# Time-space adaptive numerical methods for multi-scale reaction waves simulation

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In collaboration with S. Candel[1] and F. Laurent[1].

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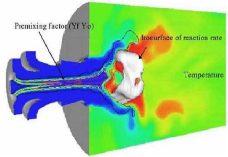
# Outline

# Context and Motivation

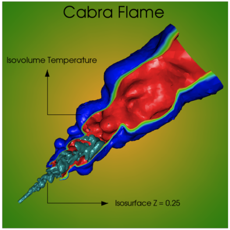
- Predictive Simulations for industrial needs
- Strong evolution of Computer Power and Modeling Tools




source: CERFACS.

Main Numerical Goals:

- Resolution of the dynamics of reaction fronts.
- Reliable accuracy control based on mathematical aspects.




source: R. Vicquelin, EM2C Lab.

**New Numerical Strategies for Time/Space Multi-scale Fronts**

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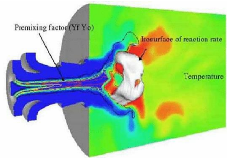
- Strong evolution of Computer Power and Modeling Tools

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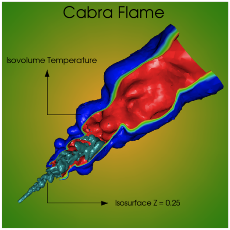


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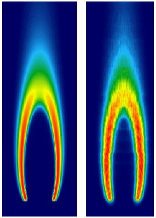
**New Numerical Strategies for Time/Space Multi-scale Fronts**

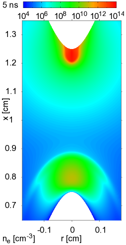
# Application Background

Flames (dynamics, pollutants, complex chemistry)

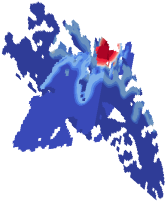


source: Yale Univ.

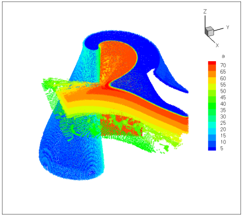
Plasma (repetitive discharges, streamers)




source: A. Bourdon EM2C



Biochemical Engineering (migraines, Rolando's region, strokes)



Chemical waves (spiral waves, scroll waves)

**Time and Space Multi-scale Phenomena**

# Numerical Strategies

Coupled resolution of large time scale spectrum

- Time explicit methods (high order in space)
- Implicit methods (adaptive time stepping)

SANDIA, ISTA/JAXA, CERFACS, ...

Alternative methods: decoupling time scale spectrum

- Partitioning methods

  G. Warnecke *et al*, ...

- Operator Splitting techniques

  J.B. Bell *et al*, M.S. Day *et al*, H.N. Najm, O.M. Knio, ...

AMR techniques for flames, detonations, reactive flows

R. Deiterding, T. Ogawa *et al*, D.W. Schwendeman *et al*, J.W. Banks *et al*, S. Paolucci *et al*, K. Schneider *et al*, ...

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# Time/Space Adaptive Numerical Strategy

Time integration method

⇓

Strang Operator Splitting

↪ based on Numerical Analysis for stiff PDEs

↪ splitting time steps larger than fastest scales

Descombes & Massot 04, Descombes *et al* 07-11

Adaptive splitting time step technique

↪ dynamic accuracy control based on NA

Descombes *et al* 11

↪ applied to instationary problems

Duarte *et al* 11

Space adaptive multiresolution technique

↪ based on wavelet transform and NA

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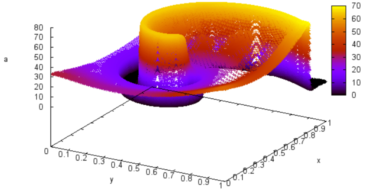
# Strang Operator Splitting

$$\partial_t u - \partial_{\mathbf{x}} \cdot \mathbf{F}(u) - \partial_{\mathbf{x}} \cdot (D(u)\, \partial_{\mathbf{x}} u) = \Omega(u)$$

$$\begin{aligned} \partial_t u &= \Omega(u) \\ \partial_t u &= \partial_{\mathbf{x}} \cdot (D(u)\, \partial_{\mathbf{x}} u) \\ \partial_t u &= \partial_{\mathbf{x}} \cdot \mathbf{F}(u) \end{aligned}$$




$$\mathcal{S}^{\Delta t} u_0 = \mathcal{R}^{\Delta t/2} \mathcal{D}^{\Delta t/2} \mathcal{C}^{\Delta t} \mathcal{D}^{\Delta t/2} \mathcal{R}^{\Delta t/2} u_0$$

$\mathcal{R}^{\Delta t_R} \rightarrow$ Radau5 (Hairer & Wanner 91)
$\mathcal{D}^{\Delta t_D} \rightarrow$ ROCK4 (Abdulle 02)
$\mathcal{C}^{\Delta t_C} \rightarrow$ OSMP3 (Daru & Tenaud 04)

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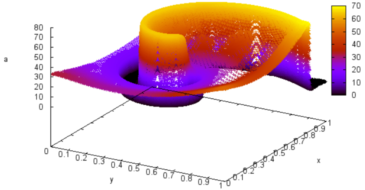


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# Time Adaptive Numerical Strategy

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Duarte *et al* 10, Tenaud *MR CHORUS*

# Adaptive Splitting Time Step

We define two time integration solvers:

$$\mathcal{S}^{\Delta t} u_0 - \mathcal{T}^{\Delta t} u_0 = \mathcal{O}(\Delta t^3) \quad \Longrightarrow \quad \text{Strang formula}$$

$$\widetilde{\mathcal{S}}^{\Delta t} u_0 - \mathcal{T}^{\Delta t} u_0 = \mathcal{O}(\Delta t^2) \quad \Longrightarrow \quad \text{embedded Strang formula}$$

and considering

$$\left\| \mathcal{S}^{\Delta t} u_0 - \widetilde{\mathcal{S}}^{\Delta t} u_0 \right\| \approx \mathcal{O}(\Delta t^2) < \eta$$

yields

$$\Delta t_{new} = \Delta t \sqrt{\frac{\eta}{\left\| \mathcal{S}^{\Delta t} u_0 - \widetilde{\mathcal{S}}^{\Delta t} u_0 \right\|}}$$

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Time integration method

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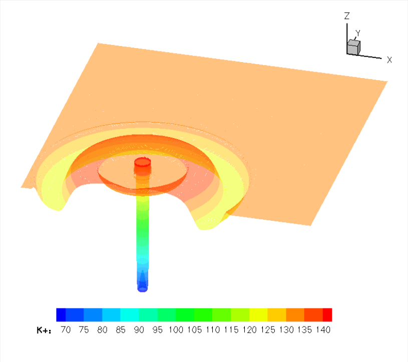
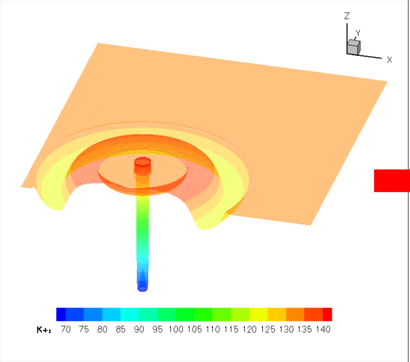
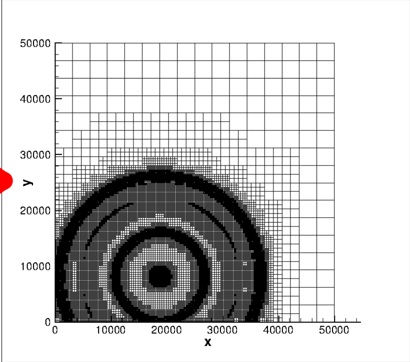



$$V^J(x,y) = V^0(x,y) + \sum_{j=1}^{J} D^j(x,y)$$

# Space Adaptive Multiresolution




$$V^J(x,y) = V^0(x,y) + \sum_{j=1}^{J} D^j(x,y)$$

$$V^J_\varepsilon(x,y)$$

$$\| V^J(x,y) - V^J_\varepsilon(x,y) \| \leq \varepsilon$$

# Time/Space Adaptive Numerical Scheme

code **MBARETE** (Duarte *et al.*)

Time integration method

$\Downarrow$

Strang Operator Splitting

$\hookrightarrow$ High order dedicated methods

Adaptive splitting time step technique

$\hookrightarrow$ Independent of stability issues

Space adaptive multiresolution technique

# Application Framework

**Combustion flames interacting with vortex structures**

$$\partial_t Y_i + \mathbf{v} \cdot \partial_\mathbf{x} Y_i = D\,\partial_\mathbf{x}^2 Y_i + \frac{\nu_i W_i}{\rho}\dot{\omega}$$

$$\partial_t T + \mathbf{v} \cdot \partial_\mathbf{x} T = D\,\partial_\mathbf{x}^2 T + \frac{\nu_F W_F Q}{\rho c_p}\dot{\omega}$$

Single step chemistry
⇓
Arrhenius law

$\mathbf{v}(\mathbf{x}, t) \Longrightarrow$ 2D vortex configuration

$$v_\theta(r,t) = \frac{\Gamma}{2\pi r}\left(1 - \exp\left(-\frac{r^2}{4\nu t}\right)\right)$$

Thermodiffusive approach
⇓
Laminar flames with constant density

# Application Framework

**Combustion flames interacting with vortex structures**

$$\begin{aligned} \partial_t Y_i + \mathbf{v} \cdot \partial_{\mathbf{x}} Y_i &= D\,\partial^2_{\mathbf{x}} Y_i + \frac{\nu_i W_i}{\rho}\dot{\omega} \\ \partial_t T + \mathbf{v} \cdot \partial_{\mathbf{x}} T &= D\,\partial^2_{\mathbf{x}} T + \frac{\nu_F W_F Q}{\rho c_p}\dot{\omega} \end{aligned}$$

Single step chemistry
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Thermodiffusive approach
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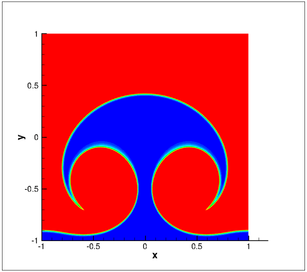
Laminar flames with constant density

# Premixed Flame with Vortex (Laverdant & Candel J. Propulsion 87)

Introducing progress variable $c(x, y, t)$

$$c = \frac{T - T_o}{T_b - T_o} = \frac{Y_{Fo} - Y_F}{Y_{Fo}}$$

$c = 1 \rightarrow$ burnt gases
$c = 0 \rightarrow$ fresh gases




$$\frac{\partial c}{\partial t_\star} + u_\star \frac{\partial c}{\partial x_\star} + v_\star \frac{\partial c}{\partial y_\star} = \frac{\partial^2 c}{\partial x_\star^2} + \frac{\partial^2 c}{\partial y_\star^2} + \mathrm{Da}(1-c)\exp\left(-\frac{T_a}{T_o(1+\tau c)}\right)$$

$$v_{\theta\star}(r_\star, t_\star) = \frac{\mathrm{Re}\,\mathrm{Sc}}{r_\star}\left(1 - \exp\left(-\frac{r_\star^2}{4\,\mathrm{Sc}\,t_\star}\right)\right)$$

# Premixed Flame with Two Vortices (Re = 1000)

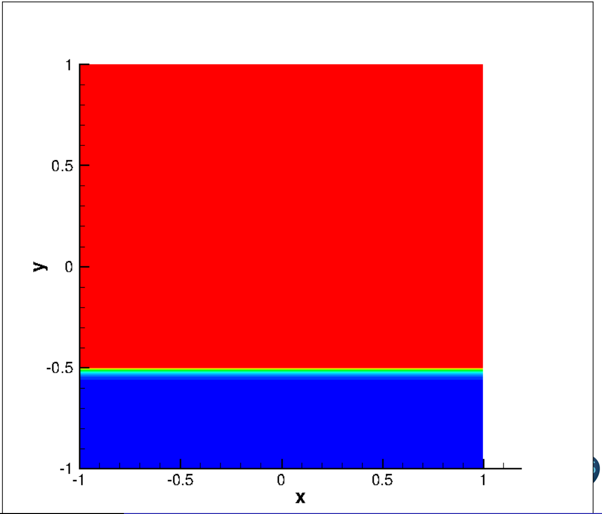
Finest Grid $= 1024^2$
CPU time $\sim 40h15$

$$\frac{\text{Active Grid}}{\text{Finest Grid}} \lesssim 9\%$$

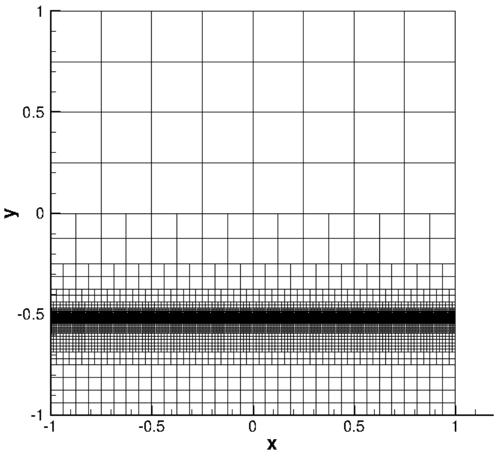
CPU time $\sim 0h57$

$$\boxed{\eta = 10^{-3}}$$

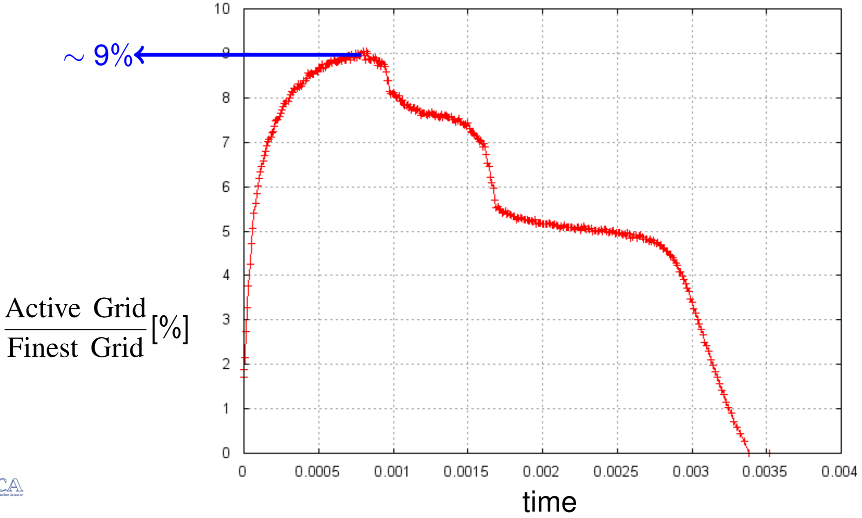
2.7 GHz AMD Shanghai
RAM memory 32 GB



# Dynamic Adaptive Grid



# Time Evolution of Data Compression



# Multiple Time Steps

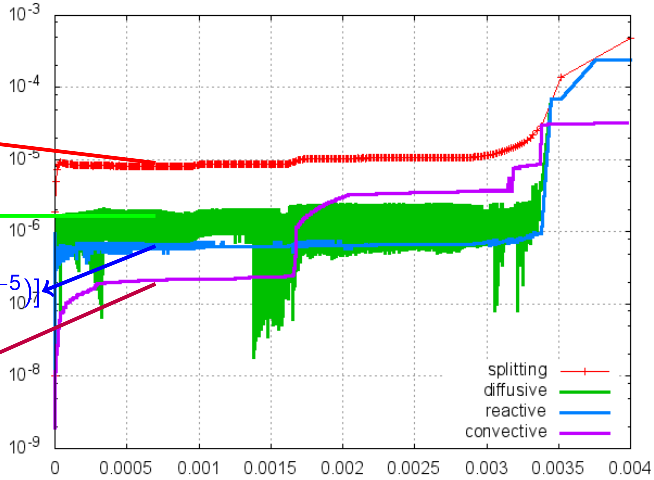
time steps

$\Delta t \sim \mathcal{O}(10^{-5})$

$\Delta t_D \sim \mathcal{O}(10^{-6})$

$\Delta t_R \sim [\mathcal{O}(10^{-7}), \mathcal{O}(10^{-5})]$

$\Delta t_C \sim \mathcal{O}(10^{-7})$




time

# Premixed Flame Toroidal Vortex (Re = 1000)

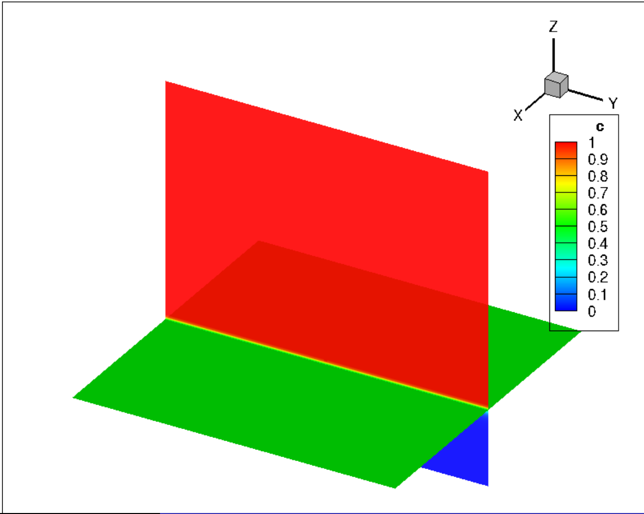
Finest Grid $= 256^3$
CPU time (out of reach)

$$\frac{\text{Active Grid}}{\text{Finest Grid}} \lesssim 17\%$$

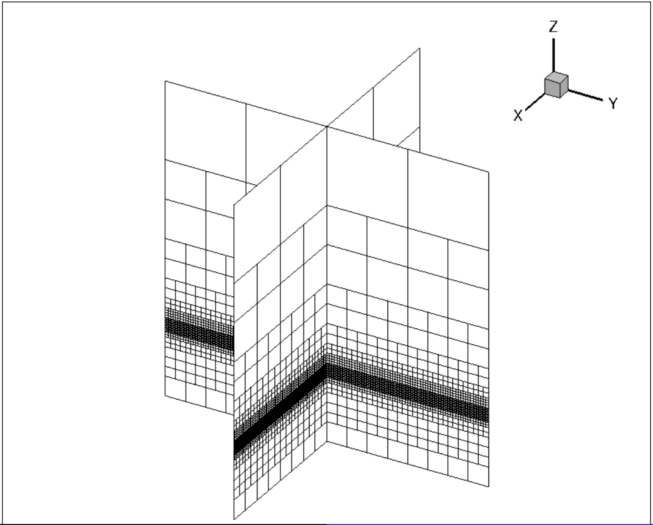
CPU time $\sim 14h40$

$$\eta = 10^{-3}$$

2.7 GHz AMD Shanghai
RAM memory 32 GB



# Dynamic Adaptive Grid



# Ignition of Diffusion Flame with Vortex (Thévenin & Candel Phys. Fluids 95)

Defining $Z(x,y,t)$ and $\theta(x,y,t)$

$$\theta = (T - T_{O0})/(T_{F0} - T_{O0}), \quad Z = \frac{\chi Y_F / Y_{F0} + \tau\theta}{\chi + \tau}$$

With dimensionless variables:

$$\frac{\partial Z}{\partial t_\star} + u_\star \frac{\partial Z}{\partial x_\star} + v_\star \frac{\partial Z}{\partial y_\star} = \frac{\partial^2 Z}{\partial x_\star^2} + \frac{\partial^2 Z}{\partial y_\star^2}$$

$$\frac{\partial \theta}{\partial t_\star} + u_\star \frac{\partial \theta}{\partial x_\star} + v_\star \frac{\partial \theta}{\partial y_\star} = \frac{\partial^2 \theta}{\partial x_\star^2} + \frac{\partial^2 \theta}{\partial y_\star^2} + F(Z,\theta)$$

$$F(Z,\theta) = \mathrm{Da}\phi\chi Y_{O0} \left[\frac{1-Z}{\phi\tau} + \frac{1}{\chi}(Z-\theta)\right]\left[Z + \frac{\tau}{\chi}(Z-\theta)\right] \exp\left(-\frac{\tau_a}{1+\tau\theta}\right)$$

# Ignition of Diffusion Flame with Vortex ($T_{O0}$ = 1000 - Re = 1000)

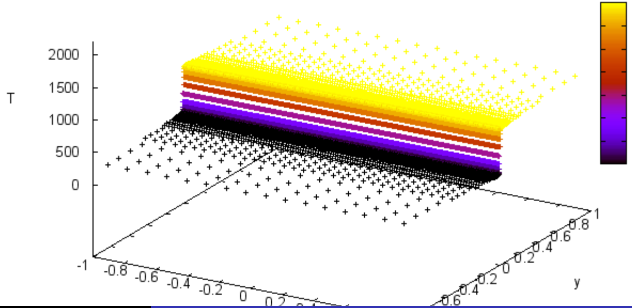
Finest Grid $= 1024^2$
CPU time $\sim 5h24$

$$\frac{\text{Active Grid}}{\text{Finest Grid}} \lesssim 6\%$$

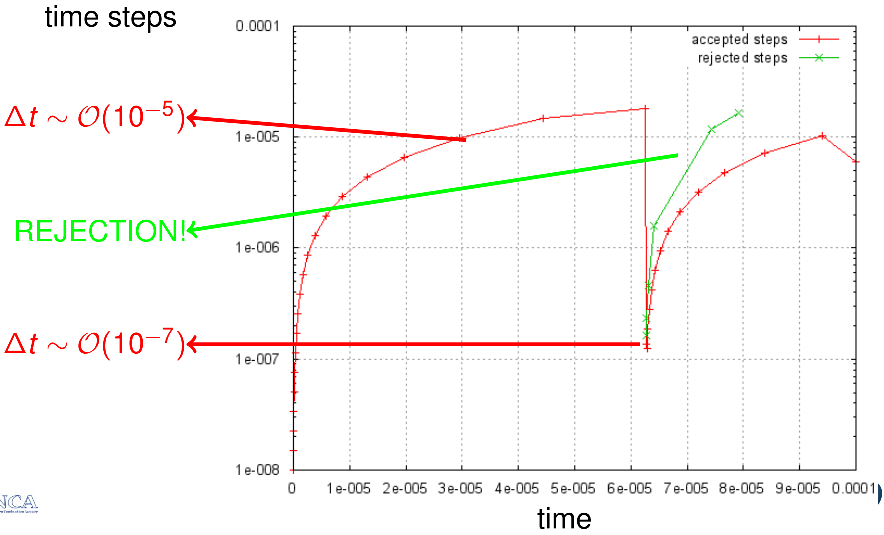
CPU time $\sim 0h08$

$$\boxed{\eta = 10^{-3}}$$

2.7 GHz AMD Shanghai
RAM memory 32 GB



# Adaptive Splitting Time Step



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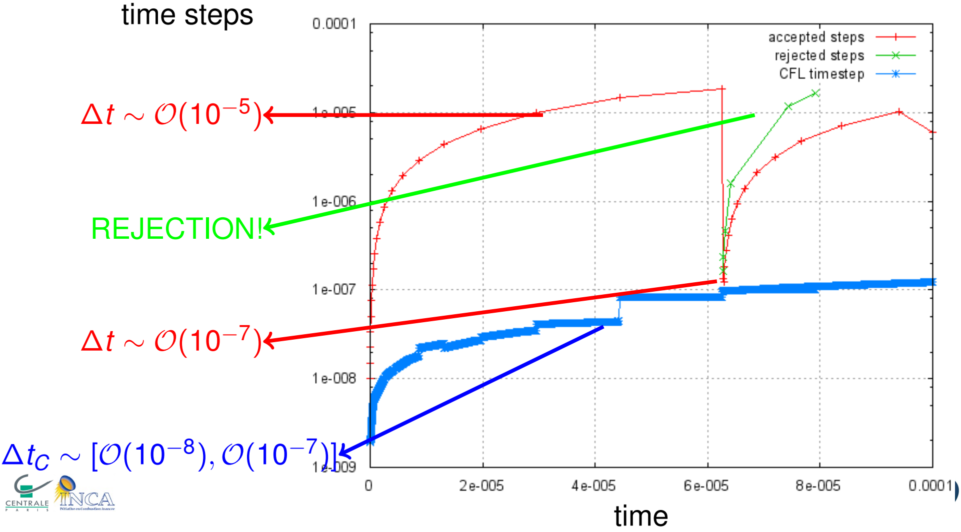

# Some Remarks and Conclusions

Concerning implementation aspects:

- Important savings in computing time and memory requirements.
- Straightforward parallelization in shared memory computing environments.
- Needs of dedicated data structures and optimized routines for MR.

Main contribution:

- Efficient time/space adaptive strategy for multi-scale phenomena.
- Time/space dynamic accuracy control.
- Mathematical background.

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- Mathematical background.

# Taking into Account Complex Chemistry

Finest Grid $= 1024^2$
49 species - 299 reactions

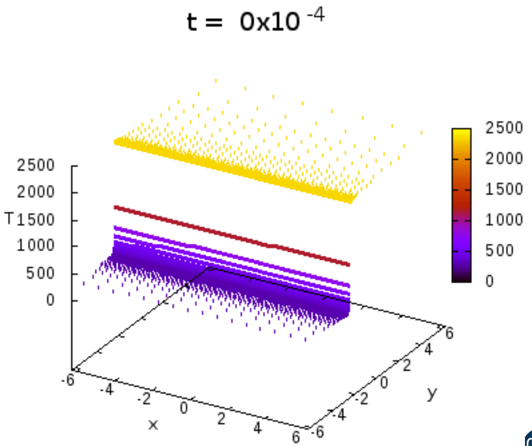
(Lindstedt *et al* 98)

$$\frac{\text{Active Grid}}{\text{Finest Grid}} \lesssim 4\%$$

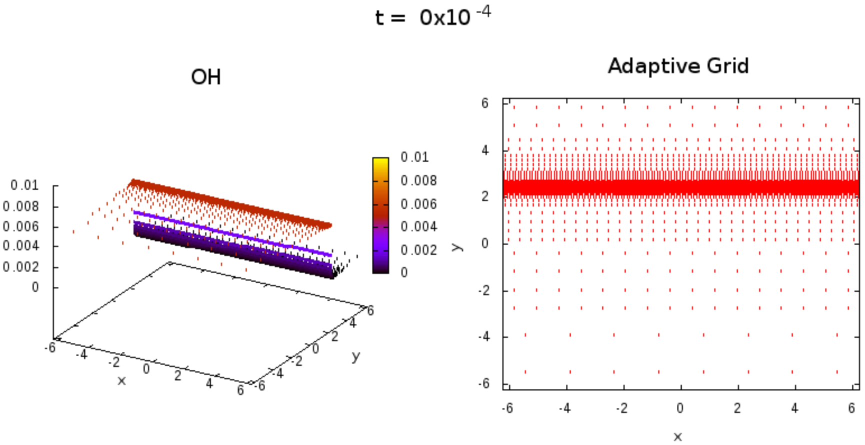
CPU time $\sim 30h30$ with 12 cores

$$\eta = 10^{-2}$$

2.7 GHz AMD Shanghai
RAM memory 48 GB



# Taking into Account Complex Chemistry



# Funds

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- DIGITEO RTRA **MUSE**, 2010-2014. Coordinator M. Massot
- ANR Blanche **SECHELLES**, 2009-2013. Coordinator S. Descombes
- **PEPS** from CNRS MIPAC, 2009-2010. Coordinator V. Louvet
- **PEPS** from CNRS, 2007-2008. Coordinators F. Laurent and A. Bourdon

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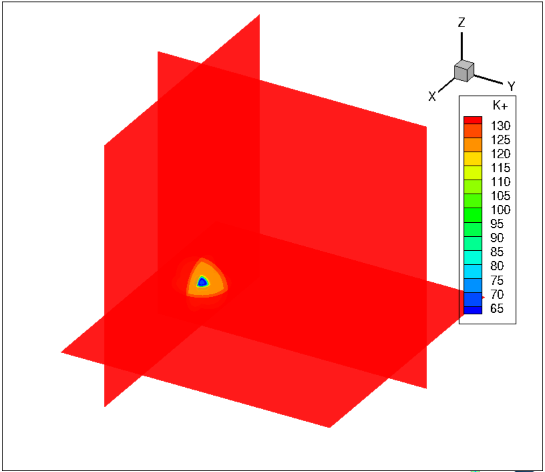
- **M. Duarte, M. Massot, S. Descombes, C. Tenaud, T. Dumont, V. Louvet and F. Laurent.** *New resolution strategy for multi-scale reaction waves using time operator splitting, space adaptive multiresolution and dedicated high order implicit/explicit time integrators.* Submitted to SIAM, available on HAL (2010)
- **T. Dumont, M. Duarte, S. Descombes, M.A. Dronne, M. Massot and V. Louvet.** *Simulation of human ischemic stroke in realistic 3D geometry: A numerical strategy.* Submitted to Bulletin of Mathematical Biology, available on HAL (2010)
- **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: Application to human ischemic stroke.* Accepted to ESAIM Proceedings (2011)
- **S. Descombes, M. Duarte, T. Dumont, V. Louvet and M. Massot.** *Adaptive time splitting method for multi-scale evolutionary PDEs.* Accepted to Confluentes Mathematici (2011)
- **M. Duarte, Z. Bonaventura, M. Massot, A. Bourdon, S. Descombes and T. Dumont.** *A new numerical strategy with space-time adaptivity and error control for multi-scale gas discharge simulations.* Submitted to J. of Comp. Physics, special issue on "Computational Plasma Physics" coordinated by Barry Koren and Ute Ebert (2011)

# Taking into Account Detailed Chemistry

- RD 21 variables model
- MR on simple geometry (Duarte *et al.* 11)
- Grid $= 512^3$
- Active Grid $\lesssim 5\%$
- CPU time $\sim 37h24$ with 8 cores - parallel gain ratio $\sim 7$
- Unfeasible with fixed grid and same computing resource



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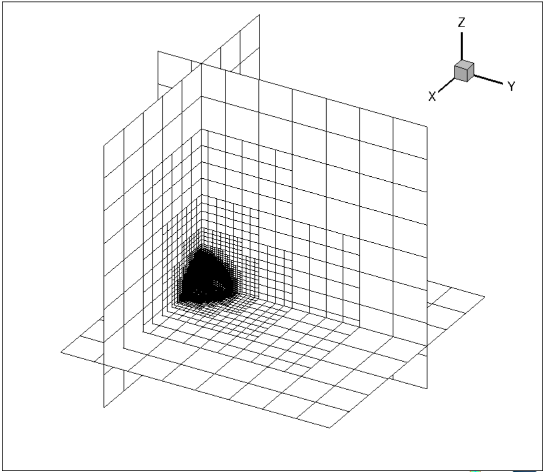
- RD 21 variables model
- MR on simple geometry (Duarte *et al.* 11)
- Grid $= 512^3$
- Active Grid $\lesssim 5\%$
- CPU time $\sim 37h24$ with 8 cores - parallel gain ratio $\sim 7$
- Unfeasible with fixed grid and same computing resource



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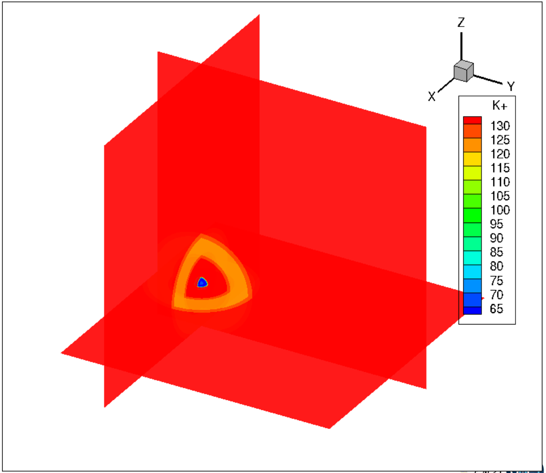

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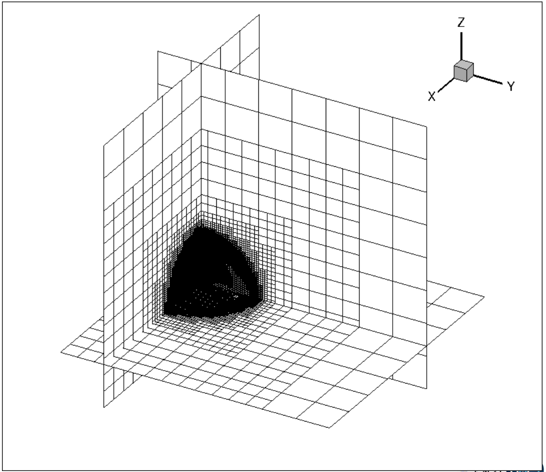

# Basis of operator splitting

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

First order methods :

**Lie Formulae.**

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

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

□

# Basis of operator splitting

Second order methods :

## Strang Formulae.

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

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

□

# Suitable Stiff Integrators

## Numerical Strategy:

$$\partial_t U + \underbrace{\nabla \cdot \mathbf{F}(U)}_{\textbf{OSMP3}} - \underbrace{\Delta U}_{\textbf{ROCK4}} = \underbrace{\Omega(U)}_{\textbf{Radau5}}$$

(Hairer & Wanner Springer-Verlag 91)

- A-stable and L-stable
- Based on RadauIIA Implicit RK with order 5
- Simplified Newton Method $\Longrightarrow$ Linear Algebra tools
- Adaptive time integration step

# Suitable Stiff Integrators

## Numerical Strategy:

$$\partial_t U + \underbrace{\nabla \cdot \mathbf{F}(U)}_{\textbf{OSMP3}} - \underbrace{\Delta U}_{\textbf{ROCK4}} = \underbrace{\Omega(U)}_{\textbf{Radau5}}$$

(Abdulle SIAM J. Sci. Comput. 02)

- Extended Stability Domain (along $\mathbb{R}^-$)
- Order 4
- Adaptive time integration step
- Explicit RK Method $\Longrightarrow$ NO Linear Algebra problems
- Low Memory Demand

# Suitable Stiff Integrators

**Numerical Strategy:**

$$\partial_t U + \underbrace{\nabla \cdot \mathbf{F}(U)}_{\textbf{OSMP3}} - \underbrace{\Delta U}_{\textbf{ROCK4}} = \underbrace{\Omega(U)}_{\textbf{Radau5}}$$

(Daru & Tenaud JCP 04)

- One-step monotonicity preserving scheme
- Order 3 at least
- Explicit Method $\Longrightarrow$ standard CFL constraint
- Low Memory Demand

# Basis of Splitting Numerical Analysis

Considering

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

and introducing Lie formalism

$$D_F G(u) = G'(u) F(u)$$

yield

$$Y^t\, U_0 = \sum_{k \geq 0} \frac{t^k}{k!} \left( D_Y^k \mathbf{Id}(U) \right) \Bigg|_{t=0} = e^{tD_Y} \mathbf{Id}\, U_0$$

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# Basis of Splitting Numerical Analysis

Hence,

$$L_2^t\, U_0 = Y^t\, X^t\, U_0 = e^{tD_X}\, e^{tD_Y} \mathrm{Id}\, U_0$$

And considering BHC formula

$$e^{tD_X}\, e^{tD_Y} = e^{L(t)} \qquad L(t) = t\,(D_X + D_Y) + \frac{t^2}{2}[D_X, D_Y] + \mathcal{O}(t^2)$$

yield

$$T^t\, U_0 - Y^t\, X^t\, U_0 = \frac{t^2}{2}[D_Y, D_X]\mathrm{Id}\, U_0 + \mathcal{O}(t^3)$$

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Considering now

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

it follows

$$S_1^t\, U_0 = Y^{t/2}\, X^t\, Y^{t/2}\, U_0 = e^{\frac{t}{2} D_Y} e^{t D_X} e^{\frac{t}{2} D_Y} \mathrm{Id}\, U_0$$

and

$$\begin{aligned} T^t\, U_0 - Y^{t/2}\, X^t\, Y^{t/2}\, U_0 &= \frac{t^3}{24}\Big[D_Y, [D_Y, D_X]\Big]\mathrm{Id}\, U_0 \\ &\quad - \frac{t^3}{12}\Big[D_X, [D_X, D_Y]\Big]\mathrm{Id}\, U_0 + \mathcal{O}(t^4) \end{aligned}$$

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# Adaptive Splitting Numerical Analysis

Defining

$$\widetilde{S}_1^t U_0 = Y^{\left(\frac{1}{2}+\varepsilon\right)t} X^t Y^{\left(\frac{1}{2}-\varepsilon\right)t} U_0$$

it follows

$$\widetilde{S}_1^t U_0 = e^{\left(\frac{1}{2}-\varepsilon\right)tD_Y} e^{tD_X} e^{\left(\frac{1}{2}+\varepsilon\right)tD_Y} \mathrm{Id} U_0$$

and

$$T^t U_0 - Y^{\left(\frac{1}{2}+\varepsilon\right)t} X^t Y^{\left(\frac{1}{2}-\varepsilon\right)t} U_0 = \varepsilon t^2 [D_Y, D_X] \mathrm{Id} U_0 + \mathcal{O}(\varepsilon t^3) + \mathcal{O}(t^3)$$

$$T^t U_0 - \widetilde{S}_1^t U_0 = \underbrace{T^t U_0 - S_1^t U_0}_{\mathcal{O}(t^3)} + \underbrace{S_1^t U_0 - \widetilde{S}_1^t U_0}_{\mathcal{O}(\varepsilon t^2)}$$

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# Wavelet Representation

Considering $J$ embedded grids $j \in [0, J]$ and the box function $\phi(x) = \chi_{[0,1)}(x)$, we define for $u(x) \in L^2$

$$P_j(u) := \sum_{k=0}^{2^j-1} \langle u, \phi_{j,k} \rangle \phi_{j,k}$$

with

$$\phi_{j,k} = 2^{j/2} \phi(2^j \cdot - k)$$

Thus, defining $\psi_{j,k} = 2^{j/2} \psi(2^j \cdot - k)$ yields

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$$\sum_{k=0}^{2^{j+1}-1} \langle u, \phi_{j+1,k} \rangle \phi_{j+1,k} = \sum_{k=0}^{2^j-1} \langle u, \phi_{j,k} \rangle \phi_{j,k} + \sum_{k=0}^{2^j-1} \langle u, \psi_{j,k} \rangle \psi_{j,k}$$

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$$(P_{j+1} - P_j)u = \sum_{k=0}^{2^j-1} d_{j,k}(u) \psi_{j,k}, \qquad d_{j,k}(u) := \langle u, \psi_{j,k} \rangle$$

# Multiresolution Transformation

(Cohen *et al.* Mathematics of Computation 01)
There is a one-to-one correspondence

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

which defines by iteration a multiscale representation of $U_J$:

$$\mathcal{M} : U_J \longmapsto M_J, \quad M_J = (U_0, D_1, D_2, \cdots, D_J)$$

And thus, thresholding is performed

$$\text{if } |d_{j,k}| < \varepsilon_j \Longrightarrow d_{j,k} = 0, \qquad \varepsilon_j = 2^{\frac{d}{2}(j-J)}\varepsilon,$$

which implies

$$\|U_J^n - V_J^n\|_{L^2} \propto n\varepsilon$$

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If the $\psi_\lambda$ have $m$ vanishing polynomial moments,

$$\langle P, \psi_{j,k} \rangle_{S_{j,k}} = 0, \qquad P \in \mathbb{P}_{m-1}$$

then,

$$|d_{j,k}(u)| = |\langle u, \psi_{j,k} \rangle| = \inf_{P \in \mathbb{P}_{m-1}} |\langle u - P, \psi_{j,k} \rangle|$$

Thus, in practice, we compute

$$d_\mu := u_\mu - \hat{u}_\mu.$$

$u_\mu \Rightarrow$ Projection: exact values computed from finer grids

$\hat{u}_\mu \Rightarrow$ Prediction: approximated values from coarser grids

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