HYDROGEN WEEK - THURSDAY

TERMINOLOGY:

WHAT IS AVAILABLE TODAY ON TNF AND WE DISCUSSED YESTERDAY: HYLON PHASE 1

WHAT WE MAY DO ON A NEW SET OF DATA IN THE FUTURE: HYLON PHASE 2

TODAY:

WE DISCUSS RESULTS OF HYLON PHASE 1 AND LESSONS LEARNED

THEN WE DISCUSS OF THE INTEREST OF AN HYLON PHASE 2 AND WHAT WE WOULD DO THERE: TO ILLUSTRATE THIS, WE DISCUSS THE WORKS OF KAUST ON HYLON AT HIGH PRESSURE BECAUSE THIS WOULD BE THE CENTER OF HYLON PHASE 2

IMFT
INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

CERFACS

9.30-11.00: CFD of hydrogen flames at high pressures: open discussion on possible models and challenges for DNS and LES (T. Poinsot + all)

11.00 COFFEE BREAK

11.30-12.00: A critical issue: from CAD to 3D printing to X tomography to CFD meshes: how to garanty that CFD experts compute the right geometry for HYLON cases. H. Magnes, S. Marragou, T. Schuller.

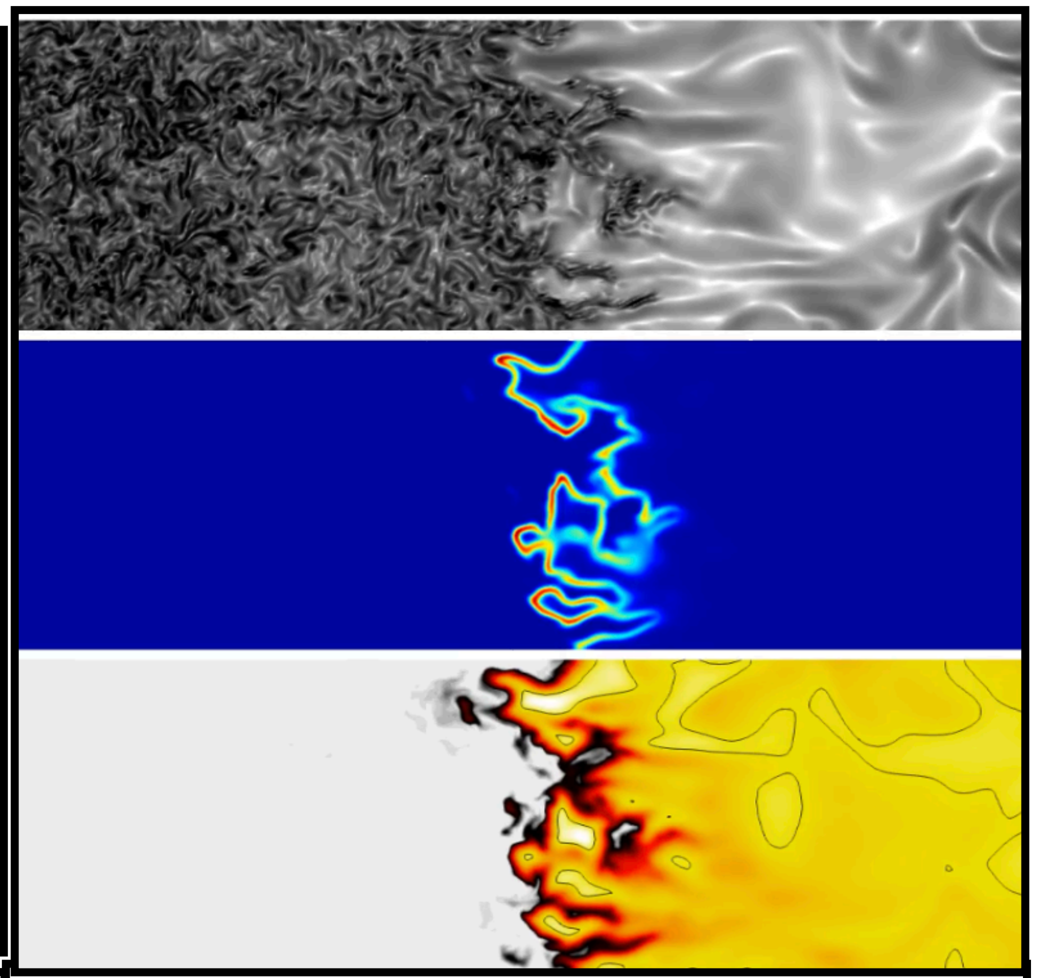
12.00-14.00 LUNCH

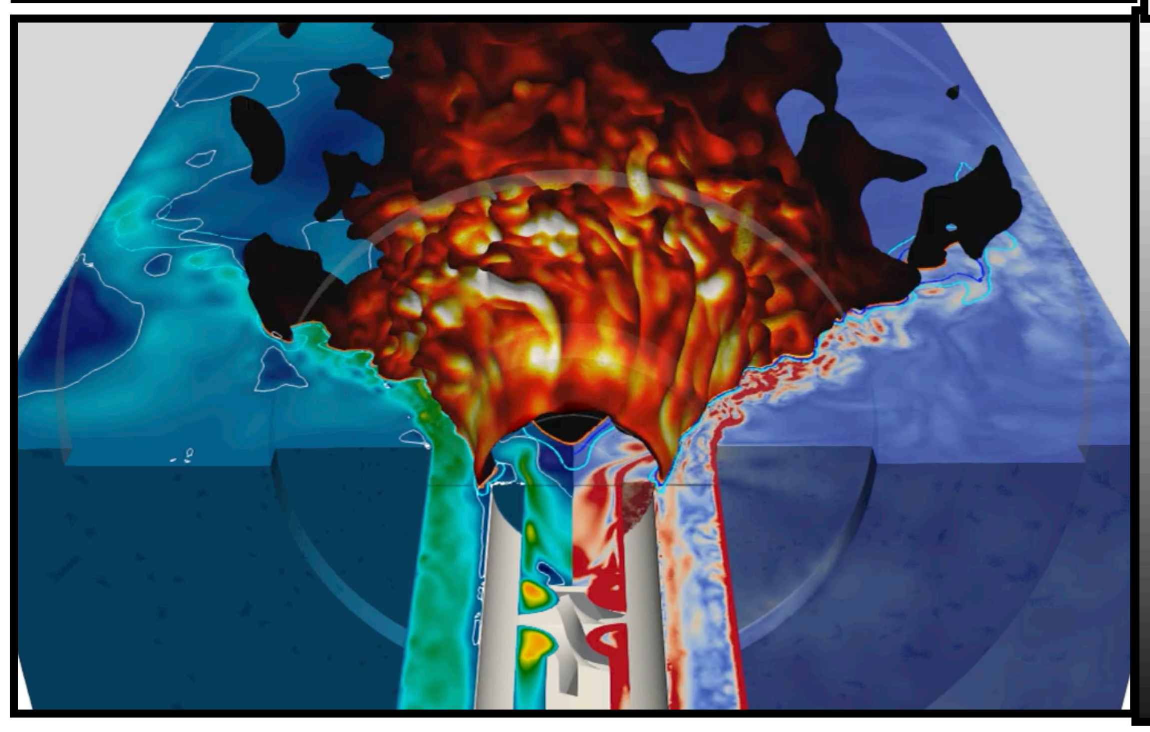
14.00-15.00 Description of the KAUST high pressure implementation of the IMFT HYLON rig (Marragou / Guiberti / Schuller)

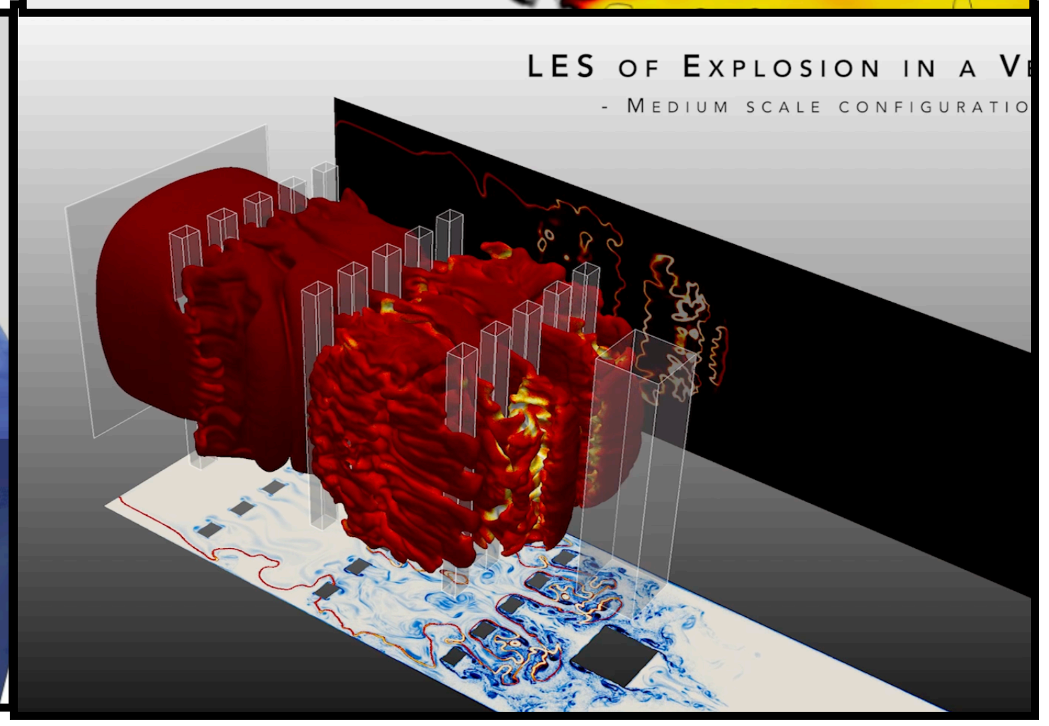
15.00-16.00 Discussion of possible addition of KAUST HYLON in the CAW H2 CFD exercise and of challenges for CFD of H2 air flames at high pressures. Links with TNF and proposed organization for future collaboration.

16.00 END OF DAY

HYDROGEN WEEK
THURSDAY
CFD FOR H2: conclusions from HYLON PHASE 1







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PROPOSAL FOR DISCUSSION OF HYLON PHASE 1

Each of us has listened to yesterdays talk and reached his own conclusions

Today: compare our opinions

Do not hesitate to interrupt and contradict…

The main issue of the day is that we'll need to go further:
- go to high pressures
- measure NOx, T and species
- go to unsteady sequences, ignition, quenching and instabilities
- predict heat load on walls

To do this, we need to think about what we achieved up to now

CONCLUSIONS OF YESTERDAY'S MEETING

MAIN OUTPUTS

- capturing the velocity fields is not that difficult: most codes do it. In fact the flame position being more or less imposed by the recirculation within the chamber, the velocity field cannot vary that much as long as we have the right temperature field. So far, so good
- what are the essential ingredients which the CFD codes should have: not so easy to determine, knowing that, up to now, most codes do the job reasonably considering the available data.
- We will try to tackle each topic in the following order:
  1. Does the code accuracy matter ? (high order ? or not)
  2. Does the mesh matter, do we need static mesh refinement, do we need dynamic mesh refinement
  3. Do we need a turbulent combustion SGS model and for which flame (anchored, lifted)
  4. Do we think that we can capture the limit between lifted and anchored flames
  5. Do we need to change the chemical schemes we use (excluding NOx), the transport models
  6. What about NOx models
  7. What about wall treatments
  8. What will happen at high pressures
  9. CPU time

1. CODE ORDER: DOES ACCURACY MATTER ?

SPACE ACCURACY: Many groups (especially coming from aerodynamics and DNS) have argued in the past that high-order codes (>4) were needed for LES in CFD. It does not seem to be the first worry of most groups here: codes have a spatial accuracy close to 2. DO WE AGREE ON THIS ?

TIME ACCURACY: yesterday, we saw a wide range of time steps. Compressible solvers use time steps close to 10 ns. Low Mach solvers go up to microseconds. That does not seem to affect results much

2 MESH, STATIC AND DYNAMIC REFINEMENTS

Smallest mesh: from 75 um to 250 microns
Noone used dynamic Mesh Refinement where the mesh follows the flame in real time: not needed here ? DO WE AGREE ?

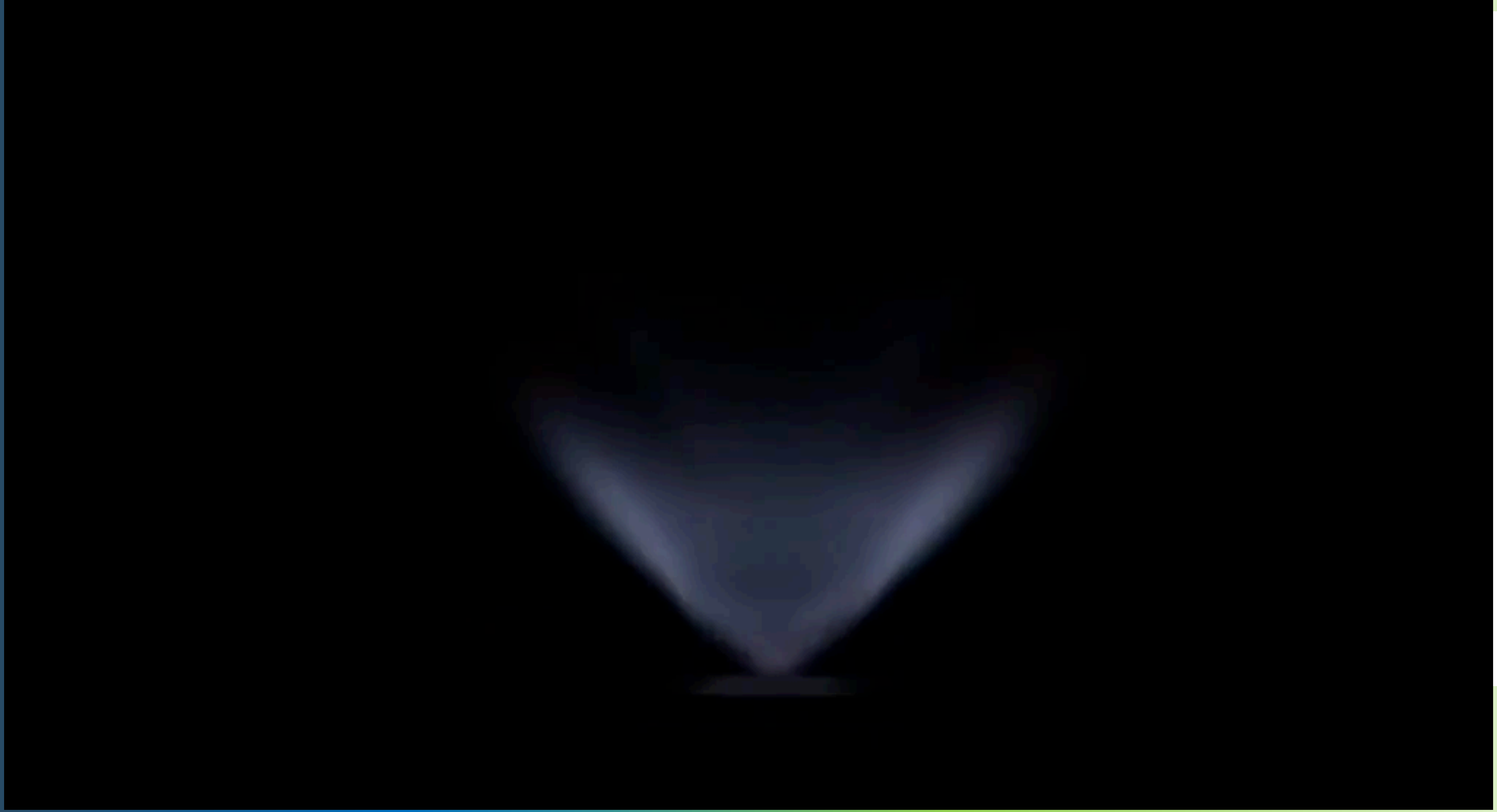
Some used static Mesh Refinement ?

What imposes the mesh size ?? The flame OR the flow in the swirler ? Most of us are combustion guys so we think this is the flame: we must resolve the flame front.

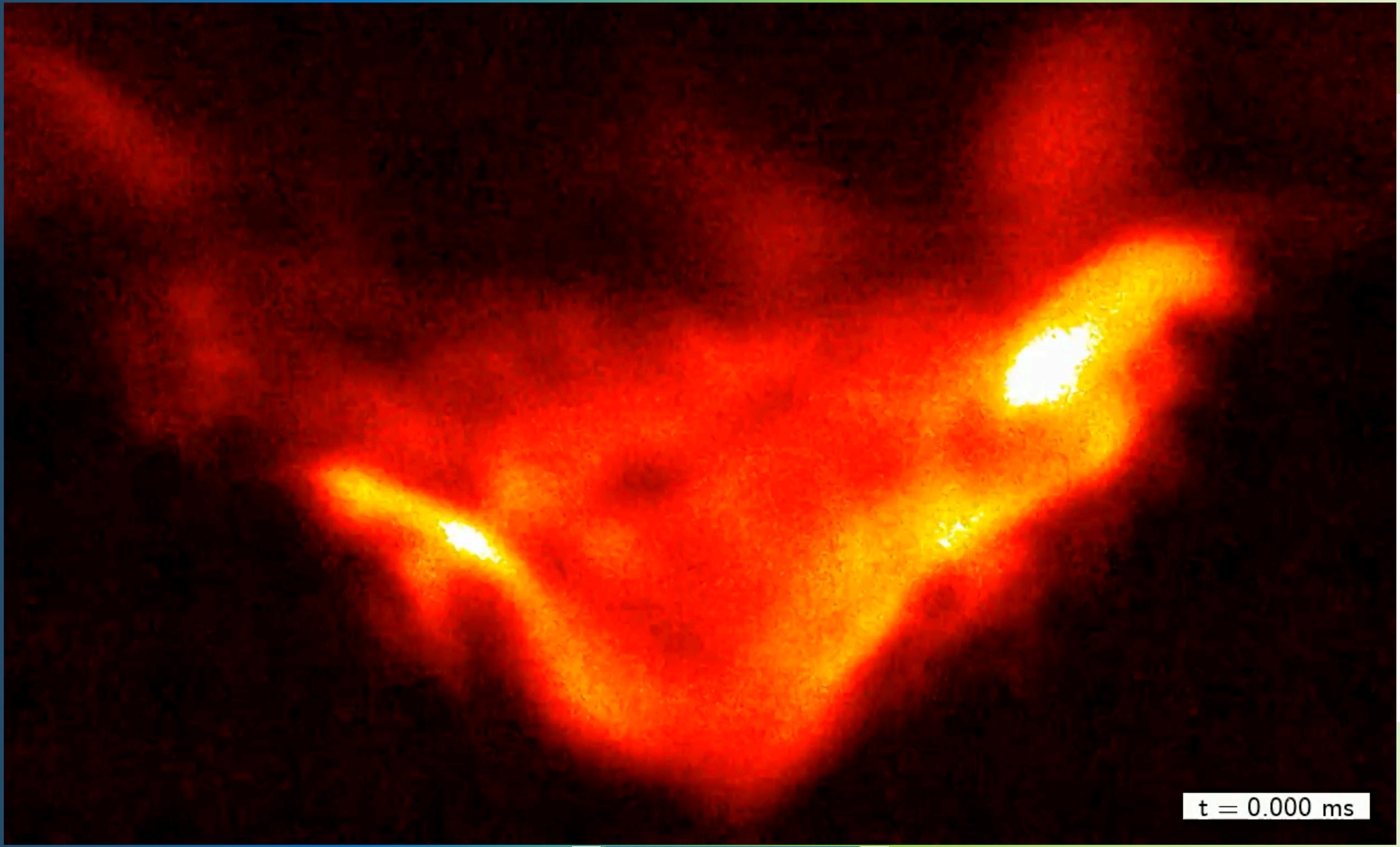
BUT…

Let us look at the transition from lifted to attached flame. Can do it experimentally and numerically

Experiment (real time)

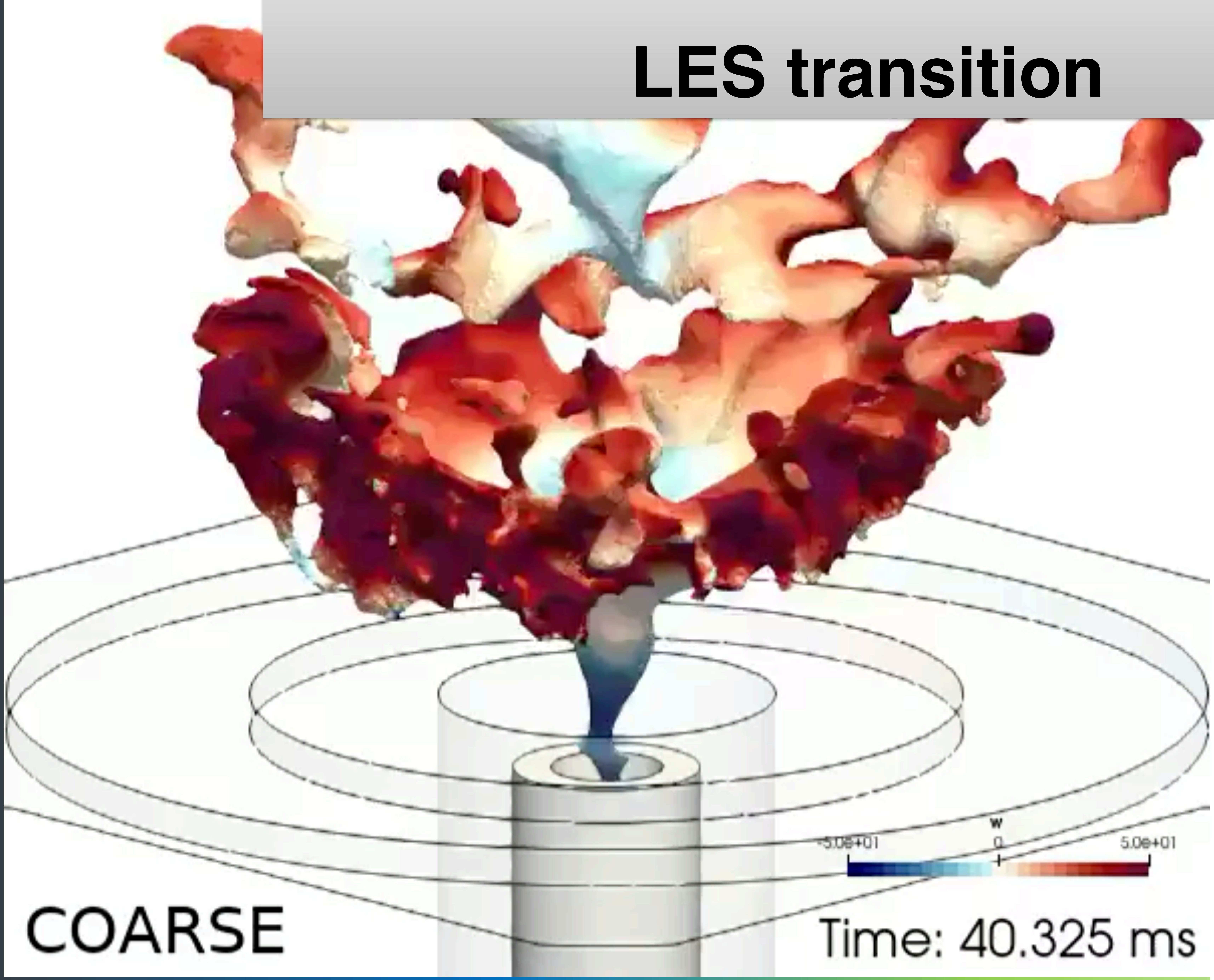


Experiment (16 kHz camera)



AIR H2 AIR

LES transition



C. Perez Arroyo

The dangerous question

A typical ‘aerodynamics post doc ‘ question:

Does this transition depend on the mesh of the swirler ?

SIMPLE TEST: refine the swirler mesh only and not the flame zone…

C. Perez Arroyo

3 TURBULENT COMBUSTION MODEL

TFLES with or without Takeno switch :

- AVBP (CERFACS)
- CONVERGE (IFPEN)
- FLUENT (UNIFI)
- FLUENT (ERGON)
- ProLB (M2P2)
- OPENFOAM (POLIMI)

FGM:

- STARCCM (LOUGHBOROUGH)

F TACLES with diffusion flamelets:

- YALES2 (CORIA, EM2C, ST)

PDF models:

- OPENFOAM (UCAM)
- BOFFIN (IMPERIAL COLLEGE)

No model at all:

- FLUENT (ANSYS)
- CONVERGE (CSI)

3 TURBULENT COMBUSTION MODEL

- Why no model at all ?

Good reasons for this:

- we don’t have a clear single model which can do premixed and diffusion at the same time. Might as well use finite rate chemistry (except we know it is wrong)
- pressure is low so maybe we are not so far from DNS -> we ll come back to this

4 - DO WE NEED TO WORRY ABOUT TRANSITION FROM LIFTED TO ANCHORED ?

Flames A and L are far from the exact conditions where the transition lifted-to-anchored occurs.

There can also be hysteresis there.

- Are we interested in capturing this transition precisely ?

- Can we do this without Conjugate Heat Transfer to know the lip temperature ?

5 - ARE OUR CHEMICAL SCHEMES SUFFICIENT ?

Schemes used yesterday:

- San Diego
- Burke
- C3 reduced to 10 species
- Boivin

5’ - ARE OUR TRANSPORT MODELS SUFFICIENT ?

Many groups use multicomponent transport models for D_k, λ, μ
In practice this is an overkill in most LES because in our codes, we never use:

D_k, λ, μ

but

Not an issue for LES: results dont change
Still: important for DNS !

D_k -

where the turbulent diffusivities D_k^t, λ^t, μ^t are both:

- VERY LARGE compared to the laminar values
- VERY WRONG: these are models for turbulent transport

$$\overline{\rho}\widetilde{\mathbf{u}''\Theta''} = -\frac{\mu_t}{Sc_t}\frac{\partial\widetilde{\Theta}}{\partial x}$$

6 - WHAT ABOUT NOx AND TEMPERATURE

NOX was NOT considered yesterday

I guess we all agree to consider it in the future

But which one ? NO, NO2 ?

This will require a proper computation of the temperature field

This raises the question of the boundary conditions to give to the CFD groups:
1/ We measure the wall temperature and use it as boundary condition for CFD
OR
2/ We let the CFD groups do the full CHT of the whole setup

We will try to provide experimental data on NOx and temperature in HYLON PHASE 2

7 - WHAT ABOUT WALL TREATMENTS

Most solvers seen yesterday use inert walls.

AVBP uses a treatment called IFHC (Comb Flame 2024) described tuesday: we still believe something must be done at the walls.

PS: note that if you use a tabulated method, you probably escape from this problem…

8 - HIGH PRESSURES

Let us go now from 1 to 20 bar.
At 1 bar, we picked a smallest mesh size between 100 and 250 micrometers and created a mesh

This choice was not guided by physics: we only did what we could…

Now, at 1 bar, the flame thickness or the triple flame thickness was 400 microns. So with the mesh we created, we are almost good: 4 points in the flame.
THIS IS A NICE COINCIDENCE. DONT TAKE IT FOR GRANTED…

Tomorrow, at 20 bar, the flame thickness will be 30 microns: no-one will use 30 microns meshes in 3D. Brute force approach will fail. Mesh Refinement will not do it -> ???

We will need LES models.

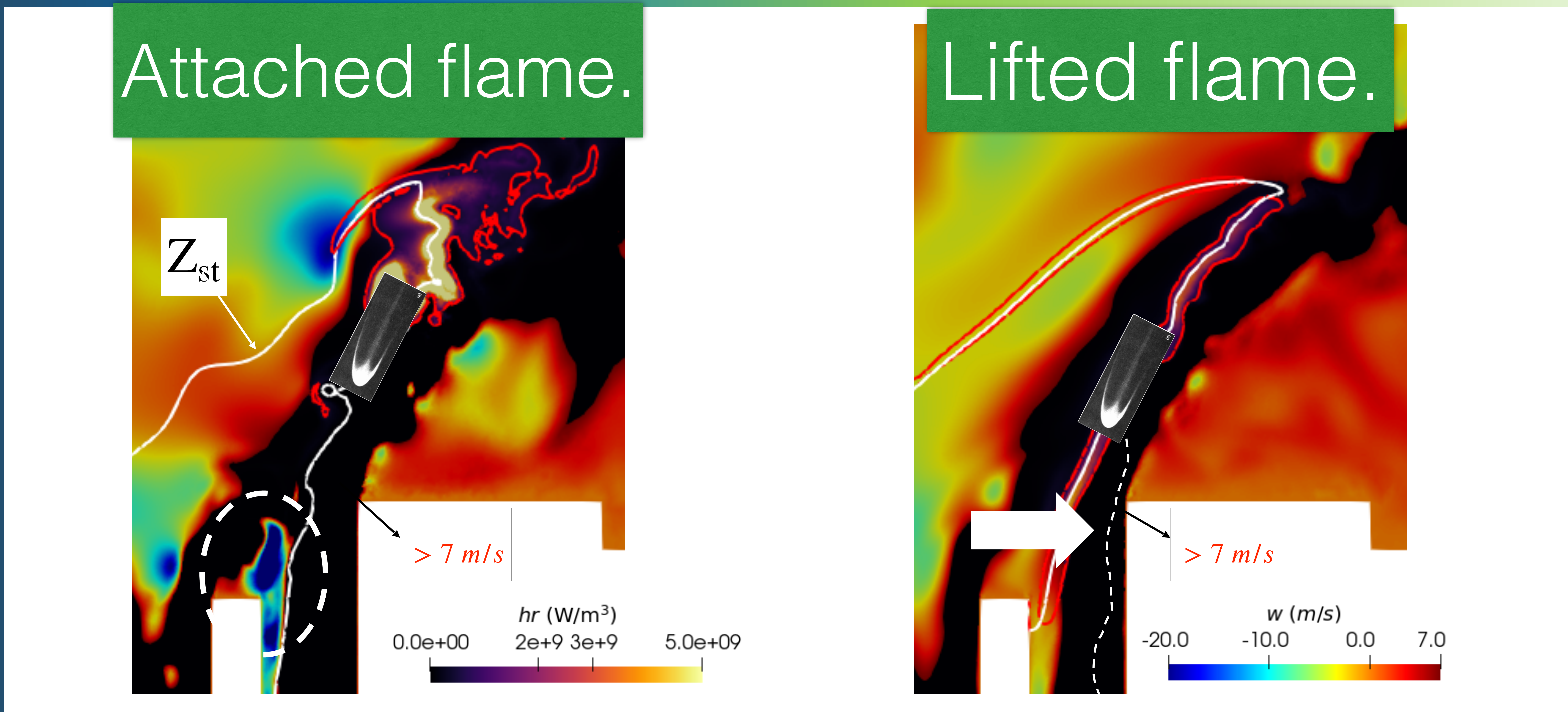
What should we do on the science side to make sure that the CFD codes will still work ?

8 - HIGH PRESSURES

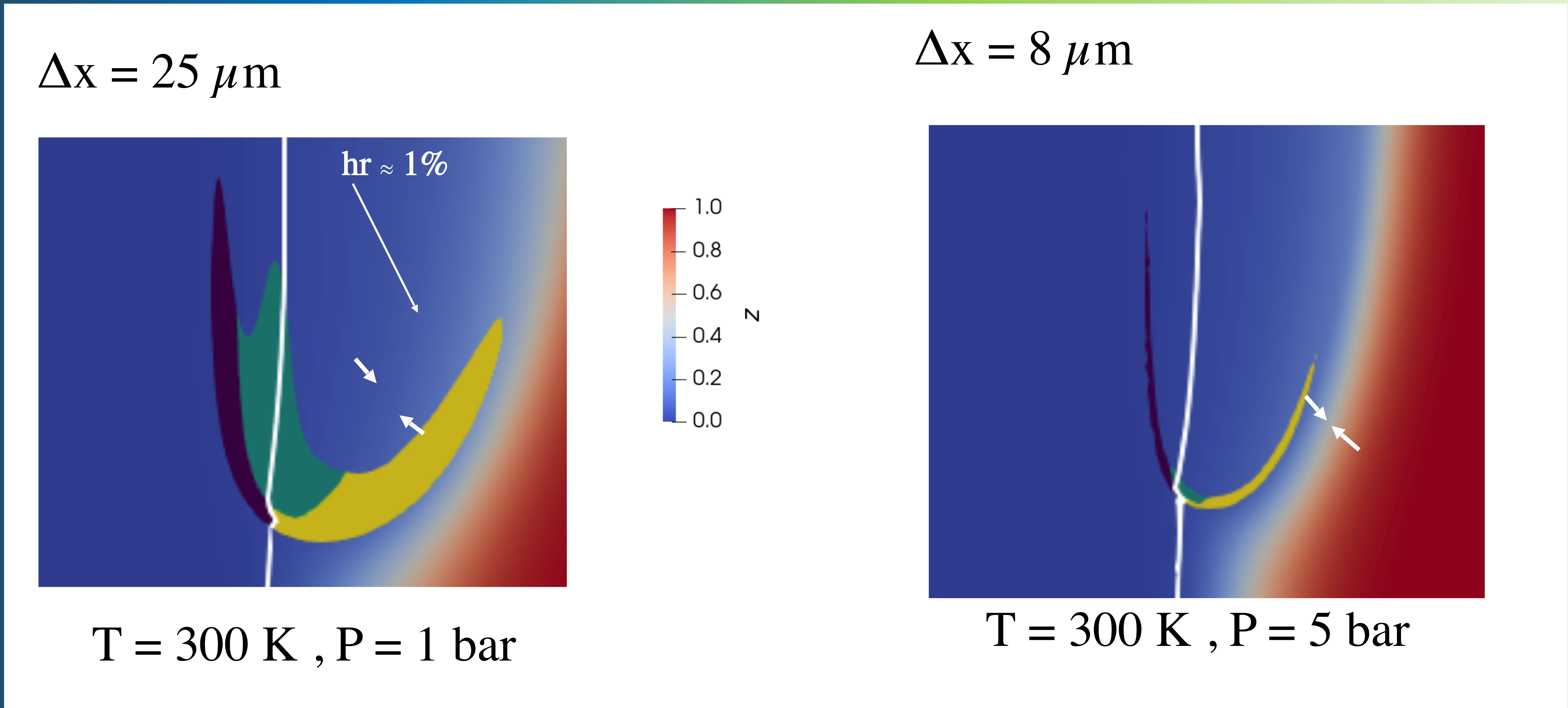
1/ NEAR THE INJECTOR LIPS: CAN WE DO IT ?

2/ IN THE FAR FIELD: SAME ISSUE

1/ NEAR THE INJECTOR LIPS:



DNS cant go to high pressures even in 2D…



Aniello's unpublished results

2/ IN THE FAR FIELD: SAME ISSUE

A sneak preview of what your LES will look like at high pressure…

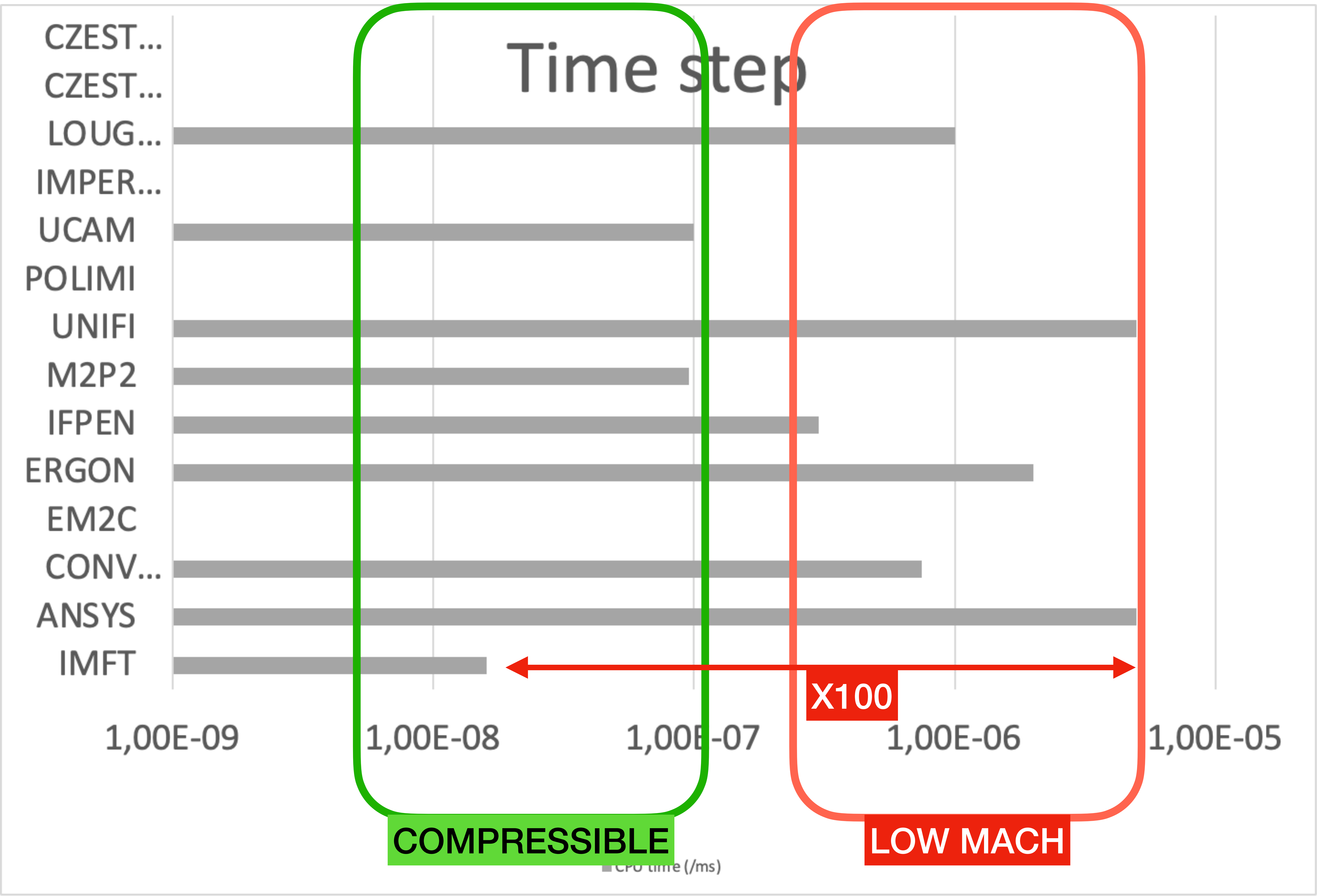
HERE WE HAD TO USE TFLES AND THE THICKENING FACTOR WENT UP TO … 50

SHORT CONCLUSION: WE HAD AN EASY TRIP AT 1 BAR. THE JOURNEY WILL BE MUCH HARDER AT HIGH PRESSURES AND WILL REQUIRE MODELS AND NOT BRUTE FORCE ONLY

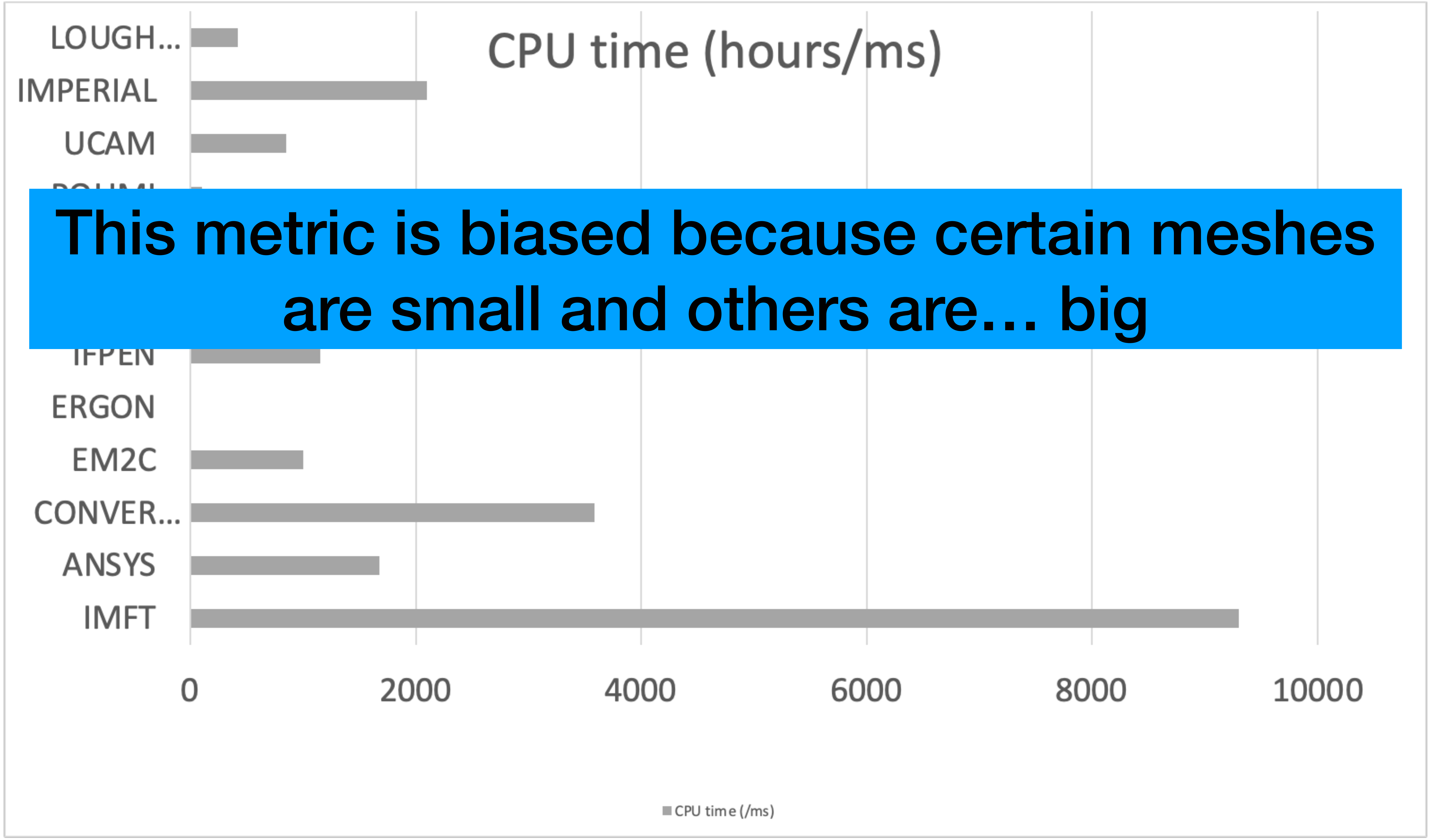
9 - CPU TIMES

Noone really tried hard to use all possible options to optimize CPU time
Everyone used a different mesh so that comparisons are also difficult
Do we want to focus on this issue now for the next round of comparisons of HYLON PHASE 1?
Let us look at orders of magnitude…

9 - CPU TIMES: time steps are vastly different !

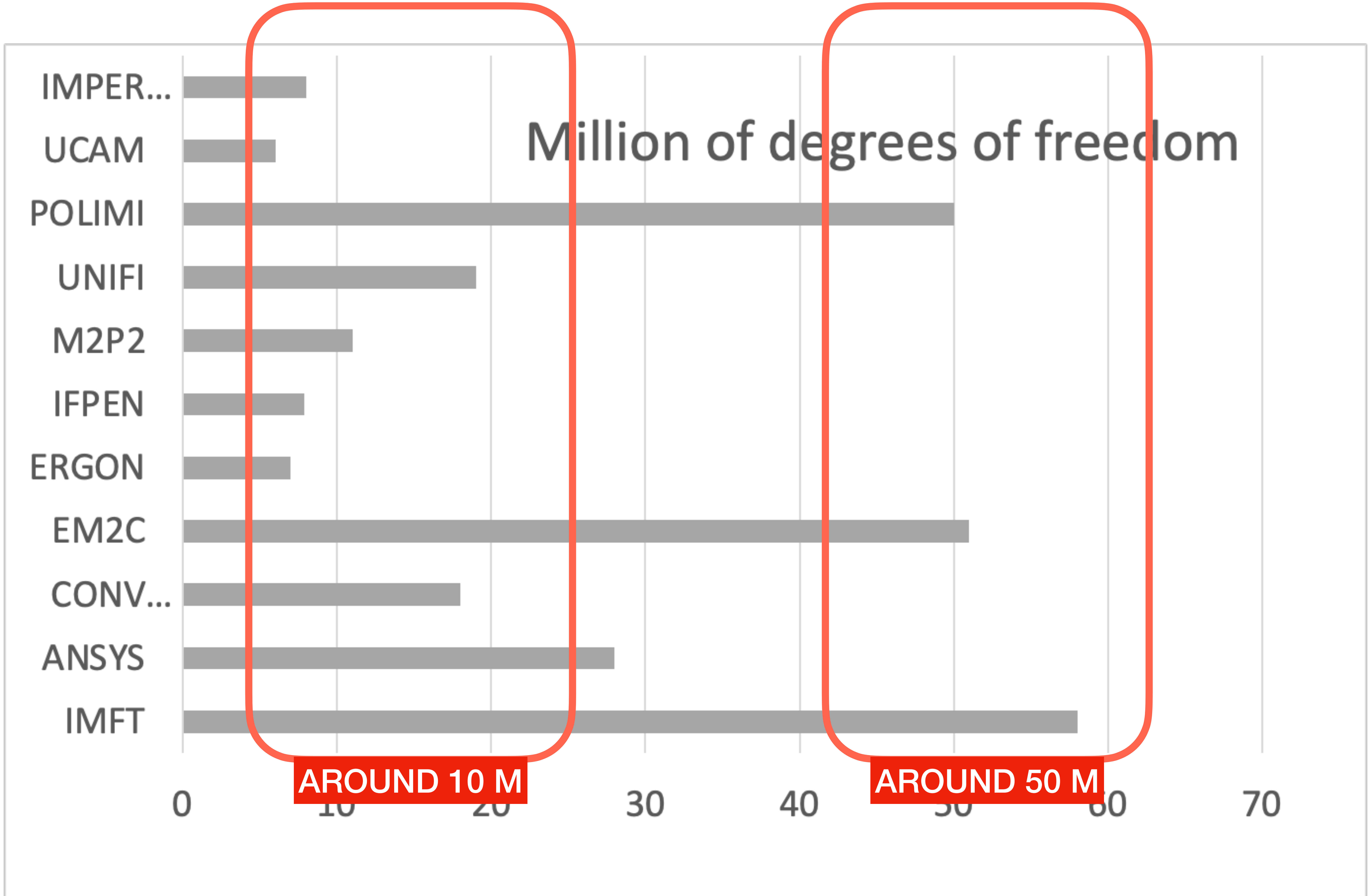


9 - CPU TIMES: CPU hours for one ms of physical time in HYLON

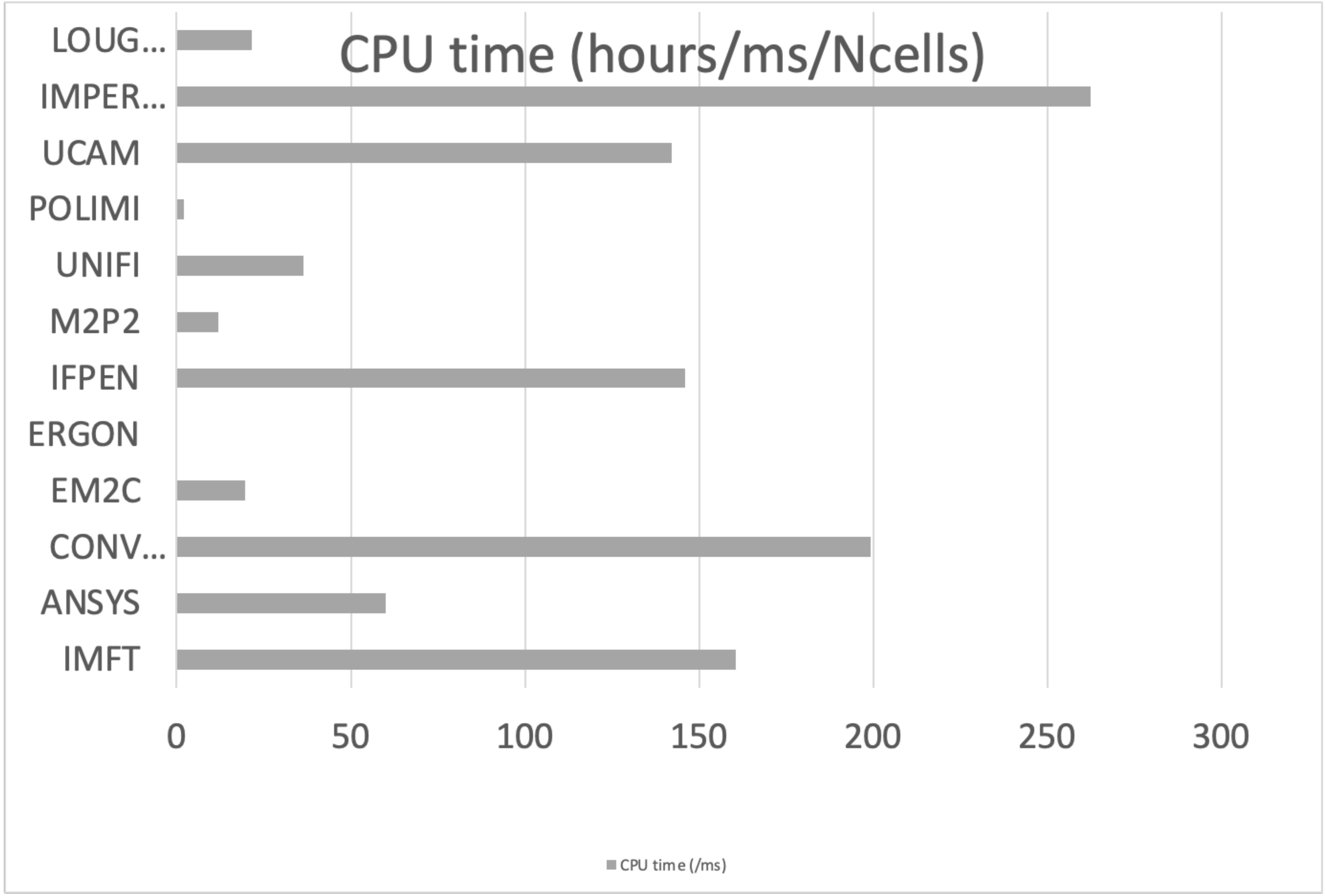


This metric is biased because certain meshes are small and others are… big

9 - CPU TIMES: Mesh sizes



9 - CPU TIMES: CPU hours for one ms of physical time in HYLON per million cells



9 - CPU TIMES: a summary -
you have what you pay for

COLD FLOW → LOW MACH REACTING FLOW → COMPRESSIBLE REACTING FLOW

CPU Hours per ms per million dof

M2P2
POLIMI

X3 to X10 →

EM2C
ANSYS
UCAM
IFPEN
UNIFI
LOUGHB.

X2 to X5 →

AVBP
CONVERGE
IMPERIAL COLLEGE