New strategies for multi-scale reaction wave : splitting methods coupled with space adaptative multiresolution and parareal algorithm

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Outline

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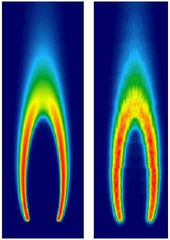
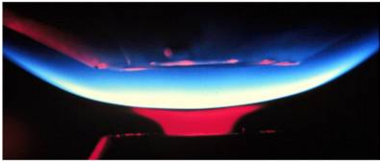
Application Background

Numerical simulation of unsteady reactive phenomena

- Flames (Instabilities, dynamics, pollutants)





- Chemical “waves” (spiral waves, scroll waves)
- Biochemical Engineering (migraines, Rolando’s region, strokes : clinical anomaly which follows an anatomic lesion of one of many cerebral blood vessels)

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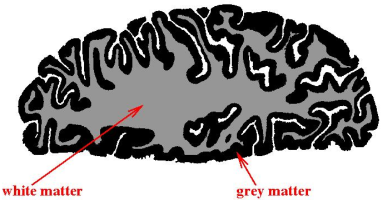

To summarize

Dynamics involving many "species" and "reactions"

Multiple scales problems

"Complex Chemistry"

Convection-diffusion coupled to chemistry

$$\partial_t U + \sum \partial_i \big(\Phi_i(U, \partial_{\boldsymbol{x}} U)\big) = \Omega(U)$$

Examples

- KPP or Fischer equation

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

- Belousov-Zhabotinsky system of equations
- Compressible flame equations with complex chemistry
- In both cases : Low diffusion ($\varepsilon \Delta$)

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$$\left\{\begin{array}{rcl}\dfrac{\partial a}{\partial \tau} - D_a \Delta a & = & \dfrac{1}{\mu}(-qa - ab + fc), \\ \dfrac{\partial b}{\partial \tau} - D_b \Delta b & = & \dfrac{1}{\epsilon}\left(qa - ab + b(1-b)\right), \\ \dfrac{\partial c}{\partial \tau} - D_c \Delta c & = & b - c,\end{array}\right.$$

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Strategies

Resolving the large scale spectrum coupled

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

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

- Reduction of chemistry (large litterature)
- Operator Splitting techniques

Outline

Operator splitting techniques

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

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 Formulae.

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

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

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$\square$

Basis of operator splitting III

Second order methods :

Strang Formulae.

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

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

□

Higher order...

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Higher order...

Error estimate

Error estimate -> Lie formalism. For an ODE $\dot{y} = f_1(y)$, we denote by φ_1^t the exact solution, we introduce the differential operator (Lie derivative)

$$D_1 = \sum_j f_{1,j} \frac{\partial}{\partial y_j}.$$

For a smooth function from $\mathbb{R}^n$ to $\mathbb{R}^n$, we have

$$\frac{d}{dt} F\left(\varphi_1^t(y_0)\right) = F'\left(\varphi_1^t(y_0)\right) f_1\left(\varphi_1^t(y_0)\right) = (D_1 F)\left(\varphi_1^t(y_0)\right)$$

Error estimate

By iterations, the Taylor's expansion of $F\left(\varphi_1^t(y_0)\right)$ in $t = 0$ gives (formally)

$$F\left(\varphi_1^t(y_0)\right) = \sum_{k\geq 0} \frac{t^k}{k!}\left(D_1^k F\right)(y_0) = e^{tD_1} F(y_0).$$

With $F =$Id, we obtain

$$\varphi_1^t(y_0) = e^{tD_1}\mathrm{Id}(y_0).$$

Error estimate

Moreover, if we introduce a second flow φ_2^t, we have :

$$\left(\varphi_2^t \varphi_1^t\right)(y_0) = e^{tD_1} e^{tD_2} \mathrm{Id}(y_0).$$

Error estimate

Then if we denote by φ_3^t the exact solution of $\dot{y} = (f_1 + f_2)(y)$, we have the following relation :

$$\varphi_3^t(y_0) - \left(\varphi_2^t \varphi_1^t\right)(y_0) = e^{t(D_1+D_2)}\mathrm{Id}(y_0) - e^{tD_1}e^{tD_2}\mathrm{Id}(y_0),$$

we then work with linear operators ! For example, for two linear operators A et B, we have

$$e^{t(A+B)} - e^{tA}e^{tB} = \frac{t^2}{2}[A, B] + O(t^3),$$

this yields,

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and $[D_1, D_2]$ is now a Lie bracket...

$$[D_1, D_2] = \sum_i \left(\sum_j \left(\frac{\partial f_{1,i}}{\partial y_j} f_{2,j} - \frac{\partial f_{2,i}}{\partial y_j} f_{1,j} \right) \right) \frac{\partial}{\partial y_i}$$

We are not limited to the finite dimension...

$$\left(D_1 = \sum_j f_{1,j} \frac{\partial}{\partial y_j} \right)$$

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Error estimate

Application to Lie et Strang formulae denoting by F the reaction term for a scalar equation.

$$T^t u_0 - Y^t X^t u_0 = \frac{t^2}{2} F''(u_0)(\partial_x u_0)^2 + O(t^3),$$

$$T^t u_0 - Y^{t/2} X^t Y^{t/2} u_0 =$$
$$\frac{t^3}{24}\left(2F^{(4)}(u_0)(\partial_x u_0)^4 + 8F^{(3)}(u_0)(\partial_x u_0)^2(\partial_{xx} u_0) + 4F''(u_0)(\partial_{xx} u_0)^2\right)$$
$$-\frac{t^3}{24}\left(\left(F(u_0)F^{(3)}(u_0) + F''(u_0)F'(u_0)\right)(\partial_x u_0)^2\right) + O(t^4)$$

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Stiffness comes into play

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

Various origins of stiffness

- Large spectrum of temp. scales in chemical source
- Large spatial gradients of the solutions

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Large spectrum of temporal scales

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

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

- 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
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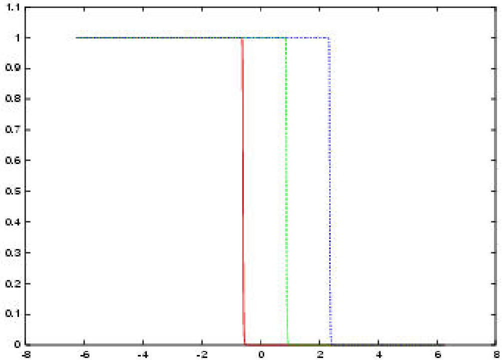

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Stability + Accuracy

Considering:

$$y' = \lambda y \quad \Longrightarrow \quad y_{n+1} = R(z) y_n \qquad z = h\lambda$$

We are particularly looking for:

- A-stable methods
- High order methods
- L-stable methods

Implicit Runge Kutta Methods

- Based on Ehle's Methods of type II: (RadauIIA)
- Order: $p = 2s - 1$ (s: stage number)
- A-stable
- L-stable

RADAU5

(Hairer & Wanner Springer-Verlag 91)

- Based on RadauIIA with $s = 3$ and $p = 5$
- Simplified Newton Method $\Longrightarrow$ Linear Algebra tools
- Adaptative time integration step

Explicit Runge-Kutta methods

We want to solve the discrete heat equation

$$\dot{u} = Au,$$

with an explicit s-stage Runge-Kutta method.

Because of the properties of the matrix A, we need to find a stable Runge-Kutta method for the simple problem

$$\dot{u} = \lambda u,$$

with λ real, negative and as big as possible...

ROCK4

(Abdulle SIAM J. Sci. Comput. 02)

- Extended Stability Domain (along $\mathbb{R}^-$) by increasing the number of stages
- Order 4 - Stability $\times s^2$.
- Adaptative time integration step
- Explicit Methods $\Longrightarrow$ NO Linear Algebra problems
- Low Memory Demand

Explicit/Implicit Operator Splitting

Numerical Strategy:

$$\partial_t U - \underbrace{\varepsilon \Delta U}_{\text{ROCK4}} = \underbrace{\Omega(U)}_{\text{RADAU5}}$$

- Reduction in Computational Time
- Reduction in Memory Demand
- Same previous accuracy established by Splitting Scheme
- Highly parallelizable - Diffusion - Reaction

Outline

Background

Consider the general nonlinear system of ODEs:

$$\begin{aligned} \boldsymbol{u}'(t) &= \boldsymbol{f}(\boldsymbol{u}(t)) \\ \boldsymbol{u}(0) &= \boldsymbol{u}^0 \end{aligned}$$

on $t \in (0, T)$ where $\boldsymbol{f} : \mathbb{R}^M \to \mathbb{R}^M$ and $\boldsymbol{u} : \mathbb{R} \to \mathbb{R}^M$.

Decomposition of the Time Direction

We decompose the time domain $\Omega = (0, T)$ into N time subdomains $\Omega_n = (T_n, T_{n+1})$ and consider for $n = 0, 1, \ldots, N-1$:

$$\begin{aligned} \boldsymbol{u}_n'(t) &= \boldsymbol{f}(\boldsymbol{u}_n(t)) \\ \boldsymbol{u}_n(T_n) &= \boldsymbol{U}_n \end{aligned}$$

on $t \in (T_n, T_{n+1})$.

Parareal Algorithm

(Lions *et al.* C. R. Acad. Sci. Paris Sér. I Math. 01)

Combination of two solvers

- Coarse Solver $\Longrightarrow$ fast (sequential calculation)
- Fine Solver $\Longrightarrow$ slow (parallel calculation)

- Convergence from a coarse approximation to the detailed dynamics
- Iterative Method

Parareal Algorithm

The parareal algorithm is based on two propagation operators : $\mathcal{G}^{\Delta T_n}(\mathbf{U})$ and $\mathcal{F}^{\Delta T_n}(\mathbf{U})$, that provide respectively a coarse and an accurate approximation of $\phi^{\Delta T_n}(\mathbf{U})$. In this way, the algorithm starts with an initial approximation $\mathbf{U_n^0}$ given for example by the sequential computation

$$\mathbf{U}_0^0 = \mathbf{u}^0, \quad \mathbf{U}_n^0 = \mathcal{G}^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^0) \; for \; n = 1, \ldots, N,$$

and then performs for $i = 1, \ldots, i_{conv}$ the correction iterations

$$\mathbf{U}_0^i = \mathbf{u}^0, \quad \mathbf{U}_n^i = \mathcal{F}^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^{i-1}) + \mathcal{G}^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^{i}) - \mathcal{G}^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^{i-1})$$

$for n = 1, \ldots, N.$

Parareal Algorithm

Based on the works of Chartier, the time decomposition method can be also interpreted as a multiple shooting method. In fact, considering $\mathbf{U} = (\mathbf{U}_0, \dots, \mathbf{U}_N)^T$ as the unknowns, the system can be written as

$$\mathbf{F}(\mathbf{U}) = \begin{pmatrix} \mathbf{U}_0 - \mathbf{u}^0 \\ \mathbf{U}_1 - \phi^{\Delta T_0}(\mathbf{U}_0) \\ \vdots \\ \mathbf{U}_N - \phi^{\Delta T_{N-1}}(\mathbf{U}_{N-1}) \end{pmatrix} = \mathbf{0}.$$

Parareal Algorithm

Solving this system with Newton's method, leads after a short calculation to

$$\mathbf{U}_0^i = \mathbf{u}^0, \quad \mathbf{U}_n^i = \phi^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^{i-1}) + \frac{\partial \phi^{\Delta T_{n-1}}(\mathbf{U}_{n-1}^{i-1})}{\partial \mathbf{U}_{n-1}^{i-1}} \left(\mathbf{U}_{n-1}^i - \mathbf{U}_{n-1}^{i-1} \right)$$

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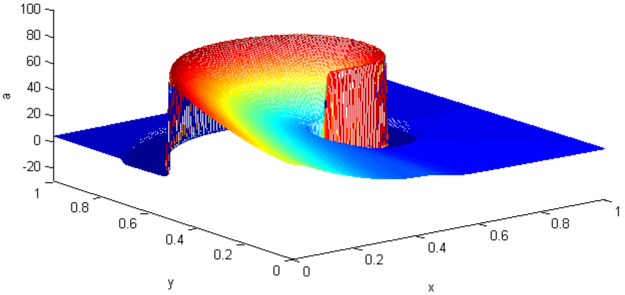
"Toy" Model

Belousov-Zhabotinsky system of equations

$$\begin{cases} \dfrac{\partial a}{\partial \tau} - D_a \Delta a &=& \dfrac{1}{\mu}(-qa - ab + fc), \\ \dfrac{\partial b}{\partial \tau} - D_b \Delta b &=& \dfrac{1}{\epsilon}\left(qa - ab + b(1-b)\right), \\ \dfrac{\partial c}{\partial \tau} - D_c \Delta c &=& b - c, \end{cases}$$

$$\epsilon = 10^{-2} \quad \mu = 10^{-5} \quad f = 1,6 \quad q = 2.10^{-3}$$
$$D_a = 2,5.10^{-3} \quad D_b = 2,5.10^{-3} \quad D_c = 1,5.10^{-3}$$

"Toy" Model



"Toy" Model - Some results

Grid	129×129		257×257	
Coarse solver	RDR Strang	Rock4	RDR Strang	Rock4
$\mathbf{N_{proc}}$	64			
$\mathbf{N_{proc}/N_{ite}}$	16	32	16	32
$\mathbf{T_{fine}/T_{para}}$	**2.16**	**3.21**	**2.02**	**2.88**

Table: Computation time ratios, 2D BZ

Conclusions

- Convergence rate diminished due to Stiff phenomena
- Parallel speedup is possible, but the speedup is modest
- Appropriate Coarse Solvers $\longrightarrow$ Cheap Stiff Integrators

Outline

Adaptive Multiresolution

(Cohen *et al.* Mathematics of Computation 01)

Principles of the MR:

- Represent a set of function data as values on a coarser grid plus a series of differences at different levels of nested grids.
- The information at consecutive scale levels are related by inter-level transformations: projection and prediction operators.
- The wavelet coefficients are defined as prediction errors, and they retain the detail information when going from a coarse to a finer grid.

Main idea: use the decay of the wavelet coefficients to obtain information on local regularity of the solution.

Multiresolution Transformation

There is a one-to-one correspondence

$$U_j \longleftrightarrow (U_{j-1}, D_j),$$

which can be implemented using the operators P^j_{j-1} and P^{j-1}_j.

By iteration of this decomposition, we obtain a multiscale representation of U_J in terms of $M_J = (U_0, D_1, D_2, \cdots, D_J)$. Using the local structure of the projection and prediction operators, we can implement the multiscale transformation

$$\mathcal{M} : \boldsymbol{U_J} \longmapsto \boldsymbol{M_J}.$$

Compression

Given a set $\Lambda \subset \nabla^J$ of indices λ, we define a truncation operator $\mathcal{T}_\Lambda$, that leaves unchanged the component d_λ if $\lambda \in \Lambda$ and replaces it by 0, otherwise.

In practice, we are typically interested in sets Λ obtained by thresholding: given a set of level-dependent threshold $(\epsilon_0, \epsilon_1, \cdots, \epsilon_J)$, we set

$$\Lambda = \Lambda(\epsilon_0, \epsilon_1, \cdots, \epsilon_J) := \{\lambda s.t. |d_\lambda| \geq \epsilon_{|\lambda|}\}.$$

Applying $\mathcal{T}_\Lambda$ on the multiscale decomposition of U_J amounts to building an approximation $\mathcal{A}_\Lambda U_J$, where the operator $\mathcal{A}_\Lambda$ is given by

$$\mathcal{A}_\Lambda := \mathcal{M}^{-1} \mathcal{T}_\Lambda \mathcal{M}.$$

Outline

1. Context and Motivation
   - Unsteady reactive phenomena
   - Time integration numerical strategies
   - Operator splitting and stiffness
2. Algorithms for multi-scale reaction waves simulation
   - Suitable Stiff Integrators - Parallelization
   - Parallelization of the Time Direction
   - One Illustrating Example
   - Space Adaptive Numerical Method
   - Adaptive Time-Space Numerical Method
   - Some illustrating examples
3. Conclusions

Adaptive Time-Space Numerical Strategy

Refinement Precautionary measure to account for possible translation or presence of finer scales in the solution.

Time Evolution Explicit/Implicit Strang RDR Operator Splitting Method.

Thresholding Wavelet Thresholding Operation:

$$\varepsilon_j = 2^{\frac{d}{2}(j-J)}\varepsilon, \quad j \in [0, J],$$

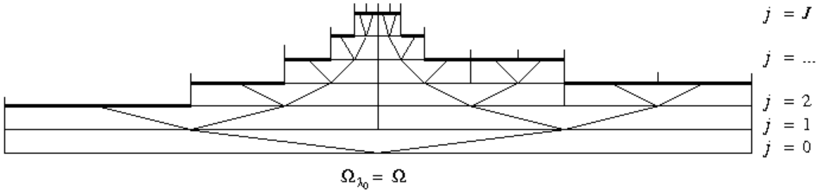
in order to ensure a thresholding error of prescribed order ε ($d =$ spatial dimension).

If $\mathcal{S}^{\Delta t}$ denotes the Strang splitting time integration operator

$$\boldsymbol{U}^{n+1} = \mathcal{S}^{\Delta t}(\mathcal{M}^{-1}\mathcal{R}\mathcal{T}_{\Lambda_\varepsilon^n}\mathcal{M}\boldsymbol{U}^n)$$

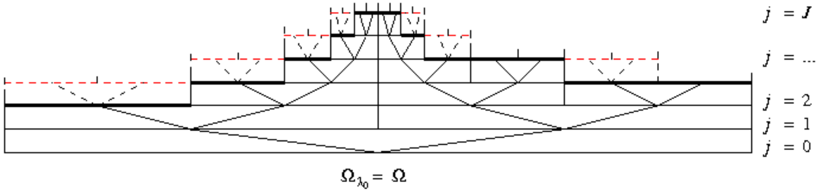
Implementing Configuration

Data Structure : Graded Tree



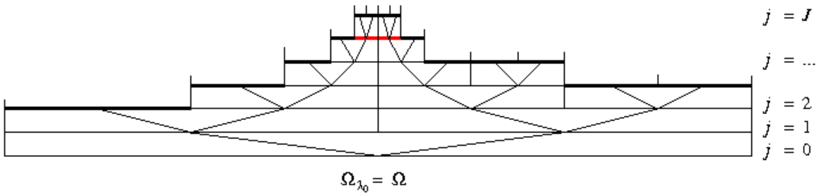
Implementing Configuration

Time Integration : Phantoms



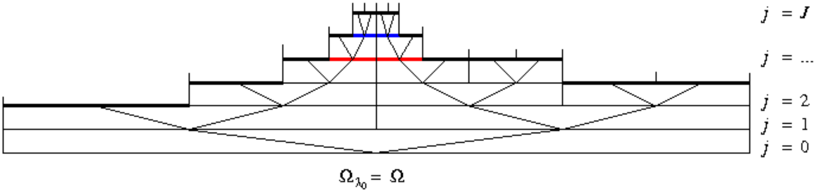
Implementing Configuration

Multiscale Transformation : Projection



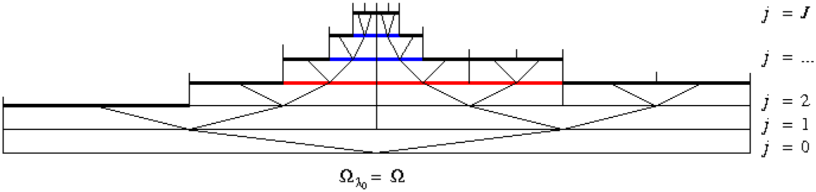
Implementing Configuration

Multiscale Transformation : Projection



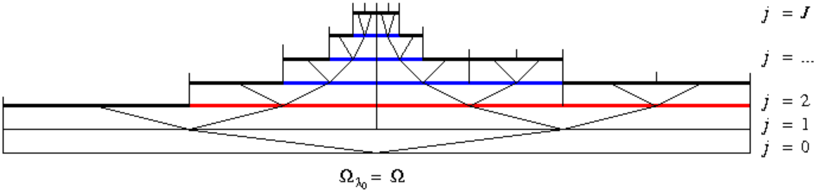
Implementing Configuration

Multiscale Transformation : Projection



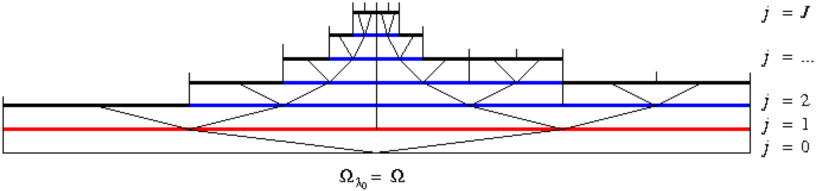
Implementing Configuration

Multiscale Transformation : Projection



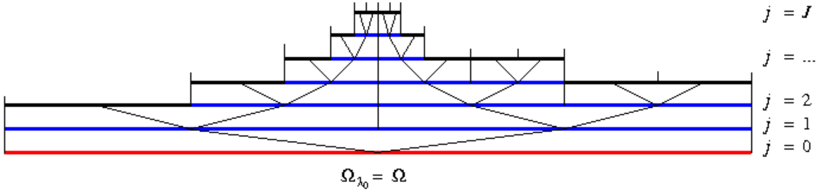
Implementing Configuration

Multiscale Transformation : Projection



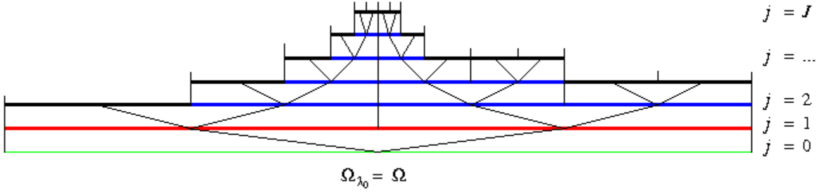
Implementing Configuration

Multiscale Transformation : Projection



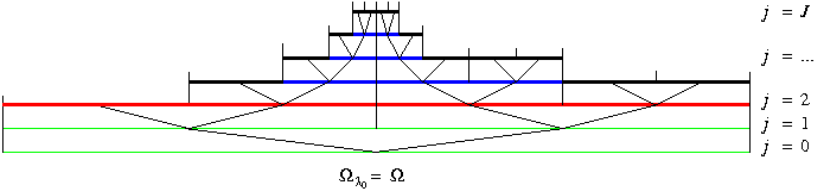
Implementing Configuration

Multiscale Transformation : Prediction



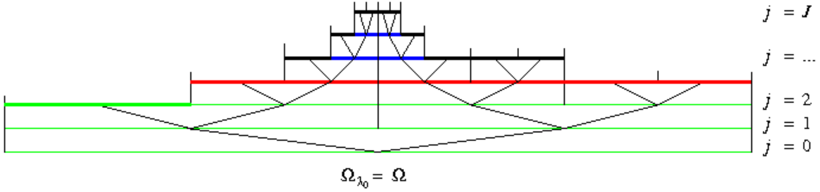
Implementing Configuration

Multiscale Transformation : Prediction



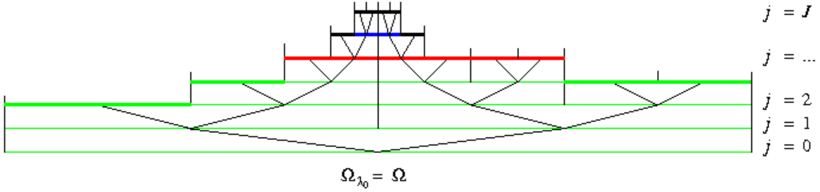
Implementing Configuration

Multiscale Transformation : Prediction



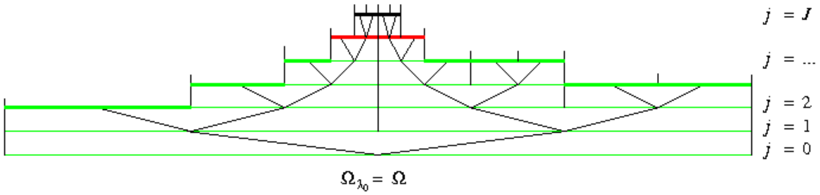
Implementing Configuration

Multiscale Transformation : Prediction



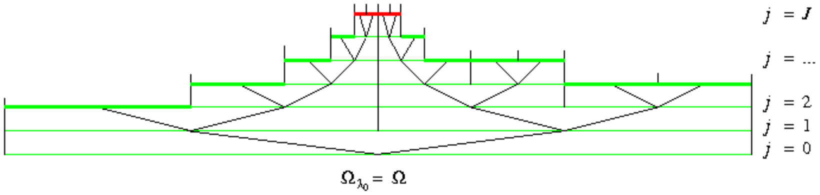
Implementing Configuration

Multiscale Transformation : Prediction



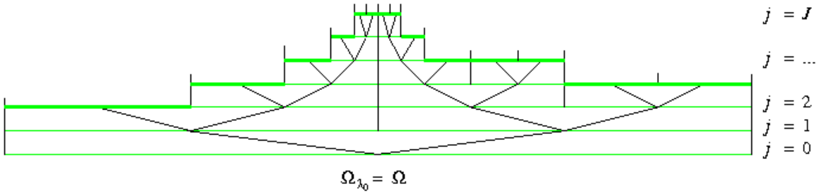
Implementing Configuration

Multiscale Transformation : Prediction



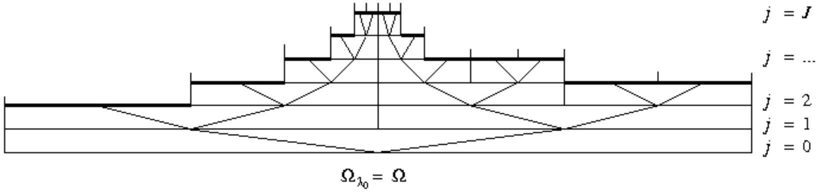
Implementing Configuration

Multiscale Transformation : Prediction



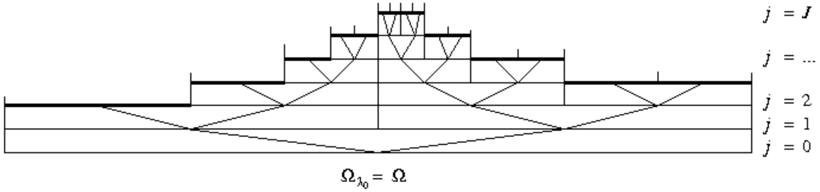
Implementing Configuration

Thresholding & Refinement



Implementing Configuration

Thresholding & Refinement



Outline

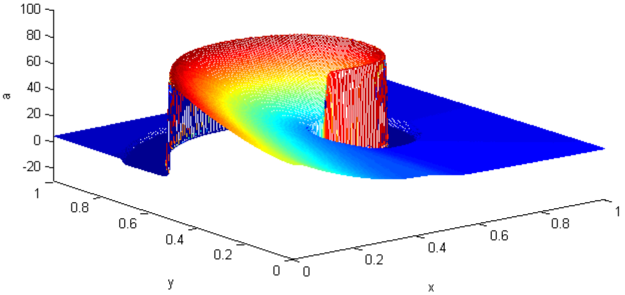
BZ Model

Belousov-Zhabotinsky system of equations

$$
\begin{cases}
\dfrac{\partial a}{\partial \tau} - D_a \Delta a = \dfrac{1}{\mu}(-qa - ab + fc), \\
\dfrac{\partial b}{\partial \tau} - D_b \Delta b = \dfrac{1}{\epsilon}\left(qa - ab + b(1-b)\right), \\
\dfrac{\partial c}{\partial \tau} - D_c \Delta c = b - c,
\end{cases}
$$

$$
\epsilon = 10^{-2} \quad \mu = 10^{-5} \quad f = 1,6 \quad q = 2.10^{-3}
$$
$$
D_a = 2,5.10^{-3} \quad D_b = 2,5.10^{-3} \quad D_c = 1,5.10^{-3}
$$

“Toy” Model

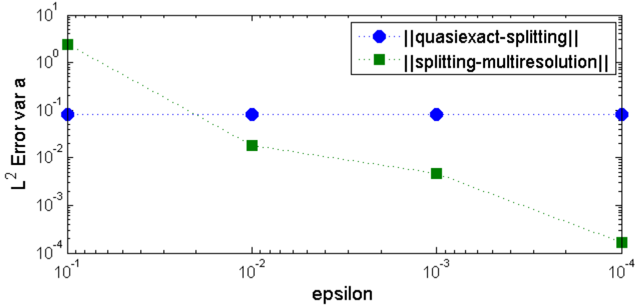


2D Configuration

- Time Domain : $T = [0, 4]$
- Spatial Domain : $\Omega = [0, 1] \times [0, 1]$
- Integration Time Step : $\Delta t = 4/1024$
- Tolerances of Time Integrators: $tol = 1.10^{-5}$
- Finest Grid Level : $J = 10$
- Number of cells at Grid J: $2^{d \times J} = 1048576 = 1024 \times 1024$

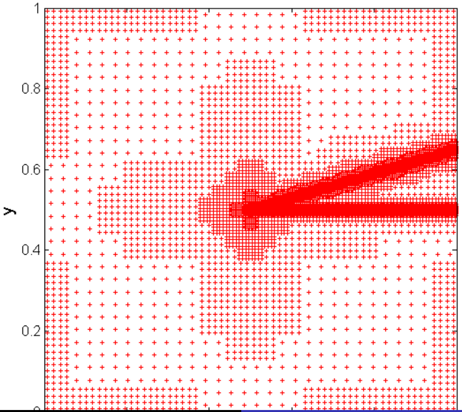
L^2 Error

$$\underbrace{\|u^J_{qe}(t) - u_{MR}(t)\|_{L^2}}_{\textit{Total Error}} \leq \underbrace{\|u^J_{qe}(t) - u^J_{split}(t)\|_{L^2}}_{\textit{Splitting Error}} + \underbrace{\|u^J_{split}(t) - u_{MR}(t)\|_{L^2}}_{\textit{MR Error}}$$



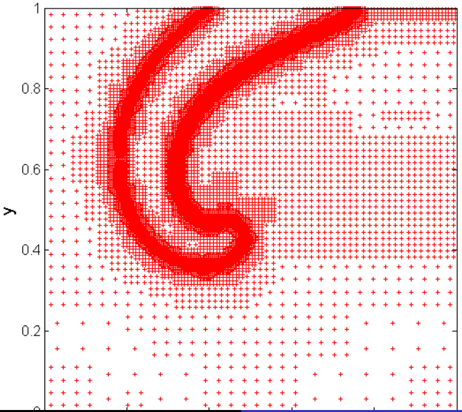
Adaptive Grid

Compression $\longrightarrow$ 1.41%



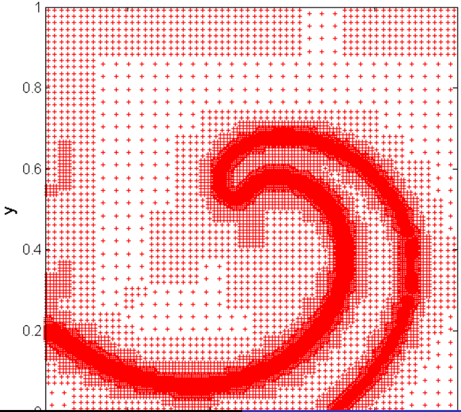
Adaptive Grid

Compression $\longrightarrow$ 2.96%



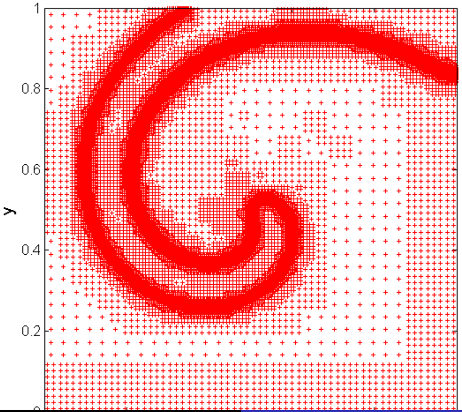
Adaptive Grid

Compression $\longrightarrow$ 3.90%



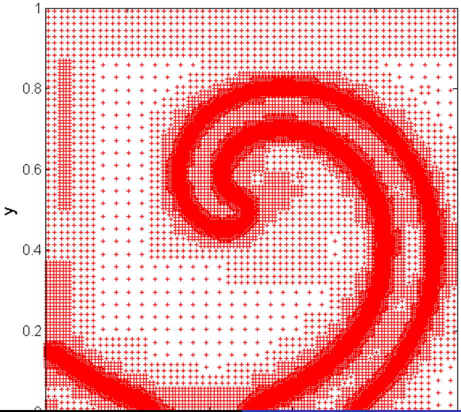
Adaptive Grid

Compression $\longrightarrow$ 4.69%



Adaptive Grid

Compression $\longrightarrow$ 5.77%



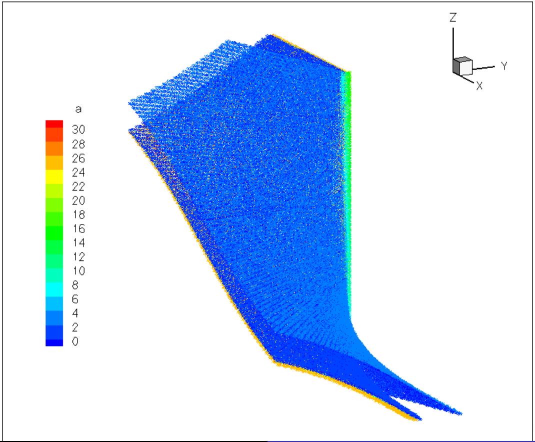
3D Configuration

- Time Domain : $T = [0, 2]$
- Spatial Domain : $\Omega = [0, 1] \times [0, 1] \times [0, 1]$
- Integration Time Step : $\Delta t = 2/256$
- Tolerances of Time Integrators: $tol = 1.10^{-5}$
- Finest Grid Level : $J = 9$
- Number of cells at Grid J:
  $2^{d \times J} = 134217728 = 512 \times 512 \times 512$

3D Configuration

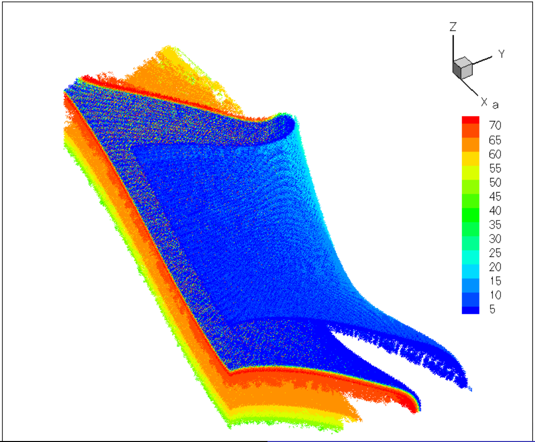
Adaptive Grid

Compression $\longrightarrow$ 4.46%



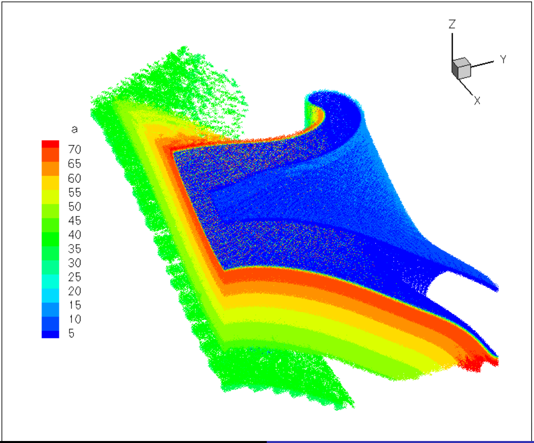
Adaptive Grid

Compression $\longrightarrow$ 10.38%



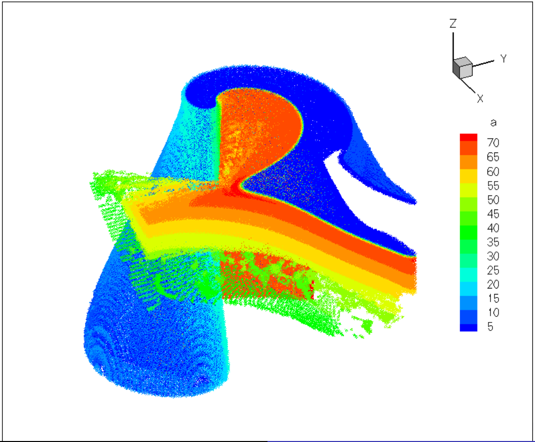
Adaptive Grid

Compression $\longrightarrow$ 17.00%



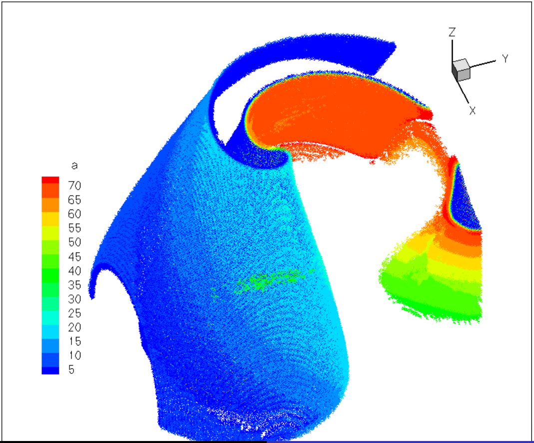
Adaptive Grid

Compression $\longrightarrow$ 12.97%



Adaptive Grid

Compression ⟶ 12.95%



Memory requirements

Radau5 $\longrightarrow$ $L_1 = 4 \times W_1 \times W_1 + 12 \times W_1 + 20$

Rock4 $\longrightarrow$ $L_2 = 8 \times W_2$

$$W = 3 \times 512 \times 512 \times 512 \approx 4.03 \times 10^8 \longrightarrow 24 \text{ Gb}$$

	W_1	W_2	$L = L_1 + L_2$	
Quasi-exact	W	0	6.5×10^{17}	$\longrightarrow$ 36 Eb
Splitting	3	W	3.2×10^9	$\longrightarrow$ 191 Gb
MR/Splitting 1.10^{-1}	3	$0.13W$	4.2×10^8	$\longrightarrow$ 25 Gb

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AVC Model - Work in progress - 0-d model

System of 19 ODEs.

Unknowns :

- ions: $(Na^+,\ K^+,\ Ca^{2+},\ Cl^-,\ glu^-)$ inside the neurons, glial cells and extracell space,
- $f_n,\ f_a,$
- V_n et V_a, potentials inside the neurons and glial cells.

In 3D, system of reaction-diffusion

- diffusion of ions in the astrocytes and in the extracell space,
- no diffusion of ions in neurons,
- no diffusion for f_n, f_a, V_n et V_a.

System of reaction-diffusion:

$$\frac{du_i}{dt} - \varepsilon_i \, \Delta \, u_i = F_i(u_1, ..., u_{19}).$$

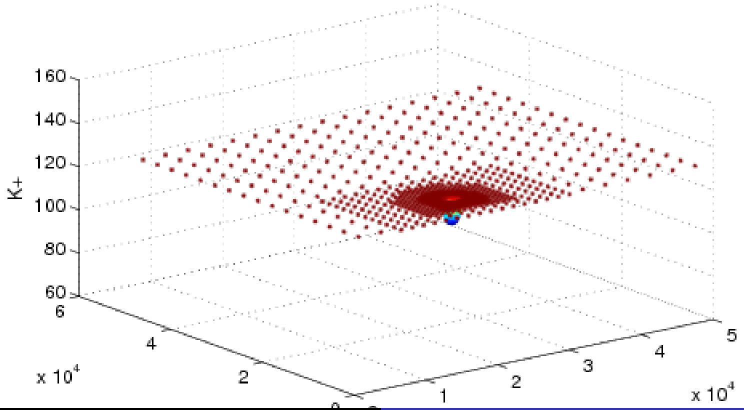
Homogeneous Neumann boundary conditions.

Configuration

- Time Domain : $T = [0, 3600]$
- Spatial Domain : $\Omega = [0, 50000] \times [0, 50000]$
- Integration Time Step : $\Delta t = 3600/360 = 10$
- Tolerances of Time Integrators: $tol = 1.10^{-5}$
- Finest Grid Level : $J = 8$
- Number of cells at Grid J: $2^{d \times J} = 65536 = 256 \times 256$

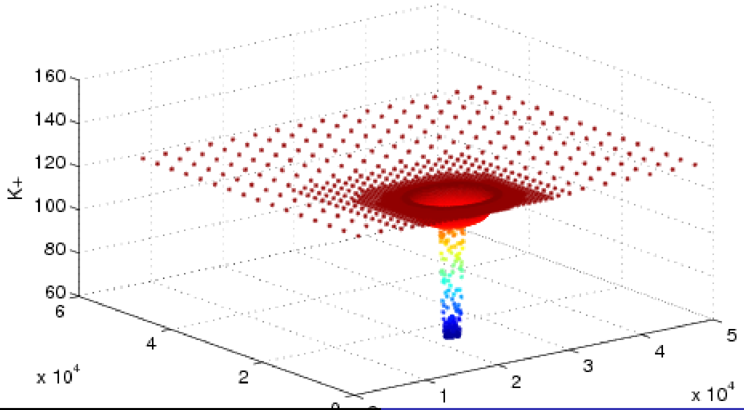
Adaptive Grid

Compression $\longrightarrow$ 1.25%



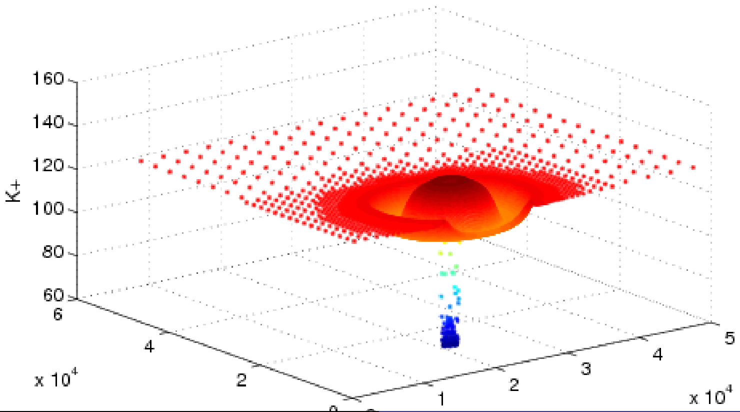
Adaptive Grid

Compression $\longrightarrow$ 7.54%



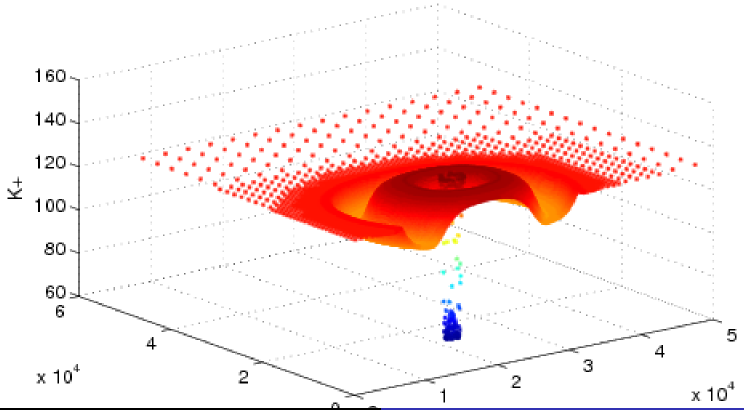
Adaptive Grid

Compression $\longrightarrow$ 16.59%



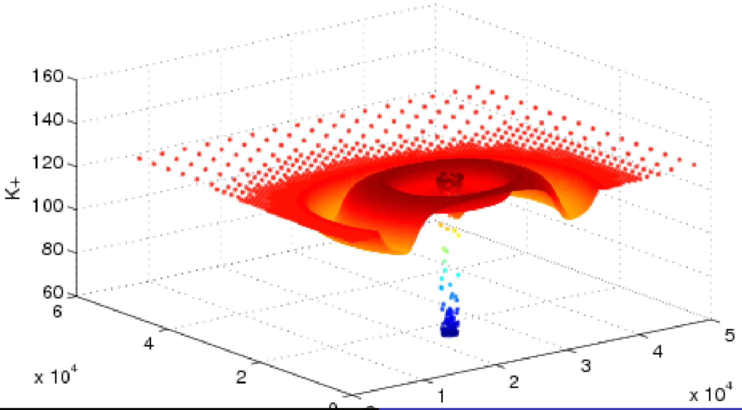
Adaptive Grid

Compression $\longrightarrow$ 28.52%



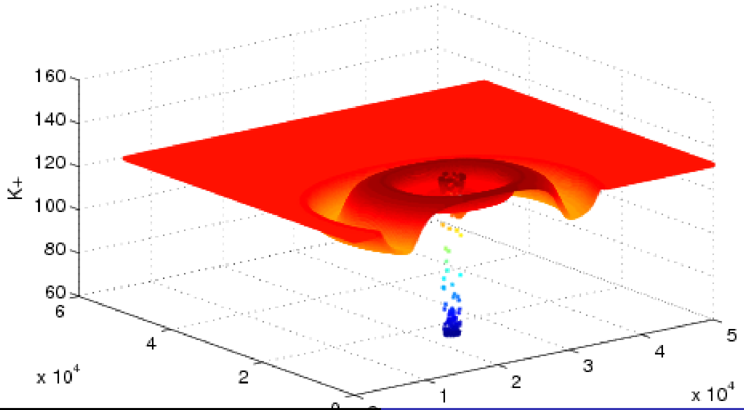
Adaptive Grid

Compression $\longrightarrow$ 35.45%



Fine Grid

Compression $\longrightarrow$ 100%



Conclusions and perspectives

- Convergence rate diminished due to Stiff phenomena
- Parallel speedup is possible, but the speedup is more modest than in space
- Reduction of the size of the system with adaptative muliresolution
- Work in progress
  - Detailed description of “waves”
  - Complex chemistry in a RD configuration
    $\longrightarrow$ detailed analysis of flame propagation
  - Multi-dimensional configurations (Brain in 3D)

Funds

- ANR CIS **PITAC**, 2006-2010. Coordinator Y. Maday
- ANR Blanche **SECHELLES**, 2009-2013. Coordinator S. Descombes
- **PEPS** from CNRS, 2007-2008. Coordinators F. Laurent and A. Bourdon
- **PEPS** from CNRS MIPAC, 2009-2010. Coordinator V. Louvet

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T. Dumont, M. Duarte, S. Descombes, M.A. Dronne, M. Massot and V. Louvet
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M. Duarte, M. Massot, S. Descombes, C. Tenaud, T. Dumont, V. Louvet and F. Laurent
New resolution strategy for multi-scale reaction waves using time operator splitting, space adaptive multiresolution and dedicated high order implicit/explicit time integrators.

References V

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Wavelet Representation

In the case where P_j^{j-1} is linear, i.e.,

$$\hat{u}_\mu := \sum_\gamma c_{\mu,\gamma} u_\gamma,$$

using the wavelet terminology, we can write

$$u_\gamma := \langle u, \tilde{\varphi}_\gamma \rangle,$$

where the dual scaling function $\tilde{\varphi}_\gamma$ is simply

$$\tilde{\varphi}_\gamma := |\Omega_\gamma|^{-1} \chi_{\Omega_\gamma},$$

and

$$d_\mu := u_\mu - \hat{u}_\mu = \langle u, \tilde{\varphi}_\mu \rangle - \sum_\gamma c_{\mu,\gamma} \langle u, \tilde{\varphi}_\gamma \rangle = \langle u, \tilde{\psi}_\mu \rangle.$$

Wavelet Representation

The dual wavelet $\tilde{\psi}_\mu$ is given by

$$\tilde{\psi}_\mu := \tilde{\varphi}_\mu - \sum_\gamma c_{\mu,\gamma} \tilde{\varphi}_\gamma.$$

To describe in a simple way the multiresolution vector, we define $\nabla^J := \bigcup_{j=0}^J \nabla_j$ with $\nabla_0 := S_0$ and write

$$\boldsymbol{M_J = (d_\lambda)_{\lambda \in \nabla^J} = (\langle u, \tilde{\psi}_\lambda \rangle)_{\lambda \in \nabla^J}}$$

where we have set $d_\lambda = u_\lambda$ and $\tilde{\psi}_\lambda = \tilde{\varphi}_\lambda$ if $\lambda \in \nabla_0$.