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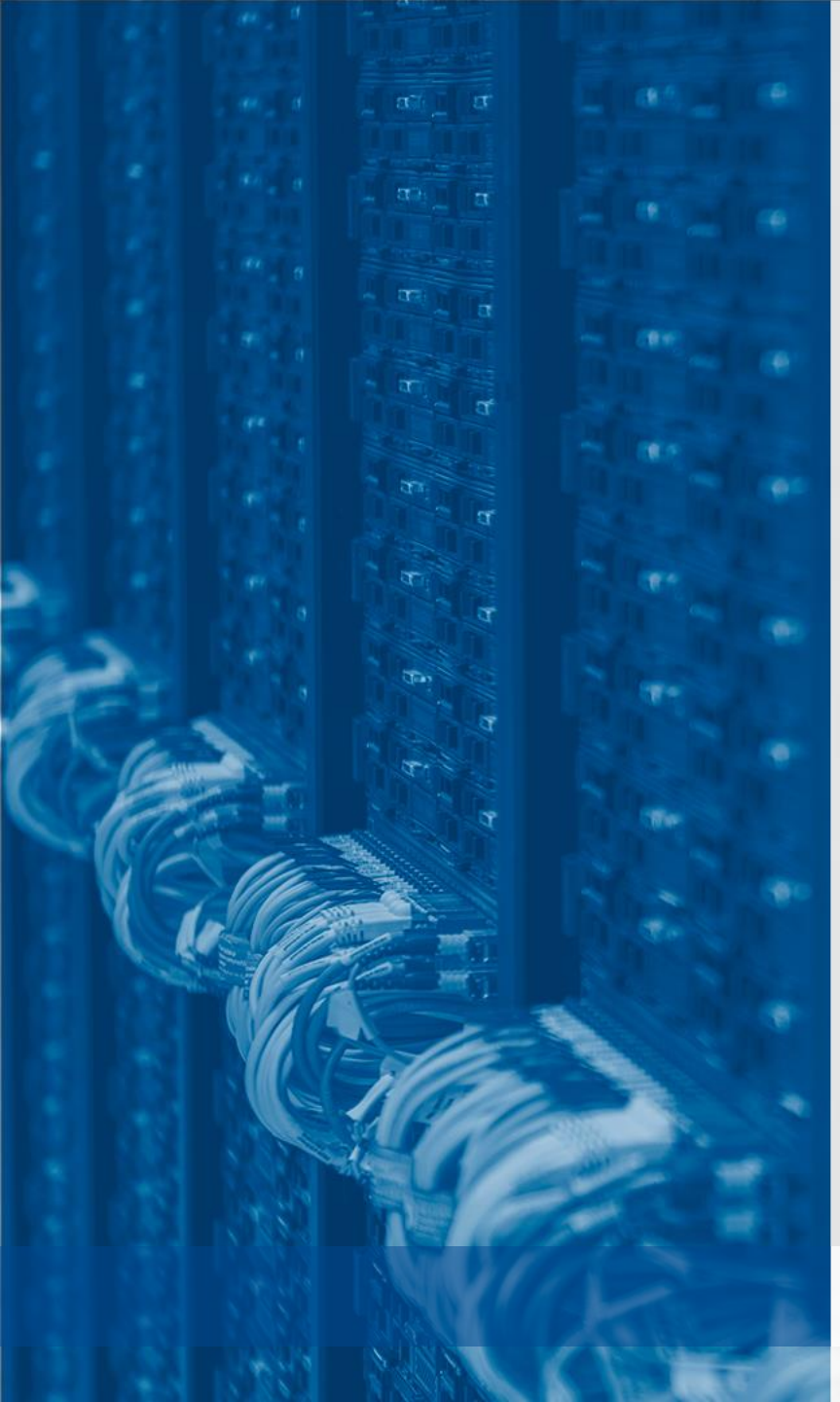
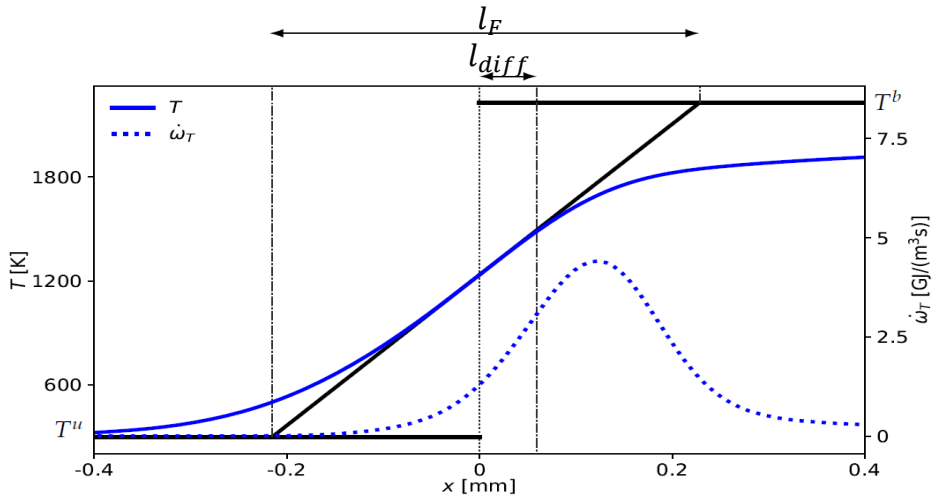


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Hands on session: CFD

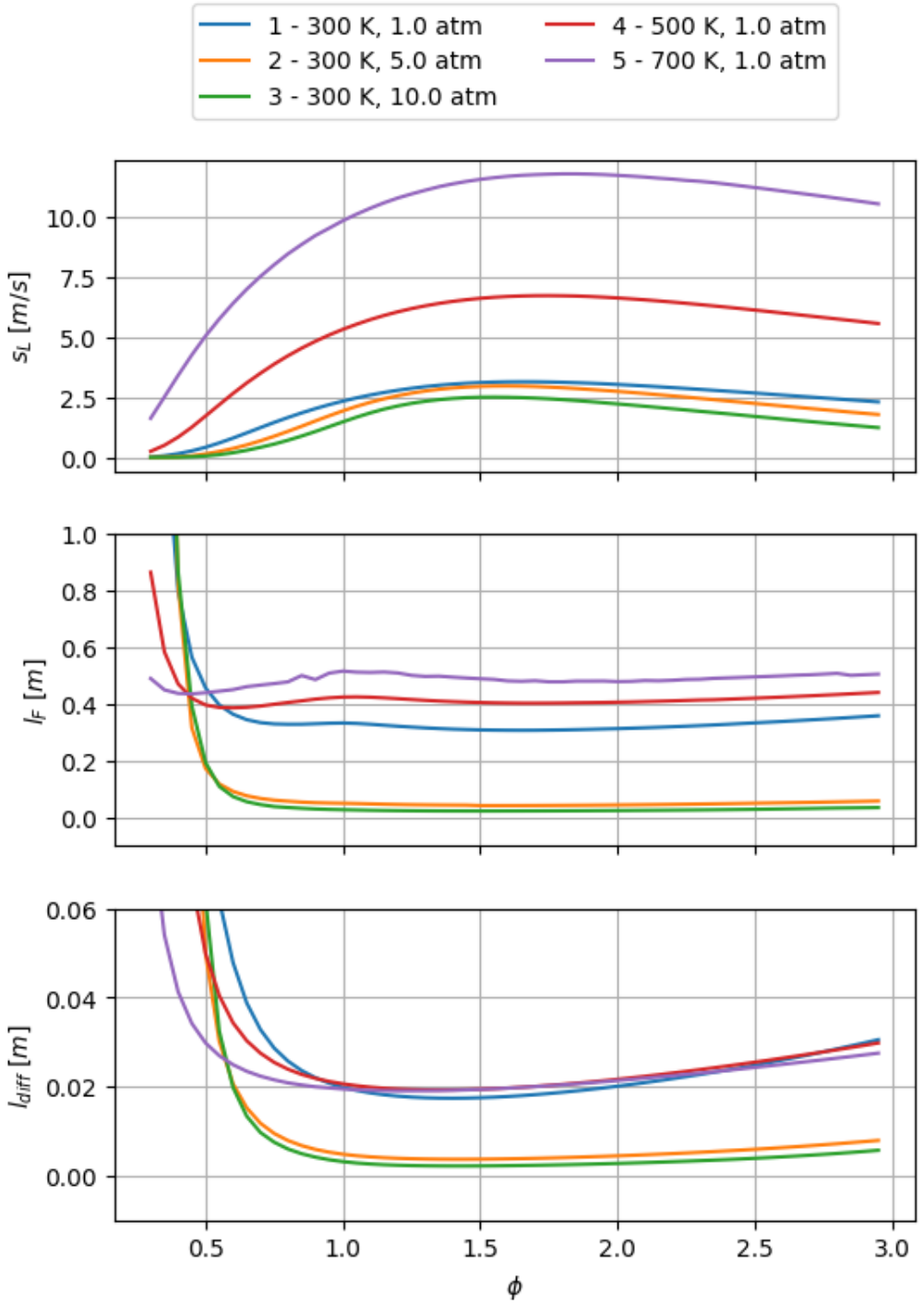
Emiliano M. Fortes, Daniel Mira

Previous results

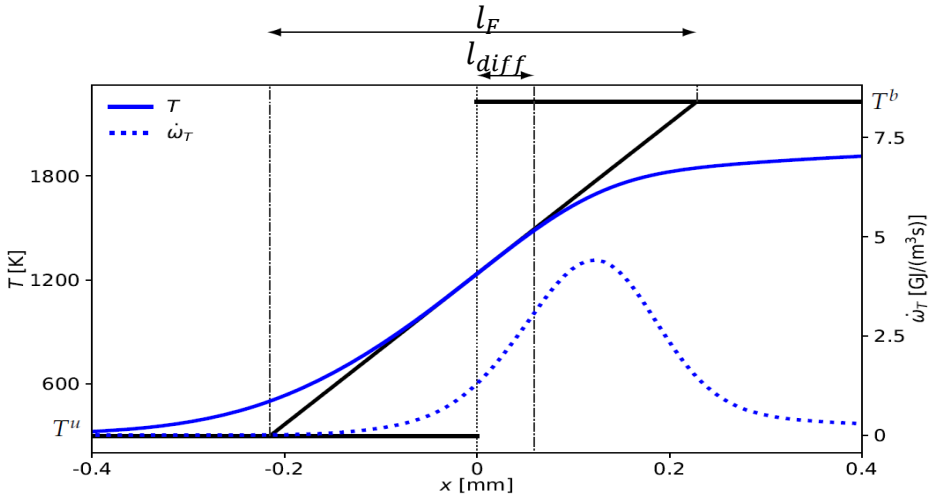


- Thermal flame thickness $l_F = \frac{T^b - T^u}{\max\left(\frac{dT}{dx}\right)}$
  - Provides a good estimate of the reaction zone size
  - Useful as length scale references and time scale reference $\tau = \frac{l_F}{s_L}$
- Diffusive thickness $l_{diff} = \frac{D_t^u}{s_L}$
  - Much lower values
  - An estimate of the scale of ignition for fresh reactants

Previous results



- Flame speed
  - Increases with temperature
  - Decreases with pressure
- Flame thickness
  - Increases with temperature
  - Decreases with pressure

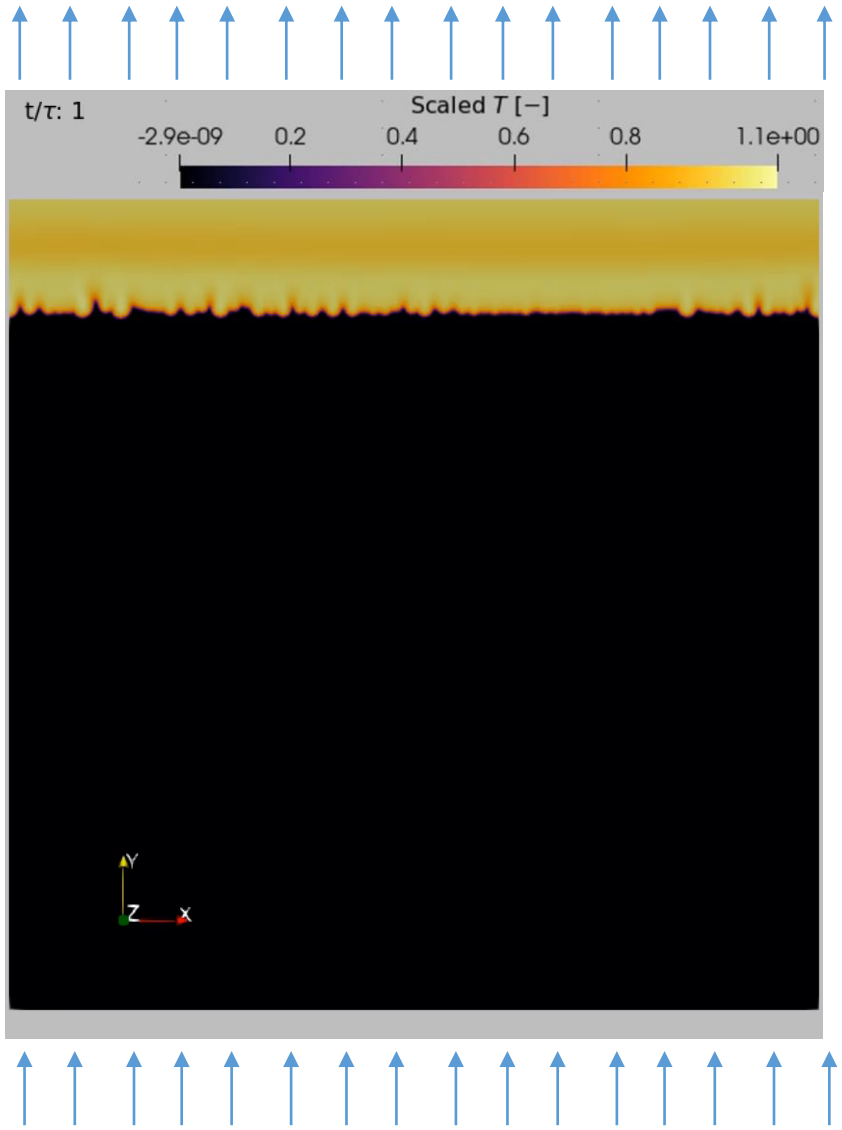


CFD Process

Today's lesson:

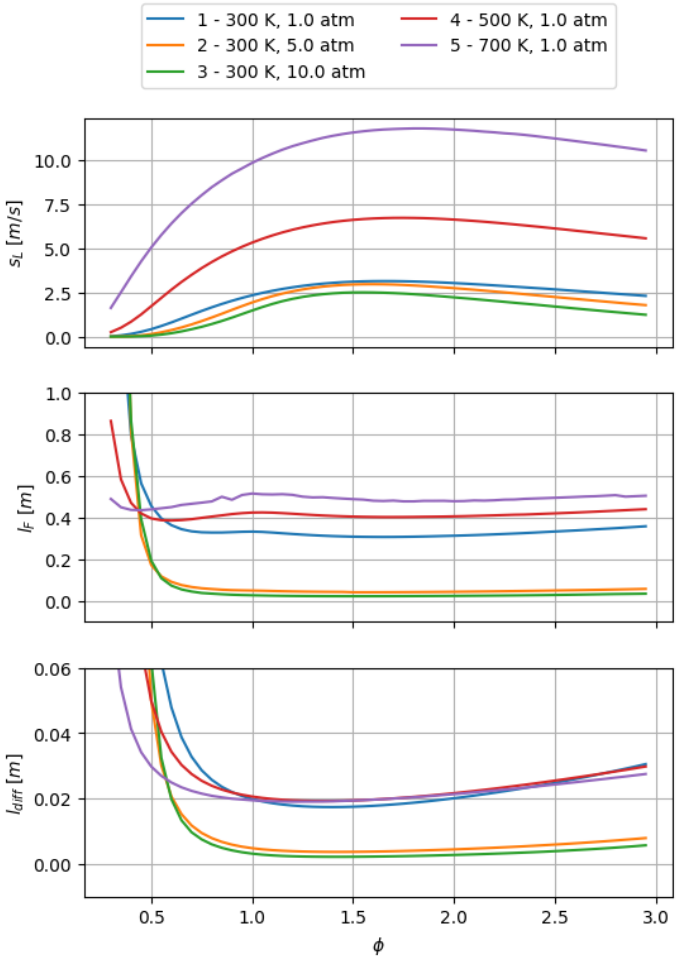
- How a CFD problem works
- Manage input files for the simulation (ALYA)
- Run timesteps of the simulation
- Postprocess data from simulation
- Visualize the data with paraview

Simulation of H2 thermo-diffusive instabilities lean mixture

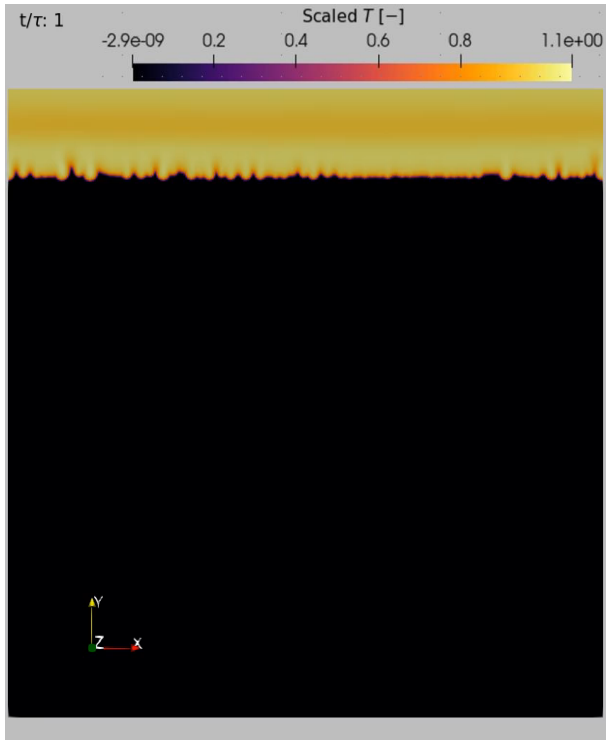


$\phi = 0.5, T = 298K, p = 1atm$

CFD Process



$T = 298, p = 1atm$

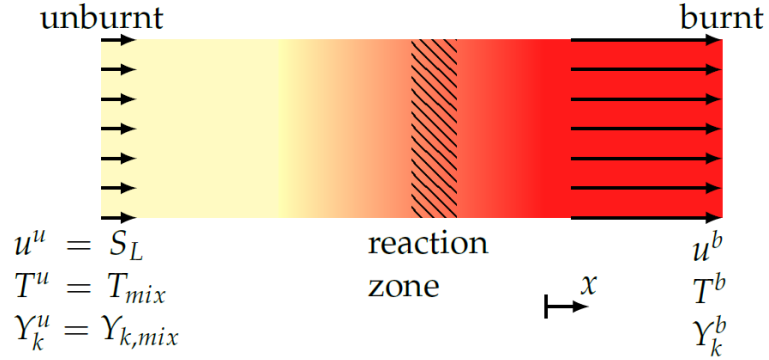


$T = 700K, p = 1atm$

$T = 298K, p = 5atm$

How a CFD problem works

- Computational simulation
  - Extend solutions outside analytical solutions in canonical cases
  - Take out the physical setup of experiments
  - Produce accurate results like experiments
  - Provides detailed results, which is hard for to measure in combustion
  - Generate lots of data to exploit with data driven techniques
  - Time expensive and easy to misunderstand results



How a CFD problem works

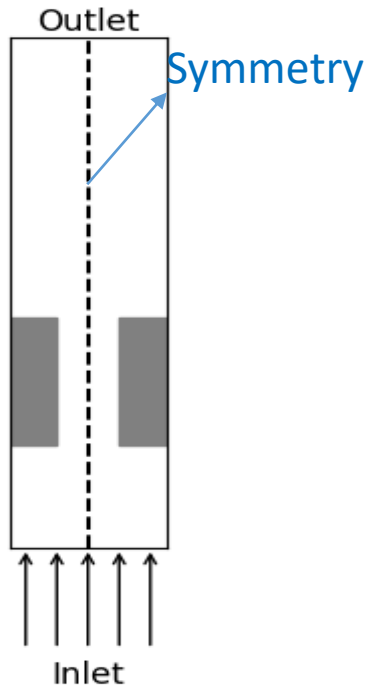
1. A burner configuration* is proposed

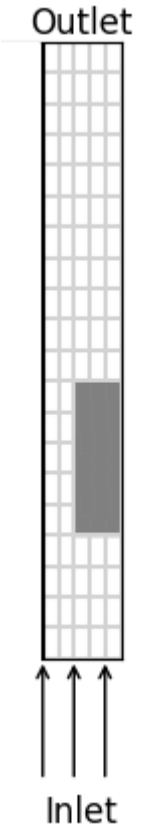
2. Meshing (Gmsh, ANSA, …)
   - Generate a geometry
   - Exploit symmetries
   - Divide into millions of tiny boxes (cells)

3. Determine boundary conditions for transport equations

4. Create initial condition fields

5. Set up numerical parameters for space and time solvers





How a CFD problem works

5. Set numerical parameters for space and time solvers
   - Space dimension:
     - Numerical simulations for transport eqs. driven mainly by convection rather than diffusion require *stabilization methods*. With the finite element method (FEM), stabilization means adding a small amount of artificial diffusion.
   - Time integration method:
     - Runge-Kutta order 3
   - Solver tolerances for convergence and steadiness

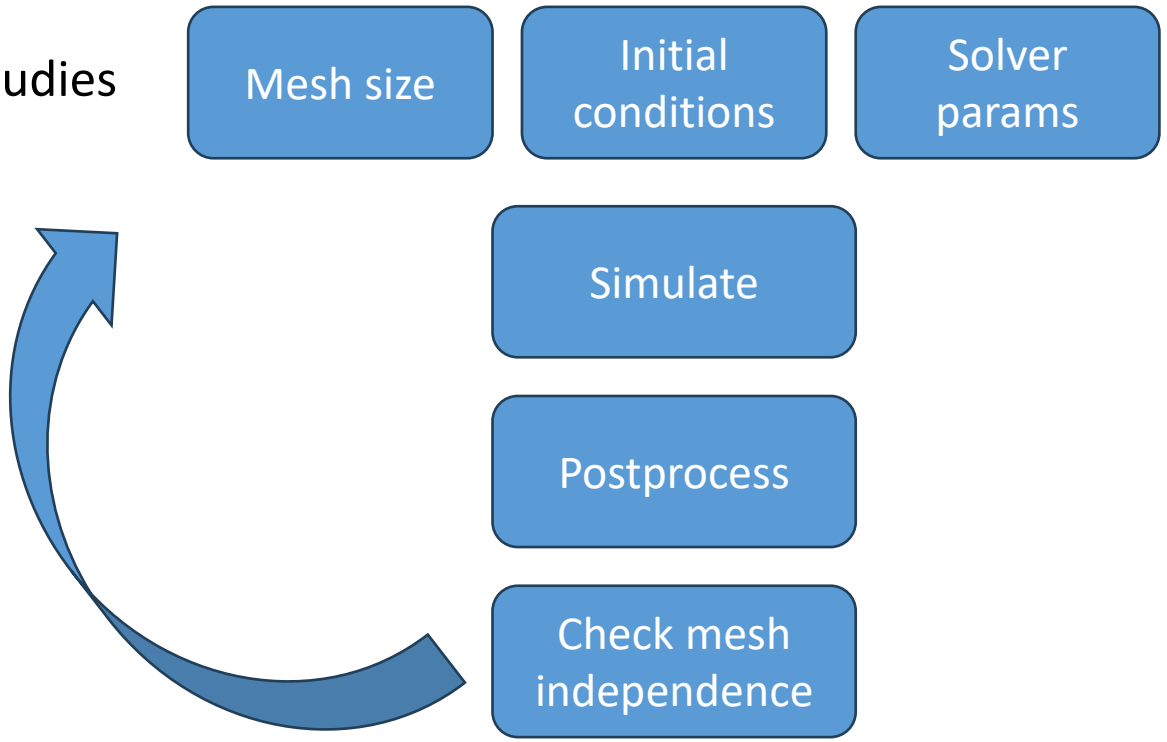
```
NUMERICAL_TREATMENT
  STABILIZATION:              ASGS
  TAU_STRATEGY:               INCLUDING
  ELEMENT_LENGTH:             Minimum
  TIME_INTEGRATION:           RUNGE, ORDER: 3
  SAFETY_FACTOR=              2.0

  COUPLING:                   MONOLITHIC
  SPLITTING:                  ORDER = 1

  STEADY_STATE_TOLERANCE   = 1e-8
  NORM_OF_CONVERGENCE      = L2
  CONVERGENCE_TOLERANCE=     1e-6

  ALGEBRAIC_SOLVER
    SOLVER:                     EXPLICIT, LUMPED
  END_ALGEBRAIC_SOLVER

END_NUMERICAL_TREATMENT
```

Numerical parameters of input file for ALYA

How a CFD problem works

1. Coarse mesh to test execution, not results

2. Define, based on bibliography and validation studies
   1. Initial condition fields
   2. Mesh size
   3. Solver parameters adjustment
3. Run the simulation, monitor results
4. Postprocess results
5. Check if results are mesh independent



6. Achieve mesh independence

Manage input files for the simulation (ALYA)

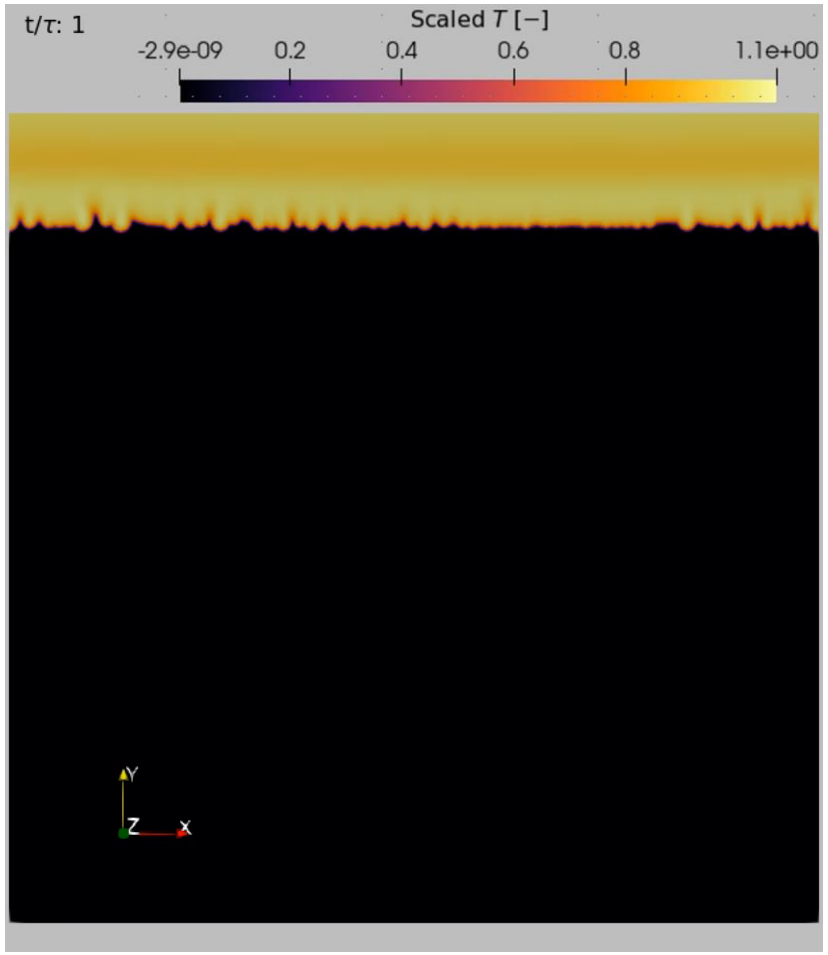
- Logging inside m
  - Open terminal (Windows: command prompt or mobaxterm in for similar experience to UNIX)
  - ssh –Y nct01XXX@mn1.bsc.es
  - Type password (GJDZFvH5.XXX)
  - (use mn2 or mn3 if input password 3 wrong times and blocked)
  - Copy simulation file

```
cp –r /gpfs/projects/nct00/nct00012/Simulation/Ref  .
```

dot

```
cd Ref
ls
```

Simulation of H2 thermo-diffusive instabilities



CFD Process: Problem setup in ALYA

- Setting up a problem in Alya:
- Input files
  - NSI.DAT (Navier-Stokes)
  - TEM.DAT (Temperature | Enthalpy)
  - CHM.DAT (Chemistry, species mass fractions)
  - KER.DAT
    - Controls the run: it contains the solvers, the input-output workflow and everything related to the mesh and geometry.
  - DOM.DAT
    - Contains properties of the mesh and elements
  - .DAT
    - Communication between modules (NSI, TEM, CHM) and general parameters (time of simulation, postprocess)
- /mesh/ directory contains the mesh of the problem
- /fields/ directory contains the initial conditions fields and boundary conditions

CFD Process: Problem setup in ALYA

- input.chm.dat – To open `vi input.chm.dat` to close `:q`

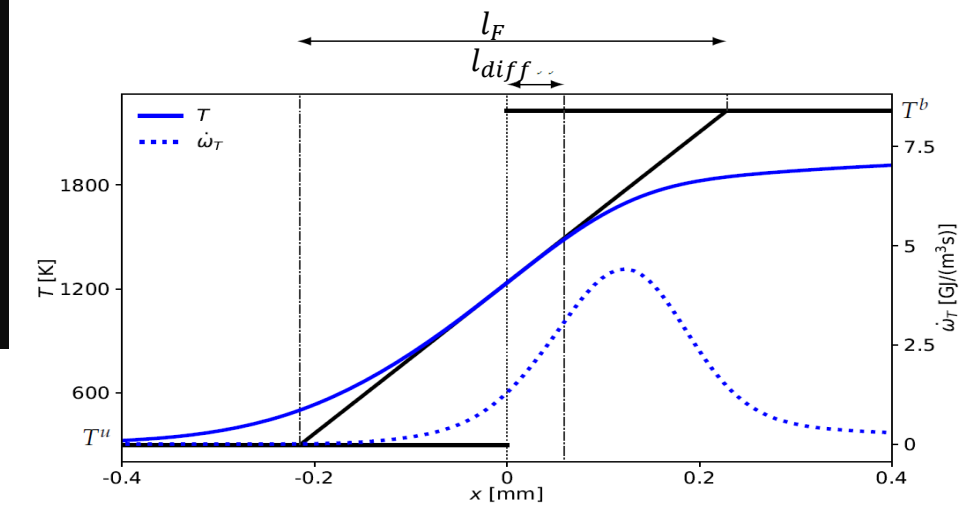
```
PHYSICAL_PROBLEM

  PROBLEM_DEFINITION
    MODEL:              FINITE_RATE
    TEMPORAL:           ON
    CONVECTION:         ON, VELOC
    DIFFUSION:          ON
    HTRAN:              DETAILED          $$ DETAILED = ENTHALPY EQUATION FOR MIXAV
    MECHANISM:          CANTERA
      ./mech_H2Burke.xml
    END_MECHANISM
  END_PROBLEM_DEFINITION

  PROPERTIES:
    THERMODYN_PRESSURE = 101325.0       $$ 1 atm
    TRANSPORT          = MIXAV          $$ LEWIS, UNITY  or MIXAV
    KINETICS           = CANTERA        $$ USER,  CANTERA
  END_PROPERTIES

  FIELDS: TEMPE= 3, SPECI = 4           $$ ALYA TECHNICALITY

END_PHYSICAL_PROBLEM
```

CFD Process: Problem setup in ALYA

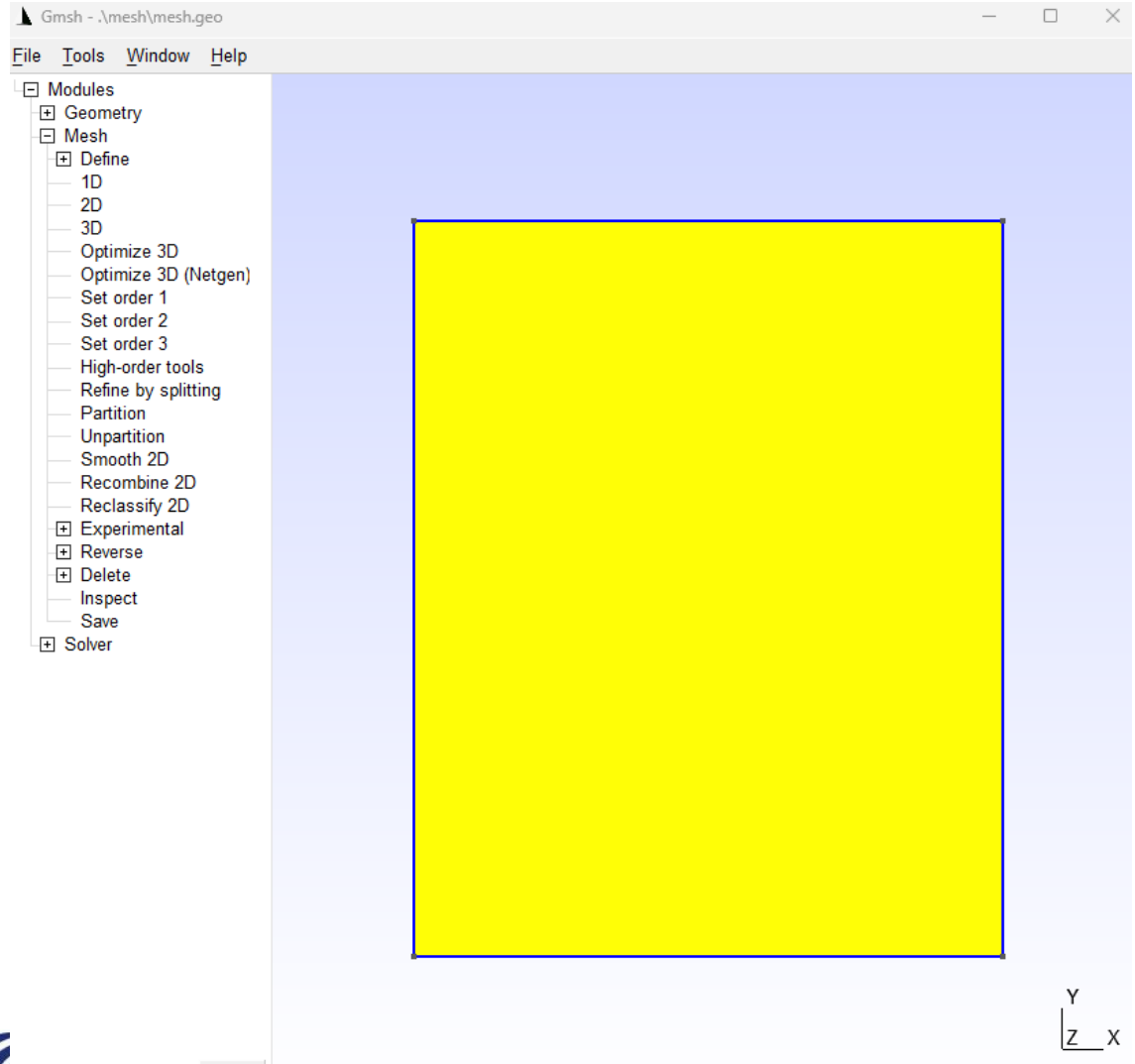
- input.dat – To open `vi input.dat` to close `:q`

```
$-----------------|-----------------------------------------------
RUN_DATA
  ALYA:                   "INPUT"
  RUN_TYPE:               CONTINUATION,PRELIMINARY,FREQUENCY=1800
END_RUN_DATA
$-------------------------------------------------------------------
PROBLEM_DATA
  TIME_COUPLING:  Global, FROM_CRITICAL
  $TIME_STEP:  5.5E-9
  NUMBER_OF_STEPS:  10
  TIME_INTERVAL:  0.0, 0.0726223 $$ 120 times the time_characteristic which is = 0.0006051856308343749

  MAXIMUM_NUMBER_GLOBAL:  1
  BLOCK_ITERATION: 1
     1 CHEMIC, TEMPER, NASTIN
  END_BLOCK_ITERATION

  CHEMIC_PROBLEM:  ON
  END_CHEMIC
  NASTIN_PROBLEM:  ON
  END_NASTIN
  TEMPER_PROBLEM:  ON
  END_TEMPER
```

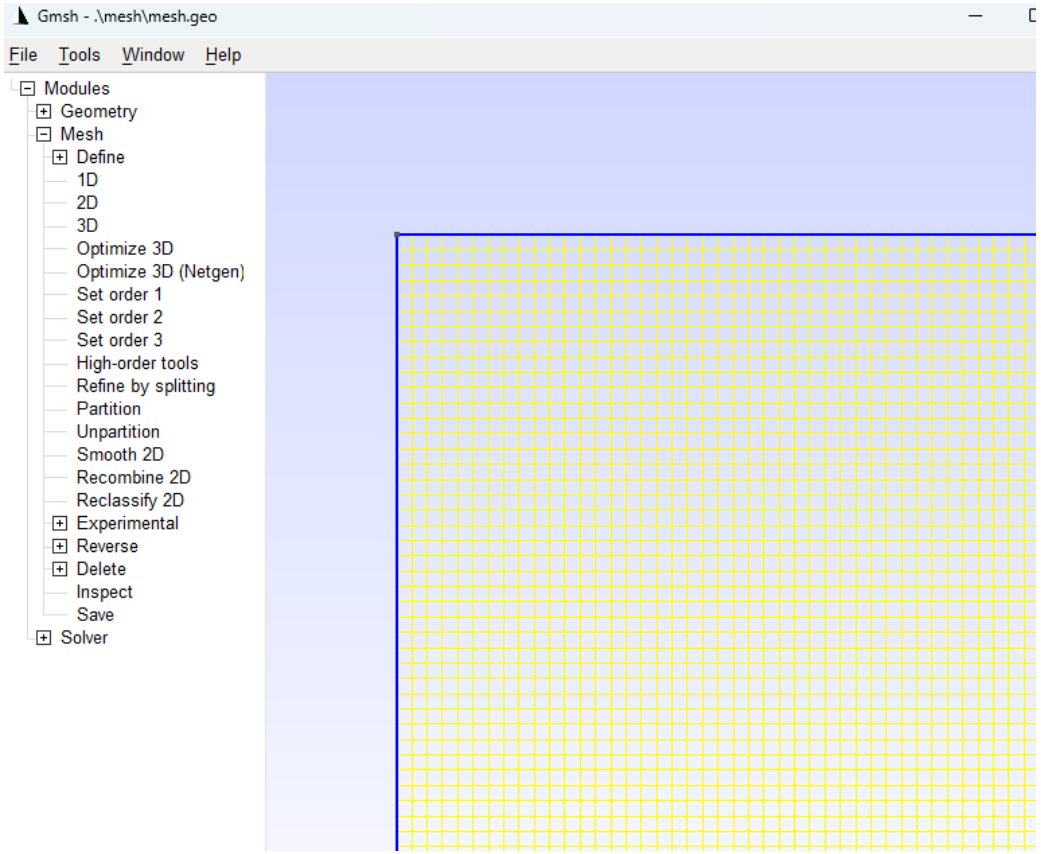
$$\tau = \frac{l_F}{u_{inlet}}$$



CFD Process: Problem setup in ALYA



- Mesh file mesh/mesh.geo using gmsh
- $\Delta x = \frac{l_F}{5}, \Delta y = \frac{l_F}{5}$

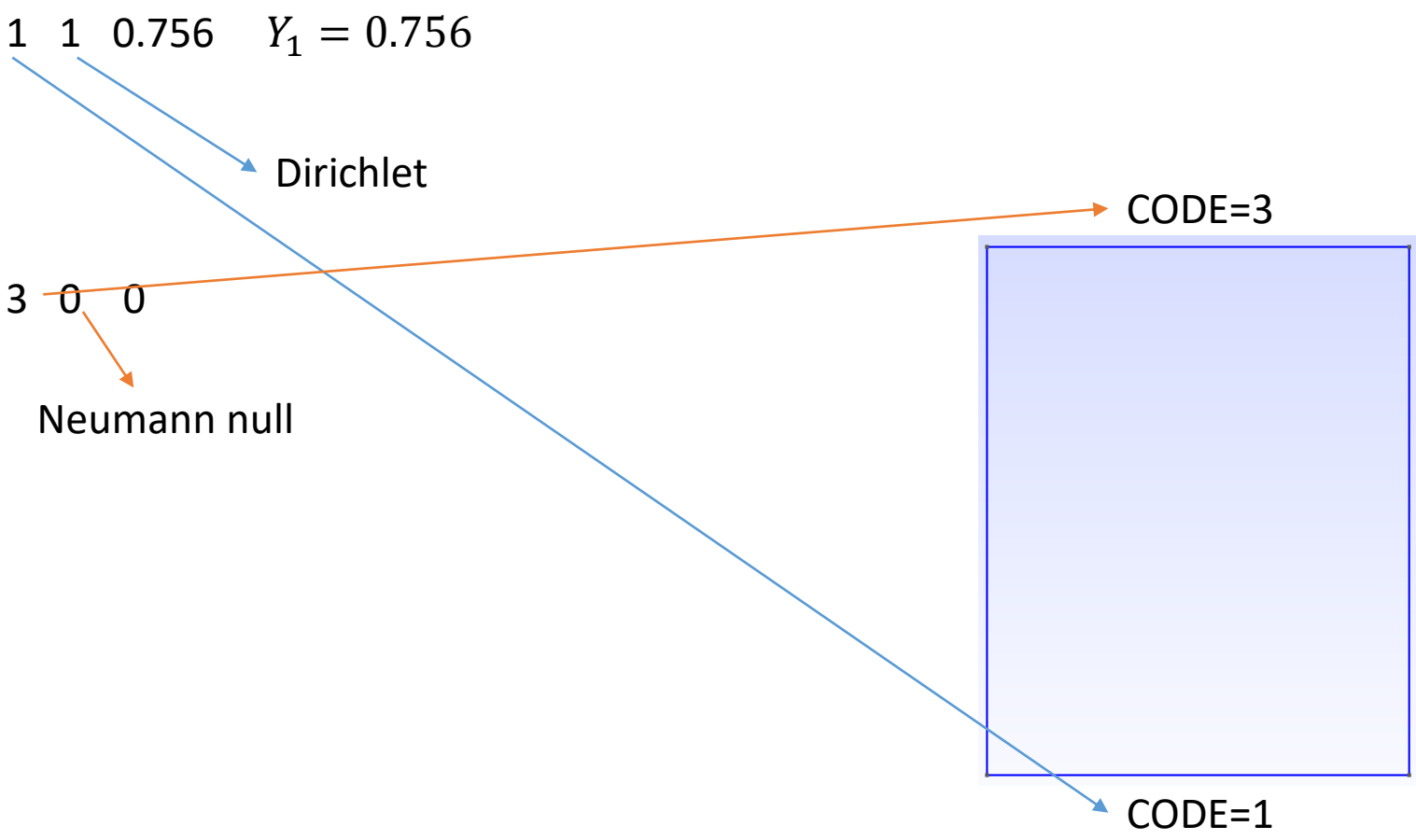


CFD Process: Problem setup in ALYA

- vi fields/boundary_species.dat

```
CODES, NODES, CLASS = 1 $$N2
   1    1  0.756
   3    0  0
END_CODES

CODES, NODES, CLASS = 2 $$H
   1    1  0.0
   3    0  0
END_CODES

CODES, NODES, CLASS = 3 $$O2
   1    1  0.22954
   3    0  0
END_CODES

CODES, NODES, CLASS = 4 $$O
   1    1  0.0
   3    0  0
END_CODES

CODES, NODES, CLASS = 5 $$OH
   1    1  0.0
   3    0  0
END_CODES

CODES, NODES, CLASS = 6 $$H2
   1    1  0.01446
   3    0  0
END_CODES
"fields/boundary_species.dat" 45L, 696C
```

CODES NODES CLASS = 1: Interpret the code on nodes to impose BC on species 1



CFD Process: Problem setup in ALYA

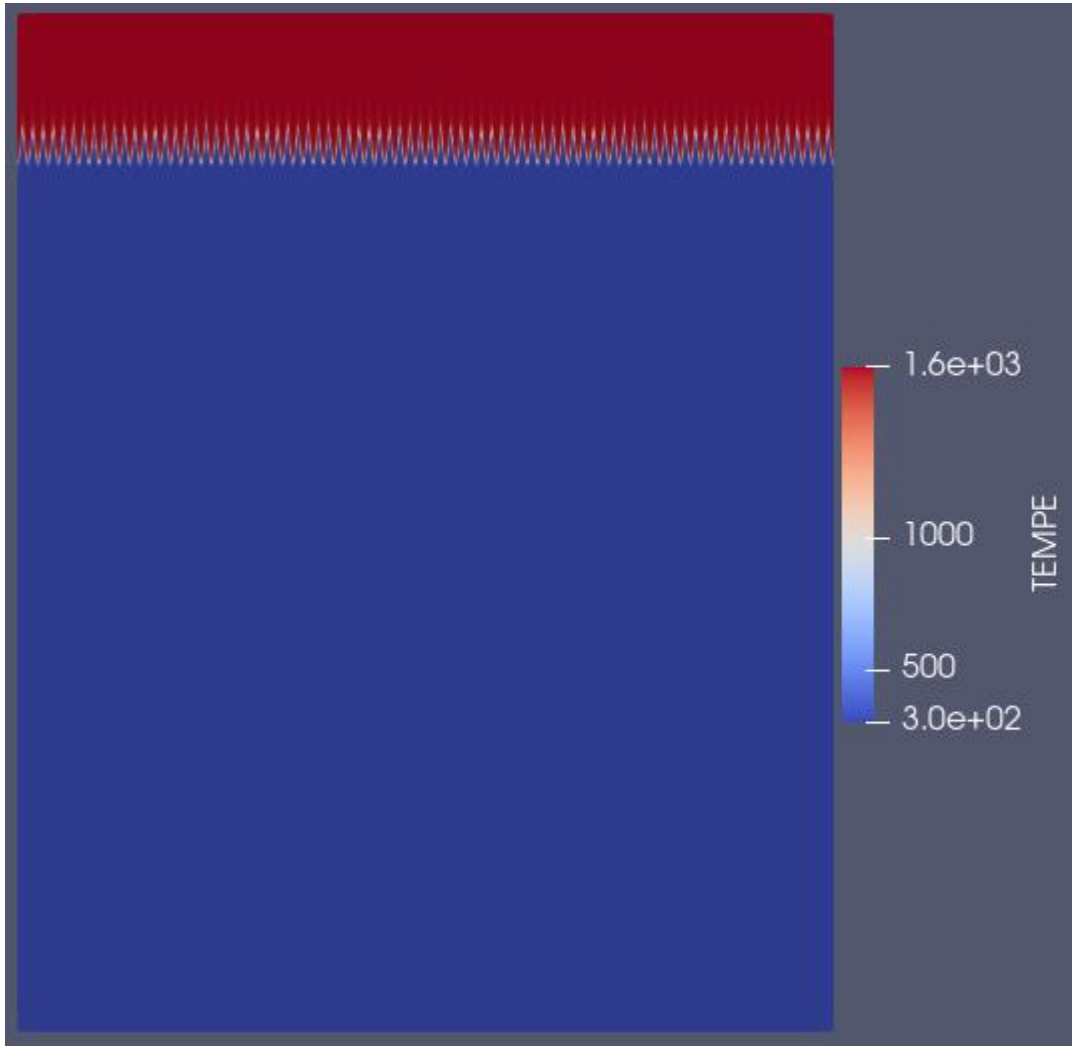
- mesh/coord.geo

NODE x y

```
1 -0.042362994158406240 -0.052953742698007800
2 0.042362994158406240 -0.052953742698007800
3 0.042362994158406240 0.052953742698007800
4 -0.042362994158406240 0.052953742698007800
5 -0.042278183359290360 -0.052953742698007800
6 -0.042193372560174480 -0.052953742698007800
7 -0.042108561761058600 -0.052953742698007800
8 -0.042023750961942730 -0.052953742698007800
9 -0.041938940162826840 -0.052953742698007800
10 -0.041854129363710960 -0.052953742698007800
11 -0.041769318564595090 -0.052953742698007800
12 -0.041684507765479200 -0.052953742698007800
13 -0.041599696966363320 -0.052953742698007800
14 -0.041514886167247450 -0.052953742698007800
15 -0.041430075368131560 -0.052953742698007800
16 -0.041345264569015690 -0.052953742698007800
17 -0.041260453769899810 -0.052953742698007800
18 -0.041175642970783920 -0.052953742698007800
19 -0.041090832171668050 -0.052953742698007800
20 -0.041006021372552240 -0.052953742698007800
21 -0.040921210573436530 -0.052953742698007800
22 -0.040836399774320830 -0.052953742698007800
23 -0.040751588975205120 -0.052953742698007800
24 -0.040666778176089410 -0.052953742698007800
25 -0.040581967376973710 -0.052953742698007800
26 -0.040497156577858000 -0.052953742698007800
27 -0.040412345778742300 -0.052953742698007800
28 -0.040327534979626590 -0.052953742698007800
29 -0.040242724180510880 -0.052953742698007800
```

- fields/TEMPE.alya

```
1 298.
2 298.
3 1642.8
4 1642.8
5 298.
6 298.
7 298.
8 298.
9 298.
10 298.
11 298.
12 298.
13 298.
14 298.
15 298.
16 298.
17 298.
18 298.
19 298.
20 298.
21 298.
22 298.
23 298.
24 298.
25 298.
26 298.
27 298.
28 298.
29 298.
"fields/TEMPE.alya"
```



Run timesteps of the simulation

- Launch simulation in debug queue2.

```
sbatch run_debug.sh
```

- Watch the job to see when it begins

```
watch squeue
```

- Once it shows no jobs, means the job got in
- See the progress

```
squeue
```

```
#!/bin/bash
#SBATCH --job-name=InstabilitiesReference
#SBATCH --output=run_%j.out
#SBATCH --error=run_%j.err
#SBATCH --mail-user=ercoftac@bsc.es
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=48
#SBATCH --time=2:00:00
#SBATCH --qos=debug

srun /gpfs/projects/nct00/nct00012/alya/build/bin/alya input
```

```
   JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
31203574 sequentia Instabil nct00012  R       0:02      1 s04r2b48
```

- A file run_31203574.out got created
- Watch it live with

```
tail –f run_31203574.out
```

```
--| ALYA  START TIME STEP 5, t=  5.306689E-06
--| ALYA     SOLVE CHEMIC (1)
--| ALYA     SOLVE TEMPER (1)
--| ALYA     SOLVE NASTIN (MC)
--| ALYA     SOLVE NASTIN (MC)
--| ALYA     SOLVE NASTIN (MSC)
--| ALYA  END TIME STEP
--| ALYA  START TIME STEP 6, t=  6.443552E-06
--| ALYA     SOLVE CHEMIC (1)
```

Run timesteps of the simulation

- Lots of new files get created
  - input.log

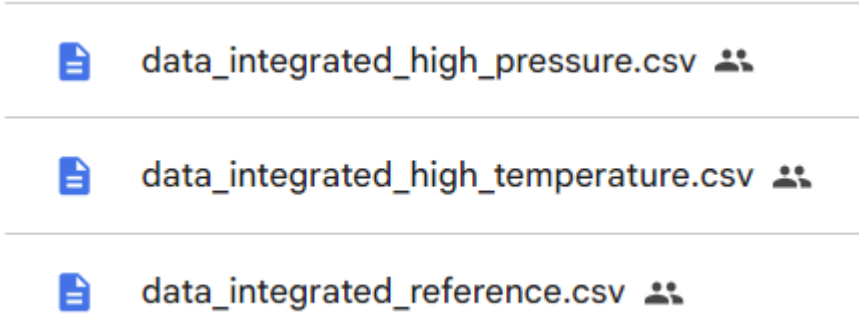
```
|- TIME STEP NUMBER:            7
   Current time step dt =  7.863E-07
   Current time t       =  7.230E-06
   CHEMIC:
   - Critical time step dtc:  4.259E-07
   - Ratio dt/dtc:            1.846E+00
   TEMPER:
   - Critical time step dtc:  9.486E-07
   - Ratio dt/dtc:            8.289E-01
   NASTIN:
   - Critical time step dtc:  8.190E-07
   - Ratio dt/dtc:            9.600E-01

   Global iteration number:     1, block number:  1
   Current CPU time:         1.114E+02
   Elapsed CPU time:         1.417E+01
   Residual of CONCENTRATION     :  1.577E-04
   Residual of TEMPERATURE       :  5.556E-02
   Residual of VELOCITY          :  7.232E+00
   Residual of PRESSURE          :  2.077E+00
```

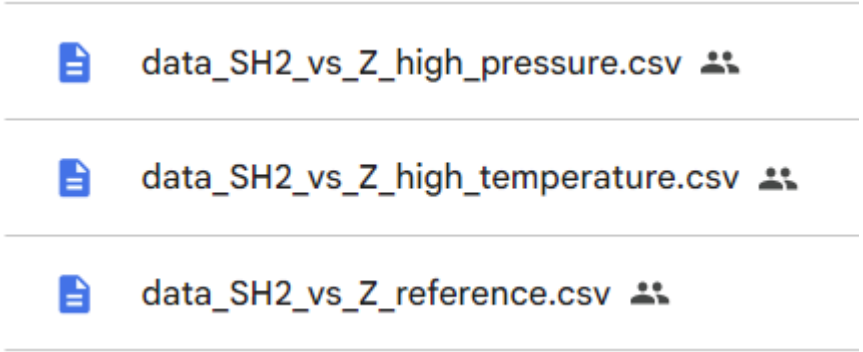
input.chm.log

```
Mixtured Average Diffusion

Reading mechanism ./mech_H2Burke.xml

# Species=           9

# Removed Species=

Species            1 =N2
Species            2 =H
Species            3 =O2
Species            4 =O
Species            5 =OH
Species            6 =H2
Species            7 =H2O
Species            8 =HO2
Species            9 =H2O2

Chemical reactions

# Reactions=          23

H + O2 <=> O + OH

H2 + O <=> H + OH

H2 + O <=> H + OH

H2 + OH <=> H + H2O
```

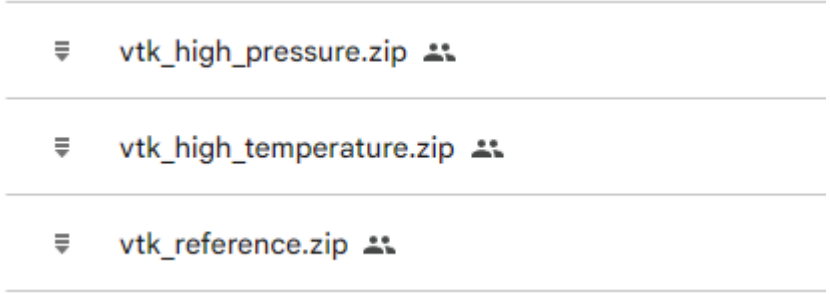
Postprocess data

- Ercoftac git: https://github.com/burn-research/ercoftac2023-workshop
- Datasets: https://drive.google.com/drive/folders/1HmD4fDx9I4drD1d5fpQWl8MeNRElGXF9
  - Part 1: Postprocess data
    - Scripts and mechanism: https://github.com/burn-research/ercoftac2023-workshop/tree/main/Instabilities





  - Part 2: Paraview



Postprocess data

- Laminar flame speed s_L

Steady state

$$\frac{\partial \rho u Y_{Fuel}}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\rho D_{Fuel}\frac{W_k}{W}\frac{\partial X_{Fuel}}{\partial x_i}\right) = \dot{\omega}_{Fuel}$$

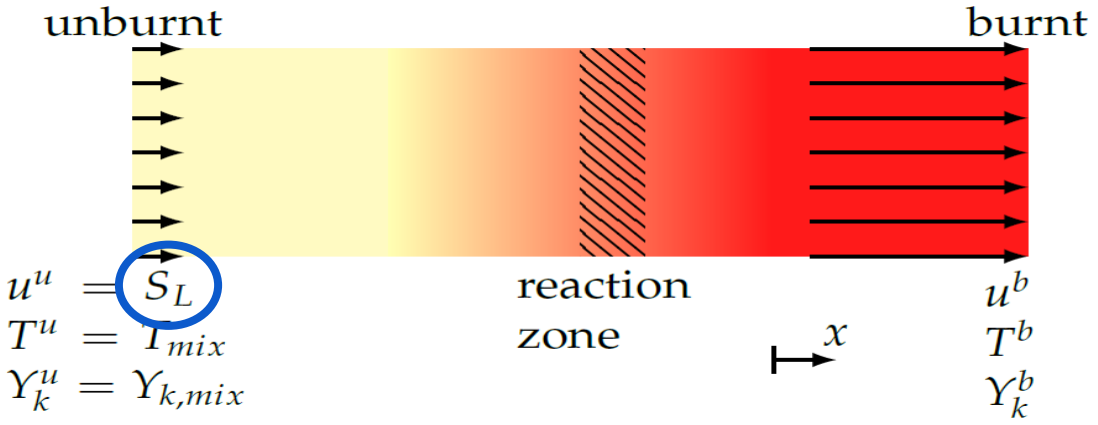
$$\int_0^L \frac{\partial \rho u Y_{Fuel}}{\partial x_i} dx \rightarrow -\rho^u s_L Y^u_{Fuel}$$

$$\int_0^L \frac{\partial}{\partial x_i}\left(\rho D_{Fuel}\frac{W_k}{W}\frac{\partial X_{Fuel}}{\partial x_i}\right) dx = 0$$

Boundaries have null diffusive flux

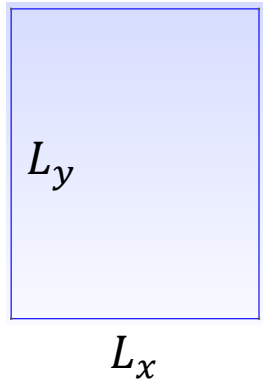
$$s_L = -\frac{1}{\rho^u Y^u_{Fuel}}\int_0^L \dot{\omega}_{Fuel} dx$$

Consumption speed s_C



$$s_C = -\frac{1}{\rho^u Y^u_{Fuel} L_x}\int \dot{\omega}_{H_2} dx dy,$$

Severely affected by the thermo-diffusive instability



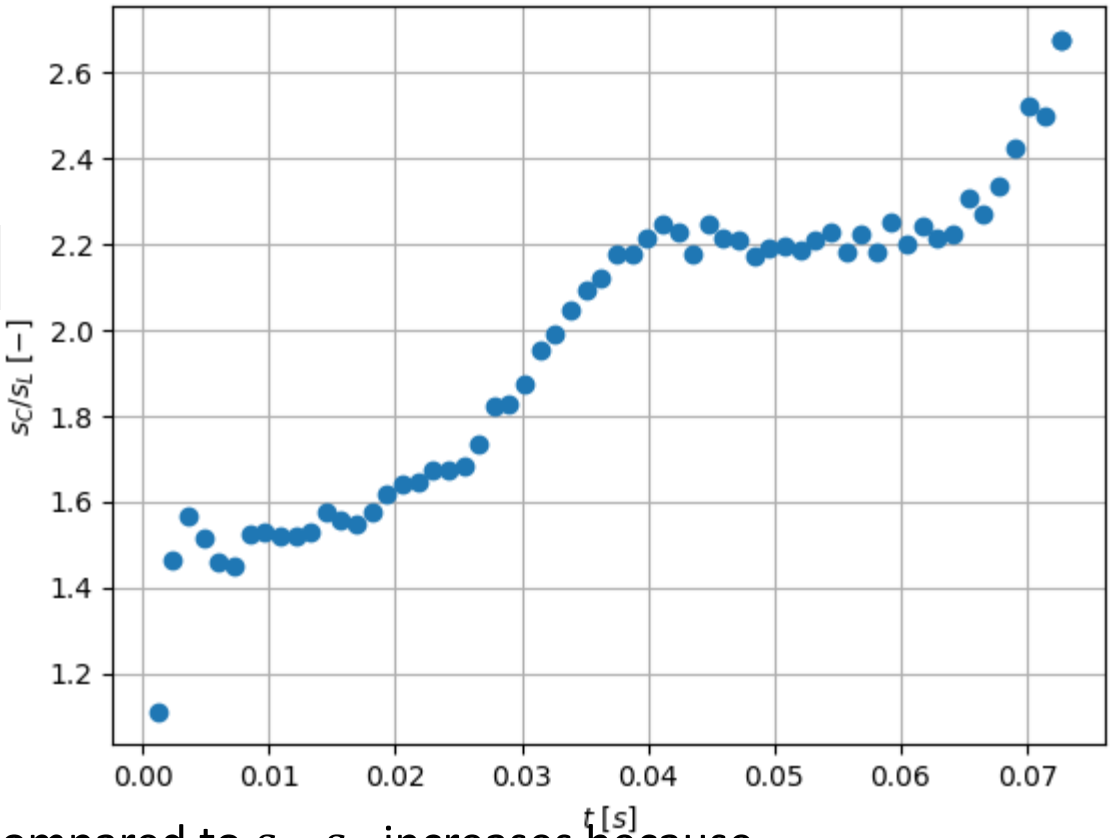
Postprocess data

- Calculate consumption speed (consumption_speed.ipynb)
- Files data_integrated_....csv contain $\int \dot{\omega}_{H_2} \mathrm{d}x\mathrm{d}y$

```
path_data = "path/to/data/data.csv"
```

```
# Reference case
s_L = 0.4913988828547467
rho_u = 0.9894
Yk_H2_u = 0.01446
L_x = 0.1058

# High temperature case
#s_L = 5.30
#rho_u = 0.4212
#Yk_H2_u = 0.01446
#L_x = 0.05

# High pressure case
#s_L = 0.22
#L_x = 0.0115
#rho_u = 4.94
#Yk_H2_u = 0.01446
```

Reference case



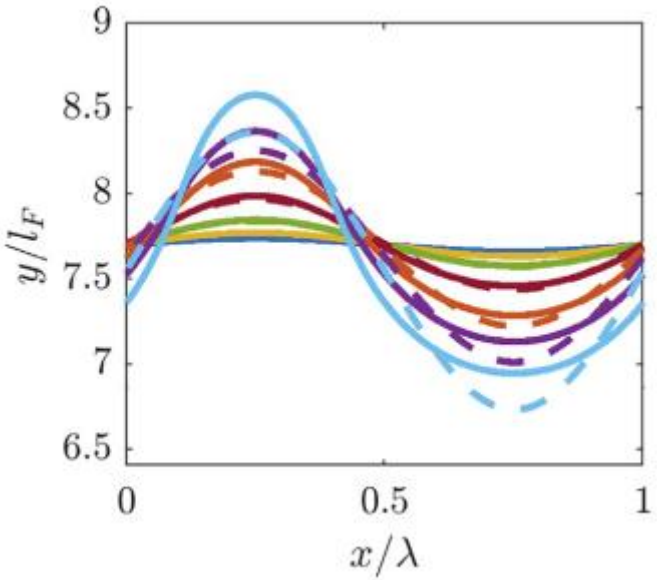
Compared to s_L, s_C increases because

- Flame front wrinkling
- variations of reaction rates

dashed: ω hydrodynamic instability

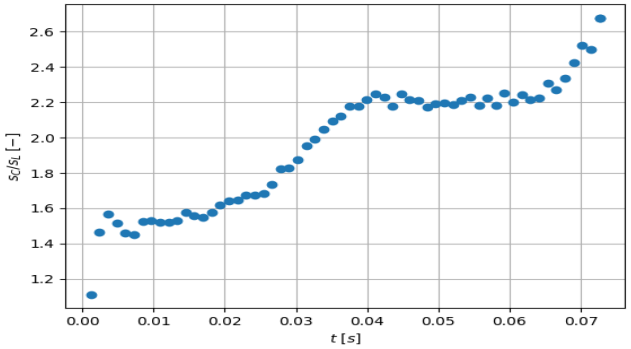
Flame speed enhancement

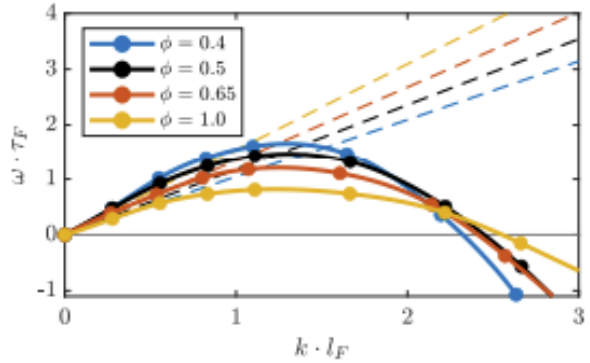
- High enhancement for Reference and high-p cases
- Not as much for high T



- $A(t) \propto e^{\omega t}$
- $\omega = \frac{\mathrm{d}\ln(A(t))}{\mathrm{d}t}$

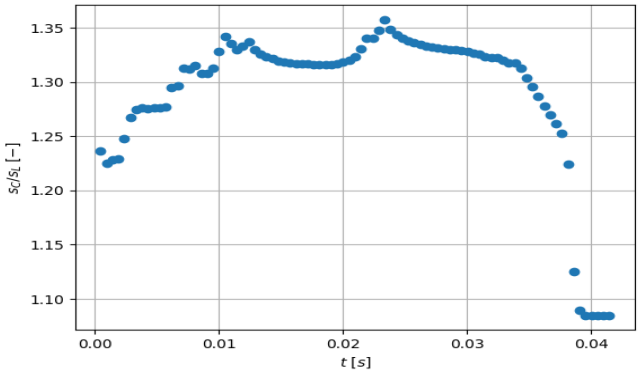
Reference

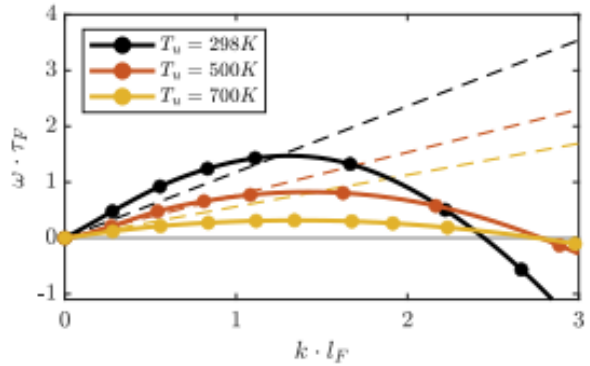




(a) ϕ-Variation at p = 1 bar and T_u = 298 K

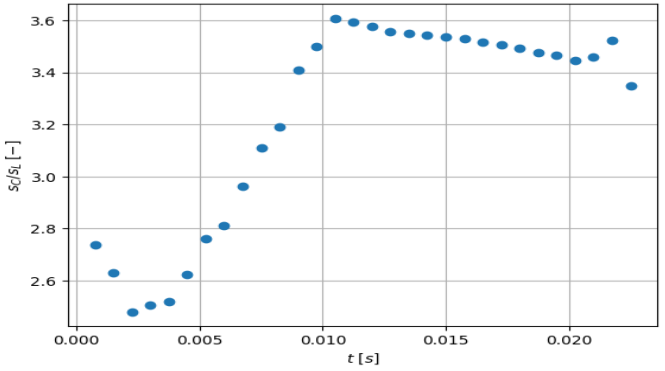
High temperature

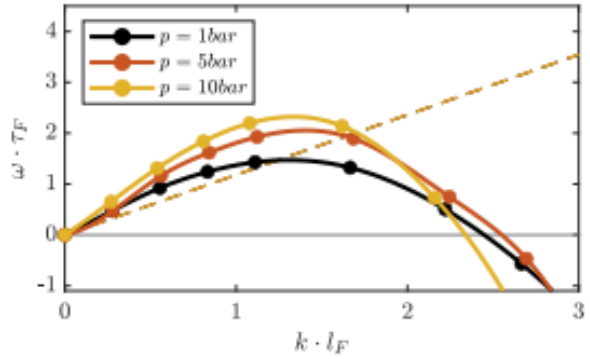




(b) T_u-Variation at ϕ = 0.5 and p = 1 bar

High pressure





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Figures from: Berger et. al. https://doi.org/10.1016/j.combustflame.2021.111935

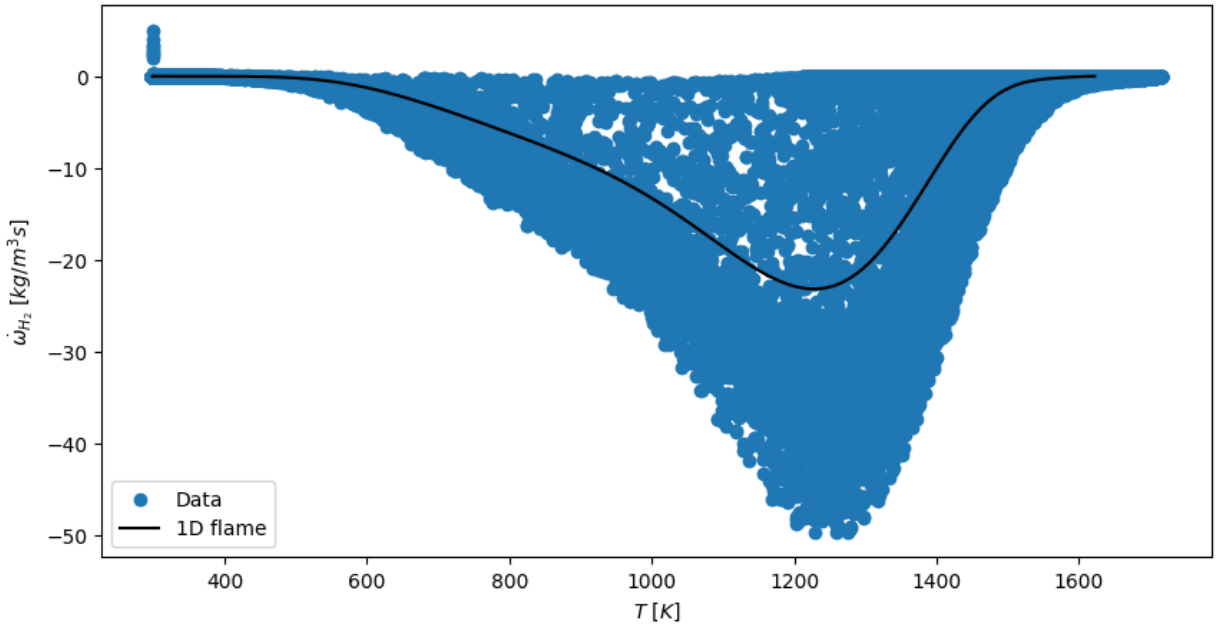
Postprocess data

- Visualize source term (source_term.ipynb)
- Files data_SH2_vs_Z_....csv contain all data from simulation at some time after wrinkling

```
path_data = "path/to/data/data.csv"
```

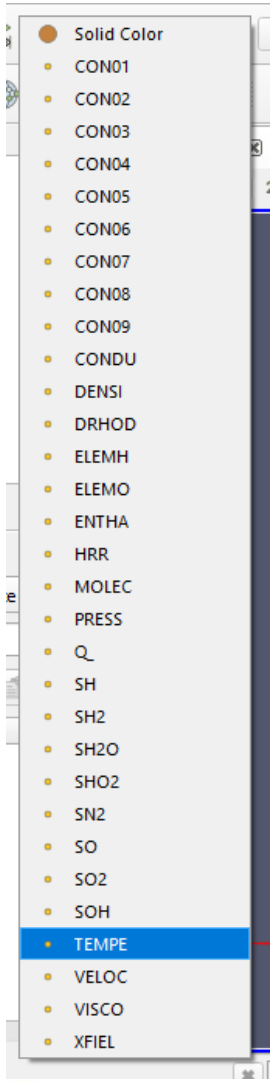
```
# Reference
T = 298
p = 1 * ct.one_atm

# High temperature
#T = 500
#p = 1 * ct.one_atm

# High pressure
#T = 298
#p = 5 * ct.one_atm
```

Reference



- Strong deviations vs the one dimensional case for the inlet mixture

Paraview



- CON01 - N2
- CON02 - H
- CON03 - O2
- CON04 - O
- CON05 - OH
- CON06 - H2
- CON07 - H2O
- CON08 - HO2
- CON09 - H2O2

- CONDU - Conductivity
- DENSI - Density
- DRHOD - $\frac{\partial \rho}{\partial t}$
- ENHTA - Enthalpy
- HRR – Heat Release Rate
- SH - $\dot{\omega}_{H2}$
- VELOC - Velocity
- VISCO - Viscosity
- XFIEL – (ALYA, IGNORE)

- ELEMH
- ELEMO

Elemental mass fractions

$$Z_{mass,m} = \sum_{k}^{Ns} \frac{a_{m,k} W_m}{W_k} Y_k$$

number of atoms of element m in species k

Curvature

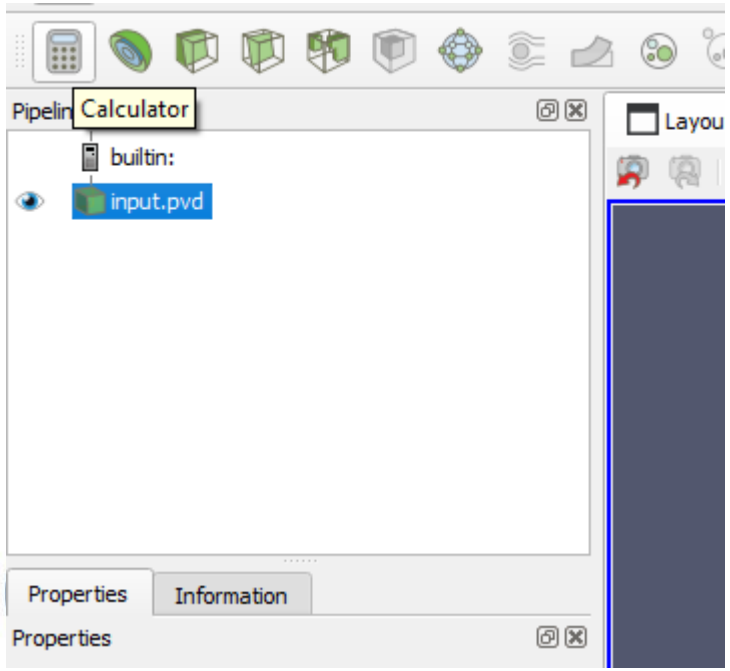
$$\hat{n} = -\frac{\nabla T}{|\nabla T|}, \qquad \kappa = \nabla \cdot \hat{n}$$

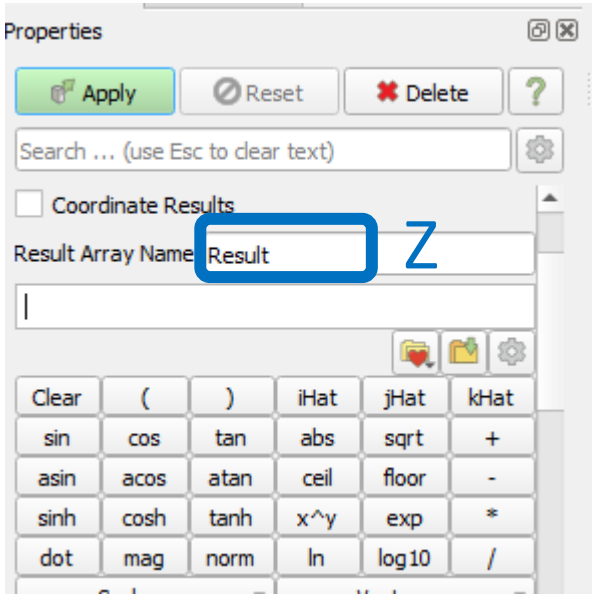
Paraview

- Hands on
  - Caulate mixture fraction field

$$Z(\phi) = \frac{b(\phi) - b_{oxidizer}}{b_{fuel} - b_{oxidizer}}$$

$$b = 2\frac{Z_{mass,C}}{W_C} + 0.5\frac{Z_{mass,H}}{W_H} - \frac{Z_{mass,O}}{W_O}$$





$Z_{mass,H}$=ELEMH

$Z_{mass,O}$=ELEMO

W_H= 1.01

W_H= 16

$b_{oxidizer}$= 0.0145

b_{fuel}= 0.496

```
((0.5*ELEMH/1.01 - ELEMO/16) + 0.0145) / (0.496 + 0.0145)
```