Méthodes numériques performantes en espace/temps pour la simulation des fluides réactifs

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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
   - One Illustrating Example with Adaptive Multiresolution
3. Conclusions and Perspectives

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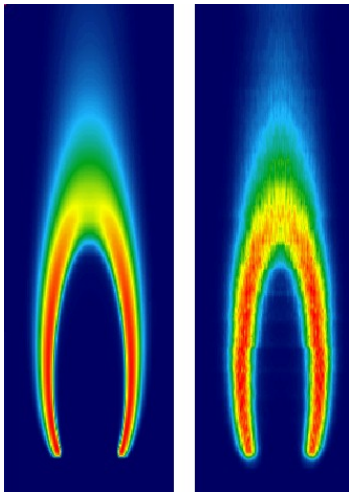
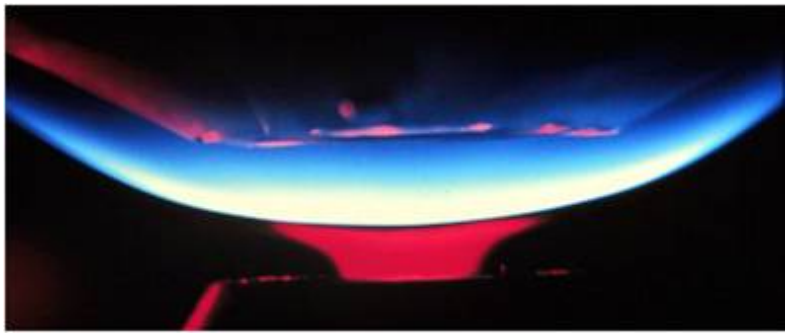
Application Background

Numerical simulation of unsteady reactive phenomena

- Flames (Instabilities, dynamics, pollutants)





- Chemical “waves” (spiral waves, scroll waves)
- Biochemical Engineering (migraines, Rolando’s region, strokes)

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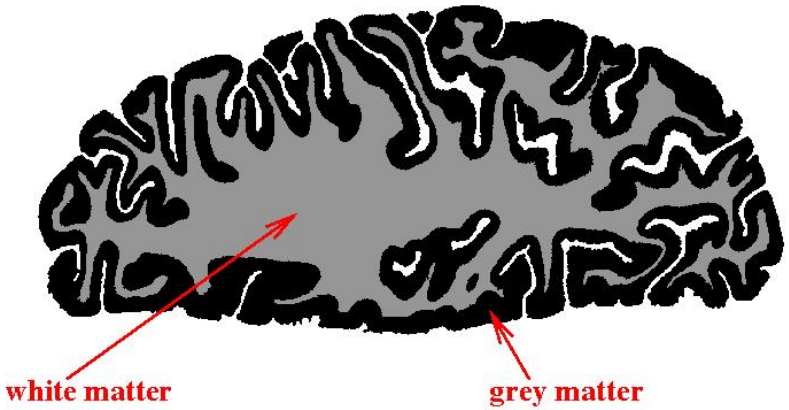

To summarize

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

Examples

- KPP or Fischer equation
- Belousov-Zhabotinsky system of equations

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

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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

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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.

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

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

Basis of operator splitting II

First order methods :

Lie Formulae.

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

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

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 estimates by Lie formalism

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 $U^\varepsilon = (u^\varepsilon, v^\varepsilon)^t$

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

- 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

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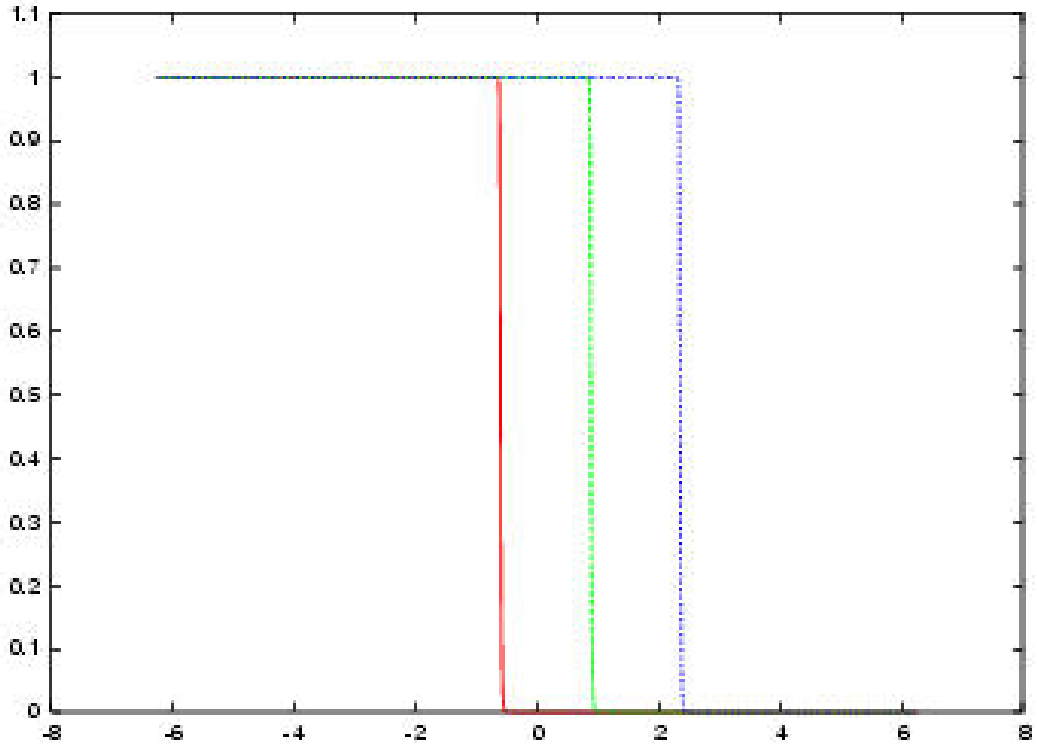
High spatial gradients

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



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

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

$$\mathbf{U_0^0} = \mathbf{u^0}, \quad \mathbf{U_n^0} = \mathcal{G}^{\Delta \mathbf{T_{n-1}}}(\mathbf{U_{n-1}^0}) \text{ for } \mathbf{n} = 1, \ldots, \mathbf{N},$$

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

$$\mathbf{U_0^i} = \mathbf{u^0}, \quad \mathbf{U_n^i} = \mathcal{F}^{\Delta \mathbf{T_{n-1}}}(\mathbf{U_{n-1}^{i-1}}) + \mathcal{G}^{\Delta \mathbf{T_{n-1}}}(\mathbf{U_{n-1}^i}) - \mathcal{G}^{\Delta \mathbf{T_{n-1}}}(\mathbf{U_{n-1}^{i-1}})$$

for n=1,. . . ,N.

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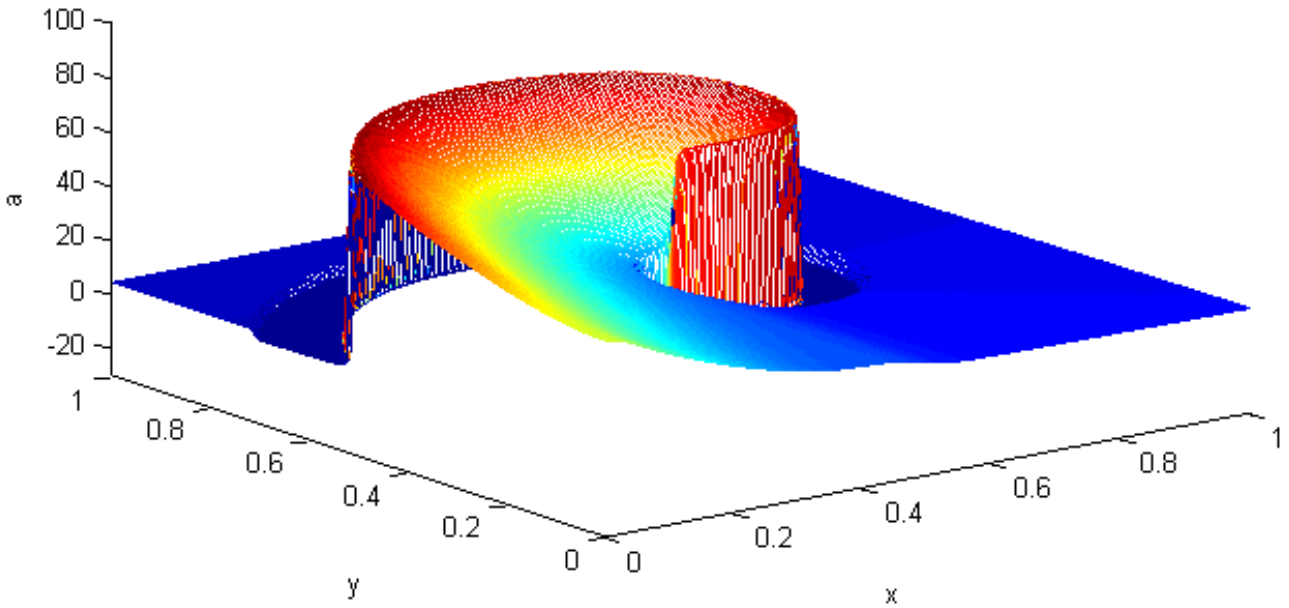
"Toy" Model

Belousov-Zhabotinsky system of equations

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

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

"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

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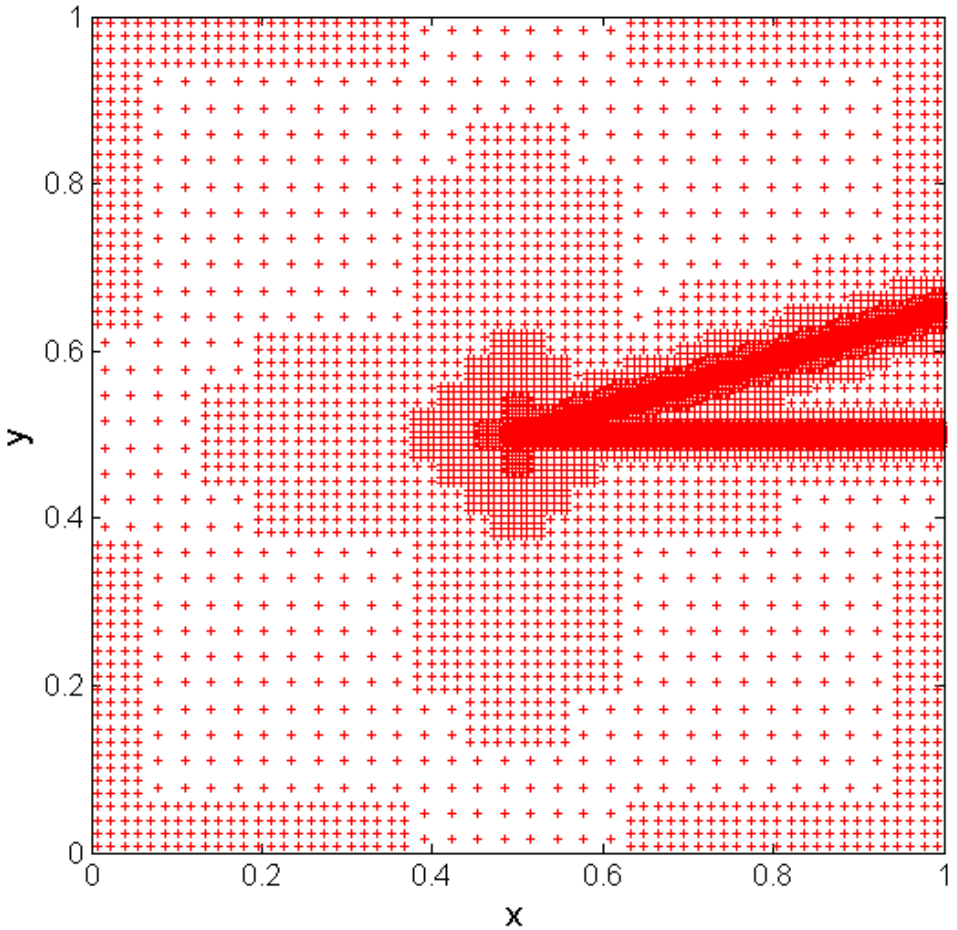
2D Configuration

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

- Time Domain : $\mathbf{T} = [0, 4]$
- Spatial Domain : $\Omega = [0, 1] \times [0, 1]$
- Integration Time Step : $\Delta \mathbf{t} = 4/1024$

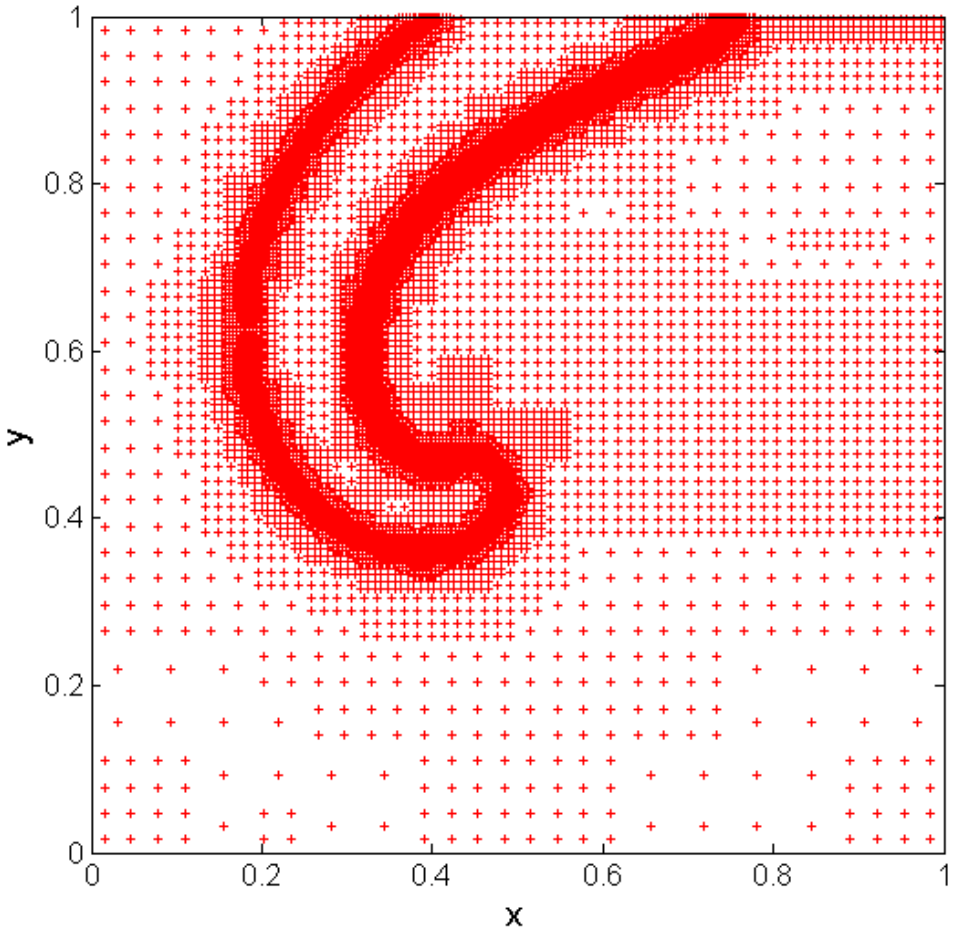
Adaptive Grid

Compression $\longrightarrow$ 1.41%



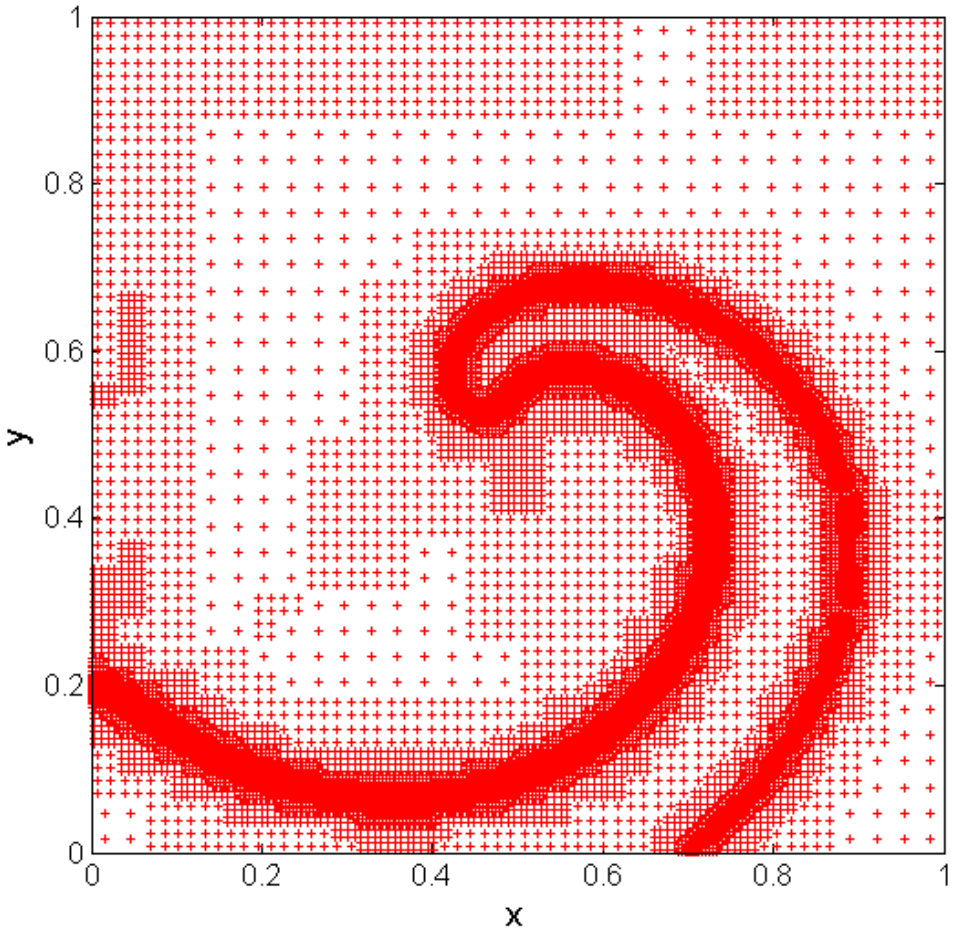
Adaptive Grid

Compression $\longrightarrow$ 2.96%



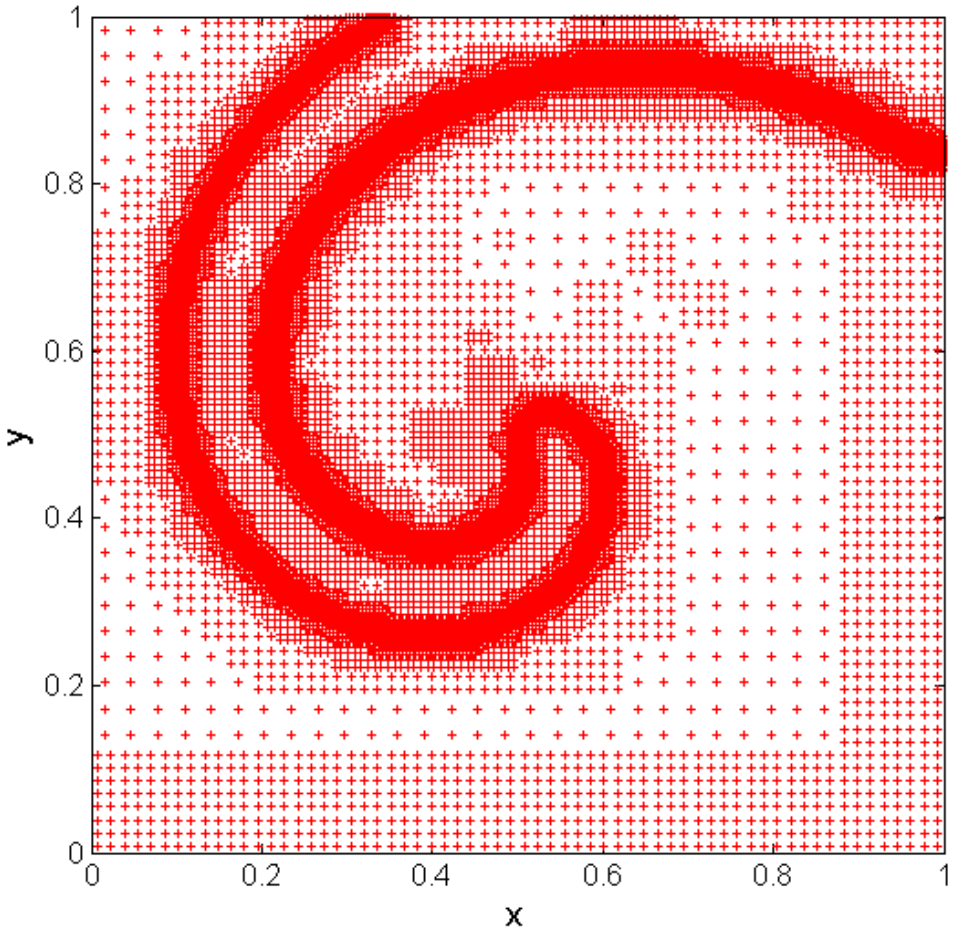
Adaptive Grid

Compression $\longrightarrow$ 3.90%



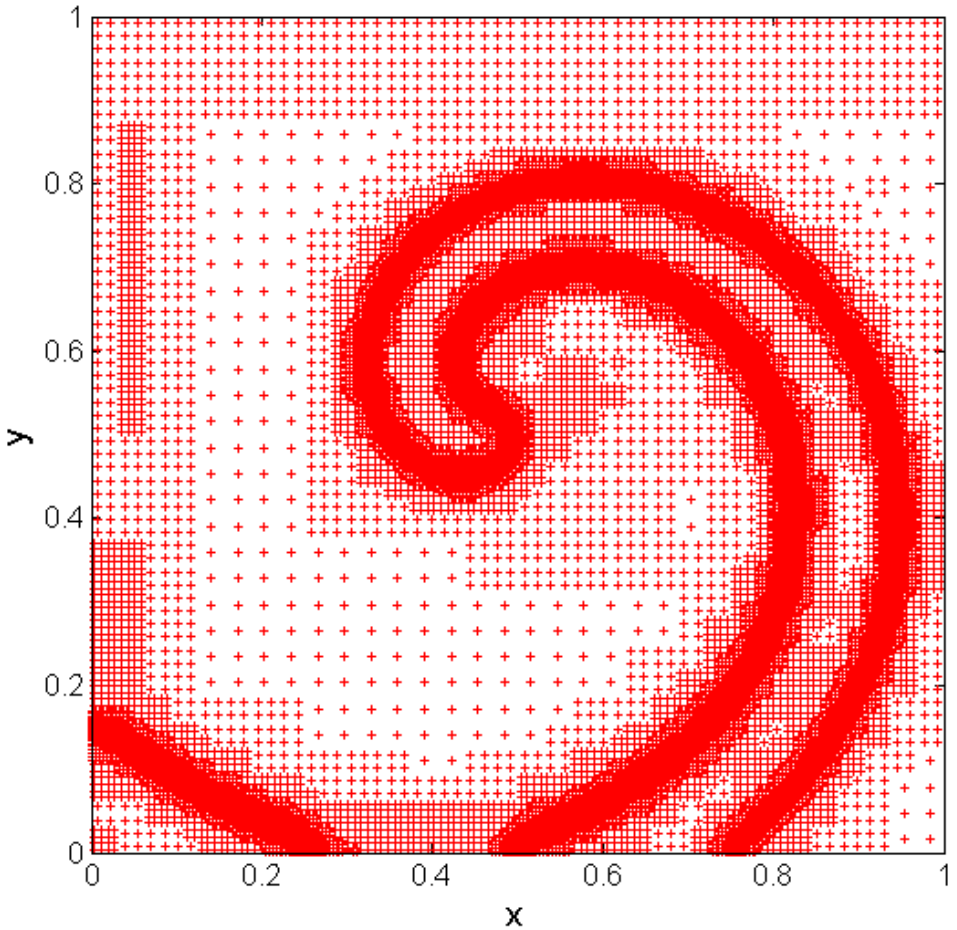
Adaptive Grid

Compression $\longrightarrow$ 4.69%



Adaptive Grid

Compression $\longrightarrow$ 5.77%

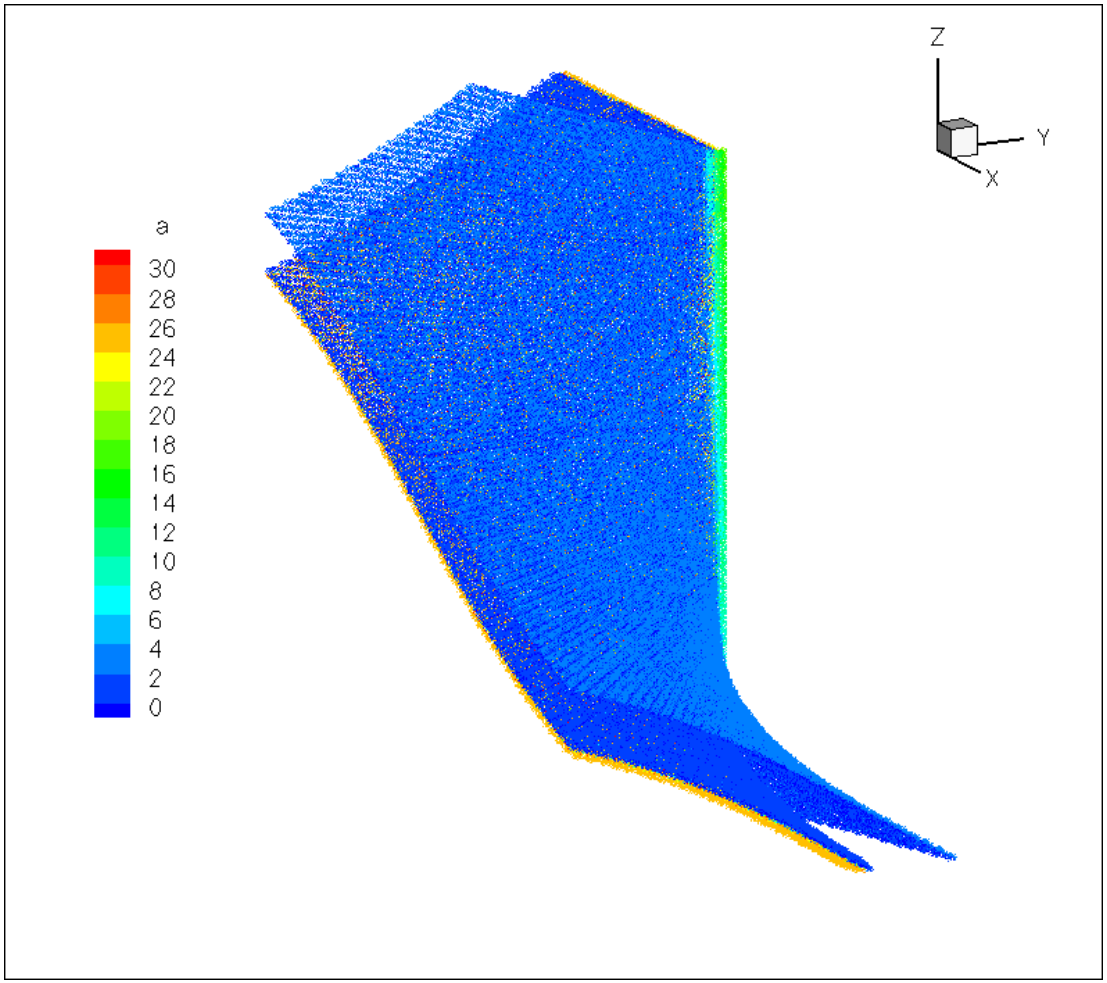


3D Configuration

- Time Domain : $\mathbf{T} = [0, 2]$
- Spatial Domain : $\Omega = [0, 1] \times [0, 1] \times [0, 1]$
- Integration Time Step : $\Delta \mathbf{t} = 2/256$

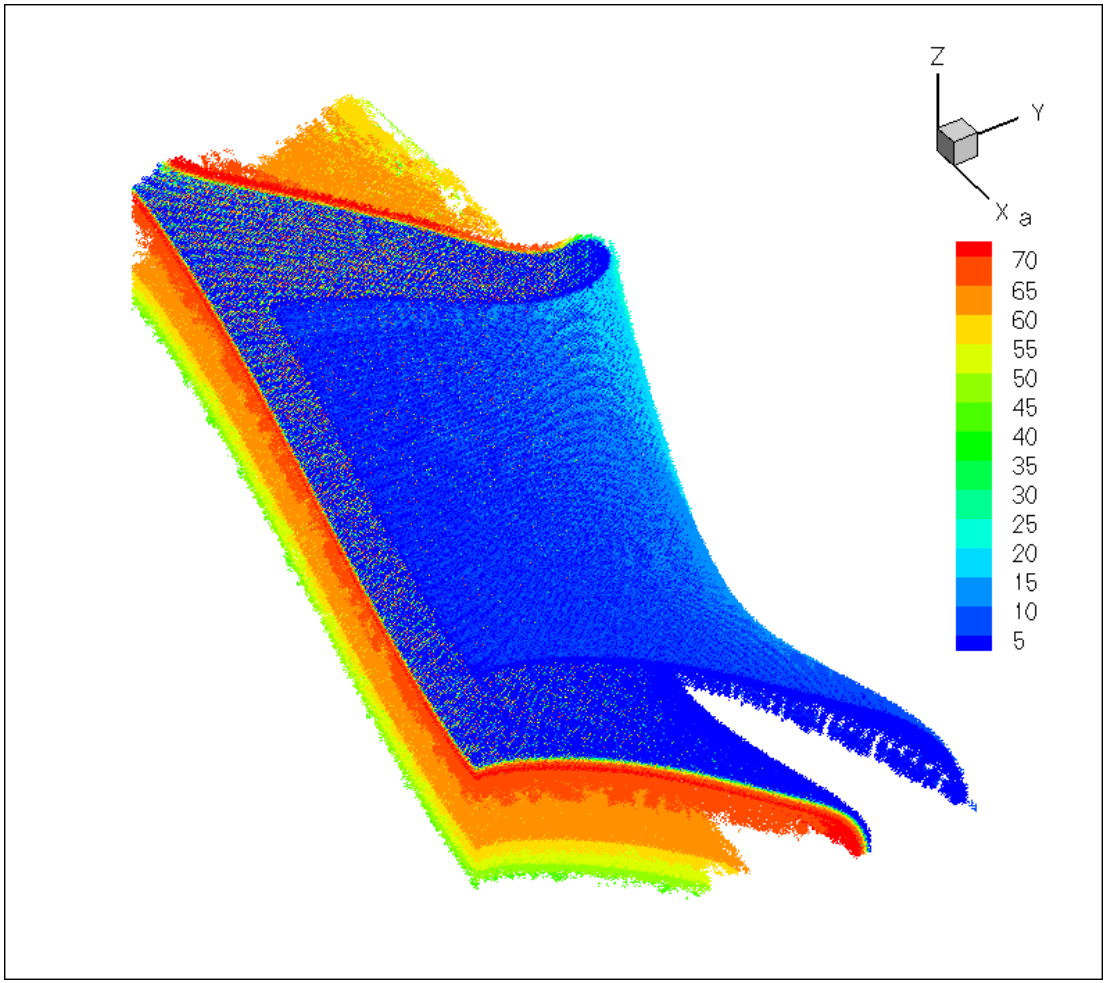
Adaptive Grid

Compression $\longrightarrow$ 4.46%



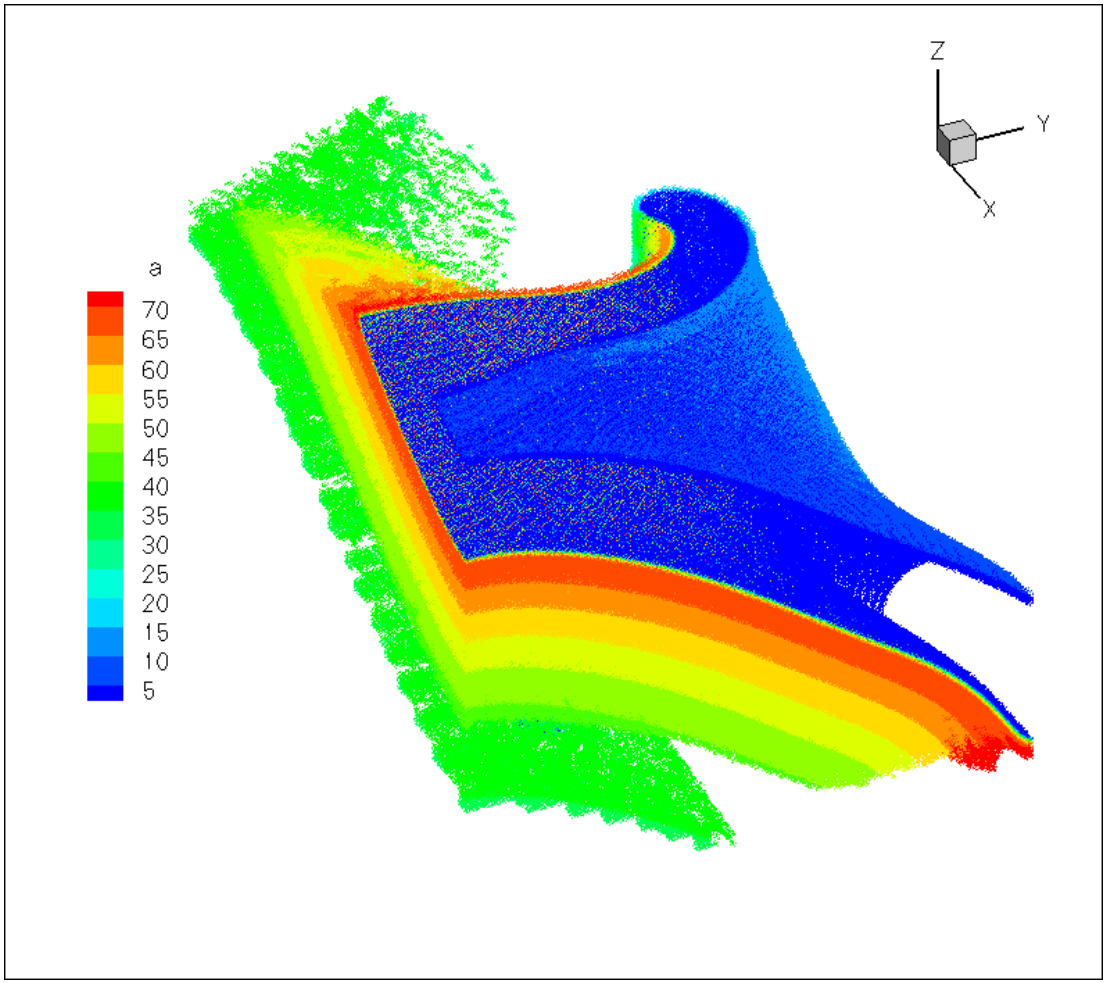
Adaptive Grid

Compression $\longrightarrow$ 10.38%



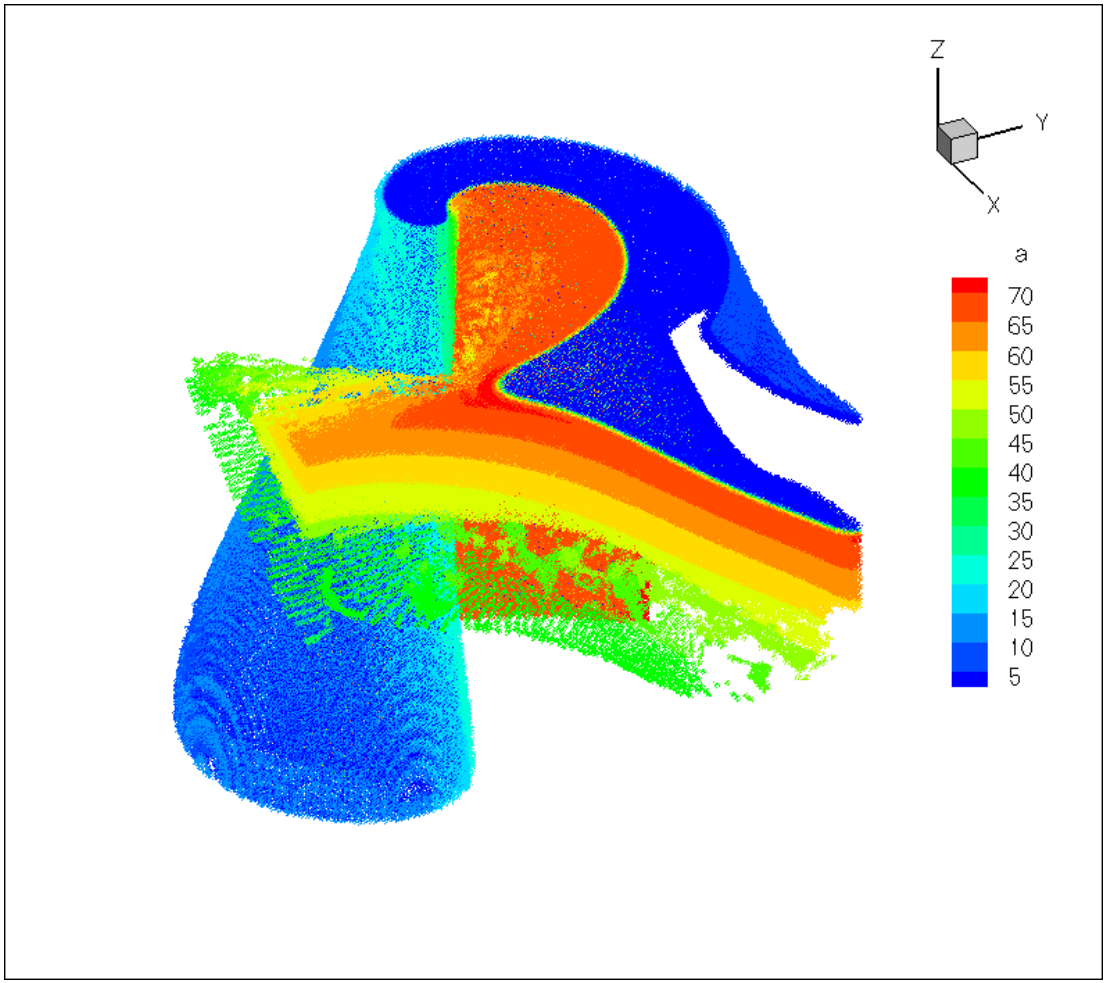
Adaptive Grid

Compression $\longrightarrow$ 17.00%



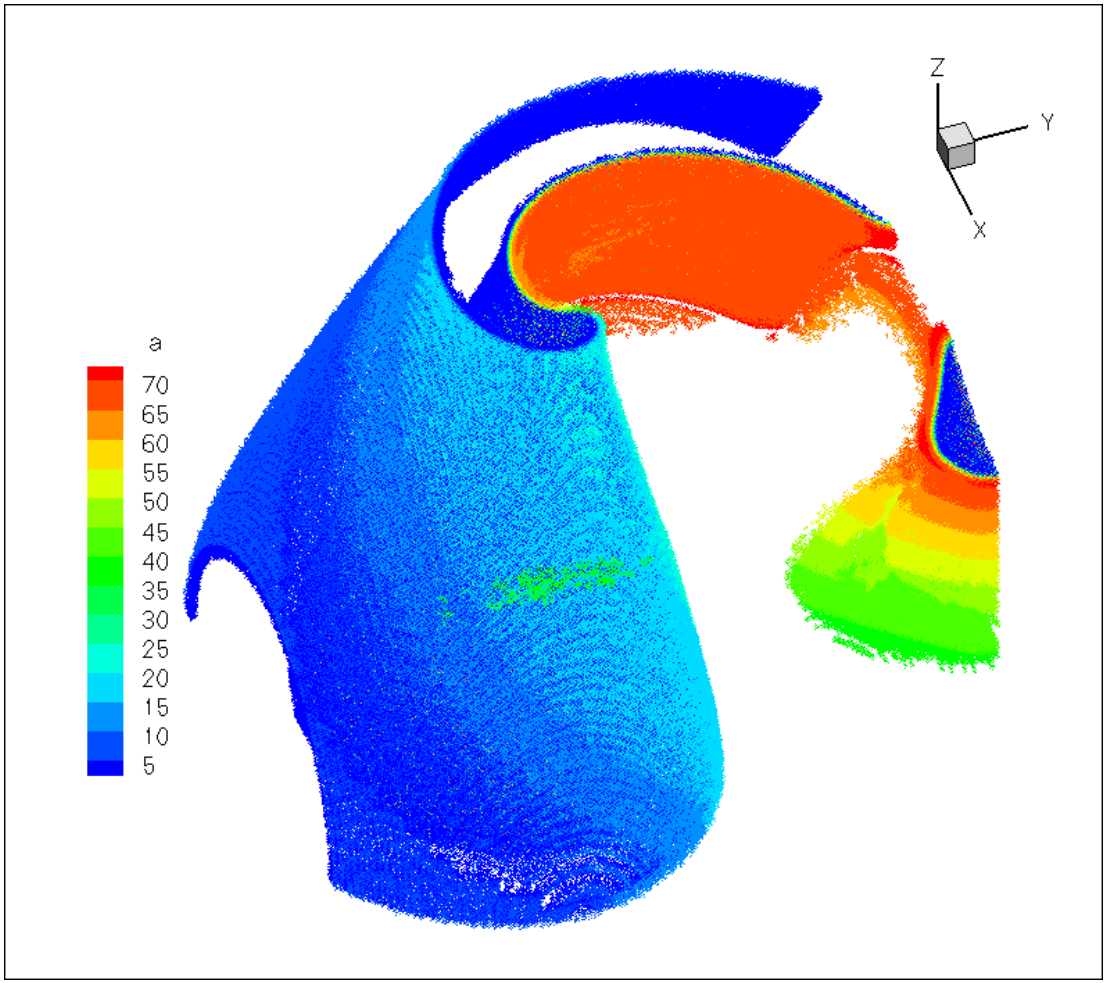
Adaptive Grid

Compression $\longrightarrow$ 12.97%



Adaptive Grid

Compression $\longrightarrow$ 12.95%



Conclusions and perspectives

- Splitting methods and efficient splitting methods
- 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
  - Real problems with Complex chemistry
  - Adaptative time step

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