Principali attività di ricerca in corso e possibili sviluppi

Mauro Valorani
Dipartimento di Ingegneria Meccanica e Aerospaziale

Incontro promozione attività di ricerca DIMA
Roma, 6 febbraio 2017

SAPIENZA
UNIVERSITÀ DI ROMA

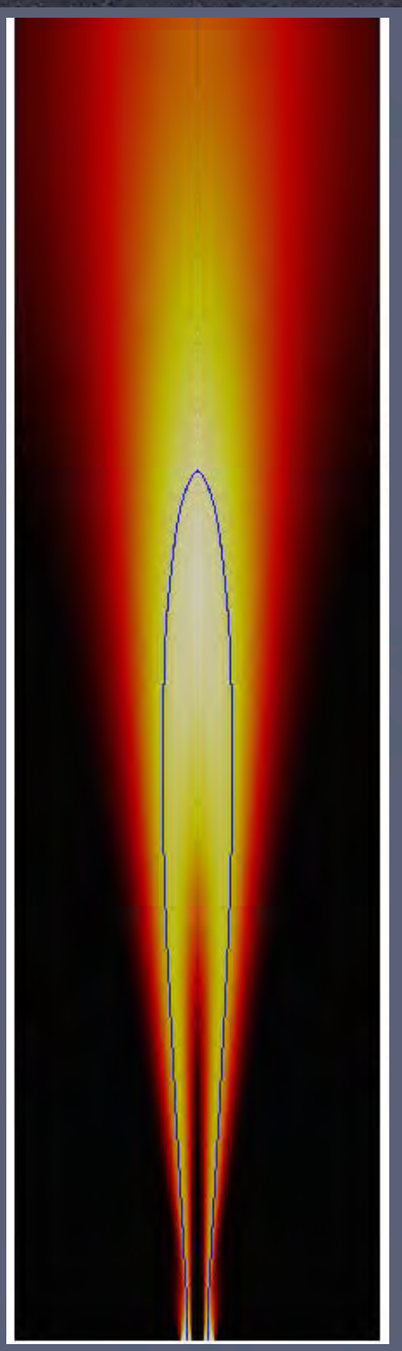
Multi-scale Simulation of Reactive Flows in Thrust Chambers

- Turbulent Combustion Closure (LES via Conditional Moment Closure)
- Ignition Transient in Combustion Chambers (URANS)
- Supercritical Combustion in LRE Chambers (RANS, URANS, LES)
- Deterministic and Probabilistic Model Reduction of Chemical Kinetics using CSPTk
- Prediction of strong and weak ignition regimes in turbulent reacting flows with temperature fluctuations
- Flame Initiation and Formation (DNS via Wavelets)
- Spray Modeling of Pressure-Swirl Atomizers using OpenFoam
- Development of the CSP Tool Kit (CSPTk) Library

An early case of Cro-SSD collaboration (06+07)

- Detached Eddy Simulation shock unsteadiness in an over-expanded planar nozzle

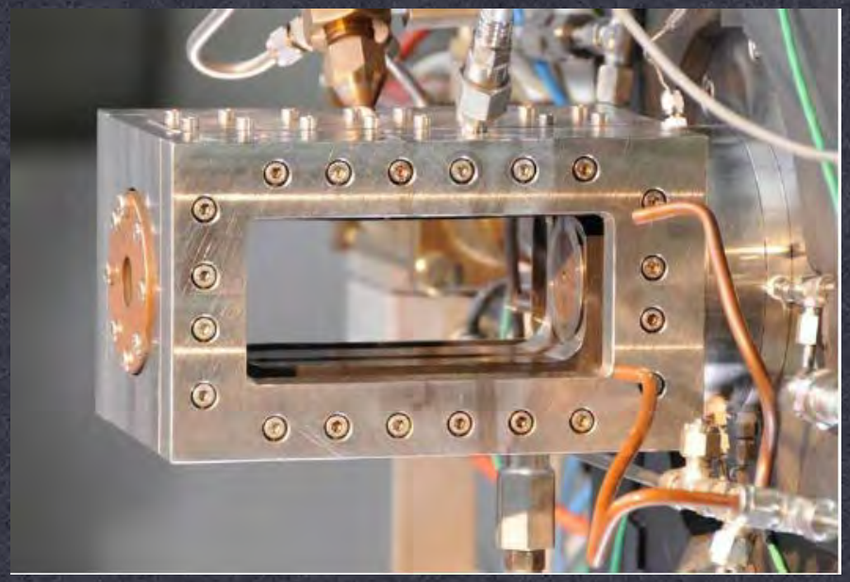
Main Topics



Target test case: Sandia flame A jet diffusion flames (www.sandia.gov/TNF/DataArch/FlameA/SandiaPilotDoc21.pdf)

Turbulent Combustion Modeling of labscale flames (KAUST)

OpenFOAM LES (P.P.Ciottoli, P.E.Lapenna, F.Creta, M.Valorani)



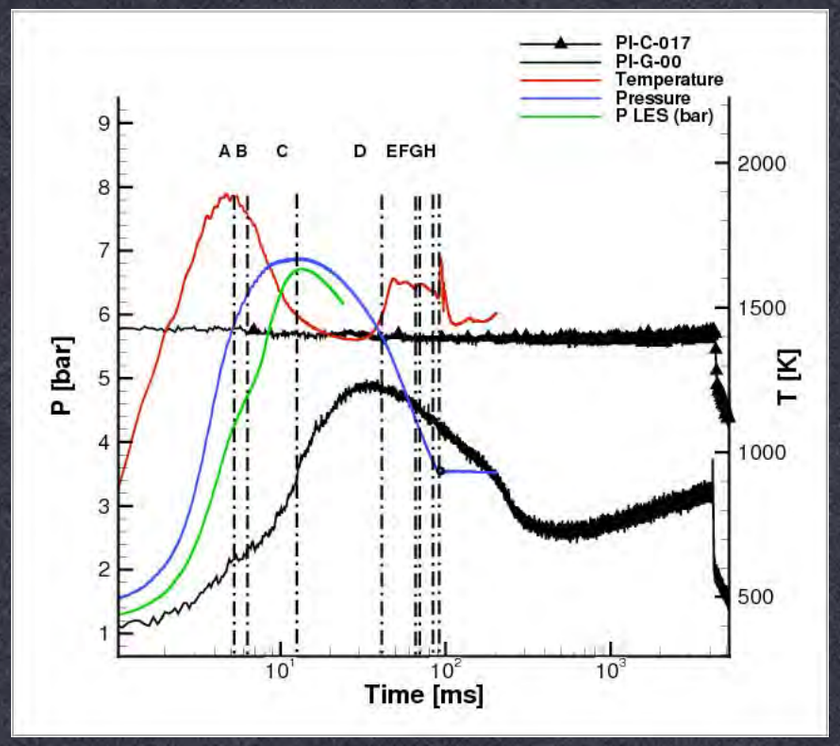
The experiment consists of triggering ignition in a well controlled gas/gas injection configuration, using a laser beam in order to control the ignition point location and energy release

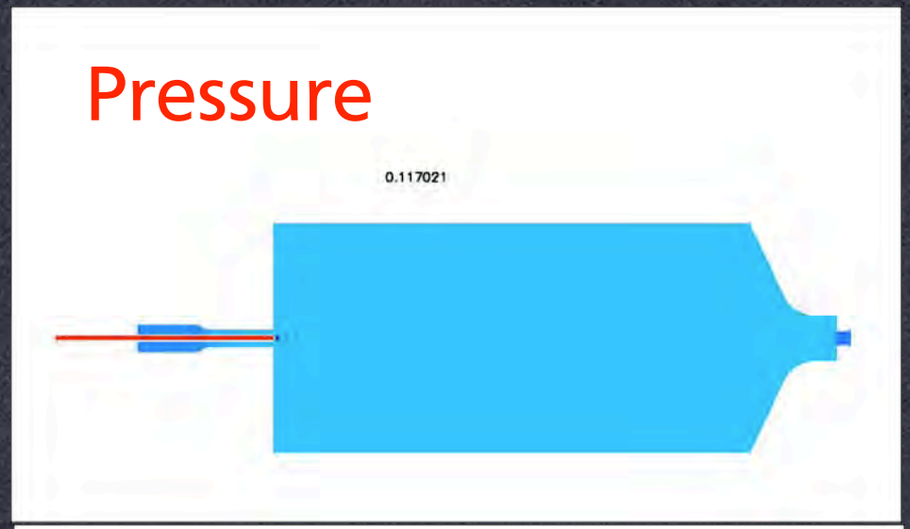
The flame kernel propagates downstream near the symmetry axis as convected by the fast central jet

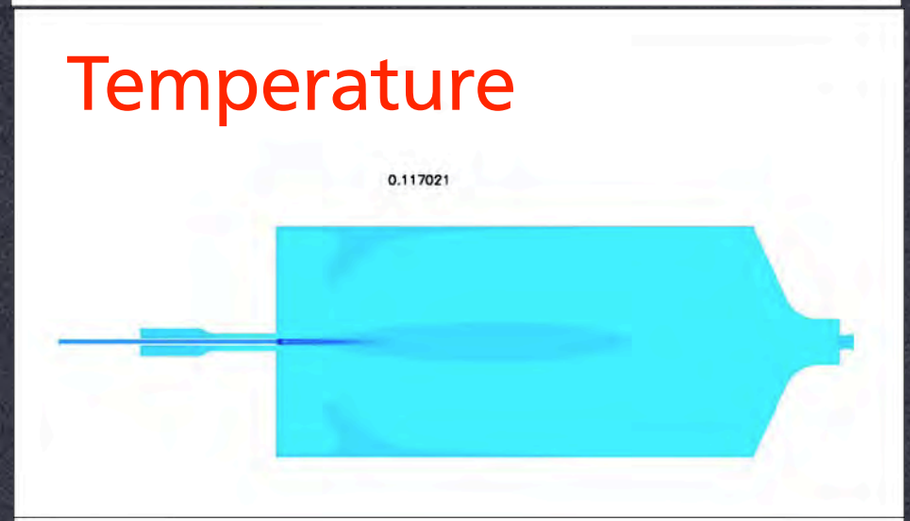
The flame kernel propagates across the recirculation region away from the axis

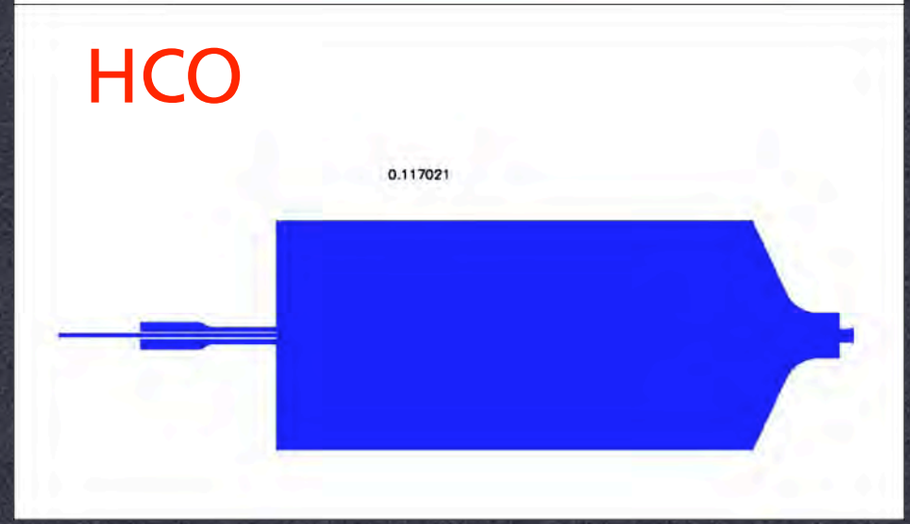
When methane is not entering the chamber anymore, the cold oxygen jet is not consumed and leaves the chamber unburned-> the temperature field at the axis becomes very cold

A significant amount of hot products is still present in the chamber ready to reignite the propellants when the chamber pressure is lowered by the mass loss through the choked nozzle



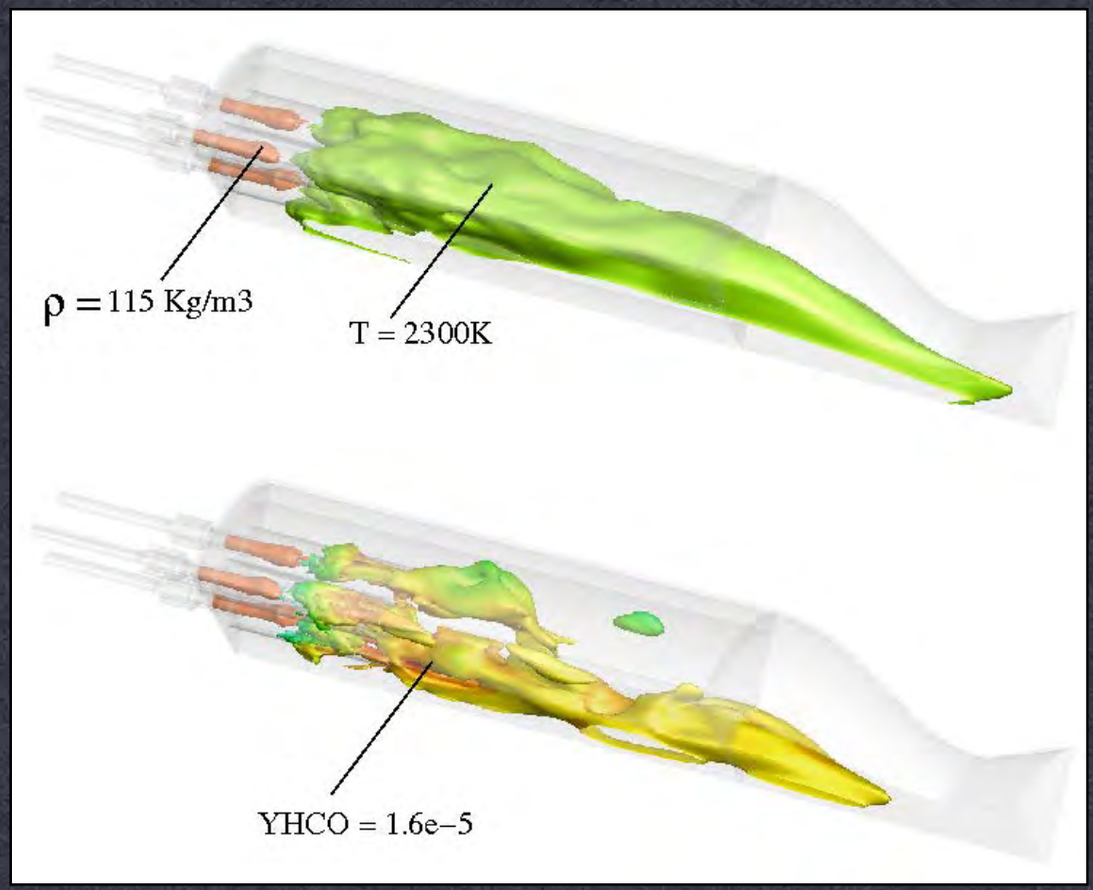


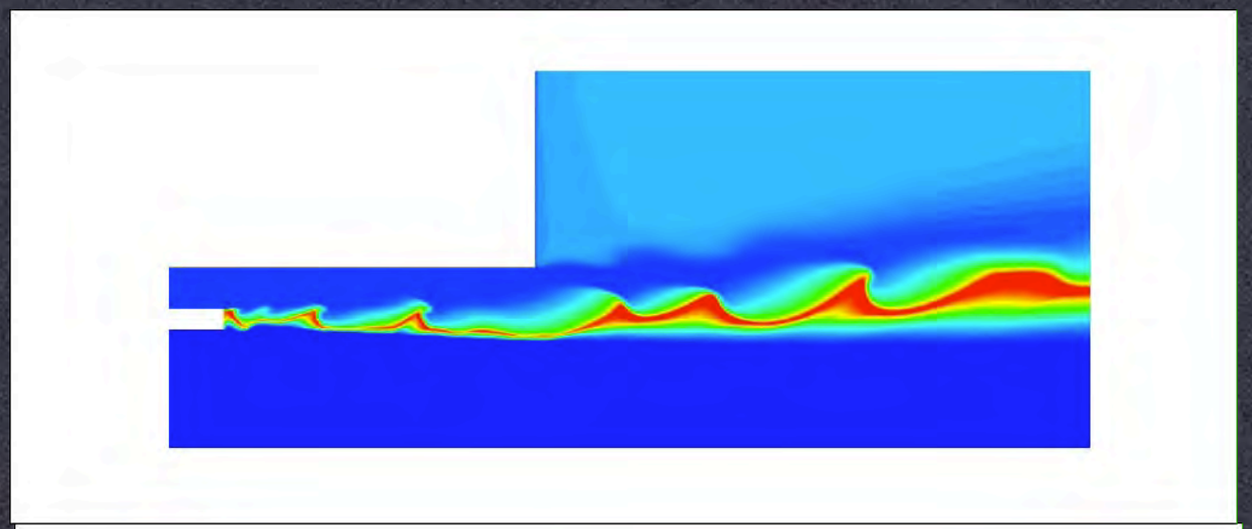


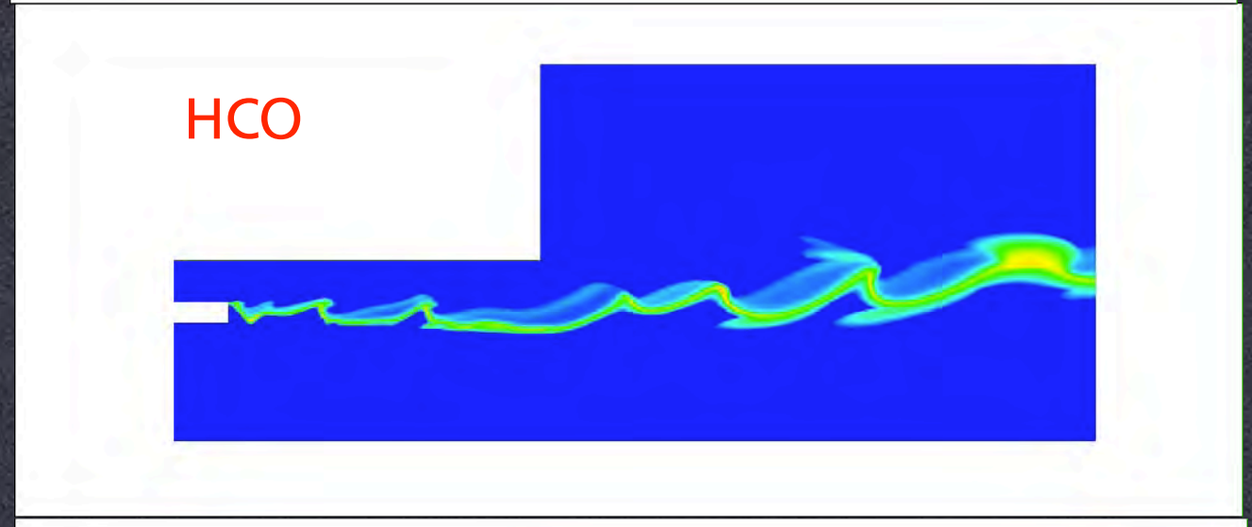


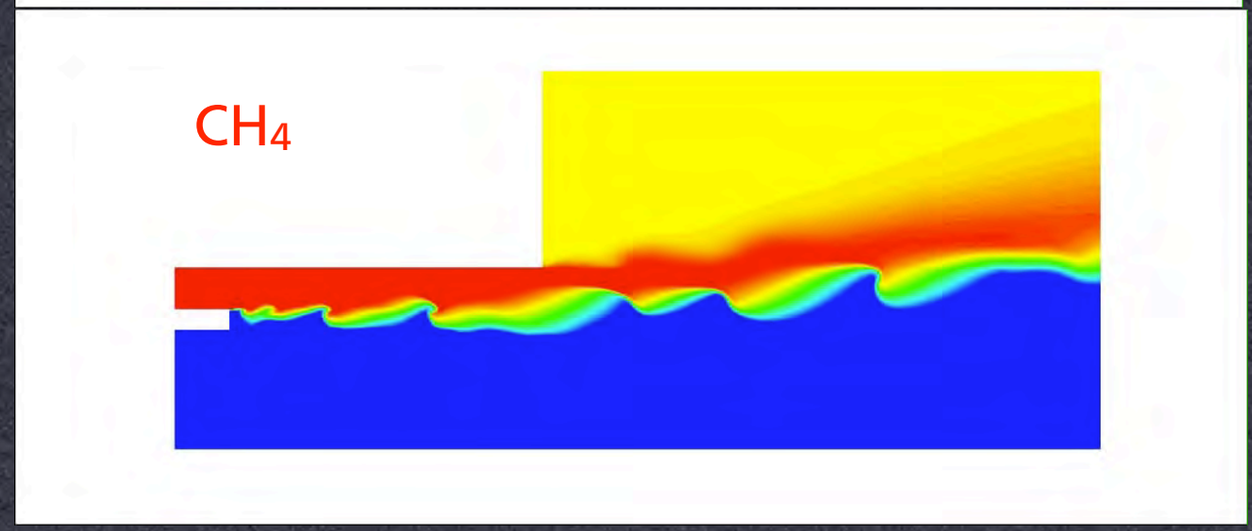
Ignition Transient in Combustion Chambers

URANS (M.Valorani, E.Martelli, P.P.Ciottoli, G.Gargiulo)









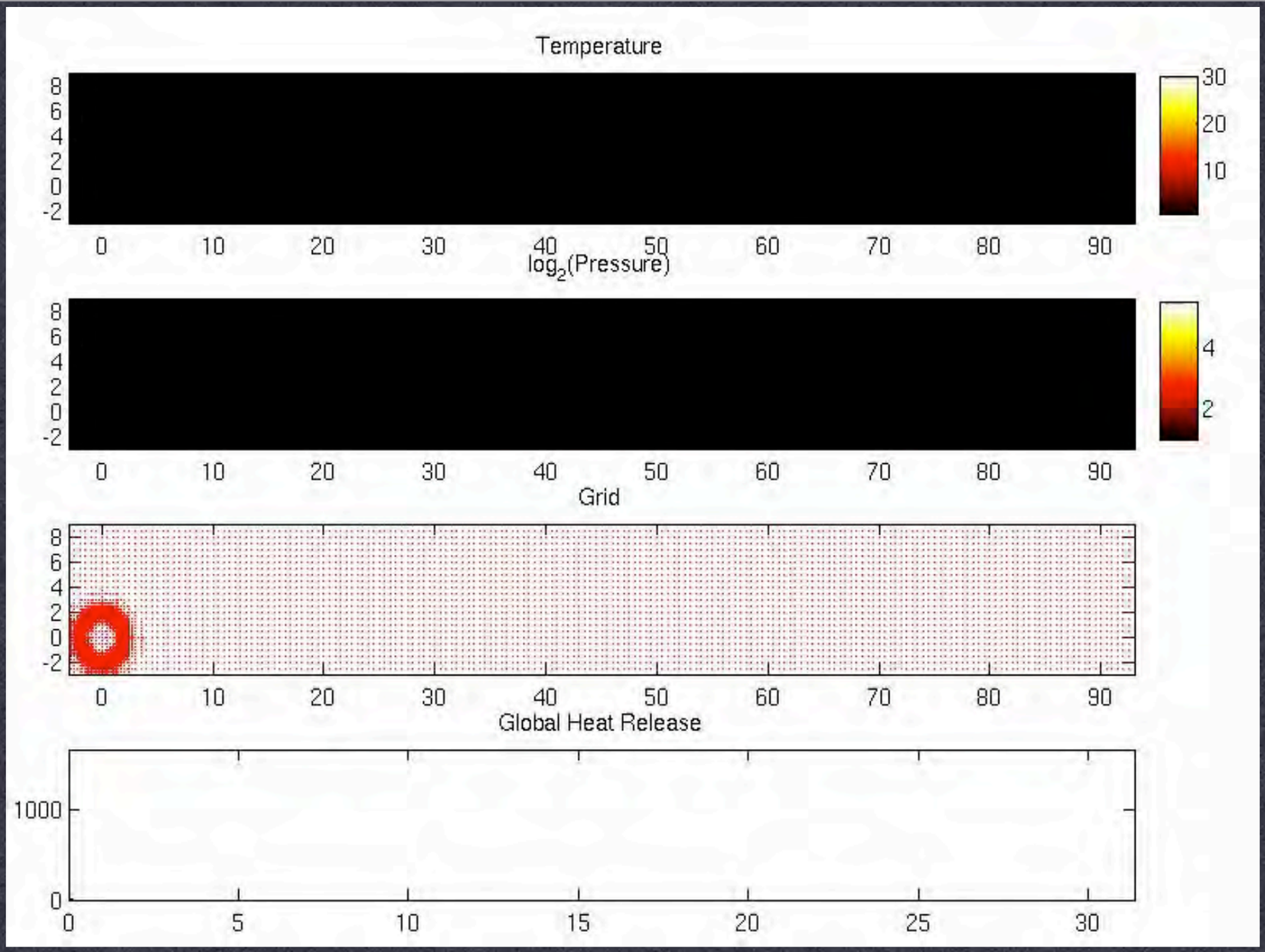
Supercritical combustion involves real gas equations of state.

Very strong density gradients occur in the mixing region formed by cryogenic oxygen and gaseous methane.

Anchoring is hindered by the high heat transfer from the flame to the cold liquid oxygen jet

Supercritical Combustion in LRE Chambers

RANS, URANS, LES (G.Gargiulo, F.Creta, M.Valorani)



IGNITION IN A CAVITY

Flames are characterized by a large spectrum of spatial and temporale scales ⇒ multi-scale problems

Direct Numerical Simulations (DNS) involves a very large number of unknowns (if a uniform mesh is used)

Dynamically adaptive wavelet collocation algorithms are ideally suited for DNS of combustion with realistic chemistry:

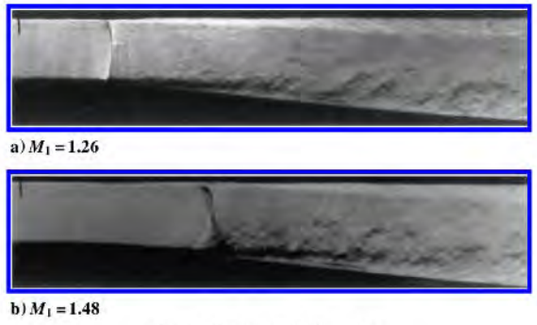
- the state functions are represented in terms of multiscale basis functions (scaling functions & wavelets), characterized by excellent localization properties both in physical and spectral space.
- adaptation is obtained by retaining only wavelets with an amplitude greater than a user defined threshold, thus providing a verified solution of prescribed accuracy and saving in computer time and memory storage.

Flame Initiation and Formation

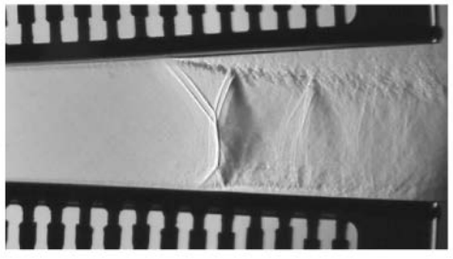
"Wavelet Adaptive Mesh Resolution" (S.Gemini,S.Paolucci, E.Martelli, M.Valorani)

Detached Eddy Simulation shock unsteadiness in an over-expanded planar nozzle

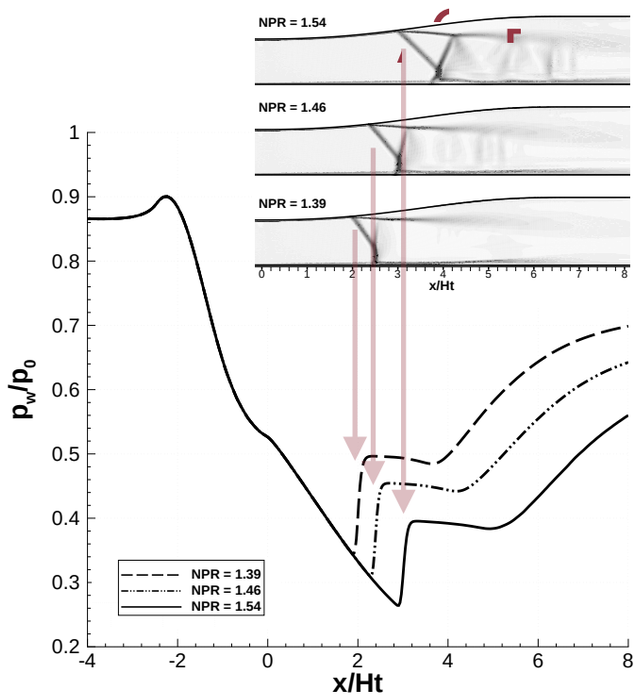
E.Martelli, P.P. Ciottoli, M. Bernardini, F. Nasuti, S. Pirozzoli, M. Valorani

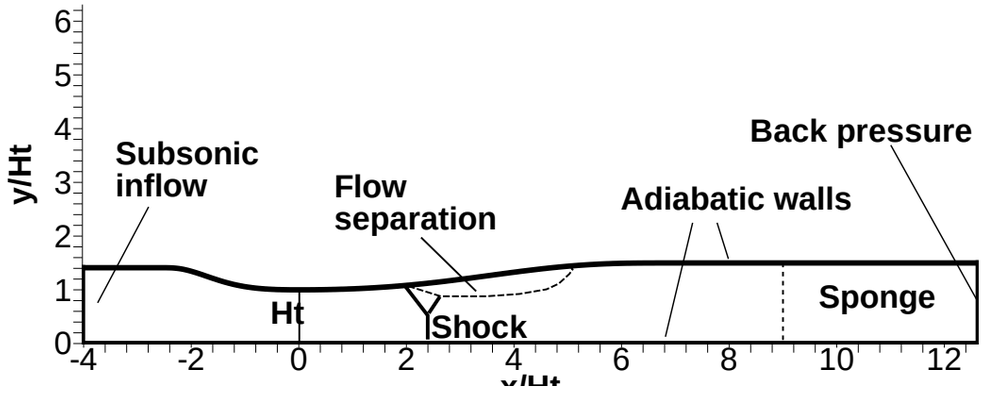


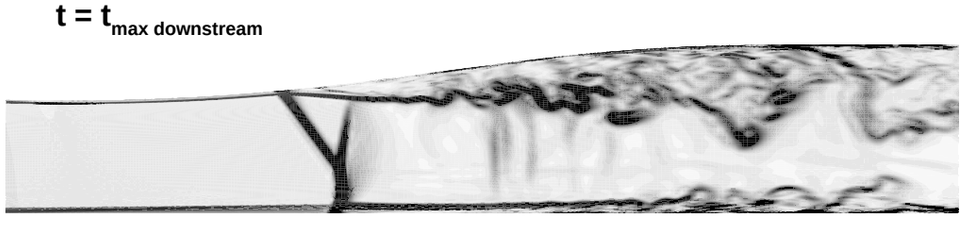
Handa, T., Masuda, M., and Matsuo, K.,

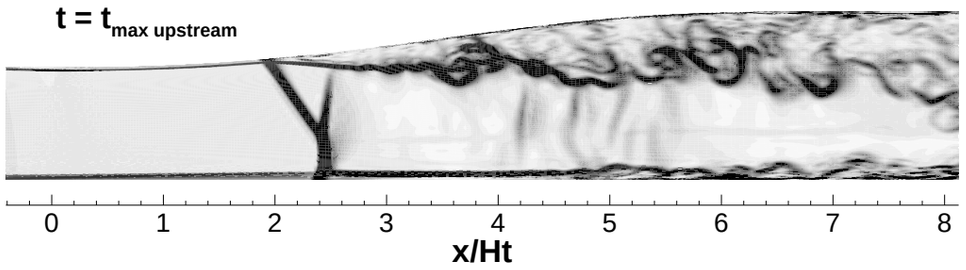


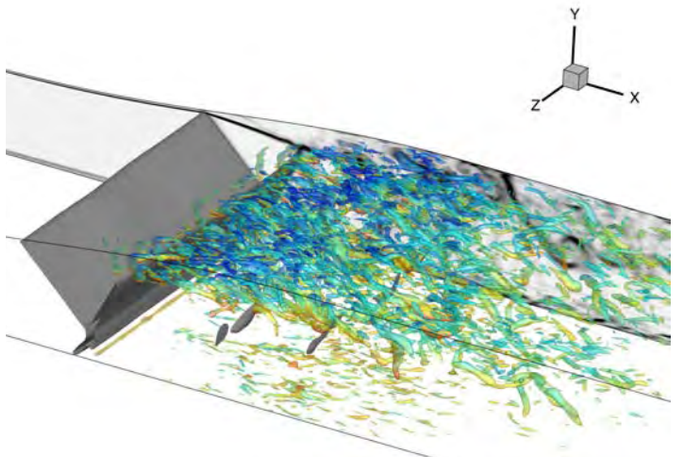
Johnson, A. D. and Papamoschou, D., “Instability

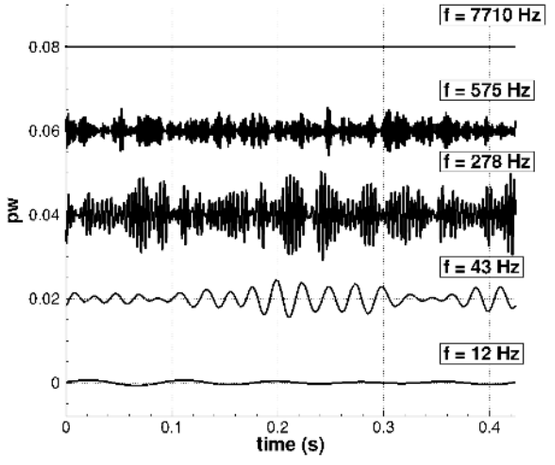


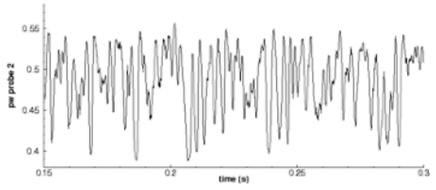


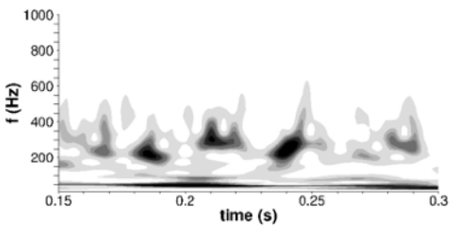




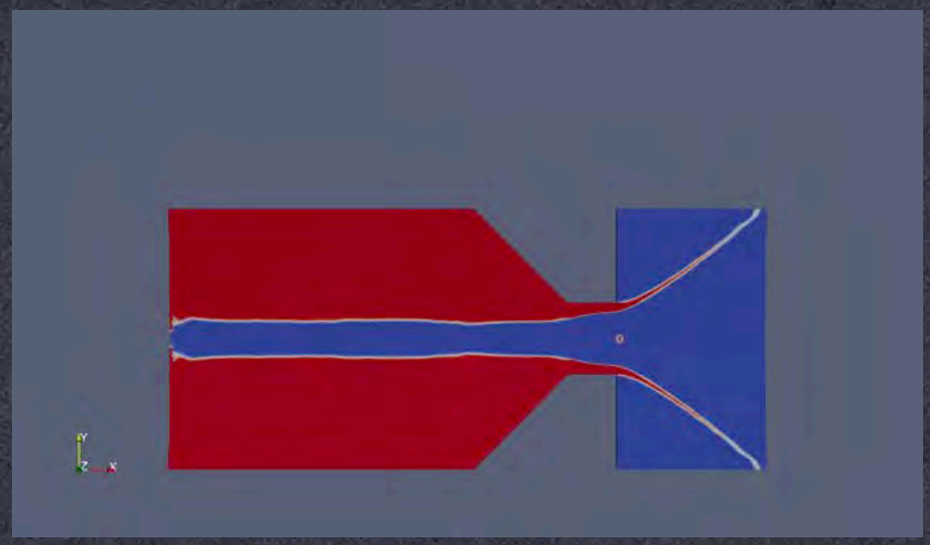








The **shock movement and the recirculating region** have been recognized to be characterized, in the time-frequency space, by a **collection of events with a modulation of the oscillation amplitude and a modulation of the frequency**



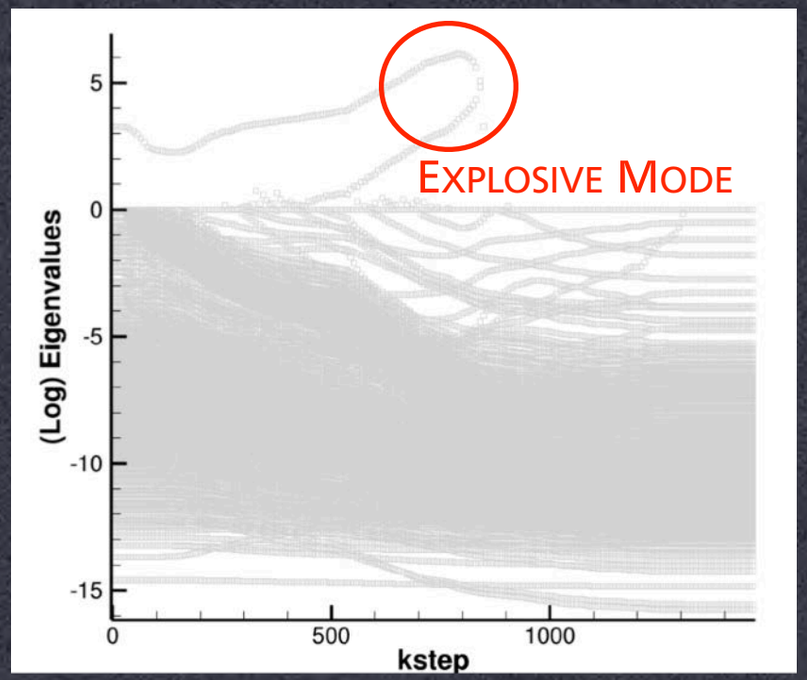
Multi-phase CFD simulations with InterFOAM solver based on the volume of fluid (VoF) method.
Top: Two dimensional axisymmetric simulation of a swirl atomizer
Bottom: Liquid jet breakup detail of the injector

Multi-Phase flow: Swirl Atomizer

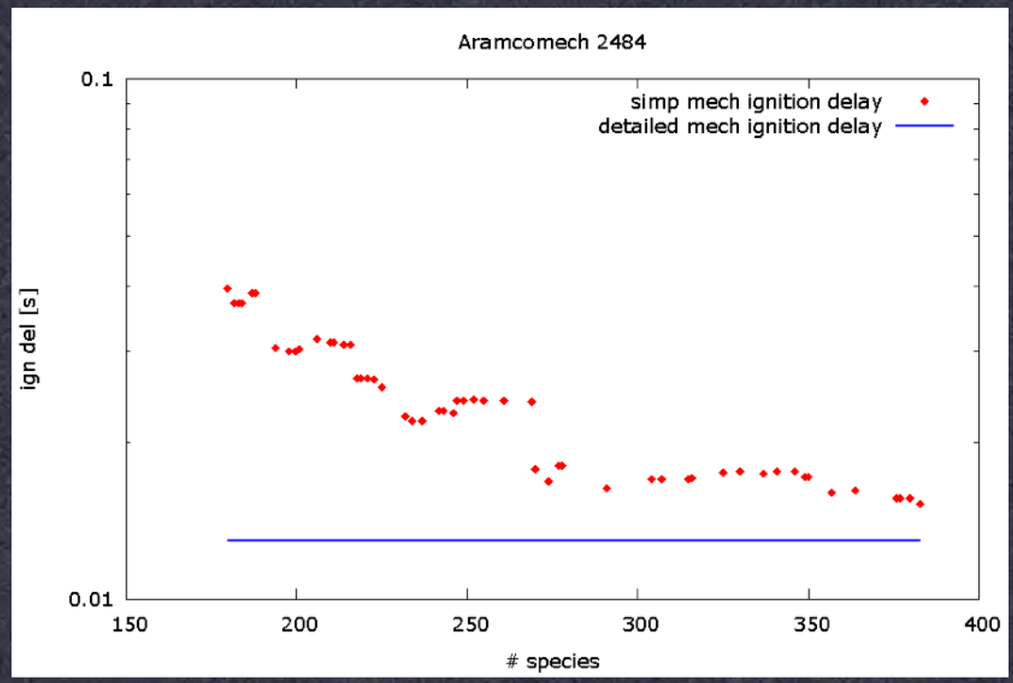
OpenFOAM RANS, LES with VoF (A. Salem, P.P.Ciottoli, M.Valorani)

Aramco Mech
2484 Species
10368 Reactions

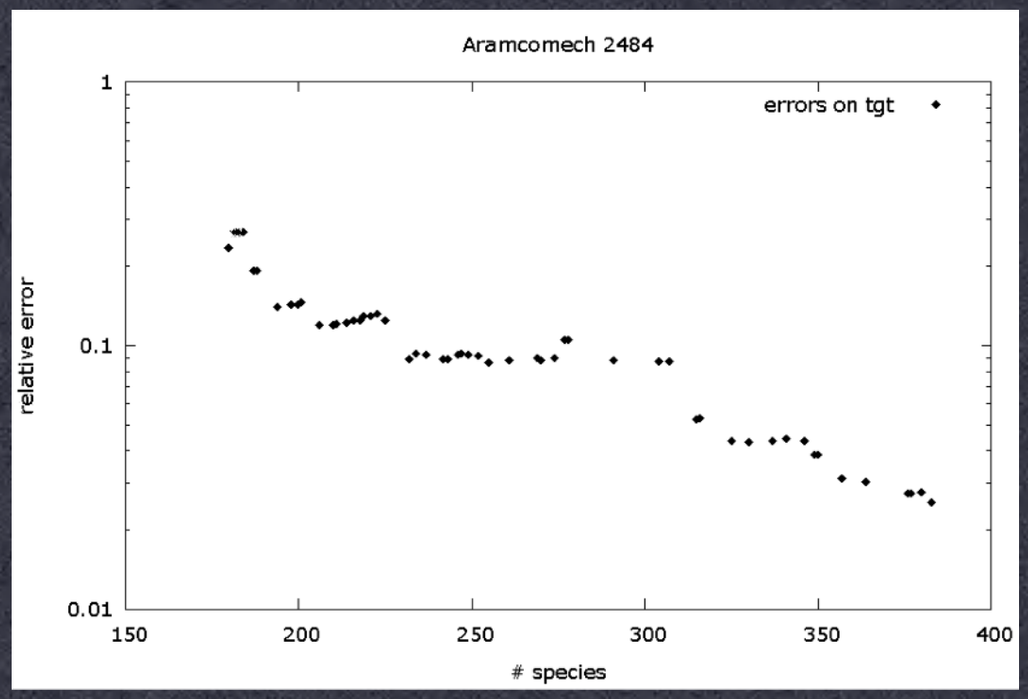
C6H5CH3	0.2923
NC7H16	0.0802
NC4H9OH	0.2756
IC8H18	0.3519



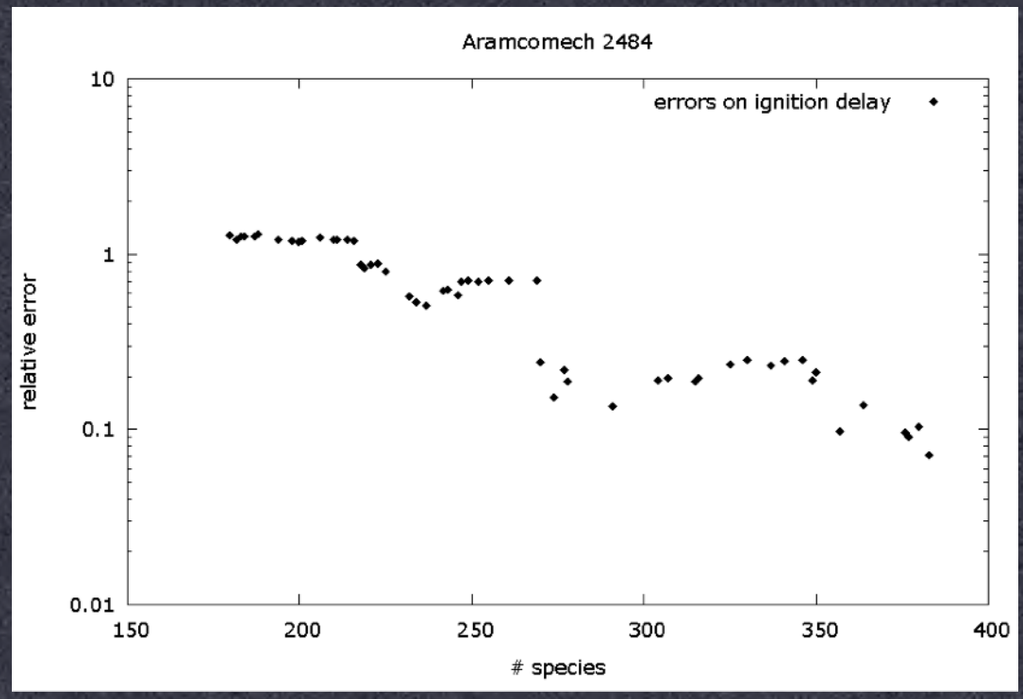
Time scales evolution



Ignition Delay Time vs Degree of Simplification



Errors on target vs # of Species



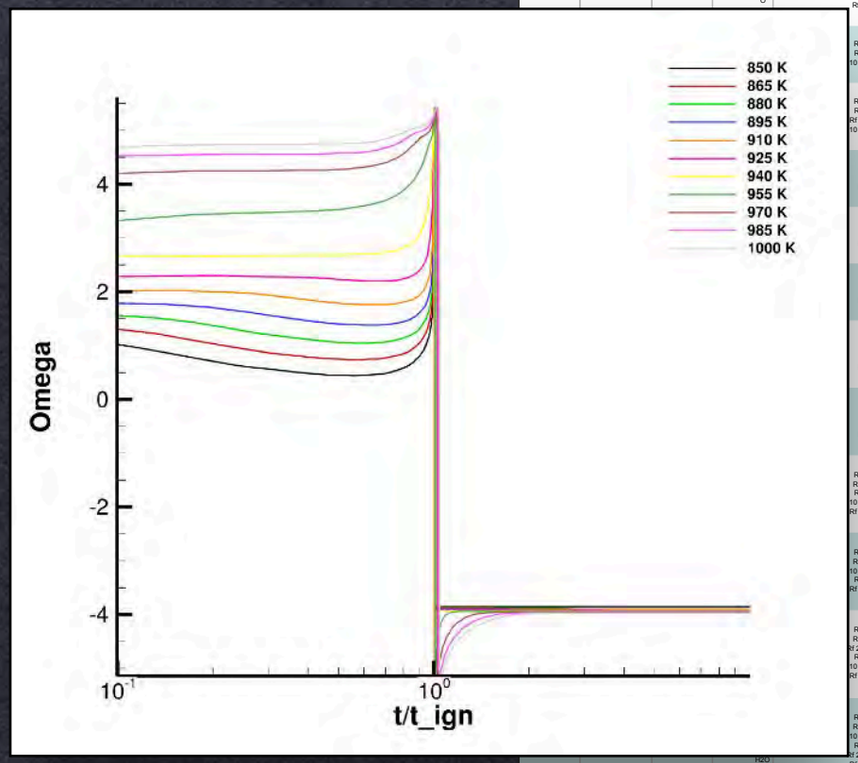
Errors on ign.time vs # of Species

Automatic Generation of Simplified Kinetic Mechanisms

M. Valorani, F. Creta, H.N. Najm, D.A. Goussis, P.P. Ciottoli, R.Malpica

Syngas Mech (H2+CO/Air)
57 Species
269 Reactions

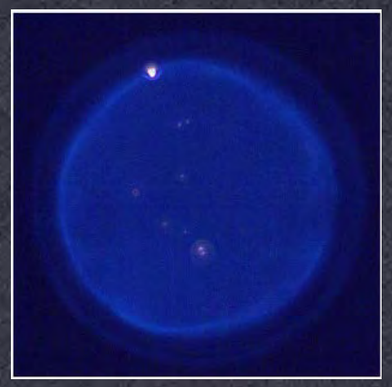
Analysis of kinetics about Crossover Temperature (950K)



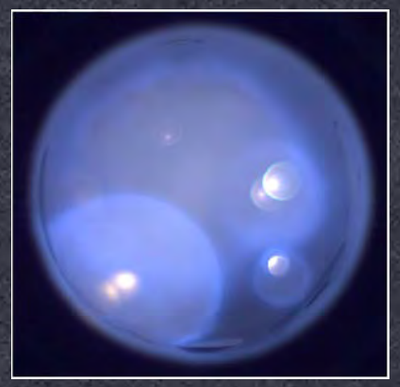
region #	time @ beginning	T @ beginning	Species	Reactions	Average PI [%]	Bar Chart
1	0.	1200.	H OH O	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O	58.36 41.38	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O
2	8.80654×10^{-8}	1200.	H OH O	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H	50.77 42.23 4.057	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H
3	2.74948×10^{-7}	1200.	H OH O	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H Rf 1 – H+O2<=>OH+O Rf 3 – H2+OH<=>H2O+H	45.27 42.58 5.46 5.173 0.6622	Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H Rf 1 – H+O2<=>OH+O Rf 3 – H2+OH<=>H2O+H
4	6.64043×10^{-7}	1200.	H O	Rf 1 – H+O2<=>OH+O Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H	27.79 26.7 26.5 12.18	Rf 1 – H+O2<=>OH+O Rb 12 – HO2+H<=>H2+O2 Rf 28 – CO+O2<=>CO2+O Rf 2 – H2+O<=>OH+H
5	4.45471×10^{-6}	1200.	H O	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H	62.88 19.39	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H
6	0.0000441018	1220.55	NaS H O	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H	51.02 21.17 11.67	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H
7	0.0000472151	1260.31	NaS H O H2	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H	42.53 20.96 13.17	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H
8	0.0000477381	1271.88	NaS H O H2	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)	40.88 20.86 13.3 5.435	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)
9	0.0000479815	1277.92	NaS H O2 O H2	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)	38.43 20.6 13.29 6.296	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)
10	0.0000491772	1314.53	NaS H O2 O H2 H2O	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)	33.3 19.67 12.75 7.762	Rf 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 3 – H2+OH<=>H2O+H Rf 10 – H+O2(+M)<=>HO2(+M)
11	0.0000493103	1319.36	NaS H O2 OH O H2 H2O	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 3 – H2+OH<=>H2O+H	30.39 18.81 12.13 10.23 8.35	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 3 – H2+OH<=>H2O+H
12	0.0000502275	1356.97	NaS H O2 OH O H2 H2O CO2	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 3 – H2+OH<=>H2O+H	27.05 17.52 11.48 10.5 8.769	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 3 – H2+OH<=>H2O+H
13	0.0000503559	1362.81	NaS H O2 OH O H2 H2O CO CO2	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 26 – CO+OH<=>CO2+H Rf 3 – H2+OH<=>H2O+H	22.94 15.26 12.63 10.64 10.45 8.447	Rf 1 – H+O2<=>OH+O Rb 1 – H+O2<=>OH+O Rf 2 – H2+O<=>OH+H Rf 10 – H+O2(+M)<=>HO2(+M) Rf 26 – CO+OH<=>CO2+H Rf 3 – H2+OH<=>H2O+H

Automatic Diagnostics of Kinetic Mechanisms

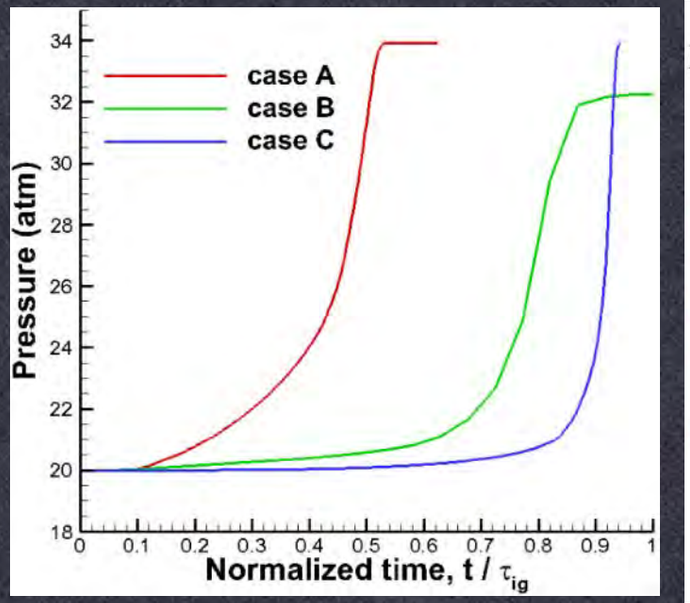
M. Valorani, P.P.Ciottoli, R.Malpica

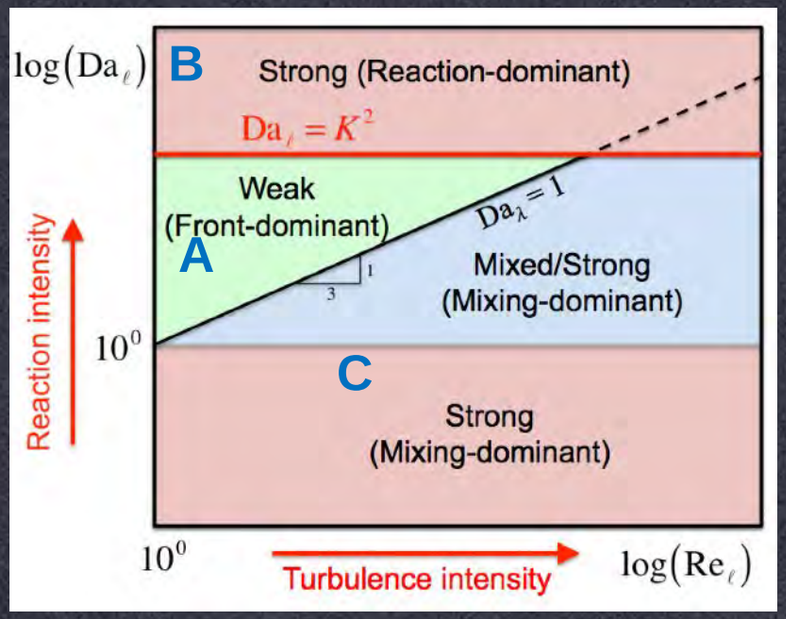


Volumetric ignition (strong)

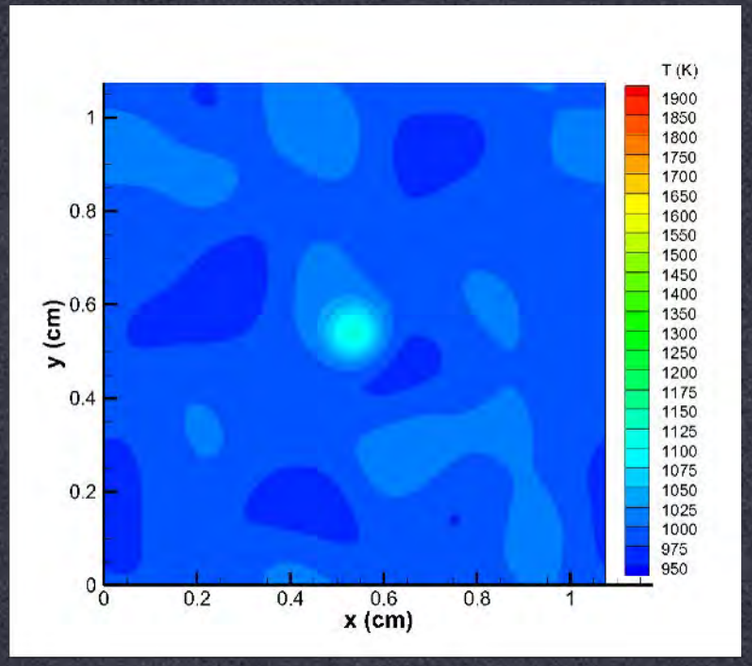


Localized ignition sites + deflagrative fronts (weak)

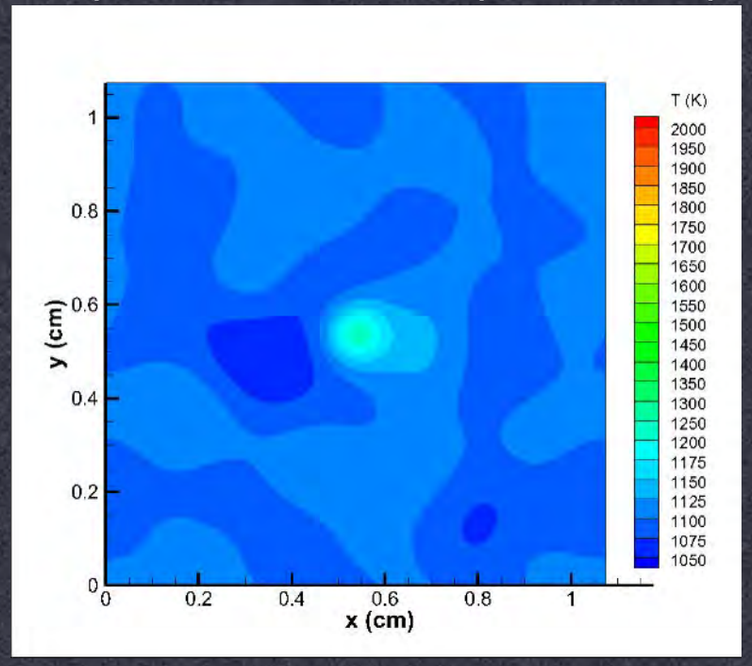




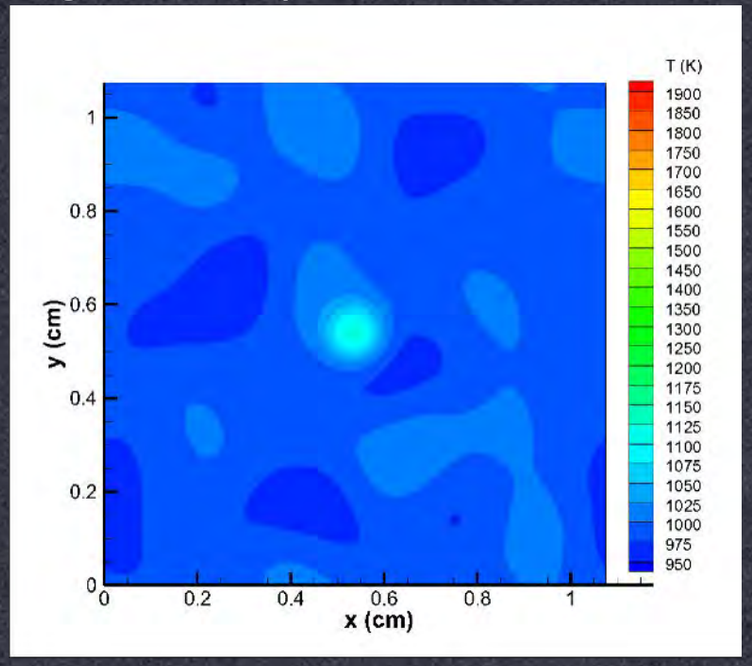
A. Weak Ignition



B. Strong Ignition (Reaction-dominant)



C. Strong Ignition (Mixing-dominant)



PREDICTION OF STRONG AND WEAK IGNITION REGIMES IN TURBULENT REACTING FLOWS WITH TEMPERATURE FLUCTUATIONS

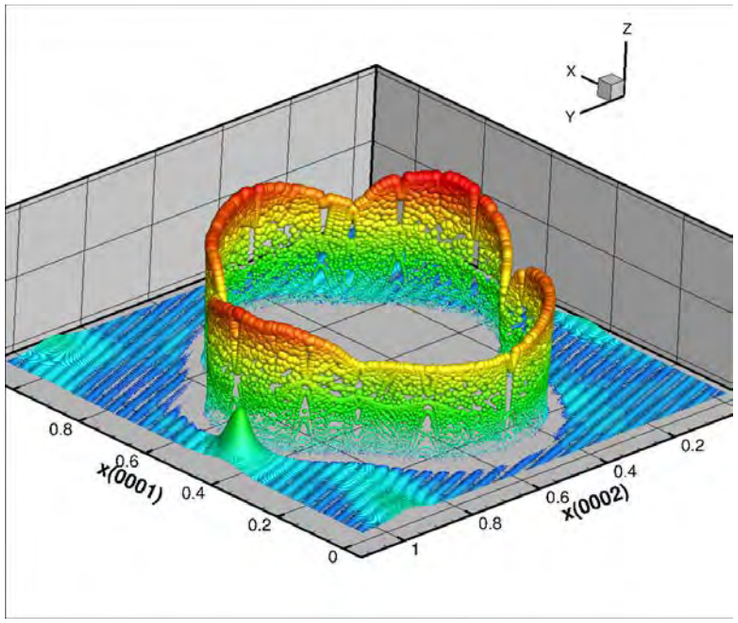
P.PINAKI, H. G. IM,P.P.CIOTTOLI,R.MALPICA,M. VALORANI

Outcomes of Year 2

Journal Articles

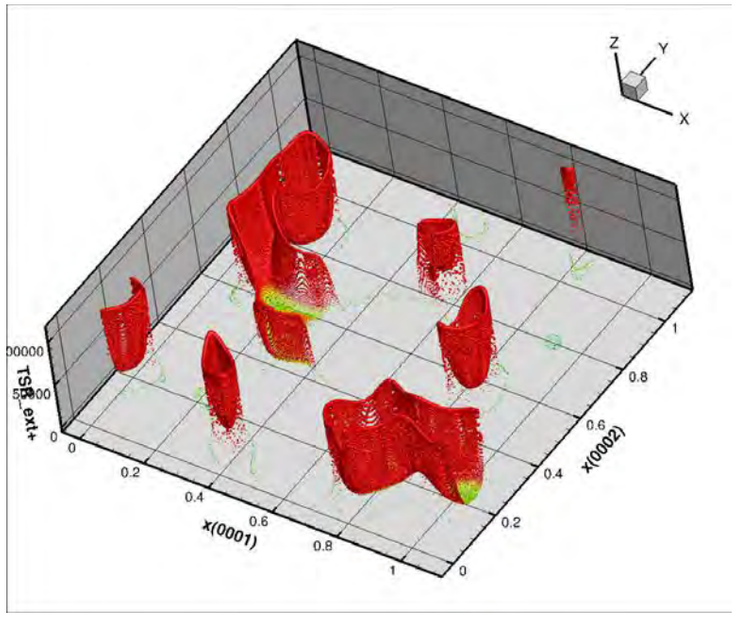
- GOAL: To predict “strong” and “weak” ignition phenomena in turbulent reacting flows with thermal inhomogeneities.

Case A
(Weak ignition)



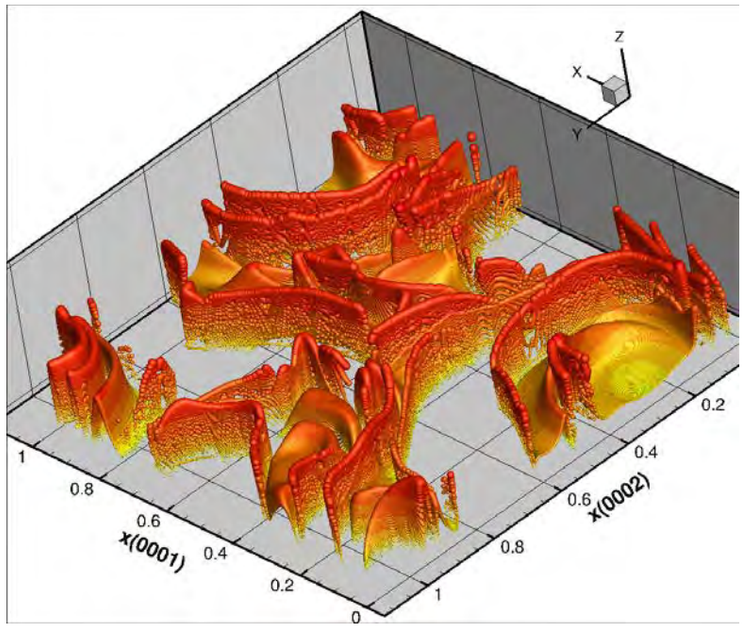
Reaction front propagates by virtue of diffusion & convection: deflagration mode

Case B
(Reaction-controlled strong ignition)



Reaction pockets occur by virtue of chemical reactions: spontaneous ignition mode

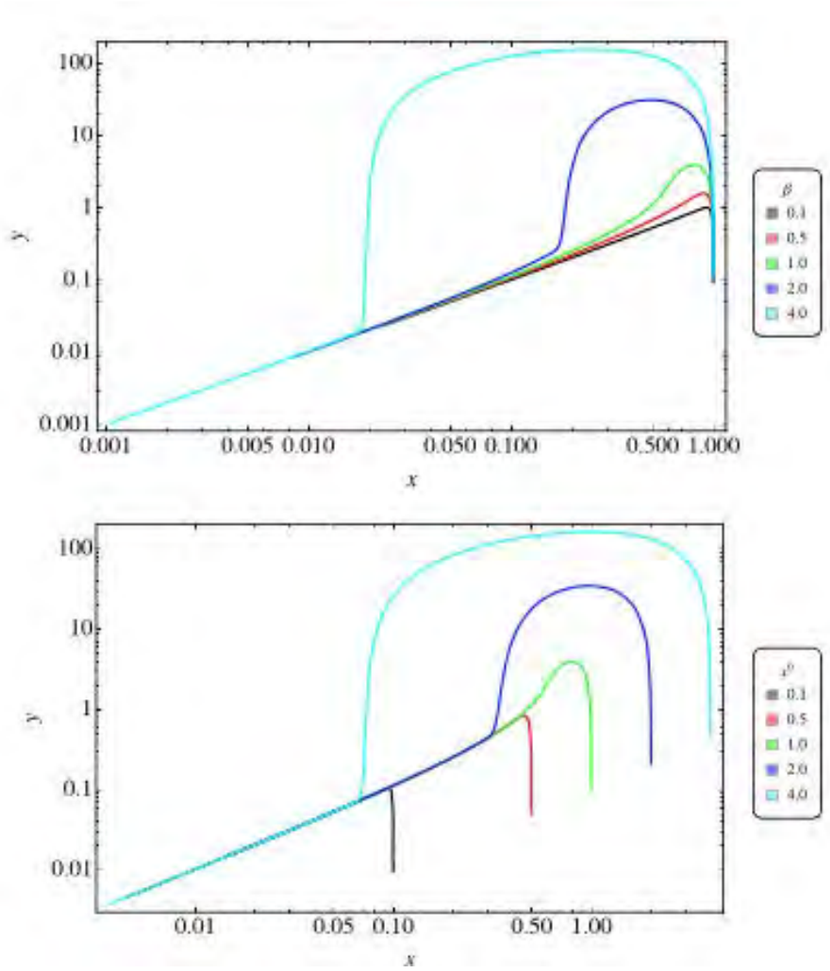
Case C
(Mixing-controlled strong ignition)



Reaction zone occur after mixing is completed: mixing-controlled strong ignition mode

Uncertain Reactive ODE Systems

- H.N.Najm, M.Valorani,“Enforcing positivity in intrusive PC-UQ methods for reactive ODE systems”, Journal of Computational Physics 270 (2014) 544–569



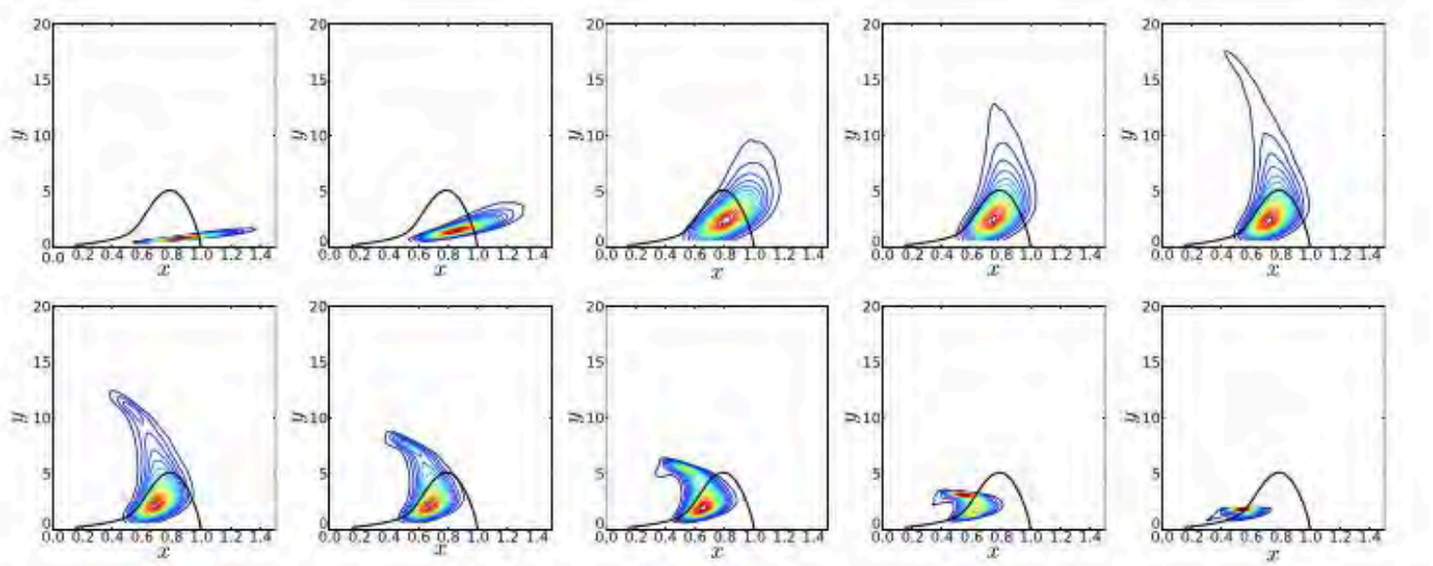


Fig. 3. Plot of the time evolution of $p(x, y)$. The frame time sequence is for $t = 0.01, 0.02, 0.04, 0.06, 0.07, 0.08, 0.09, 0.10, 0.12, 0.15$, ordered left to right and top to bottom. The frames are all on the same scale, with the horizontal axis showing $x \in [0, 1.5]$, and the vertical axis showing $y \in [0, 20]$. Using MC sampling, for the Case 1, superposed on the mean (x, y) trajectory.

Chemical Model Reduction under Uncertainty

- R.Malpica Galassi, M.Valorani, H.N.Najm, C.Safta, M.Khalil, P.P.Ciottoli, "Chemical Model Reduction under Uncertainty", paper submitted to 36th Symposium Combustion 2016.

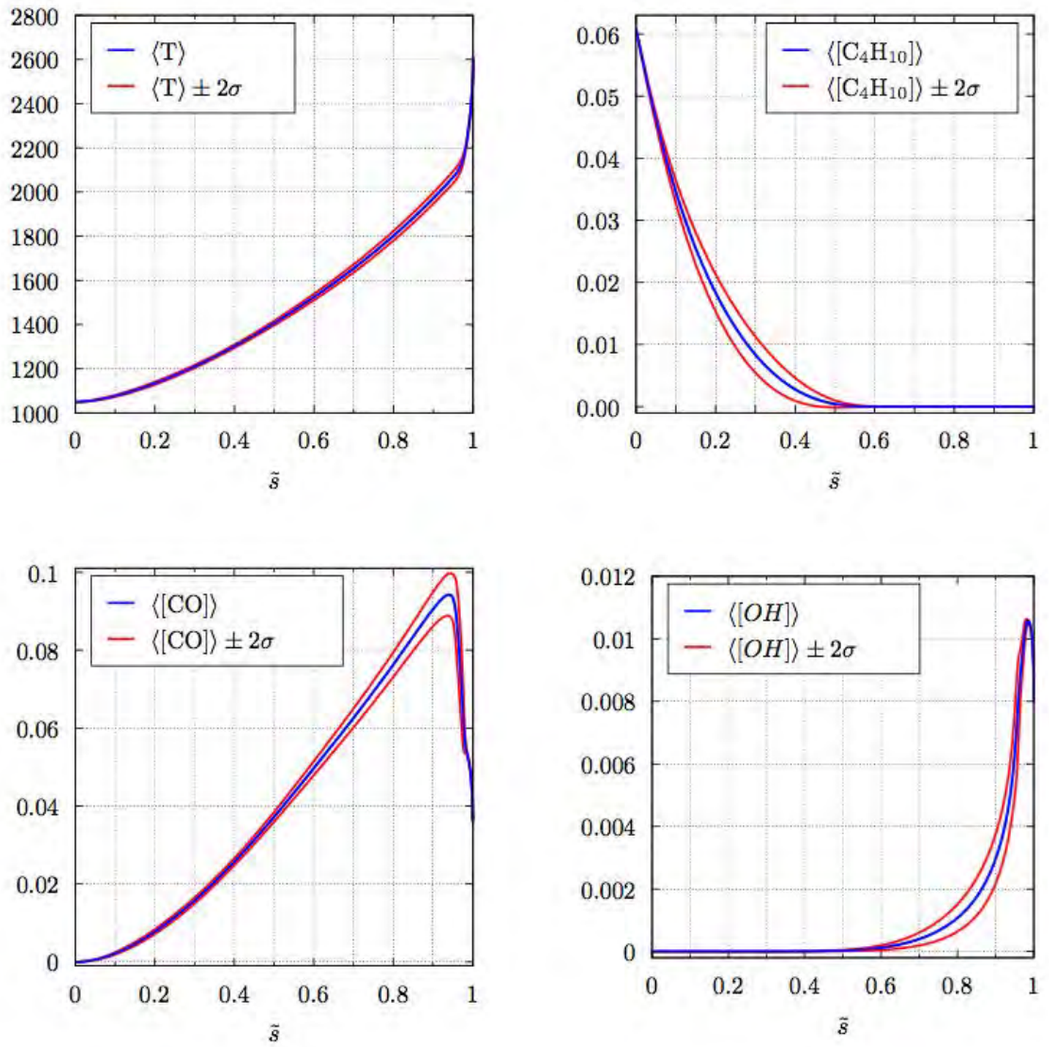


Figure 1: Average temperature, C_4H_{10}, CO and OH trajectories, with 2 standard deviation bounds

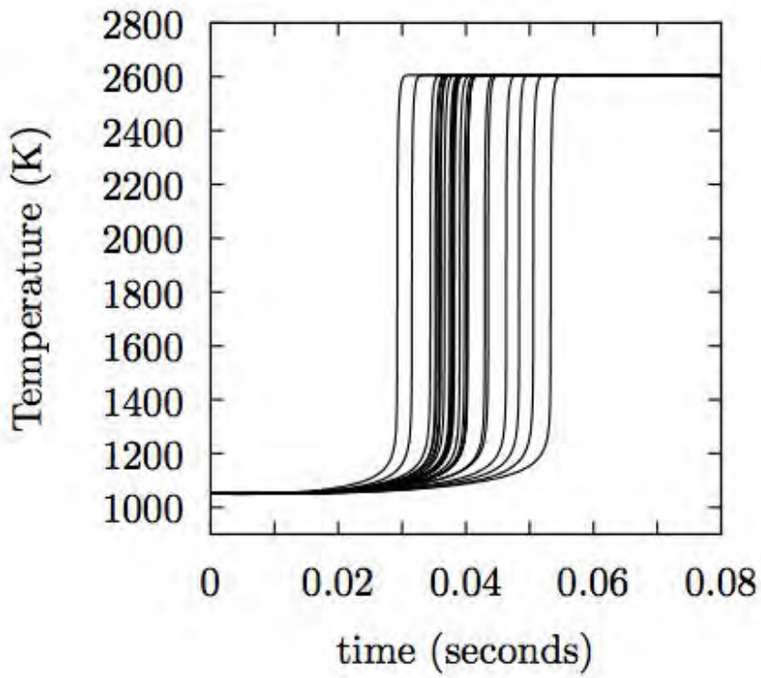


Figure 2: Temperature evolution in time for a number of samples

Chemical Model Reduction under Uncertainty

- R.Malpica Galassi, M.Valorani, H.N.Najm, C.Safta, M.Khalil, P.P.Ciottoli, "Chemical Model Reduction under Uncertainty", paper submitted to 36th Symposium Combustion 2016.

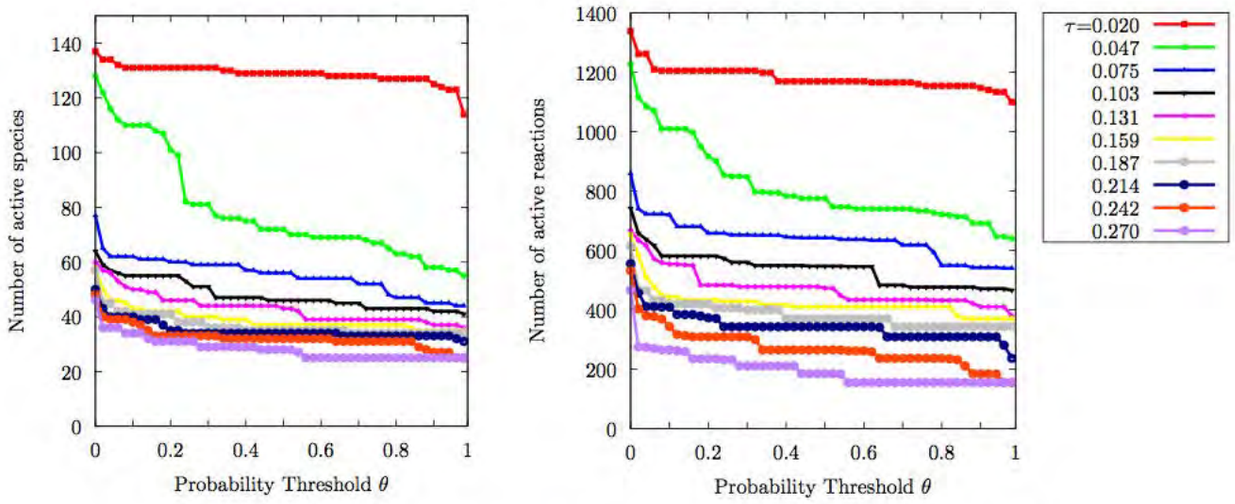
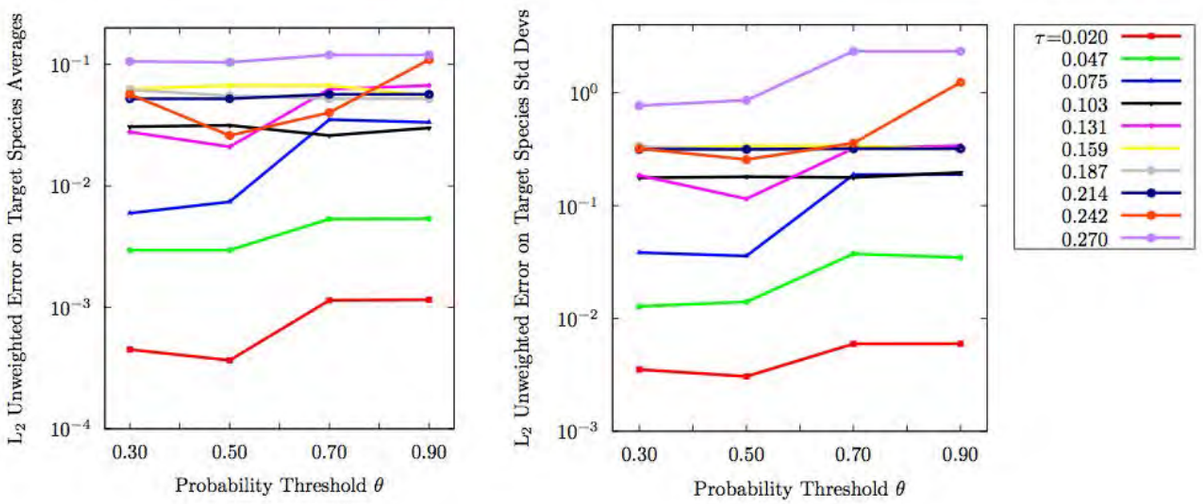
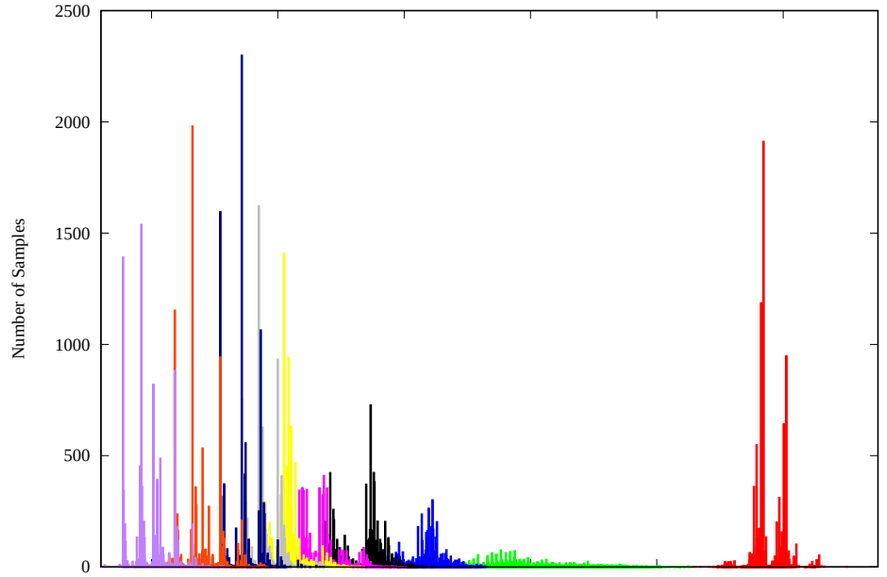


Figure 4: Number of retained/active species and reactions with increasing τ and θ

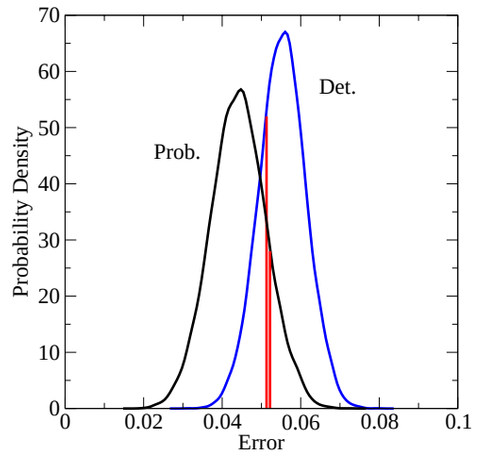


(a) (b)

Figure 6: Average over the target species of the L_2 un-weighted relative errors of the mean (left) and standard deviation (right) transient evolution against θ thresholds for given τ tolerances



PDF of mechanism size at different threshold of importance



Performance of deterministic vs probabilistic reduction

Solvers for Systems of Stiff ODEs

- G-Scheme with re-use of CSP basis

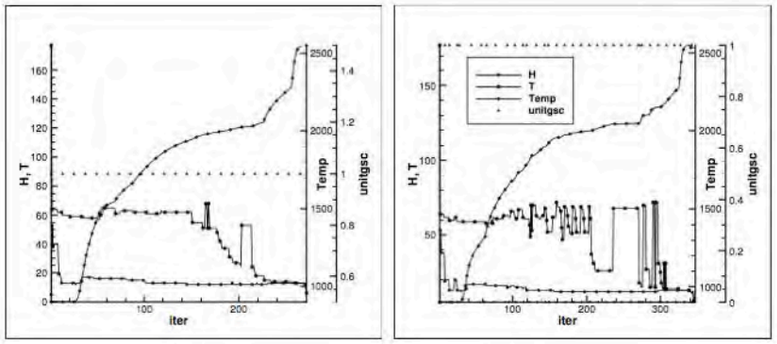


Figure 17: n-Butane. Without (left) and with (right) reuse of Jacobian and Basis. Evolution of head (square symbols) and tail (circle) dimensions; temperature evolution (diamond) and update(1)/reuse(0) (gradient)

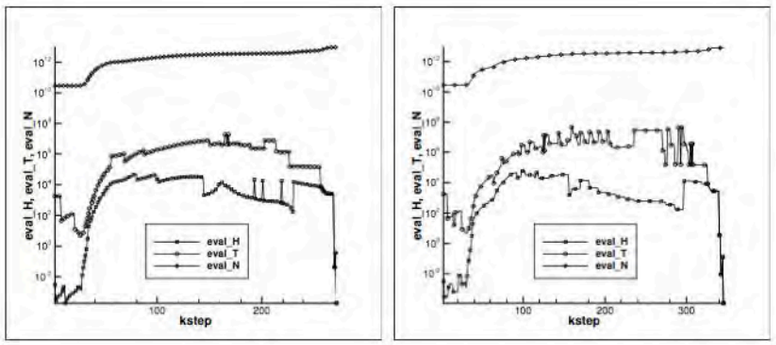


Figure 18: n-Butane. Without (left) and with (right) reuse of Jacobian and Basis. Evolution of head (square symbols), tail (circle), and fastest (diamond) time scales (reciprocal).

CPU Time: number of state variables N = N_s +1 (Temperature); rtol = 10^{-4}, 10^{-3}, 10^{-2}

N vars	CVODE N Iters	GSC N Iters	CPU CVODE (s)	CPU GSC (s)	CPU GSC/CVODE
33	1161	233	0.05013	0.063311	1.26294
54	1310	251	0.095707	0.152625	1.59471
119	1675	298	0.290572	0.705717	2.42872
177	1615	281	0.489075	1.96473	4.01724
562	1434	308	4.65785	47.7425	10.2499

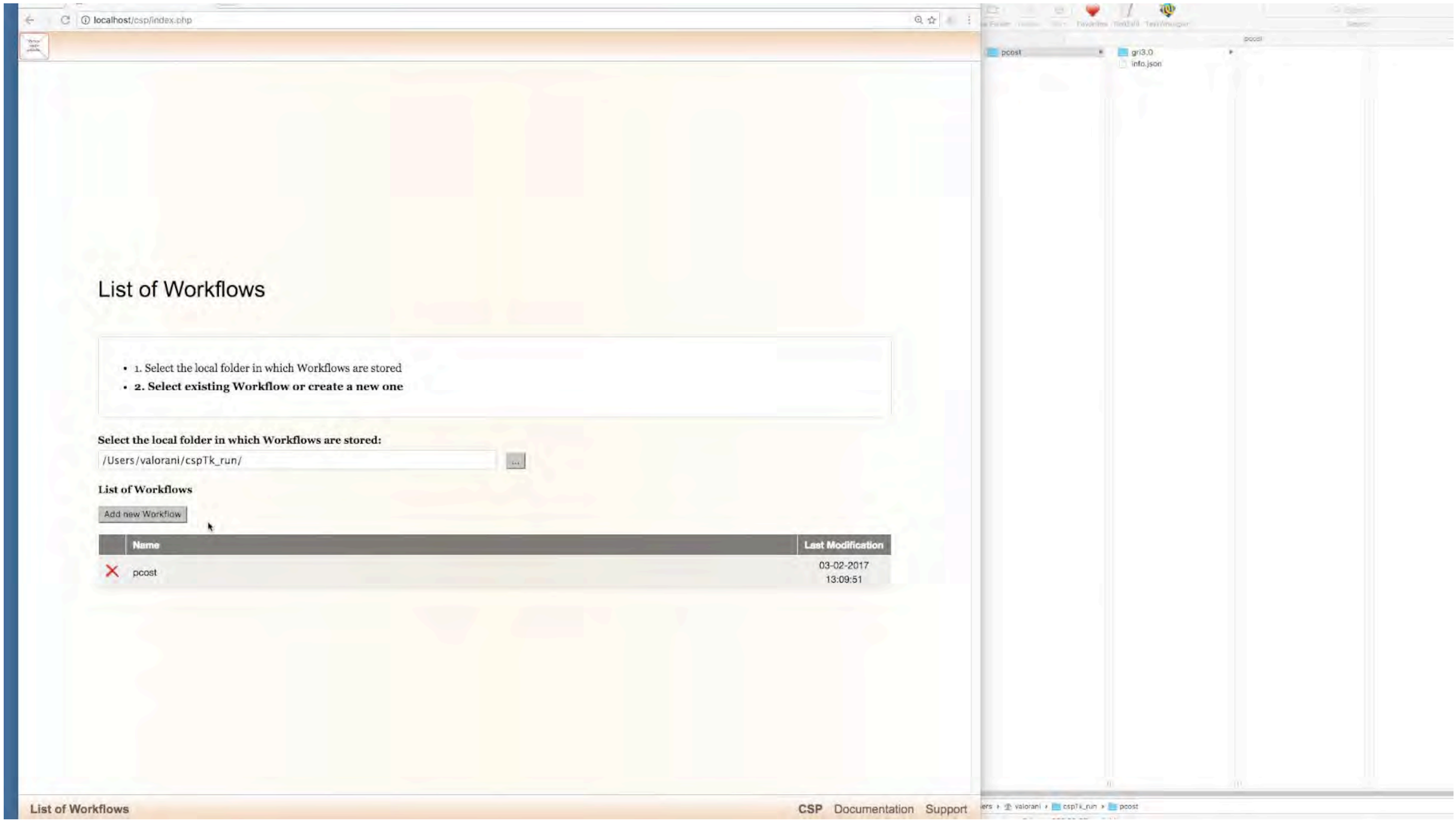
N vars	CVODE N Iters	GSC N Iters	CPU CVODE (s)	CPU GSC (s)	CPU GSC/CVODE
33	1161	200	0.05013	0.055073	1.0986
54	1310	200	0.095707	0.13264	1.3859
119	1675	217	0.290572	0.571197	1.96577
177	1615	203	0.489075	1.60425	3.28017
562	1434	227	4.65785	36.8613	7.9138

N vars	CVODE N Iters	GSC N Iters	CPU CVODE (s)	CPU GSC (s)	CPU GSC/CVODE
33	1161	592	0.05013	0.123645	2.46649
54	1310	497	0.095707	0.241588	2.52425
119	1675	323	0.290572	0.680094	2.34054
177	1615	376	0.489075	2.00814	4.10599
562	1434	327	4.65785	39.2042	8.4168

N vars	CVODE N Iters	GSC N Iters	CPU CVODE (s)	CPU GSC (s)	CPU GSC/CVODE
33	1161	619	0.05013	0.133874	2.67054
54	1310	563	0.095707	0.267126	2.79108
119	1675	656	0.290572	0.980779	3.37534
177	1615	598	0.489075	2.54091	5.19534
562	1434	411	4.65785	41.4817	8.90577

Uniroma1 & NTUA Contribution

How CSPTk runs



Uniroma1 & NTUA Contribution

What comes out from CSPTk