Numerical analysis of operator splitting techniques for the numerical simulation of reaction waves with multiple scales

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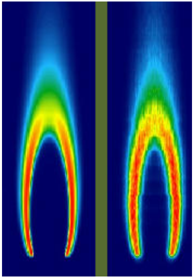
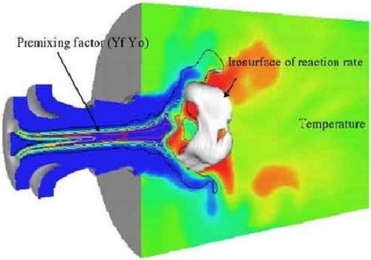
Outline

Application Background

Numerical simulation of unsteady reactive phenomena

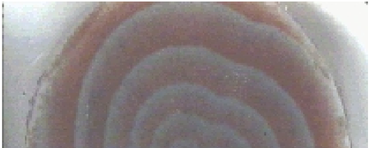
- Flames (Instabilities, dynamics, pollutants)





Yale University and CERFACS

- Chemical "waves" (spiral waves, scroll waves)



Convection-diffusion coupled to chemistry

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

Examples

- KPP or Fischer equation

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

- Belousov-Zhabotinsky system of equations

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

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

- Compressible flame equations with complex chemitry

Aim and scope

Examples

- Low Mach Number approximation / complex chemistry
  (J.B. Bell, M.S. Day LBNL)
- DNS of non-premixed turbulent flames
  (2D or 3D with chemistry of “simple” fuel, Y. Mizobuchi, T. Takeno et al., CERFACS- NTMIX-CHEMKIN)
- Scroll waves, heart fibrillation
  (F. Fenton, A. Karma, Hofstra University)
- Blocking of Migraines by Rolando sulcus
  (E. Grenier, J.P. Boissel et al., IMTH and ENS Lyon)

Need for dedicated solver for “DNS”-like simulations

Strategies

Resolving the large scale spectrum coupled

- Explicit methods in time (high order in space)
- Fully implicit methods with adaptative 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)
- Operator Splitting techniques

Purpose of the presentation

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

What about **fast scales**?

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

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".

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

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

□

Basis of operator splitting II

First order methods, Lie formalism :

Lie Formulae.

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

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

□

Basis of operator splitting III

Second order methods, Strang formalism :

Strang Formulae.

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

$$S_2^t\, U_0 = X^{t/2}\, Y^t\, X^{t/2}\, U_0 \qquad S_2^t - T^t = O(t^3),$$

□

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

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
- Large spatial gradients of the solutions

Large spectrum of temporal scales

- A “model” problem for the fast scales for $U^\varepsilon = (u^\varepsilon, v^\varepsilon)^t$

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

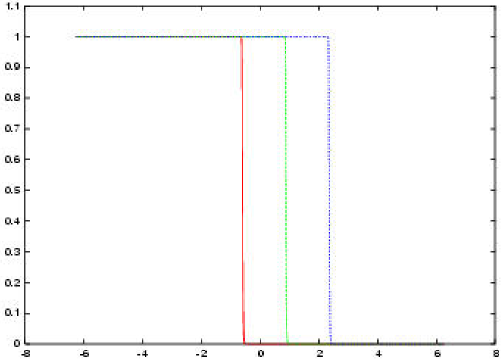
- The entropic structure of the RD system of equations
  $\Rightarrow$ Dynamics on the partial equilibrium manifold

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

- Order reduction due to fast scales
  - Diag. diffusion : Lie RD order 0 fast variable only
  - Diag. diffusion : Strang DRD order 0 fast variable only
  - Non-diag. diffusion : Lie DR and RD order 0
  - Non-diag. diffusion : Strang RDR order 1, DRD order 0

High spatial gradients

- Initial data with high gradient (L^2 norm)

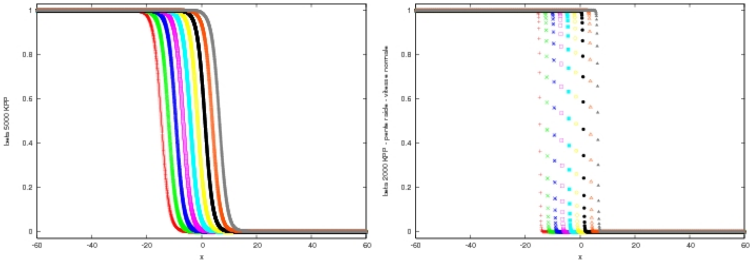


- High constant in the error estimate
  $O(t^2) = C(||U_0||_{H^1})\ t^2$
- Exact error estimate (differential geometry)

$$e^{(-t\,(A+B))} - e^{(-t\,A)}e^{(-t\,B)} = -\int^{t}\int^{s} e^{(-(t-s)\,(A+B))}$$

KPP

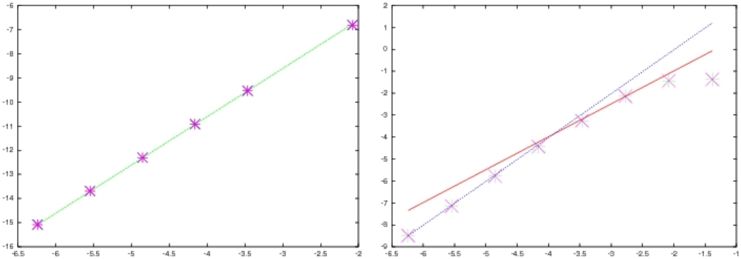
$$\partial_t \beta - \partial_{xx} \beta = \beta^2 (1 - \beta), \qquad \partial_t \beta^{st} - \mathbf{0.1}\, \partial_{xx} \beta^{st} = \mathbf{10}\, {\beta^{st}}^2 (1 - \beta^{st})$$



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

Splitting second order is lost

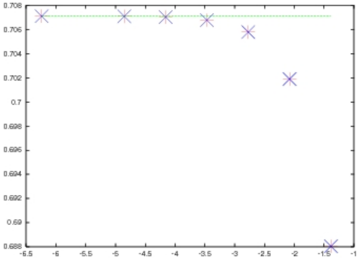
The global error for both KPP and stiff KPP

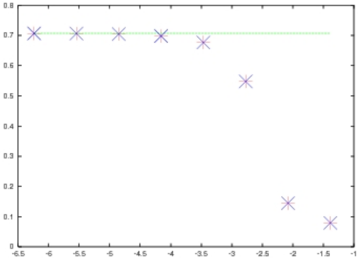


Reproduces the local error predicted by the theory

KPP wave velocity

The two graph look similar but...

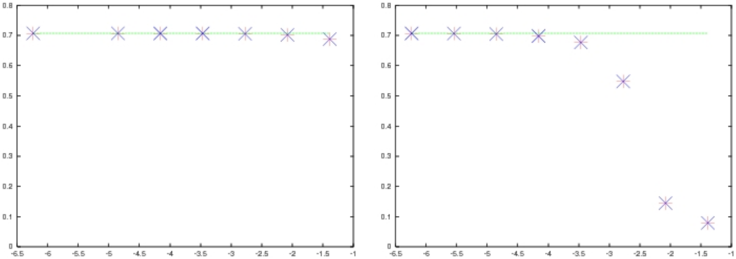




Scale on the left [0.688,0.708], on the right [0,0.7]

KPP wave velocity

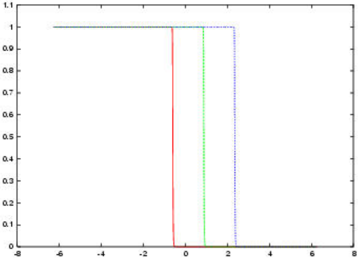
The two graph look similar but...

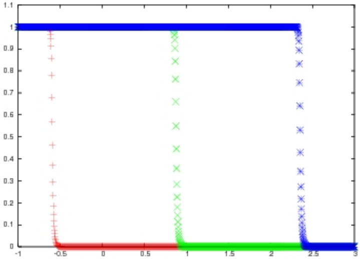


Stiffness ⇒ bad resolution of the wave speed!

Methane plane flame

Simple chemistry (Veynante - Poinsot 2005) Lewis = 1

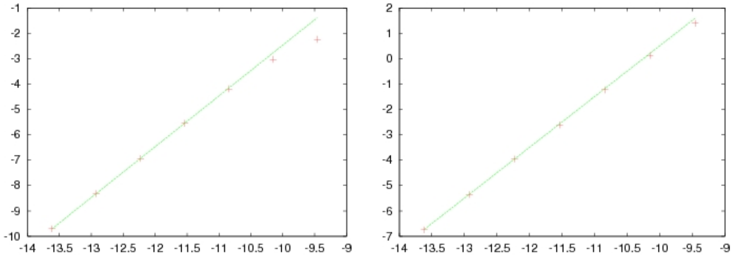




The phase space diagram is similar to the one of stiff KPP

Strang splitting RDR

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

Conclusion and perspectives

- Numerical analysis of temporal and spatial origins of order loss
  - fast temporal scales in the reaction source term
    $\longrightarrow$ dynamics on an “equilibrium manifold”
    $\longrightarrow$ effect of non-diagonal diffusion
  - high spatial variation of the solution
- Work in progress
  - Temporal and spatial discretization
  - Detailed description of “waves”
  - Complex chemistry in a RD configuration
    $\longrightarrow$ detailed analysis of flame propagation
  - Multi-dimensional configurations

References and Grants I

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