methods. Introduced in [**1**] by Crouzeix et *al*, the idea is to combine implicit and explicit multistep schemes to discretize (1.1) in time: implicit schemes are used for discretizing the diffusion part and explicit schemes for the reaction part. More precisely, denoting by Δt a constant time step, $t_n = n\,\Delta t$, $n = 0, \ldots, N$, $T = N\,\Delta t$, one defines a sequence of approximations $(U_\varepsilon^n, V_\varepsilon^n)$, of (u, v) at time t_n by

$$\sum_{i=0}^{q} \alpha_i \begin{pmatrix} U^{n+i} \\ V^{n+i} \end{pmatrix} - \Delta t \sum_{i=0}^{q} \beta_i \Delta \begin{pmatrix} U^{n+i} \\ V^{n+i} \end{pmatrix} = \Delta t \sum_{i=0}^{q-1} \gamma_i \begin{pmatrix} f(U^{n+i}, V^{n+i}) \\ \dfrac{g}{\varepsilon}(U^{n+i}, V^{n+i}) \end{pmatrix},$$

where α_i, β_i , $i = 1, \ldots, q$ and δ_i , $i = 1, \ldots, q-1$ are real numbers. In the case of $\varepsilon = O(1)$, as we mention in the Introduction, it has been shown in [**1**] under some conditions on the coefficients α_i, β_i , $i = 1, \ldots, q$, δ_i , $i = 1, \ldots, q-1$, that the resulting schemes are stable, consistent and very efficient, since their implementation requires at each time step the solution of a linear system with the same matrix for all time levels.

A simple example of implict-explicit method is the following

$$\frac{1}{\Delta t} \begin{pmatrix} U^{n+1} \\ V^{n+1} \end{pmatrix} - \frac{1}{\Delta t} \begin{pmatrix} U^{n} \\ V^{n} \end{pmatrix} - \Delta \begin{pmatrix} U^{n+1} \\ V^{n+1} \end{pmatrix} = \begin{pmatrix} f(U^n, V^n) \\ \dfrac{g}{\varepsilon}(U^n, V^n) \end{pmatrix},$$

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it is of order one. A more precise implicit-explicit scheme (i.e. of order 2) is a two-steps scheme defined by the following coefficients :

$$\alpha_0 = \frac{1}{2} \qquad \alpha_1 = -2 \qquad \alpha_2 = \frac{3}{2}, \tag{2.1}$$

$$\beta_0 = 0 \qquad \beta_1 = 0 \qquad \beta_2 = -1, \tag{2.2}$$

$$\gamma_0 = -1 \qquad \gamma_1 = 2. \tag{2.3}$$

We use this scheme in our numerical simulations.

2.2. Splitting methods. Let us introduce the classical decoupling of the diffusion and reaction parts of (1.1). More precisely, we denote by $X^t(u_0,\, v_0)$ the solution of the diffusion equation :

$$\begin{cases} \dfrac{\partial u_d^\varepsilon}{\partial t} - \Delta u_d^\varepsilon = 0, \quad x \in \mathbb{R}^d,\, t > 0, \\ \dfrac{\partial v_d^\varepsilon}{\partial t} - \Delta v_d^\varepsilon = 0, \quad x \in \mathbb{R}^d,\, t > 0, \end{cases} \tag{2.4}$$

with initial data $u_d(0,.) = u_0(.)$ and $v_d(0,.) = v_0(.)$; we also denote by $Y_\varepsilon^t(u_0,\, v_0)$ the solution of the reaction part where the x coordinate can be considered as a parameter :

$$\begin{cases} \dfrac{\partial \bar{u}_r^\varepsilon}{\partial t} = f(\bar{u}_r^\varepsilon, \bar{v}_r^\varepsilon), \quad x \in \mathbb{R}^d,\, t > 0, \\ \dfrac{\partial \bar{v}_r^\varepsilon}{\partial t} = \dfrac{g(\bar{u}_r^\varepsilon, \bar{v}_r^\varepsilon)}{\varepsilon}, \quad x \in \mathbb{R}^d,\, t > 0, \end{cases} \tag{2.5}$$

with initial data $\bar{u}_r^\varepsilon(0,.) = u_0(.)$ and $\bar{v}_r^\varepsilon(0,.) = v_0(.)$.

The two Lie approximation formulae of (1.1) are defined by :

$$L_{1\varepsilon}^t(u_0, v_0) = X^t Y_\varepsilon^t(u_0, v_0) \tag{2.6}$$

and

$$L_{2\varepsilon}^t(u_0, v_0) = Y_\varepsilon^t X^t(u_0, v_0) \tag{2.7}$$

and the two Strang approximation formulae of (1.1) [**13**] [**14**] are defined by :

$$S_{1\varepsilon}^t(u_0, v_0) = X^{t/2} Y_\varepsilon^t X^{t/2}(u_0, v_0) \tag{2.8}$$

and

$$S_{2\varepsilon}^t(u_0, v_0) = Y_\varepsilon^{t/2} X^t Y_\varepsilon^{t/2}(u_0, v_0). \tag{2.9}$$

When $\varepsilon = O(1)$, it is well know that Lie formulae (resp. Strang formulae) are an approximation of order 1 (reps. 2) of (1.1). But it has been shown in [**3**] that these schemes suffer from order reductions when ε is a small parameter, in fact the formal order of the scheme is less than

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the one obtained by the theory. We give in the next section a simple example of this order reduction.

2.3. An example of order reduction for splitting methods. We are considering a very simple case of an ordinary differential equation in $\mathbb{R}^3$, let A and P be the matrices defined by

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and } P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The system that we consider is the following

$$\begin{cases} \dot{U}_\varepsilon = AU_\varepsilon - \dfrac{P}{\varepsilon} U_\varepsilon, \\ U_\varepsilon(0) = U_0, \end{cases} \tag{2.10}$$

with exact solution

$$U_\varepsilon(t) = e^{t(A-P/\varepsilon)} U_0. \tag{2.11}$$

The Lie and Strang approximations of the previous system are defined by

$$\begin{aligned} L_{1\varepsilon}(t) =& e^{tA} e^{-tP/\varepsilon} U_0,\ L_{2\varepsilon}(t) = e^{-tP/\varepsilon} e^{tA} U_0, \\ S_{1\varepsilon}(t) =& e^{tA/2} e^{-tP/\varepsilon} e^{tA/2} U_0,\ S_{2\varepsilon}(t) = e^{-tP/2\varepsilon} e^{tA} e^{-tP/2\varepsilon} U_0. \end{aligned}$$

Introducing the matrix Q defined by $P+Q = \mathrm{Id}$, we have the following result :

THEOREM 2.1. *Let $t > 0$, for ε sufficiently small satisfying $\varepsilon << t$, we have the following estimates*

$$U_\varepsilon(t) - L_{1\varepsilon}(t) = -tPAQU_0 + O(e^{-t/\varepsilon}) \tag{2.12}$$

$$U_\varepsilon(t) - L_{2\varepsilon}(t) = -tQAPU_0 + O(e^{-t/\varepsilon}) \tag{2.13}$$

$$U_\varepsilon(t) - S_{1\varepsilon}(t) = \frac{t}{2}(2QAQ - QA - AQ) + O(e^{-t/\varepsilon}) \tag{2.14}$$

$$U_\varepsilon(t) - S_{2\varepsilon}(t) = -\frac{t^2}{2} QAPAQU_0 + O(e^{-t/\varepsilon}) \tag{2.15}$$

PROOF. We only prove estimate (2.15), the others can be obtain by the same ideas. By definition we have

$$e^{-tP/2\varepsilon} = \begin{pmatrix} e^{-t/2\varepsilon} & 0 & 0 \\ 0 & e^{-t/2\varepsilon} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.16}$$

thus

$$e^{-tP/2\varepsilon} = e^{-t/2\varepsilon} P + Q,$$

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this relation allows us to obtain

$$S_{2\varepsilon}(t) = Qe^{tA}QU_0 + O(e^{-t/2\varepsilon}). \tag{2.17}$$

We now perform the same computations with system (2.10). The decomposition

$$A - P/\varepsilon = \begin{pmatrix} 1-1/\varepsilon & 0 & 0 \\ 0 & 1-1/\varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = C + D,$$

with $[C, D] = 0$ allows us to write

$$e^{t(A-P/\varepsilon)} = e^{tD}e^{tC}$$

and finally

$$U_\varepsilon(t) = e^t e^{tD}QU_0 + O(e^{-t/\varepsilon}), \tag{2.18}$$

and thanks to the relation $e^t e^{tD}QU_0 = e^{tQAQ}QU_0$, we have

$$U_\varepsilon(t) = e^{tQAQ}QU_0 + O(e^{-t/\varepsilon}). \tag{2.19}$$

Thanks to (2.17) and (2.19), we obtain

$$\begin{aligned} U_\varepsilon(t) - S_{2\varepsilon}(t) &= e^{tQAQ}QU_0 - Qe^{tA}QU_0 + O(e^{-t/\varepsilon}) \\ &= U_0 - U_0 + t(QAQ - QAQ)QU_0 \\ &\quad + \frac{t^2}{2}(QAQAQU_0 - QA^2Q)QU_0 + O(e^{-t/\varepsilon}) \end{aligned}$$

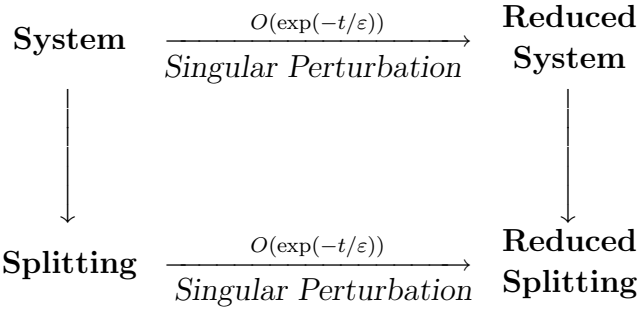
and this yields

$$U_\varepsilon(t) - S_{2\varepsilon}(t) = -\frac{t^2}{2}QAPAQU_0 + O(e^{-t/\varepsilon})$$

which proves (2.15). □

Remark 2.2. This theorem shows that in the presence of stiffness, Strang formula ending with the stiff part is the best candidate.

Remark 2.3. The proof of order reduction is based on the study of the difference of the two reduces problems and in fact follows the diagram



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The key point of this proof is the singular perturbation hypothesis (as in [**11**]) : the reduced problems are well-posed and the differences between all the problems and their reduced problems behave like $O(\exp(-t/\varepsilon))$.

In the next subsection, we study the eventual order reduction for Strang formula for the approximation of (1.1).

2.4. Local order study of the Strang formula. Since in our numerical simulations we use a Crank-Nicolson approximation of (2.4) defined by

$$\frac{1}{\Delta t}\begin{pmatrix} U^{n+1} \\ V^{n+1} \end{pmatrix} - \frac{1}{\Delta t}\begin{pmatrix} U^{n} \\ V^{n} \end{pmatrix} = \frac{1}{2}\Delta \begin{pmatrix} U^{n+1}+U^{n} \\ V^{n+1}+V^{n} \end{pmatrix},$$

it is suitable to study the scheme still denoted $S^t_{2\varepsilon}$ and defined by

$$S^t_{2\varepsilon}(u_0,v_0) = Y^{t/2}_{\varepsilon} X^t_{\mathrm{cn}} Y^{t/2}_{\varepsilon}(u_0,v_0) \tag{2.20}$$

with X^t_{cn} defined by

$$X^t_{\mathrm{cn}}(u_1,v_1) = \begin{pmatrix} L(t) & 0 \\ 0 & L(t) \end{pmatrix}\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}$$

with

$$L(t) = \left(\mathrm{Id} + \frac{t}{2}\Delta\right)\left(\mathrm{Id} - \frac{t}{2}\Delta\right)^{-1}.$$

For $\varepsilon = O(1)$, if we assume that f and g are C^∞ Lipschitz functions and that u_0 and v_0 belong to $H^2(\mathbb{R}^d)$, it has been shown in [**4**] that $S^t_{2\varepsilon}$ is an approximation of order 2 in time of (1.1), i.e. we have locally

$$\|T^t_{\varepsilon}(u_0,v_0) - S^t_{2\varepsilon}(u_0,v_0)\|_{L^2} = O(t^3). \tag{2.21}$$

An interesting result is that the order of approximation is the same even if ε is small.

THEOREM 2.4. *Assume that ε is a small parameter, under the previous hypothesis and assuming, as in* [**3**]*, that the reduced problems are well-posed in the sense of singular perturbation analysis, the approximation $S^t_{2\varepsilon}$ does not suffer from order reduction and* (2.21) *remains true.*

PROOF. We first introduce the reduced problem $T^t u_0$ associated to (1.1), there exists a unique C^∞ function h such that $g(u,v) = 0$ is equivalent to $v = h(u)$, the reduced problem (which only depends on

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u_0) reads :

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = G(u), & x \in \mathbb{R}^d,\ t > 0, \\ u(0,x) = u_0(x), & x \in \mathbb{R}^d, \\ v(t,x) = h(u(t,x)), & x \in \mathbb{R}^d,\ t \geq 0; \end{cases} \tag{2.22}$$

to simplify the notations, we have written $G(u) = f(u, h(u))$. The reduced system of the reaction term can be written :

$$\begin{cases} \dfrac{d\bar{u}}{dt} = G(\bar{u}) & t > 0, \\ \bar{u}(0) = \bar{u}_0, \\ \bar{v}(t) = h(\bar{u}(t)), & t \geq 0, \end{cases} \tag{2.23}$$

we denote by $Y_u^t u_0$ the first component of the solution $(\bar{u}(t), \bar{v}(t))$ of (2.23). To study the order of approximation of T_ε^t by the Strang formula $S_{2\varepsilon}^t$, we first investigate the order of approximation of T^t by the reduced splitting scheme. We thus define :

$$(u_{\text{err}}, v_{\text{err}}) = T^t u_0 - S_2^t u_0.$$

By definition u_{err1} is the difference between u solution of (2.22) and the term $Y_u^{t/2} X_{\text{cn}}^t Y_u^{t/2} u_0$ thus u_{err1} is the usual error between the Strang (modified with Crank-Nicolson scheme) formula and u. Thanks to the result of [**4**], the estimate (2.21) remains true for the slow variable u. Let us mention that the key point is that the diffusive part does not couple the slow and fast variables.

We now turn to the results for the fast variable : for t sufficently small, the local error for the Strang formula on the fast variable satisfies :

$$v_{\text{err}} = h(u) - h(Y_u^{t/2} X_{\text{cn}}^t Y_u^{t/2} u_0),$$

and since h is a C^∞ Lipschitz function, it is clear that v_{err} has the same behaviour as u_{err}. Let us now come back to the case $\varepsilon \neq 0$, we have

$$\begin{aligned} T_\varepsilon^t(u_0, v_0) - S_{2\varepsilon}^t(u_0, v_0) =& T_\varepsilon^t(u_0, v_0) - (T^t u_0, h(T^t u_0))^t + (u_{\text{err}}, v_{\text{err}})^t \\ &+ (Y_u^{t/2} X_{\text{cn}}^t Y_u^{t/2} u_0, h(Y_u^{t/2} X_{\text{cn}}^t Y_u^{t/2} u_0))^t - S_{2\varepsilon}^t(u_0, v_0). \end{aligned}$$

The second term of the right hand side is estimated in the previous result and coupling the results of [**2**] and [**3**], the two others term are bounded by $O\left(\exp\left(-Ct/\varepsilon\right)\right) + O(\varepsilon)$. This concludes the proof of theorem 2.4. □

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3. Numerical illustrations

In this section, we are concerned with the numerical approximation of some models coming from nonlinear chemical dynamics, the Belousov-Zhabotinski reaction, a catalyzed oxidation of an organic species by acid bromate ion, for more details in illustations, see [**5**]. We first consider the two-variable Oregonator model, studied in [**6**], it has solutions that represent propagation of a steep wave front by interplay of $HBrO_2$ (hypobromous acid) diffusion with an autocatalytic reaction that quickly generates $HBrO_2$ (using bromide ions Br^- as an intermediary species that remains always in equilibrium with local instantaneous $HBrO_2$). Denoting by $b = [HBrO_2]$ and $c = [Br^-]$, we consider the following model :

(3.1)
$$\begin{cases} \dfrac{\partial b}{\partial t} - D_b \Delta b = \dfrac{1}{\varepsilon}\left(b - b^2 - f\,c\,\left(b + \dfrac{q}{b-q}\right)\right), & x \in \mathbb{R}^2,\ t > 0, \\ \dfrac{\partial c}{\partial t} - D_c \Delta c = b - c, & x \in \mathbb{R}^2,\ t > 0, \end{cases}$$

with

$$D_b = 2,5.10^{-3},\ D_c = 1,5.10^{-3}\ f = 1.6\ q = 2.10^{-3}\ \varepsilon = 10^{-2}.$$

A more refined model, introduced in [**7**] and coming from the classic work of Field, Körös and Noyes (FKN)(1972), takes into account not only the two species $HBrO_2$ and Br^- but also the cerium(IV). Denoting by $a = [\text{Ce(IV)}]$, we obtain a vey stiff system of three partial differential equations

(3.2)
$$\begin{cases} \dfrac{\partial a}{\partial t} - D_a \Delta a = \dfrac{1}{\mu}\left(a\,b - a\,q - f\,c\right), & x \in \mathbb{R}^2,\ t > 0, \\ \dfrac{\partial b}{\partial t} - D_b \Delta b = \dfrac{1}{\varepsilon}\left(b - b^2 - a\,(b+q)\right), & x \in \mathbb{R}^2,\ t > 0, \\ \dfrac{\partial c}{\partial t} - D_c \Delta c = b - c, & x \in \mathbb{R}^2,\ t > 0, \end{cases}$$

with

$$D_a = 2,5.10^{-3},\ \mu = 10^{-5}.$$

We have computed an "exact" solution of the two problems by finite difference discretization in space on a 120×120 grid and the use of LSODE for solving the system of ODE obtained after discretization. The following pages contain the graphs of the various variables involved in both models with two and three chemical species as well as the comparison between the exact solution and the solutions computed

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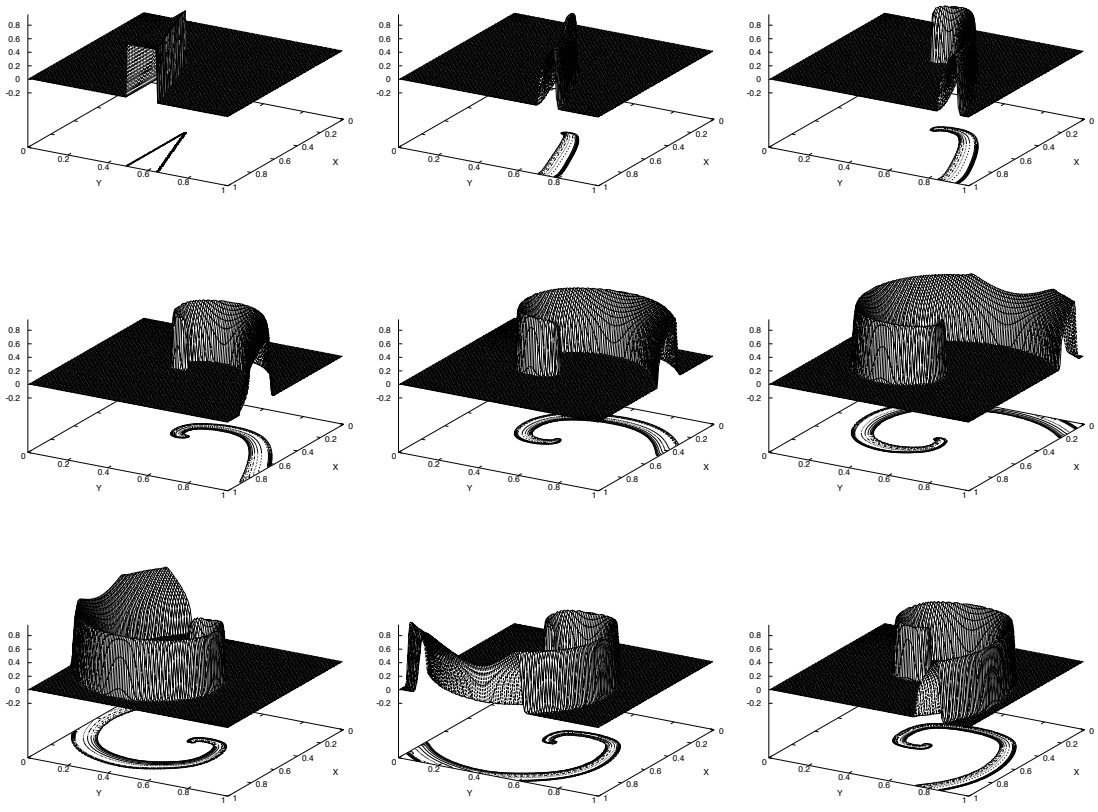


FIGURE 1. Two-variables system, evolution of the variable b.

either with the Strang splitting or the implicit-explicit method. The time interval considered for this purpose is $[0, 4]$; the initial data are discontinuous and can not be handled by the implicit-explicit method whereas this case can be treated by the splitting method. Consequently for comparaison purposes, we have chosen to start the simulations with both numerical methods from the time $t = 0.5$ and to evaluate the difference with the "exact" solution at further times.

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	Splitting method		Implicit-explicit method	
t	Variable b	Variable c	Variable b	Variable c
1.0	0.00032390	0.00011732	0.00021633	7.9144e-05
1.5	0.00041503	0.00015030	0.00024652	8.9992e-05
2.0	0.00061965	0.00023190	0.00042127	0.00015898
2.5	0.00087475	0.00031532	0.00065399	0.00023631
3.0	0.00070172	0.00026740	0.00053277	0.00020293
3.5	0.00078809	0.00025690	0.00058653	0.00019151
4.0	0.00076141	0.00029546	0.00054120	0.00021087

TABLE 1. Errors in the computations when $\Delta t = 1.25\ 10^{-4}$

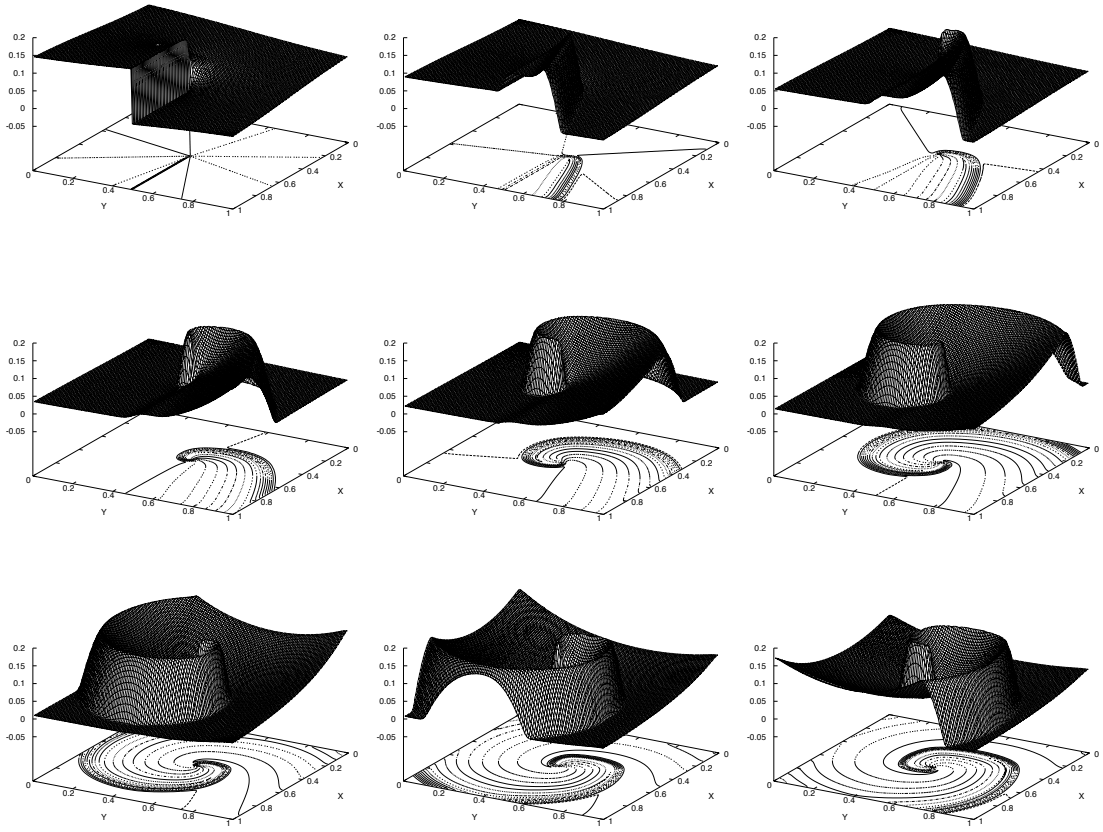


FIGURE 2. Two-variables system, evolution of the variable c.

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	Splitting method		Implicit-explicit method	
t	Variable b	Variable c	Variable b	Variable c
1.0	0.0017115	0.0006101	nan	
1.5	0.0031170	0.0011470	nan	
2.0	0.0052246	0.0019515	nan	
2.5	0.0072773	0.0026890	nan	
3.0	0.0073482	0.0028322	nan	
3.5	0.0097870	0.0033560	nan	
4.0	0.0122379	0.0046812	nan	

TABLE 2. Errors in the computations when $\Delta t = 10^{-3}$

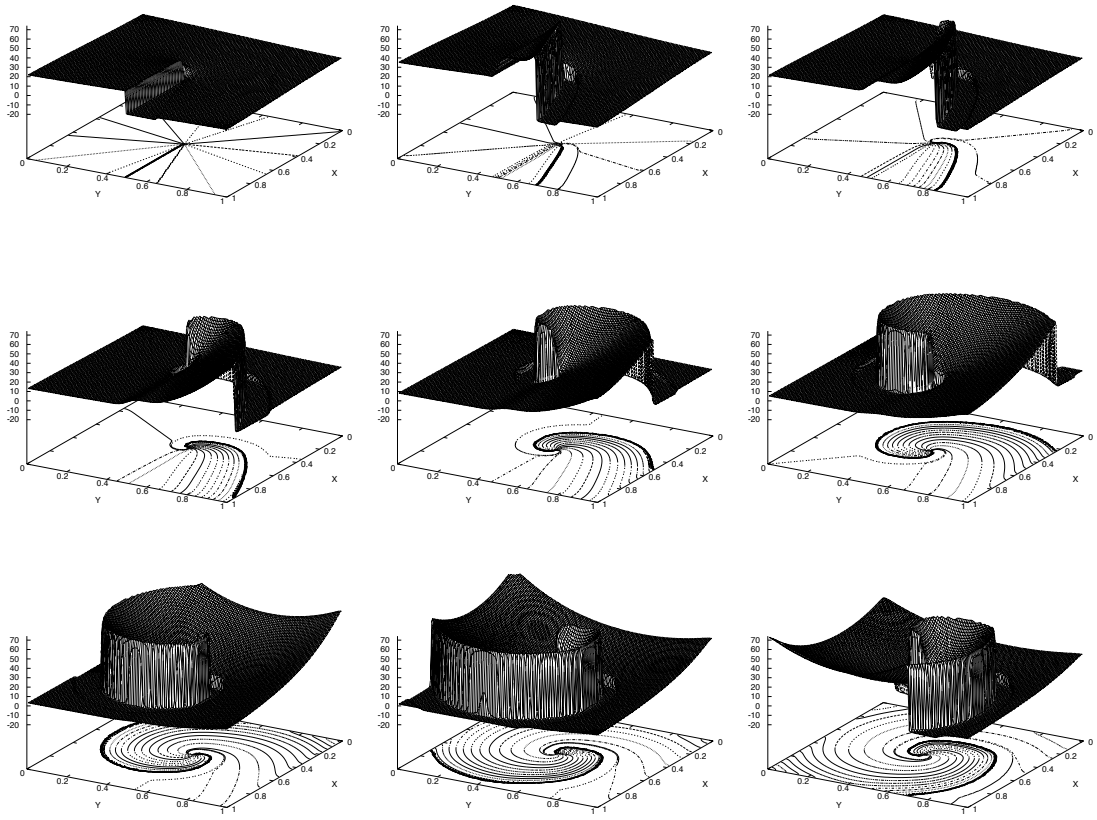


FIGURE 3. Three-variables system, evolution of the variable a.

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	Splitting method			Implicit-explicit method		
t	Variable a	Variable b	Variable c	Var. a	Var. b	Var. c
1.0	0.0005289	0.00030128	0.00011420	nan		
1.5	0.0005724	0.00035616	0.00013211	nan		
2.0	0.0009549	0.00058686	0.00021545	nan		
2.5	0.0018741	0.00087294	0.00030569	nan		
3.0	0.0012878	0.00068979	0.00025623	nan		
3.5	0.0014290	0.00069288	0.00024154	nan		
4.0	0.0010484	0.00070439	0.00028174	nan		

TABLE 3. Errors in the computations when $\Delta t = 1.25\ 10^{-4}$

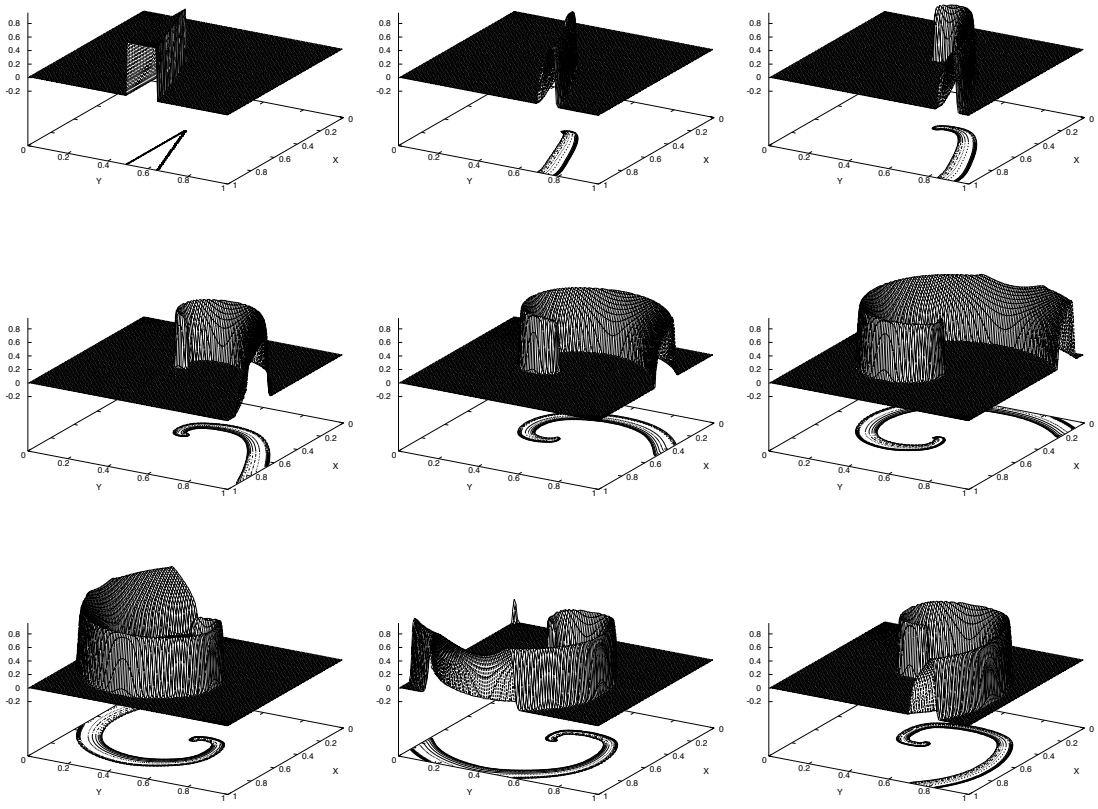


FIGURE 4. Three-variables system, evolution of the variable b.

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	Splitting method			Implicit-explicit method		
t	Variable a	Variable b	Variable c	Var. a	Var. b	Var. c
1.0	0.0021828	0.0012266	0.00046654	nan		
1.5	0.0021897	0.0014792	0.00054826	nan		
2.0	0.0042770	0.0032539	0.0011895	nan		
2.5	0.0107966	0.0053699	0.0018828	nan		
3.0	0.0099095	0.0056984	0.0021364	nan		
3.5	0.0126072	0.0073398	0.0025357	nan		
4.0	0.0131397	0.0089194	0.0035895	nan		

TABLE 4. Errors in the computations when $\Delta t = 10^{-3}$

In conclusion, we can notice that the implict-explicit method requires in the two-variables case a very small step time, having in fact the same order of magnitude as ε, a condition which becomes irrealistic in the second case since $\mu = 10^{-5}$. On the contrary, the splitting method is shown to be very robust; it gives good results in all cases and in the second case, the very stiff one, we can see a very good approximation of the wave speed. As far as the computational cost is concerned, the time required to solve the diffusion phenomenon is the same for both methods; the reactive part, however requires only one evaluation of the source term in the implicit explicit method, whereas it takes many evaluations in the splitting method for the newton iterations. Consequently, even if the splitting method required much less time than would require a fully implicit method, it is comparable but longer than the implicit-explicit method for a single time step. Nevertheless, it becomes much more efficient in the configuration we have chosen since the splitting time step can be taken 100 time bigger than the one for the implicit-explicit method. Moreover, the resolution of the reactive part could be very easily parallelized and would provide a nice improvement if the number of chemical species would increase a lot. It has to be noticed that the system with three variables is a very difficult problem; the splitting method behaves remarkedly well in this case and reveals itself as a very good candidate in order to treat problems involving complex chemistry with large time scale spectra. In such a case, the reference solver will be the fully implicit one with

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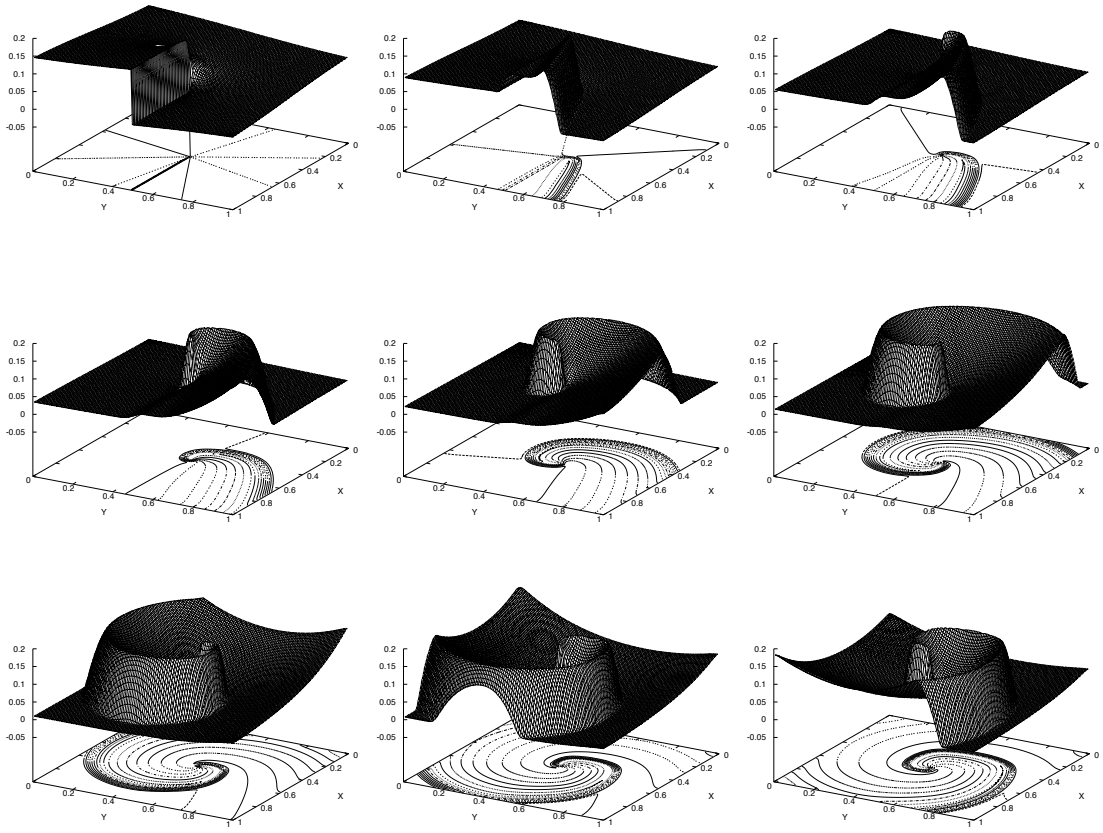


FIGURE 5. Three-variables system, evolution of the variable c.

adaptive time steps and we would need the possibility to adapt the splitting time step for comparison purposes; this is the topic of our current research.

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