Computational perspectives to hydrogen combustion using open-source code

Physics/chemistry views

Hydrogen Breakfast Seminar 4, Wednesday, May 29th 2024
Otaniemi, Espoo

Fig: I. Morev

Associate Prof. Ville Vuorinen
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BUSINESS FINLAND

Research Council of Finland

CSC

Aalto Science-IT project

Contents of the talk

1) Motivation

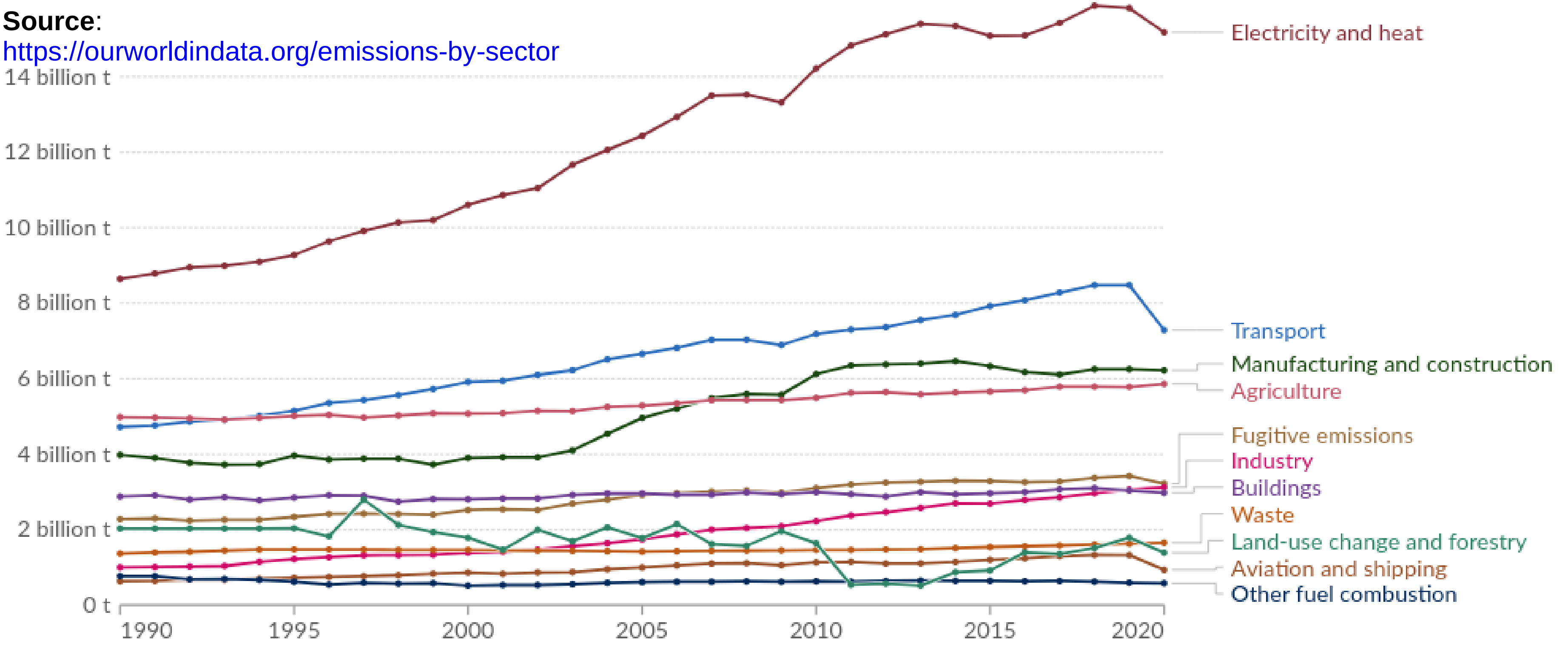
We have a problem...

Source:
https://ec.europa.eu/eurostat/web/products-eurostat-news/w/DDN-20230515-2

Green house gas emissions by sector

Measured in terms of CO2-equivalents over 100 year span

Source:
https://ourworldindata.org/emissions-by-sector



Extreme vision: there would be a great potential to even full decarbonization i.e. replacement of fossil fuels with hydrogen + e-fuels

Electrolysis → Hydrogen+ e-fuels → **Full decarbonization (H_2 + e-fuels)**

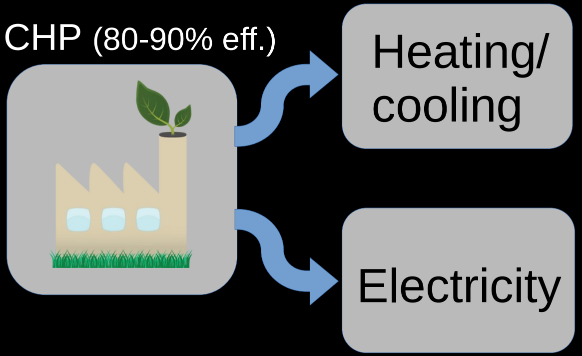
- Combustion engine
- Gas turbine
- Combustor
- Fuel cell

↑

High demand to re-design energy conversion devices for H_2

Example: combined heat and power (CHP) plants

CHP (80-90% eff.)



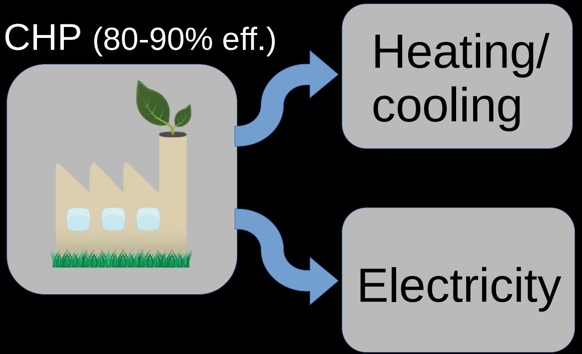
Combustion device (e.g. engine)

CFD direct numerical simulation of reactive flow in gas engine cylinder by HPC (high-performance comp.)

Credit: George Giannakopoulos

$$\vec{U}=\vec{U}(x,y,z,t) \qquad \rho=\rho(x,y,z,t)$$
$$T=T(x,y,z,t) \qquad p=\rho R T$$

Example: combined heat and power (CHP) plants



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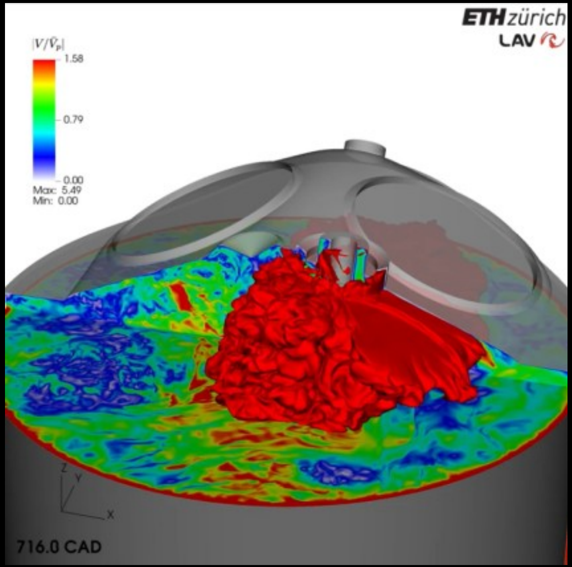

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$$\vec{U}=\vec{U}(x,y,z,t) \qquad \rho=\rho(x,y,z,t)$$
$$T=T(x,y,z,t) \qquad p=\rho R T$$

HPC + CFD caveats

→ CFD is computationally quite heavy

→ Requires HPC i.e. either a cluster or a supercomputer

→ CFD requires highly educated/experienced users

→ CFD of reactive flows extremely heavy

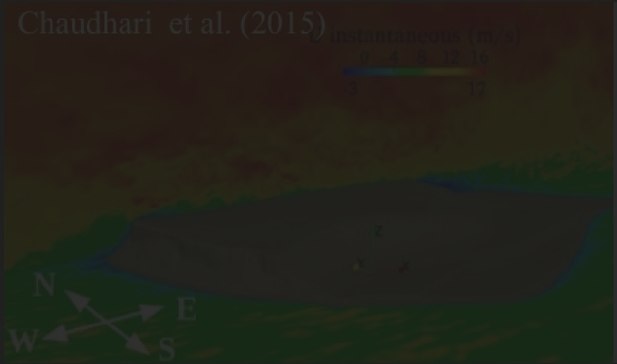
→ CFD of reactive flows highly multidisciplinary: engineering + physics + chemistry + software + HPC + data management

2) Computational fluid dynamics at Aalto/ENG

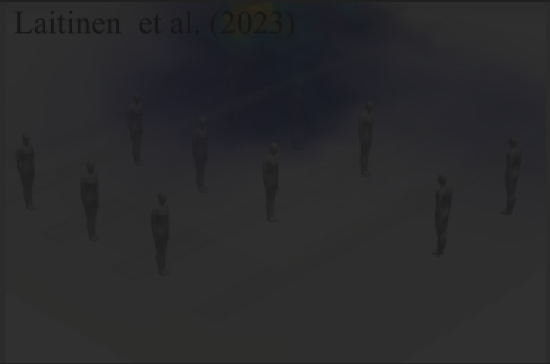
Computational fluid dynamics team at Aalto University/ENG, Finland

- Prof. V.Vuorinen + Prof. O.Kaario + 20 researchers
- 15 supervised PhD’s, 100+ journal papers
- Hydrogen, e-fuels, reactive multiphase flow, heat transfer, gas-/hydrodynamics
- OpenFOAM, StarCCM+, STAR-CD, LES/DNS/RANS/DES, DLBFoam


Wind power efficiency in landscapes

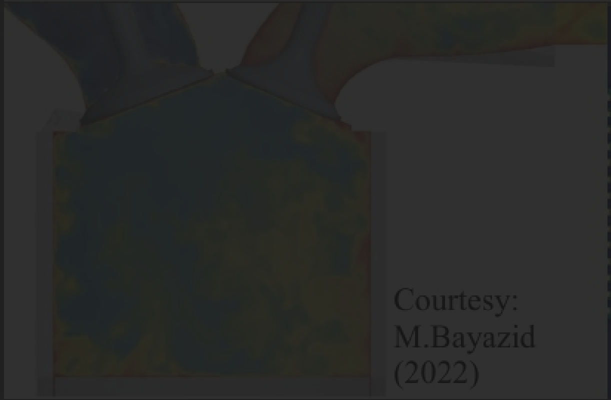


Healthy indoor air/vertical farming



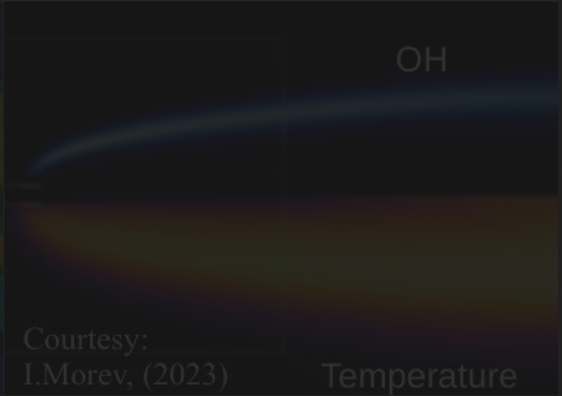
Energy conversion to H2/burners

Energy conversion to H2/engines



Heat transfer and energy

Hydrogen flame physics/chemistry



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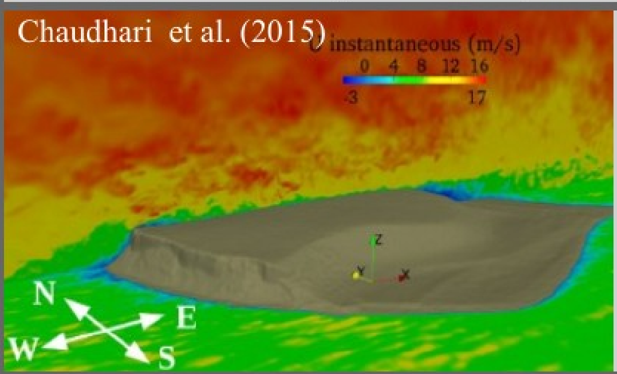
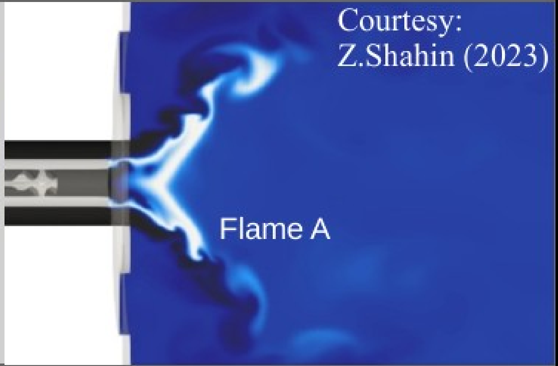
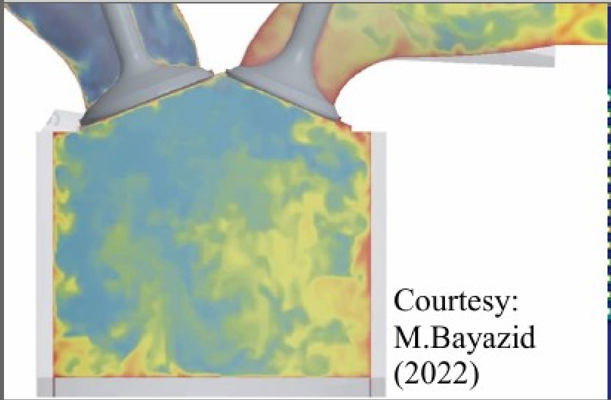


Healthy indoor air/vertical farming

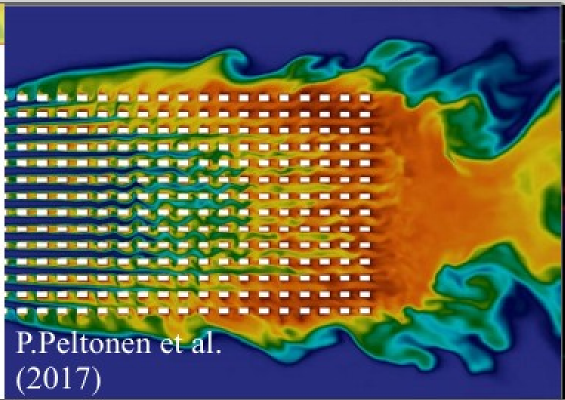
Energy conversion to H2/burners



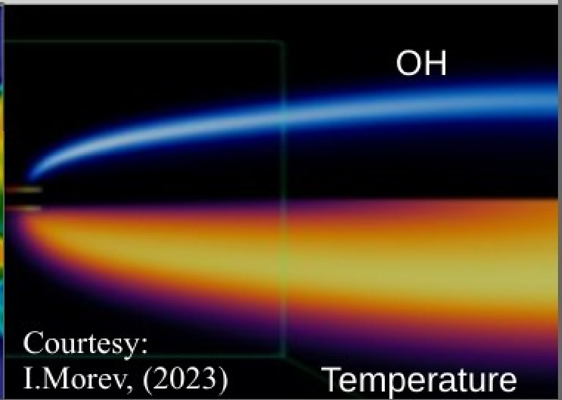
Energy conversion to H2/engines



Heat transfer and energy



Hydrogen flame physics/chemistry



OpenFOAM: the world's largest open-source code for computational fluid dynamics (CFD)

Governing equations in reactive flow CFD simulation

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = \bar{S}_\rho, \quad (1)$$

Mass conservation (1 eqn)

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(-\bar{p}\delta_{ij} + \bar{\rho}\tilde{u}_i\tilde{u}_j - \bar{\rho}\widetilde{u_i u_j} + \bar{\tau}_{ij}\right) + \bar{S}_{u,i}, \quad (2)$$

Momentum conservation (3 eqs)

$$\frac{\partial(\bar{\rho}\tilde{Y}_k)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{Y}_k)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\tilde{Y}_k - \bar{\rho}\widetilde{u_i Y_k} + \bar{\rho}\tilde{D}\frac{\partial \tilde{Y}_k}{\partial x_i}\right) + \bar{S}_{Y_k} + \bar{\dot{\omega}}_k, \quad (3)$$

Species conservation (~10-30 eqs for H_2)

$\sim N_{species}$

$$\frac{\partial(\bar{\rho}\tilde{h}_t)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{h}_t)}{\partial x_j} = \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{h}_s - \bar{\rho}\widetilde{u_j h_s} + \frac{\bar{\lambda}}{\bar{c}_p}\frac{\partial \tilde{h}_s}{\partial x_j}\right) + \bar{S}_h + \bar{\dot{\omega}}_h, \quad (4)$$

Reactions $\sim N^2$
→ bottle-neck

Energy conservation (~1 eqn)

The world's 3rd most powerful supercomputer: CSC's LUMI in Kajaani

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Aalto University

DLBFoam: open-source code to radically accelerating the chemistry bottle-neck in OpenFOAM CFD simulations

Solution: We developed DLBFoam: finite rate chemistry code with Dynamic Load Balancing in order to accelerate the chemistry. Utilizes analytical Jacobian evaluation via pyJac.
pyJac: https://slackha.github.io/pyJac/
DLBFoam: https://github.com/Aalto-CFD/DLBFoam

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ELSEVIER

DLBFoam: An open-source dynamic load balancing model for fast reacting flow simulations in OpenFOAM ☆,☆☆

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Physics of Fluids TUTORIAL scitation.org/journal/phf

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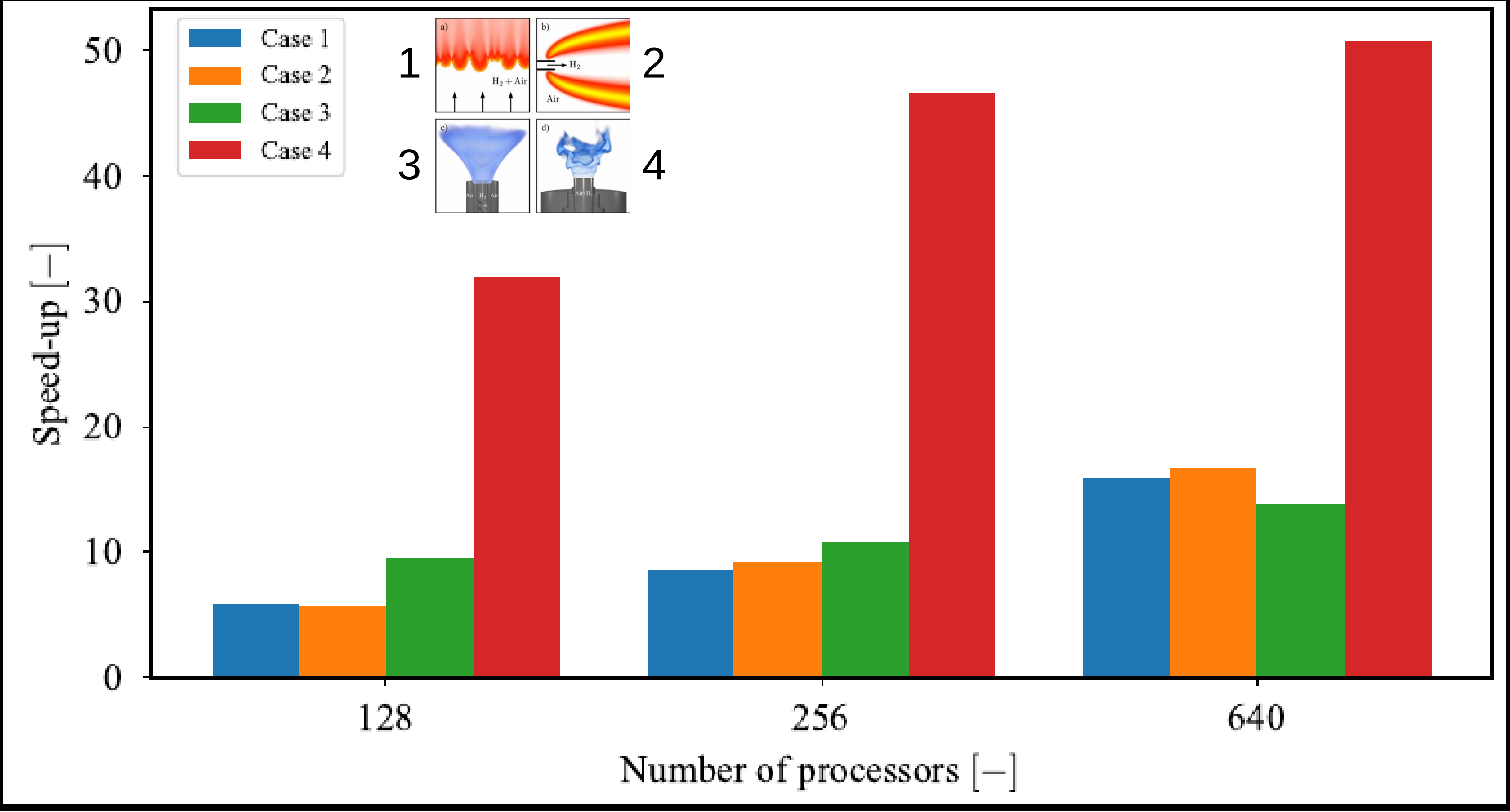
Examples on recent publications where DLBFoam is used

[1] M.Gadalla, S.Karimkashi, I.Kabil, O.Kaario, T.Lu and V.Vuorinen, Embedded direct numerical simulation of ignition kernel evolution and flame initiation in dual-fuel spray assisted combustion, Combustion and Flame, 259, 113172, (2024).
[2] S.Karimkashi, M.Gadalla, J.Kannan, B.Tekgul, O.Kaario, and V.Vuorinen, Large-eddy simulation of diesel pilot spray ignition in lean methane-air and methanol-air mixtures at different ambient temperatures, International Journal of Engine Research, 24, 3, (2023).
[3] A.Shahanaghi, S.Karimkashi, O.Kaario and V.Vuorinen, Efficient two-dimensional simulation of primary reference fuel ignition under engine-relevant thermal stratification, Physics of Fluids, 35, 126102, (2023).
[4] P.Tamadonfar, S.Karimkashi, O.Kaario and V.Vuorinen, A Numerical Study on Premixed Turbulent Planar Ammonia/Air and Ammonia/Hydrogen/Air Flames: An Analysis on Flame Displacement Speed and Burning Velocity, Flow, Turbulence and Combustion, 111, 717–741, (2023).
[5] S.Karimkashi, M.Gadalla, J.Kannan, B.Tekgul, O.Kaario, and V.Vuorinen, Large-eddy simulation of diesel pilot spray ignition in lean methane-air and methanol-air mixtures at different ambient temperatures
[6] B.Tekgul, P.Peltonen, H.Kahila, O.Kaario and V.Vuorinen, DLBFoam: An open-source dynamic load balancing model for fast reacting flow simulations in OpenFOAM, Computer Physics Communications, 267, 108073 (2021).
[7] M.Gadalla, J.Kannan, B.Tekgul, S.Karimkashi, O.Kaario and V.Vuorinen, Large-eddy simulation of tri-fuel combustion Diesel spray assisted ignition of methanol-hydrogen blends, International Journal of Hydrogen Research, 46, 41, (2021).
[8] J.Kannan, M.Gadalla, O.Kaario, S.Karimkashi, B.Tekgul and V.Vuorinen, Large-eddy simulation of tri-fuel ignition diesel spray-assisted ignition of lean hydrogen–methane–air mixtures, Combustion Theory and Modelling, 25, 3, (2021).
[9] B.Tekgul, S.Karimkashi, H.Kahila, Z.Ahmad, J.Hyvönen, E.Lendormy, O.Kaario and V.Vuorinen, Large-eddy simulation of spray assisted dual-fuel ignition under reactivity-controlled dynamic conditions, FUEL, 293, 120295, (2021).
[10] B.Tekgul, V.Vuorinen et al. Large-eddy simulation of dual-fuel spray ignition at different ambient temperatures, Combustion and Flame, 215, (2020).
[11] S.Karimkashi, H.Kahila, O.Kaario, M.Larmi, and V.Vuorinen, A numerical study on combustion mode characterization for locally stratified dual-fuel mixtures, Combustion and Flame, 214, (2020).
[12] H.Kahila, Z.Ahmad, O.Kaario, M.Ghaderi-Masouleh, M.Larmi, and V.Vuorinen, Large-eddy simulation of dual-fuel ignition: Diesel spray injection into a lean methane-air mixture, Combustion and Flame, 191, 142-159, (2019).

DLBFoam: computational speed-up for H_2 for 4 different flame cases 1-4 (~5-50x speed-up)



3) Remarks about hydrogen

Oversimplification:

$$H_2 + ½O_2 \rightarrow H_2O$$

"Hydrogen + Oxygen → Water"

Hydrogen combustion is complex and also produces nitric oxide emissions

E.g. Westbrook et al. (2004)
→ 19 chemical reactions
→ 11 molecule species

	Reaction	A	n	E_a	Ref.
	H_2/O_2 Chain Reactions				
1	$\dot{H} + O_2 = \dot{O} + \dot{O}H$	1.91×10^{14}	0.00	16.44	[39]
2	$\dot{O} + H_2 = \dot{H} + \dot{O}H$	5.08×10^{4}	2.67	6.292	[40]
3	$\dot{O}H + H_2 = \dot{H} + H_2O$	2.16×10^{8}	1.51	3.43	[41]
4	$\dot{O} + H_2O = \dot{O}H + \dot{O}H$	2.97×10^{6}	2.02	13.4	[42]
	H_2/O_2 Dissociation/Recombination Reactions				
5[a]	$H_2 + M = \dot{H} + \dot{H} + M$	4.57×10^{19}	−1.40	105.1	[43]
6[b]	$\dot{O} + \dot{O} + M = O_2 + M$	6.17×10^{15}	−0.50	0.00	[43]
7[c]	$\dot{O} + \dot{H} + M = \dot{O}H + M$	4.72×10^{18}	−1.00	0.00	[43]
8[d,e]	$\dot{H} + \dot{O}H + M = H_2O + M$	4.50×10^{22}	−2.00	0.00	[43] ×2.0
	Formation and consumption of $H\dot{O}_2$				
9[f,g]	$\dot{H} + O_2 + M = H\dot{O}_2 + M$	3.48×10^{16}	−0.41	−1.12	[44]
	$\dot{H} + O_2 = H\dot{O}_2$	1.48×10^{12}	0.60	0.00	[45]
10	$H\dot{O}_2 + \dot{H} = H_2 + O_2$	1.66×10^{13}	0.00	0.82	[6]
11	$H\dot{O}_2 + \dot{H} = \dot{O}H + \dot{O}H$	7.08×10^{13}	0.00	0.30	[6]
12	$H\dot{O}_2 + \dot{O} = \dot{O}H + O_2$	3.25×10^{13}	0.00	0.00	[46]
13	$H\dot{O}_2 + \dot{O}H = H_2O + O_2$	2.89×10^{13}	0.00	−0.50	[46]
	Formation and Consumption of H_2O_2				
14[h]	$H\dot{O}_2 + H\dot{O}_2 = H_2O_2 + O_2$	4.2×10^{14}	0.00	11.98	[47]
	$H\dot{O}_2 + H\dot{O}_2 = H_2O_2 + O_2$	1.3×10^{11}	0.00	−1.629	[47]
15[i,f]	$H_2O_2 + M = \dot{O}H + \dot{O}H + M$	1.27×10^{17}	0.00	45.5	[48]
	$H_2O_2 = \dot{O}H + \dot{O}H$	2.95×10^{14}	0.00	48.4	[49]
16	$H_2O_2 + \dot{H} = H_2O + \dot{O}H$	2.41×10^{13}	0.00	3.97	[43]
17	$H_2O_2 + \dot{H} = H_2 + H\dot{O}_2$	6.03×10^{13}	0.00	7.95	[43]×1.25
18	$H_2O_2 + \dot{O} = \dot{O}H + H\dot{O}_2$	9.55×10^{06}	2.00	3.97	[43]
19[h]	$H_2O_2 + \dot{O}H = H_2O + H\dot{O}_2$	1.0×10^{12}	0.00	0.00	[50]
	$H_2O_2 + \dot{O}H = H_2O + H\dot{O}_2$	5.8×10^{14}	0.00	9.56	[50]

O'Connaire, M., H. J. Curran, J. M. Simmie, W. J. Pitz, and C. K. Westbrook,
"A Comprehensive Modeling Study of Hydrogen Oxidation,"
Int. J. Chem. Kinet., 36:603-622, 2004 (UCRL-JC-152569).

Hydrogen is actually quite different from other fuels.

Not only diffusive/light but also very high flame speed.

Hydrogen (H_2) has very different combustion properties when compared to hydrocarbons e.g. methane (CH_4) or propane (C_3H_8)

Table 1
Thermal properties and fundamental combustion characteristics of ammonia and hydrocarbon fuels. Data of boiling point and condensation point are from NIST database [8].

Fuel	NH_3	H_2	CH_4	C_3H_8
Boiling temperatureat 1 atm (°C)	−33.4	−253	−161	−42.1
Condensation pressure at 25 °C (atm)	9.90	N/A	N/A	9.40
Lower heating value, LHV (MJ/kg)	18.6	120	50.0	46.4
Flammability limit (Equivalence ratio)	0.63∼1.40	0.10∼7.1	0.50∼1.7	0.51∼2.5
Adiabatic flame temperature (°C)	1800	2110	1950	2000
Maximum laminar burning velocity (m/s)	0.07	2.91	0.37	0.43
Minimum auto ignition temperature (°C)	650	520	630	450

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H. Kobayashi et al. / Proceedings of the Combustion Institute 37 (2019) 109–133

Flame speed is very important concept affecting fluid dynamical design of combustion devices.

E.g. try to avoid “flashback” vs “blow-out”

Simulated premixed H_2 combustion/AHEAD burner

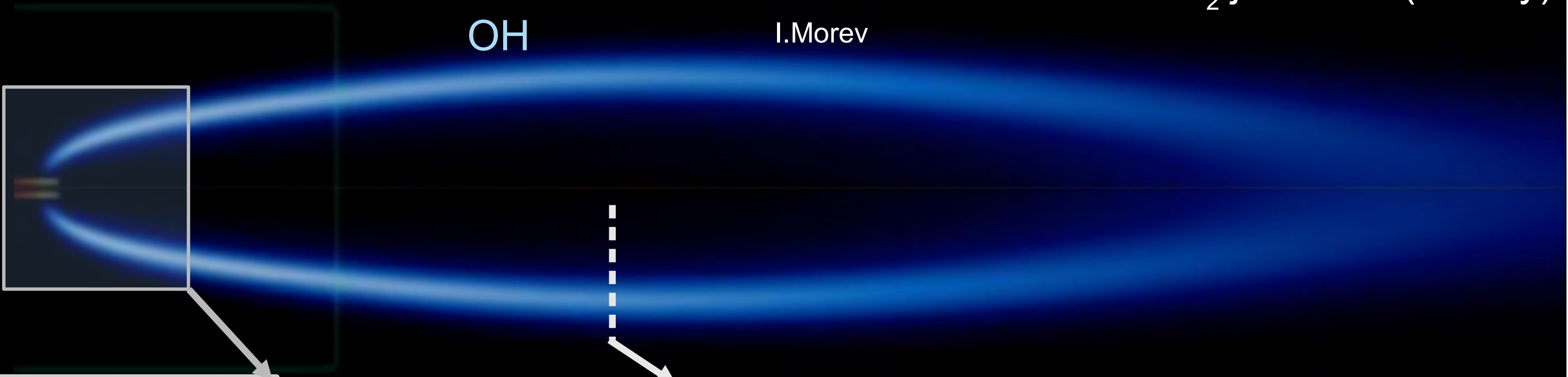
To be submitted

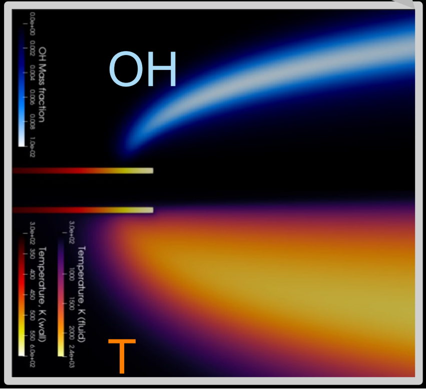
Courtesy:
A.Haider/
Aalto

How do you know your simulation is correct?
→ Compare 3D flame structure sim. vs exp.

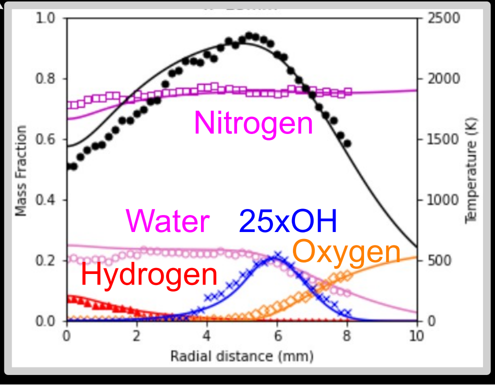
"Case 2": Simulated H_2 jet flame (steady)

I.Morev





Zoom to injector

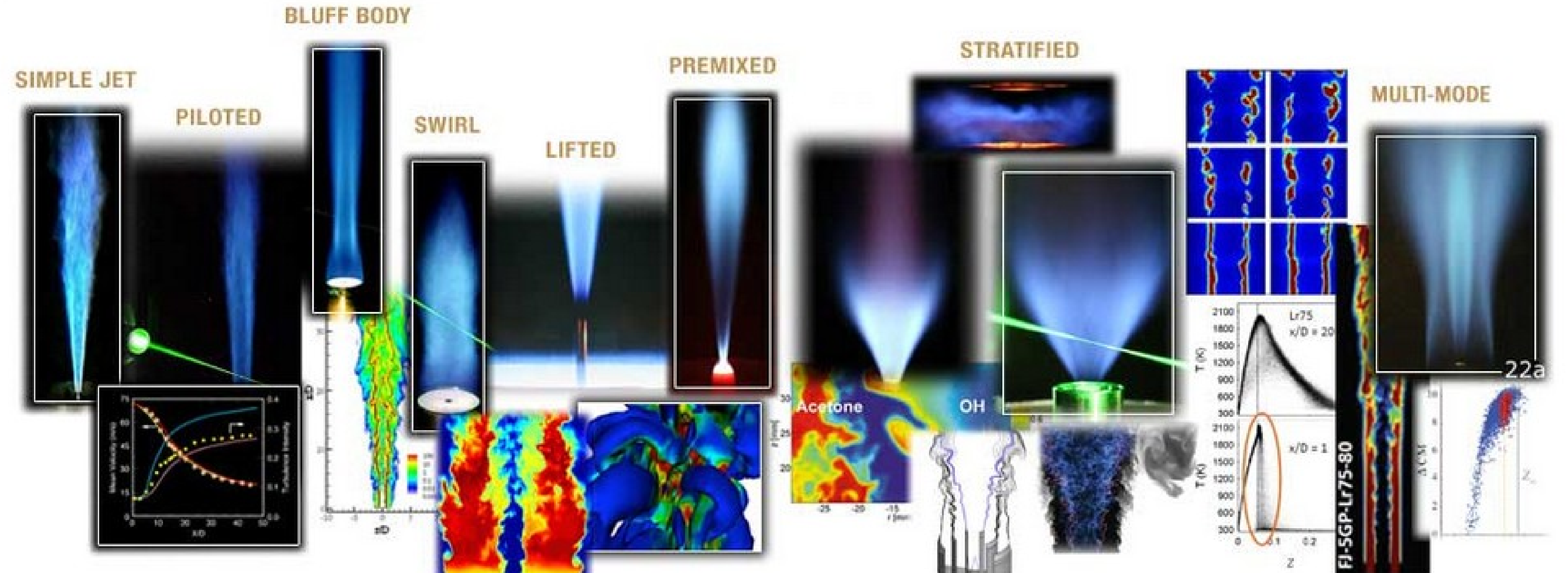


Experiment vs simulation

4) Aalto/ENG + international efforts to model hydrogen flames

TNF Workshop

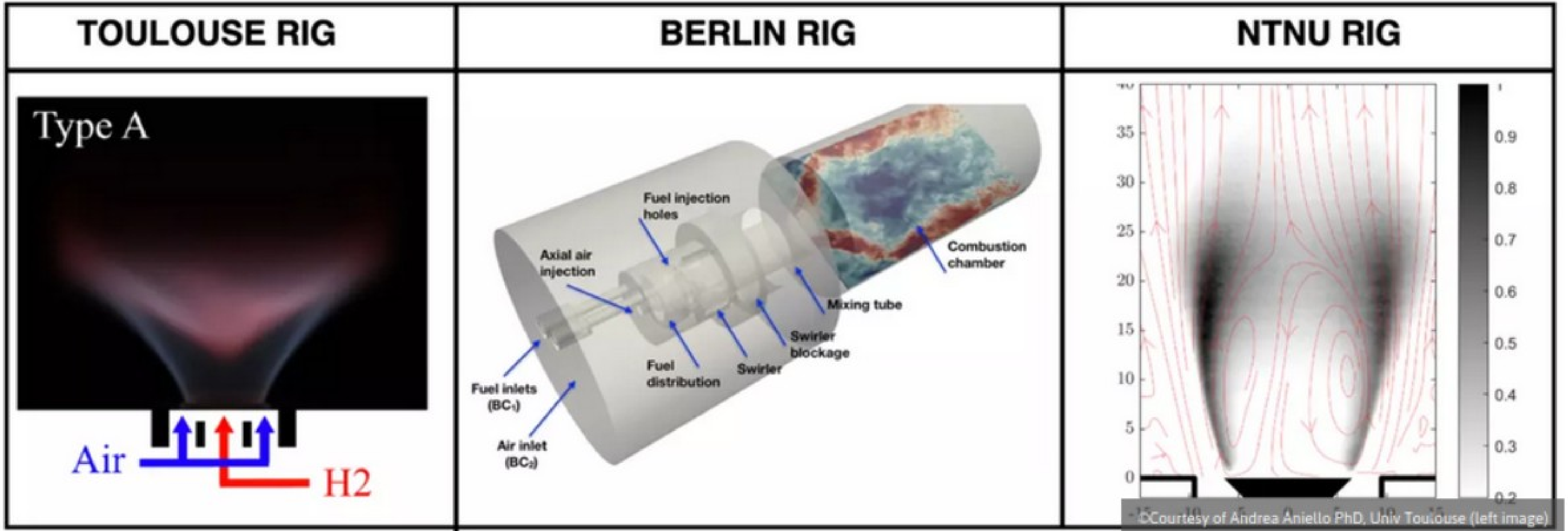
International Workshop on Measurement and Computation of Turbulent Flames



May 2023: International initiative to compare different CFD codes against high quality experimental data on three hydrogen flame rigs

Clean Aviation working group on CFD codes for hydrogen-air combustion

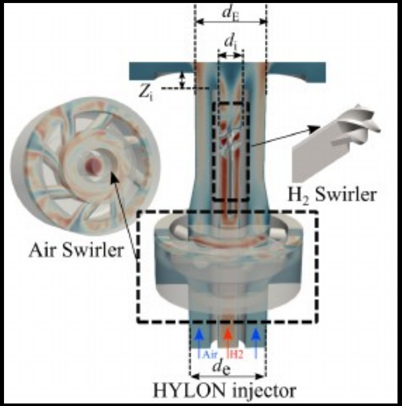
Experimental, high-precision data will be made available from **three experiments**: the **HYLON rig** in Toulouse, the **TU Berlin rig** in Berlin and the **NTNU rig** in Trondheim. Only pure hydrogen-air flames will be considered in the frame of this workshop.



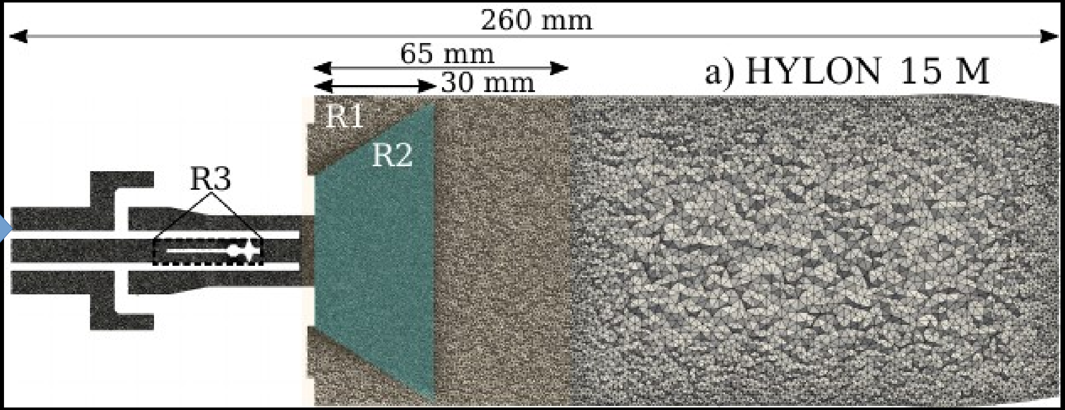
©Courtesy of Andrea Aniello PhD, Univ Toulouse (left image)

Computational modeling steps before H_2 flame CFD simulations

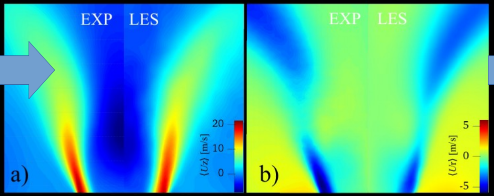
Step 1: 3D CAD model



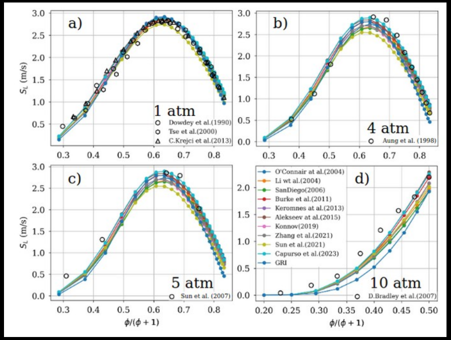
Step 2: 3D meshing

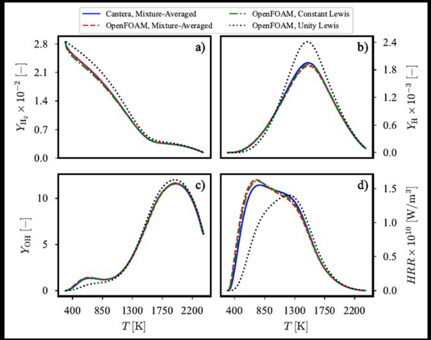


Step 3: Cold flow validation (3d)

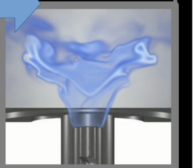


Step 4: Chemistry+diffusion validation/verification (0d/1d)



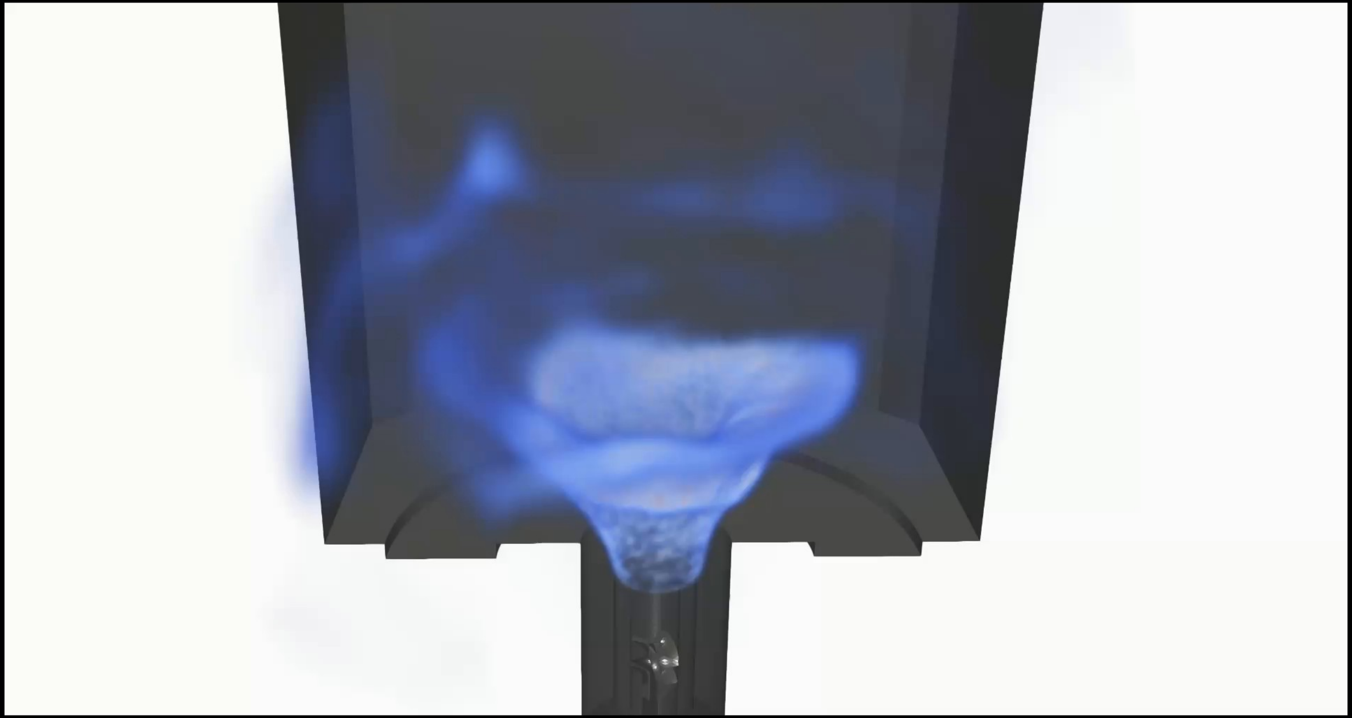


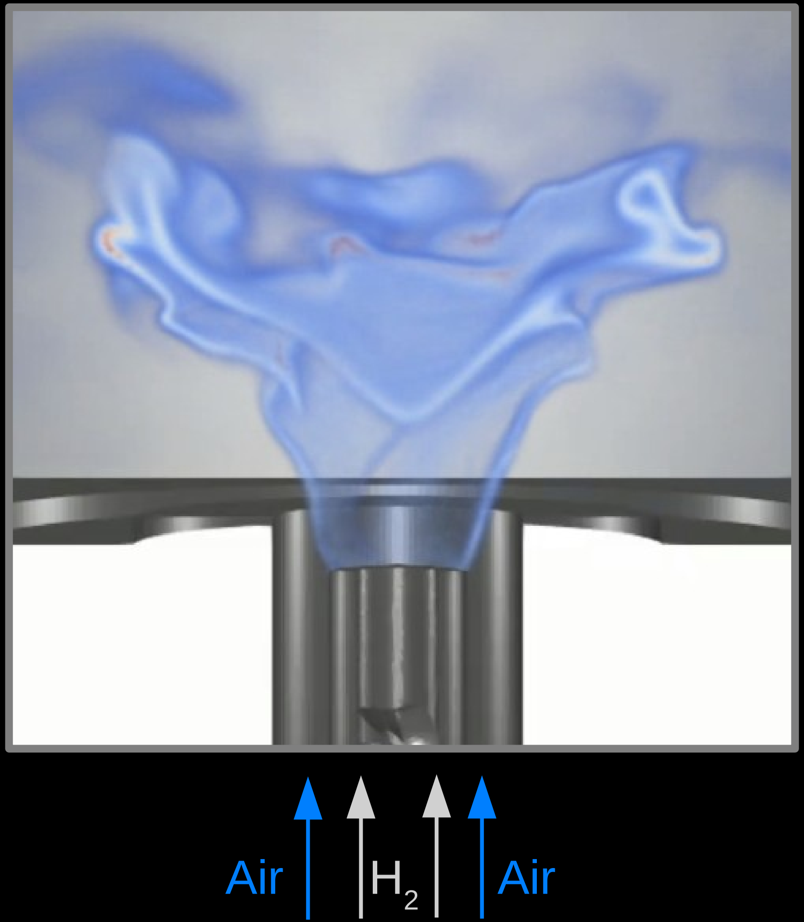
Step 5: Reactive flow (3d)



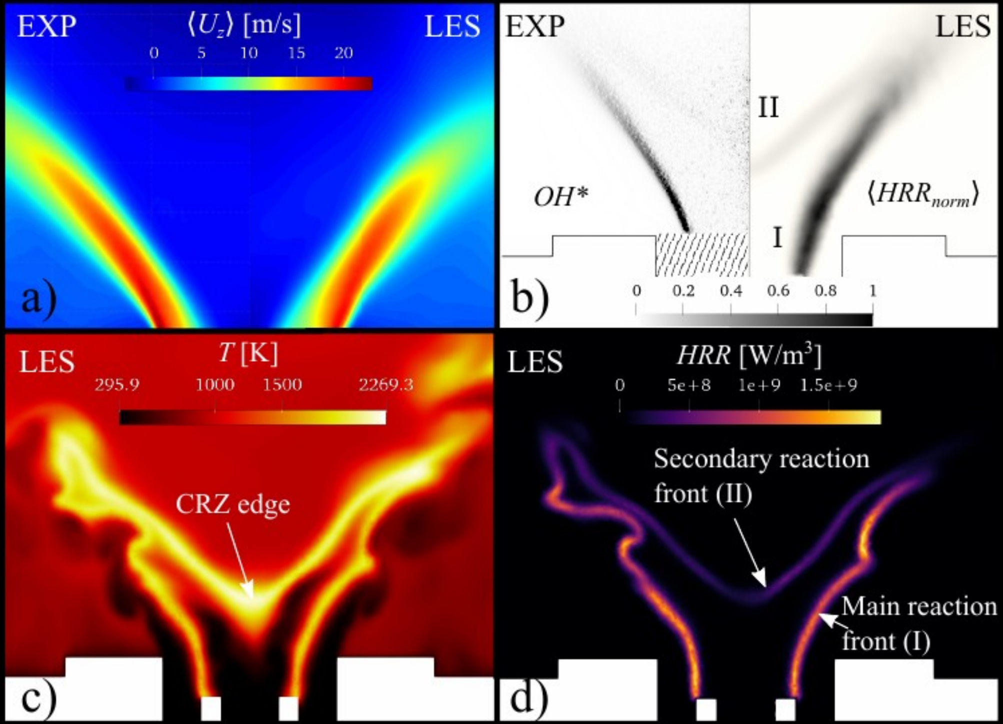
Large-eddy simulation of HYLON Flame A setup (TOULOUSE rig): non-premixed hydrogen combustion

Courtesy: Z.Shahin (M.Sc. thesis 2023)




Air
H_2
Air

HYLON Flame A: comparison of present simulation (LES/CFD) against experimental data



Courtesy: Z.Shahin (M.Sc. thesis 2023)

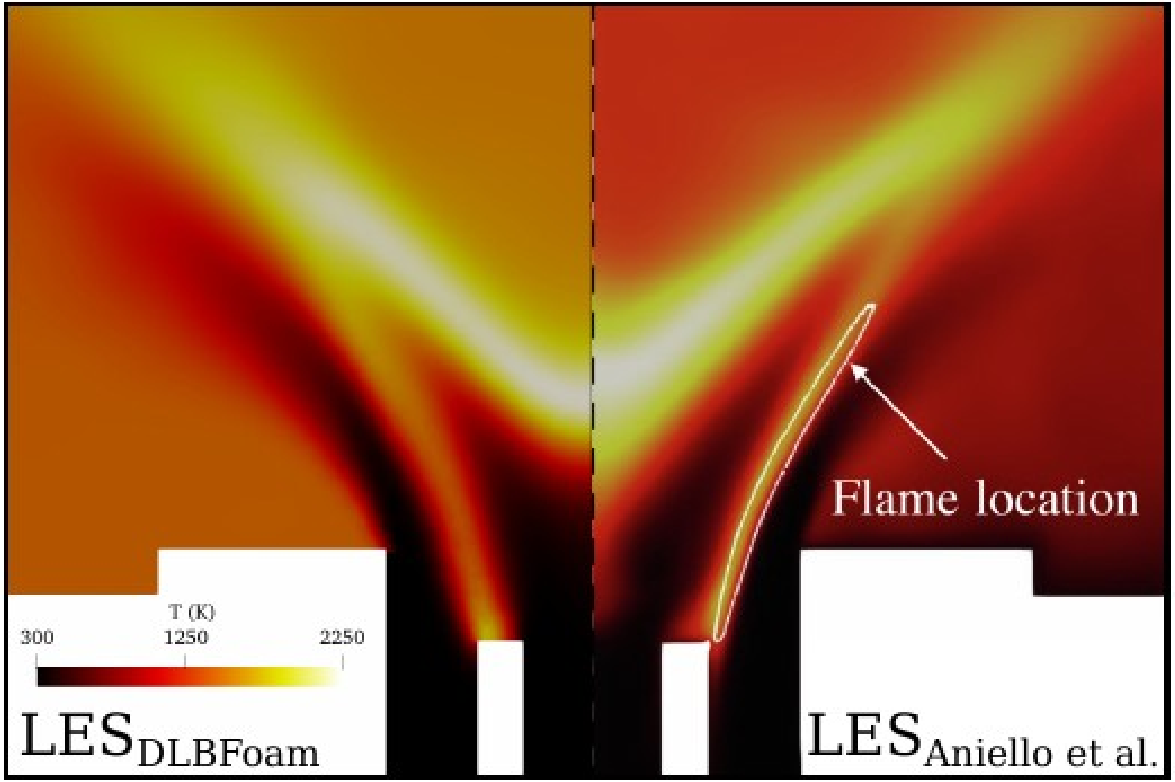
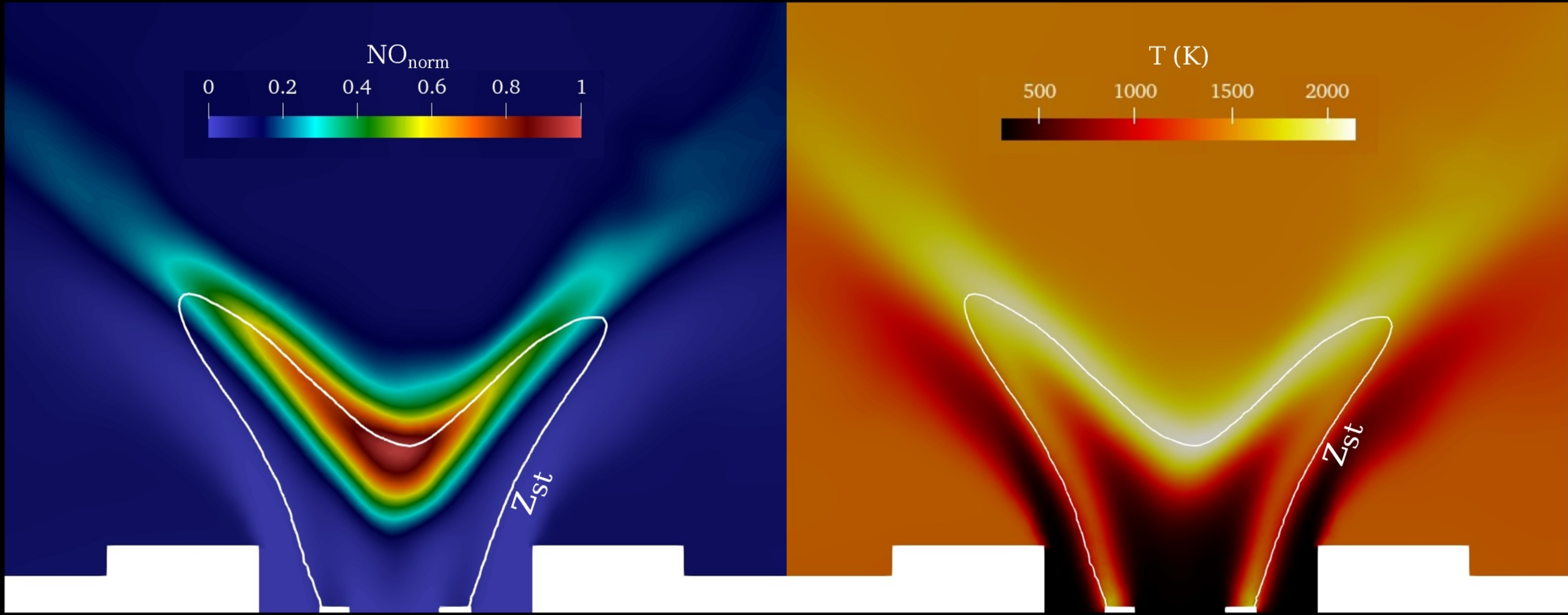


Figure 36: Contour map of the the temperature observed from the current work a) and the LES values from [14]b) for the anchored flame A.

NOx emissions vs local temperature



Courtesy: Z.Shahin (M.Sc. thesis 2023)

5) Concluding remarks

Personal experiences from our team on solving very difficult computational problems

1) show that it is possible to solve a problem

2) do it more efficiently

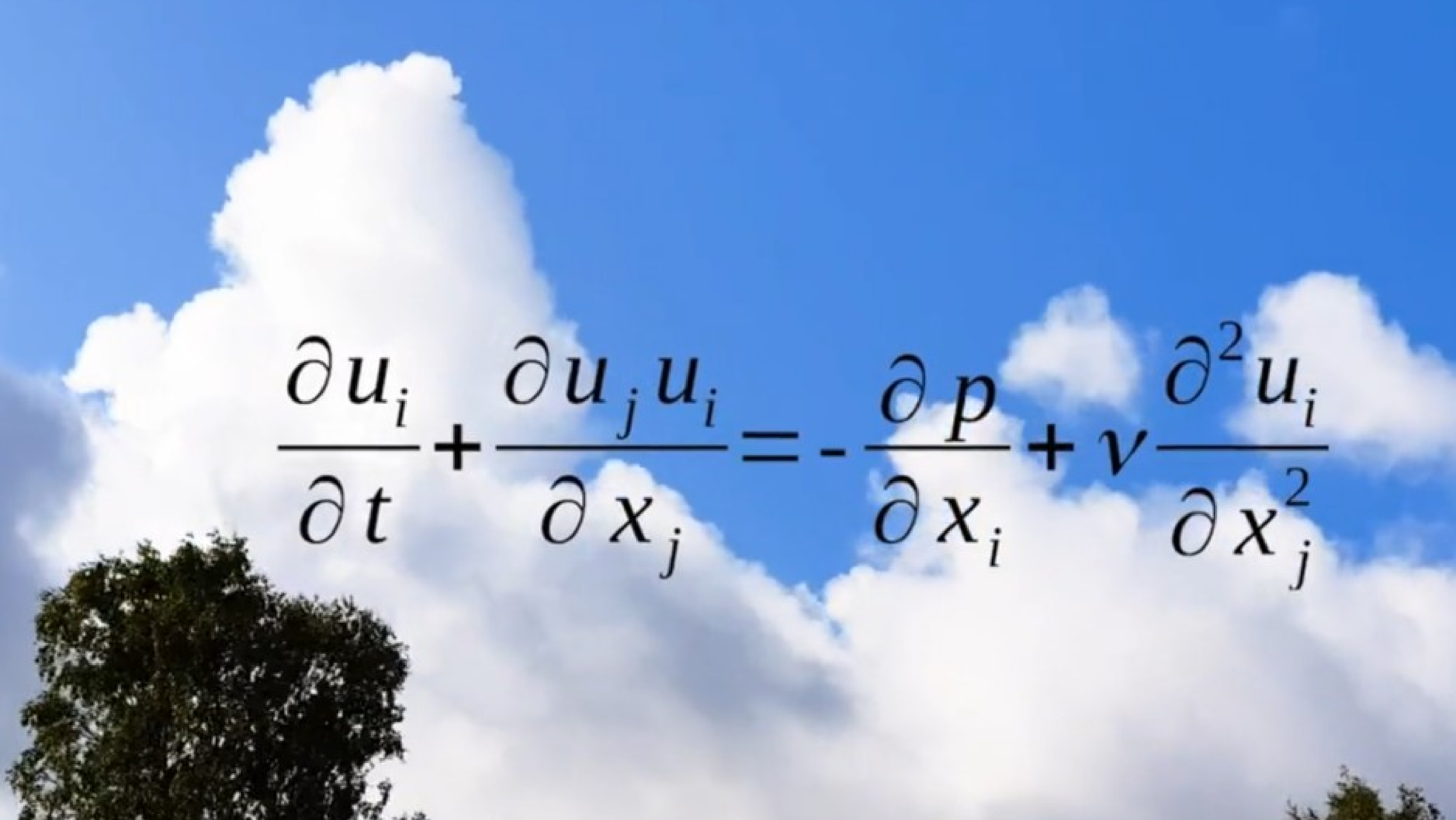
3) make your code/setups open to everyone

4) trust on the power of community efforts e.g. “OpenFOAM”

5) go back to 1)

→ **This talk:** open-source CFD (OpenFOAM+DLBFoam) R&D potential shown for complex H_2 combustion devices.

“Simulation has become the third scientific pillar alongside theory and experiments” (Prof. C.Hasse/Nov. 6th 2023)



$$\frac{\partial u_i}{\partial t}+\frac{\partial u_j u_i}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 u_i}{\partial x_j^2}$$

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