LES OF PREMIXED COMBUSTION WITH THE THICKENED FLAME MODEL COUPLED TO AMR

C. MEHL[1], S. LIU[2], Y. C. SEE[2], O. COLIN[1]

[1] IFPEN, 1-4 avenue du Bois-Préau, Rueil-Malmaison, 92500, France
[2] Convergent Science, 6400 Enterprise Ln, Madison, WI 53719, USA

INTRODUCTION

- LES is now routinely used in gas turbines combustion
- **Main challenge for industrials:** perform accurate simulations of complex burners at affordable computational costs
- An important factor for computational costs is the number of nodes required in the numerical mesh

INTRODUCTION

- Issues regarding the meshing of industrial gas turbines:
  - Position of the flame is not known *a priori*
  - Flame is non-stationary and thus moves in the domain

- **Common practice in other CFD codes:** large area of refined meshes

- Opportunity to optimize the refined mesh region: **Adaptive Mesh Refinement (AMR)**
  - Use of refined elements only where it is needed
  - No a priori knowledge on the flame position required
  - Temporal adaptation of the mesh to follow flame movements

Questions:

- How to define an adaptive refinement strategy ?
- Do we still need a turbulent combustion model or is stand-alone AMR sufficient ?

ISSUE: How to couple AMR with turbulent combustion simulations?

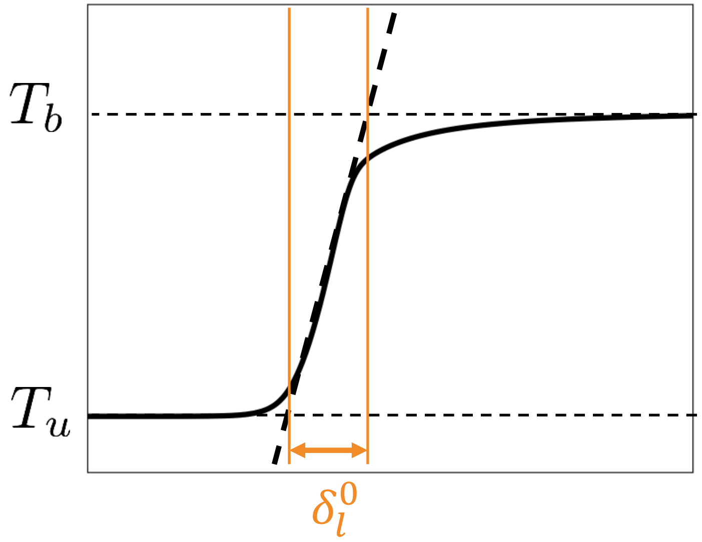
First analysis: Focus on turbulent **premixed** combustion

SUMMARY OF THE PRESENTATION

I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

- **Premixed combustion:** a laminar flame thickness δ_l^0 is defined as

$$\delta_l^0 = \frac{T_b - T_u}{\max(|\nabla T|)}$$



I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

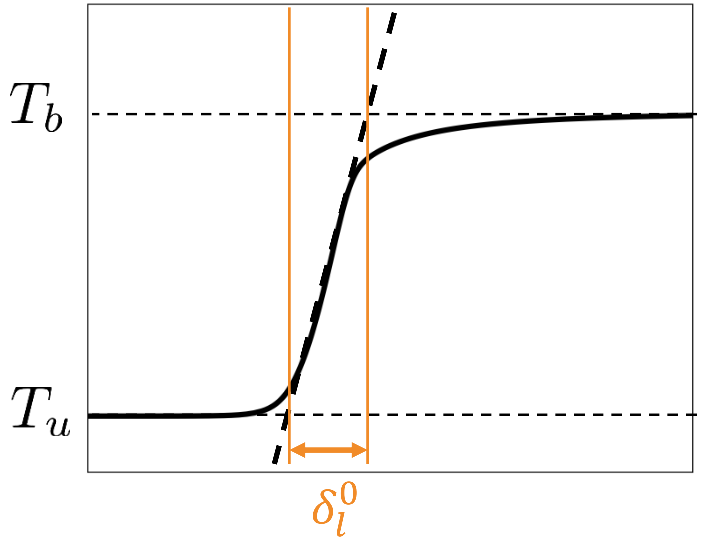
- **Premixed combustion:** a laminar flame thickness δ_l^0 is defined as

$$\delta_l^0 = \frac{T_b - T_u}{\max(|\nabla T|)}$$

- **Typical values of flame thickness:** $\approx 0.5\ mm$ for ambiant CH_4/air flames at $\phi = 0.75$

=> Smaller than typical LES mesh size !

Question: How many points are required in the flame front for an accurate simulation ?



I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

- **Evaluation of resolution:** often done by considering the flame consumption speed (in m/s),

$$S_c(t) = \frac{1}{\rho_u\left(Y^u_{fuel} - Y^b_{fuel}\right)} \int_{x=-\infty}^{+\infty} \rho\dot{\omega}_{fuel}(x,t)dx$$

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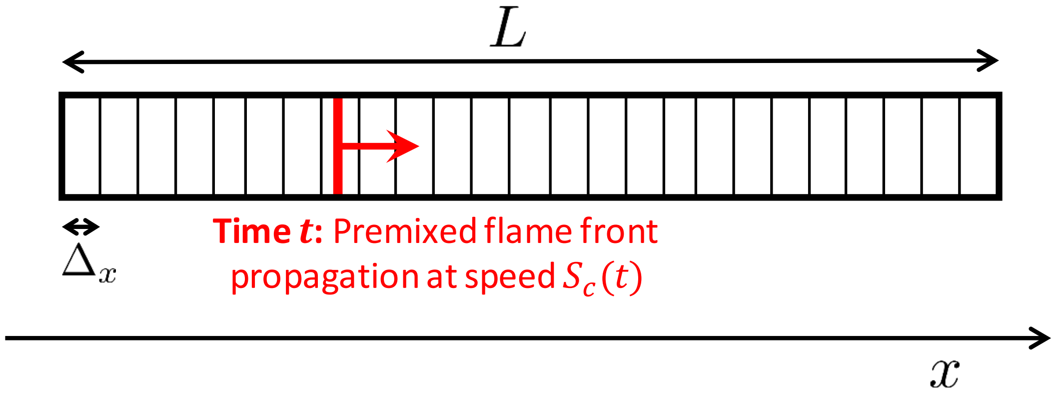
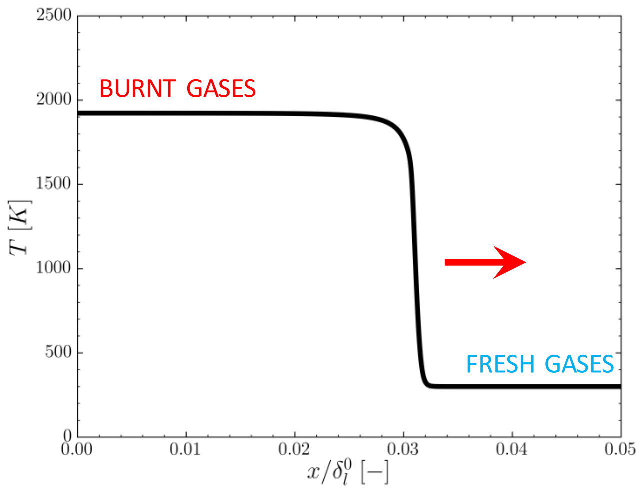
- **Canonical set-up:** laminar premixed flame propagating in a 3-D box

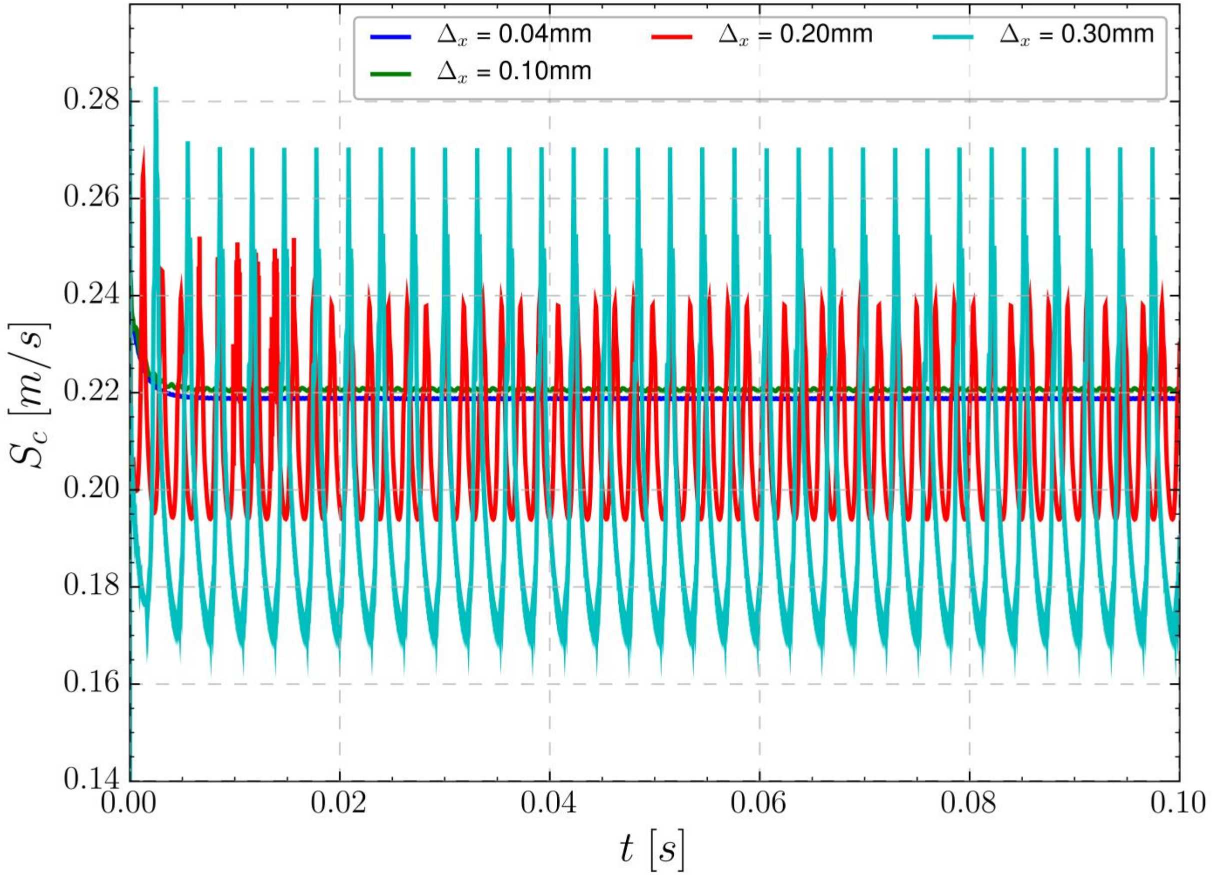




Numerical set-up:
- Solver: CONVERGE
- 2-step global mechanism
- Equivalence ratio: $\phi = 0.75$
- Varying grid resolution Δ_x

I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

Flame propagation evolution in time for different grid sizes



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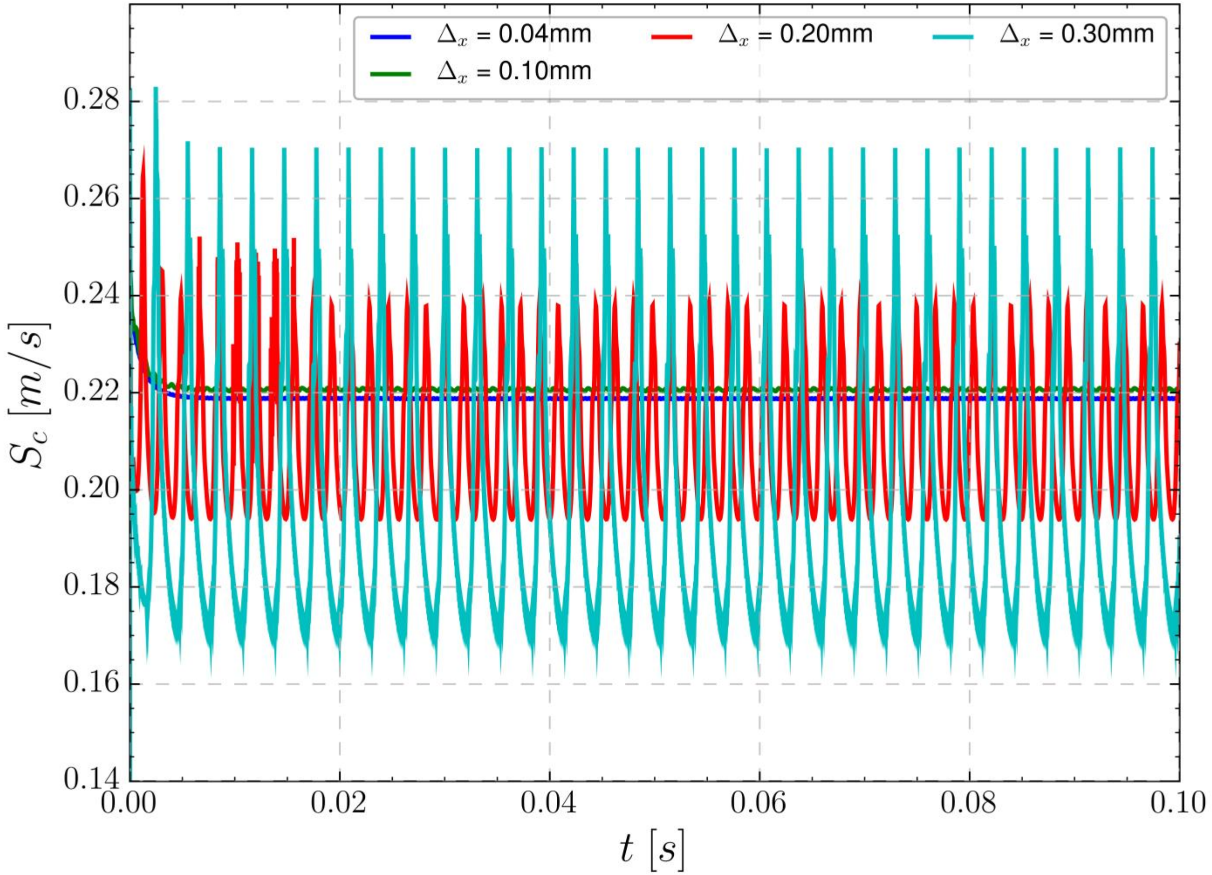
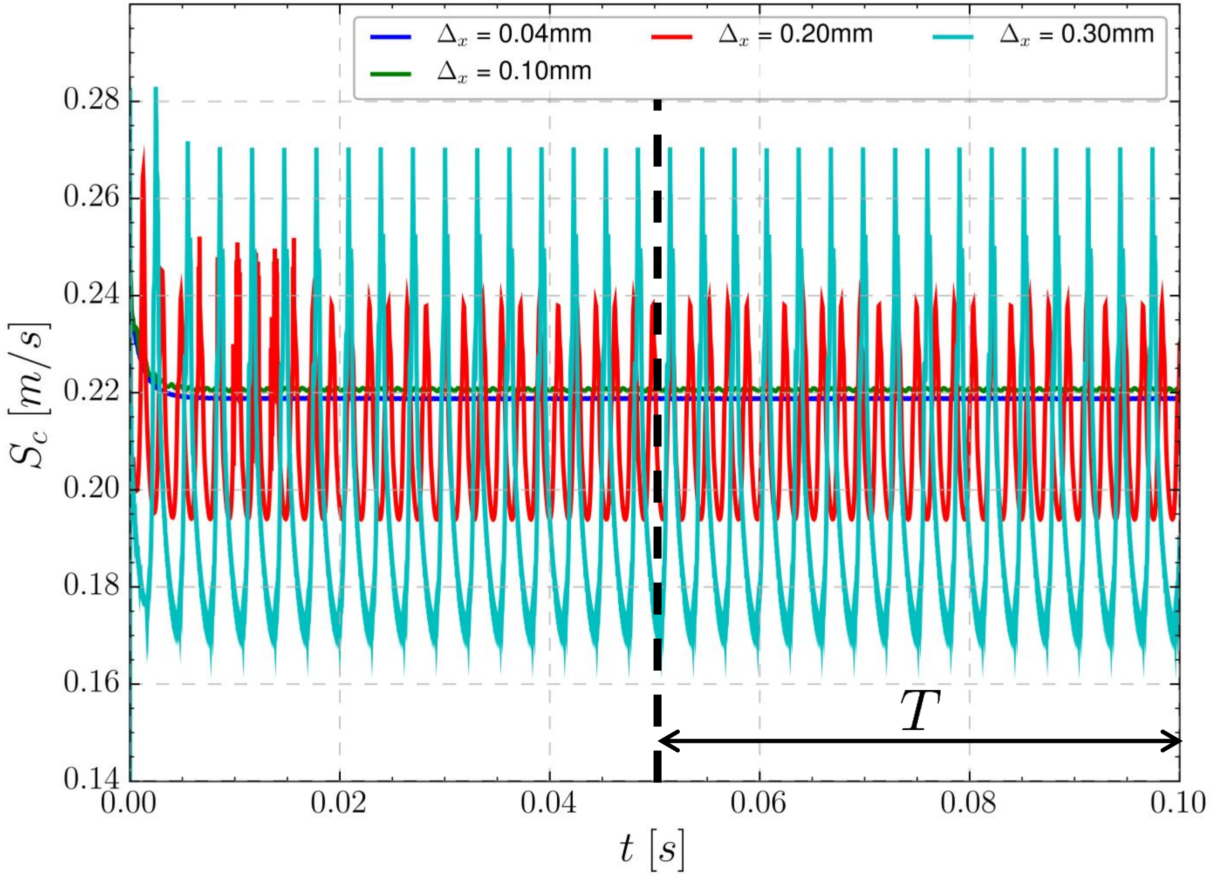


=> Large mesh size involves strong non-physical oscillations of the flame propagation speed

Flame propagation evolution in time for different grid sizes



ADDITIONAL POST-PROCESSING

Error on mean flame propagation speed:

$$\hat{S} = \frac{1}{T}\int_0^T S_c(t)dt$$

$$\varepsilon = 100 \times \frac{\hat{S} - S_c^{ref}}{S_c^{ref}} \text{ (in \%)}$$

Oscillations amplitude:

$$\delta S_c = 100 \times \frac{\max_{t \geq T}[S_c(t)] - \min_{t \geq T}[S_c(t)]}{\hat{S}} \text{ (in \%)}$$

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I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

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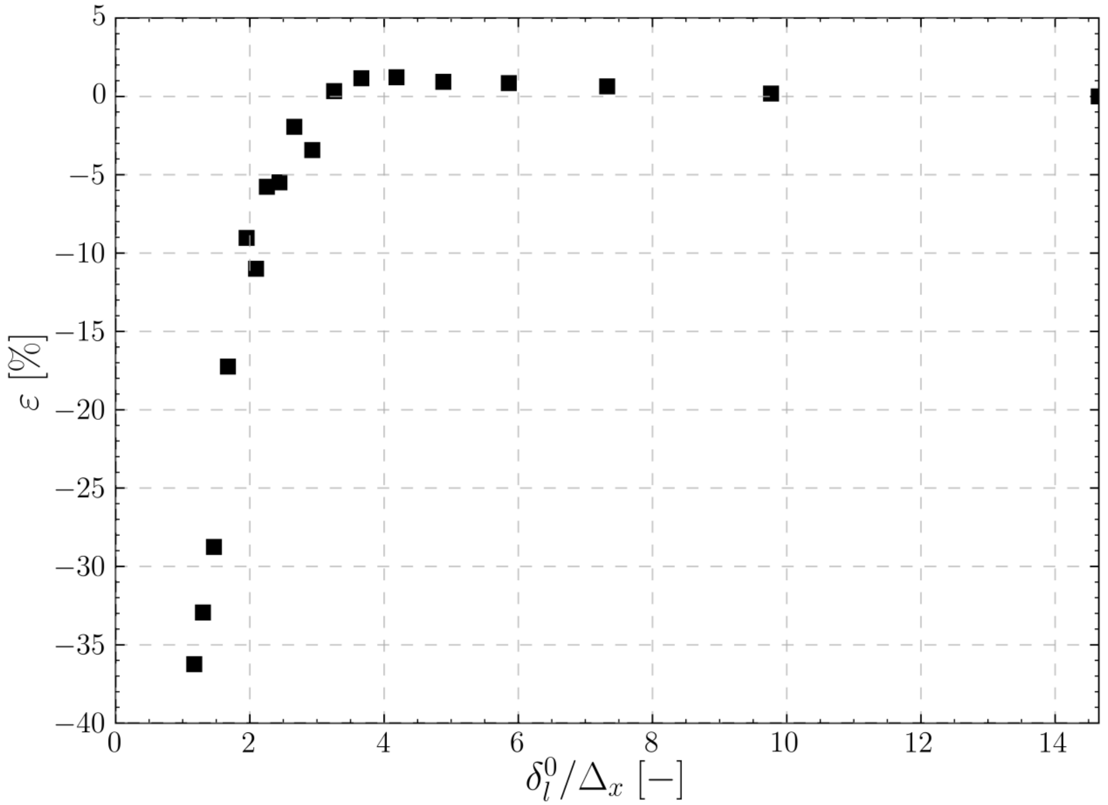
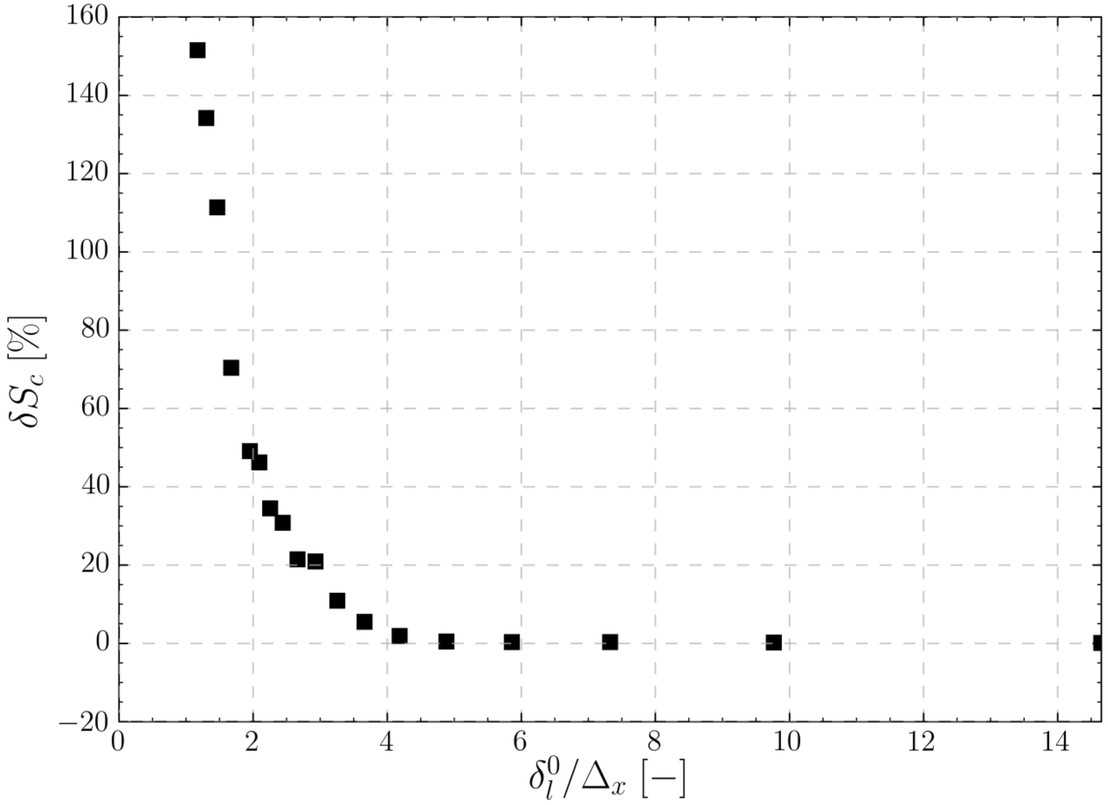


Oscillations amplitude



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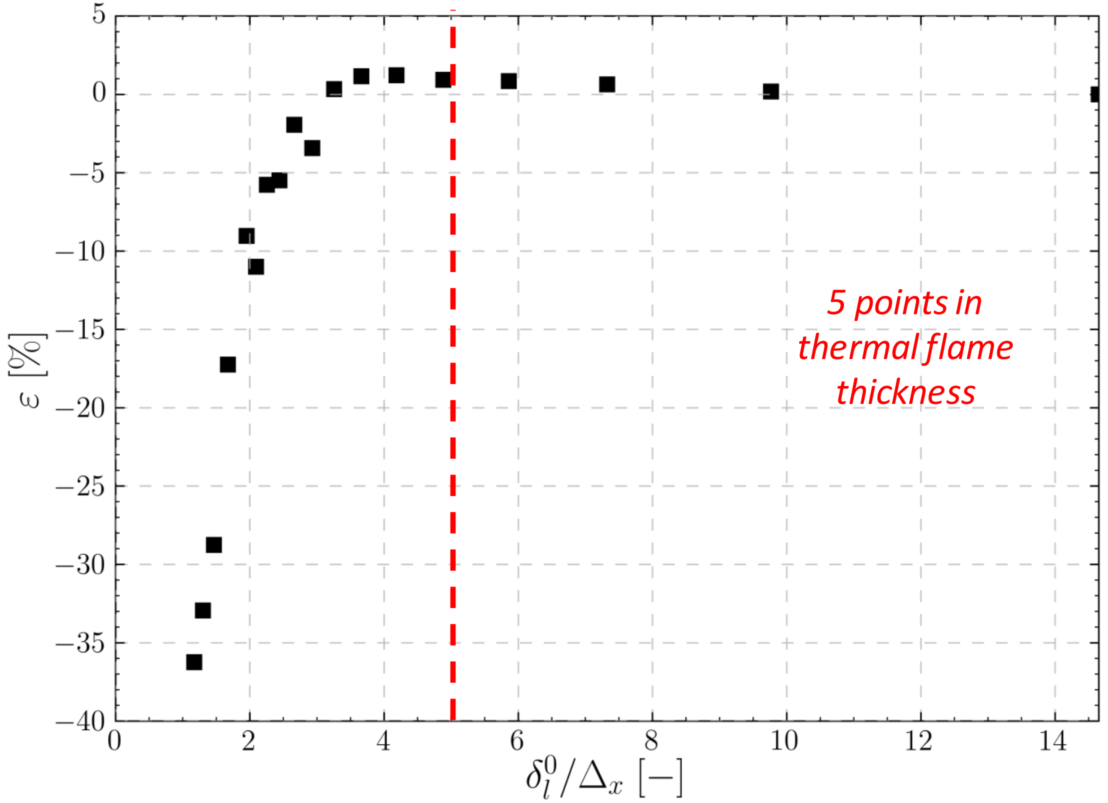
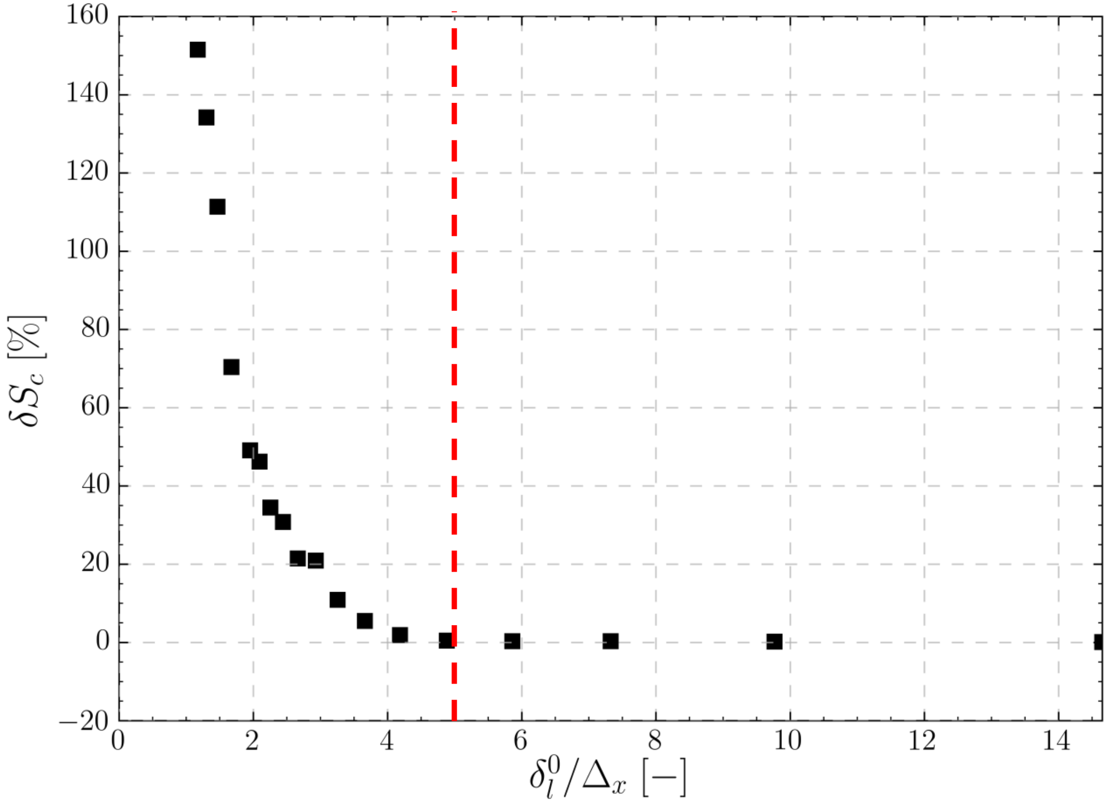


Oscillations amplitude



i. δ_l^0/Δ_x *represents the number of points in the thermal flame thickness (flame front resolution)*

ii. *Error on flame speed and oscillations amplitude decrease as the flame resolution increases*

iii. *Good resolution choice is around* $\delta_l^0/\Delta_x \approx 5$

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- **Issue:** 5 points in the flame front implies $\Delta_x \approx 0.1mm$ for this case => difficult to reach in realistic LES, **even using AMR !**
  - $\Rightarrow$ **Additional modeling is thus required to predict premixed propagation accurately**

I. MODELING CHALLENGES: FLAME FRONT RESOLUTION

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  - $\Rightarrow$ **Additional modeling is thus required to predict premixed propagation accurately**

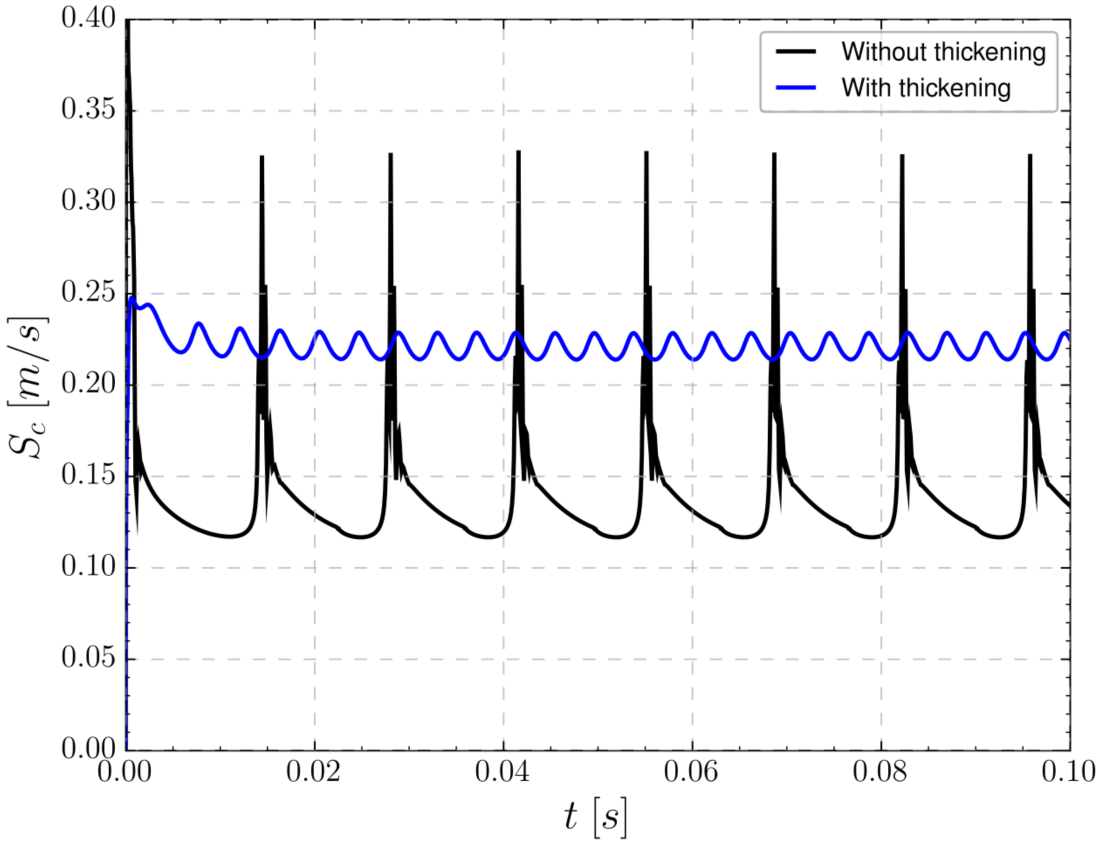
- Methodology to deal with resolution in premixed LES: **flame thickening** (Colin et al., 2000)

- **Principle:** artificially broaden the flame front by a factor $\mathcal{F} = \max\left(\frac{n_{res}\Delta_x}{\delta_l^0(\phi)}, 1\right)$

Where n_{res} is the number of grid points in the flame thickness.

I. MODELING CHALLENGES: FLAME THICKENING

Illustration of the impact of thickening:

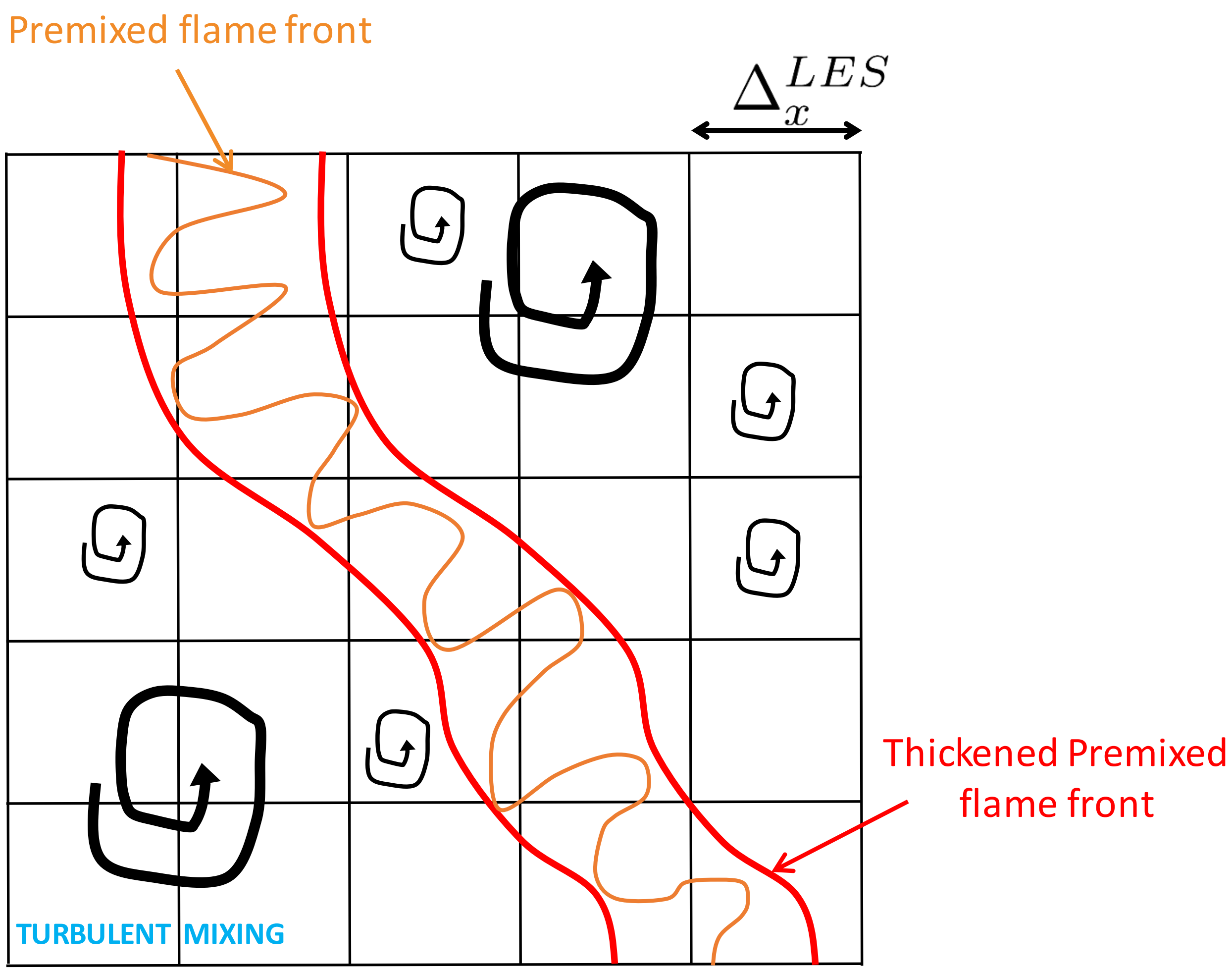


$$\Delta_x = 0.5mm \approx \delta_l^0$$

$$n_{res} = 5$$

=> Significant decrase of flame speed oscillations when thickening the flame front

I. MODELING CHALLENGES: FLAME / TURBULENCE INTERACTIONS



Issues:

1) Thickening affects turbulent mixing outside the flame region

2) Thickened flame front is not wrinkled by (unresolved) small eddies and flame surface is reduced

=> Flame dynamics not reproduced

ISSUE 1) :

- Thickening equations outside the flame region artificially increases turbulent mixing !

- Problem tackled by introducing a flame sensor $\hat{S}$ with the following properties: $\boldsymbol{\hat{S} = 0}$ **outside the flame region and** $\boldsymbol{\hat{S} = 1}$ **in the flame front**

- Thickening computed as:

$$\mathcal{F} = \mathcal{F}_{max} + (\hat{S} - 1)\mathcal{F}_{max}$$

where,

$$\mathcal{F}_{max} = \max\left(\frac{n_{res}\Delta_x}{\delta_l^0(\phi)}, 1\right)$$

ISSUE 2) :

- Loss of subgrid flame surface compensated by increasing the flame speed: $S_T = \Xi_\Delta S_l^0$

- Model for the subgrid scale wrinkling (Wang et al., 2011):

$$\Xi_\Delta = \left(1 + \min\left[\frac{\Delta}{\delta_l^0} - 1, \Gamma_\Delta\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{S_l^0}, Re_\Delta\right)\frac{u'_\Delta}{S_l^0}\right]\right)^\beta$$

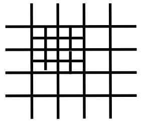
=> Thickened Flame Model (TFM)

II. TFM-AMR MODELING STRATEGY: PRINCIPLE

AMR inputs

- AMR sensor
- AMR level

Updated refined mesh



AMR algorithm

Generation of new grid using user-defined criterion

LES SOLVER

- Equations solved on current AMR mesh
- Solving TFM model equations:

$$\frac{\partial \bar{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u}\widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x}\left(\mathcal{F}\Xi_\Delta \frac{\mu}{Sc} + (1-\hat{S})\frac{\mu_t}{Sc_t}\frac{\partial \widetilde{Y}_k}{\partial x}\right) + \frac{\Xi_\Delta}{\mathcal{F}}\bar{\rho}\widetilde{\dot{\omega}}_k$$

Resolved fields and modeling variables

$$\widetilde{Y}_k,\ \widetilde{T},\ \widetilde{u},\ \mathcal{F},\ldots$$

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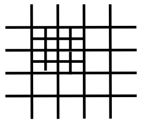

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Resolved fields and modeling variables

$$\widetilde{Y}_k, \ \widetilde{T}, \ \widetilde{u}, \ \mathcal{F}, \ldots$$

QUESTION: How to choose the AMR sensor and the AMR level ?

II. TFM-AMR MODELING STRATEGY: AMR SENSOR

- **Objective:** activate the AMR in the flame front, where high resolution is required.
- In TFM model: flame reactive zone localized by the flame sensor $\widehat{\mathcal{S}}$.
- Hence the following AMR sensor:

AMR is activated when $\widehat{S} > 0$ (equivalently: $\mathcal{F} > 1$)

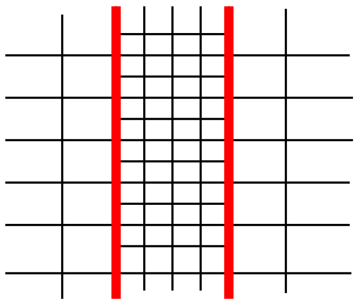
II. TFM-AMR MODELING STRATEGY: AMR LEVEL

- AMR mesh size in CONVERGE: $\Delta_x = \Delta_x^{Base} / 2^{n_{AMR}}$

  => Thickening factor in flame region: $\mathcal{F}_{max} = \max\left(\frac{n_{res}\Delta_x^{Base}}{2^{n_{AMR}}\delta_l^0(\phi)}, 1\right)$

- **Default strategy:** set a constant AMR refinement level when the AMR sensor is active

$\phi = 0.75$



Flame front

$\delta_l^0 \approx 0.5mm$
$\Delta_x = 0.5mm$
$\mathcal{F} = 5$

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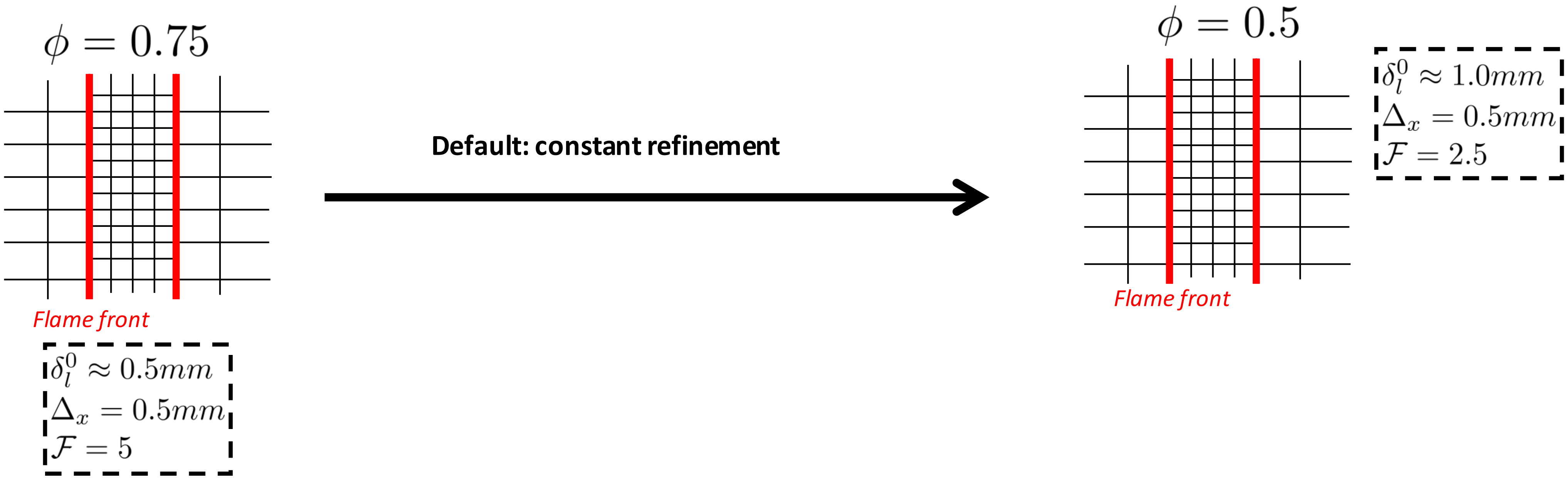

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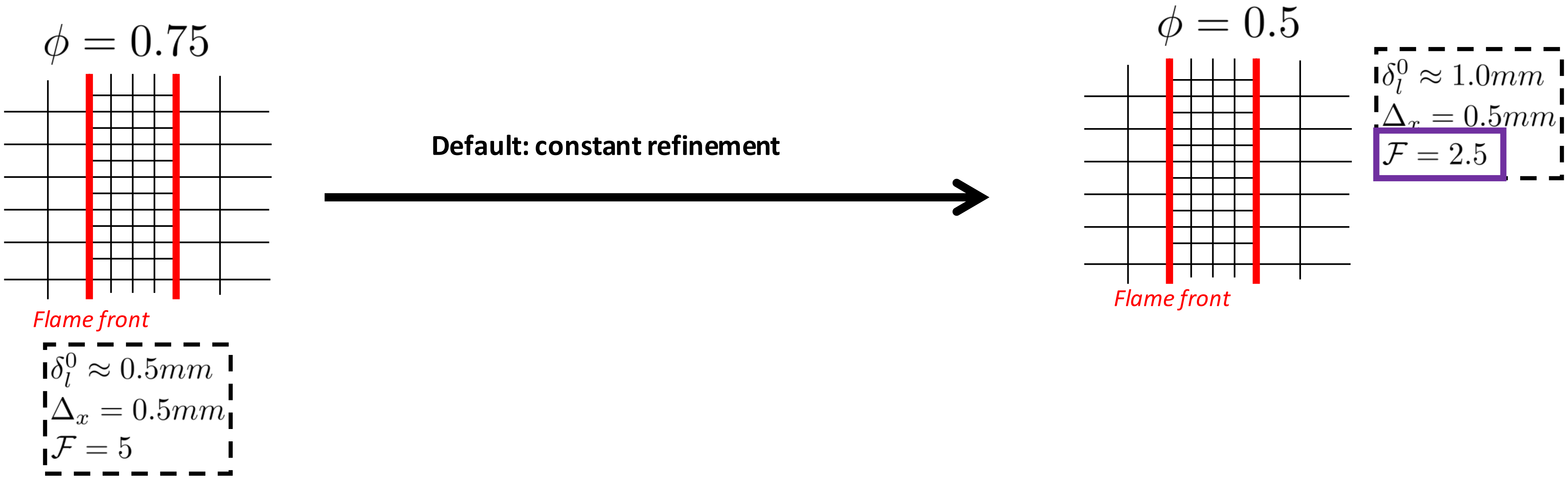

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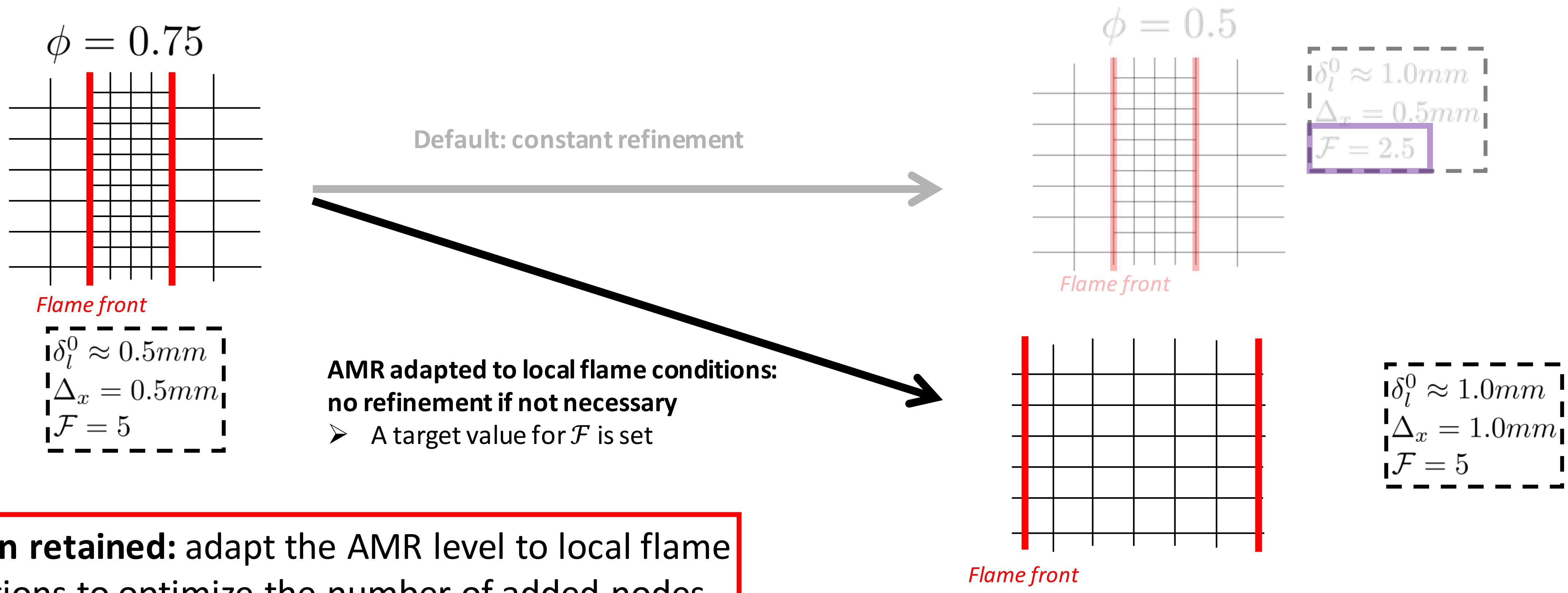


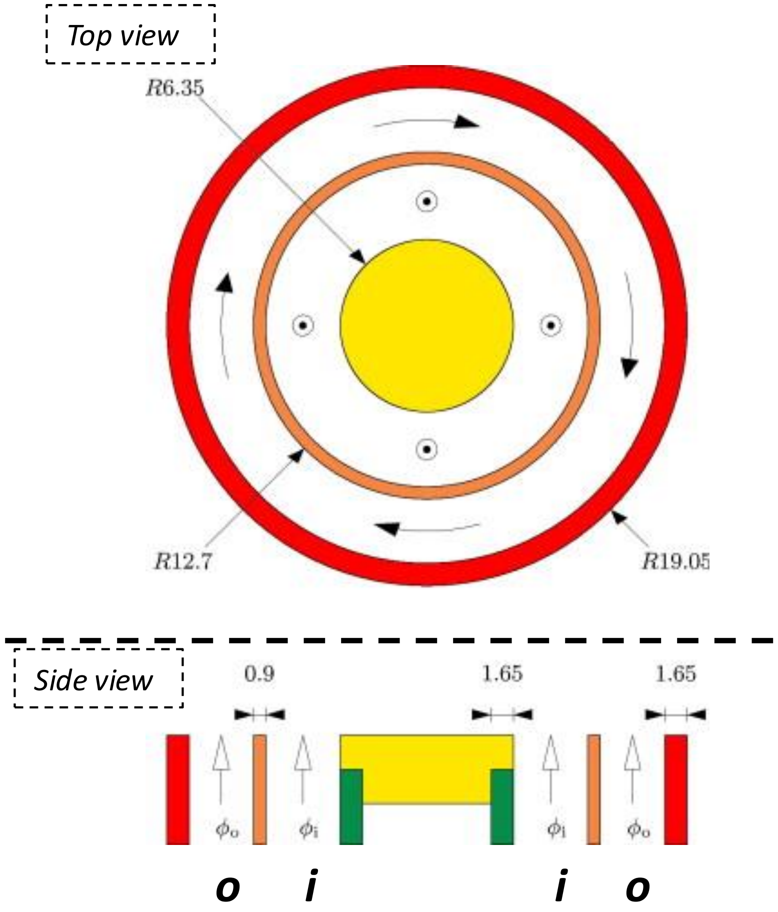
AMR adapted to local flame conditions: no refinement if not necessary

- ➢ A target value for $\mathcal{F}$ is set

Solution retained: adapt the AMR level to local flame conditions to optimize the number of added nodes.

III. VALIDATION ON A 3-D BURNER: EXPERIMENTAL SET-UP

Cambridge SwB burner (Sweeney et al., 2012):



OPERATING CONDITIONS

Flame:

- Premixed configuration: $\phi_i = \phi_o = 0.75$

Flow:

- No swirl
- Inner/Outer tube speeds: $U_i = 8.31$, $U_o = 18.7$
- Reynolds numbers: $Re_i = 5960$, $Re_o = 11500$

EXPERIMENTAL MEASUREMENTS

- Flow diagnostics: PIV, LDA
- Scalar diagnostics: Rayleigh & Raman scattering, CO-LIF, OH-PLIF

III. CHEMICAL FORMALISM

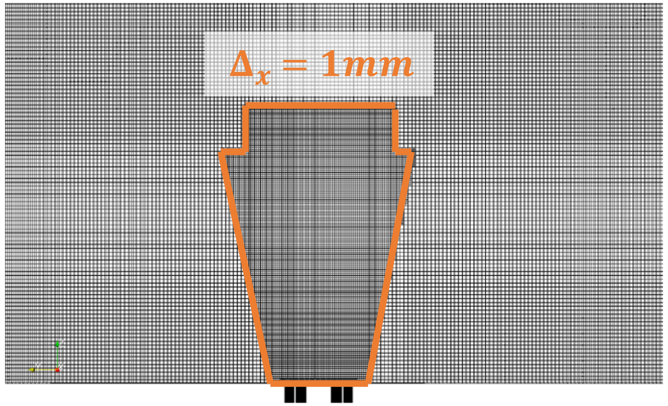
- Global chemical mechanism: 2S-CM2 mechanism (Boudier, 2007)

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$
$$CO + 0.5O_2 \leftrightarrow CO_2$$

- Adaptive zoning to accelerate chemistry calculations

III. VALIDATION STRATEGY

Non-reacting flow simulation on coarse LES grid



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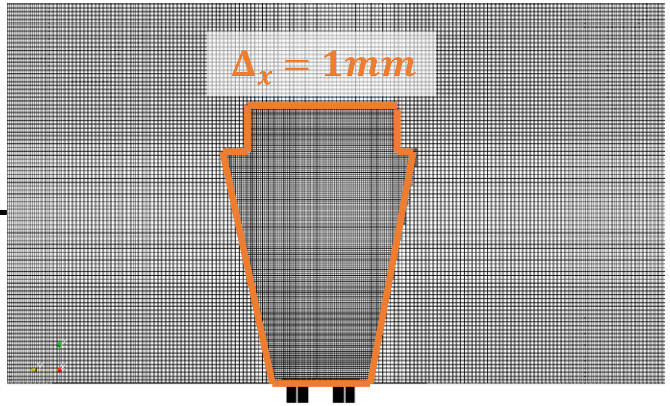
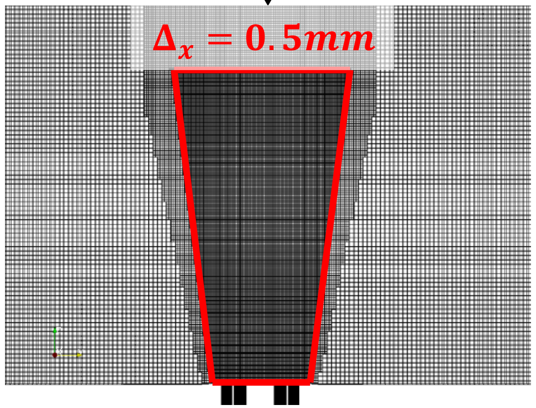


Default option (used in other CFD codes): *embedding in a large area*



Flame simulation with TFM and embedded refined grid

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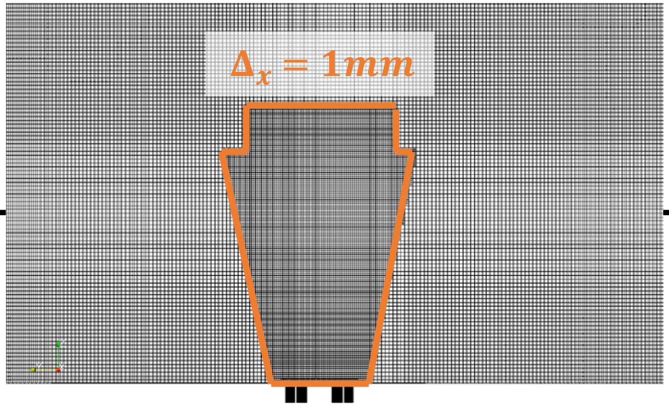

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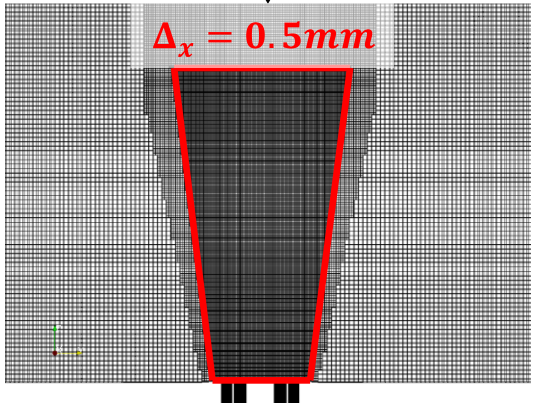
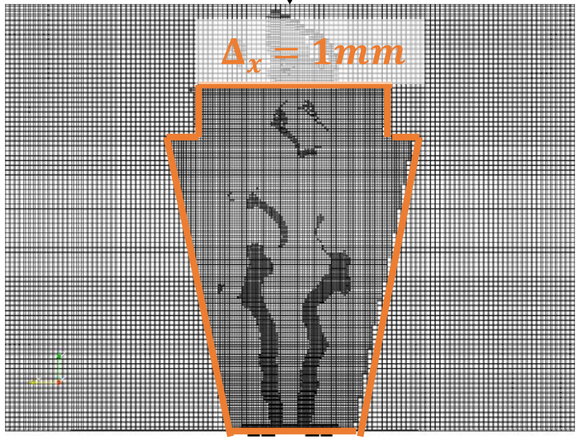
New methodology: *AMR on coarse LES grid*



Flame simulation with TFM and embedded refined grid



Flame simulation with TFM and AMR

$\mathcal{F}_{target} = \mathbf{5} \Rightarrow \Delta_x = 0.5mm$ for $\phi = 0.75$

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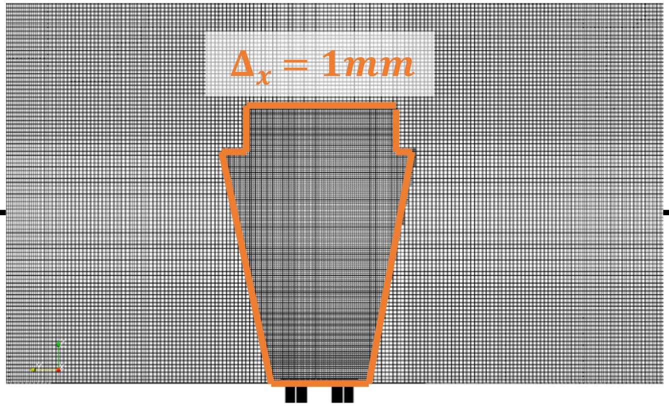

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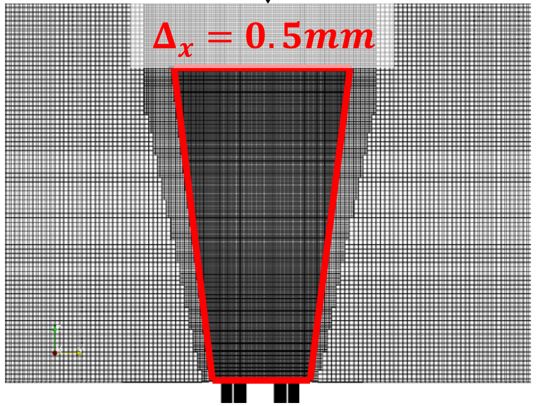
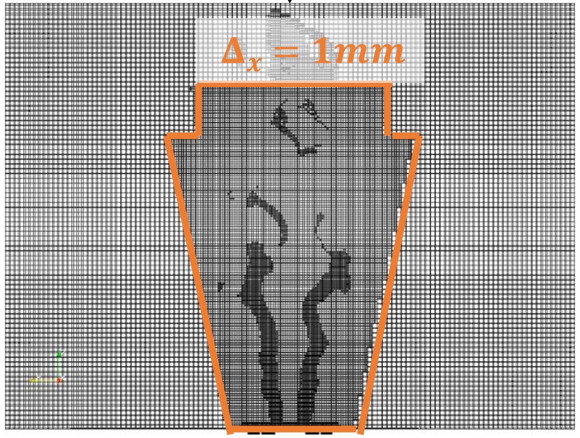


Flame simulation with TFM and embedded refined grid

Comparison to validate the TFM-AMR strategy



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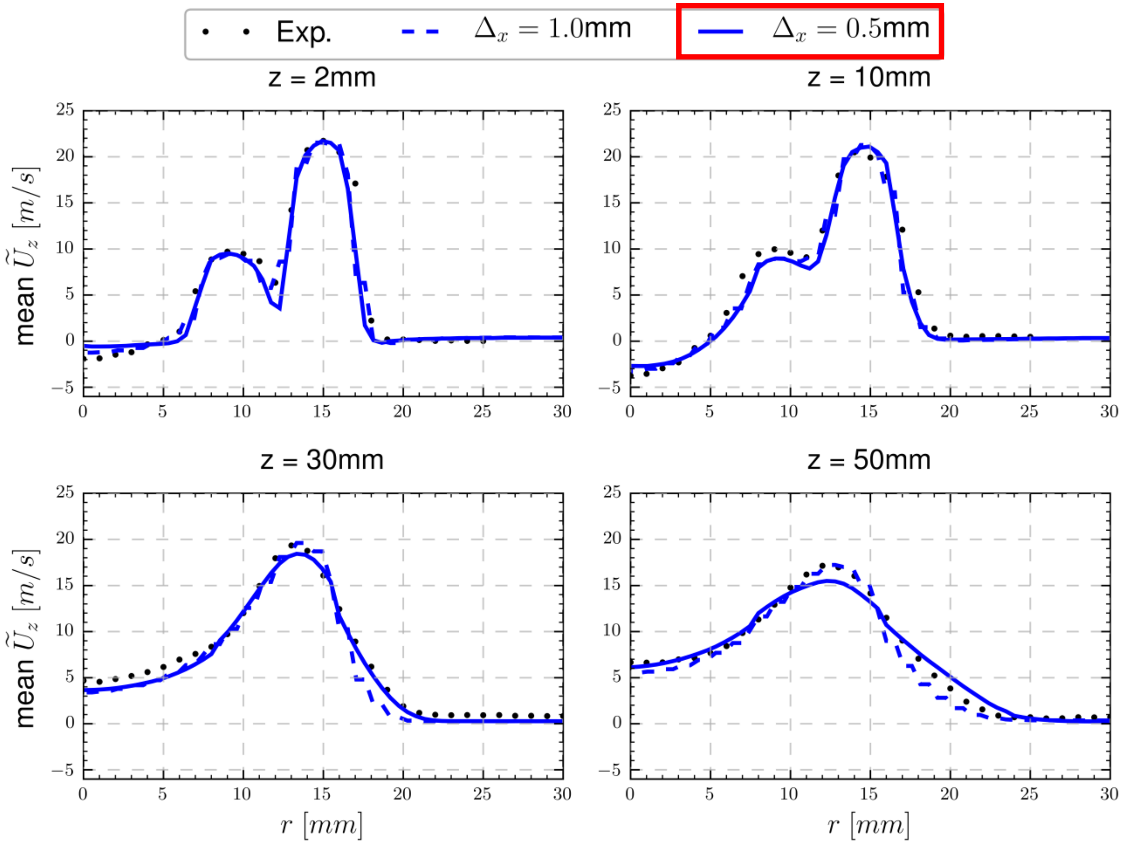
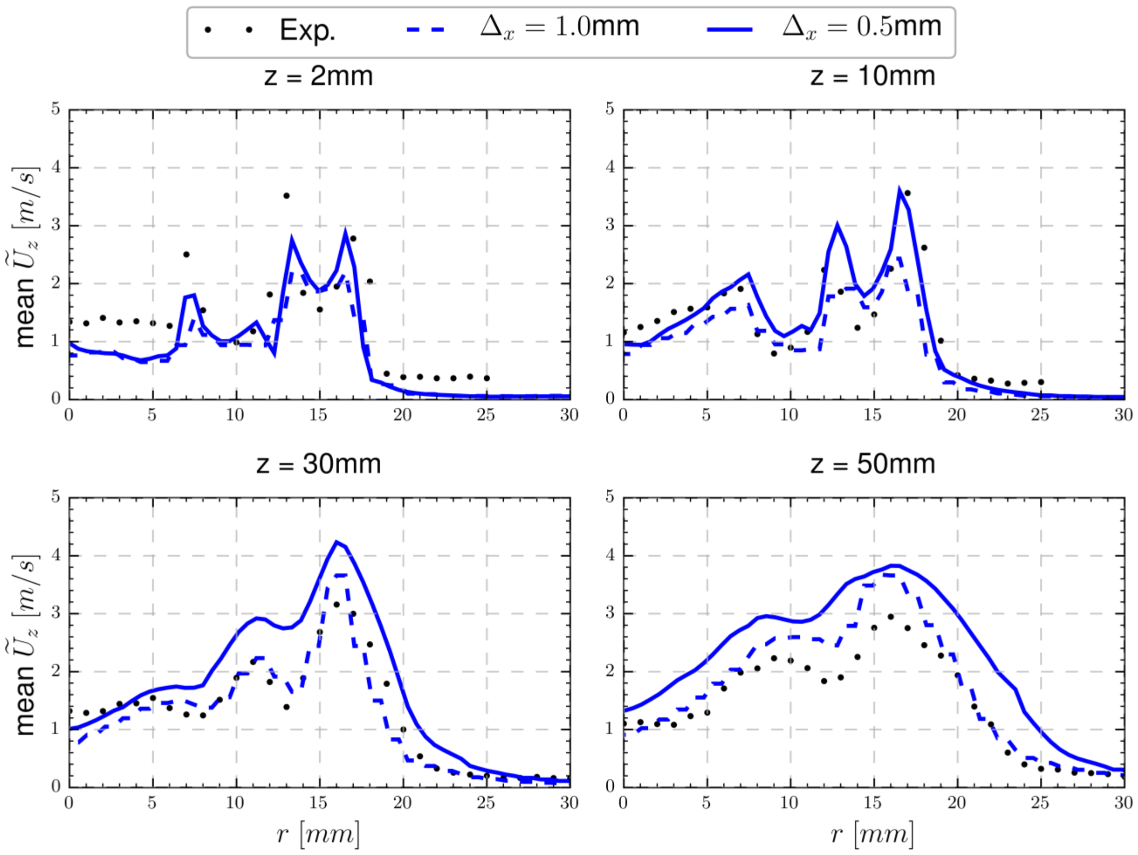
III. RESULTS: NON-REACTING FLOW

High resolution added to show grid-convergence



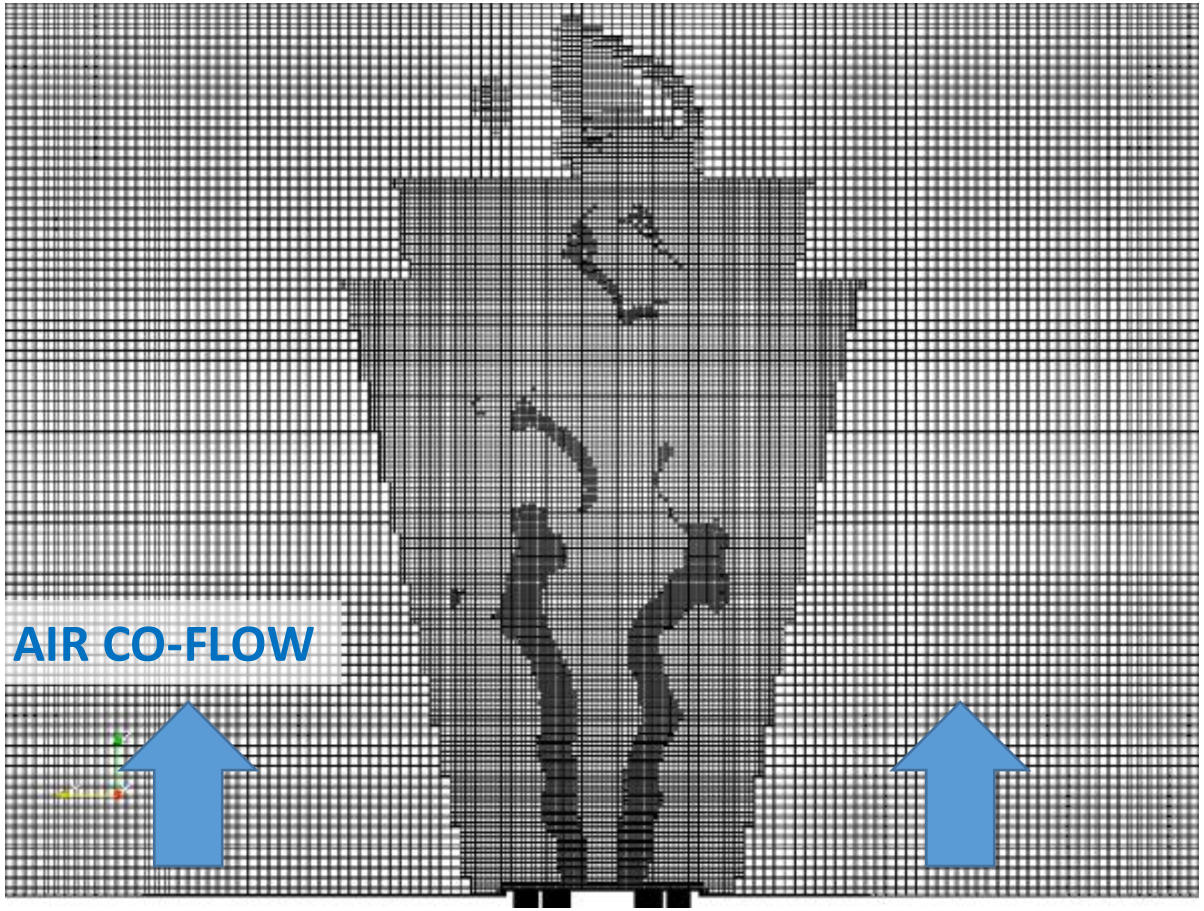


i. *Mean non-reacting speeds are well predicted*

ii. *Axial velocity RMS are lower for the coarse grid; but agreement is satisfying for both resolutions*

III. RESULTS ON REACTING FLOW: AMR BEHAVIOR

Analyzing the behavior of AMR:



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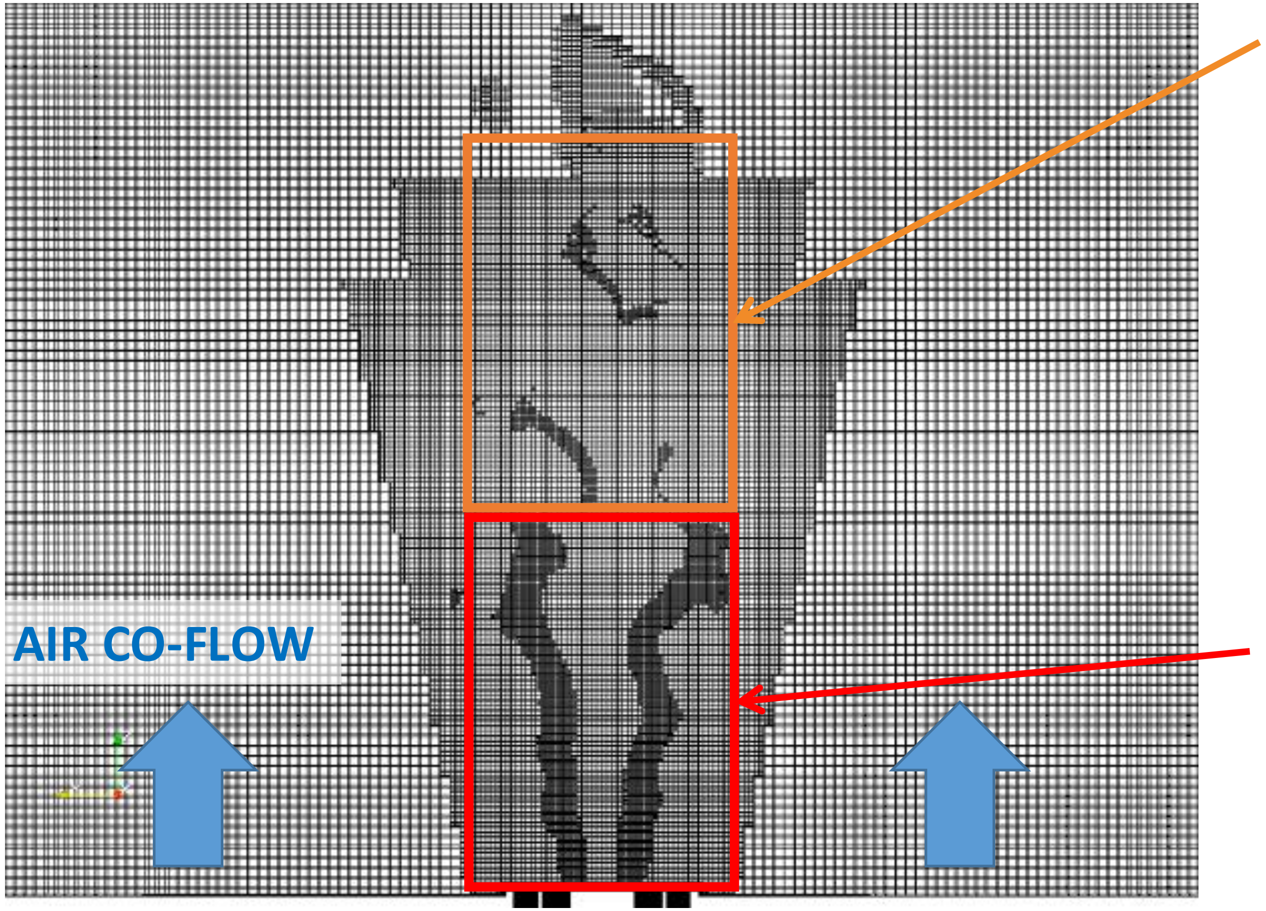
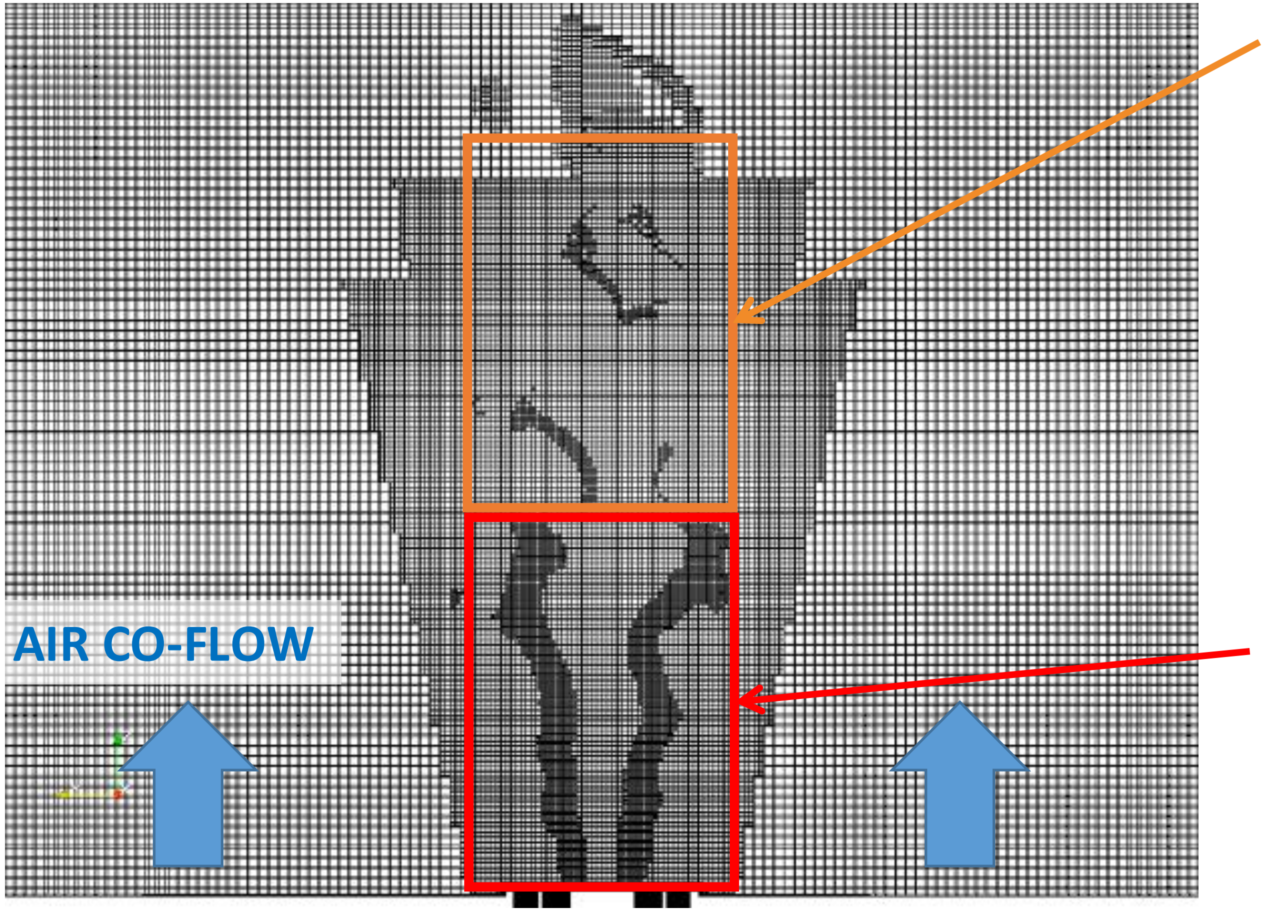


Dilution by air co-flow
=> ϕ is decreased
=> $n^*_{AMR} \approx 1$

Region of premixed burning
($\phi = 0.75$)
=> $n^*_{AMR} = 2$

Analyzing the behavior of AMR:



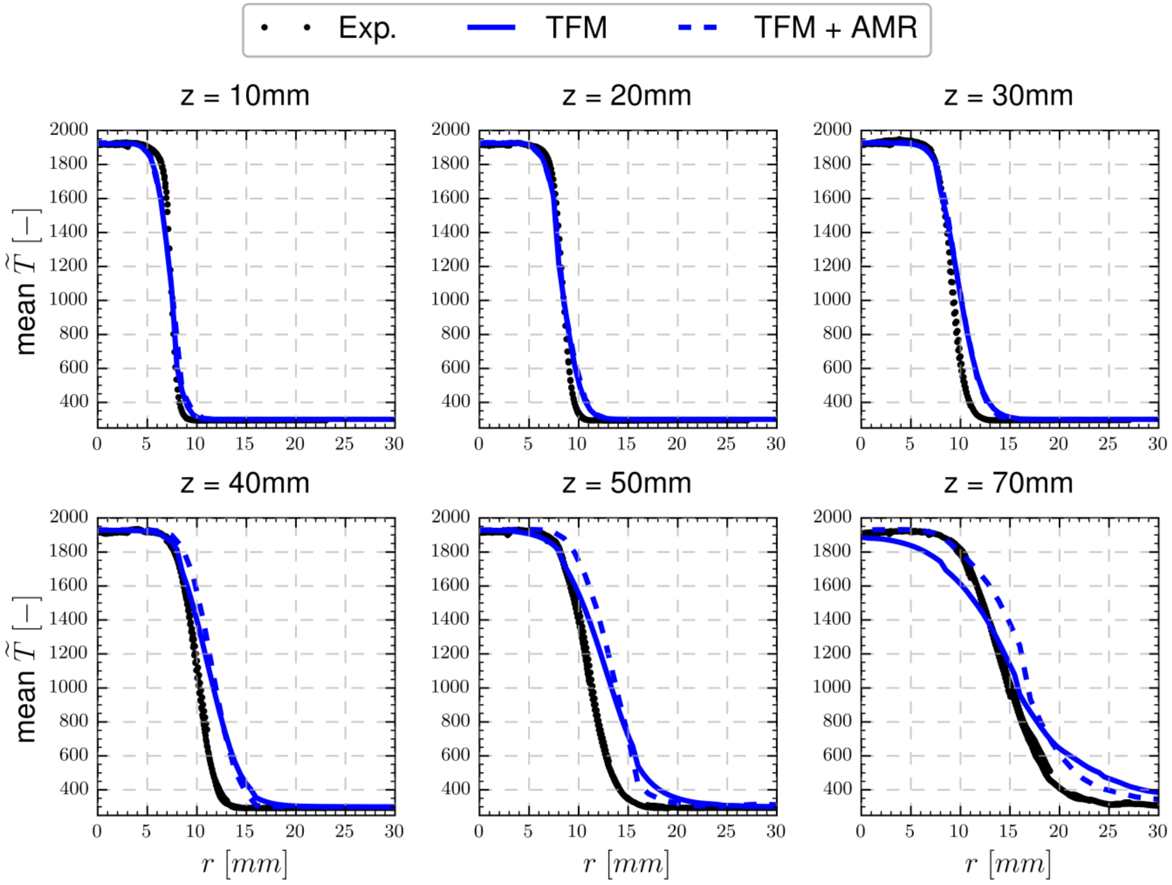
Dilution by air co-flow
=> ϕ is decreased
=> $n^*_{AMR} \approx 1$

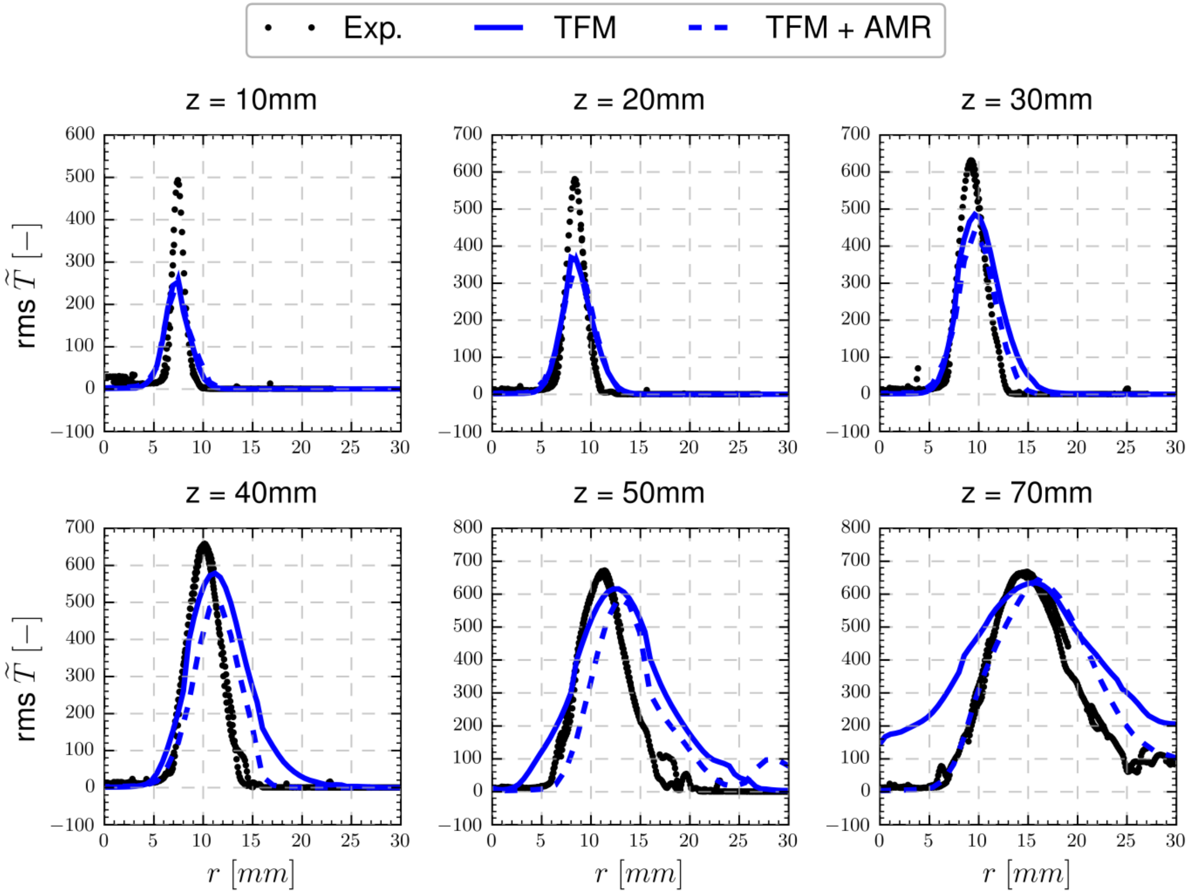
Simulation	Number of nodes
Non-reacting	6 760 008
TFM with embedding	+ 3 695 236
TFM with AMR	+ 373 942

=> Decrease by a factor ≈ 10 !

Region of premixed burning
$(\phi = 0.75)$
=> $n^*_{AMR} = 2$

III. RESULTS ON REACTING FLOW: STATISTICS





i. *Overall good agreement between experimental and numerical results for both TFM and TFM-AMR models*

ii. *TFM and TFM-AMR in good agreement*

IV. SUMMARY AND PERSPECTIVES

- Adaptive Mesh Refinement (AMR) is selected as a method to simulate turbulent flames without *a priori* knowledge of the flame position; and following its dynamics

- AMR is coupled to a TFM model to provide high accuracy at low computational costs

- A strategy to adapt AMR to the local flame thickness has been developed and successfully validated on a simple 3-D academic burner.
  - In practice: $p \approx 20 - 30\ bar$ => Flames are much thinner and the model will be much more important

- **Benefits for industrial applications:**
  - Be able to perform simulations not possible with classical embedding
  - At iso-computational costs: perform simulation with lower $\mathcal{F}$ (=> more accurate results)

- **Perspectives:** simulation with detailed chemistry to predict pollutants and complex chemistry effects (ignition, LBO,…)

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REFERENCES

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FLAME THICKENING

- **Thickening factor:** the flame is broadened by a factor $\mathcal{F} = \max\left(\frac{n_{res}\Delta_x}{\delta_l^0(\phi)}, 1\right)$

Where n_{res} is the number of grid points in the flame thickness

- **Scaling laws:** $\delta_l^0 \propto \sqrt{\frac{D_{th}}{\dot{\Omega}}}$ **and** $S_l^0 \propto \sqrt{D_{th}\dot{\Omega}}$

D_{th}: Heat diffusivity
$\dot{\Omega}$: Mean reaction rate

- **Modeling requirements:** $\delta_l^0 \rightarrow \mathcal{F}\delta_l^0$ and $S_l^0 \rightarrow S_l^0$
  - **Diffusion multiplied by $\mathcal{F}$ and reaction rates by $1/\mathcal{F}$**

- **Transport equation for species mass fractions:**

$$\frac{\partial \bar{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u}\widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x}\left(\mathcal{F}\frac{\mu}{Sc}\frac{\partial \widetilde{Y}_k}{\partial x}\right) + \frac{1}{\mathcal{F}}\bar{\rho}\widetilde{\dot{\omega}}_k$$

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SPECIES MASS FRACTIONS TRANSPORT EQUATIONS

- Final transport equation for species mass fractions (TFM model):

$$\frac{\partial \overline{\rho} \widetilde{Y}_k}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u} \widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x} \left(\mathcal{F} \Xi_\Delta \frac{\mu}{Sc} + (1 - \hat{S}) \frac{\mu_t}{Sc_t} \frac{\partial \widetilde{Y}_k}{\partial x} \right) + \frac{\Xi_\Delta}{\mathcal{F}} \overline{\rho} \widetilde{\dot{\omega}}_k$$

- ✓ Resolution of the flame front thickness
- ✓ Accurate turbulent propagation speed
- ✓ Only flame front is thickened

TFM-AMR MODELING STRATEGY: AMR LEVEL COMPUTATION

- Principle:
  - Setting a target flame thickening value $\mathcal{F}_{target}$
  - Computing the theoretical AMR level n^*_{AMR} to reach the $\mathcal{F}_{target}$ value

- Relationship between n^*_{AMR} and $\mathcal{F}_{target}$:

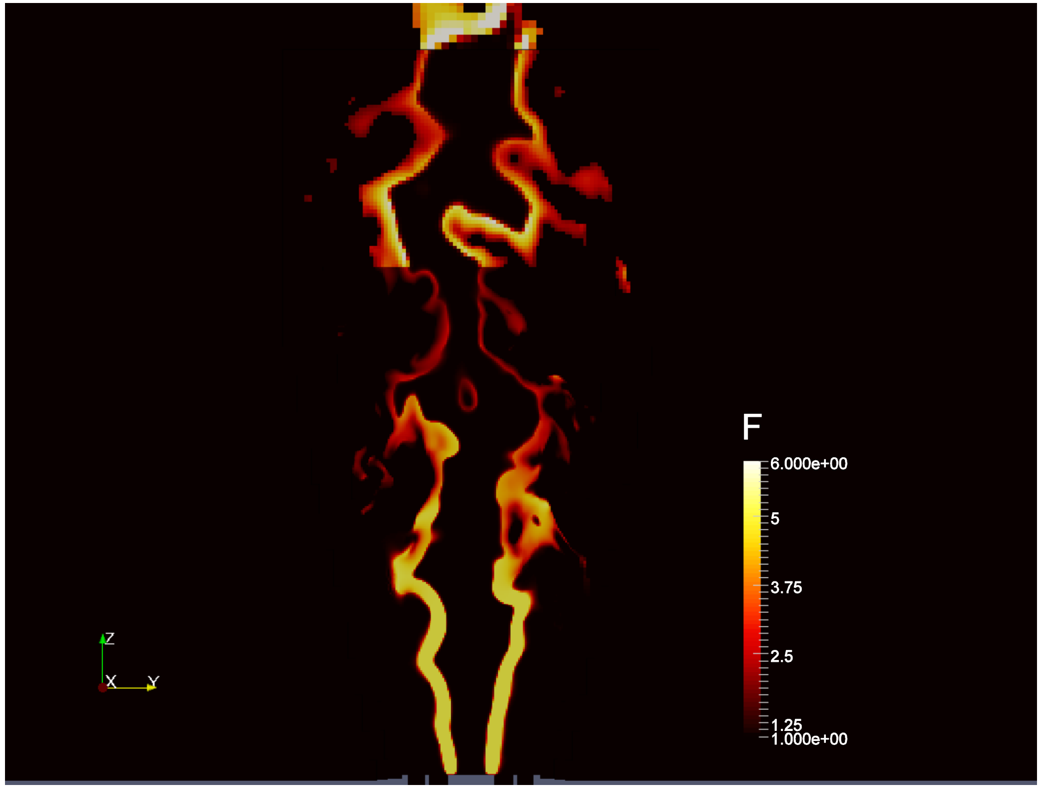
$$\frac{\delta_l^0(\phi)\mathcal{F}_{target}}{n_{res}} = \frac{\Delta_x^{Base}}{2^{n^*_{AMR}}}$$

- Theoretical AMR level:

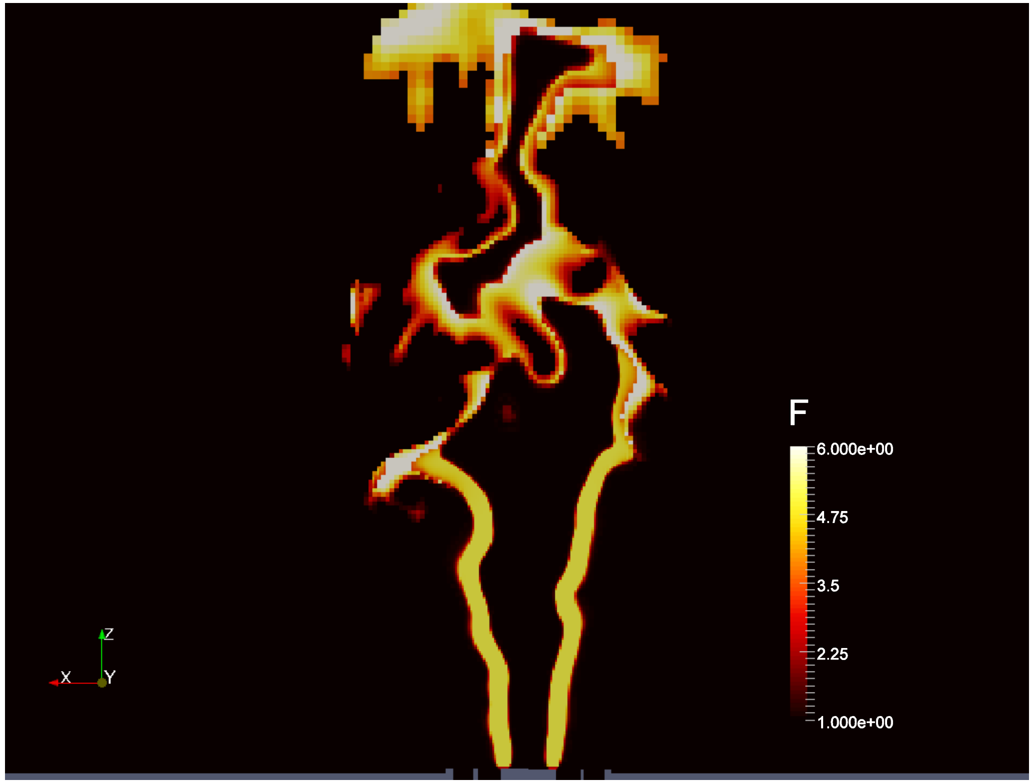
$$n^*_{AMR} = \frac{1}{log(2)} log\left(\frac{n_{res}\Delta_x^{Base}}{\delta_l^0(\phi)\mathcal{F}_{target}}\right)$$

RESULTS ON REACTING FLOW: THICKENING FACTORS

Classic TFM



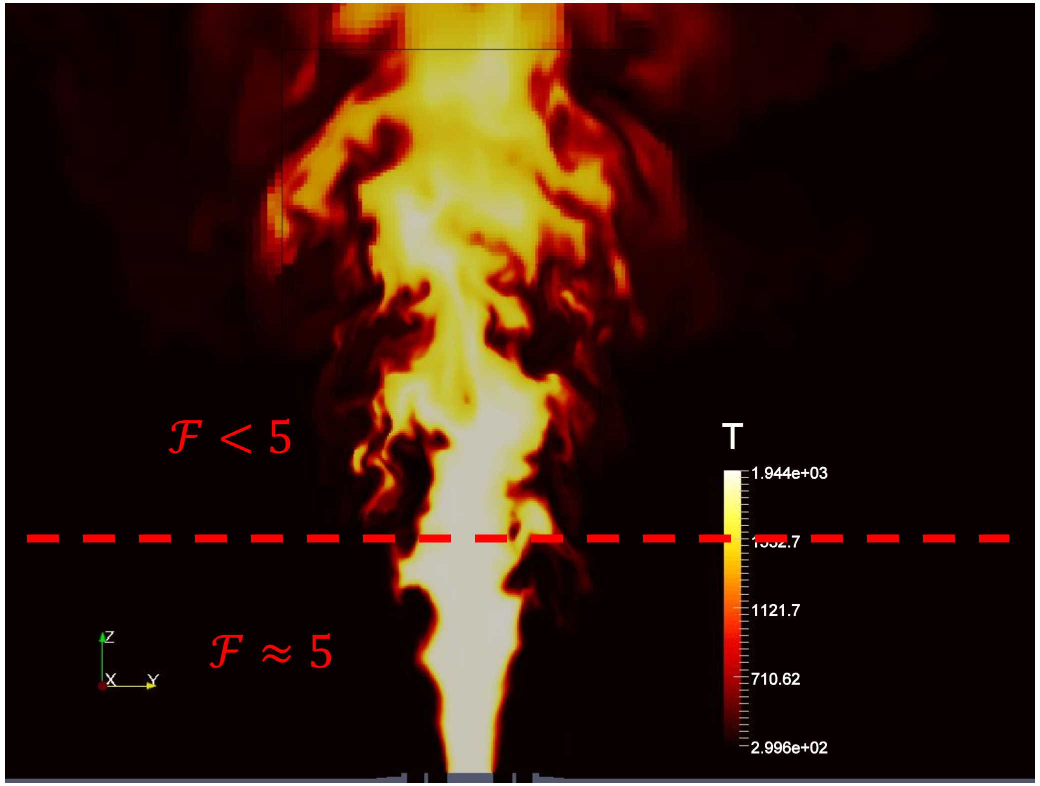
TFM + AMR



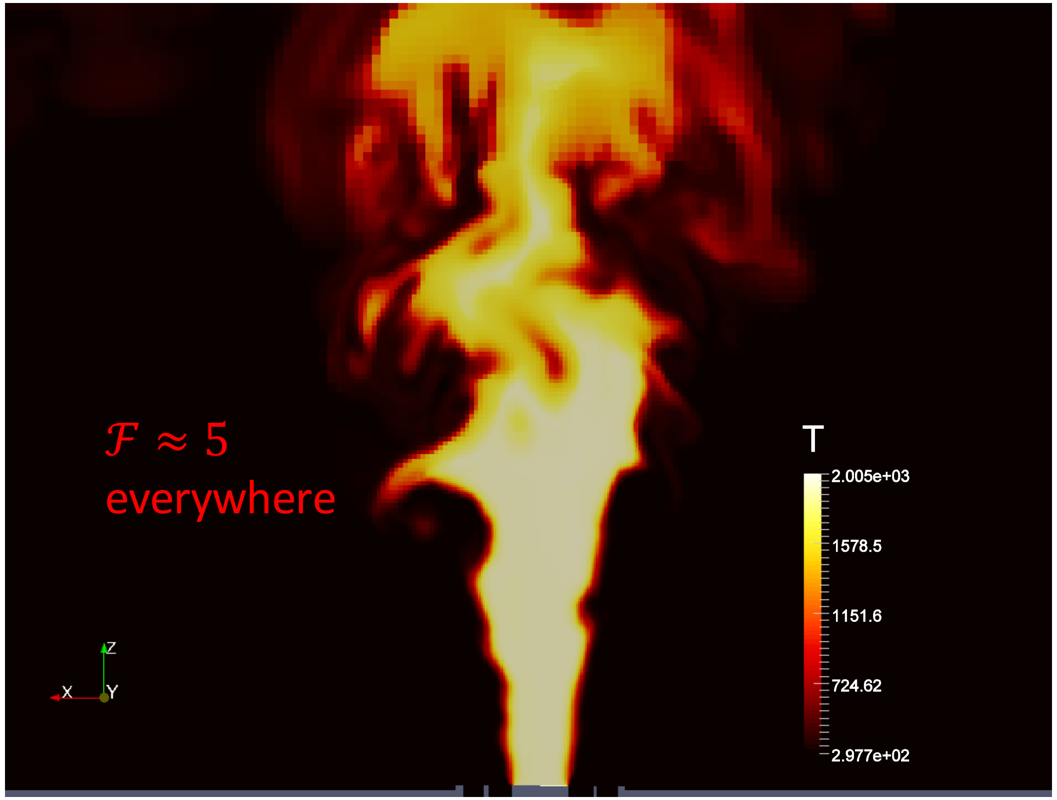
Comment: Thickening factor field is more uniform with TFM AMR model -> the mesh is released in regions where it is not necessary to have high resolution

RESULTS: COMPARISON OF TEMPERATURE FIELDS

Classic TFM



TFM + AMR



Comment: Flame looks more wrinkled when using classic TFM. This is partly due to the fact that lower thickening factors (due to higher resolution) is present at the top of the flame in classic TFM. This has to be further analyzed.

RESULTS ON REACTING FLOW: STATISTICS