Analysis of operator splitting order reduction in the non-asymptotic regime for reaction-diffusion equations

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Centre de Mathématiques Appliquées, Ecole Polytechnique

MAP551. Systèmes dynamiques pour la modélisation et la simulation des milieux réactifs multi-échelles (2018-2019)

Outline

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Application Background

Numerical simulation of unsteady reactive fronts

- Flames (Instabilities, dynamics, pollutants)
- Chemical "waves" (spiral waves, scroll waves)
- Biochemical Engineering (migraines, Rolando's region, Strokes)

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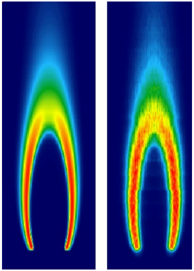

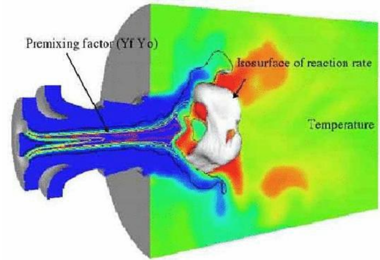

Yale University and CERFACS

Unsteady flames (S. Ducruix, S. Candel, N. Tran, EM2C)

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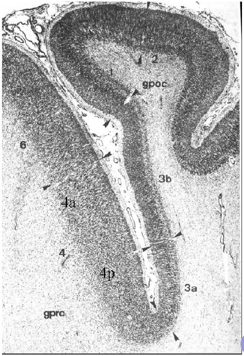

Potassium ions during stroke (T. Dumont, ICJ)

Characterization of such systems

$\hookrightarrow$ Dynamics involving many species and reactions : **complex chemistry**

$\hookrightarrow$ Solution with **high spatial gradients** associated with the presence of fronts

Time and space multi-scales unsteady problems

Pagoda Flame (D. Durox, S. Ducruix, S. Candel)

Need for **dedicated solver** able to solve a large scale spectrum and large spatial gradients on multi-dimensional configuration

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Convection-diffusion coupled to chemistry

$$\partial_t U + \sum_{i \in C} \partial_i \big(\Phi_i(U, \partial_{\boldsymbol{x}} U)\big) = \Omega(U)$$

- KPP or Fischer equation

$$\partial_t \beta - \partial_{xx} \beta = \beta^2 (1 - \beta)$$

Explicit travelling wave solution with velocity $c = 1/\sqrt{2}$ and maximal gradient $1/\sqrt{32}$.
Phase space analysis :

$$\mathrm{d_x} \beta^{\mathrm{TW}} = \beta^{\mathrm{TW}} (1 - \beta^{\mathrm{TW}})/\sqrt{2}$$

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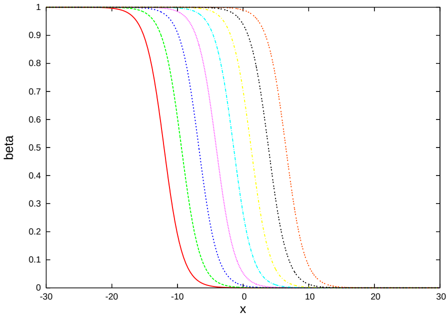

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$$\partial_t b - D_b \, \Delta \, b = \frac{1}{\varepsilon} \left(b - b^2 - f\, c \, (\frac{b+q}{b-q}) \right)$$

$$\partial_t c - D_c \, \Delta \, c = b - c$$

$\varepsilon = 0.01$, $D_b = 1.0$, $D_c = 0.6$, $f = 1.6$, $q = 0.002$ $\mu = 10^{-5}$

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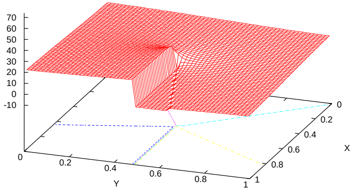

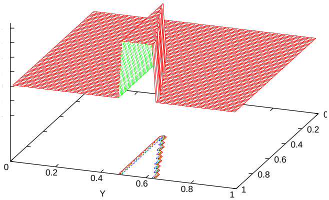

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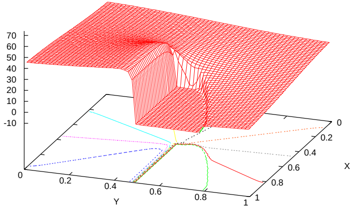

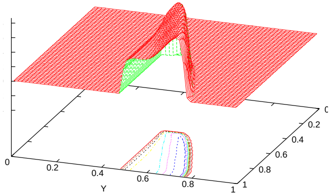

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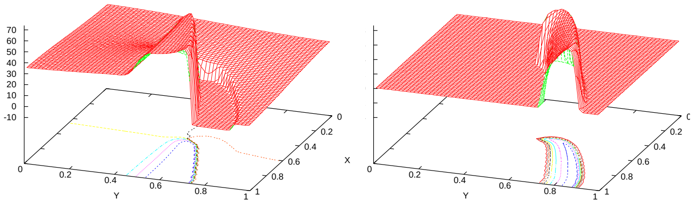

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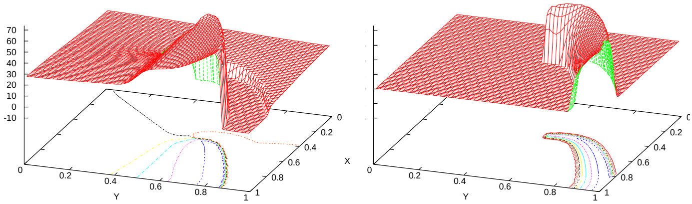

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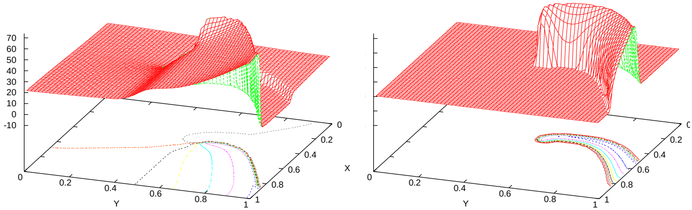

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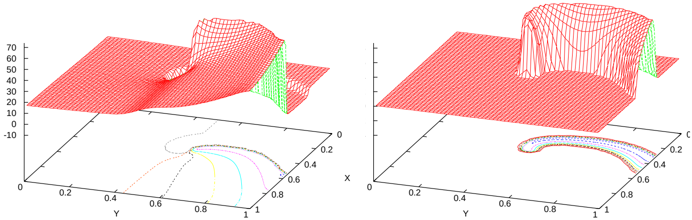

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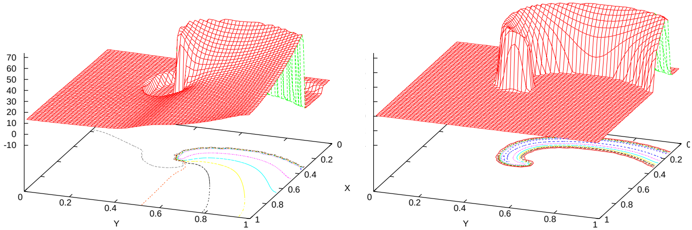

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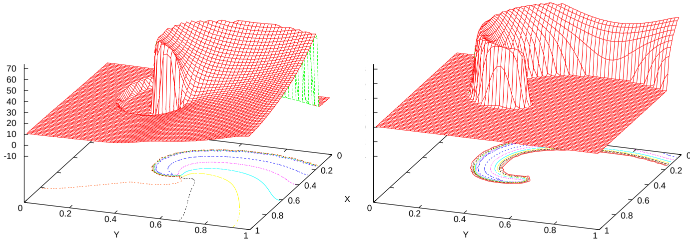

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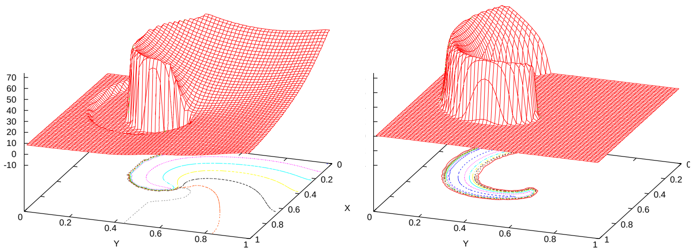

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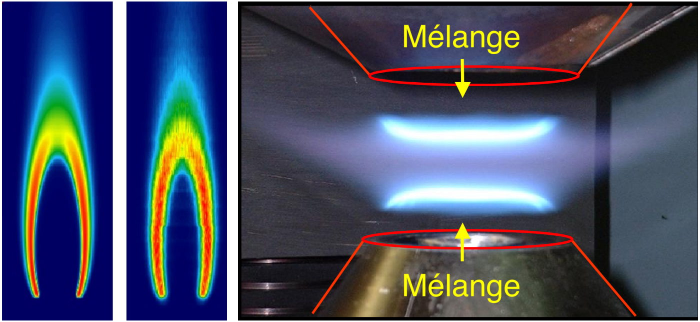
- Low Mach number reacting flows
  (low speed deflagrations : premixed flames - Yale University - EM2C)



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- Low Mach - planar flame with simple chemistry (Veynante - Poinsot 2005) Le = 1

$$\partial_t \theta - \partial_{xx} \theta = -\omega(\theta, \bar{Y}_F, \bar{Y}_O)$$

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$$\omega(\theta) = \exp\left(-T_a/(T_0 + \frac{Q}{C_p} Y_F^0 \theta)\right) \frac{L^2}{\kappa} B\, \bar{Y}_F \bar{Y}_O^{1/2}$$

$T_a = 10055K$, $T_0 = 300K$, $L = 4mm$, $Q/C_p = 34550K$, $Y_F^0 = 0.0583$, $Y_O^1 = 0.29167$, $\kappa = 2.26 10^{-5} m^2.s^{-1}$, $\phi = 0.8$, $B_1 = 10^7$

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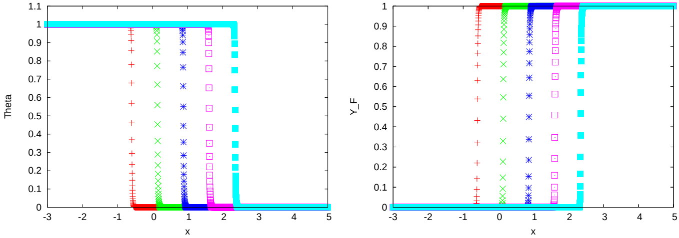

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Temperature Field ignited by a hot spot Fuel Mass Fraction

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Exemples des besoins de simulations intensives

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- DNS de flammes turbulentes non-prémélangées (3D with chemistry of “simple” fuel, Y. Mizobuchi et al.)
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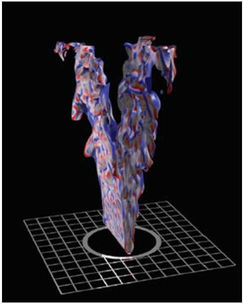

Besoin de solveurs dédié de type “simulation directe”

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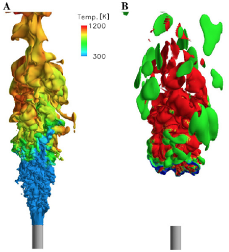

Fig. 12. Overview of the simulated hydrogen jet lifted flame. (A) Instantaneous iso-surface of the hydrogen mole fraction at 60% with the temperature distribution on the surface. (B) Instantaneous iso-surface of hydrogen consumption rate at 10^4 mol/s/m^3, where the surface color presents the combustion mode: red, rich premixed; blue, lean premixed; and green, diffusive.

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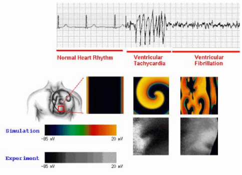

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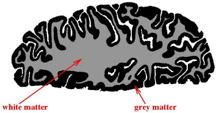

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Outline

1. Context and Motivation
   - Unsteady reactive fronts
   - Reaction-Convection-Diffusion Systems
   - Time integration numerical strategies
2. Operator splitting and stiffness
   - Standard numerical analysis of operator splitting
   - Stiffness comes into play
   - Splitting local error analysis for PDEs
3. Illustrating numerical simulations
   - “Toy” system with and without cross-diffusion
   - BZ system in two dimensions
   - KPP, Stiff KPP and Combustion waves with simple chemistry
   - Premixed counterflow flames with complex chemistry and transport

Strategies

Resolving the large scale spectrum coupled

- Explicit methods in time (high order in space)
- Fully implicit methods with adaptive time stepping
- Semi-implicit methods (source explicit in time)
- Method of lines coupled to a stiff ODE solver

The computational cost and memory requirement have suggested the study of alternative methods : decoupling

- Reduction of chemistry (large litterature)
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Operator splitting : separate convection-diffusion and chemistry

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- Allow the use of dedicated solver for each step
- Yield lower storage and optimization capability

This methods are already used for flame computation

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Bring some **theoretical insight** using **numerical analysis for model REACTION-DIFFUSION systems**

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Bring some **theoretical insight** using **numerical analysis for model REACTION-DIFFUSION systems**

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Operator splitting : separate convection-diffusion and chemistry

- High order methods exist
- Allow the use of dedicated solver for each step
- Yield lower storage and optimization capability

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Outline

Basis of operator splitting I

Reaction-diffusion system to be solved (t : time interval)

$$U(t) = T^t U_0 \quad \begin{cases} \partial_t U - \Delta U = \Omega(U) \\ U(0) = U_0 \end{cases}$$

Two elementary "blocks".

$$V(t) = X^t V_0 \quad \begin{cases} \partial_t V - \Delta V = 0 \\ V(0) = V_0 \end{cases}$$

$$W(t) = Y^t W_0 \quad \begin{cases} \partial_t W = \Omega(W) \\ W(0) = W_0 \end{cases}$$

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Basis of operator splitting II

First order methods, Lie formalism :

Lie Formulae.

$$L_1^t\, U_0 = X^t\, Y^t\, U_0 \qquad L_1^t - T^t = O(t^2),$$

$$L_2^t\, U_0 = Y^t\, X^t\, U_0 \qquad L_2^t - T^t = O(t^2),$$

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Basis of operator splitting III

Second order methods, Strang formalism :

Strang Formulae.

$$S_1^t\, U_0 = Y^{t/2}\, X^t\, Y^{t/2}\, U_0 \qquad S_1^t - T^t = O(t^3),$$

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Higher order

$$Z^t = \frac{4}{3}\, S^{t/2}\, S^{t/2} - \frac{1}{3}\, S^t \qquad Z^t - T^t = O(t^5),$$

Key assumption : continuity at $t = 0$
i.e. no faster scales than the splitting time step t

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Outline

Background

- Detected by the beginning of 90'
  (Hairer Wanner 91, D'Angelo Larrouturou 95)
- Numerical analysis of linear model ODEs
  (Verwer Sportisse 00)
- Ropp et al., SANDIA

Various origins of stiffness

- **Large spectrum of temp. scales in chemical source** (see reference Descombes, Massot, Numerische Mathematik, 2004)
- **High spatial gradient** (see reference Descombes, Dumont, Louvet, Massot, International Journal of Computer Mathematics, 2007)

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Outline

1. Context and Motivation
   - Unsteady reactive fronts
   - Reaction-Convection-Diffusion Systems
   - Time integration numerical strategies
2. Operator splitting and stiffness
   - Standard numerical analysis of operator splitting
   - Stiffness comes into play
   - Splitting local error analysis for PDEs
3. Illustrating numerical simulations
   - "Toy" system with and without cross-diffusion
   - BZ system in two dimensions
   - KPP, Stiff KPP and Combustion waves with simple chemistry
   - Premixed counterflow flames with complex chemistry and transport

Singular perturbation

On montre que le système de réaction diffusion général peut se mettre sous la forme $U^\varepsilon = (u^\varepsilon, v^\varepsilon)^t$

$$\begin{cases} \partial_t u^\varepsilon - \partial_x \cdot (B^u(u^\varepsilon, v^\varepsilon)\, \partial_x U^\varepsilon) & = f(u^\varepsilon, v^\varepsilon), \quad x \in \mathbb{R}^d \\ \partial_t v^\varepsilon - \partial_x \cdot (B^v(u^\varepsilon, v^\varepsilon)\, \partial_x U^\varepsilon) & = \dfrac{g(u^\varepsilon, v^\varepsilon)}{\varepsilon}, \quad x \in \mathbb{R}^d \end{cases}$$

- La structure entropique permet de définir proprement le modèle réduit et la théorie de perturbation singulière pour le système d'EDP

$$\partial_t u - \partial_x \cdot \left(B^u(u, h(u))\, \partial_x \begin{pmatrix} u \\ h(u) \end{pmatrix} \right) = f(u, h(u)),$$

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Analyse Numérique : Principe

$$
\begin{tikzcd}
\textbf{Système} \arrow[rr, "O(\varepsilon)+O(\exp(-\delta t/\varepsilon))", "\textit{Pert. Sing.}"'] \arrow[d, "\textit{Sép.}"'] & & \textbf{Système Réduit} \arrow[d, "\textit{Sép.}"'] \\
\textbf{Système Séparé} \arrow[rr, "O(\varepsilon)+O(\exp(-\delta t/\varepsilon))", "\textit{Pert. Sing.}"'] & & \textbf{Système Séparé/Réduit}
\end{tikzcd}
$$

Analyse Numérique : Notations

$$U^\varepsilon(t) = \begin{pmatrix} u^\varepsilon \\ v^\varepsilon \end{pmatrix} = T^t_\varepsilon \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \qquad \begin{cases} \partial_t u^\varepsilon - \Delta u^\varepsilon = f(u^\varepsilon, v^\varepsilon) \\ \partial_t v^\varepsilon - \Delta v^\varepsilon = \dfrac{g(u^\varepsilon, v^\varepsilon)}{\varepsilon} \end{cases}$$

$$V(t) = \begin{pmatrix} u \\ v \end{pmatrix} = X^t V_0 \qquad \partial_t V - \Delta V = 0$$

$$\bar{U}^\varepsilon(t) = \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix} = Y^t_\varepsilon \bar{U}_0 \qquad \begin{cases} \partial_t \bar{u}^\varepsilon = f(\bar{u}^\varepsilon, \bar{v}^\varepsilon) \\ \partial_t \bar{v}^\varepsilon = \dfrac{g(\bar{u}^\varepsilon, \bar{v}^\varepsilon)}{\varepsilon} \end{cases}$$

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Erreur sur les systèmes réduits

Théorème :

$$\begin{pmatrix} u_{err1} \\ v_{err1} \end{pmatrix} = T^t - X^t\, Y^t \begin{pmatrix} u_0 \\ h(u_0) \end{pmatrix}$$

$$||u_{err1}||_{L^2} = O(t^2), \quad v_{err1} = -t\, h''(u_0)(\partial_x u_0)^{\otimes 2} + O(t^2)$$

$$\begin{pmatrix} u_{err2} \\ v_{err2} \end{pmatrix} = T^t - Y^t\, X^t \begin{pmatrix} u_0 \\ h(u_0) \end{pmatrix}$$

$$||u_{err2}||_{L^2} = O(t^2), \quad ||v_{err2}||_{L^2} = O(t^2)$$

Erreur sur les systèmes réduits

Théorème :

$$\begin{pmatrix} u_{err3} \\ v_{err3} \end{pmatrix} = T^t - X^{t/2}\, Y^t\, X^{t/2} \begin{pmatrix} u_0 \\ h(u_0) \end{pmatrix}$$

$$||u_{err3}||_{L^2} = O(t^3),\; v_{err3} = -t/2\, h''(u_0)(\partial_x u_0)^{\otimes 2} + O(t^2)$$

$$\begin{pmatrix} u_{err4} \\ v_{err4} \end{pmatrix} = T^t - Y^{t/2}\, X^t\, Y^{t/2} \begin{pmatrix} u_0 \\ h(u_0) \end{pmatrix}$$

$$||u_{err4}||_{L^2} = O(t^3), \quad ||v_{err4}||_{L^2} = O(t^3)$$

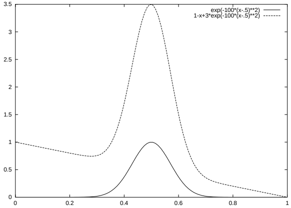
Outline

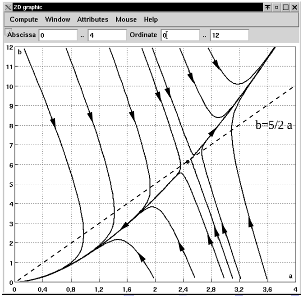
"Toy" model

$$
\begin{cases}
\partial_t a - \Delta a \quad -\eta \Delta b = k_a \left(b - \frac{5}{2} a\right), \\
\partial_t b \qquad\qquad - \quad \Delta b = k_b \dfrac{a^2 - b}{\varepsilon}, \\
\quad b(0,x) \quad = \exp\left(-100\,(x - \frac{1}{2})^2\right), \\
\quad a(0,x) \quad = 1 - x + 3\, b(0,x),
\end{cases}
$$

Cross-diffusion : $\eta = 0$ or $\eta = 1/5$

100 pts, time 0.1, $\Delta t = 0.1/16 - 0.1/256$





"Toy" model

Slow variable a

$t * 100$	*DRD withoutdiff*	*RDR withoutdiff*	*DRD withdiff*	*RDR withdiff*
1.25	1.9081	1.8793	1.1007	0.9874
2.50	1.8603	1.9031	1.0195	1.0168
3.75	1.7997	1.9577	1.0291	1.0164
5.00	1.7383	2.0297	1.0021	1.0185
6.25	1.6894	2.1004	0.9527	1.0294
7.50	1.6560	2.1476	0.9184	1.0397
8.75	1.6339	2.1793	0.9151	1.0485

Diag. Diffusion : no order loss on the slow variable!
Cross-diffusion : 1 order is lost for both DRD and RDR

"Toy" model

Fast variable b

$t * 100$	*DRD withoutdiff*	*RDR withoutdiff*	*DRD withdiff*	*RDR withdiff*
1.25	1.0255	2.0065	1.1026	0.9903
2.50	1.0029	1.9407	1.0411	1.0124
3.75	0.9829	1.8247	1.0147	1.0116
5.00	0.9513	1.7432	1.0119	1.0111
6.25	0.9054	1.6876	1.0025	1.0199
7.50	0.8525	1.6523	0.9866	1.0305
8.75	0.8293	1.6297	0.9643	1.0405

Diag. Diffusion : no order loss for RDR - order loss for DRD!
Cross-diffusion : 1 order is lost for both DRD and RDR

Outline

Belousov-Zhabotinsky system of equations

Belousov-Zhabotinsky system of equations
Nonlinear chemical dynamics

(Dpt Chemical Engineering Leeds - Ferroin on a nafion membrane)

Belousov-Zhabotinsky system of equations

Two variables b semi-fast and c slow:

$$\partial_t b - D_b \, \Delta \, b = \frac{1}{\varepsilon} \left(b - b^2 - f \, c \, (\frac{b+q}{b-q}) \right)$$

$$\partial_t c - D_c \, \Delta \, c = b - c$$

Three variables a fast, b semi-fast and c slow:

$$\partial_t a - D_a \, \Delta \, a = \frac{1}{\mu} \left(a \, (b - q) - f \, c \right)$$

$$\partial_t b - D_b \, \Delta \, b = \frac{1}{\varepsilon} \left(b - b^2 - a \, (b + q) \right)$$

$$\partial_t c - D_c \, \Delta \, c = b - c$$

(Oregonator model Jahnke Skaggs Winfree 89, Epstein Pojman 98, Gray Scott 94) b : hypobromous acid, c : bromide ions – a :cerium IV (Field Köros Noyes 72)
$\varepsilon = 0.01$, $D_b = 1.0$, $D_c = 0.6$, $f = 1.6$, $q = 0.002$, $\mu = 1.e-5$

Belousov-Zhabotinsky system of equations

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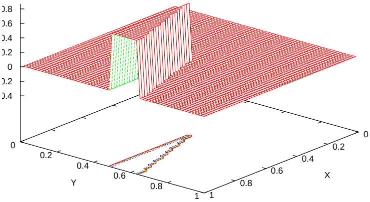
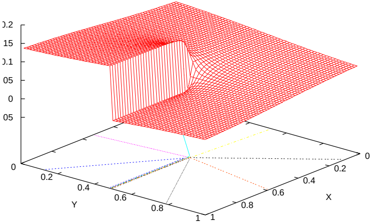
BZ "quasi-exact" solution

Belousov-Zhabotinsky system of equations with two variables *b* and *c*





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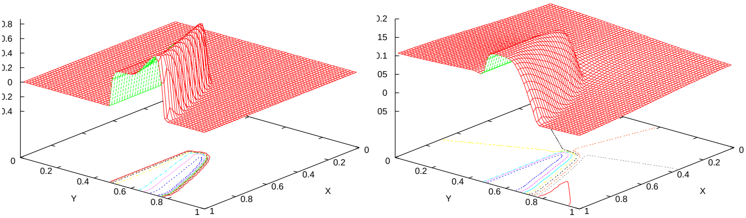

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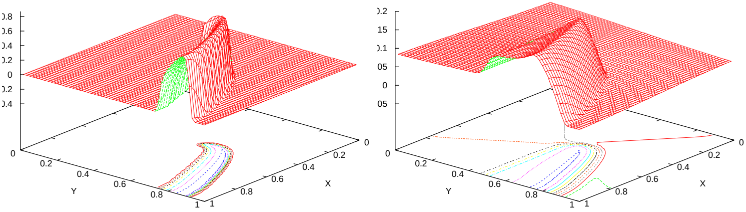

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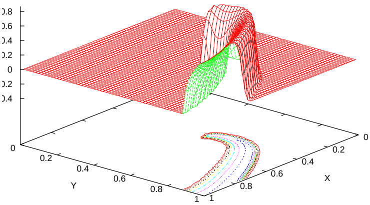

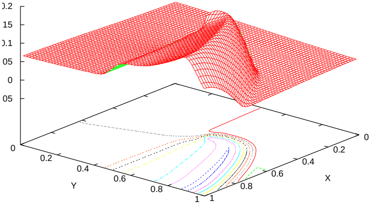

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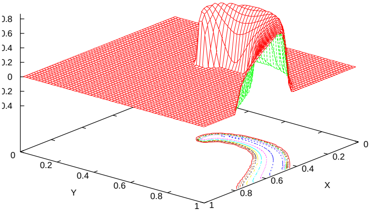

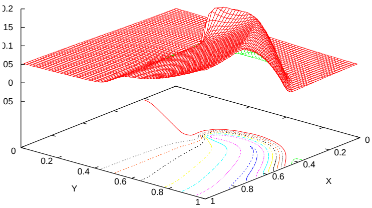

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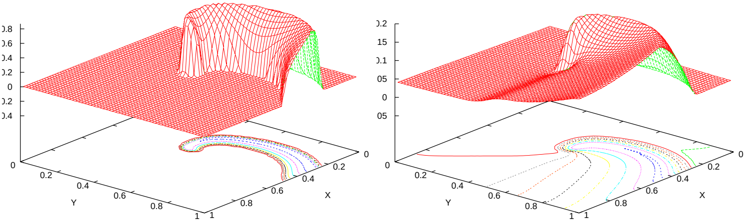

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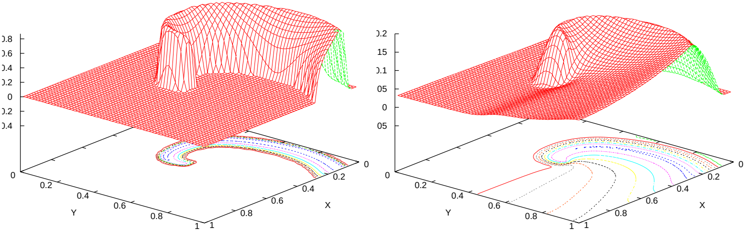

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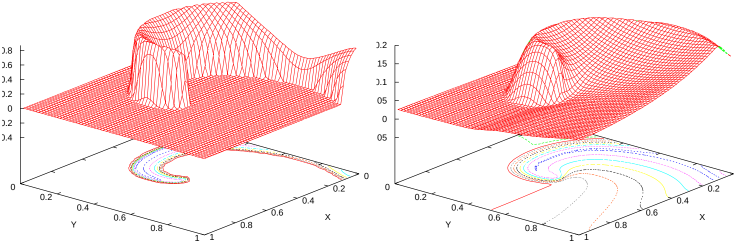

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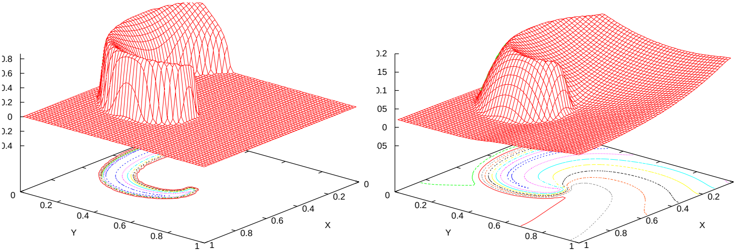
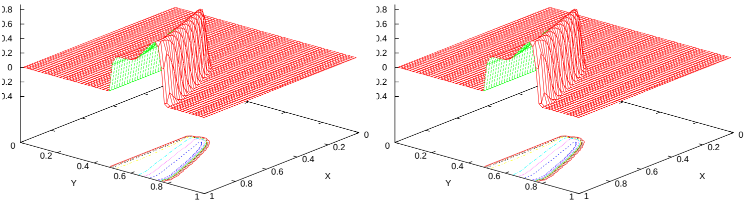


BZ with Strang Splitting RDR

BZ system with 2 variables
Strang Splitting for the *b* variable $\Delta t = 2/256$



BZ with Strang Splitting RDR

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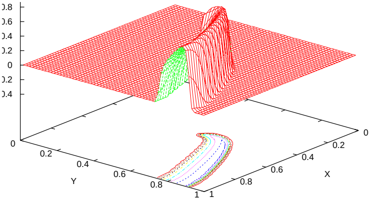
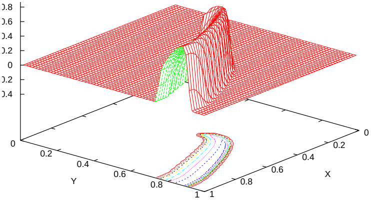
Strang Splitting for the b variable $\Delta t = 2/256$





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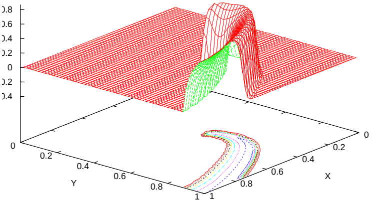

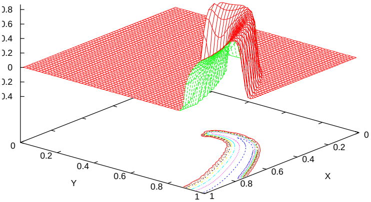

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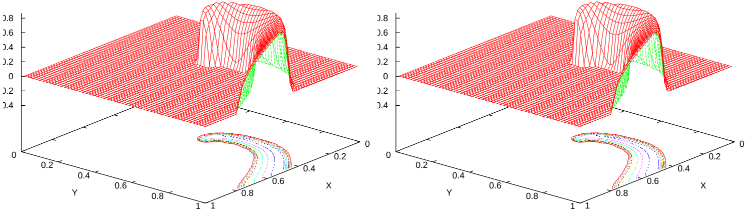

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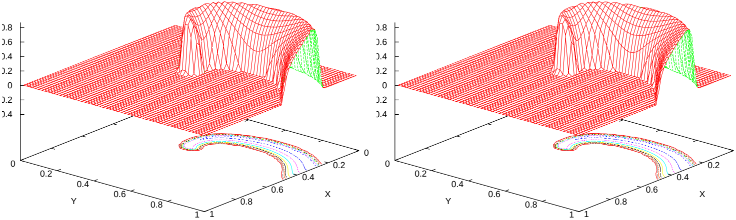

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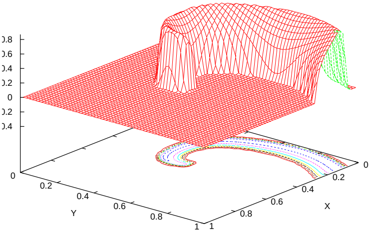

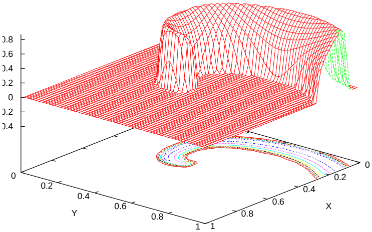

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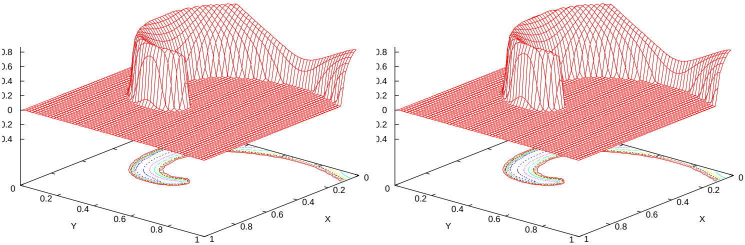

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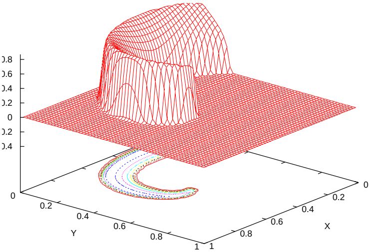
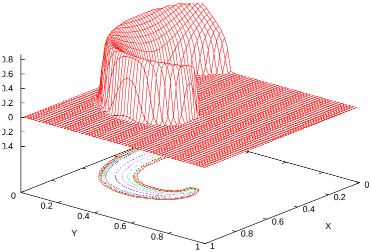
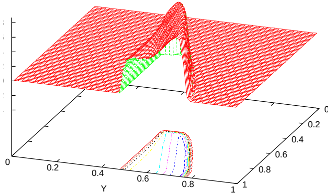
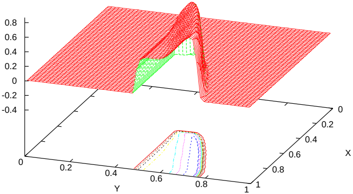




BZ with Strang Splitting RDR

BZ system with 3 variables
Strang Splitting for the b variable $\Delta t = 2/256$





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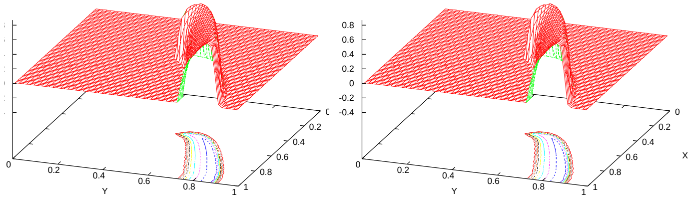

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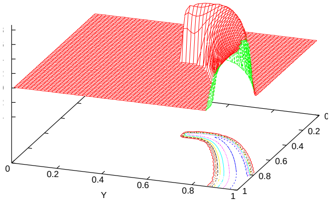

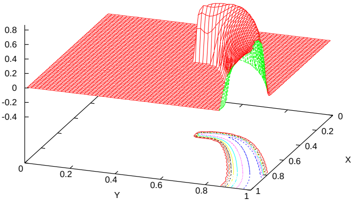

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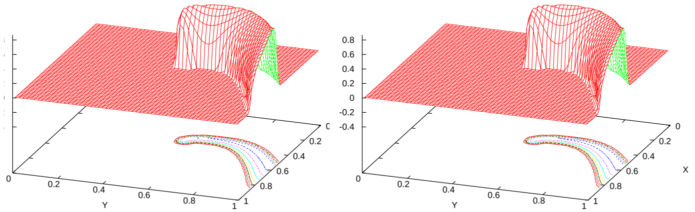

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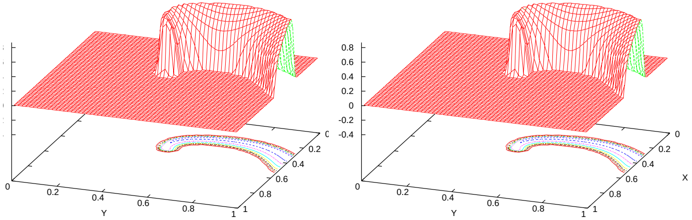

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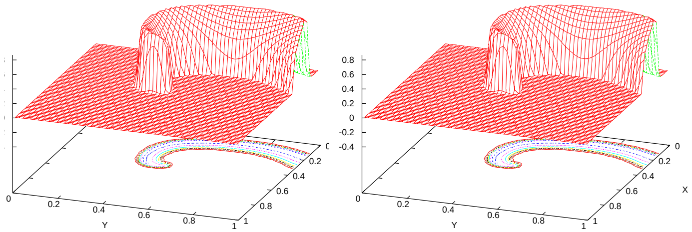

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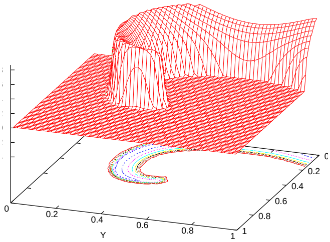

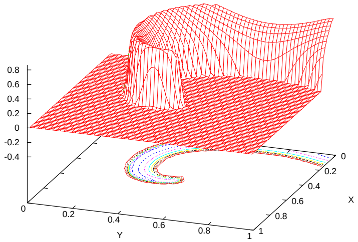

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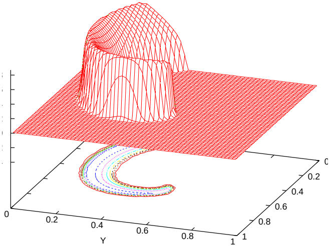
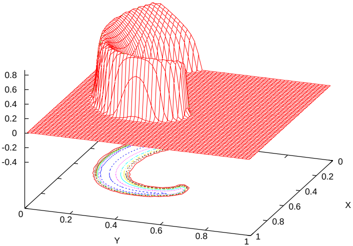
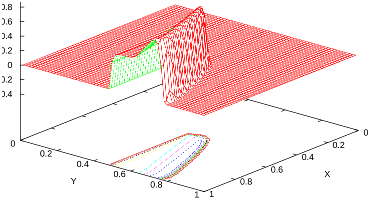
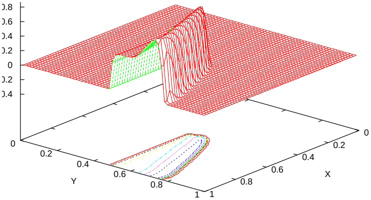




BZ with Strang Splitting RDR

BZ system with 2 variables
Strang Splitting for the *b* variable $\Delta t = 2/64$





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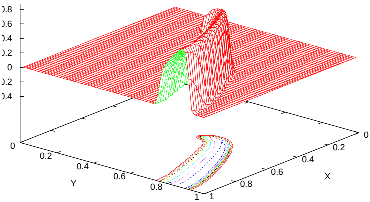

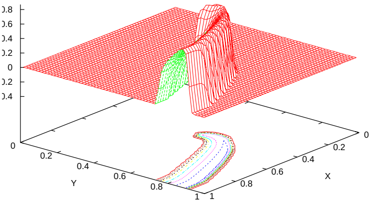

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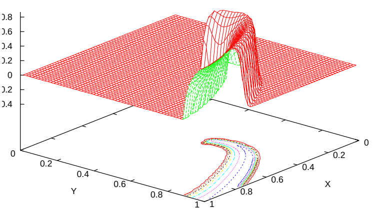

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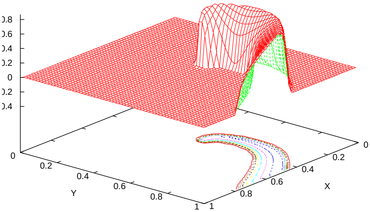

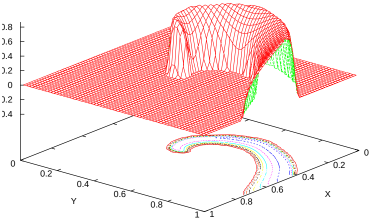

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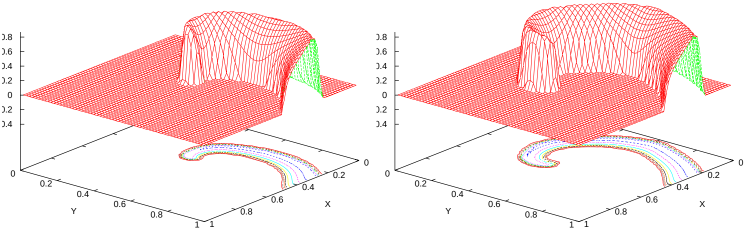

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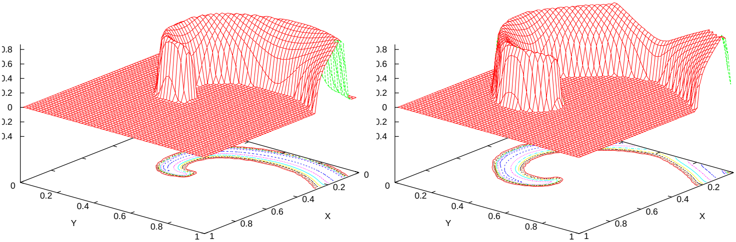

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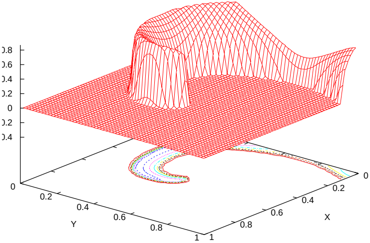

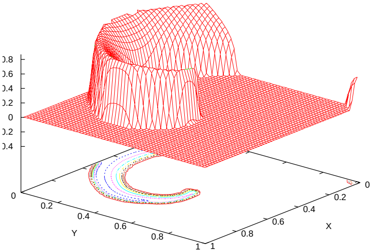

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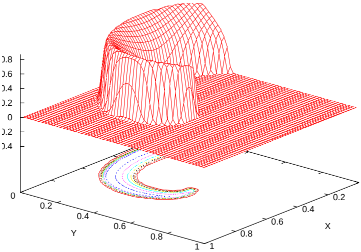
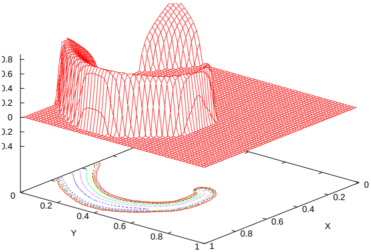
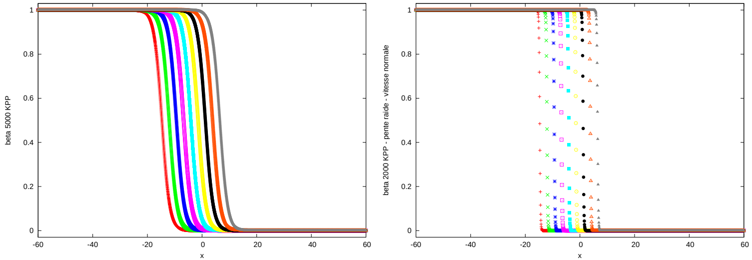




Outline

KPP

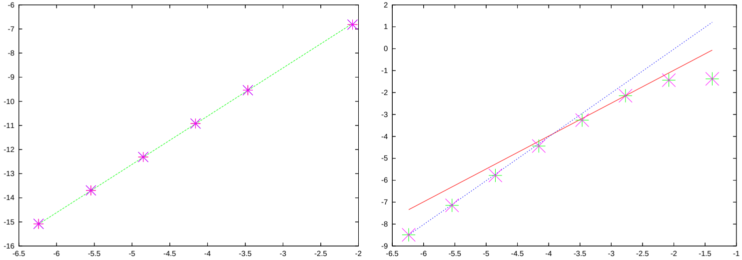
$$\partial_t \beta - \partial_{xx}\beta = \beta^2(1-\beta), \qquad \partial_t \beta^{st} - \mathbf{0.1}\, \partial_{xx}\beta^{st} = \mathbf{10}\, {\beta^{st}}^2(1-\beta^{st})$$



Two analytical solutions with the same velocity.
β^{st} has a gradient 10 times bigger.

Strang Splitting second order is lost

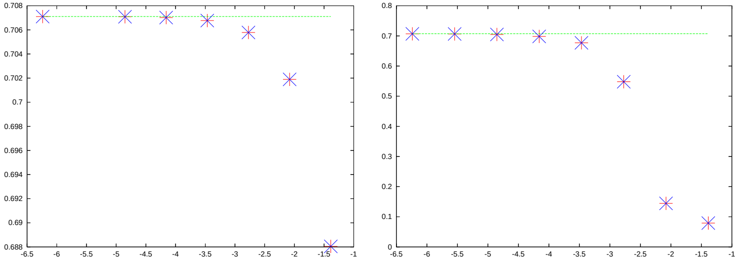
The global error for both KPP and stiff KPP



Reproduces the local error predicted by the theory

KPP wave velocity

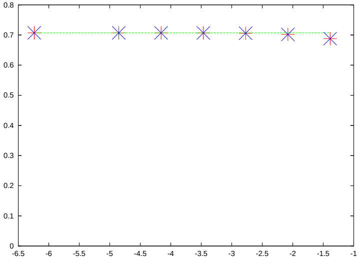
The two graph look similar but...

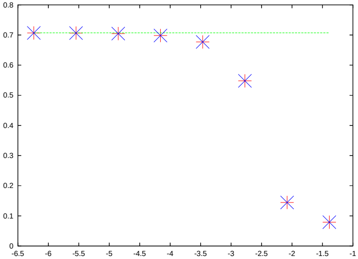


Scale on the left [0.688,0.708], on the right [0,0.7]

KPP wave velocity

The two graph look similar but...





Stiffness $\Rightarrow$ bad resolution of the wave speed!

Combustion system of equations

Methane planar flame with simple chemistry (Veynante - Poinsot 2005)

$$\partial_t \theta - \partial_{xx}\,\theta = -\omega(\theta, \bar{Y}_F, \bar{Y}_O)$$

$$\partial_t \bar{Y}_F - \frac{1}{Le_F}\partial_{xx}\,\bar{Y}_F = \omega(\theta, \bar{Y}_F, \bar{Y}_O)$$

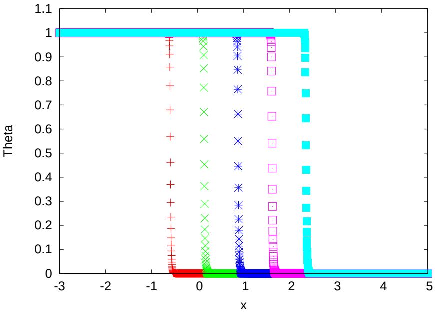
$$\partial_t \bar{Y}_O - \frac{1}{Le_O}\partial_{xx}\,\bar{Y}_O = \phi\,\omega(\theta, \bar{Y}_F, \bar{Y}_O)$$

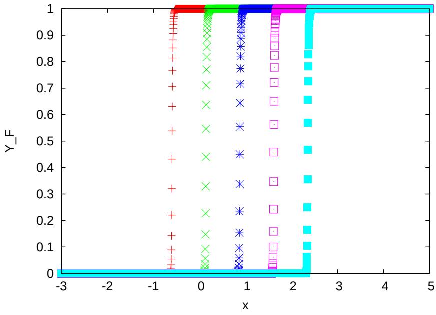
$$\omega(\theta) = \exp\left(-T_a/(T_0 + \frac{Q}{C_p}\,Y_F^0\theta)\right)\,\frac{L^2}{\kappa}\,B\,\bar{Y}_F\,\bar{Y}_O^{1/2}$$

$T_a = 10055K$, $T_0 = 300K$, $L = 4mm$, $Q/C_p = 34550K$, $Y_F^0 = 0.0583$, $Y_O^1 = 0.29167$, $\kappa = 2.2610^{-5} m^2.s^{-1}$, $\phi = 0.8$, $B_1 = 10^7$

Combustion quasi-exact solution

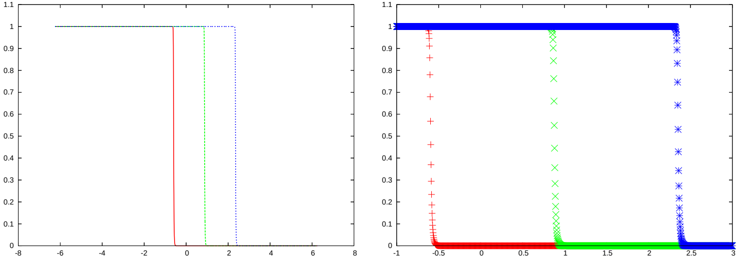
Planar flame (simple chemistry, $Le = 1$, 4000 pts, $t \in [0, 0.04]$





Strang splitting RDR

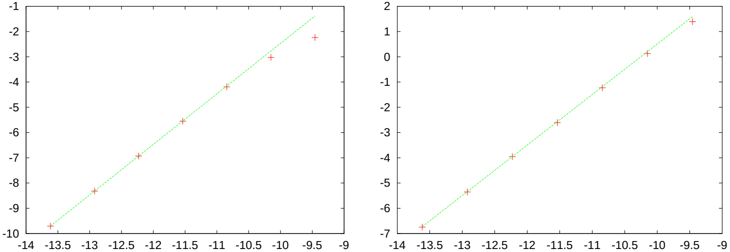
Same behavior as the stiff KPP equation



The phase space diagram is similar to the one of stiff KPP

Planar flame with Strang Splitting RDR

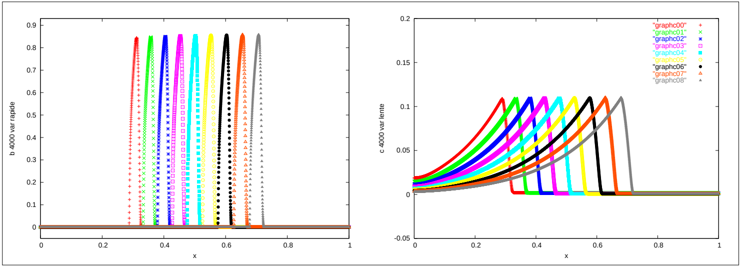
Simple chemistry $Le = 1$ - $\Delta t = 0.04/256$-$0.04/32768$
Same behavior as the stiff KPP equation



Log of l^2 norm of error and Log of wave velocity error versus Log of time step

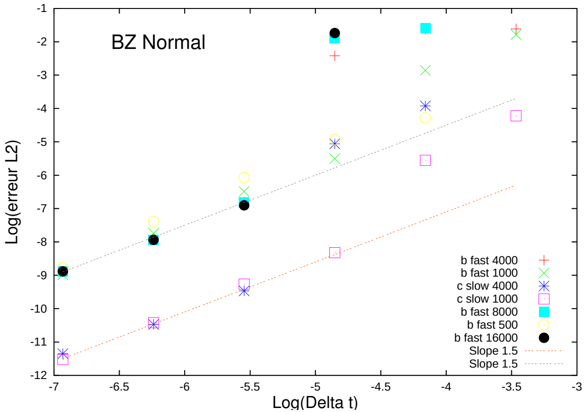
BZ "quasi-exact" solution in 1D

Belousov-Zhabotinsky system of equations with two variables b and c



BZ with Strang Splitting RDR

BZ system with 2 variables



Outline

1. Context and Motivation
   - Unsteady reactive fronts
   - Reaction-Convection-Diffusion Systems
   - Time integration numerical strategies
2. Operator splitting and stiffness
   - Standard numerical analysis of operator splitting
   - Stiffness comes into play
   - Splitting local error analysis for PDEs
3. Illustrating numerical simulations
   - "Toy" system with and without cross-diffusion
   - BZ system in two dimensions
   - KPP, Stiff KPP and Combustion waves with simple chemistry
   - Premixed counterflow flames with complex chemistry and transport

Stiffness comes into play

- order reduction due to fast scale (see reference Descombes, Massot, Numerische Mathematik, 2004)
- order reduction due to high spatial gradient (see reference Descombes, Dumont, Louvet, Massot, International Journal of Computer Mathematics, 2007)

Stiffness comes into play

Error behaviour.

In case of fast scale, the local error for Lie and Strang formalism behave like :

$$\|E_L(t)U_0\|_2 \leq \left(\frac{C_{L0}\, t^2}{2} + \frac{C_{L1}\, t\sqrt{t}}{3\sqrt{2e}} \right) \|U_0\|_2$$

$$\|E_S(t)U_0\|_2 \leq \frac{(C_{S0} + 2C_{S1})\, t^3}{12} + \frac{C_{S2}\, t^2\sqrt{t}}{15\sqrt{2e}} + \frac{C_{S3}\alpha\, t\sqrt{t}}{4}$$

In case of high spatial gradient, for Lie Formalism, there exists an explicit constant $\theta > 0$ depending on $\|\sqrt{A}U_0\|_2$ such that for $t \leq \theta$, $\|E_L(t)U_0\|_2$ behaves like t^2 and for $t \geq \theta$, $\|E_L(t)U_0\|_2$ behaves like $t\sqrt{t}$. □

Assumptions

- Complex chemistry
- Detailed transport
- 2D axisymetrical configuration
- Similarity assumption :

$$\rho = \rho(z,t) \qquad T = T(z,t) \qquad Y_k = Y_k(z,t)$$

$$\rho u_z = V(z,t) \qquad u_r = rU(z,t) \qquad \tilde{p} = -J(t)\frac{r^2}{2} + \hat{p}(z,t)$$

↪ Experimental studies in EM2C laboratory, Ecole Centrale Paris (T. Schuller, P. Duchaine)

- See N. Darabiha, "Transient behaviour of laminar counterflow hydrogen-air diffusion flames with complex chemistry", Combust. Sci. and Tech., 1992

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Isobaric Flame Equations

System of equation.

$$
\begin{aligned}
\rho c_p \frac{\partial T}{\partial t} + c_p V \frac{\partial T}{\partial z} - \frac{\partial}{\partial z}\left(\lambda \frac{\partial T}{\partial z}\right) &= -\sum_{k=1}^{n_S} h_k m_k \omega_k \\
&\quad - \sum_{k=1}^{n_S} \rho Y_k c_{p,k} \mathcal{V}_{z,k} \frac{\partial T}{\partial z}, \\
\rho \frac{\partial Y_k}{\partial t} + V \frac{\partial Y_k}{\partial z} + \frac{\partial}{\partial z}\left(\rho Y_k \mathcal{V}_{z,k}\right) &= m_k \omega_k, \\
\frac{\partial J}{\partial z} &= 0, \\
\rho \frac{\partial U}{\partial t} + \rho U^2 + V \frac{\partial U}{\partial z} &= J + \frac{\partial}{\partial z}\left(\mu \frac{\partial U}{\partial z}\right), \\
\frac{\partial \rho}{\partial t} + 2\rho U + \frac{\partial V}{\partial z} &= 0.
\end{aligned}
$$

Application of splitting method : chemical correction I

- Eliminating chemical terms : important variation of the temporal derivative of the density ρ, instant perturbation of the velocity field.
- Necessity to take into account the chemical contribution in the diffusion-convection step

$$\rho c_p \frac{\partial T}{\partial t} = -\sum_{k=1}^{n_S} h_k m_k \omega_k$$

$$\rho \frac{\partial Y_k}{\partial t} = m_k \omega_k$$

Application of splitting method : chemical correction I

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$$\rho \frac{\partial Y_k}{\partial t} = m_k \omega_k$$

Application of splitting method : chemical correction II

- Using the ideal gas law, chemical contribution on the temporal derivative of the density :

$$\left(\frac{\partial \rho}{\partial t}\right)_{chemical} = \frac{1}{\rho c_p} \cdot \sum_{k=1}^{n_S} h_k m_k \omega_k - m \sum_{k=1}^{n_S} \omega_k$$

- This contribution must be added to the convection-diffusion step

Density equation of the convection-diffusion system.

$$\frac{\partial \rho}{\partial t} + \left(\frac{\partial \rho}{\partial t}\right)_{chimie} + 2\rho U + \frac{\partial V}{\partial z} = 0$$

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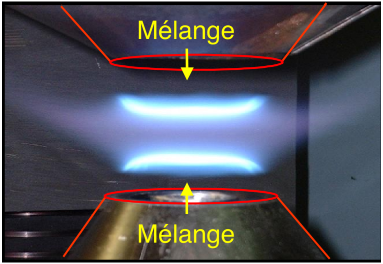
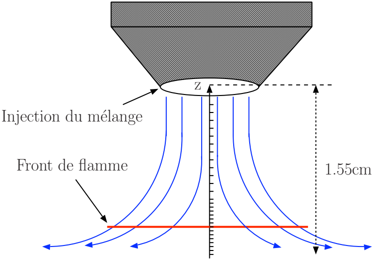
Numerical Resolution

- Finite difference spatial discretization :
  - diffusion : centered schemes
  - convection : upwind schemes
- Boundary value problem solved by Newton method
- Time discretization :
  - convection-diffusion : 2nde order implicit finite difference scheme
  - reaction : radauIIA, implicit Runge Kutta

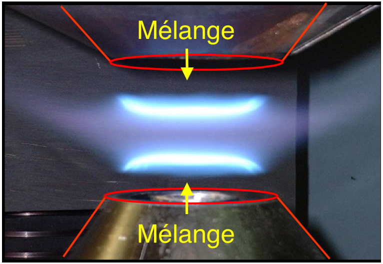
Dynamics of a pulsated premixed methane flame

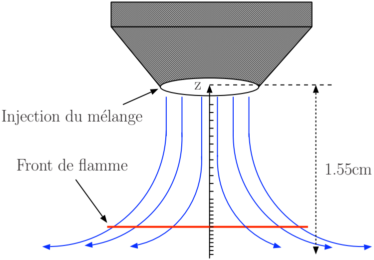




Pulsated premixed methane-air flame at 100Hz - 10% - Acoustic mode
Comparaisons with the experimental measurements at Lab. EM2C (P. Duchaine, C. Goefpert, P. Palies et T. Schuller)

Dynamics of a pulsated premixed methane flame

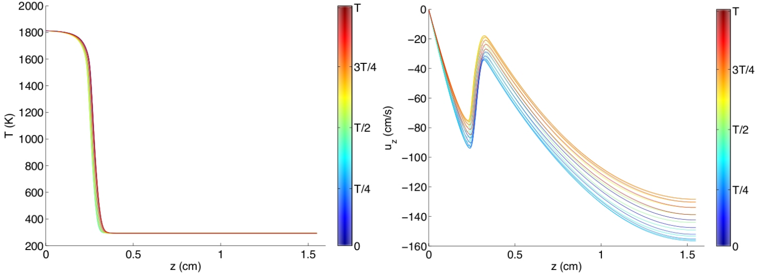




Low Mach number approximation - autosimilarity assumption - 1D detailed modeling
Ideal configuration for the evaluation of numerical methods on a model with complex chemistry and detailed transport (45 species 250 reactions)

Flame Dynamics

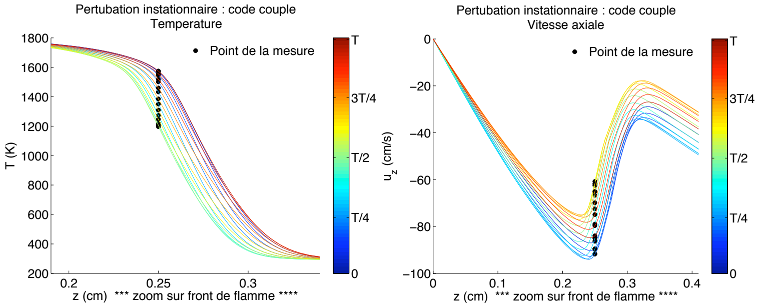
Code Couplé



Pulsation de la flamme de type acoustique conforme aux mesures expérimentales

Flame Dynamics

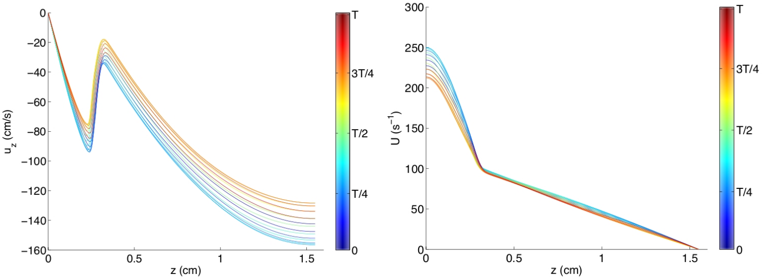
Code Couplé



Pulsation de la flamme de type acoustique conforme aux mesures expérimentales

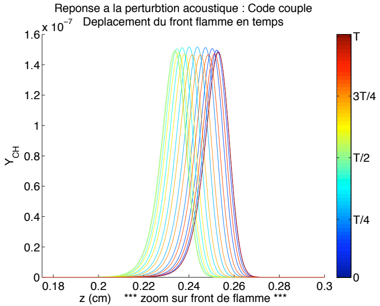
Numerical Results I

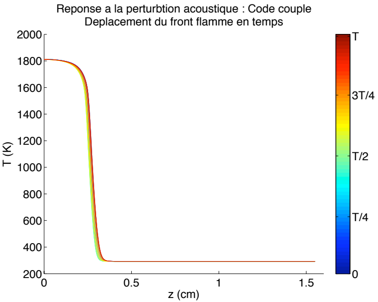
Unstationary simulations : the perturbation of the flame is a sinusoidal acoustic oscillation



Some axial velocity and reduced radial velocity profiles for a value of the period T of the sinusoidal perturbation from 10% of the inlet velocity at a frequency of 100Hz.

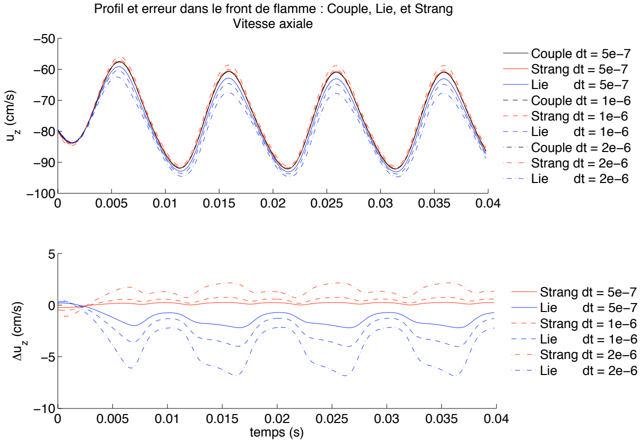
Numerical Results II





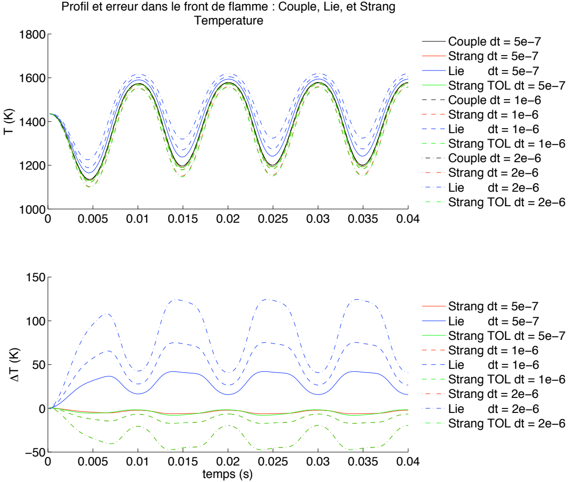
Some mass fraction Y_{CH} and Temperature profiles for a value of the period T of the sinusoidal perturbation from 10% of the inlet velocity at a frequency of 100Hz.

Splitting Errors



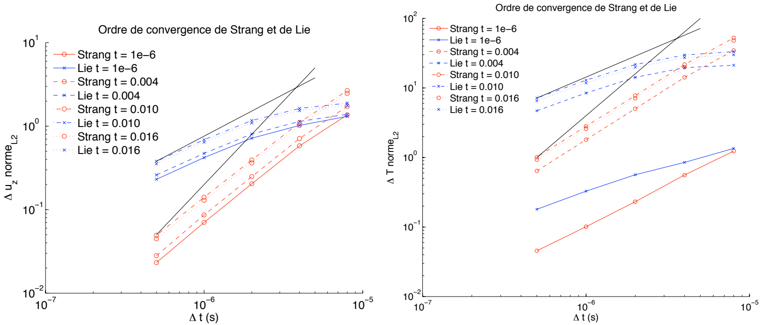
Dynamics is preserved Axial velocity

Splitting Errors



Dynamics is preserved Temperature

Convergence order



$\hookrightarrow$ Reduction order as predicted by the theory (Descombes et al, SIAM Numerical Analysis 2014)

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- Grants
  - Young Investigator Award (S. Descombes, M. Massot)
    "New Interfaces of Mathematics" (ACI NIM),
    French Ministry of Research 2003-2006
  - Projet Exploratoire Pluridisciplinaires (Dpt ST2I et MPPU du CNRS) 2007-2008 (F. Laurent et A. Bourdon - EM2C)
  - Projet ANR Séchelles (S. Descombes, M. Massot - 2009-2014)
  - Projet DIGITEO MUSE (M. Massot, 2010-2014)
  - Projet Labex LASIPS/LMH NEMESIS (M. Massot, 2015-2019)