An adaptive multiresolution algorithm for parabolic PDEs

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Outline

- Introduction
- Governing equations for thermodiffusive flames
- Adaptive multiresolution method for parabolic PDEs
- Numerical validation
- Application to thermodiffusive flame instabilities
- Conclusions and perspectives

Introduction

- Active research on combustion instabilities
  - Theoretical (Zeldovich 1938, Sivashinsky 1977, Joulin-Clavin 1979)
  - Experimental (Boyer *et al* 1980, Ronney 1984, Pearlman-Ronney 1994)
  - **Numerical** (Denet-Haldenwang 1992, Bockhorn-Fröhlich-Schneider 1999)

- Problems with numerical combustion: stiffness space and time
  - Very fine grids required, but only around the moving flame front

- Solution: Adaptive techniques
  - Adaptive Mesh Refinement (Berger *et al* 1984, Haldenwang-Pignol 2002)
  - Adaptive wavelet methods (Liandrat *et al* 1990, FS 1994, ...)

Introduction

- Multiresolution schemes (Harten 1995)
  - solution on fine grid → solution on coarse grid + details
  - Details "small" ⇒ interpolation, no computation (CPU time Reduced)
  - 2D non-linear hyperbolic problems e.g. shock computations (Bihari-Harten 1996, Abgrall-Harten 1996, Chiavassa-Donat 2001, Dahmen *et al* 2001)
- Adaptive multiresolution schemes (Müller 2001, Cohen *et al* 2002)
  - Details "small" ⇒ remove from memory (Memory also Reduced)
  - 2D non-linear hyperbolic problems
- **Objectives: for combustion, 3D non-linear parabolic problems**

Introduction

- Combustion of lean gaseous mixtures:

  Hydrodynamic and **thermodiffusive** instabilities may appear

  - Thermodiffusive case: *cellular* flames, *pulsating* flames
  - Instabilities observed experimentally in flame balls (Ronney 1990) and simulated numerically (Schneider 1996, Gerlinger *et al* 2003)
  - Different scenarios of evolution: spherical growth, splitting, extinction, steady

- **Objectives**:

  - **Investigation of pulsating instabilities for large values of the activation energy (very thin reaction zone)**
  - **Interaction of flame balls with e.g. adiabatic walls or vortices**

Governing equations

Hypothesis

- Combustion of premixed perfect gases
- Simple chemical reaction $\mathcal{A}_1 + \mathcal{A}_2 \rightarrow \mathcal{A}_3$
- $\mathcal{A}_1$ and $\mathcal{A}_3$ highly diluted in $\mathcal{A}_2$ $(Y_1 = Y,\ Y_3 = 1 - Y)$
- One-step kinetics (Arrhenius)
- Activation energy large, but finite
- Constant density approximation
- Constant transport coefficients
- No gravity
- Black-body radiation model (Stefan-Boltzmann)

Governing equations

Non-dimensional thermodiffusive equations

$$\begin{aligned} \partial_t T + \vec{v}\cdot\vec{\nabla}T - \nabla^2 T &= \omega - s && (1)\\ \partial_t Y + \vec{v}\cdot\vec{\nabla}Y - \frac{1}{Le}\nabla^2 Y &= -\omega && (2) \end{aligned}$$

$$\omega(T,Y) = \frac{Ze^2}{2\,Le} Y \exp\left[\frac{Ze(T-1)}{1+\alpha(T-1)}\right] \text{ (reaction rate)}$$

$$s(T) = \gamma\left[\left(T+\alpha^{-1}-1\right)^4 - \left(\alpha^{-1}-1\right)^4\right] \text{ (heat loss due to radiation)}$$

$+$ initial and boundary conditions

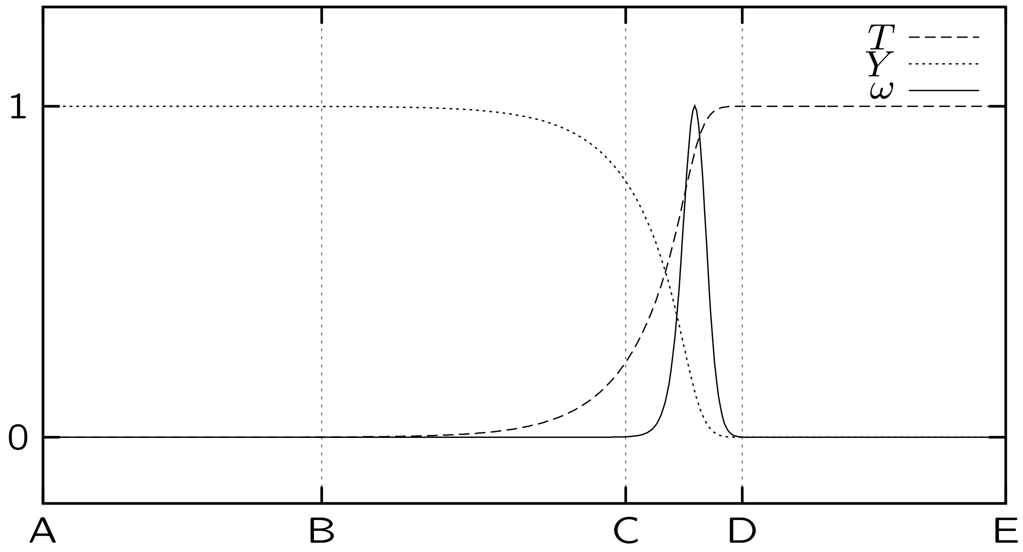
$Y = Y_1$, $T = \dfrac{\bar{T}-\bar{T}_u}{\bar{T}_b-\bar{T}_u}$, $Le = \dfrac{\kappa}{D}$ (Lewis), $\alpha = \dfrac{\bar{T}_b-\bar{T}_u}{\bar{T}_b}$, $Ze = \alpha\dfrac{E_a}{RT_b}$ (Zeldovich)

$\vec{v}$ given by the incompressible NS equations. When the fluid is at rest, $\vec{v} = \vec{0}$.

Governing equations

Planar flames

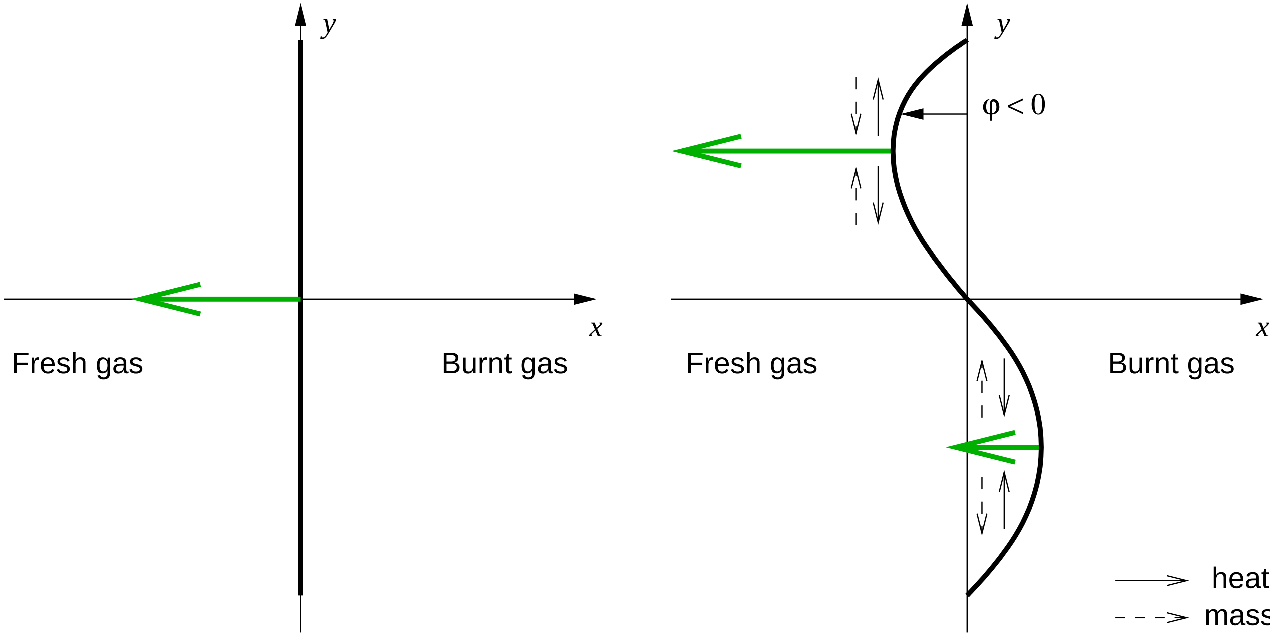
- Flame propagation at the velocity v_f
- When the fresh mixture is advected at $v = -v_f \Rightarrow$ **steady planar flame**



AB: *fresh mixture*, BC: *preheat zone*, CD: *reaction zone* $d = O(Ze^{-1})$, DE: *burnt mixture*

Governing equations

Thermodiffusive instability



Stable: ω for $Le = 1$, $Ze = 10$ (animation) - Unstable: ω for $Le = 0.3$, $Ze = 10$ (animation)

Asymptotic theory for $Ze >> 1$ (Sivashinsky 1977, Joulin-Clavin 1979)

1) $Ze(Le - 1) < -2$: cellular flames 2) $Ze(Le - 1) > 16$: pulsating flames

2D Flame front

Temperature

Reaction rate

Adaptive grid

stable
Le = 1.0

Unstable
Le = 0.3

Adaptive multiresolution method

Discretization of the thermodiffusive equations

- *Thermodiffusive equations: non-linear parabolic equations of the form*

$$\partial_t U = \mathcal{D}(U), \; U = (T, Y)^t, \text{ and } \mathcal{D}(U) = -\nabla \cdot f(U) + \nu \nabla^2 U + S(U) \qquad (3)$$

- **Explicit time integration:** 2^{nd}*-order Runge-Kutta scheme*

$$\begin{aligned} U^* &= U^n + \Delta t\, \mathcal{D}(U^n) && (4) \\ U^{n+1} &= \frac{1}{2}\left(U^n + U^* + \Delta t\, \mathcal{D}(U^*)\right) && (5) \end{aligned}$$

- **Space discretization**: *finite volume formulation (2^{nd}-order)*
  ENO upwind scheme for advective terms, centered for diffusive ones

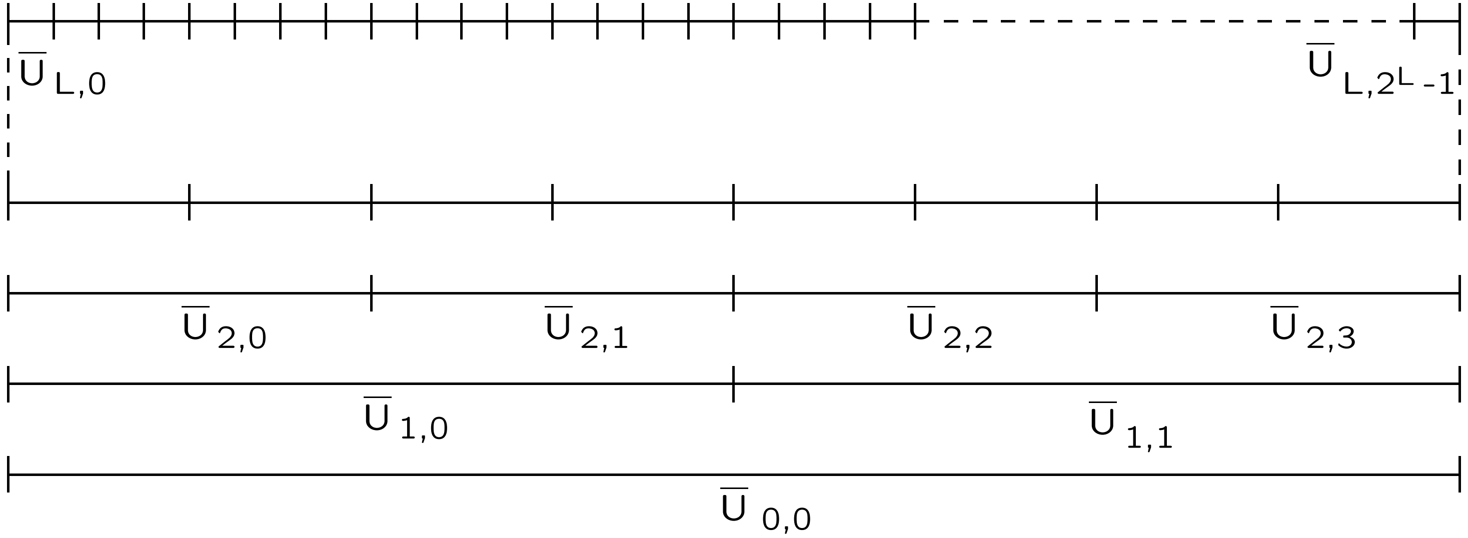
$$\text{Domain: } \Omega = (\Omega_i)_{i \in \Lambda}. \qquad \forall i \in \Lambda, \; \partial_t \bar{U}_i = \bar{\mathcal{D}}_i \text{ with } \bar{U}_i = \frac{1}{|\Omega_i|} \int_{\Omega_i} U \, d\mathcal{V} \qquad (6)$$

$$\text{and } \bar{\mathcal{D}}_i := \frac{1}{|\Omega_i|} \int_{\Omega_i} \mathcal{D} \, d\mathcal{V} = -\frac{1}{|\Omega_i|} \int_{\partial \Omega_i} (f(U) - \nu \nabla U) \cdot n_i \, ds + \bar{S}_i$$

Adaptive multiresolution method

Multiresolution: nested dyadic grids $\Omega = (\Omega_{l,i})_{0 \leq i < 2^l}$, $0 \leq l \leq L$

Data: Cell-average value on $\Omega_{l,i}$: $\bar{U}_{l,i} = \dfrac{1}{|\Omega_{l,i}|} \displaystyle\int_{\Omega_{l,i}} U \, d\mathcal{V}$



We denote by $\bar{U}_l = (U_{l,i})_{0 \leq i < 2^l}$.

Adaptive multiresolution method

Multiresolution decomposition for cell-average values

Projection : (or restriction) $\bar{U}_{l-1} = \mathbf{P}_{l \to l-1} \bar{U}_l$
Prediction : (or prolongation) $\widehat{U}_{\,l+1} = \mathbf{P}_{l \to l+1} \bar{U}_l$

$\mathbf{P}_{l \to l+1}$ is **local** and **consistent with** $\mathbf{P}_{l \to l-1}$, i.e.

$$\mathbf{P}_{l \to l-1}\, \mathbf{P}_{l \to l+1} \;=\; \mathrm{Id}$$

Details: $D_{l,i} = \bar{U}_{l,i} - \widehat{U}_{l,i}$. If $\mathbf{P}$ is consistent, they are redundant .

The knowledge of $\bar{U}$ for the N children is **equivalent** to the knowledge of $\bar{U}$ for the parent and $N-1$ details: $\bar{U}_l \leftrightarrow (\bar{U}_{l-1}, D_l)$.

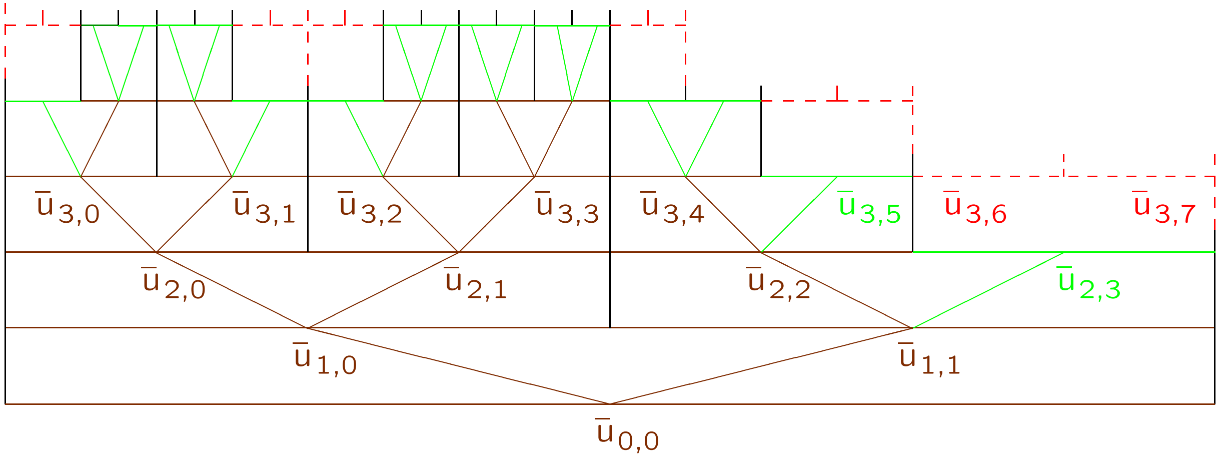
Multiresolution transform : $\bar{\mathrm{M}} : \bar{U}_L \mapsto (\bar{U}_0, D_1, \ldots, D_L)$

Adaptive multiresolution method

Thresholding : Delete $D_{l,i}$ if $|D_{l,i}| < 2^{d(l-L)}\,\epsilon$, $d =$ dimension

$\Rightarrow$ error controlled

Data : graded tree structure $\bar{U}_l = (\bar{u}_{l,i})_{0 \leq l \leq L,\, i \in \Lambda_l}$



- nodes **- leaves** **- virtual leaves**

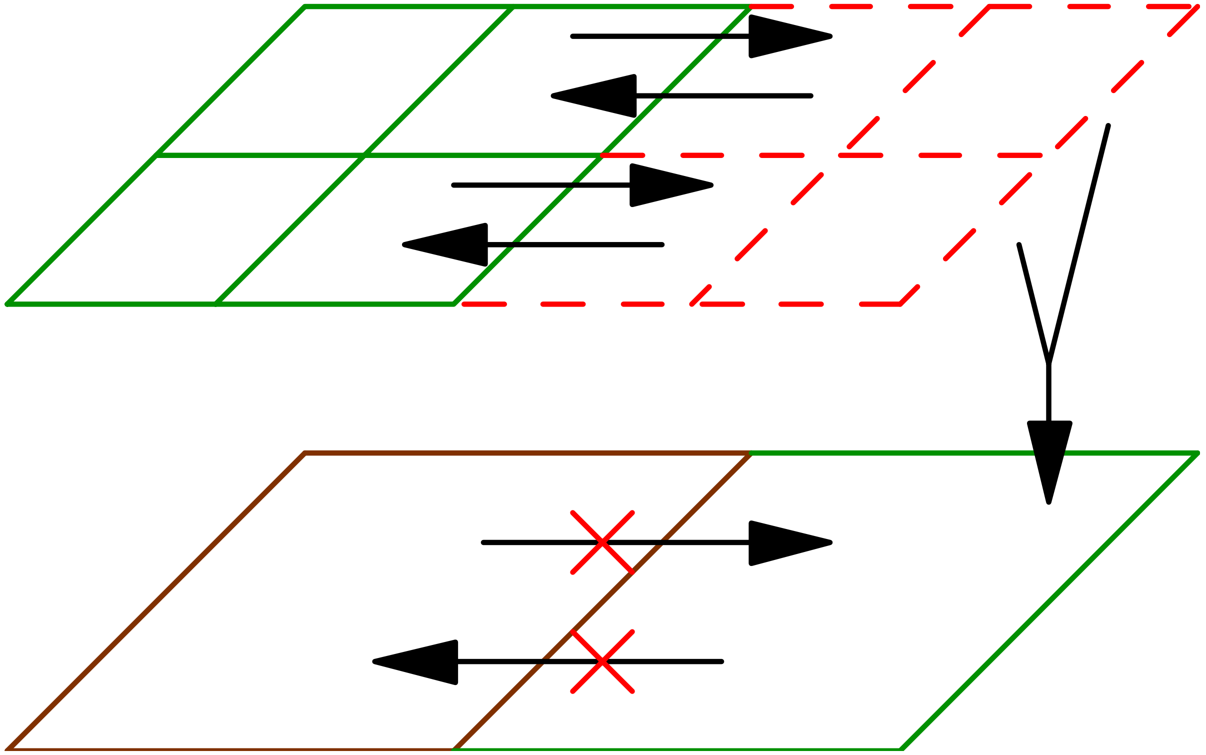
Adaptive multiresolution method

Algorithm

$$\bar{U}^{n+1} = \bar{\mathbf{M}}^{-1}\,\mathbf{T}(\epsilon)\,\bar{\mathbf{M}}\,\mathbf{E}(\Delta t)\,\bar{U}^{n}$$

- *Thresholding:* $\mathbf{T}(\epsilon)$
  - After thresholding, **one more level is added** ⇒ undelete details
- *Time evolution*: $\mathbf{E}(\Delta t)$
  - Only on leaves. Virtual leaves are used for the *flux computation*.
  - To ensure **conservativity** : flux always computed on the *higher level*
- *Complexity*: $O(N \log N)$, N = number of degrees of freedom

Conservative flux computation



Ingoing and outgoing flux computation in 2D for two different levels

Numerical validation

Error analysis

- *Stability*
  Convection-diffusion equation: $\partial_t u + \partial_x u = \frac{1}{Pe}\partial^2_{xx} u$, TVD if (Bihari 1996)

$$\Delta t \leq \frac{\Delta x^2}{4Pe^{-1} + \Delta x}\ , \ \Delta x \propto 2^{-L} \tag{7}$$

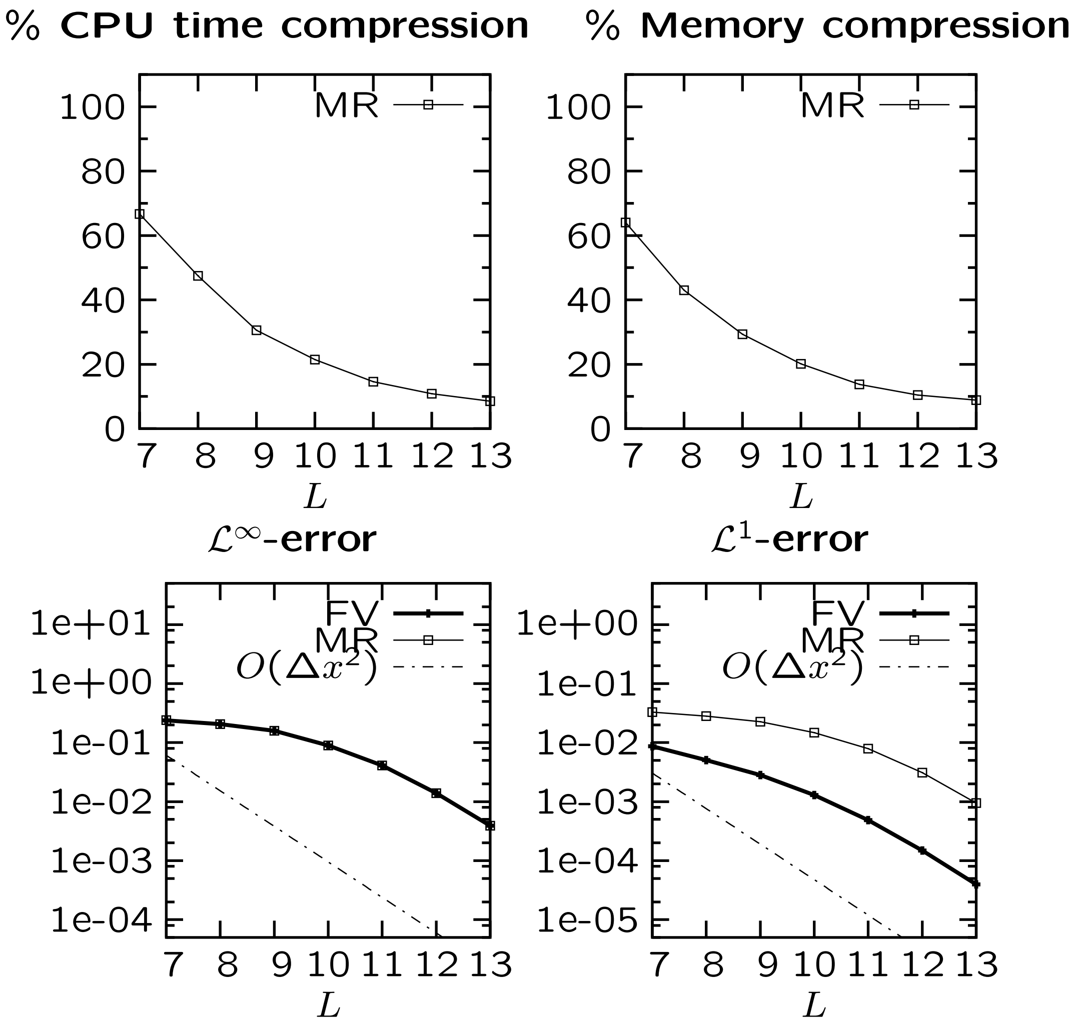
- *Accuracy*

$$||\bar{u}^L_{ex} - \bar{u}^L_{MR}|| \leq ||\bar{u}^L_{ex} - \bar{u}^L_{FV}|| + ||\bar{u}^L_{FV} - \bar{u}^L_{MR}|| \tag{8}$$

Discretization error: $||\bar{u}^L_{ex} - \bar{u}^L_{FV}|| \propto 2^{-\alpha L}$
Perturbation error: $||\bar{u}^L_{FV} - \bar{u}^L_{MR}|| \propto n\epsilon = \frac{T}{\Delta t}\epsilon$ (Cohen *et al* 2002)

We want the perturbation error to be **of the same order** as the discretization error. Therefore we choose

$$\boxed{\epsilon = C\frac{2^{-(\alpha+1)L}}{Pe + 2^{L+2}}\ , \ C > 0} \tag{9}$$

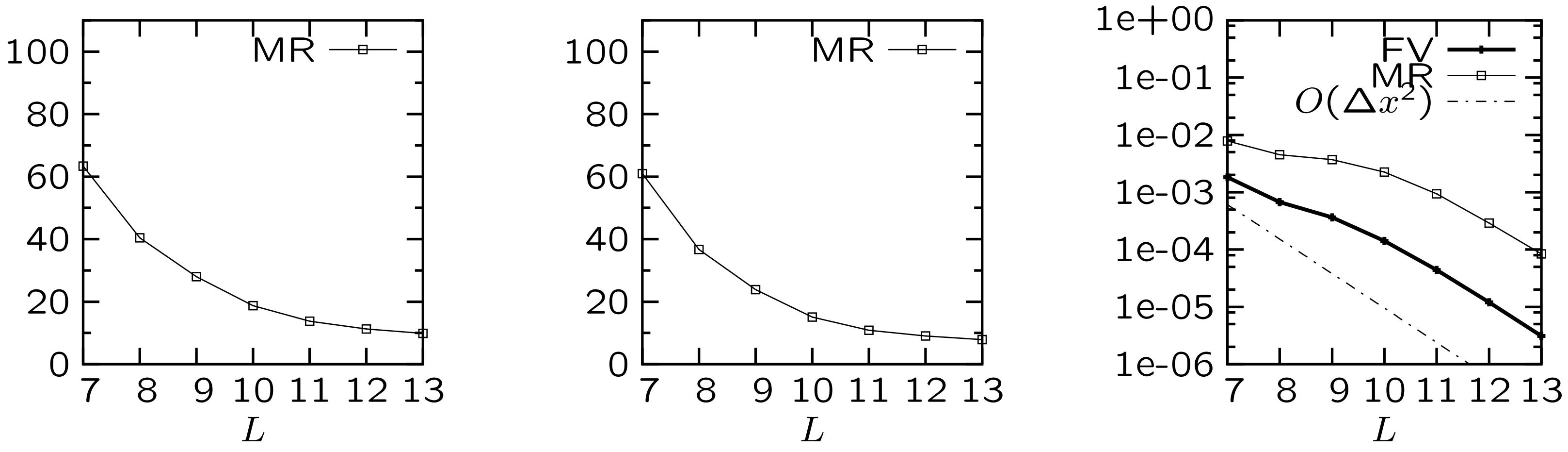


Convection-diffusion: $Pe = 10000$, $t = 0.2$, $C = 5.10^8$

Numerical validation

Viscous Burgers equation: $\partial_t u + \partial_x \left(\frac{u^2}{2}\right) = \frac{1}{Re}\partial_{xx}^2 u$
Analogously, we set

$$\epsilon = C \frac{2^{-(\alpha+1)L}}{Re + 2^{L+2}} \ , \ C > 0 \tag{10}$$



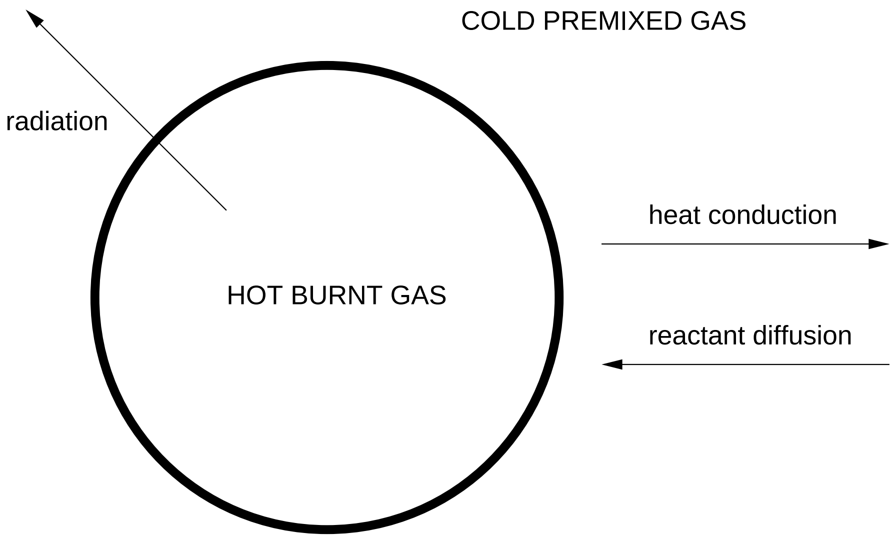
% CPU time compression **% Memory compression** **$\mathcal{L}^1$-error**

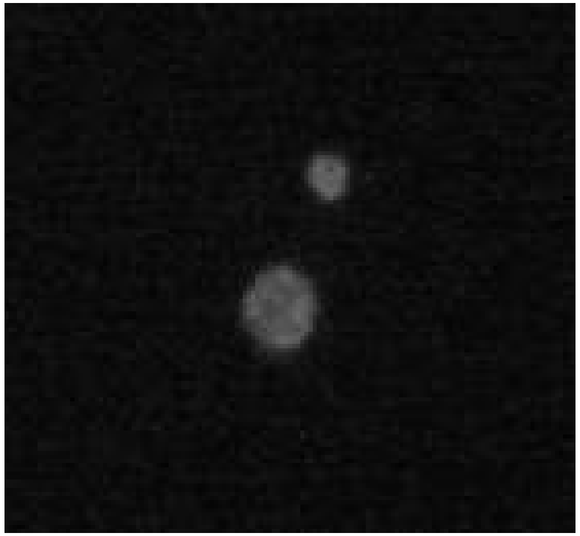
$Re = 1000$, $t = 0.2$, $C = 5.10^8$

Application to TD flames

The flame ball configuration

- Simplest experiment to study the interaction of chemistry and transport of gases (experimental: Ronney 1984, theory: Buckmaster-Joulin-Ronney 1990-91)
- Enables to study the flammability limit of lean gaseous mixtures





- Problem: the combustion chamber is finite ⇒ **Interaction with wall**

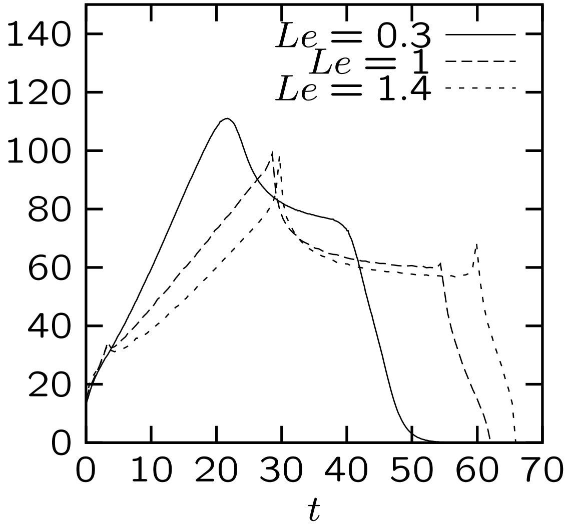
Application to TD flames

Interaction flame ball-adiabatic wall

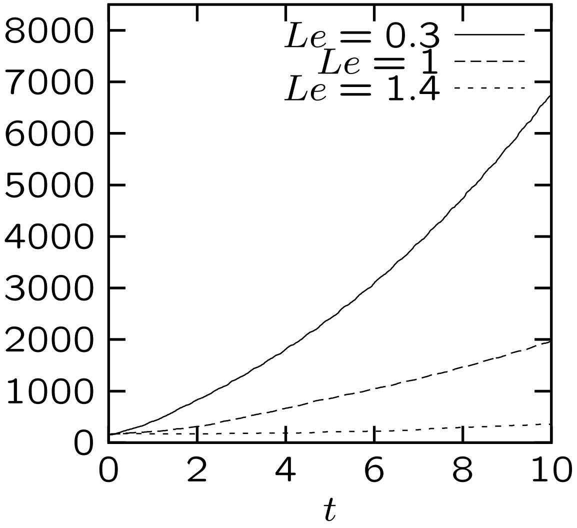
- Radiation neglected, $Ze = 10$, $\alpha = 0.64$, $\Omega = [-50, 50]^d$
- Adiabatic walls $\Rightarrow$ Neuman boundary conditions
- At $t = 0$, the radius of the flame ball is $r_0 = 2$.
- 2D: Evolution of T and mesh for $Le = 0.3$ (animations 1-2)
- 2D: Evolution of T for $Le = 1$ (animation 3)
- 2D: Evolution of T for $Le = 1.4$ (animation 4)
- 3D: Evolution of T and mesh for $Le = 1$ (animations 5-6)
- Analogy with capillarity for a fluid droplet

Application to TD flames

Interaction flame ball-adiabatic wall



$\mathcal{R} = \int \omega \, d\Omega$ in 2D



$\mathcal{R} = \int \omega \, d\Omega$ in 3D

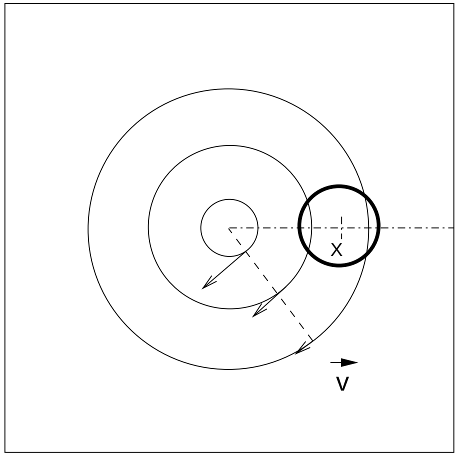
Application to TD flames

Interaction flame ball-adiabatic wall: Performances

d	Le	N_{max}	% CPU	% Mem
2	0.3	256^2	25.50%	14.10%
2	1	256^2	21.50%	11.75%
2	1.4	256^2	21.00%	11.10%
3	1	128^3	12.98%	4.38%

Application to TD flames

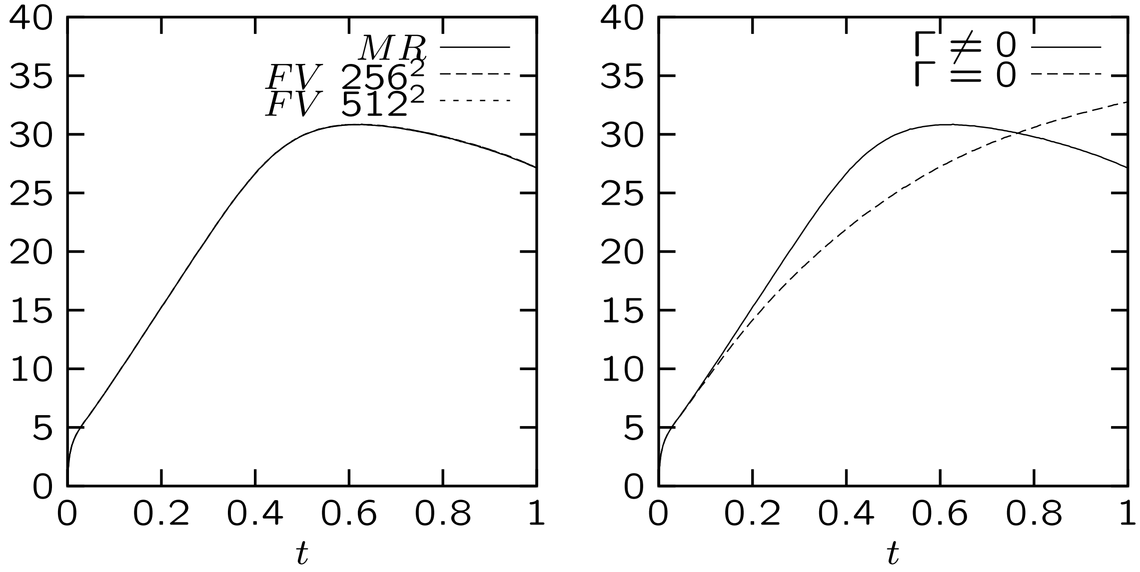
Interaction flame ball-vortex



- Phenomenon which happens e.g. in furnaces
- Thermodiffusive model, $\vec{v}$ analytic solution of Navier-Stokes
- Evolution of T and mesh for $Ze = 10$, $Le = 0.3$, no radiation (animations)

Application to TD flames

Interaction flame ball-vortex



$\mathcal{R} = \int \omega \, d\Omega$: for MR and FV methods with and without vortex

3D flame ball, Le = 1

Temperature

Adaptive grid

Conclusion and perspectives

Summary

- New adaptive multiresolution algorithm for 3D parabolic problems
- Efficiency and accuracy shown on prototype parabolic equations (convection-diffusion, viscous Burgers)
- Application to several thermodiffusive flame instabilities
- *Pulsating planar flames:*
  - For large Ze, numerical results confirm the asymptotic theory
  - For large Le and moderate Ze, stable flames can exist
- *Flame balls:*
  - Interaction with adiabatic walls: analogy with capillarity
  - Interaction with a vortex: perturbation amplified, global reaction rate Reduced

Conclusion and perspectives

Work in progress

- Parallelization for realistic 3D computations: concept of *forest* structure

Perspectives

- Extension to reactive Navier-Stokes to take into account hydrodynamics
- Coherent Vortex Simulation (CVS) of turbulent reactive flows
  (for non-reactive turbulent flows, see Farge-Schneider 2001)
- Complex geometries (penalization, structured or unstructured meshes)
  (for 2D hyperbolic problems, see Angot 1999, Müller 2001, Cohen *et al* 2002)
- Adaptivity in time: time step per scale

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