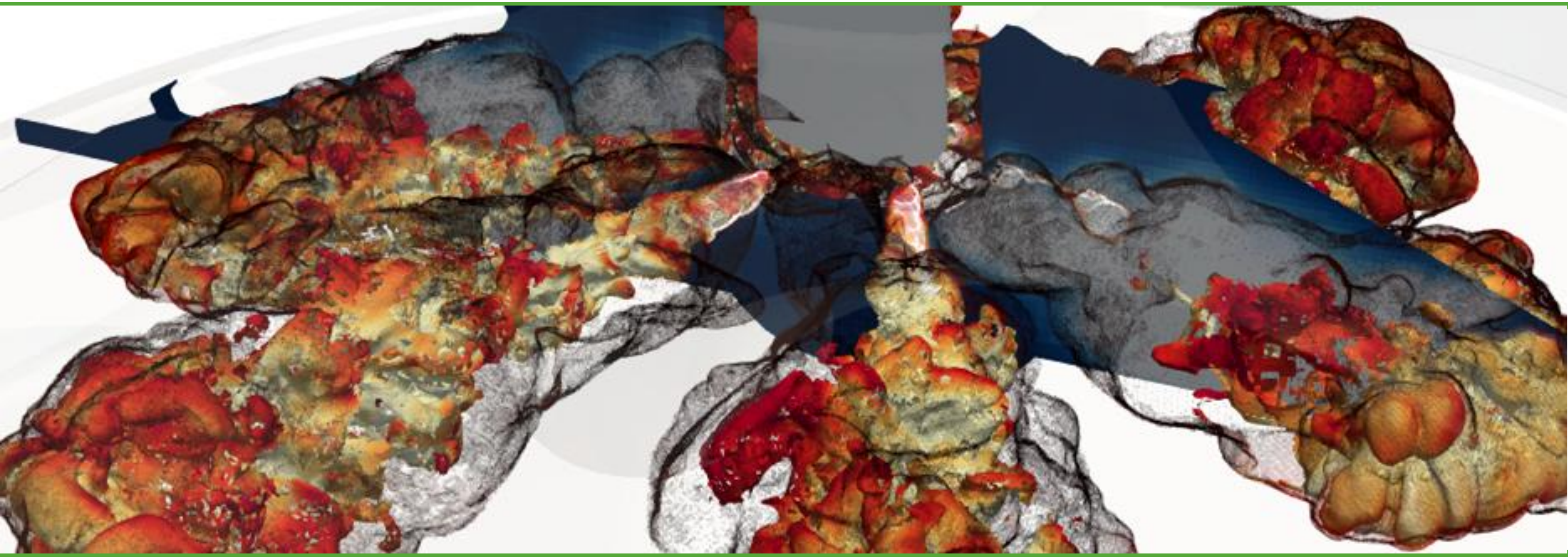

SEMINAR

CFD SIMULATION OF REACTIVE FLOWS: BRIDGING FUNDAMENTAL RESEARCH AND INDUSTRIAL APPLICATIONS

J. Gómez Soriano (jogoso1@mot.upv.es)

CMT – Clean Mobility & Thermofluids - Universitat Politècnica de València

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Clean Mobility & Thermofluids

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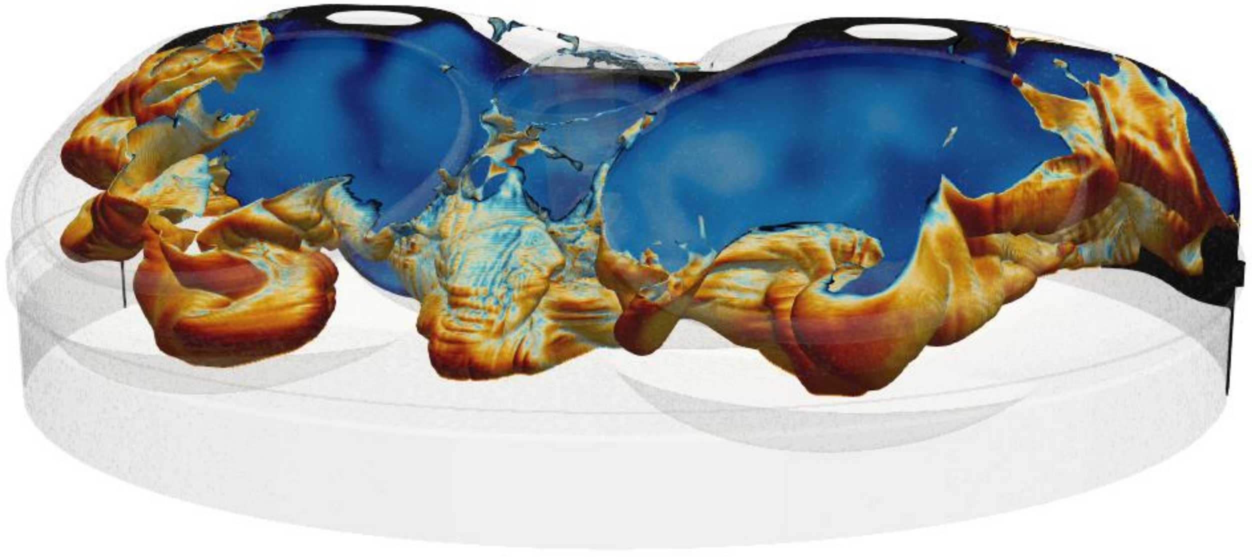

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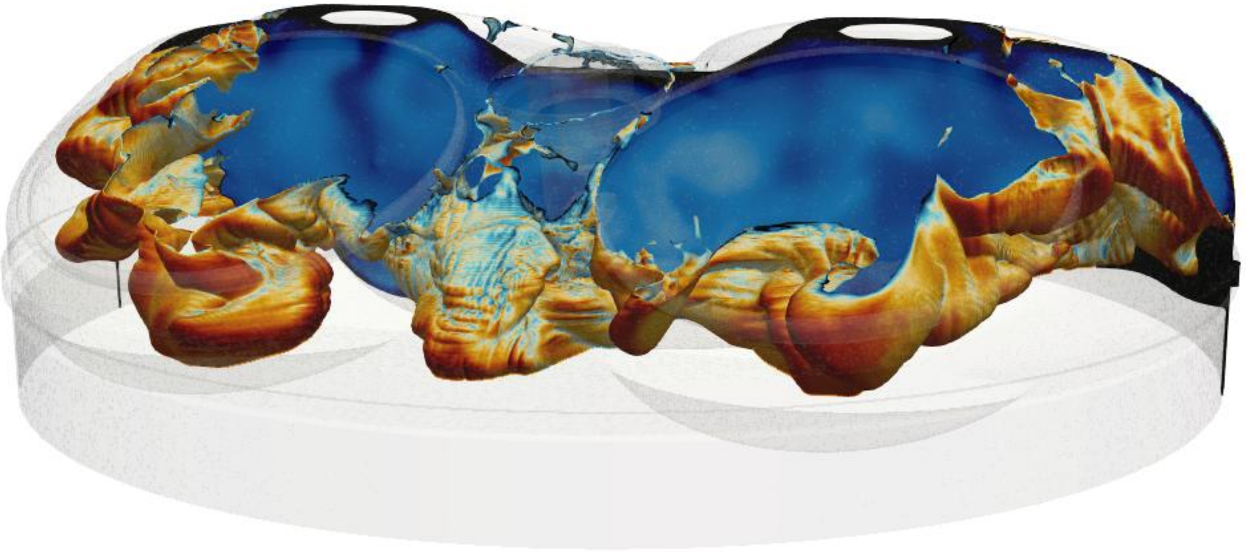
  - URANS of hydrogen combustion
  - URANS/LES of hydrogen injection
  - LES for combustion noise source characterization
- **CFD for applied research**
  - LES for optimization of pre-chamber ignition systems
  - URANS coupled with optimization techniques



INTRODUCTION

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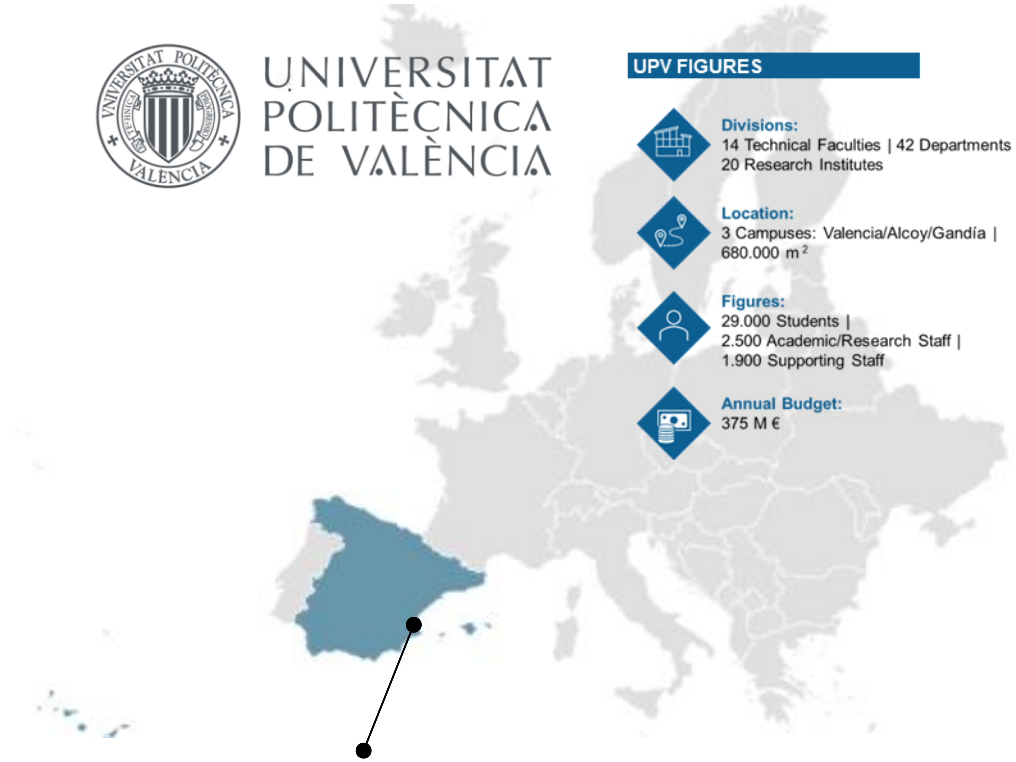

Clean Mobility & Thermofluids

STAFF

60	25	70
Faculty / Researchers	Testing Engineers	MSc and PhD Students

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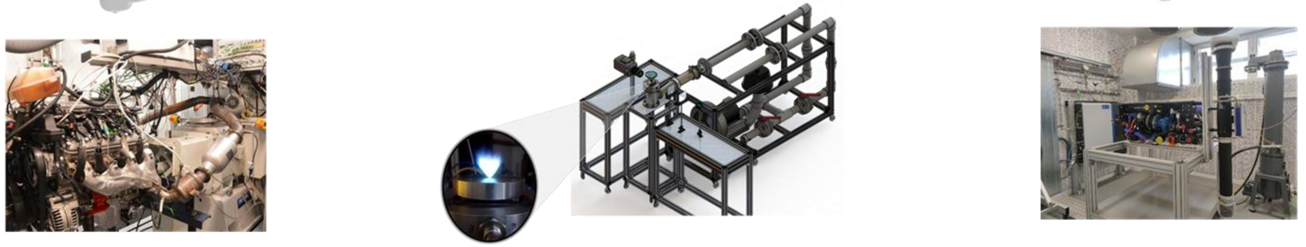
Clean Mobility & Thermofluids

Key experimental environment



Target application

ICE	GT	FC
Transportation (road & marine) Power generation	Transportation (aero) Power generation	Transportation (road & aero) Power generation

Research Institute R+D+i

⇕

University Advanced Training

→

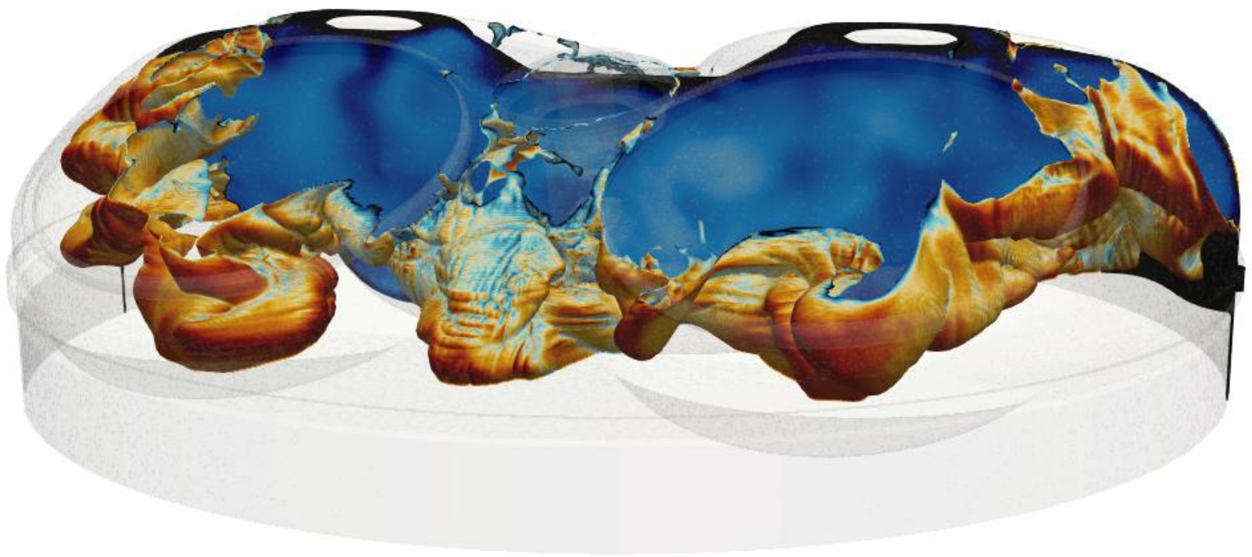
ICE

GT

FC

- Basic knowledge generation
- Systems analysis and evaluation
- Systems integration and optimization
- Final solution evaluation (LCA/TCO)
- Knowledge transfer to industry & society

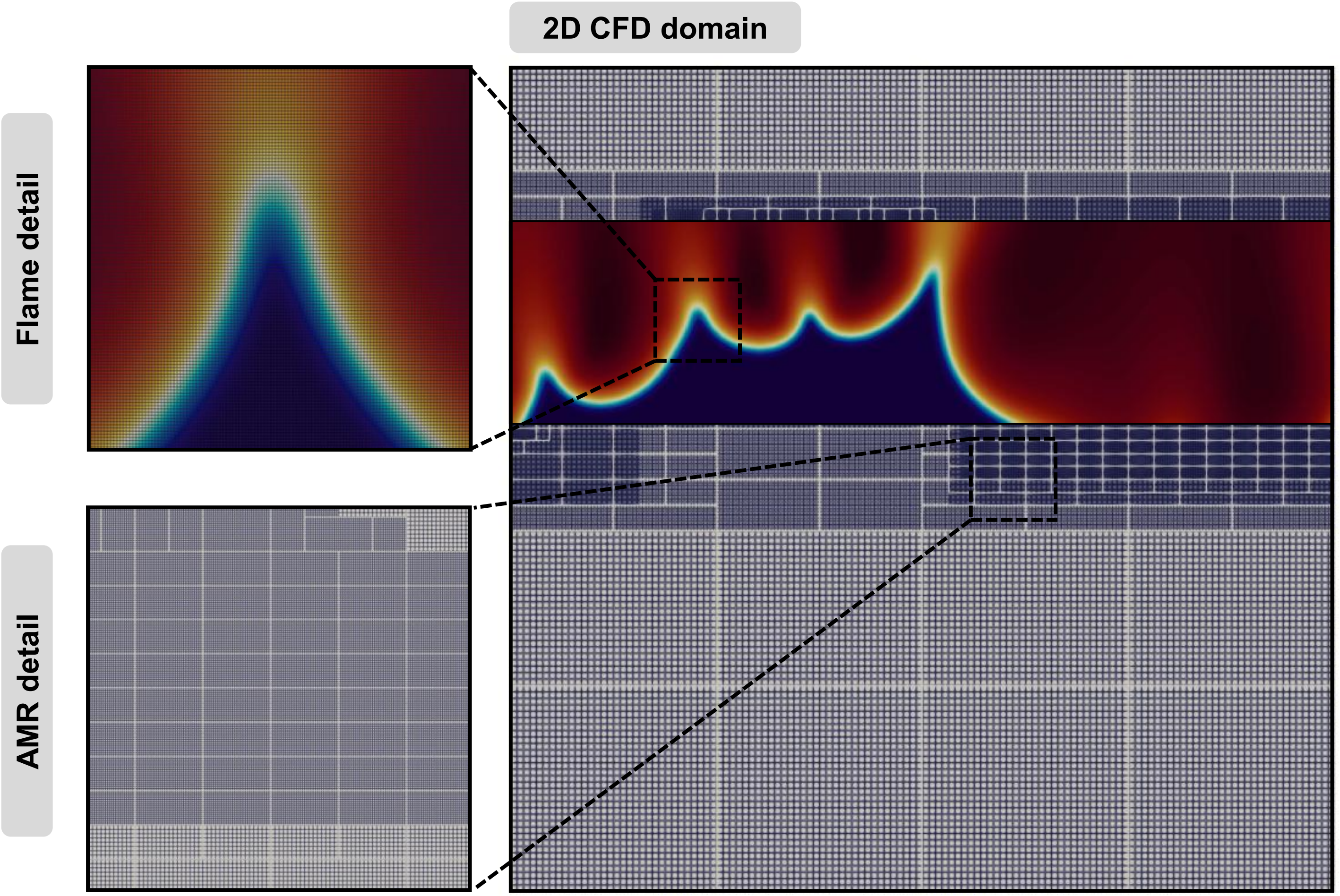
CONTENTS



CFD FOR FUNDAMENTAL UNDERSTANDING

DNS of unstable hydrogen flames

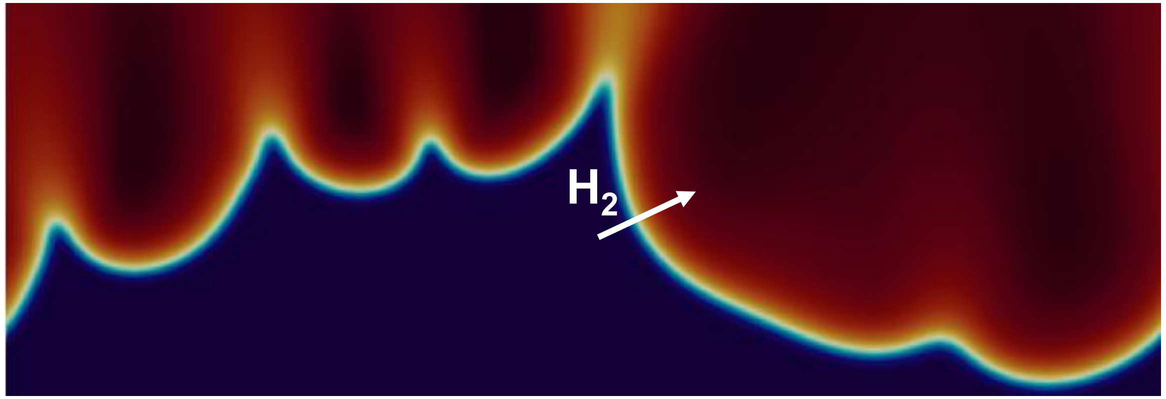
- Problem definition
  - Lean hydrogen flame
    - T_u = 298 K
    - p = 1 bar
    - φ = 0.5
  - Lewis number (α/D) < 1
  - Laminar conditions (Re↓↓)
- Case setup
  - 2D DNS with AMR
  - Detailed chemical kinetics
  - Domain size:
    - 60 x l_F (18x18 mm)
    - Base cell size: 140 μm
    - ~1 million total cell count
  - Minimum cell size:
    - 17.5 μm
    - ~25 cells within thermal flame thickness (l_F)

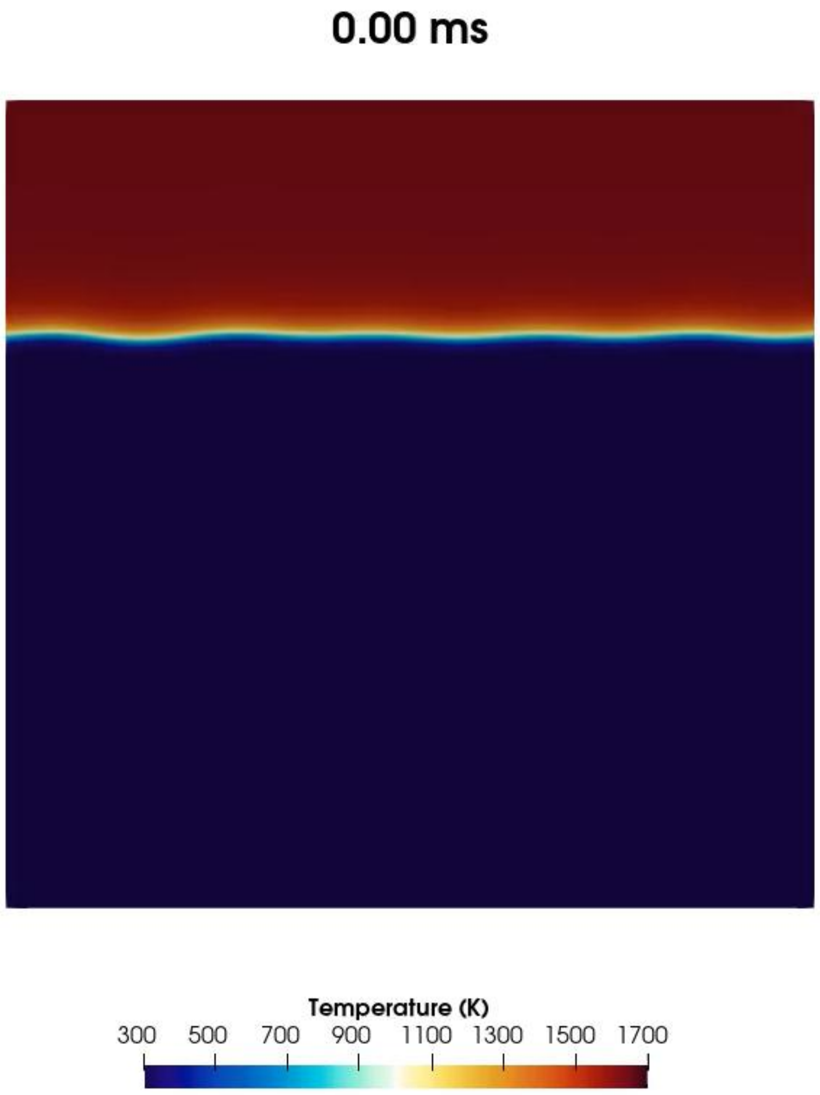


CFD FOR FUNDAMENTAL UNDERSTANDING

DNS of unstable hydrogen flames

- HPC resources
  - UPV cluster (Sirius)
  - GPU (NVIDIA HGX H100)
  - Return time: ~2 weeks
- Thermo-diffusive instabilities characterization
  - Caused by high mobility of H_2 molecules
  - Effective flame velocity increased (~ x 2)
  - Wavelength of flame perturbations (~ 6 x l_F)





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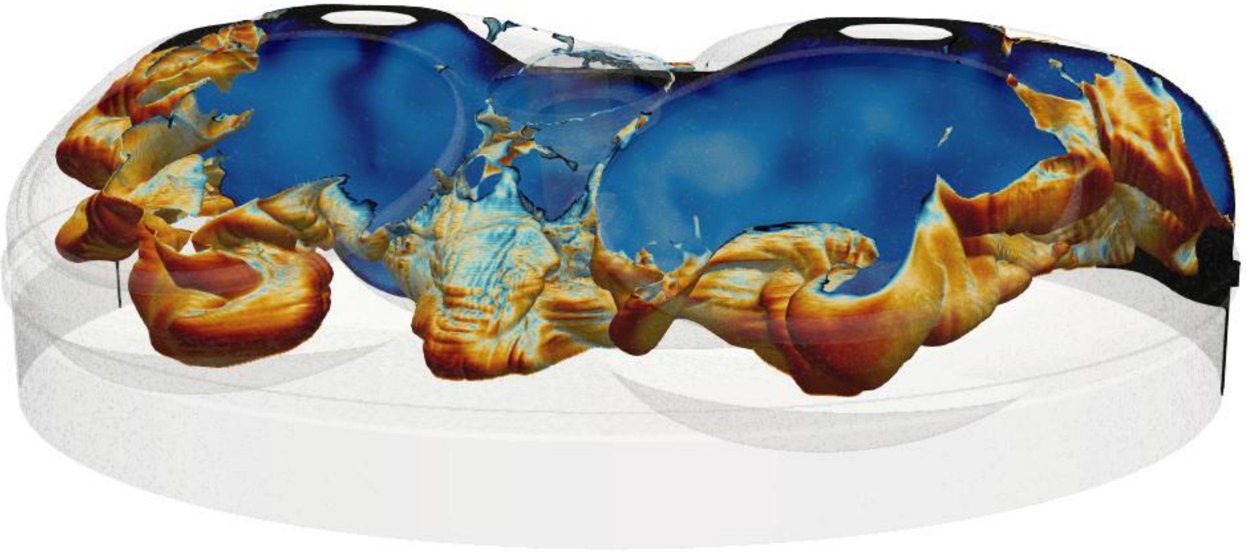
  - LES for optimization of pre-chamber ignition systems
  - URANS coupled with optimization techniques

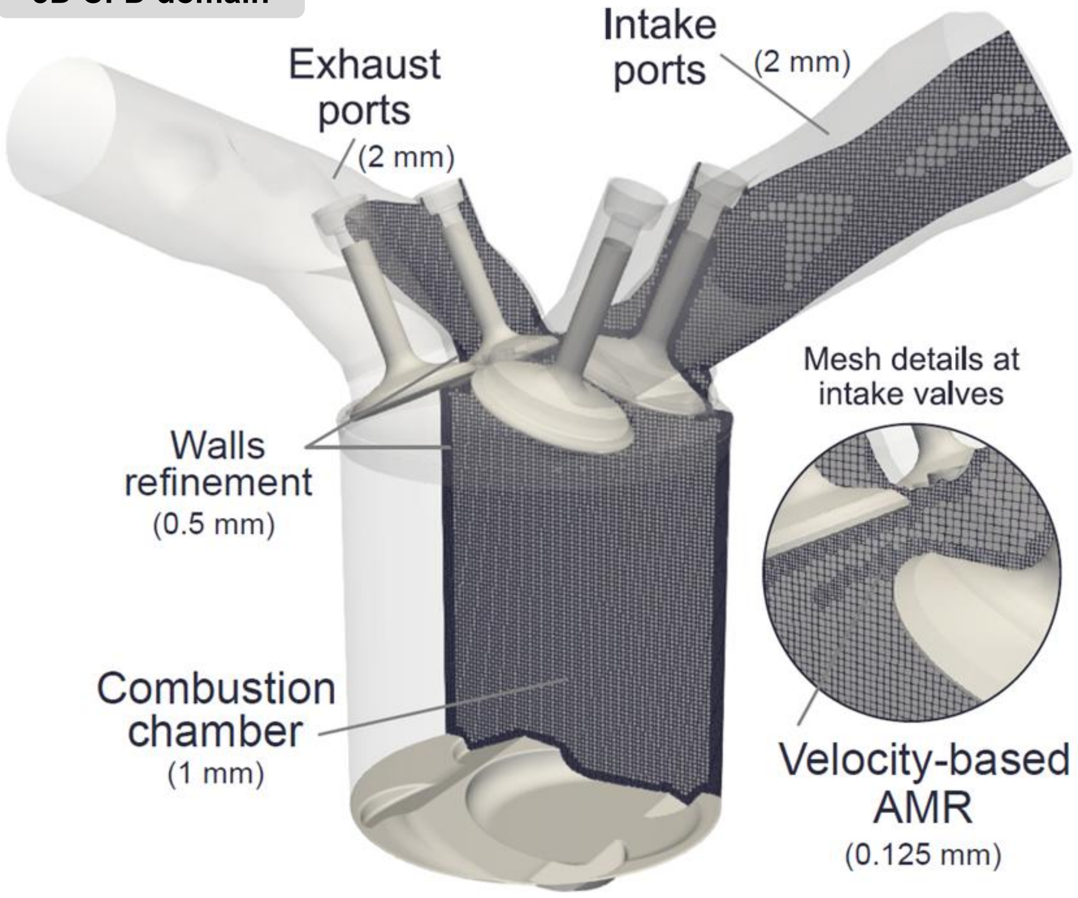


CFD FOR FUNDAMENTAL UNDERSTANDING

URANS of hydrogen combustion: from DNS to URANS models

- Thermo-diffusive instabilities characterization from DNS
  - New H_2 combustion models: development and implementation
- Numerical model setup
  - CONVERGE v3.0.28
  - Turbulence modeling: URANS, RNG k-ε
  - Cell sizes
    - AMR: Velocity (0.125 mm), Temperature (0.125 mm)
    - Spark embedding: 0.0625 mm around the spark
    - Total cell count: varied between 1 and 5 million
  - Specific sub-models/features
    - G-Equation + SAGE (in/on/out of the flame)
    - Tabulated laminar flame speed (s_L)
      - Corrected with **thermo-diffusive instabilities effects**
    - Chemical mechanism
      - Kéromnès et al. (10.1016/j.combustflame.2013.01.001)
    - Molecular diffusion modeling
      - Mixture averaged

3D CFD domain



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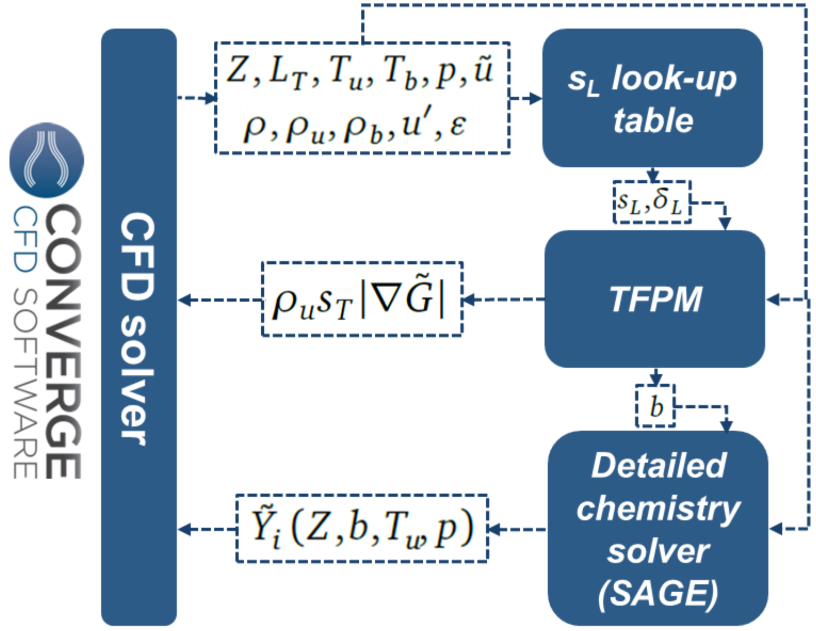
CFD FOR FUNDAMENTAL UNDERSTANDING

URANS of hydrogen combustion: from DNS to URANS models

- Thermo-diffusive instabilities characterization from DNS
  - New H_2 combustion models: development and implementation



$$\frac{\partial \rho \tilde{G}}{\partial t} + \nabla(\rho \tilde{u} \tilde{G}) = -\rho D_t \tilde{\kappa} |\nabla \tilde{G}| + \rho_u s_T |\nabla \tilde{G}|$$

Turbulent flame propagation

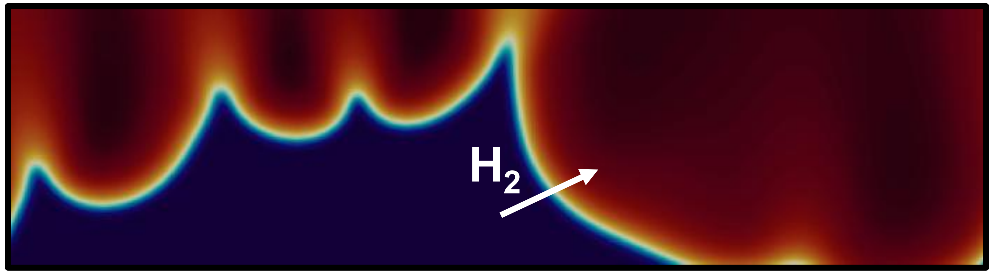
Peters' correlation

$$\frac{s_T}{s_L} = 1 - \frac{a_4 b_3^2}{2 b_1} \frac{L_T}{\delta_L} + \left[\left(\frac{a_4 b_3^2}{2 b_1} \frac{L_T}{\delta_L} \right)^2 + a_4 b_3^2 \frac{u'}{s_L} \frac{L_T}{\delta_L} \right]^{1/2}$$

Correction for thermo-diffusive instabilities

- A correction can be applied to the unstretched laminar flame speed

$$s_M = I_0 \cdot s_L \qquad I_0 = \begin{cases} \exp(0.08\omega_2) & \text{if } \Pi < \Pi_c, \\ 1 + 0.47\omega_2 & \text{otherwise.} \end{cases}$$

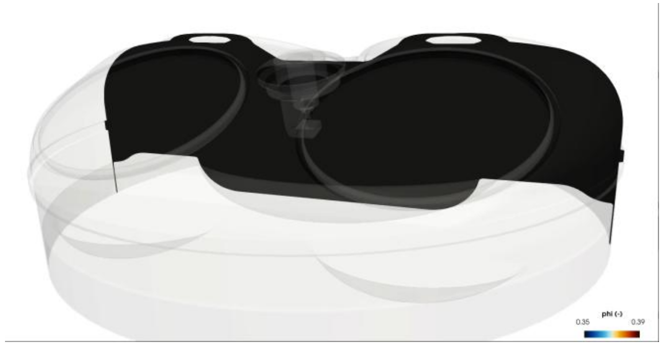


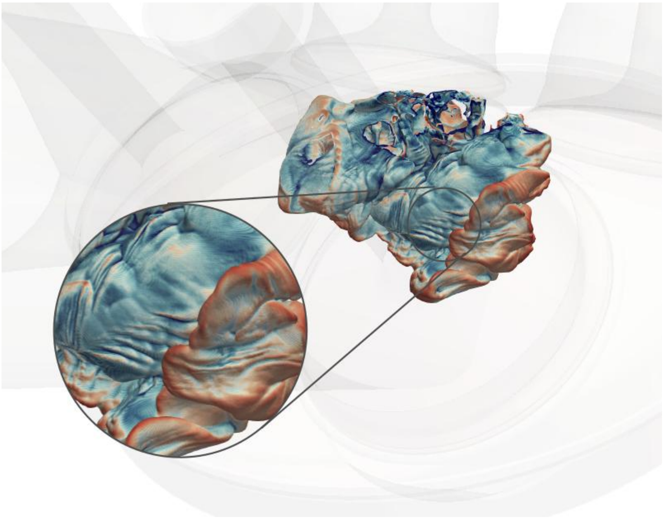
CFD FOR FUNDAMENTAL UNDERSTANDING

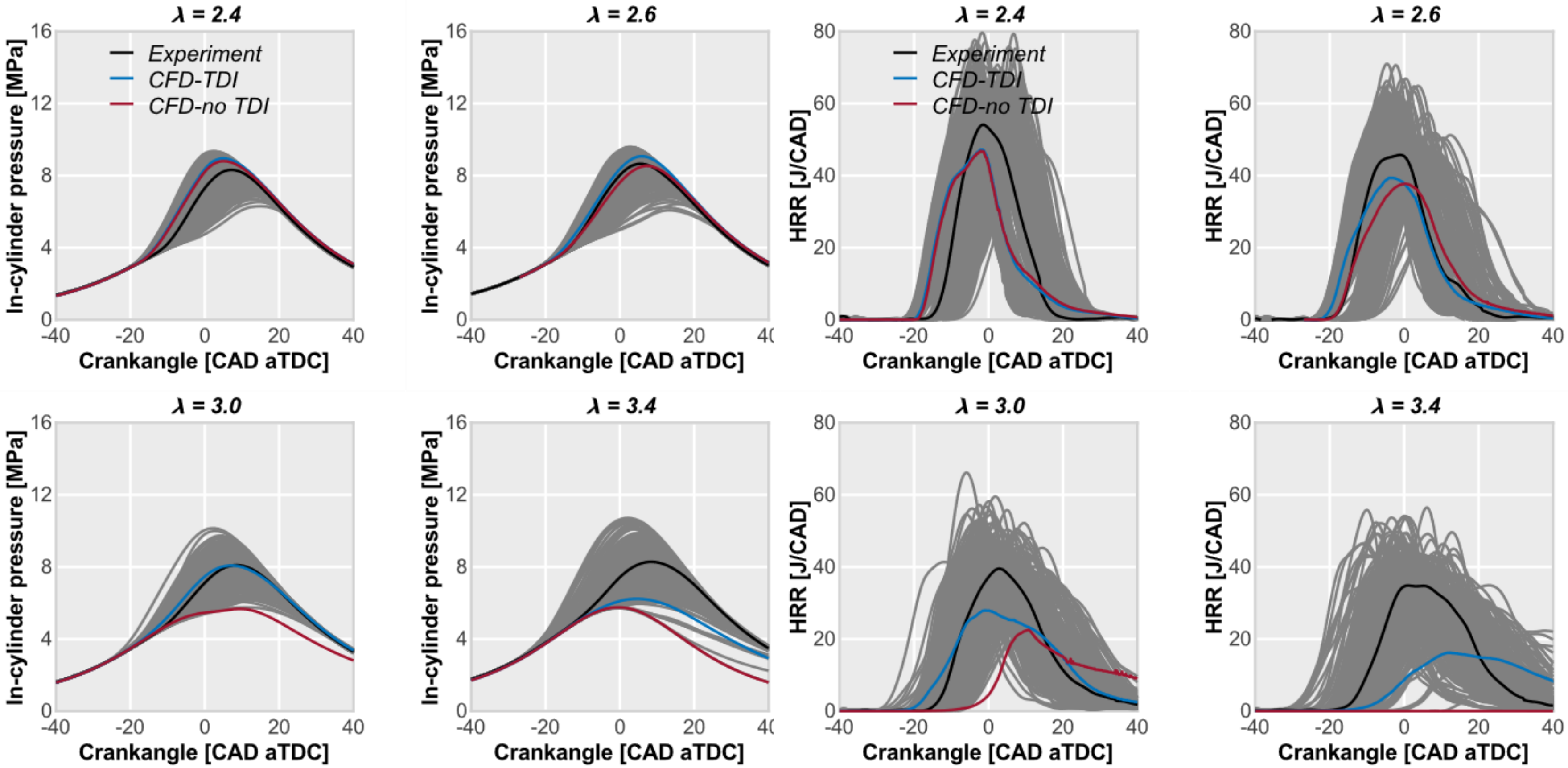
URANS of hydrogen combustion: from DNS to URANS models

- Validation: comparison with experimental results
  - ➢ In-cylinder pressure and HRR profiles

1500 rpm @ 8.5 bar of IMEP
4 dilution levels (λ)
Calibration case: **λ = 2.6**
Same constants are applied to all OP







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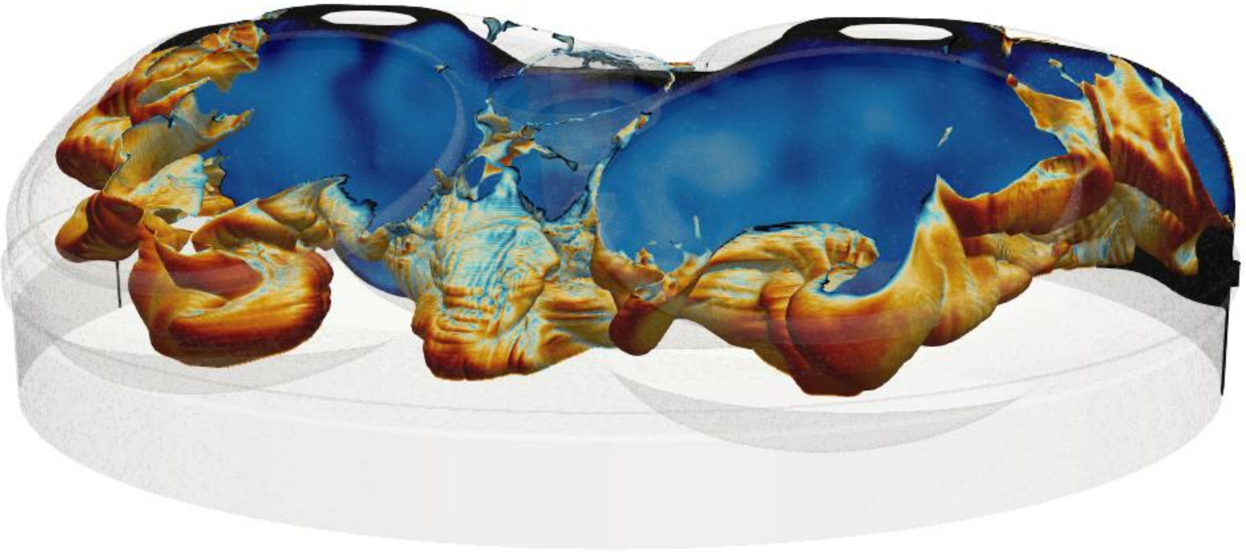
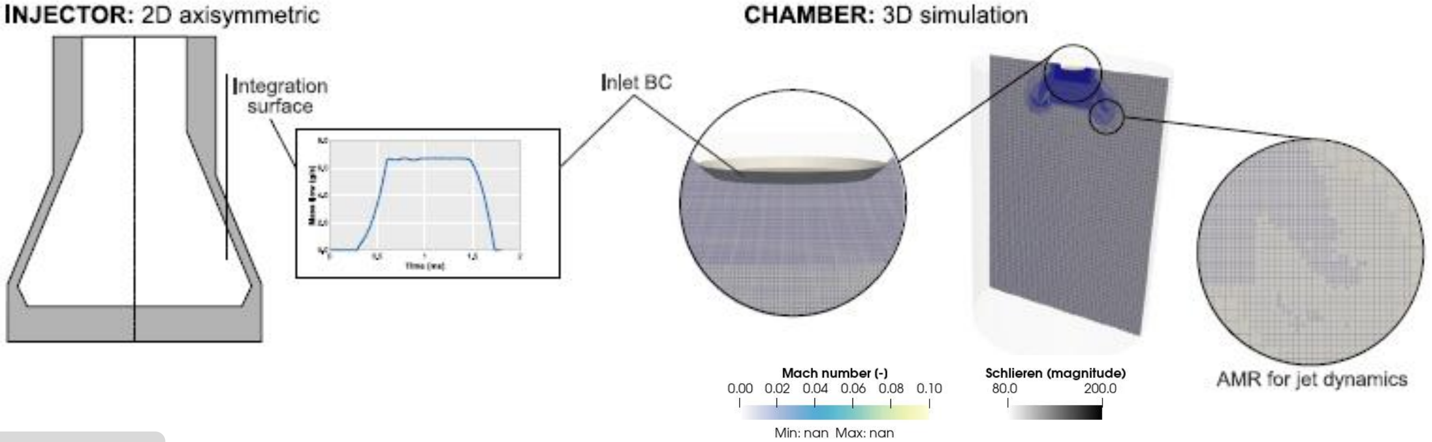
  - ➢ LES for combustion noise source characterization
- CFD for applied research
  - ➢ LES for optimization of pre-chamber ignition systems
  - ➢ URANS coupled with optimization techniques



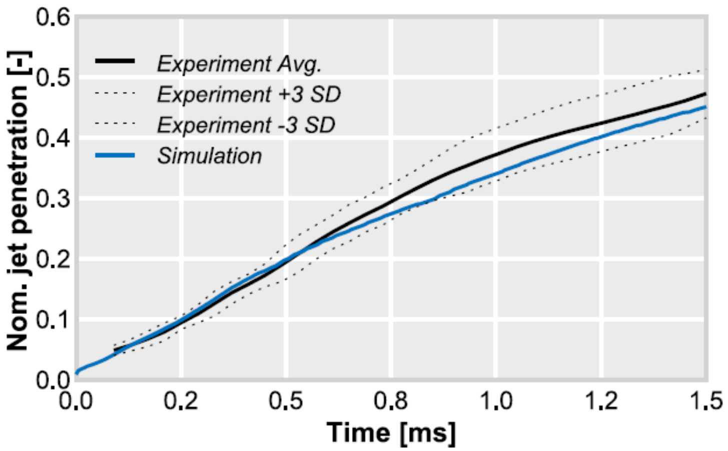
CFD FOR FUNDAMENTAL UNDERSTANDING

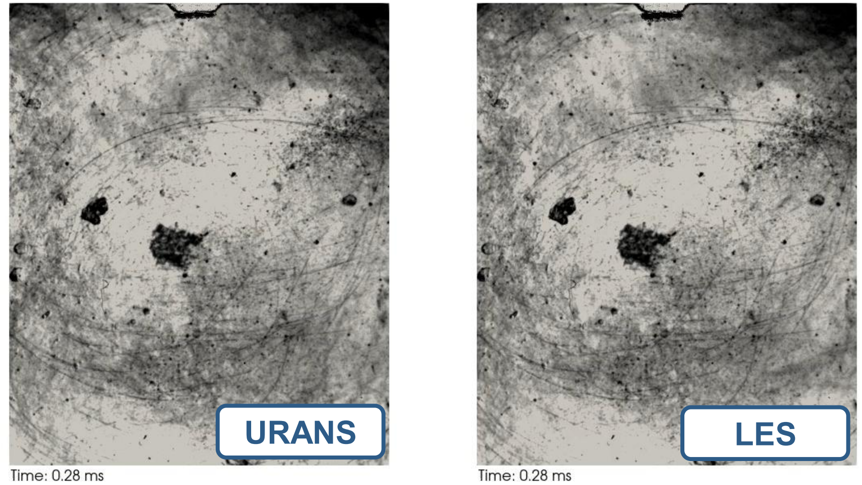
URANS/LES of hydrogen injection

- Modeling hydrogen injection under critical conditions
  - ➢ Combination of different modeling approaches

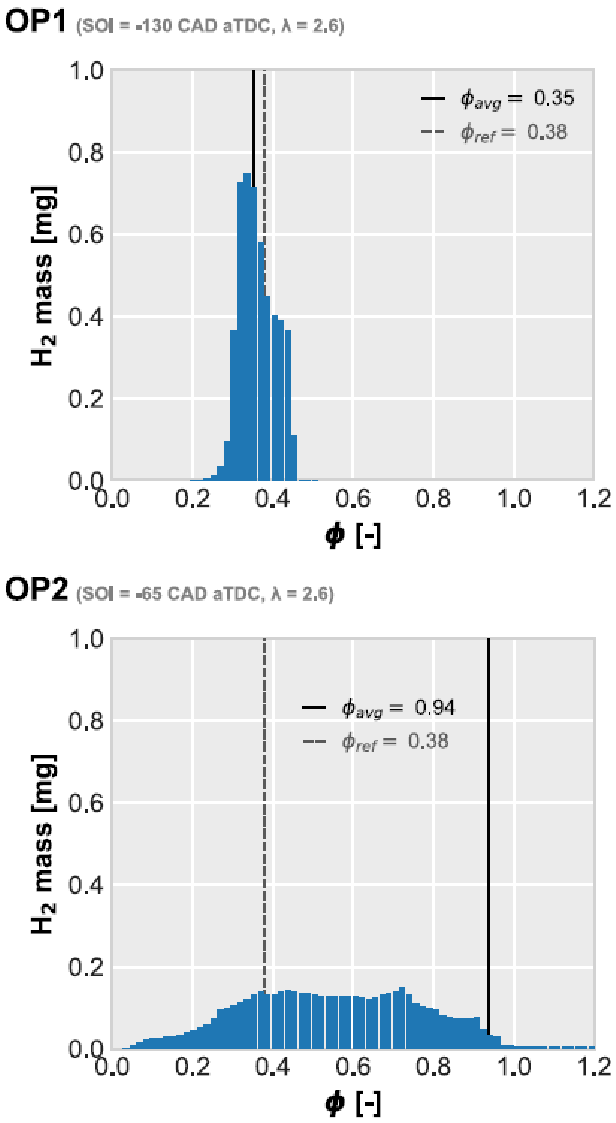


Validation





Results & distribution analysis



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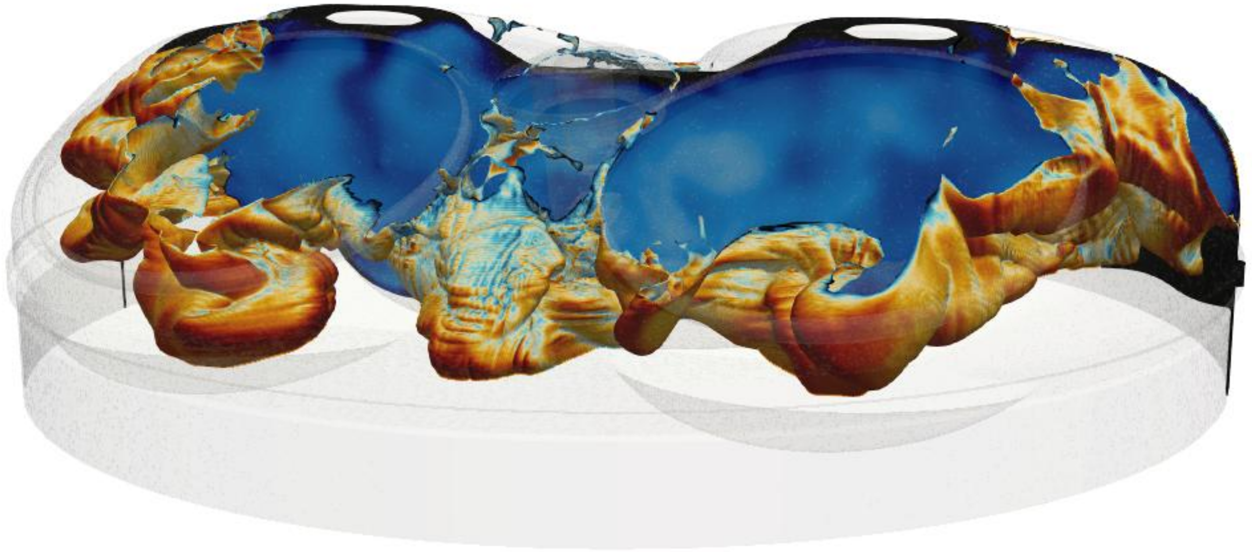
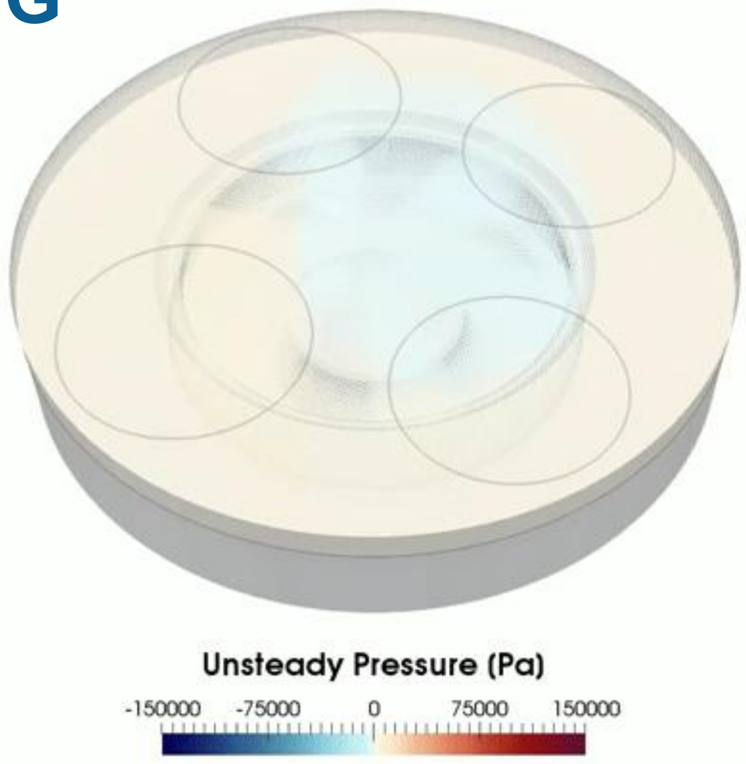
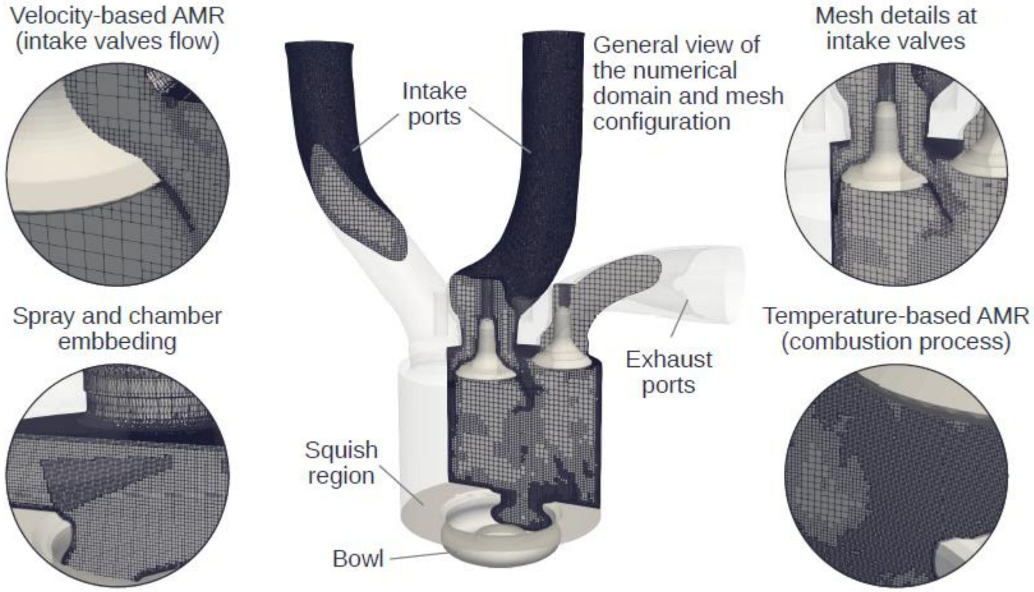


CFD FOR FUNDAMENTAL UNDERSTANDING

LES for combustion noise source characterization

- Problem definition
  - CC resonance in CI engines
  - Characterization of sources
  - Assessment of simulation complexity and cost
- Case setup
  - 3D LES/URANS with AMR
  - Detailed chemical kinetics



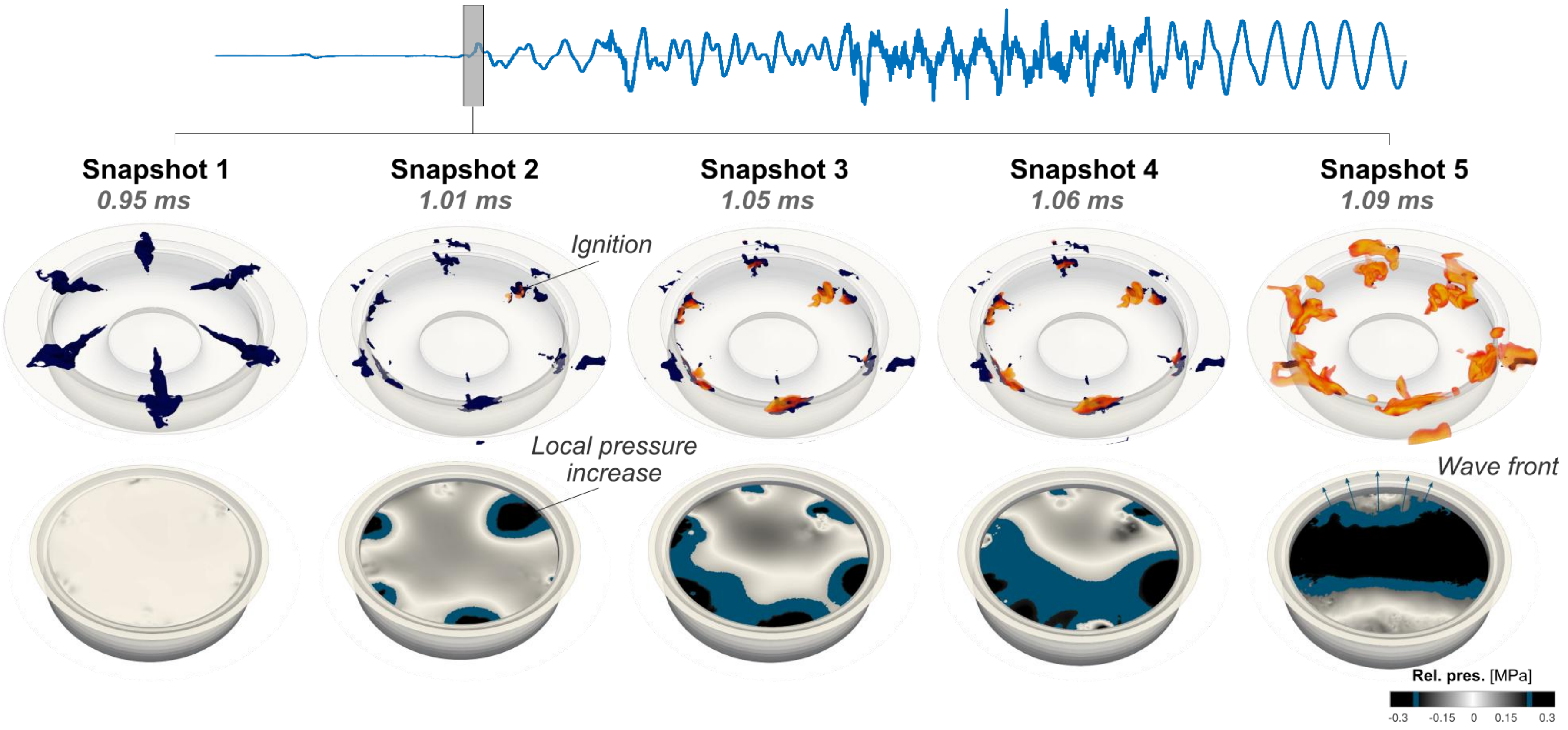


Configuration	URANS-Coarse[a]	URANS-Fine	LES
Domain		Full geometry[b]	
Base size	3 mm	3 mm	2.2 mm
Walls refinement	3 (0.375 mm)	3 (0.375 mm)	3 (0.275 mm)
Spray refinement	3 (0.375 mm)	3 (0.375 mm)	3 (0.275 mm)
Chamber refinement	2 (0.75 mm)	2 (0.75 mm)	2 (0.55 mm)
AMR	3 (0.375 mm)	4 (0.188 mm)	4 (0.138 mm)
Sonic CFL number		< 1	
Initialization		Non-uniform[c]	
Turbulence modelling	URANS RNG k-ϵ		Dynamic structure LES

CFD FOR FUNDAMENTAL UNDERSTANDING

LES for combustion noise source characterization

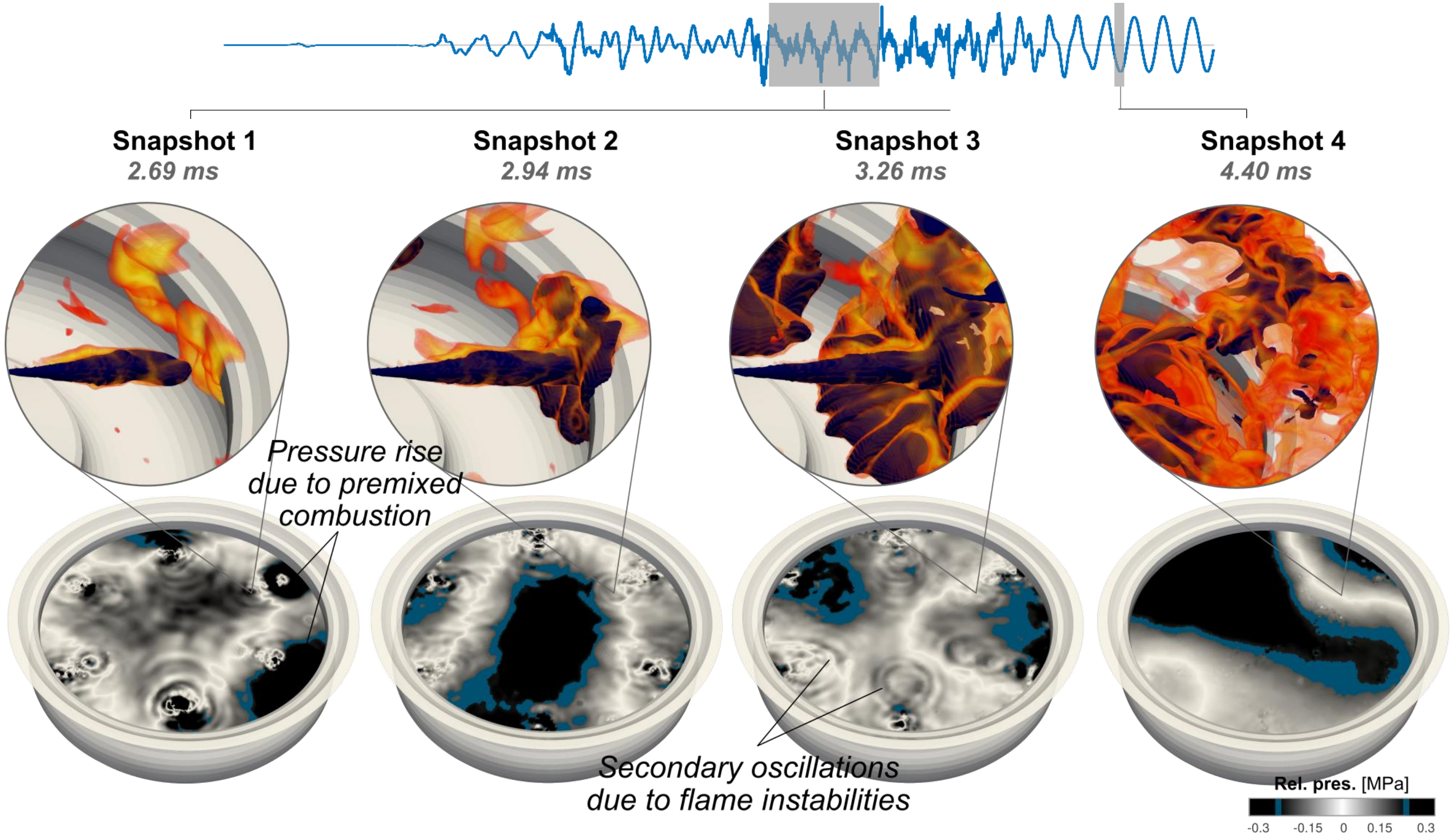
- Phenomenological analysis of combustion noise sources
  - Premixed combustion phase



CFD FOR FUNDAMENTAL UNDERSTANDING

LES for combustion noise source characterization

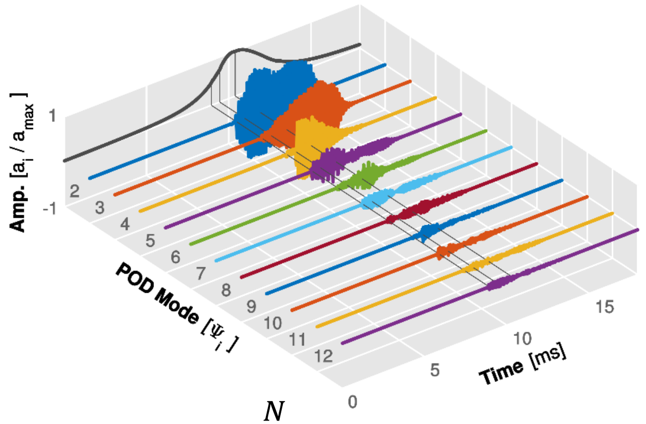
- Phenomenological analysis of combustion noise sources
  - Diffusive combustion phase

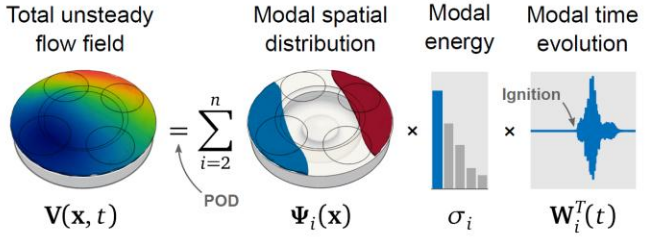


CFD FOR FUNDAMENTAL UNDERSTANDING

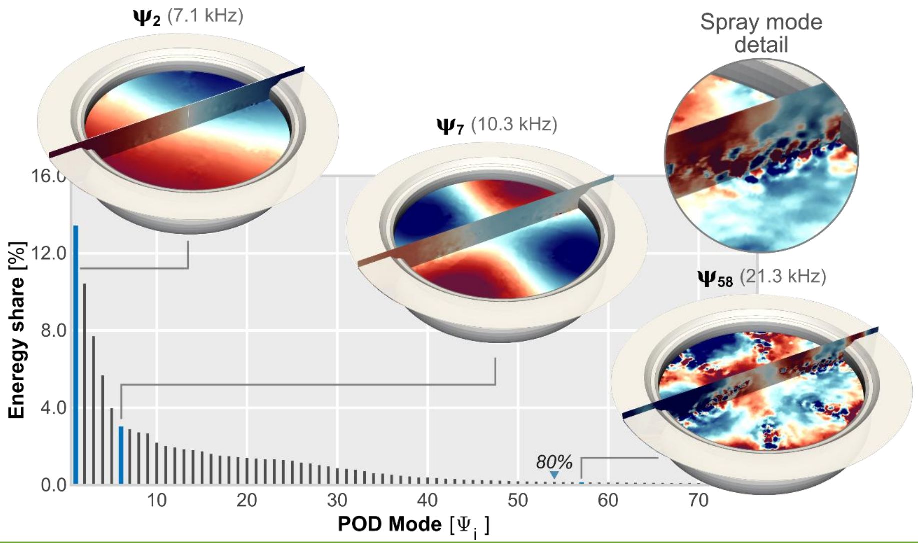
LES for combustion noise source characterization

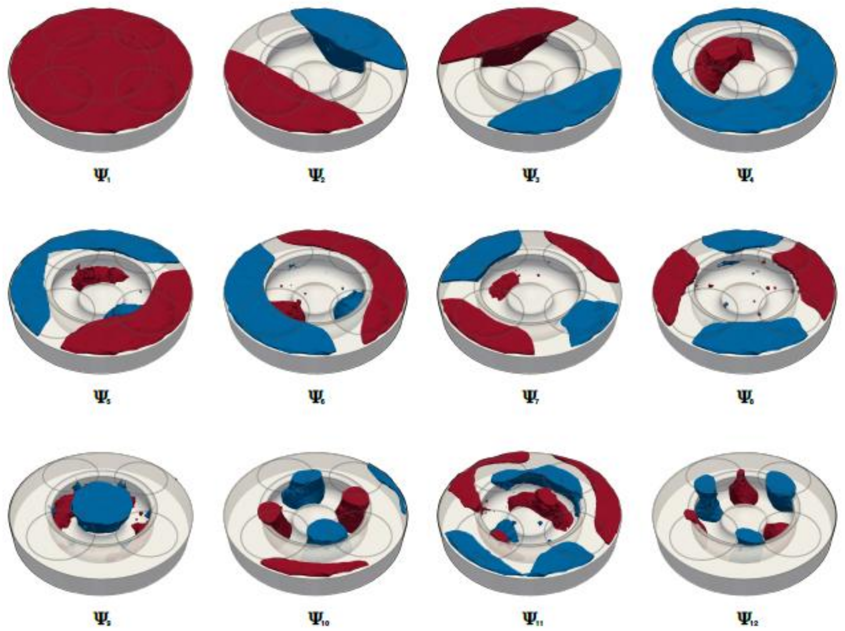
- Phenomenological analysis of combustion noise sources
  - ➢ Modal decomposition techniques
    - **P**roper **O**rthogonal **D**ecomposition
      - ○ Spatial oscillation pattern
      - ○ Time evolution
      - ○ Energy contribution
  - ➢ The size of the oscillation structures correlates with the energy contribution
    - **Large-scale oscillation structures** gather **80% of the energy**
    - **Jet-induced structures** only constitute **20% of the energy**





$$\boldsymbol{P}(\boldsymbol{x},t) \overset{SVD}{\Longrightarrow} \sum_{i=1}^{N} \boldsymbol{\Psi}_i(x) \cdot \sigma_i \cdot \boldsymbol{W}^T(t)$$





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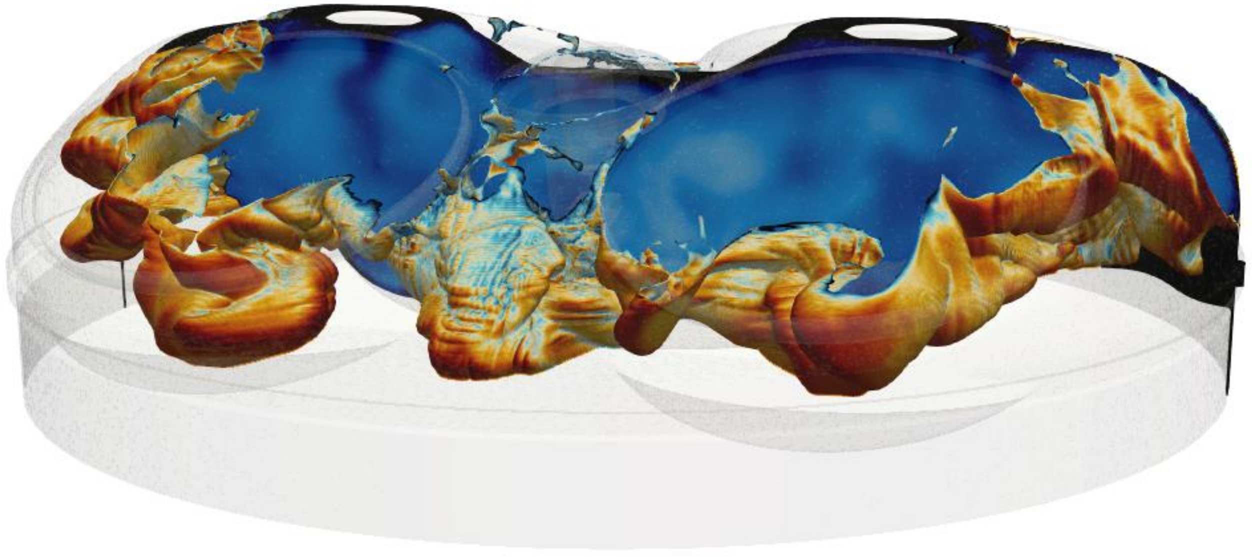
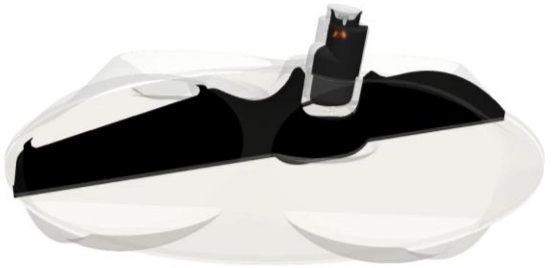
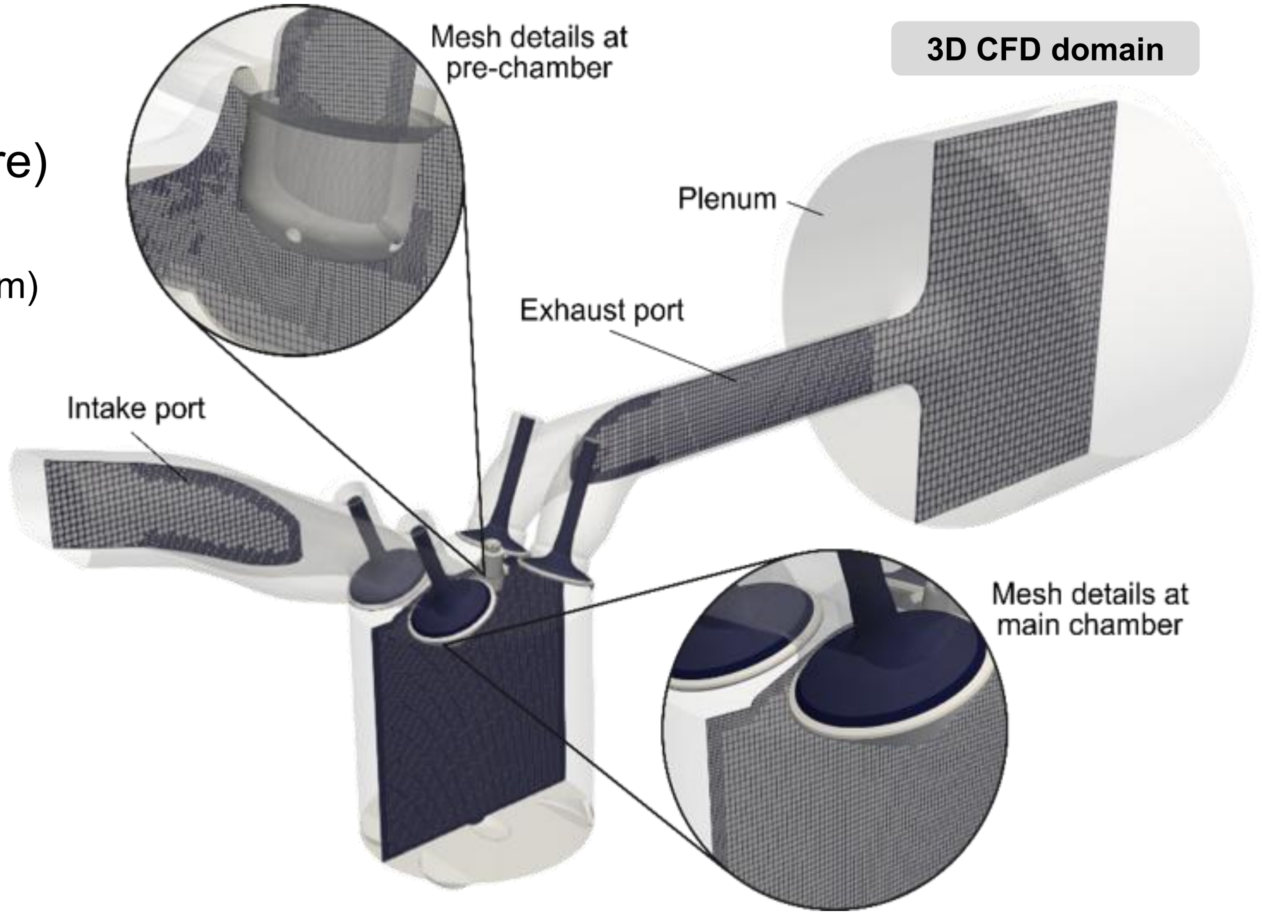


CFD FOR APPLIED RESEARCH

LES for optimization of pre-chamber ignition systems



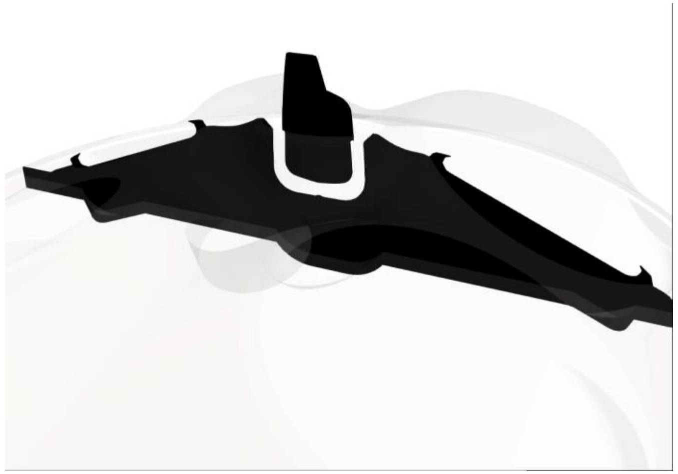
- Problem definition
  - ➢ Pre-chamber ignition concept modelling
- Numerical model setup
  - ➢ CONVERGE v3.0.28
  - ➢ Turbulence modeling: LES (dynamic structure)
  - ➢ Cell sizes
    - AMR: Velocity (0.0625 mm), Temperature (0.625 mm)
    - Spark embedding: 0.0312 mm around the spark
    - Total cell count: varied between 10 and 15 million
  - ➢ Specific sub-models/features
    - G-Equation + SAGE (in/on/out of the flame)
    - Tabulated laminar flame speed (s_L)
    - Chemical mechanism
      - Liu et al. (gasoline fuel)

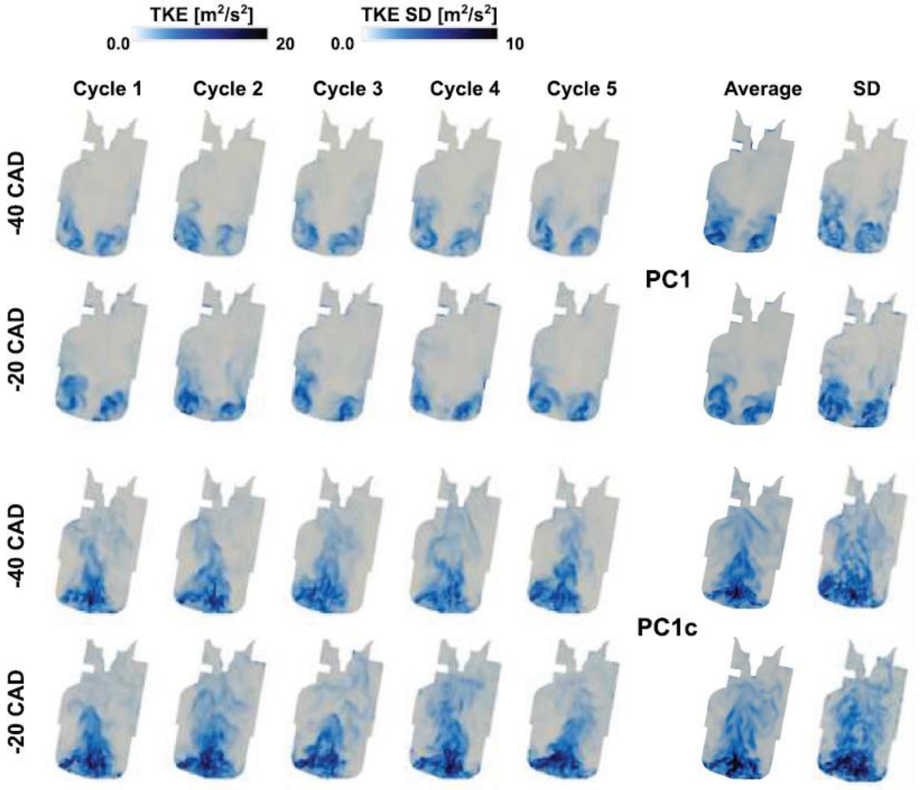


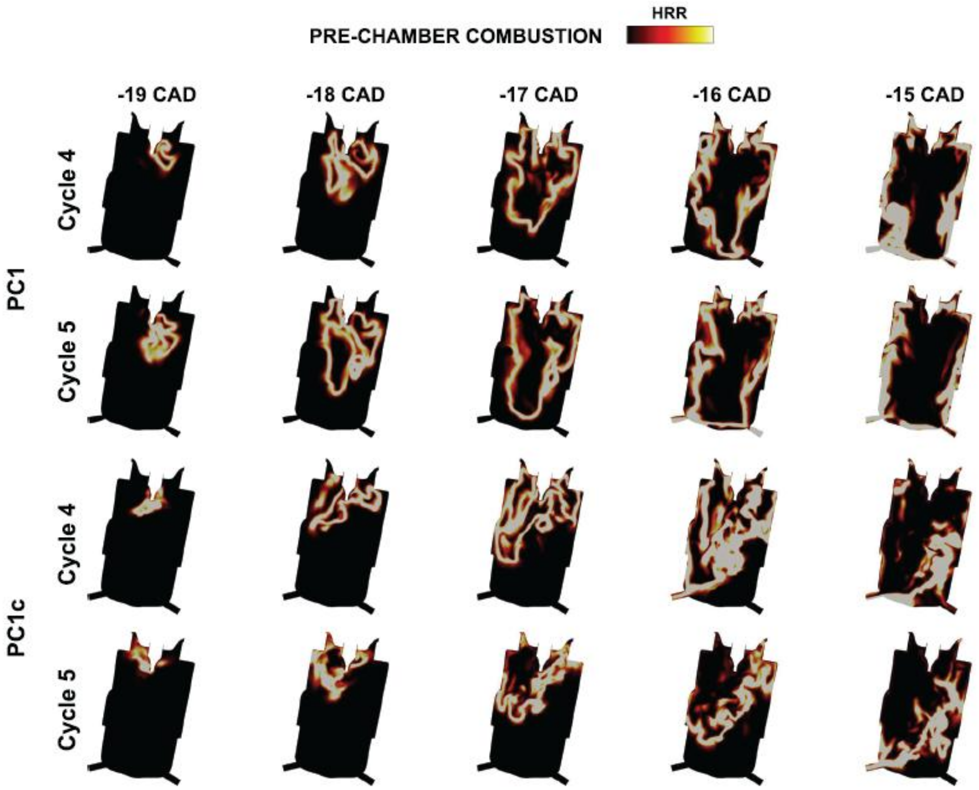
CFD FOR APPLIED RESEARCH

LES for optimization of pre-chamber ignition systems

- Analysis of cycle-to-cycle variability
  - Pre-chamber flow patterns
  - Combustion progress inside the pre-chamber
  - Uniformity of flame patterns and nozzle distribution

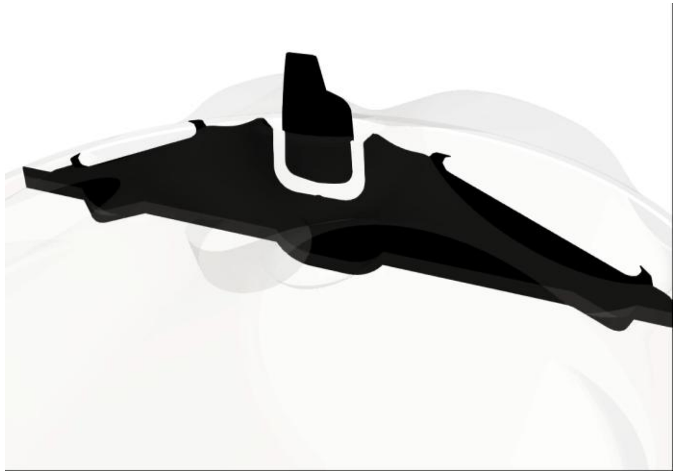






CFD FOR APPLIED RESEARCH

LES for optimization of pre-chamber ignition systems



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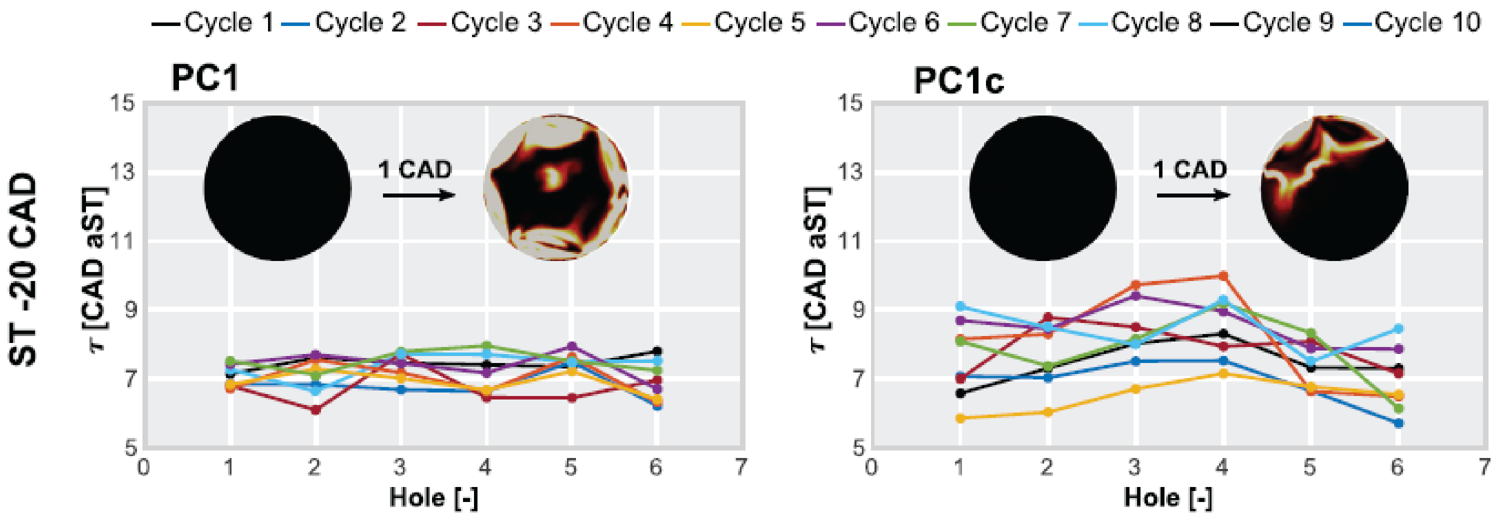

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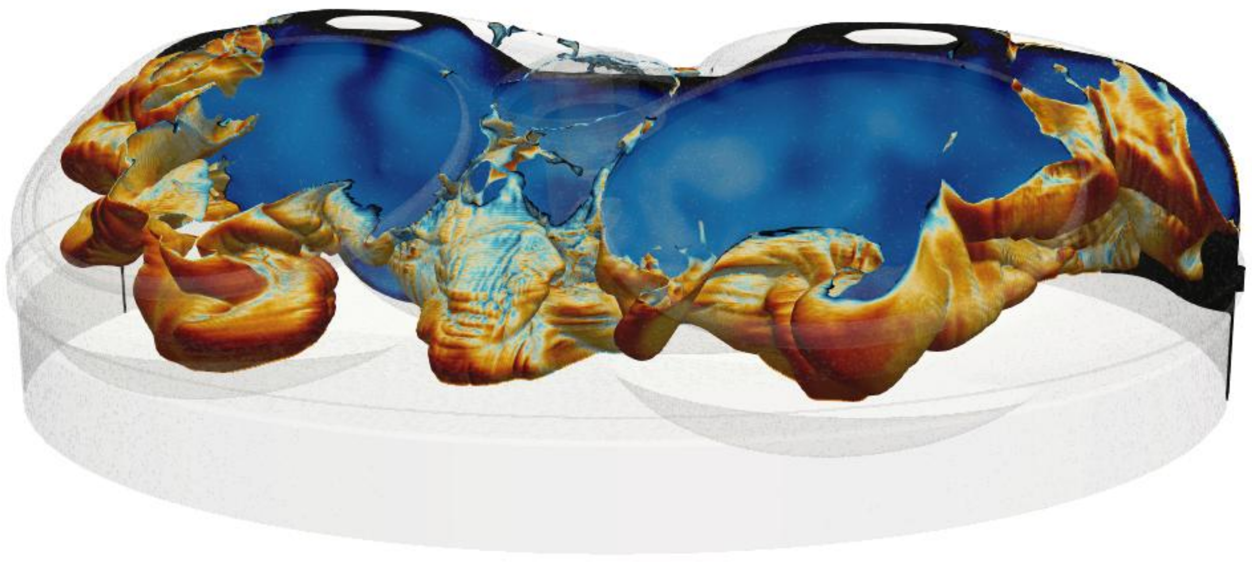


CFD FOR APPLIED RESEARCH

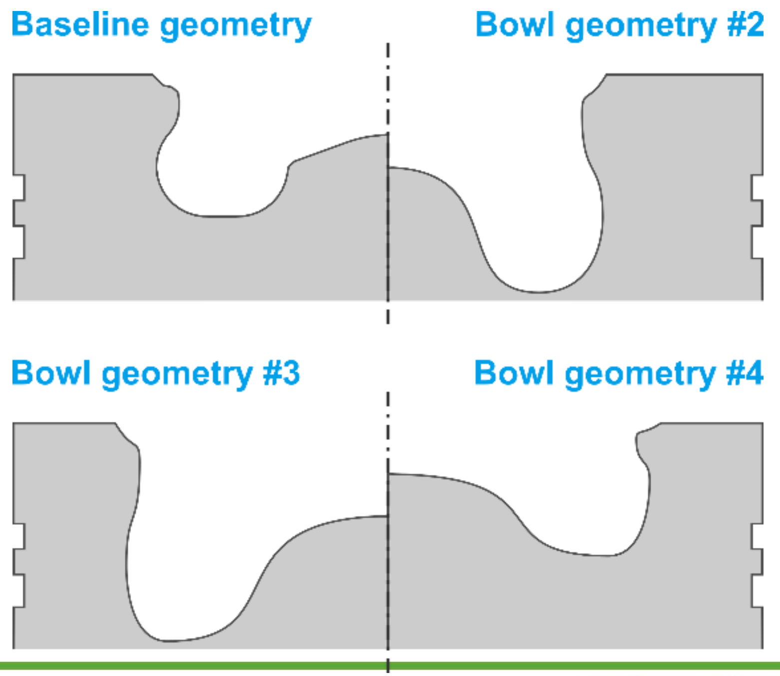
URANS coupled with optimization techniques

- Noise optimization - GA optimization methodology
  - ➢ Combustion system design
  - ➢ Evolutionary optimization method (genetic algorithms)
    - **8 optimizing parameters**
      - 5 geometric parameters for piston bowl
      - Included angle, number of nozzle holes
      - 1 parameter for intake port config. (swirl)
    - **Constraints**
      - Controlled emissions: NOx and soot
    - **Objectives**
      - Minimize resonance energy → Noise ↓↓
      - Minimize ISFC → Efficiency ↑

Ranges of the optimizing parameters

Geometric parameter 1 [-]	0.01–0.99
Geometric parameter 2 [-]	0.01–0.99
Geometric parameter 3 [-]	0.01–0.99
Geometric parameter 4 [-]	0.01–0.99
Geometric parameter 5 [-]	0.01–0.99
Number of injector nozzles [-]	4–12
Spray included angle [-]	80–180
Swirl number at IVC [-]	0.0–2.0

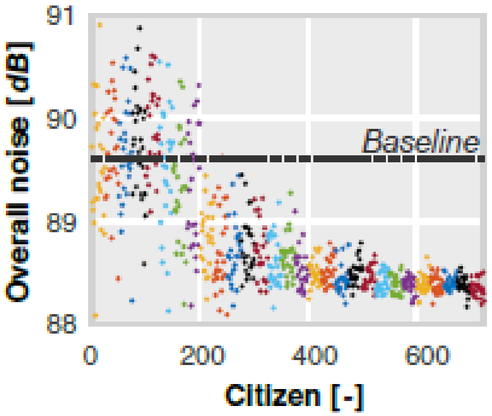
Example of different bowl profiles obtained by the Bezier polynomial method

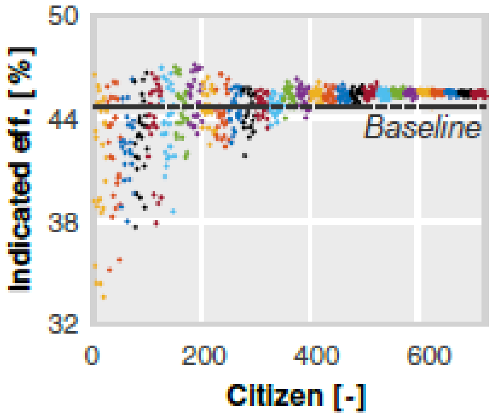


CFD FOR APPLIED RESEARCH

URANS coupled with optimization techniques

- Noise optimization - GA optimization methodology
  - ➢ Solution convergence
    - Reached after 725 simulations (25 citizens x 29 generations)
  - ➢ Synthesis of the results
    - **Constraints**
      - Pollutant levels are maintained below the predefined limits
    - **Objectives → clear improvements in:**
      - Noise level (~1.4 dB) → resonance energy ↓
      - Efficiency (~0.8%) → fuel consumption ↓

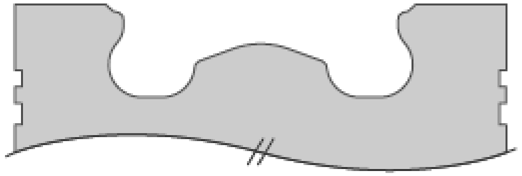




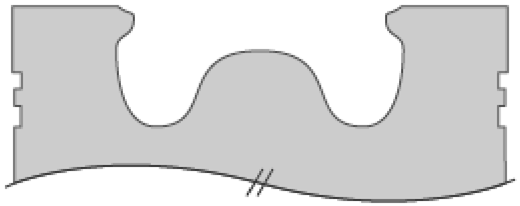
Optimized configuration

Configuration	Baseline	Optimized
Spray included angle [deg]	75.0	83.4
Number of nozzle holes [-]	6	12
Swirl number [-]	1.26	1.69

Baseline bowl geometry



Optimized bowl geometry

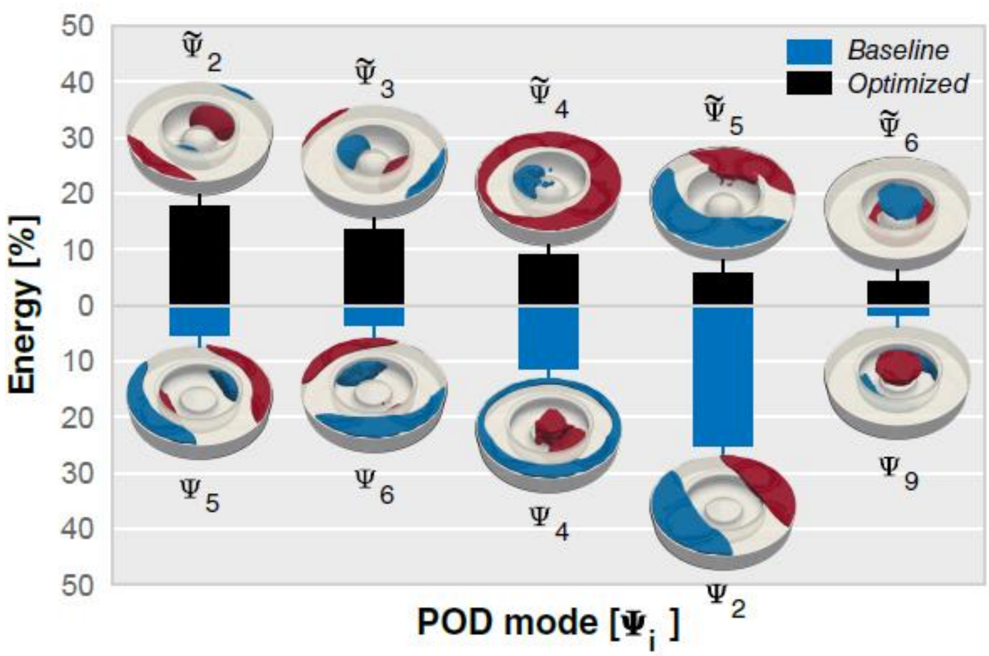


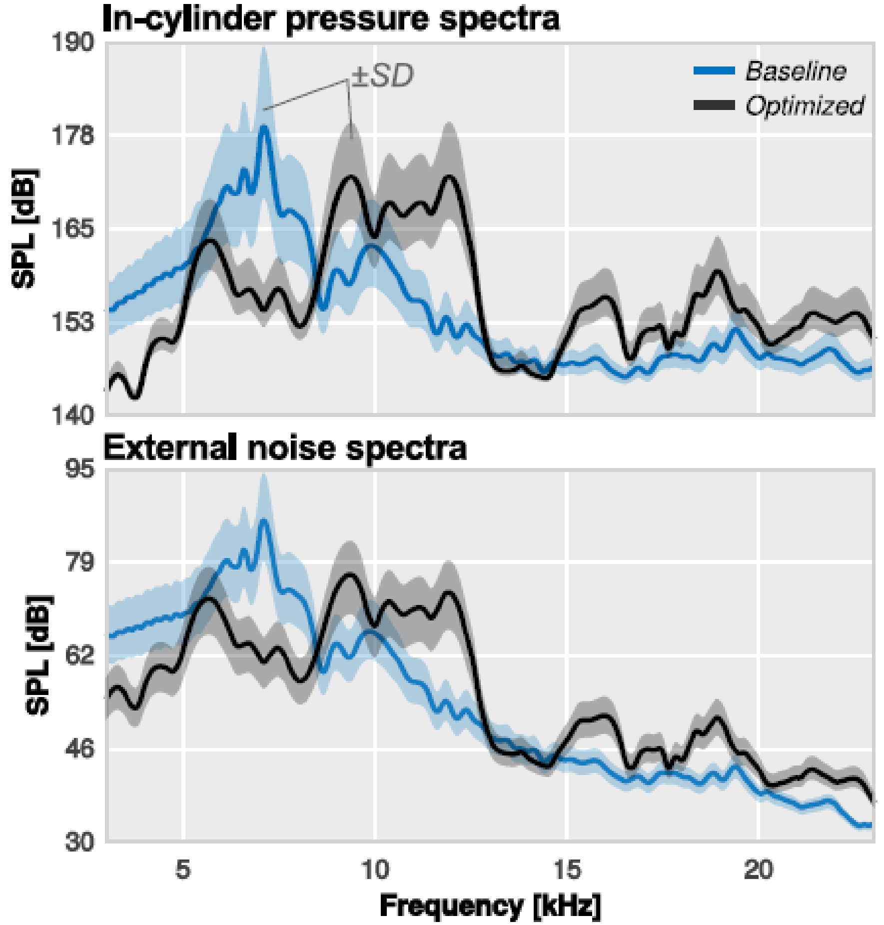
Configuration	Baseline	Optimized
E_{res} [$kPa^2 \cdot s$]	5.95	1.53
ISFC [g/kWh]	188.3	184.9
NO_x [mg/s]	7.54	7.48
Soot [mg/s]	0.16	0.12
Overall noise [dB]	89.6	88.2
Indicated eff. [%]	44.7	45.5

CFD FOR APPLIED RESEARCH

URANS coupled with optimization techniques

- Noise optimization - GA optimization methodology
  - Acoustic energy distribution (FFT analysis)
    - The acoustic energy is shifted towards higher frequencies
    - Resonant modes experience a notable amplitude lowering
    - Therefore, the overall resonant noise is reduced





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Thank you for your attention!

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