CERFACS

CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

B. Vanbersel

F. Meziat

LARGE EDDY SIMULATIONS OF A HYDROGEN-AIR EXPLOSION IN AN OBSTRUCTED CHAMBER USING ADAPTIVE MESH REFINEMENT

Vanbersel, B.[1], Meziat Ramirez, F.A.[1,2], Vermorel, O.[1], Jaravel, T.[1], Douasbin, Q.[1] and Dounia, O.[1]

[1] CERFACS, CFD Team, Toulouse, Cedex 01 31057, France, vanbersel@cerfacs.fr
[2] Air Liquide – Paris Innovation Campus, Les Loges-en-Josas, 78354, France

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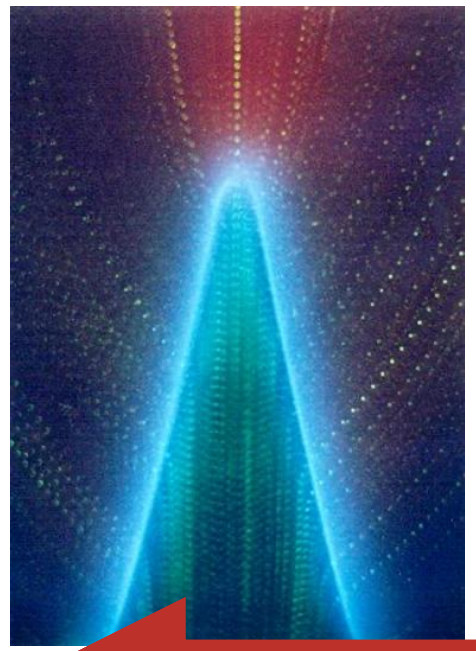
TotalEnergies GRTgaz Air Liquide

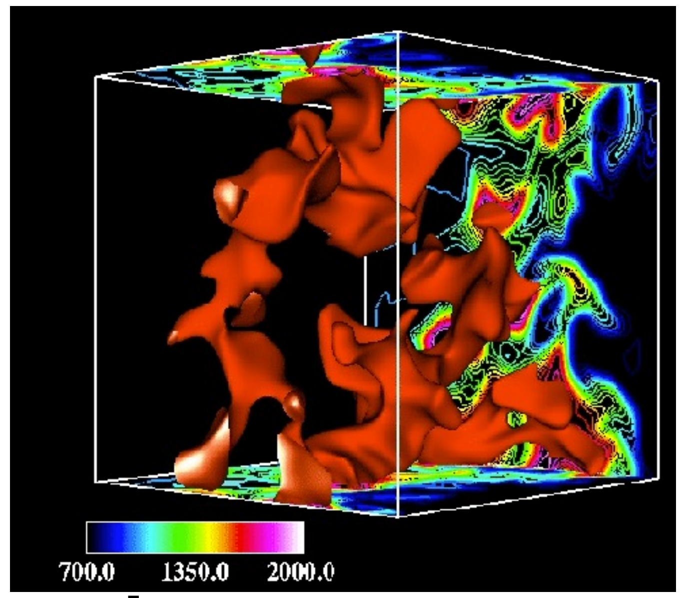
CFD for Explosions: the main challenge

Explosions are highly multi-scale phenomena

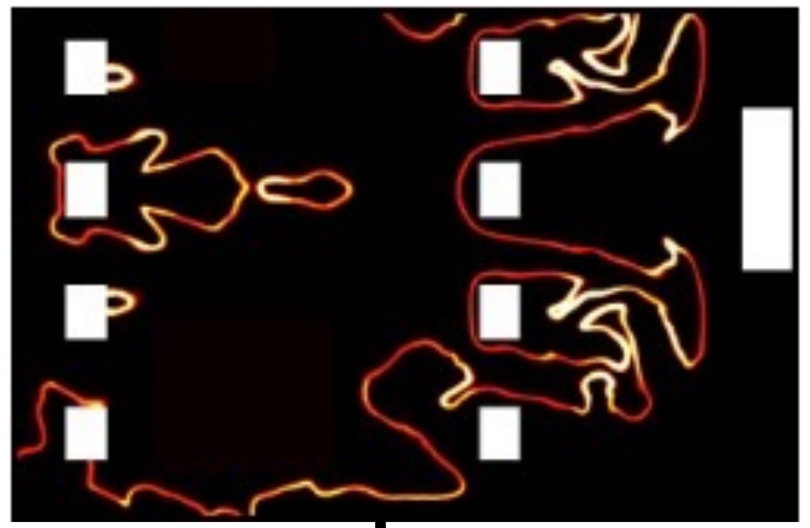
Chemical reactions



Turbulence



Flame/Obstacle interaction



Real-world safety scenarios

Relevant scales for real-world applications

Spatial Scale

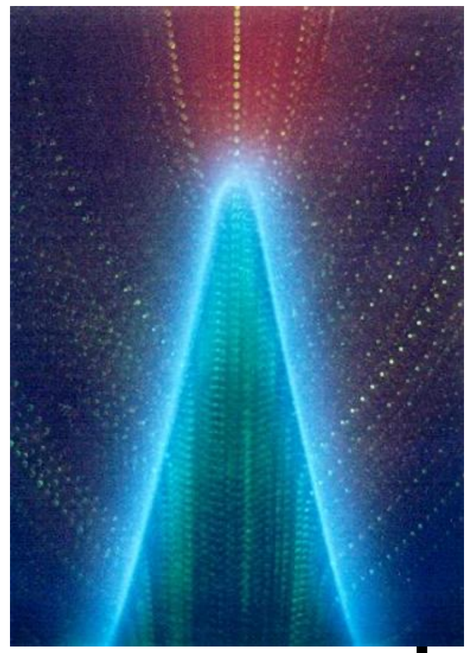
~100 µm | ~1 mm | ~10 mm | ~100 mm | ~1 m | ~10 m | ~100 m

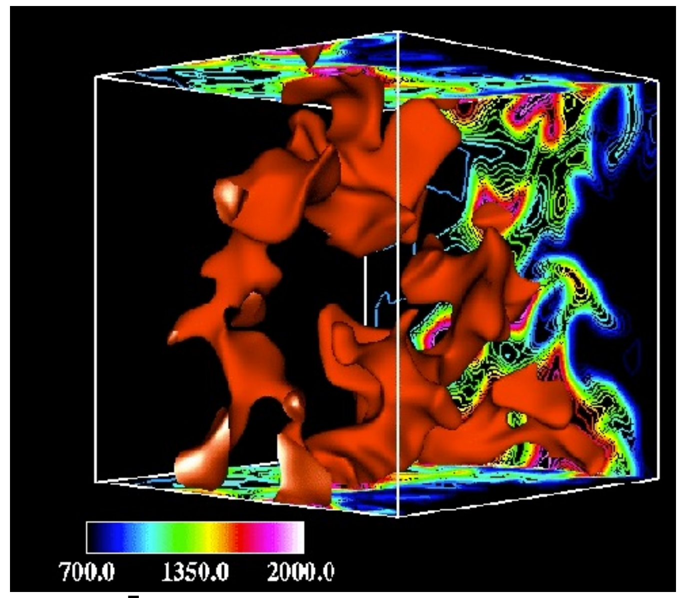
Explosion physics: the main challenge

Explosions are highly multi-scale phenomena

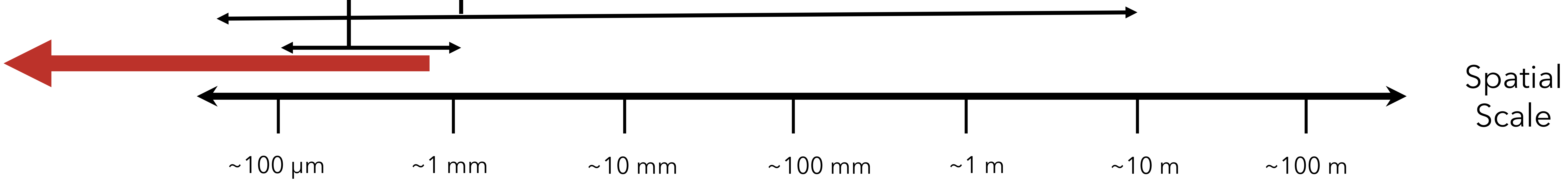
Chemical reactions

Turbulence





Chemical and turbulent scales constantly evolving



LES for High-fidelity prediction of relatively large scale explosions

DNS

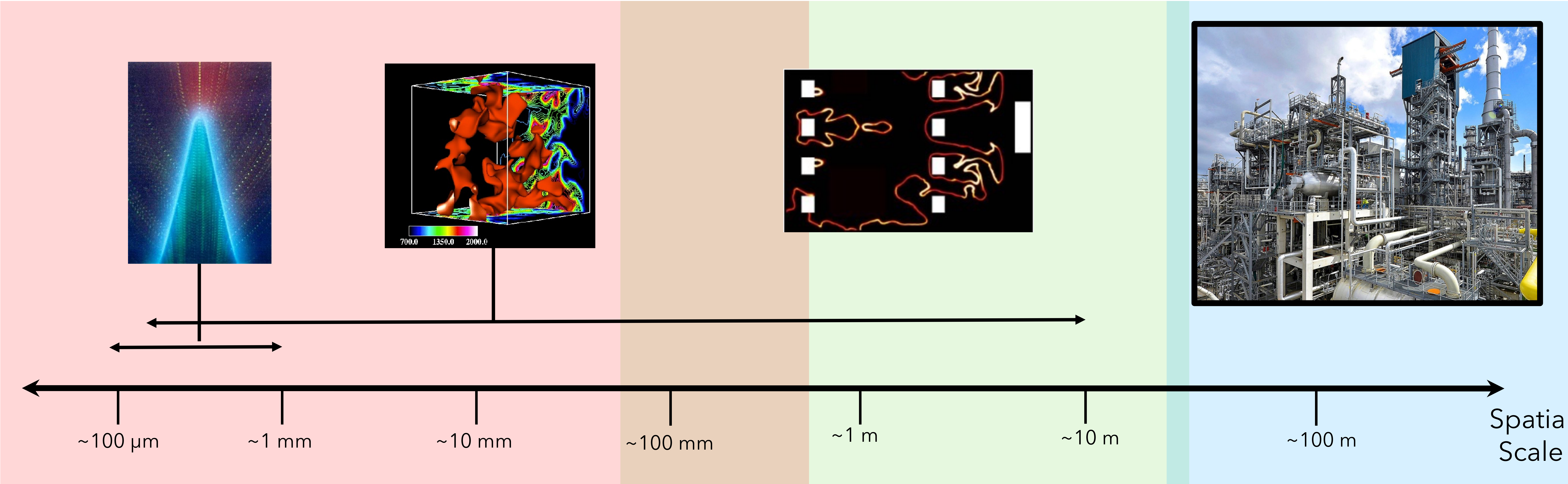
Subgrid-scale models

Large Eddy Simulation (LES) :

- Bridge the gap between DNS and URANS range of applications
- Towards industrial relevance

=> need for a massively parallel and efficient LES code

URANS



LES solver: AVBP

AVBP

Unstructured LES/DNS solver

- Unstructured (hex., tet., prisms, hybrid)
- Explicit in time
- Massively parallel
- Multi-phase (Lagrangian & Eulerian coupling)
- Chemistry: tabulated, reduced, detailed
- Other state-of-art numerical techniques

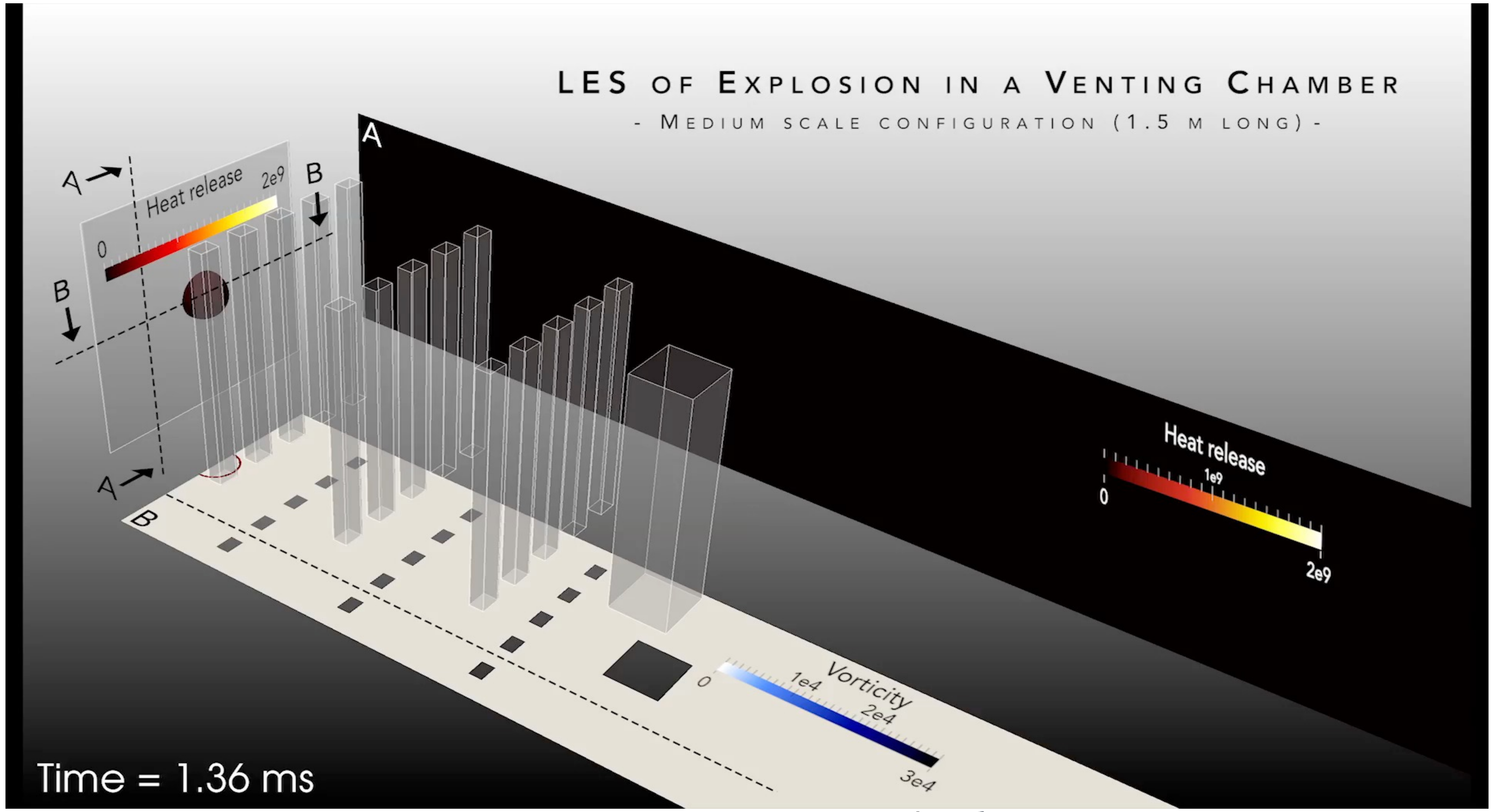
For explosion applications

- **Numerics**
  - 3rd order (space and time)
  - artificial dissipation for shock handling
  - Dynamic Adaptive Mesh Refinement
- **LES Modeling**
  - Flow: Smagorinsky, WALE, Sigma, …
  - Combustion:
    - *Thickened flame model (TFLES)*
    - Colin/Charlette efficiency functions

Operating point

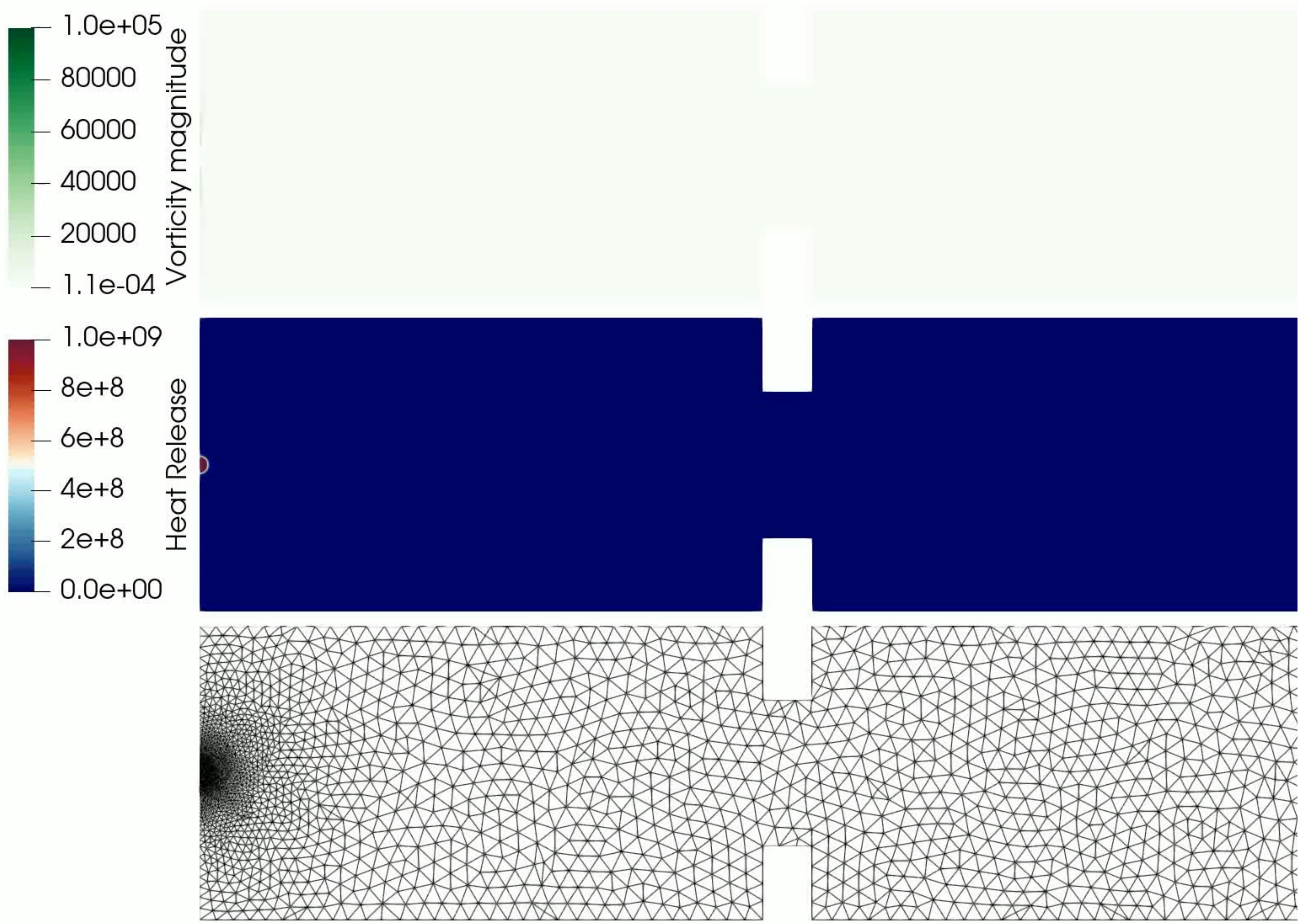
- Premixed mixture (C_3H_8/Air)
- No initial turbulence
- Equivalence ratio: $\Phi = 1$
- One central square obstruction
- Turbulence generating grids
- Laser ignition at the closed end

- 30 x 30 x **150** cm

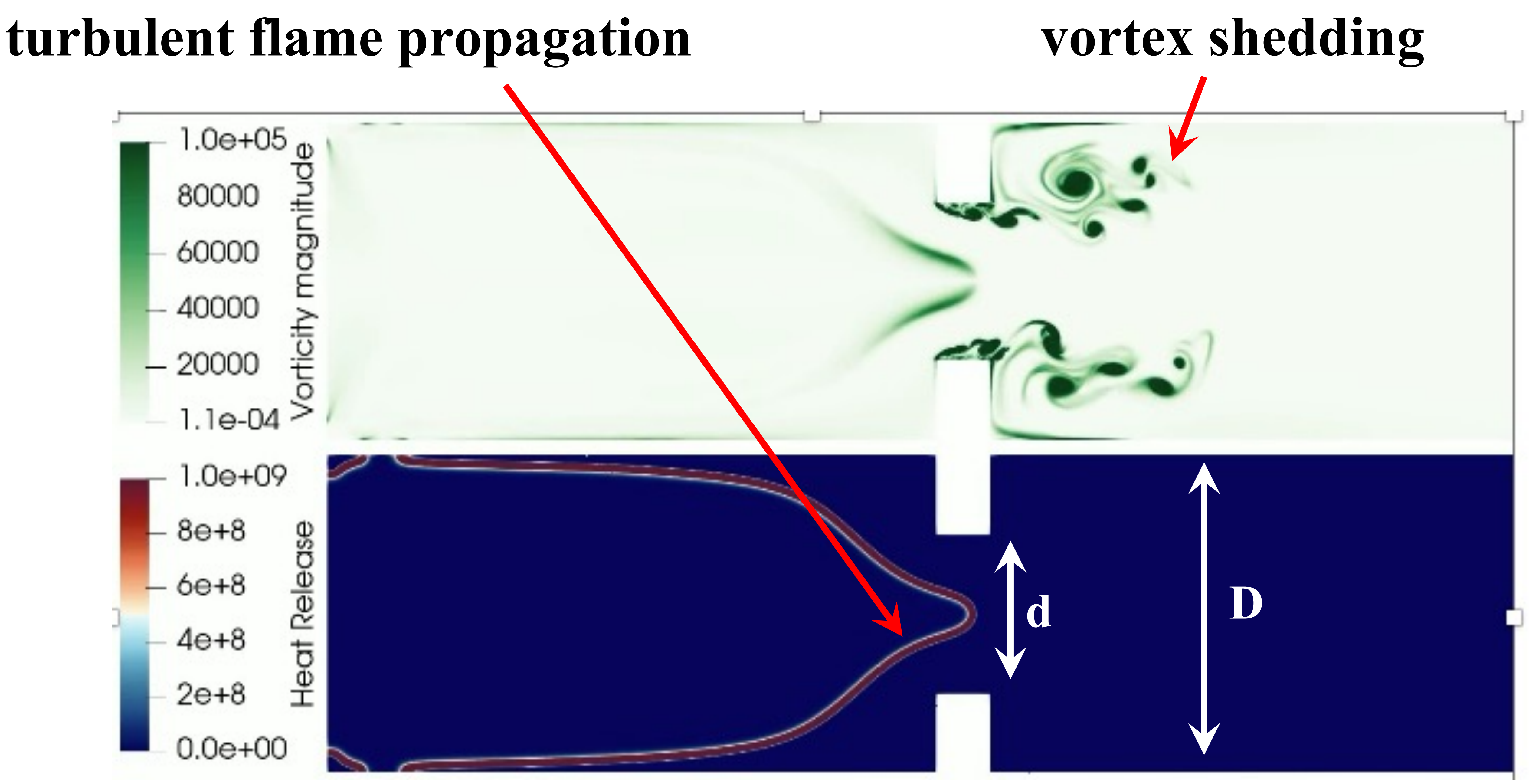


Combine LES with Dynamic Mesh Refinement for flame acceleration problems

Flame/Obstacle interaction problem



Good resolution needed to accurately predict:



⇒Large scale problem + Static mesh => Not affordable

=> Combine LES with Dynamic Mesh Refinement

AMR library for unstructured grids:
YALES2[1]/Kalpataru(CERFACS) + MMG3D [2]

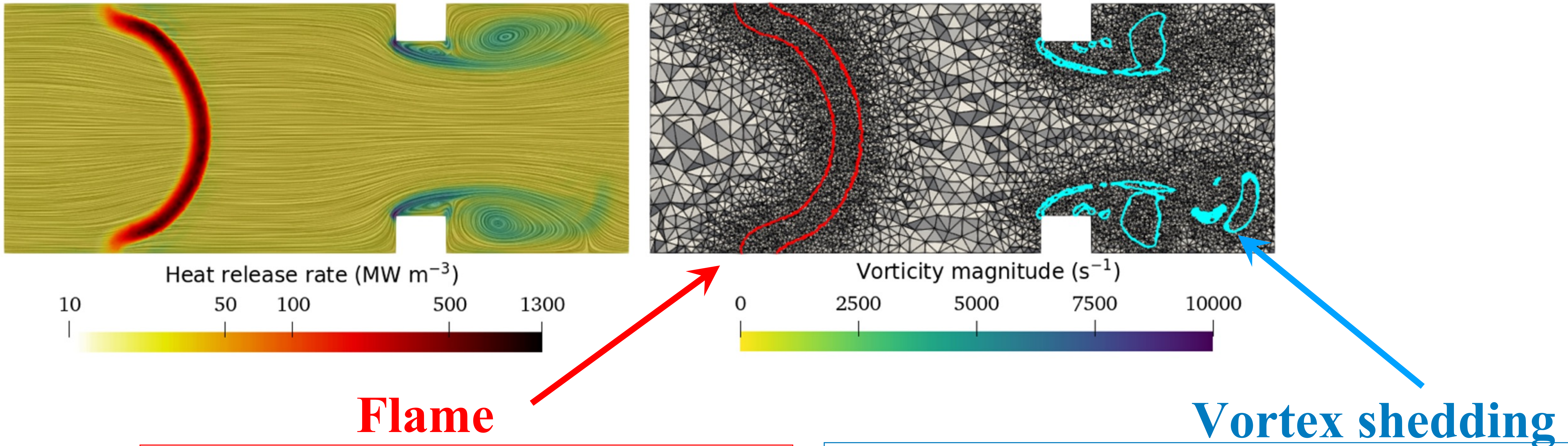
[1] P. Benard, et al, *International Journal for Numerical Methods in Fluids* **81**, 719 (2016).
[2] C. Dapogny, et al, *Journal of Computational Physics* **262**, 358 (2014).

Objectives:

- **Develop an AMR strategy for LES of fast deflagrations in large scale configurations (+ unstructured grids constraint)**
- **Get rid (AMAP) of user defined parameters**

1. **AMR recipe for high-fidelity LES of gas explosions**
2. **Validation on a fast deflagration case (Gravent)**

AMR recipe for high-fidelity LES [1/2]



Regions of interest:

- **Metric :** θ_F[7] (from the DTFLES model)
- **Resolution: Δx_1**
  - **F ~ [10-30]**
  - **Relatively thin flame: $F\delta_L$ << d**

- **Metric :**Ω[8] to detect regions where
  - **rotation overtakes deformation**
- **Resolution: Δx_1**
  - **all regions of interest share the same Δx_1** [9]

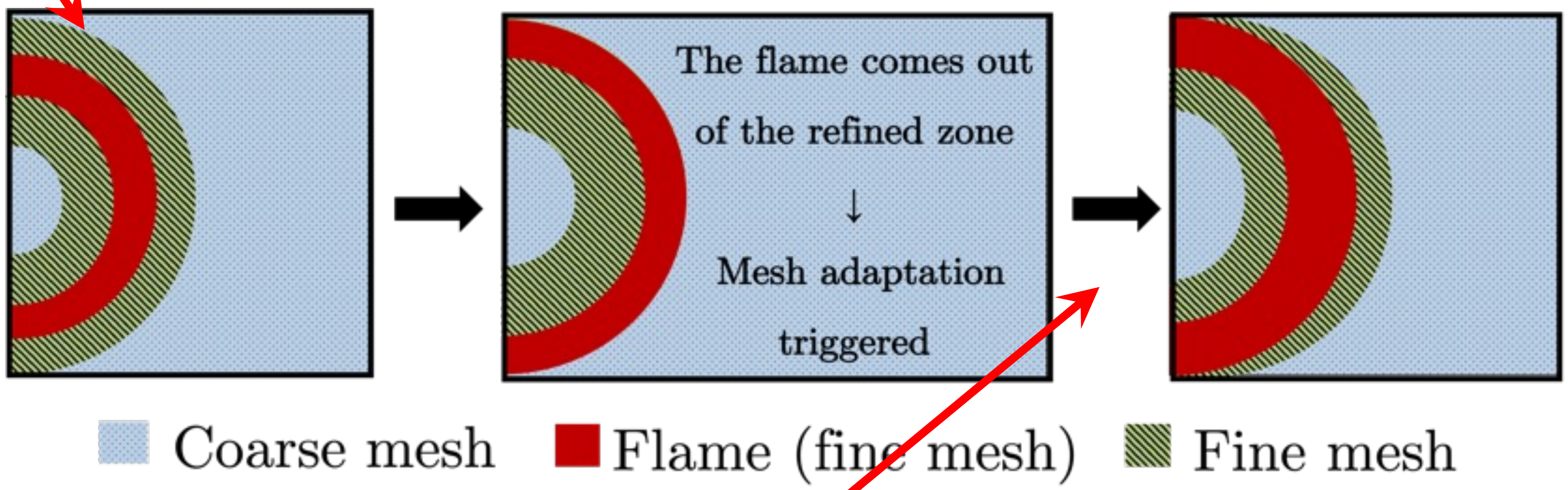
Outside Regions of interest:

Sufficient resolution to capture:
- **Flow contraction**
- **flow profiles in un-obstructed regions**

[7] J. P. Legier et al., *Proceedings of the Summer Program, CTR, 2000.*
[8] C. Liu et al., *Science China: Physics, Mechanics and Astronomy, 2016*
[9] C. Mehl, S. Liu, O. Colin, FTACS, 2021

AMR recipe for high-fidelity LES [2/2]

Mask dilatation (1 cell) : ensures the QoI stays inside the RoI



Automatic mesh triggering:

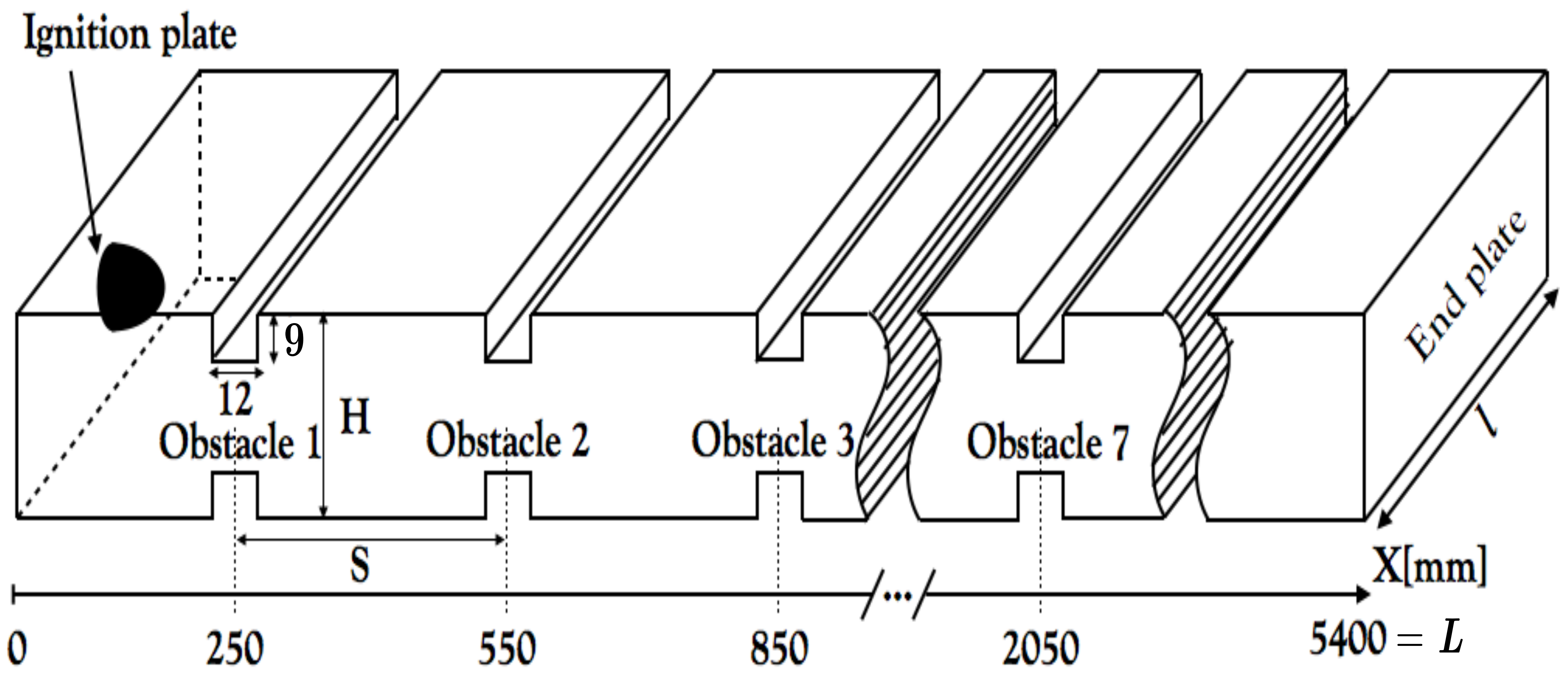
- **when the flame reaches the limit of the RoI**
- **No user-defined parameter**

QoI: Quantity of Interest
RoI: Region of Interest

1. **AMR recipe for high-fidelity LES of gas explosions**
2. **Validation on a fast deflagration case (Gravent)**

Gravent BR30hS300 Test case[2,4]

- Entirely closed rectangular channel (5.4 (L) x 0.3 (l) x 0.06 m (H)),
- Seven obstacles (BR=30%, S=300mm)
- H_2-air perfectly premixed: $\phi = 0.52, \mathrm{P} = 1\mathrm{atm}, \mathrm{T} = 300\mathrm{K}$
- Validation of the AMR strategy: Focus on Flame acceleration



GraVent BR30hS300 configuration[3]

[2] L. Boeck et al., The gravent ddt database, Shock Waves 26 (2016).
[3] O. Dounia, Ph.D. thesis, INP Toulouse (2018).
[4] L. Boeck, Ph.D. thesis, Technische Universität München (2015).

Numerical setup

- LW convection scheme[4]: 2nd order in space and time.
- Isothermal Walls with law of the wall
- LES:
  - Subgrid turbulent stresses: WALE [5]
  - Flame thickening DTFLES
  - Turbulent combustion: Colin [6]
- **Meshes: fully unstructured tetrahedral meshes**

- Chemistry: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

ϕ	s_L^0 (ms^{-1})	T_{ad} (K)	δ_L^0 (m)
0.52	0.59	1657	$2.03 \cdot 10^{-4}$

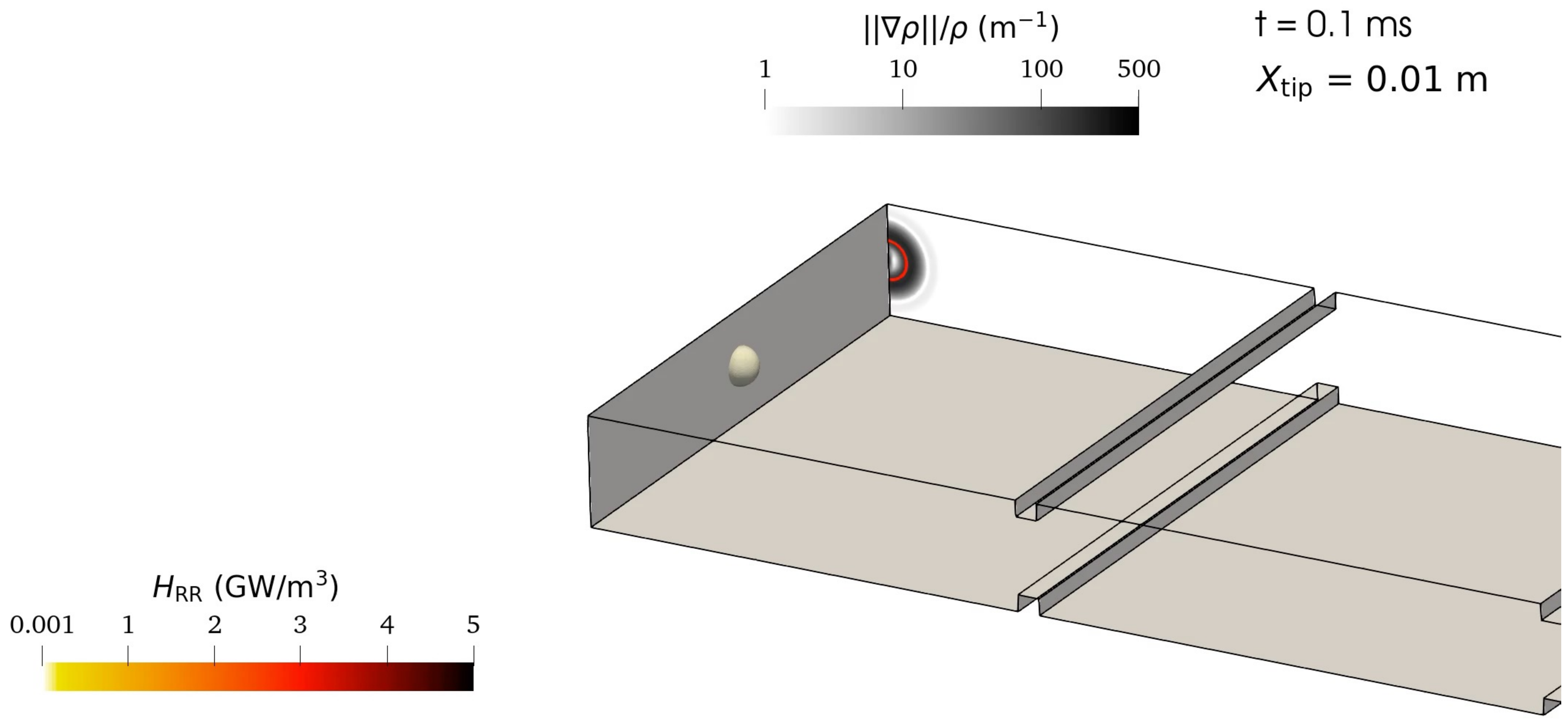
Table 1: Laminar H_2-air flame characteristics at $T_0 = 300\,\mathrm{K}$ and $p_0 = 1\,\mathrm{atm}$ for the single-step chemical scheme.

- Static REF (**380Mcells**):
  - $\mathbf{\Delta x = 1\ mm} = \boldsymbol{d/42}$, $\boldsymbol{F \approx 25}$
  - $\mathbf{\Delta x = 10\ mm = D/6}$

- Dynamic AMR
  - $\Delta_x^{min} = d/42 = 1\ \mathrm{mm}$, $\Delta_x^{max} = d/10 \approx 4mm$, $F \approx 25$
  - $\Delta_x^{min} = d/42 = 1\ \mathrm{mm}$, $\Delta_x^{max} = D/6 = 10mm$

1. [4] P. Lax and B. Wendroff, *Communications on Pure and Applied Mathematics* 1960.
2. [5] F. Nicoud and F. Ducros, *Flow, Turbulence and Combustion* 1999.
3. [6] O. Colin, et al., Physics of Fluids, 2000.

Validation of the AMR strategy



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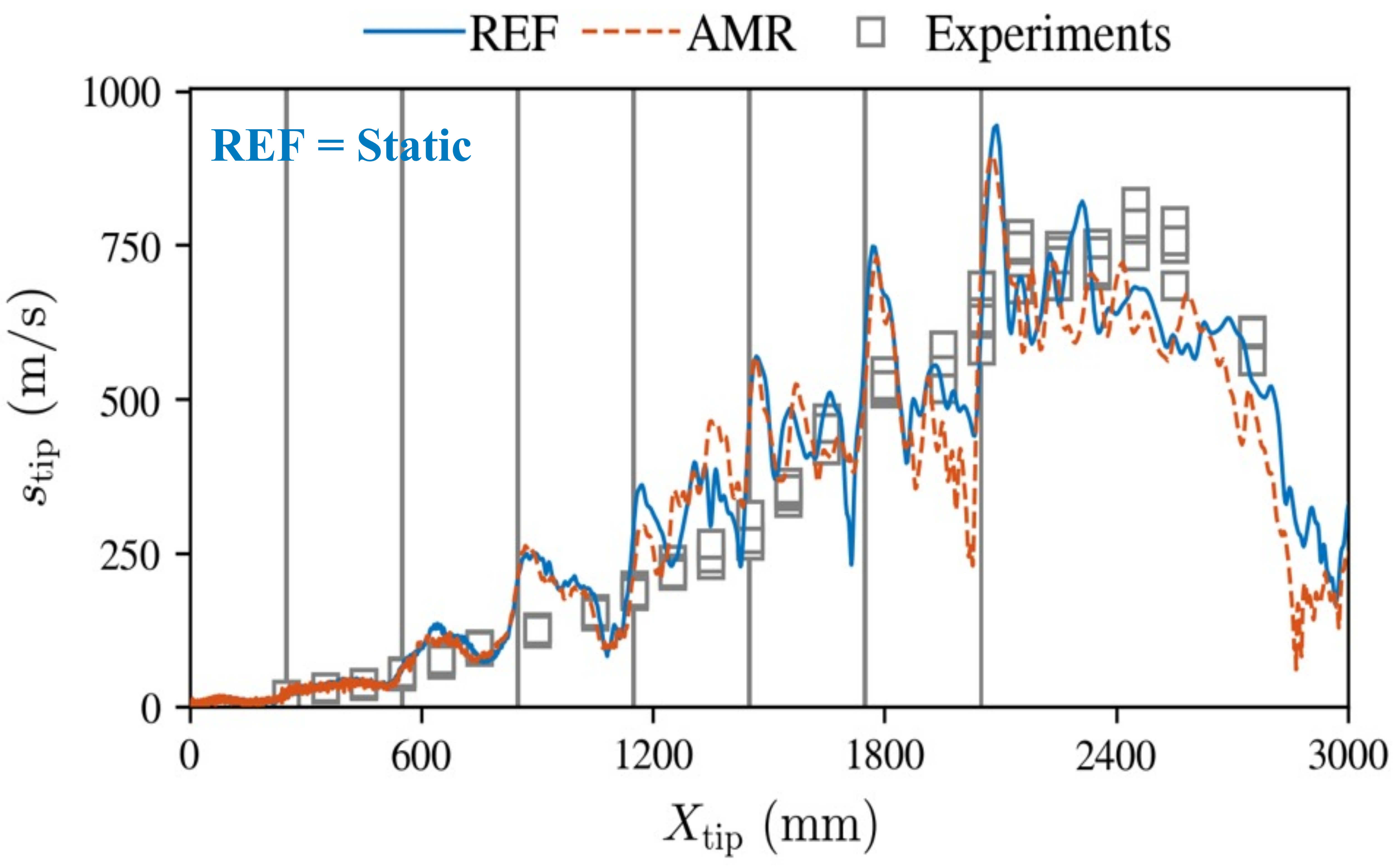
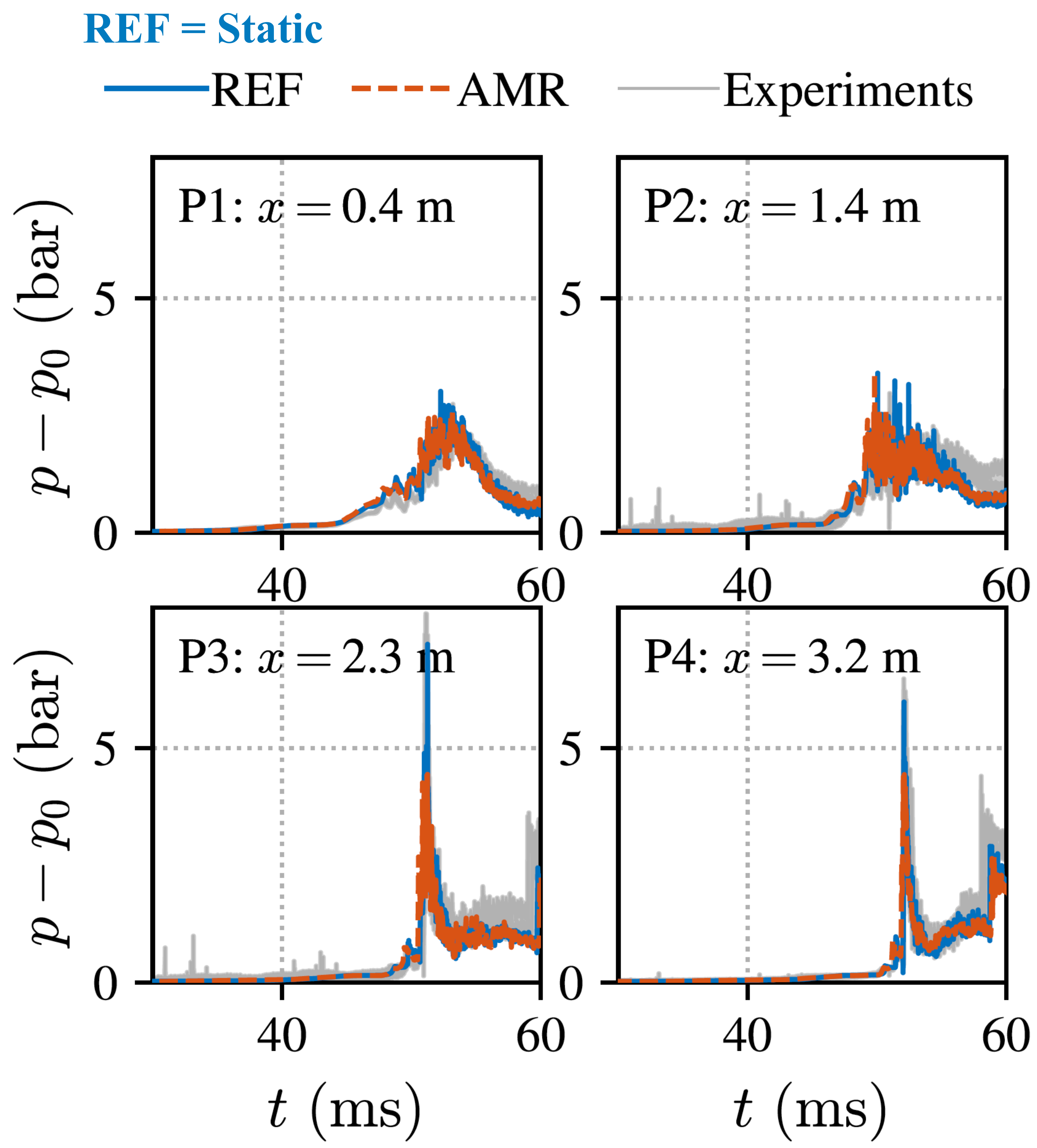
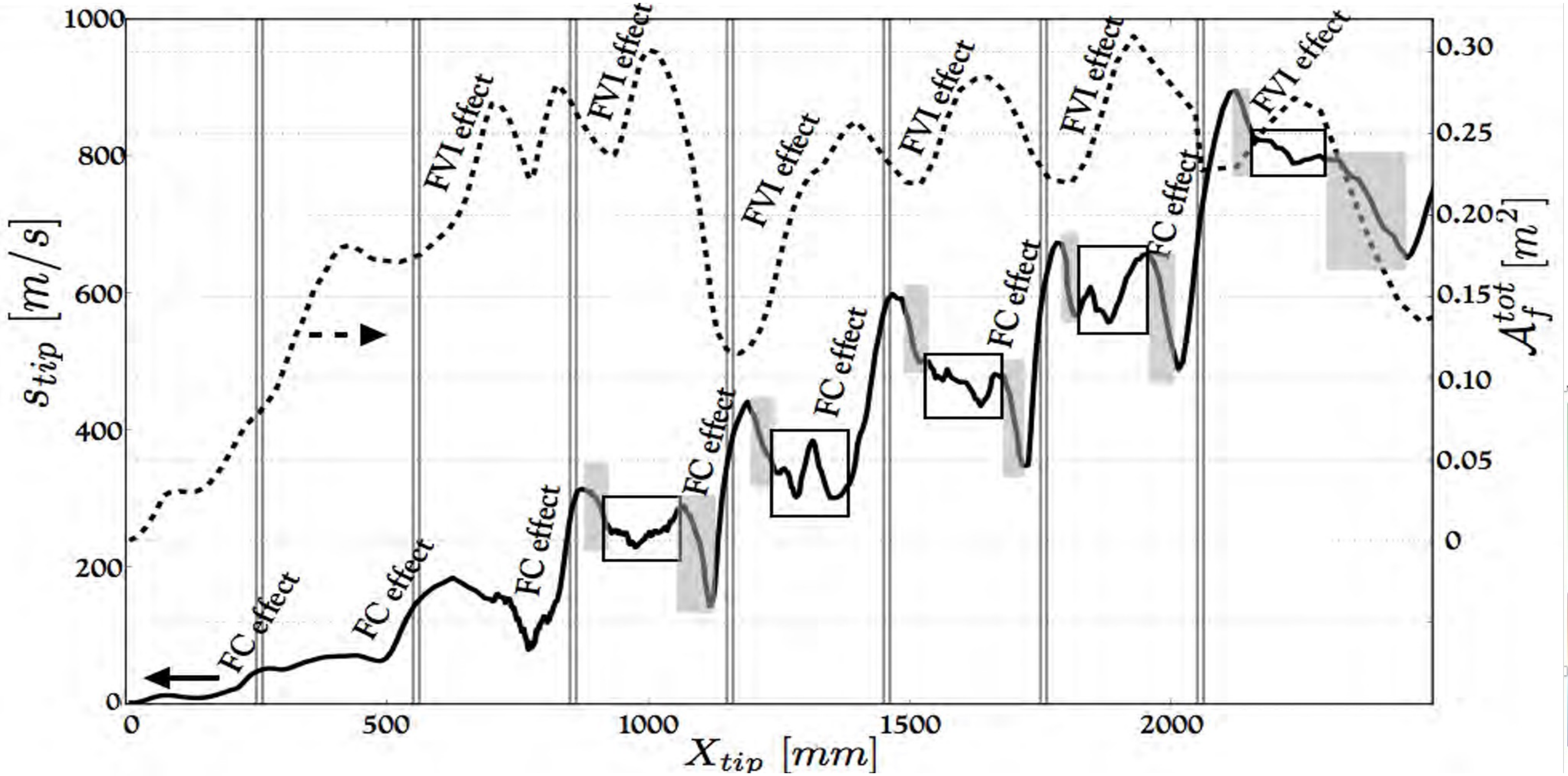


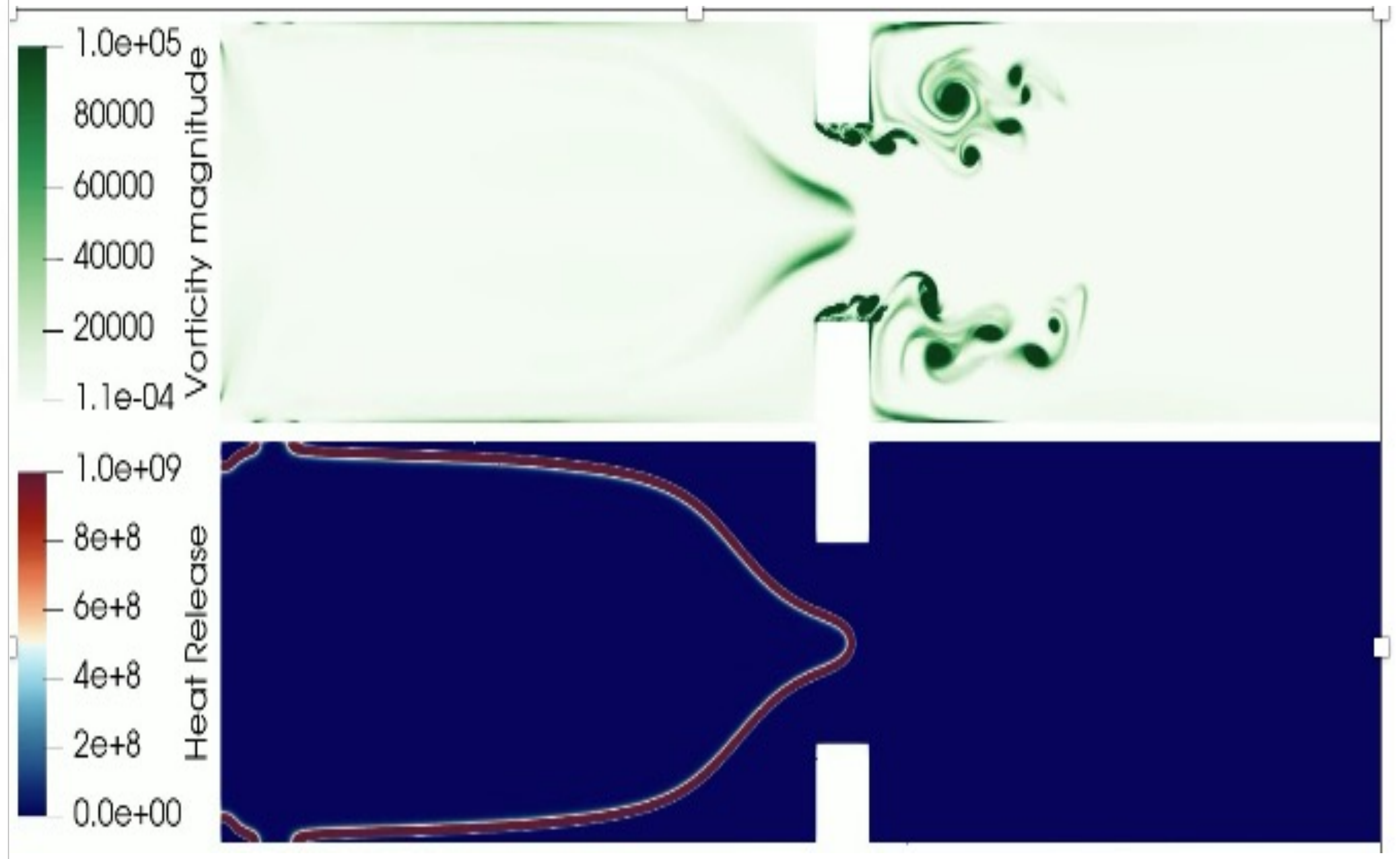


- Very good agreement between AMR and Static:
  - **Flame acceleration**
  - **Shock formation and overpressure production**

FA mechanisms

Flow contraction (FC) + Flame/Vortex interaction (FVI)

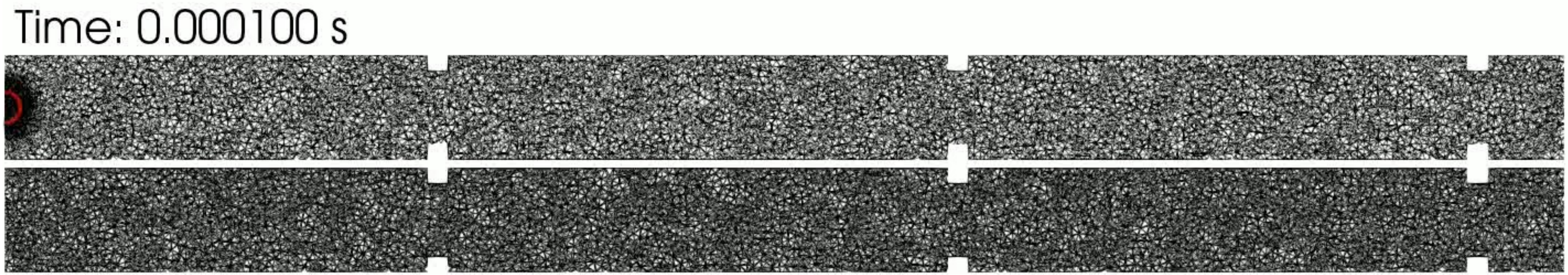




Flame propagation speed s_{tip} (solid line) and total flame surface A_f^{tot} (dashed line) as a function of the flame tip position X_{tip}.[3]

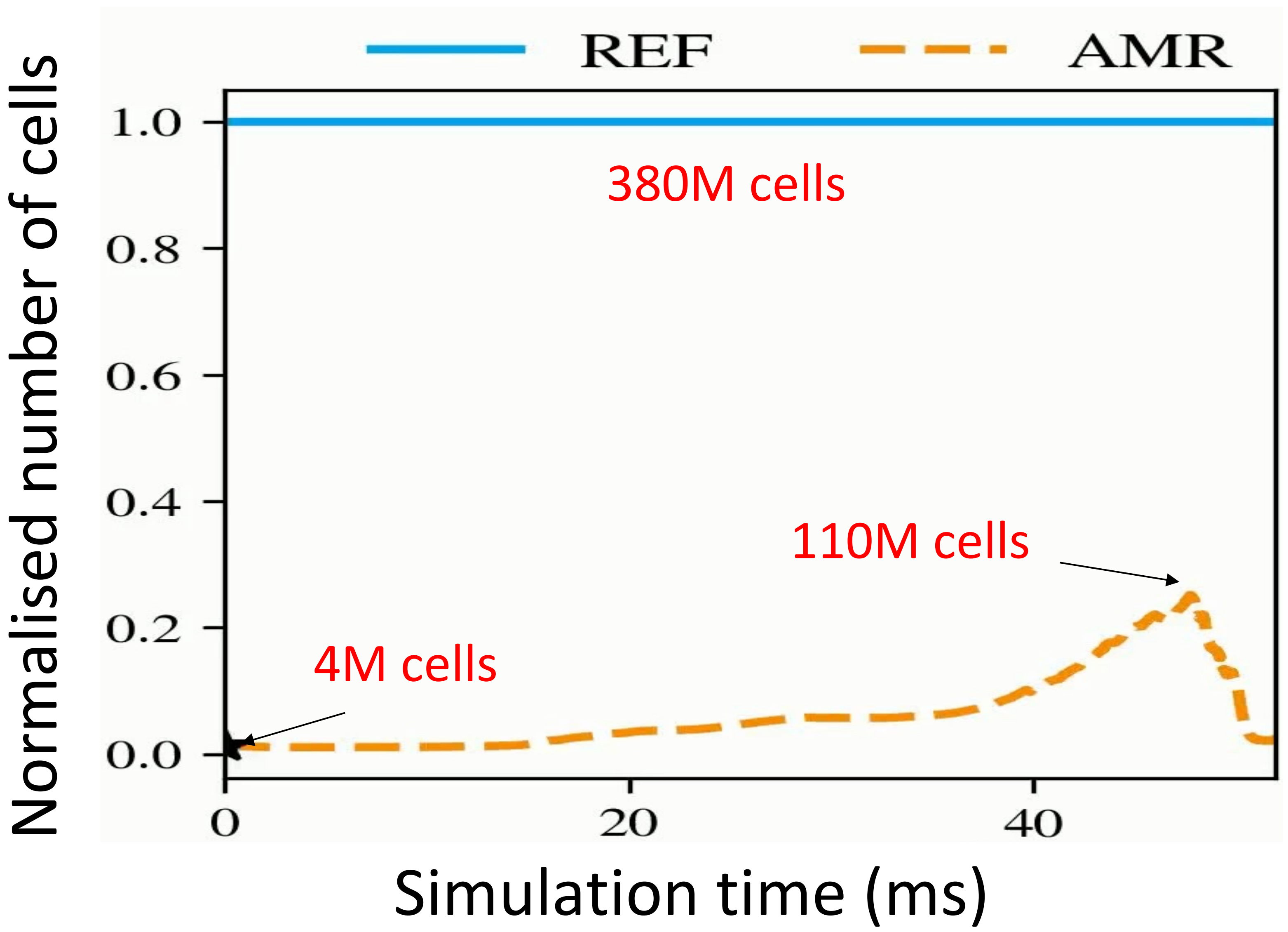
[3] O. Dounia, Ph.D. thesis, INP Toulouse (2018).

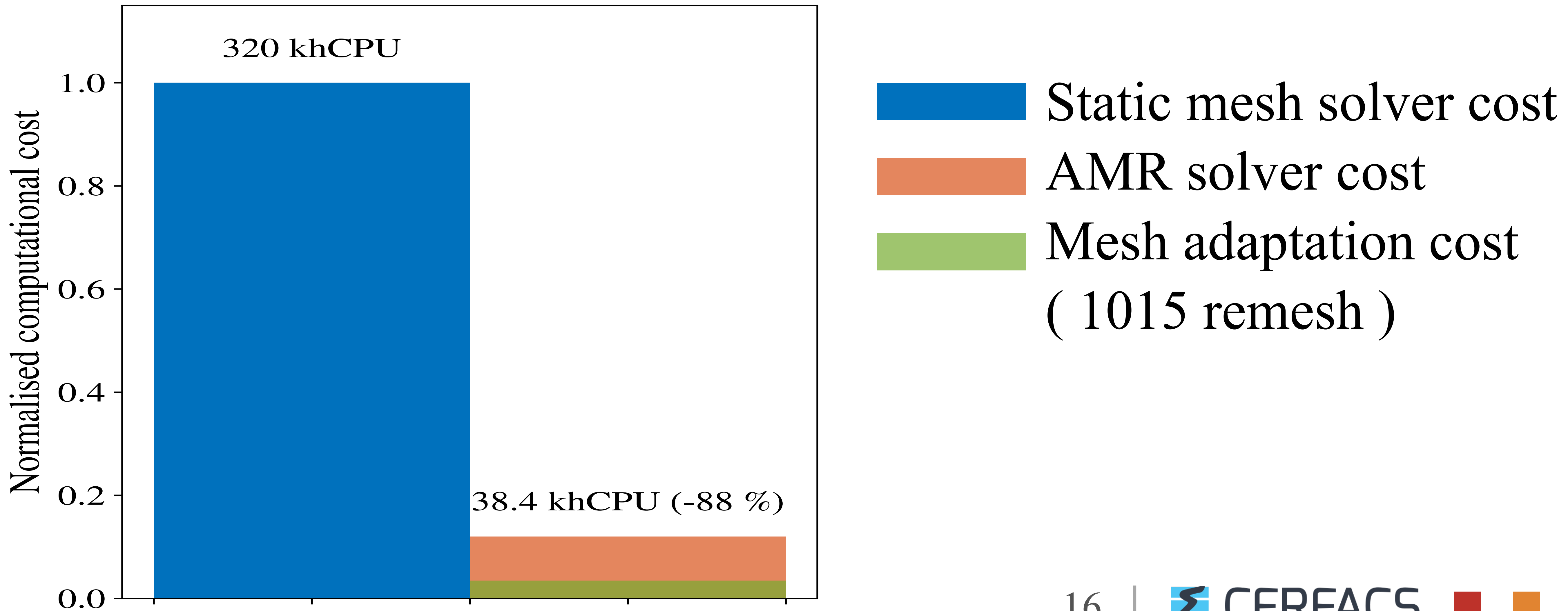
Computational efficiency of AMR



- Increase of mesh size with FA
- **Mesh size <= 0.3 x (Static mesh size)**

- 88% reduction in computational time
- **Cost of remeshing low**





Conclusion

Takeaways

- A feature-based dynamic mesh refinement strategy was developed:
  - Suited for LES on unstructured grids
  - Does not rely on user-defined parameters for its sensors (flame, shocks, vortex structures)
  - Automatic remeshing triggering
- Validation against a fast deflagration case:
  - Good agreement with experiments and static mesh results
  - Drastic gain in computational efficiency compared to the static mesh approach
- Validation against other cases not shown here
- Working towards application in larger-scale explosions

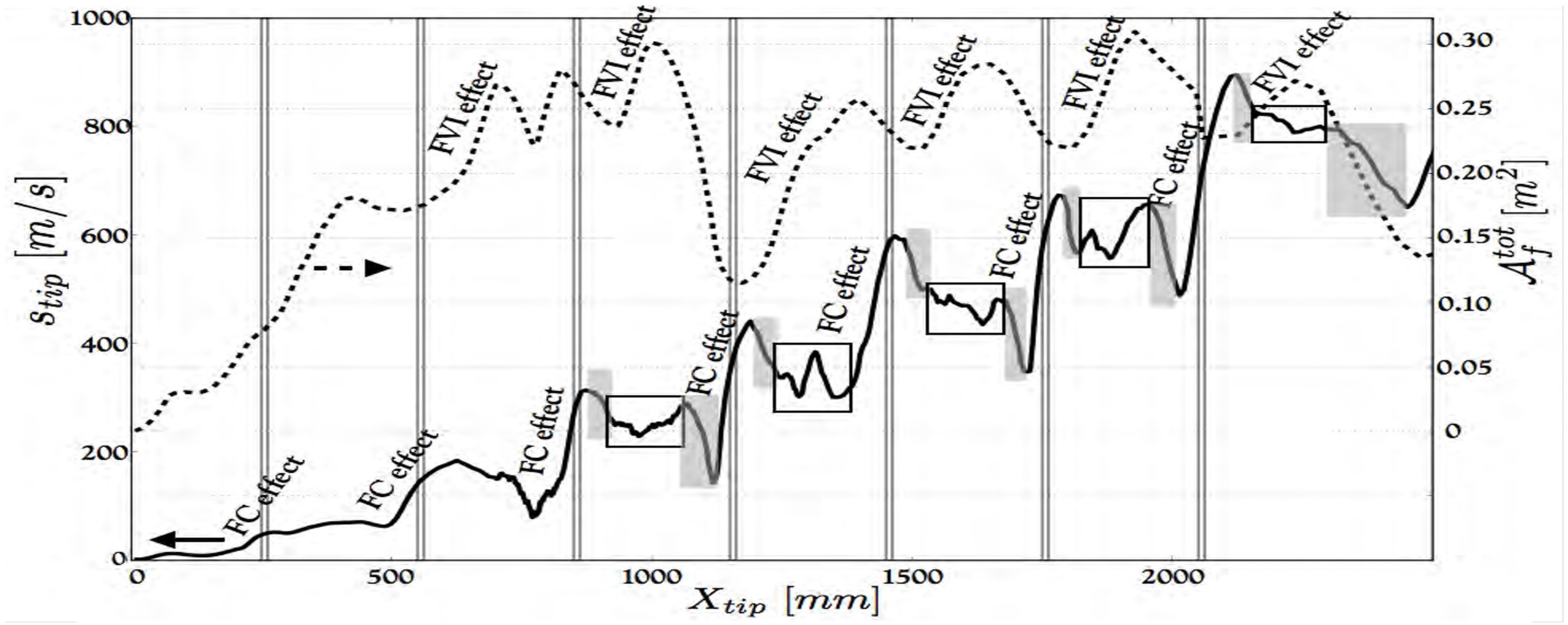
Funding acknowledgement

LES FOR EXPLOSIONS (LEFEX)

TotalEnergies GRTgaz Air Liquide

Goal of the project: Develop a high-fidelity LES code for explosion prediction in large/complex geometries.

Gravent BR30hS300 Test case[2]



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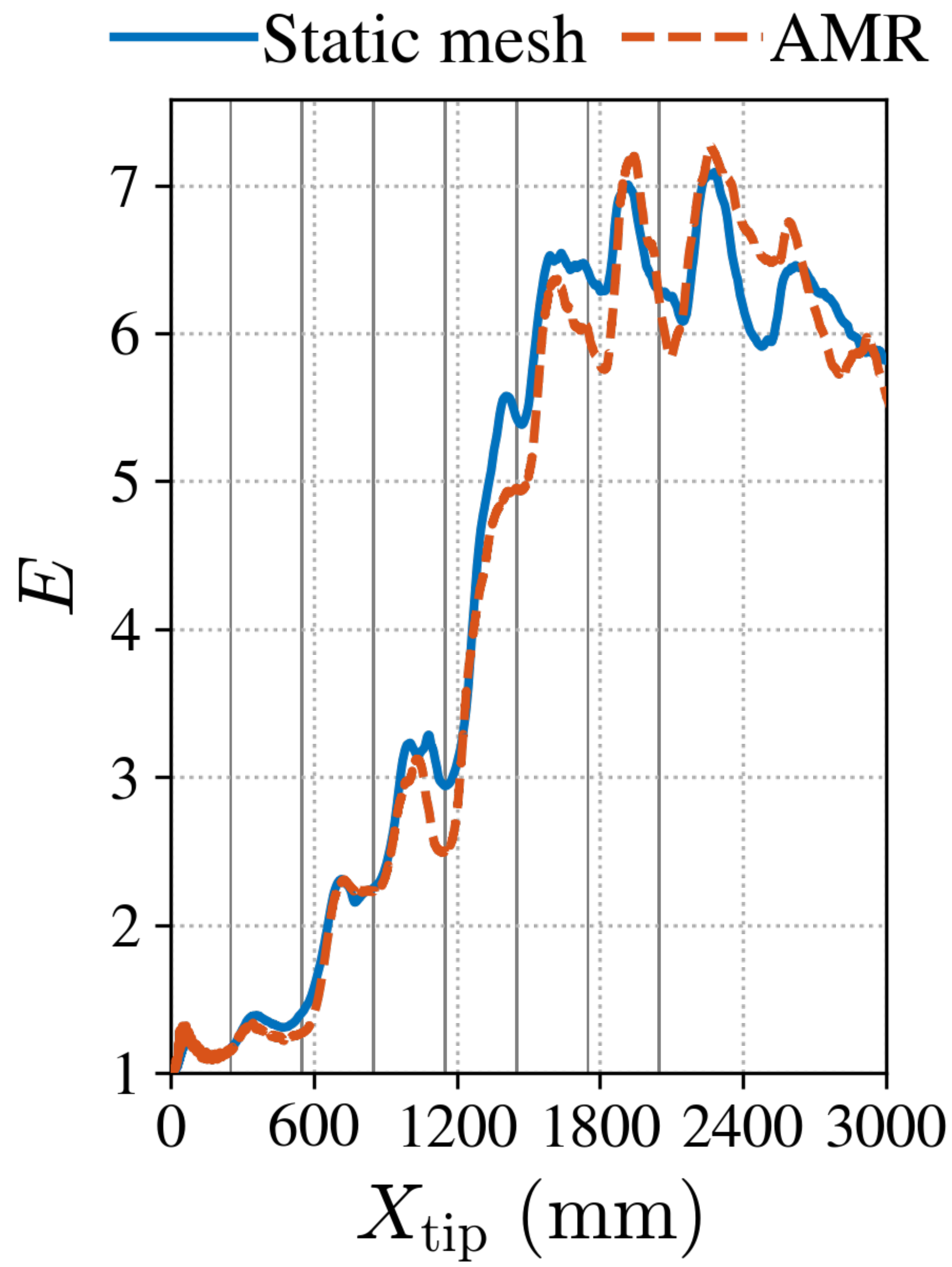
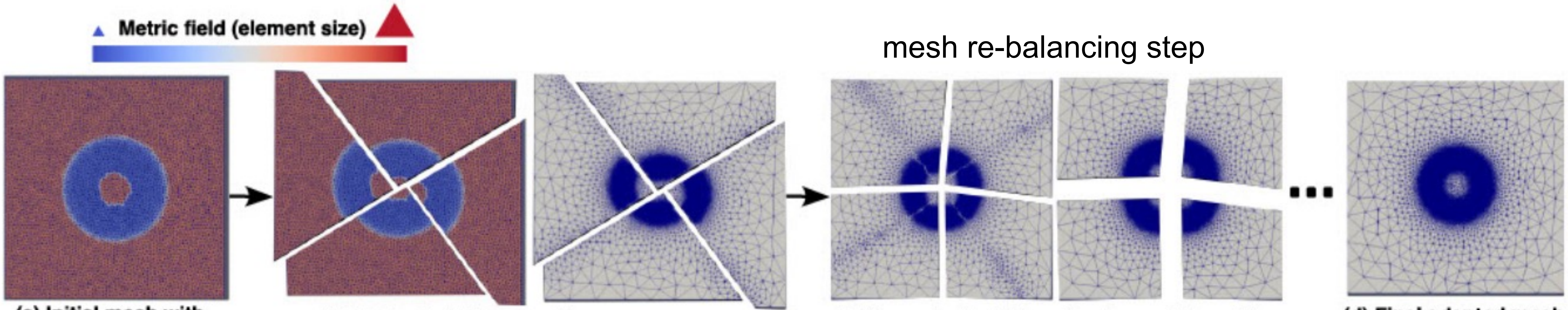


[2] L. Boeck et al., The gravent ddt database, Shock Waves 26 (2016).
[3] O. Dounia, Ph.D. thesis, INP Toulouse (2018).
[4] L. Boeck, Ph.D. thesis, Technische Universität München (2015).

Parallel Kalpataru AMR library

Topology-Aware adaptive Refinement and load-balancing framework for Unstructured meshes

- Couples the load-balancing tool with the remeshing library MMG3D
- Iterative approach



(a) Initial mesh with metric field

(b) First adaptation step (frozen processor boundaries)

(c) Second adaptation step (re-partition with edge/vertex weights at processor boundaries)

(d) Final adapted mesh satisfies metric field