OpenFOAM Training: Combustion
3-5 July 2017, Brussels

Use of external libraries for chemistry: Getting started with OpenSMOKE++

Alberto Cuoci

Download the training session material

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https://github.com/acuoci/OpenFOAMTrainingCombustion

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```

or download the corresponding zip file:

```
https://github.com/acuoci/OpenFOAMTrainingCombustion/archive/master.zip
```

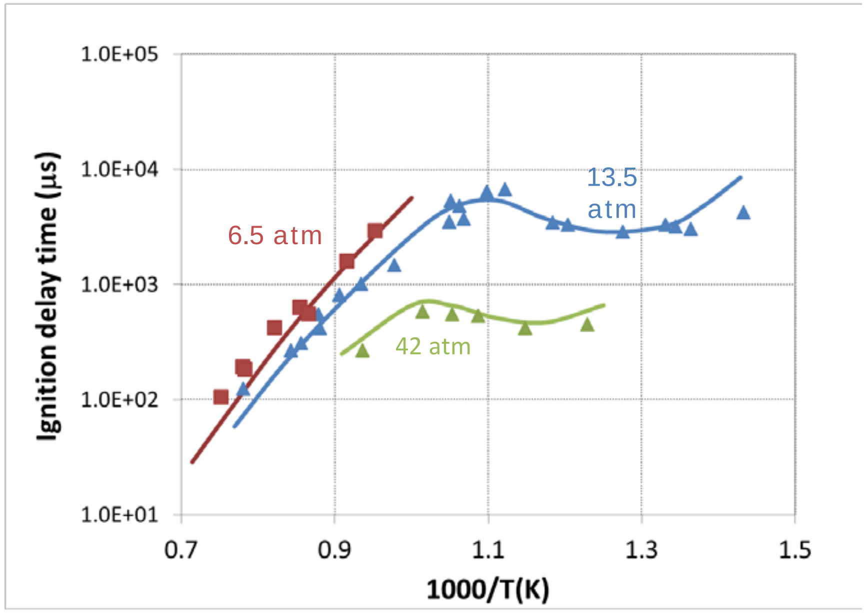
Outline

Outline

Detailed combustion chemistry (I)

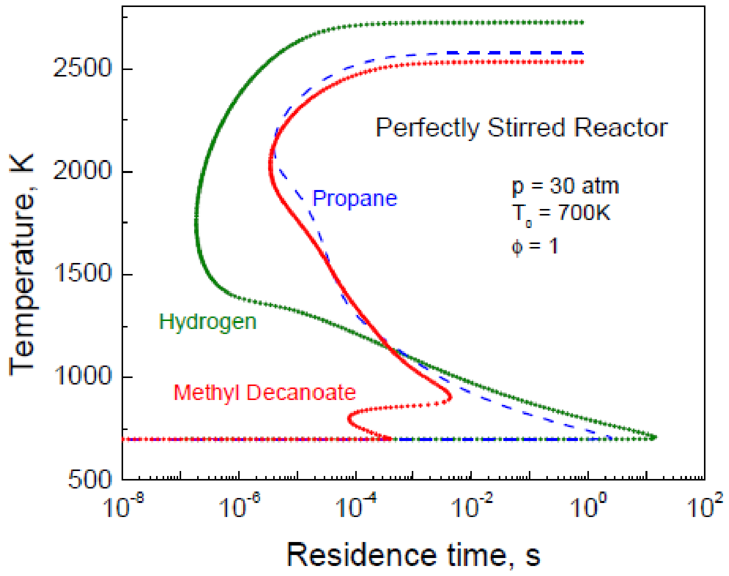
Detailed combustion chemistry is important for: ignition, extinction, instabilities …

Negative temperature Coefficients (NTC)



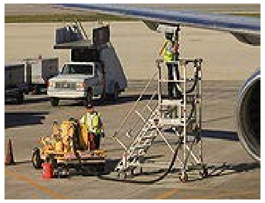
Experimental data from:
Ciezki H.K. and Adomeit G., *Shock-tube investigation of self-ignition of n-heptane-air mixtures under engine relevant conditions*, Combustion and Flame 93 p. 421–433 (1993)

Combustion "S"-curves



Plot from:
Lu T., *Computational Tools for Diagnostics and Reduction of Detailed Chemical Kinetics*, Princeton-CEFRC Summer School on Combustion (2012)

Detailed combustion chemistry (II)

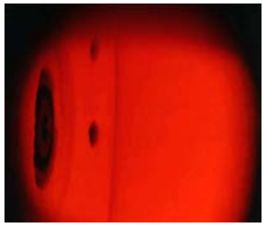


Real fuels and surrogate mixtures

need of modeling synergistic effects between the different components

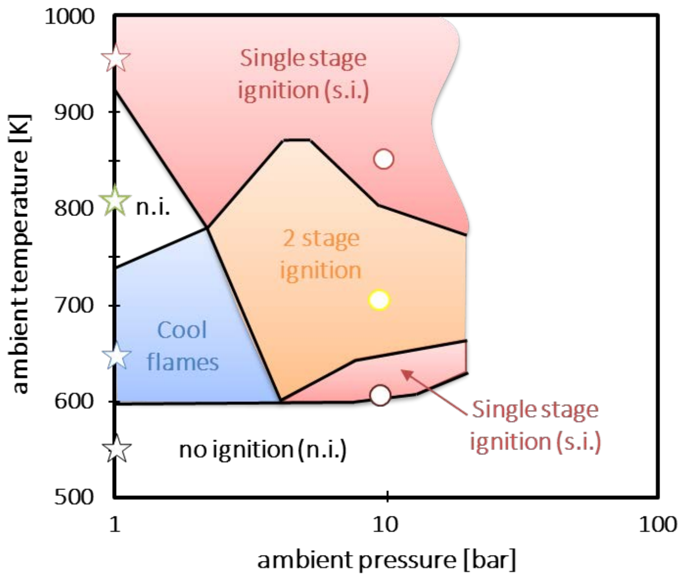
Biofuels

Bio-alcohols, biodiesel, green diesel, bio-ethers



Flameless combustion

(low Damkholer number, slow chemistry)



Auto-ignition regimes of n-alkanes droplets

Tanabe et al., 26th Symposium (International) on Combustion, p. 1637-1643 (1996)

Cuoci A. et al., Proceedings of The Combustion Institute, 2015

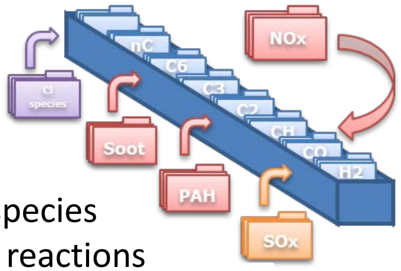
CFD and Combustion with detailed chemistry

1. Number of equations
Since detailed kinetic mechanisms involve hundreds or thousands of species, the number of coupled equations can be very large, especially when multidimensional geometries are simulated

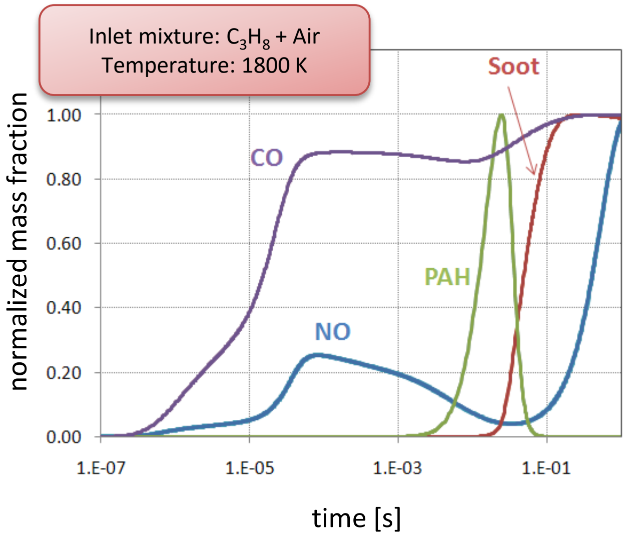
2. Non-linearity
The transport equations of species and energy are very non-linear, because of reaction rates expressions (power-law and exponential)

3. Stiffness
The characteristic times of species involved in a kinetic scheme cover several orders of magnitudes.

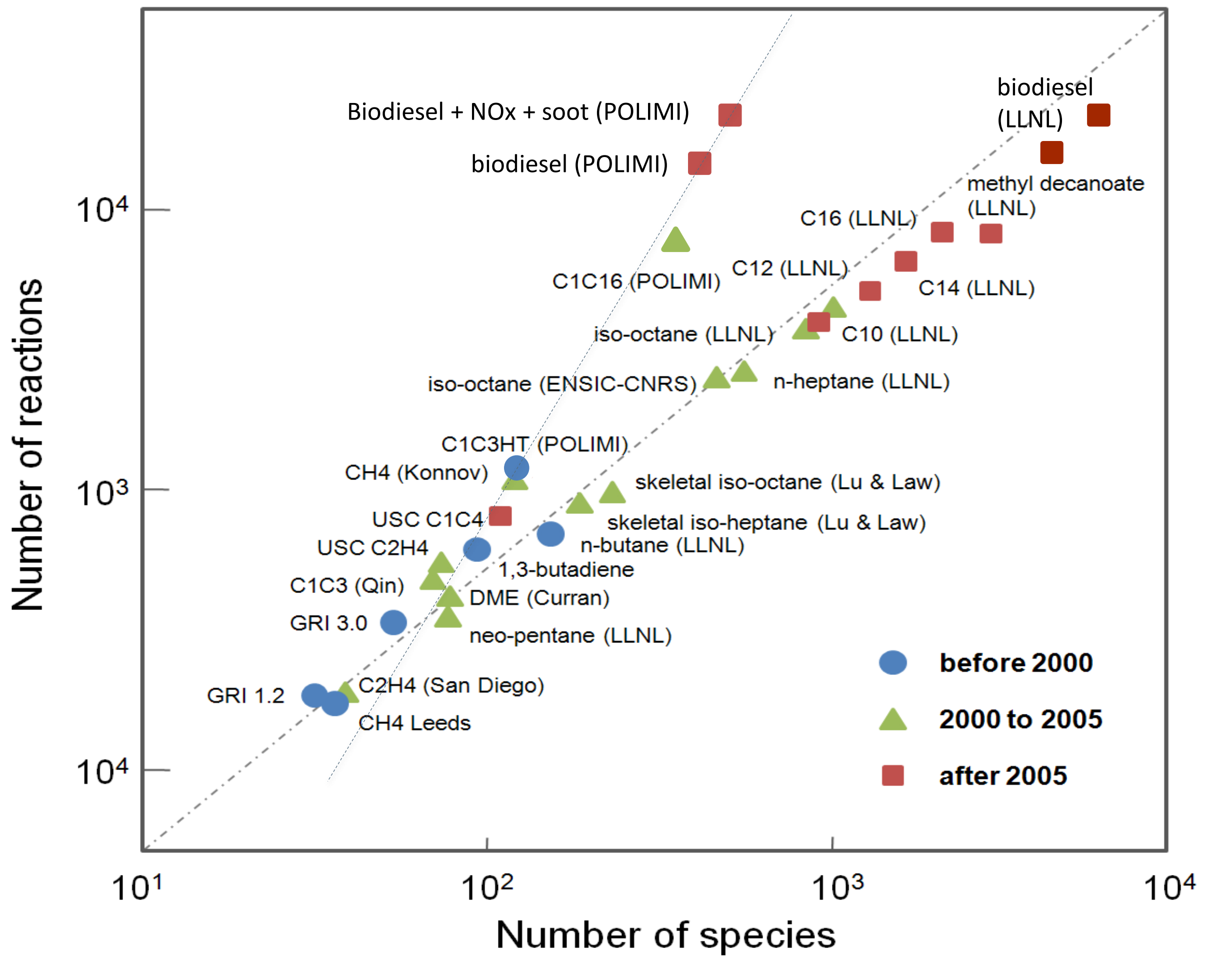
Detailed kinetic schemes



~ 1,000 species
~ 10,000 reactions

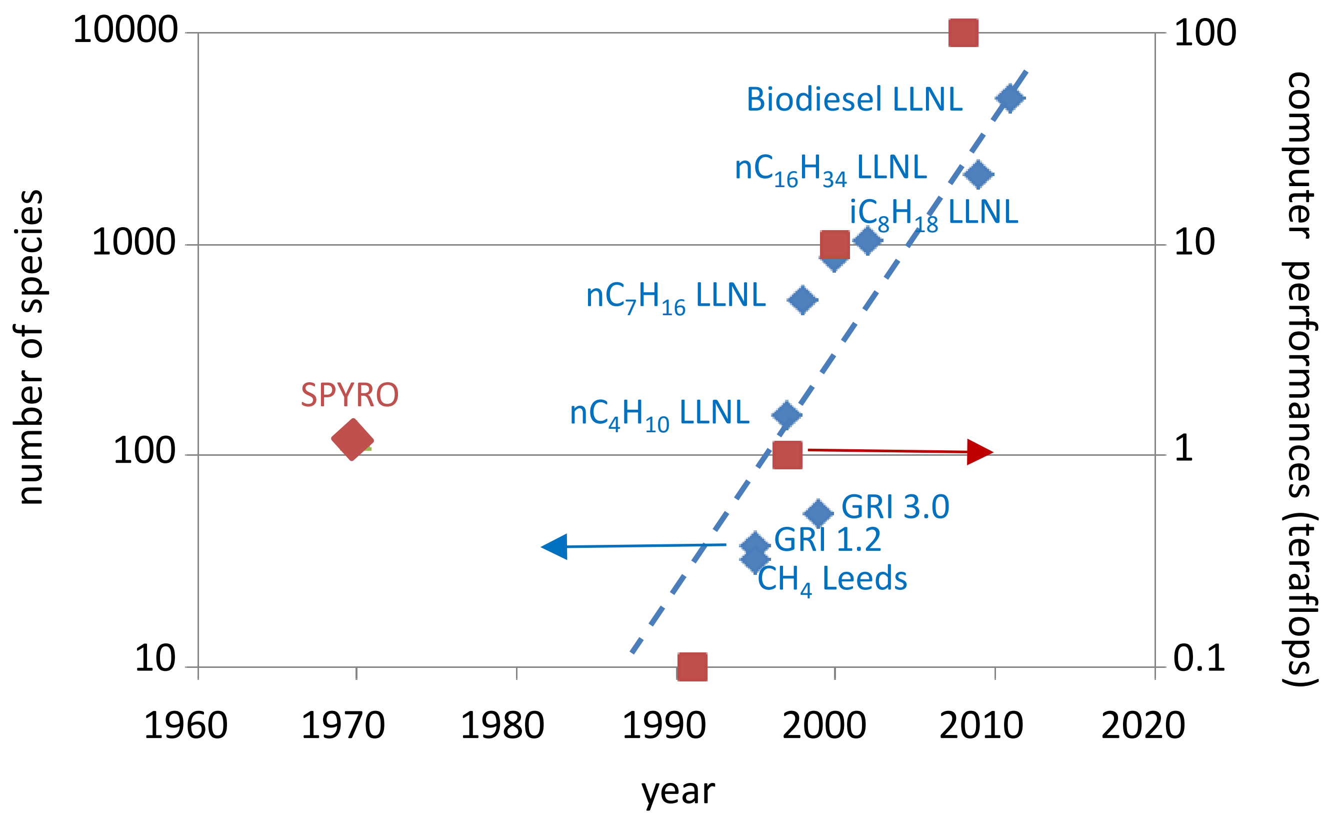


Combustion chemistry is very complex (I)



Adapted from: **T.F. Lu, C.K. Law**, *Toward accommodating realistic fuel chemistry in large-scale computations,* Progress in Energy and Combustion Science, 35, p. 192–215 (2009)

Combustion chemistry is very complex (II)



Adapted from:

T. Faravelli, *Numerical Modeling of Pollutant Emissions with Detailed Kinetics: from Ideal Reactors to Flames*, Invited Lecture at 14th ICNC 2013, San Antonio (TX)

Combustion chemistry is strongly non linear

A reaction in general form:

$$\upsilon_1^f S_1 + \upsilon_2^f S_2 + \cdots + \upsilon_K^f S_K = \upsilon_1^b S_1 + \upsilon_2^b S_2 + \cdots + \upsilon_K^b S_K$$

υ_j^f forward stoichiometric coefficients

υ_j^b backward stoichiometric coefficients

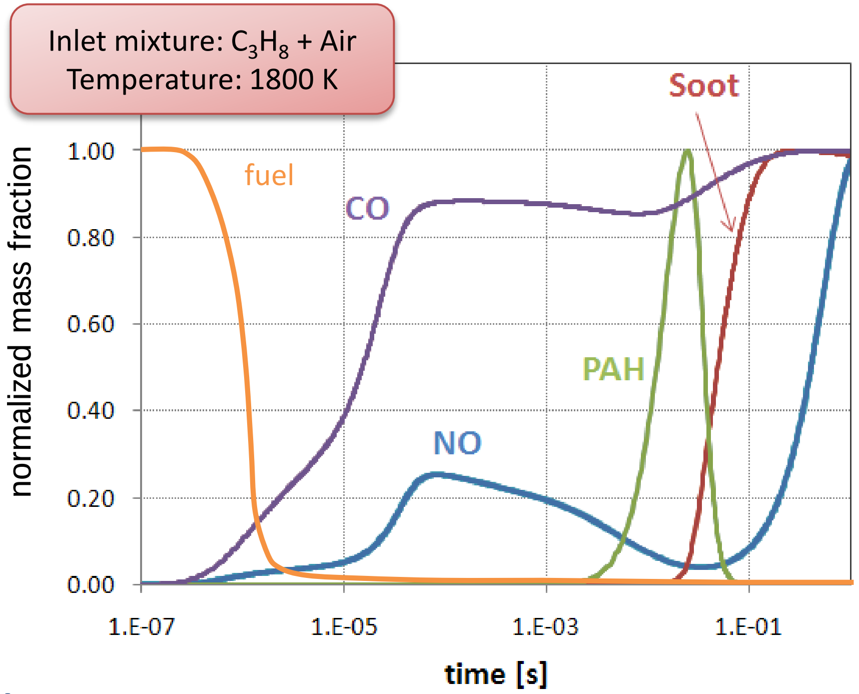
The reaction rates are strongly non-linear!

$$\dot{\Omega}_f = k_f(T) \prod_j C_j^{\upsilon_j^f} \qquad \dot{\Omega}_r = k_r(T) \prod_j C_j^{\upsilon_j^b}$$

$$k_f(T) = AT^n exp\left(-\frac{E}{RT}\right) \qquad k_r(T) = \frac{k_f(T)}{K_{eq}(T)}$$

Adapted from:
Lu T., *Computational Tools for Diagnostics and Reduction of Detailed Chemical Kinetics*, Princeton-CEFRC Summer School on Combustion (2012)

Combustion chemistry is stiff



1. **Slow reactions:**

NOx and soot formation

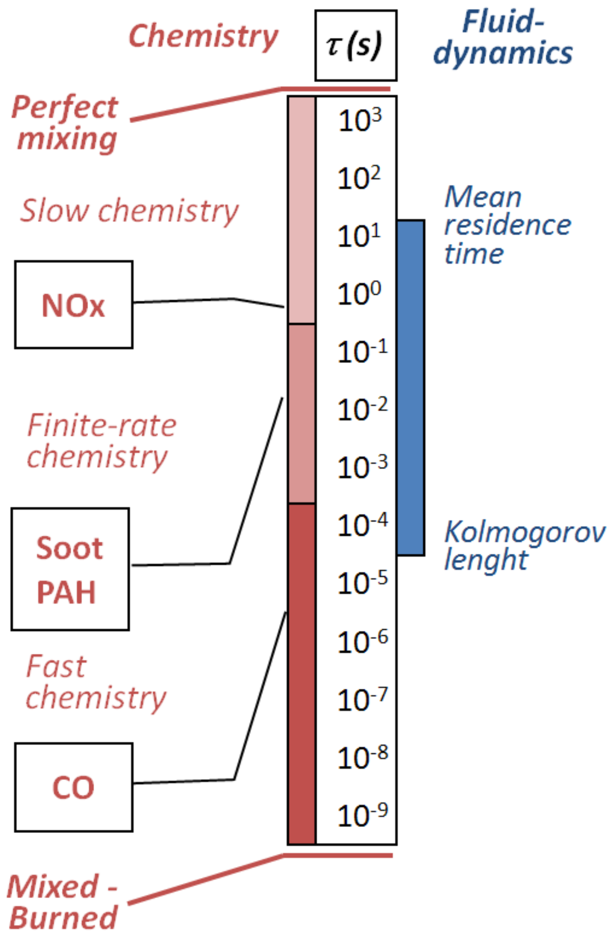
$CO \rightarrow CO_2$ (often rate limiting)

2. **Fast reactions:**

Reactions involving highly reactive radicals (H, O, OH, …)

$HCO \rightarrow CO$

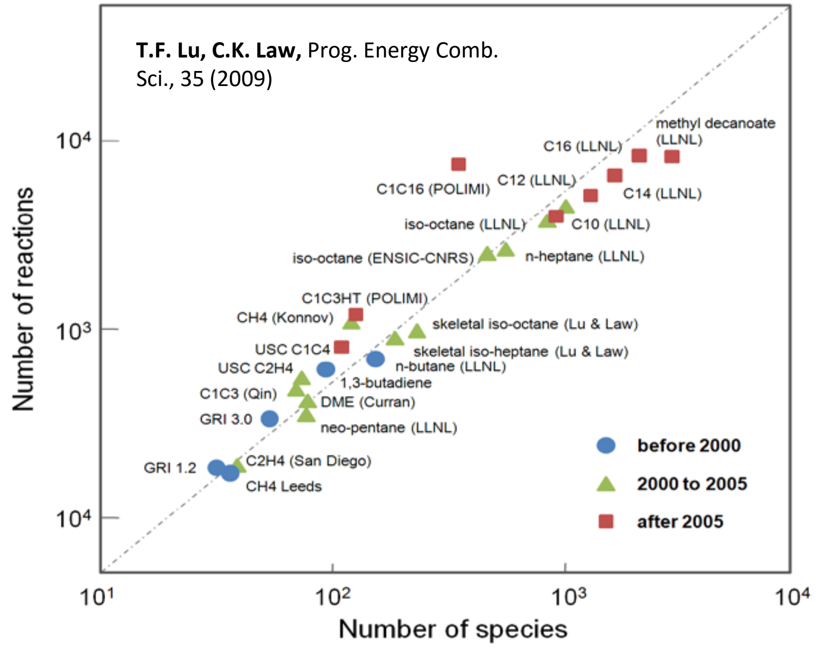
$CH_3O \rightarrow CH_2O$



Adapted from:
R. Fox, *"Computational models for turbulent reacting flows"*, Cambridge University Press (2002)

Outline

Motivations



more complex reaction mechanisms in simulation of combustion processes

development of reaction mechanisms with different levels of **detail and comprehensiveness**

computational cost associated with such mechanisms is usually very high

need of **computational tools** to:

1. **manage** large kinetic mechanisms
2. **integrate** them in new and/or existing numerical codes

OpenSMOKE++ Framework

Object oriented

User friendly

CPU efficient

Extensible

The OpenSMOKE++ Framework

C++ Object-Oriented Programming

OOP produces code that is easier to write, validate, and maintain than procedural techniques. C++ is better suited for complex and highly dynamic data structures.

Templates and Policies

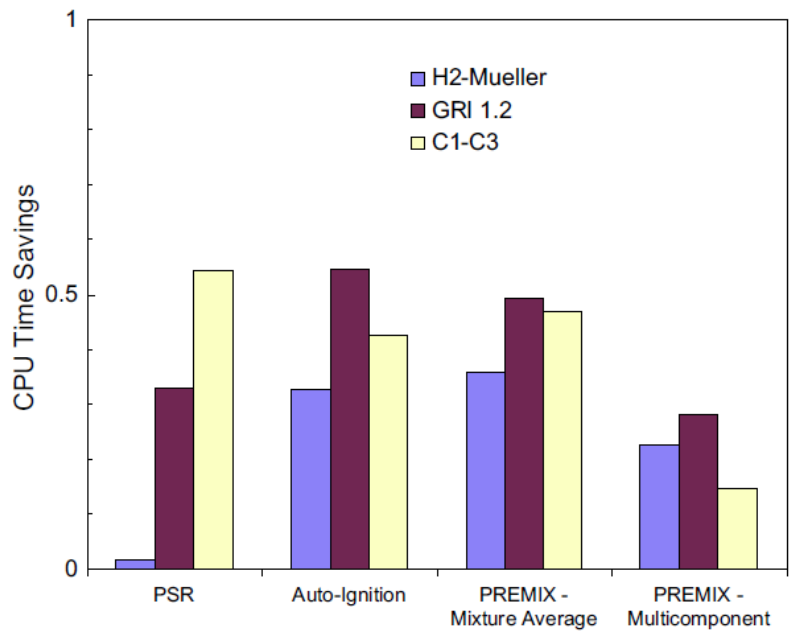
based on ***template programming*** and strongly relies on the concept of *policies* and ***policy classes***, an important class design technique that enable the creation of flexible, highly reusable libraries.

Computation Cost Minimization (CCM)

- **code reformulation:** many parts of the numerical algorithms are reformulated in a less intuitive way in order to minimize the number of flops needed to perform some calculations
- **caching:** the code is written in order to cache as much as possible, which means storing items for future use in order to avoid retrieving or recalculating them
- **object pools:** they are a technique for avoiding the creation and deletion of a large number of objects during the code execution
- **optimized functions:** the numerical algorithms are often reformulated in order to exploit the Intel® MKL Vector Mathematical Functions Library (VML)

CCM: an example of code reformulation

Calculated savings in CPU time with CCM normalized by that of detailed mechanisms



Plot from: **T.F. Lu, C.K. Law**, Prog. Energy Comb. Sci., 35 (2009)

Natural implementation

$$k = AT^n exp\left(-\frac{E}{RT}\right)$$

1 power: ~50 flops
1 exponentiation : ~50 flops
5 multiplications: ~5 flops
Total: ~105 flops

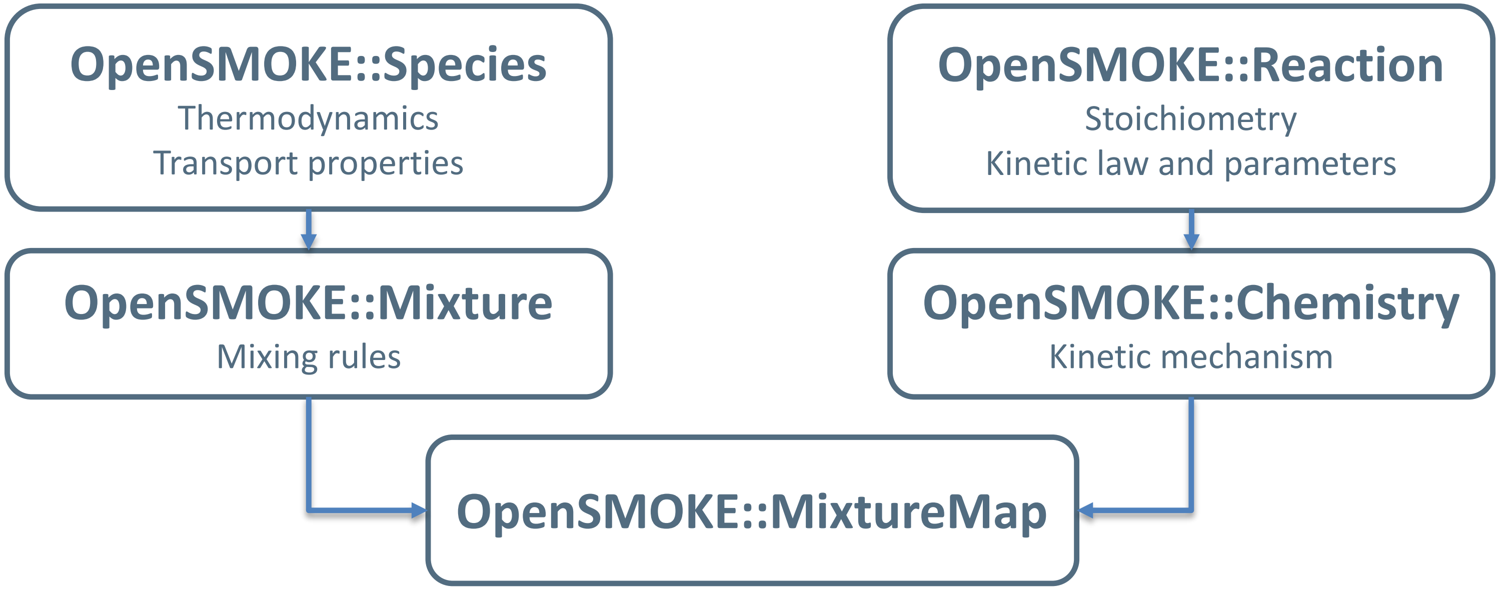
Smart implementation

$$k = exp(ln(A) + \alpha ln(T) - E/RT)$$

1 exponentiation: ~50 flops
3 multiplications: ~5 flops
2 additions: ~2 flops
Total: ~57 flops

The *ln(T)* term above only has to be evaluated once for each call of the rate evaluation subroutine, and the *ln(A)* and *E/R* terms can be pre-evaluated.

OpenSMOKE++ Maps



```
OpenSMOKE::MixtureMap *map = new OpenSMOKE::MixtureMap(fileName);

map->updateStatus(T,P,y);                  // update status
R = map->formationRates();                 // formation rates
r = map->reactionRates();                  // reaction rates
J = map->Jacobian();                       // Jacobian matrix
ropa = map->ROPA();                        // Rate of Production Analysis
```

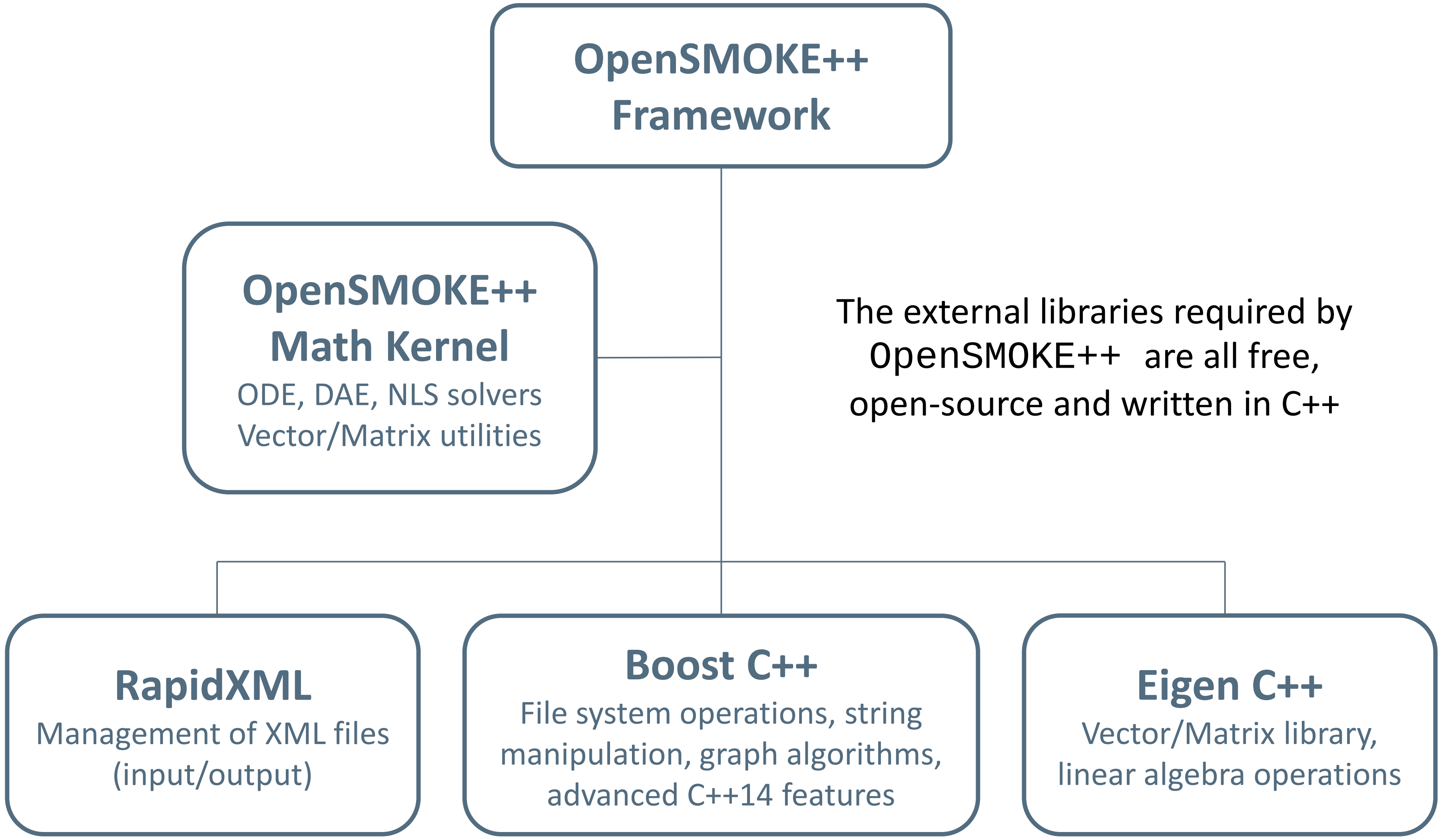
Relevant features of OpenSMOKE++

- Fully compatible with `CHEMKIN` format
- Heterogeneous catalytic reactions (`CHEMKIN` format)
- Detailed transport properties
- Species bundling (efficient calculations of diffusion coefficients)
- Semi-analytical Jacobian evaluation
- Dense and sparse (direct and iterative) linear solvers
- Coupling to a wide range of external ODE, DAE, and NLS solvers
- On-the-fly sensitivity and rate of production analysis

Work in progress

- Stefan-Maxwell approach for estimation of transport properties
- On-the-fly mechanism reduction (through DRG)
- On-the-fly stiffness removal
- Parallelization of ODE and DAE solvers (based on OpenMP®)

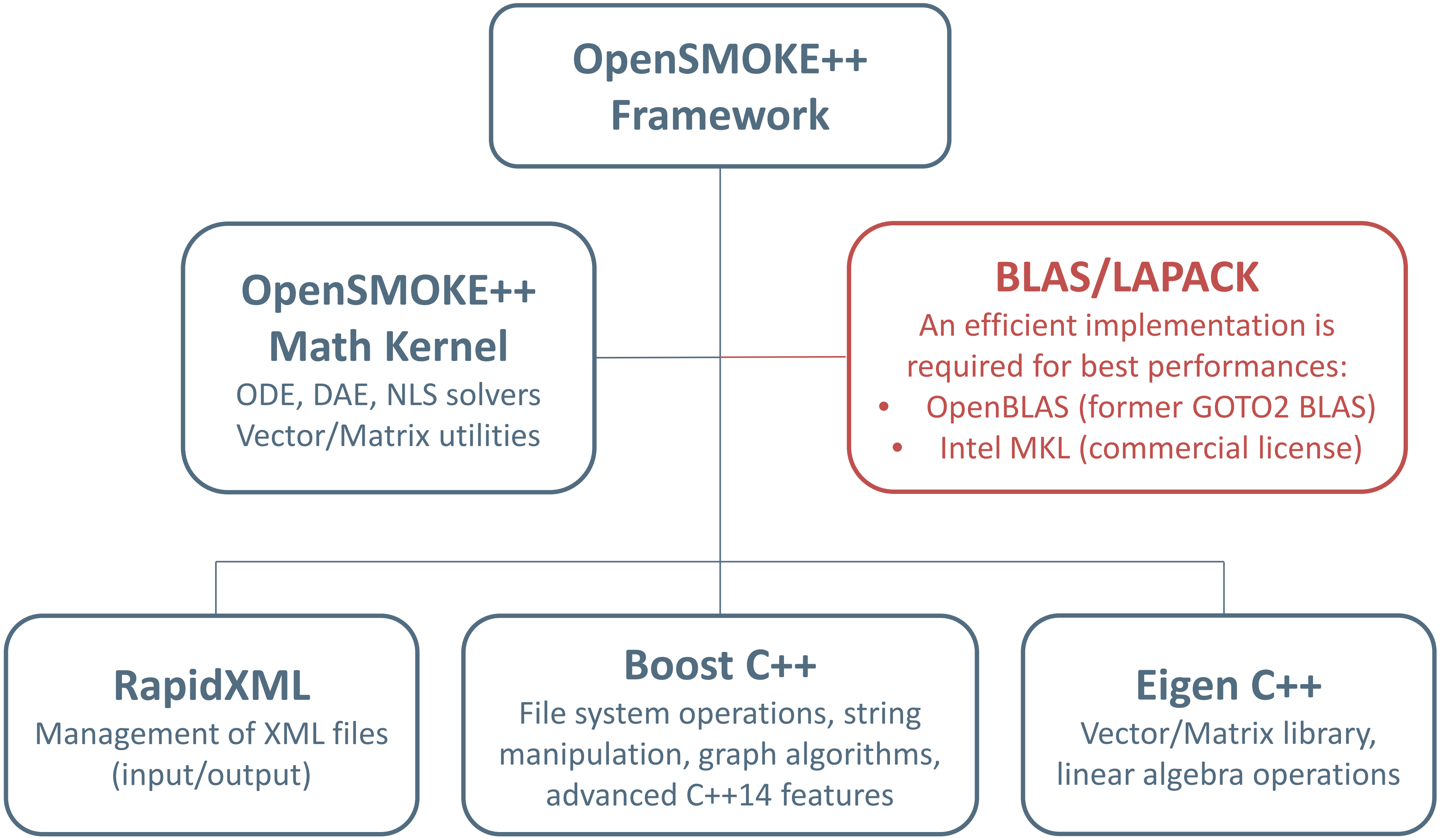
External dependencies



OpenSMOKE++ Framework
OpenSMOKE++ Math Kernel
ODE, DAE, NLS solvers
Vector/Matrix utilities
RapidXML
Management of XML files (input/output)
Boost C++
File system operations, string manipulation, graph algorithms, advanced C++14 features
Eigen C++
Vector/Matrix library, linear algebra operations

The external libraries required by `OpenSMOKE++` are all free, open-source and written in C++

External dependencies



OpenSMOKE++ Framework

OpenSMOKE++ Math Kernel
ODE, DAE, NLS solvers
Vector/Matrix utilities

BLAS/LAPACK
An efficient implementation is required for best performances:
- OpenBLAS (former GOTO2 BLAS)
- Intel MKL (commercial license)

RapidXML
Management of XML files (input/output)

Boost C++
File system operations, string manipulation, graph algorithms, advanced C++14 features

Eigen C++
Vector/Matrix library, linear algebra operations

Additional external libraries (optional)

OpenSMOKE++ Framework

Sundials
Solvers for stiff ODE, DAE, and NL systems

ODEPACK
Solvers for stiff and non stiff ODE systems
(DLSODE, DLSODA, DVODE)

DASPK
Solver for DAE systems

RADAU
Solvers for stiff ODE systems

SuiteSparse
Solvers and utilities for linear sparse systems

SuperLU
Solvers and utilities for linear sparse systems

Outline

1. **Presentation of OpenSMOKE++**
    1. Introduction
    2. The OpenSMOKE++ Framework
    3. **The OpenSMOKE++ Suite**
    4. Coupling with OpenFOAM

2. **Training**
    1. Introduction (environment preparation, organization, …)
    2. Preprocessing of thermodynamics, transport and kinetics
    3. OpenSMOKE++ Maps for thermodynamics, transport and kinetics
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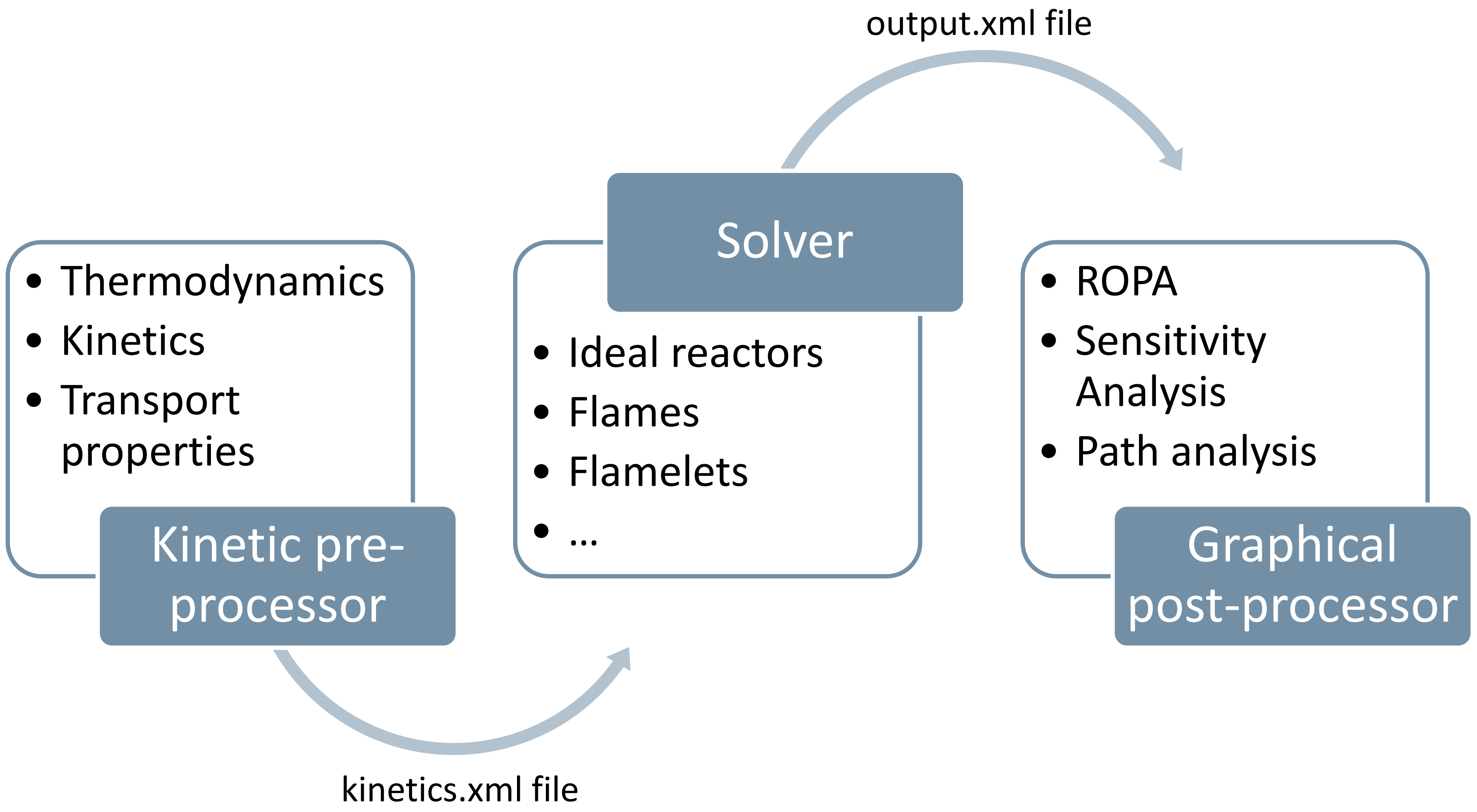
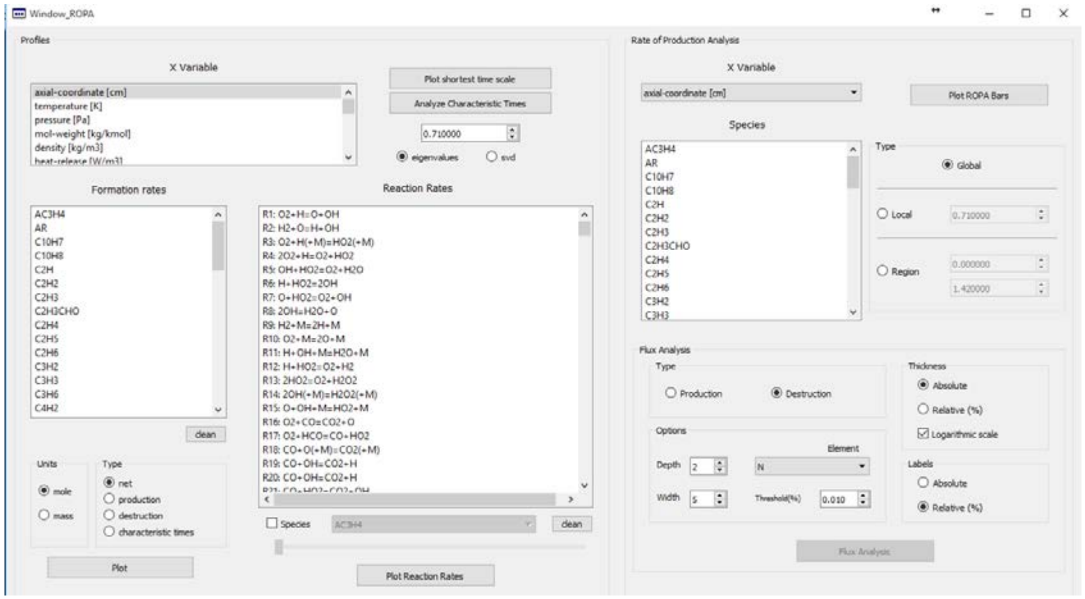
The OpenSMOKE++ Suite (II)

1. Kinetic preprocessor
   Fully compatible with CHEMKIN standard
2. Ideal reactors
   Batch, plug flow, CSTR, shock-tube, rapid compression machine
3. Laminar flames
   1D premixed flat flames, counterflow diffusion flames, burner stabilized stagnation flames
4. Laminar flamelets
   Steady-state flamelet generator, look-up table generator
5. Heterogeneous catalytic reactors
   Batch, plug-flow, honeycomb, CSTR
6. Reduction of kinetic mechanisms
   `DoctorSMOKE++` (flux-based (DRG with error propagation) and sensitivity analyses)

The OpenSMOKE++ Suite (III)



The Graphical Post-Processor (GPP)



```
Window_ROPA

Profiles
X Variable
axial-coordinate [cm]
temperature [K]
pressure [Pa]
mol-weight [kg/kmol]
density [kg/m3]
heat-release [W/m3]

[Plot shortest time scale]
[Analyze Characteristic Times]
0.710000
[✓ eigenvalues]  svd

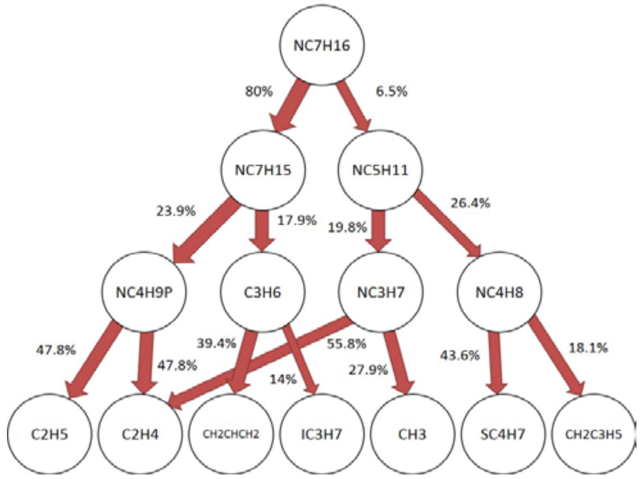
Formation rates
AC3H4
AR
C10H7
C10H8
C2H
C2H2
C2H3
C2H3CHO
C2H4
C2H5
C2H6
C3H2
C3H3
C3H6
C4H2
[clean]

Units: [✓ mole]  mass
Type: [✓ net]  production  destruction  characteristic times
[Plot]

Reaction Rates
R1: O2+H=O+OH
R2: H2+O=H+OH
R3: O2+H(+M)=HO2(+M)
R4: 2O2+H=O2+HO2
R5: OH+HO2=O2+H2O
R6: H+HO2=2OH
R7: O+HO2=O2+OH
R8: 2OH=H2O+O
R9: H2+M=2H+M
R10: O2+M=2O+M
R11: H+OH+M=H2O+M
R12: H+HO2=O2+H2
R13: 2HO2=O2+H2O2
R14: 2OH(+M)=H2O2(+M)
R15: O+OH+M=HO2+M
R16: O2+CO=CO2+O
R17: O2+HCO=CO+HO2
R18: CO+O(+M)=CO2(+M)
R19: CO+OH=CO2+H
R20: CO+OH=CO2+H
Species  AC3H4  [clean]
[Plot Reaction Rates]

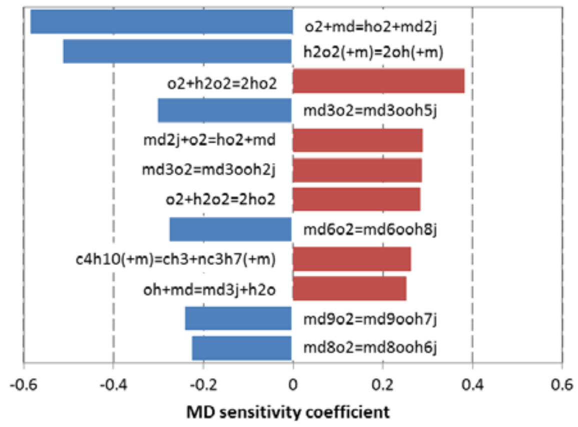
Rate of Production Analysis
X Variable
axial-coordinate [cm]
[Plot ROPA Bars]
Species
AC3H4
AR
C10H7
C10H8
C2H
C2H2
C2H3
C2H3CHO
C2H4
C2H5
C2H6
C3H2
C3H3
Type: [✓ Global]
Local  0.710000
Region  0.000000  1.420000

Flux Analysis
Type: Production  [✓ Destruction]
Options
Depth 2    Element N
Width 5    Threshold(%) 0.010
Thickness: [✓ Absolute]  Relative (%)  [✓ Logarithmic scale]
Labels: Absolute  [✓ Relative (%)]
[Flux Analysis]
```



adiabatic batch reactor (1 atm, 1200 K, Φ=1) burning a mixture of nC7 and air (276 species, 8439 reactions)

adiabatic batch reactor (2 atm, 750 K, Φ=1) burning a mixture of MD and air (460 species, 16,000 reactions)



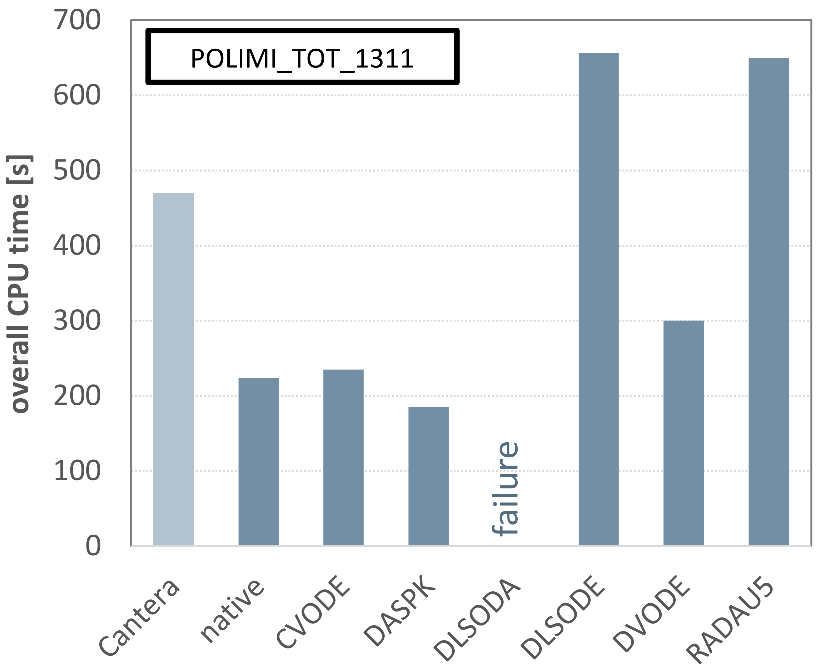
Automatic generation of bar charts and time/space profiles:

- Sensitivity analysis
- ROPA (Rate of Production Analysis)

Automatic generation of flux diagrams:

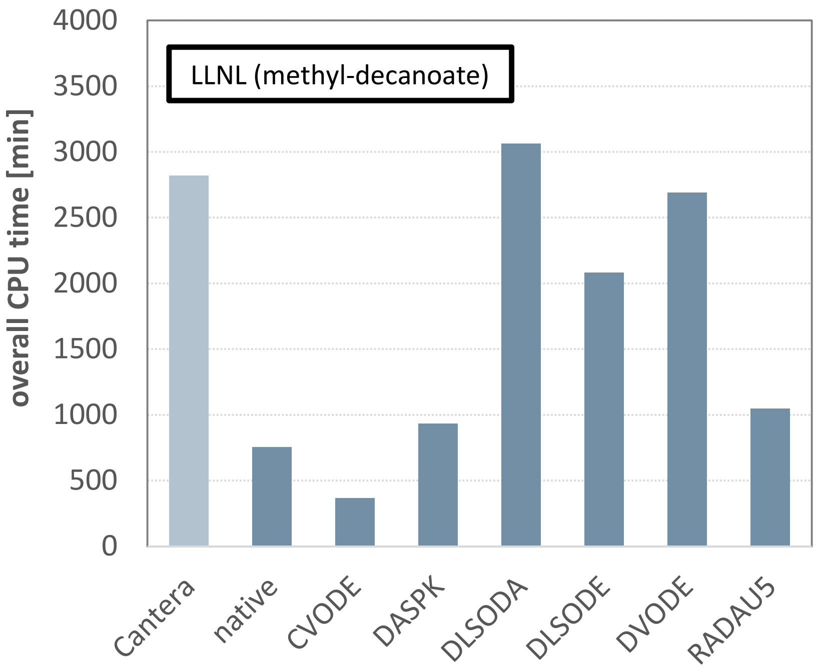
- Reaction Path Analysis

Performances



Constant volume, adiabatic batch reactors burning a mixture of methyl-decanoate and air (460 species, 16,000 reactions)

Pressures: 2-20 atm
Temperatures: 750-1500 K
Equivalence ratios: 0.5-2



Constant volume, adiabatic batch reactors burning a mixture of methyl-decanoate and air (2878 species, 8,855 reactions)

Pressures: 2-20 atm
Temperatures: 750-1500 K
Equivalence ratios: 0.5-2

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Coupling with OpenFOAM®

OpenFOAM®

Unstructured, multidimensional meshes
Spatial discretization of transport equations
Density/Pressure coupling algorithms
Input/Output management
MPI Parallelization
Turbulence models (RANS, LES)

+

OpenSMOKE++

Thermodynamics and detailed kinetics
Multicomponent transport properties
ODE solvers for stiff chemistry
Tools for kinetic analysis (ROPA)

laminarSMOKE

- Simulation of reacting flows in laminar conditions (coflow flames, burner stabilized stagnation flames, …)

flameletSMOKE

- Simulation of turbulent flames based on the steady-state laminar flamelet

edcSMOKE

- Simulation of turbulent flames based on the Eddy Dissipation Concept (EDC) model

catalyticFOAM

- Simulation of catalytic heterogeneous (gas/solid) reactors (in cooperation with M. Maestri, Energy Dep. Polimi)

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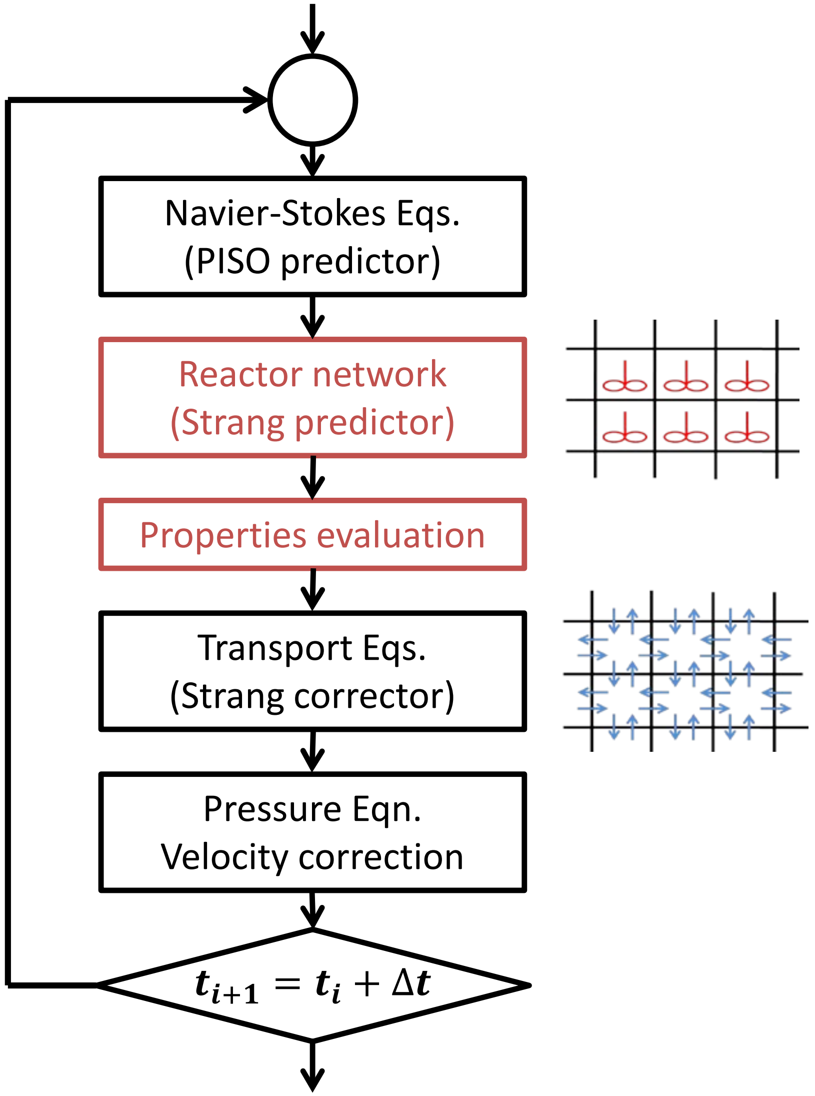
Operator-splitting algorithm



```
while (runTime.run())
{
        #include "readTimeControls.H"
        #include "readPISOControls.H"
        #include "compressibleCourantNo.H"
        #include "setDeltaT.H"

        runTime++;

        #include "rhoEqn.H«

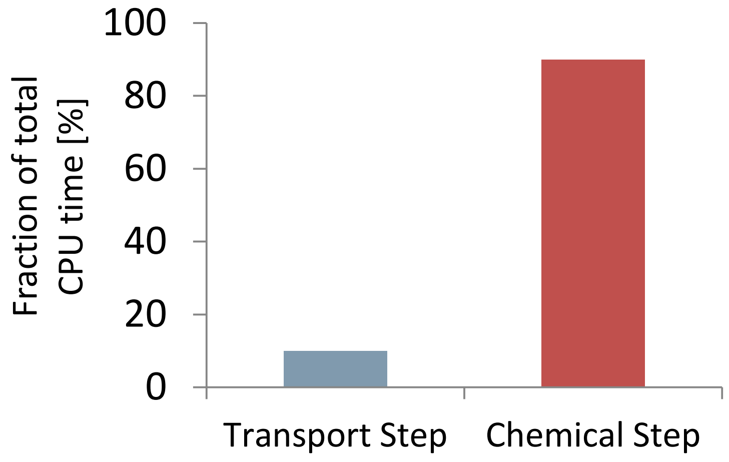
        for (label k=1;k<=nOuterCorr;k++)
        {
                #include "UEqn.H"
                #include "chemistry.H"
                #include "properties.H"
                #include "YEqn.H"
                #include "TEqn.H"

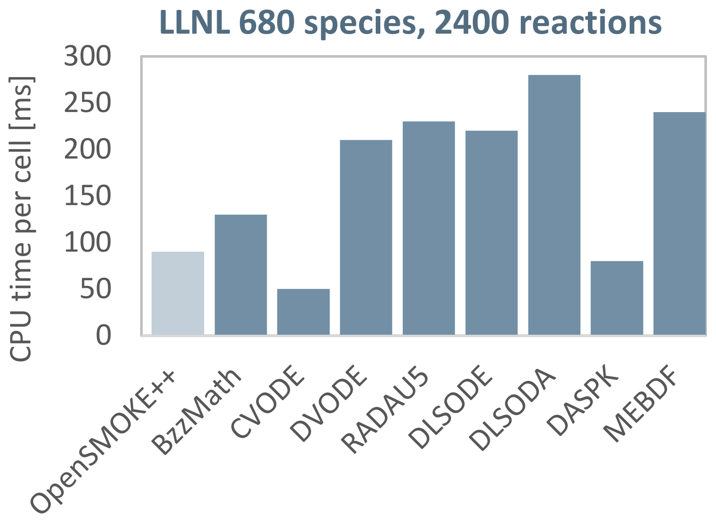
                for (int j=1;j<=nCorr;j++)
                        #include "pEqn.H"
        }

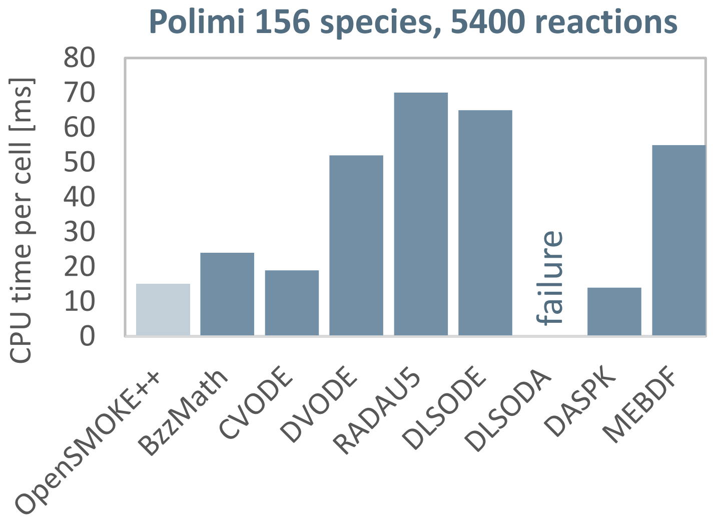
        #include "write.H"
}
```

Performances

Most of the CPU Time (80-90%) is spent for the numerical integration of the ODE systems corresponding to the network of batch reactors



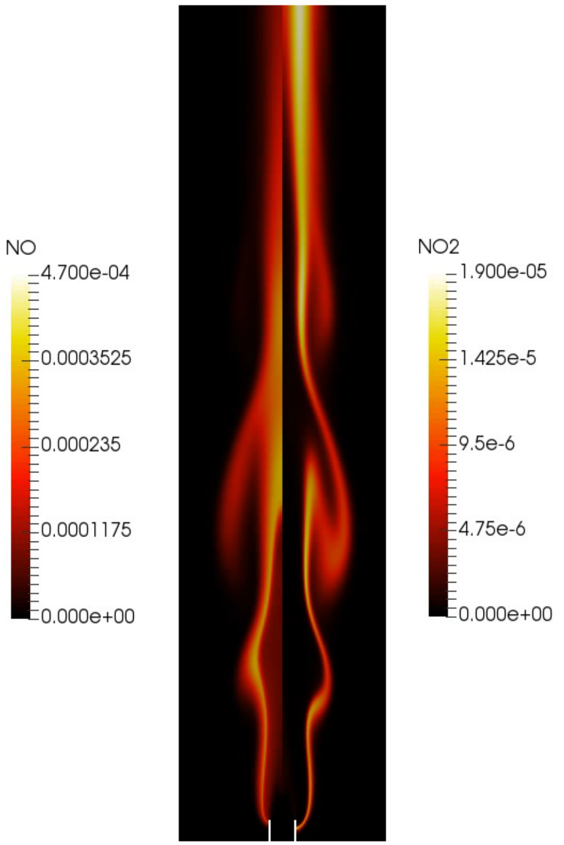




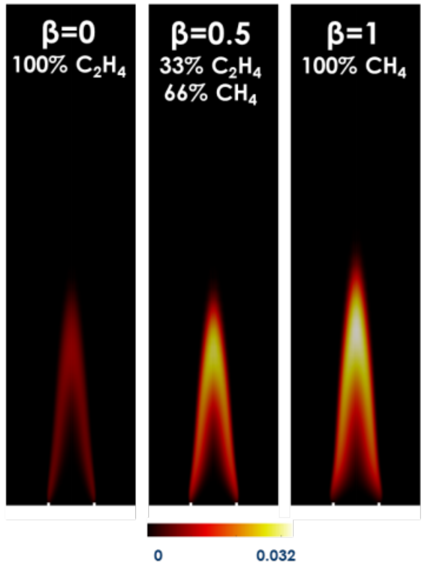
The best ODE solver depends on the features of the kinetic mechanism adopted:

- ✓ number of species
- ✓ species/reactions ratio
- ✓ lumped reactions

Examples

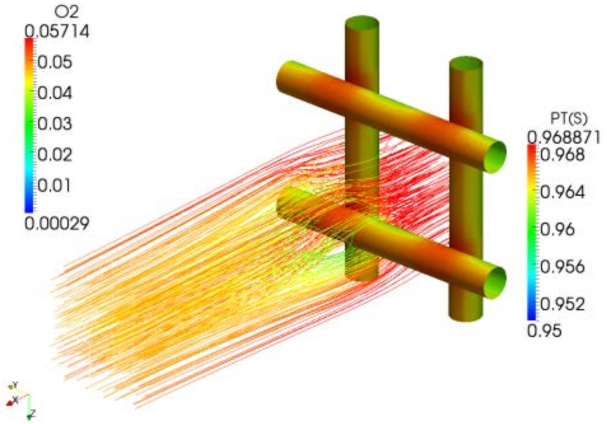


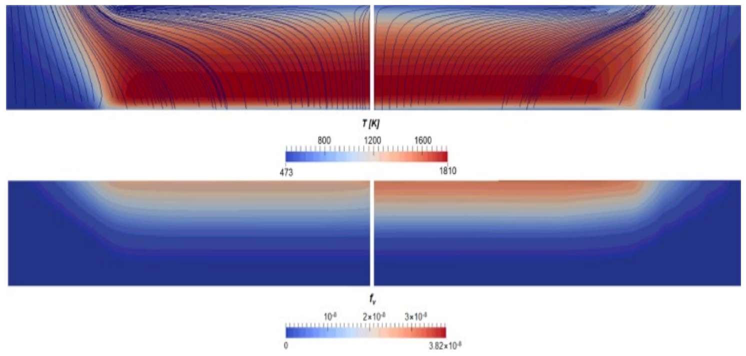
Naturally flickering coflow flame fed with propane in air



Laminar coflow flames fed with CH4/C2H4 mixtures

Catalytic Partial Oxidation of CH4 over a Pt gauze





Soot formation in a burner stabilized stagnation flame

Naturally flickering flame (I)

Example of naturally flickering buoyancy-dominated diffusion flame

https://www.youtube.com/watch?v=w5zWkSuYflY

Naturally flickering buoyancy-dominated diffusion flames exhibit natural flicker as a result of a **buoyancy-induced flow instability**, which leads to the formation of strong vortical motions that subsequently interact with the combusting regions of the flame.

Naturally occurring flickering flames are **difficult to investigate experimentally** because, even though the **flickering frequency** is well defined, there exist cycle-to-cycle variations. These variations lead to spatial and temporal averaging with a resulting loss in resolution.

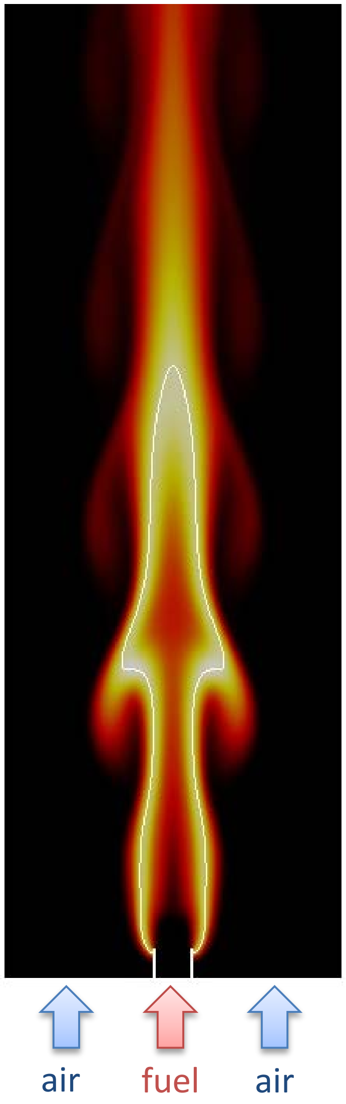
Naturally flickering flame (II)

Chrystie & Chung (2014) Combustion Science and Technology, 186:4-5, 409-420, DOI: 10.1080/00102202.2014.883202

Fuel stream
Composition: 100% C3H8
Temperature: 298 K
Velocity: 10 cm/s

Oxidizer stream
Composition: 21% O2+79% N2
Temperature: 298 K
Velocity: 7 cm/s

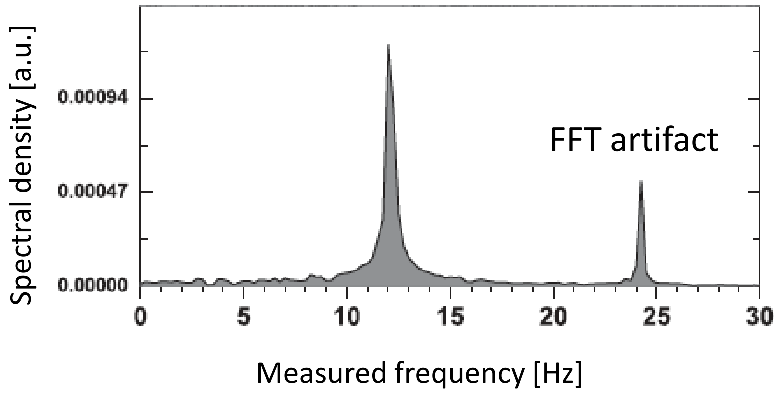
Burner
Diameter: 9 mm
Thickness: 0.8 mm



Under normal gravity conditions, laminar coflow diffusion flames have a well defined **oscillation frequency f**, which is inversely proportional to the square root of the burner diameter, D (in m):

$$f \sim \frac{1.5}{\sqrt{D}}$$

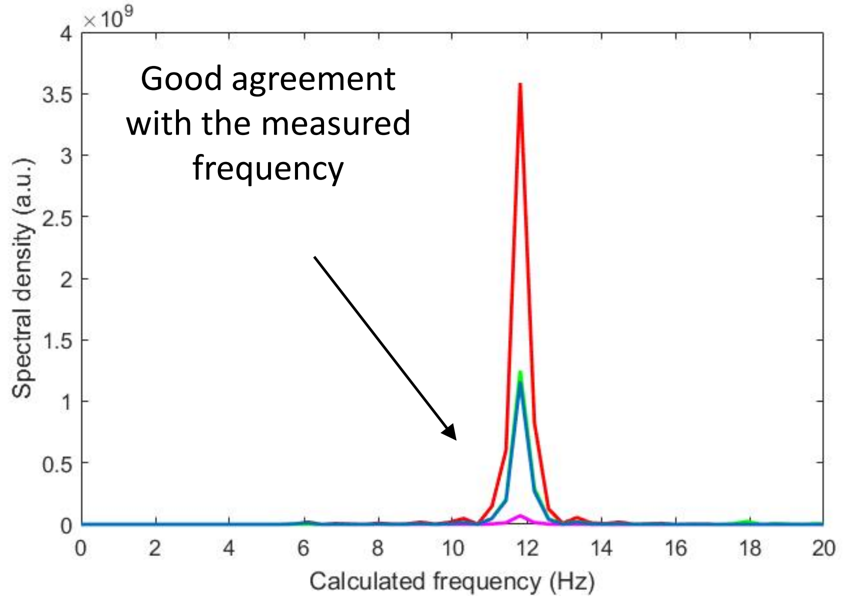
FFT decomposition of the frequencies (exp.)

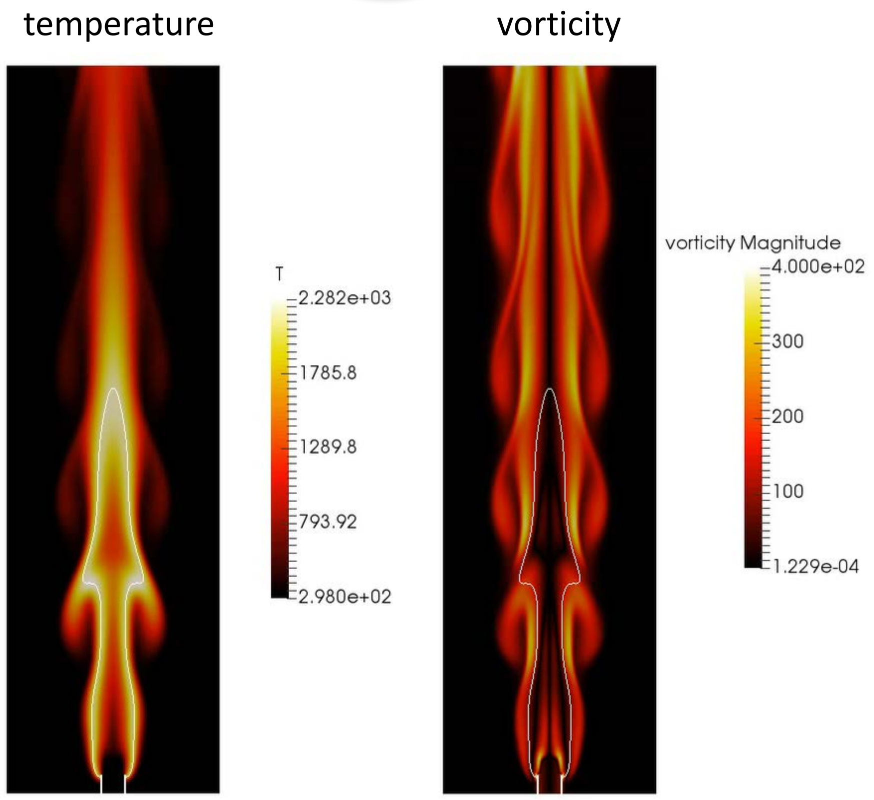


Naturally flickering flame (III)

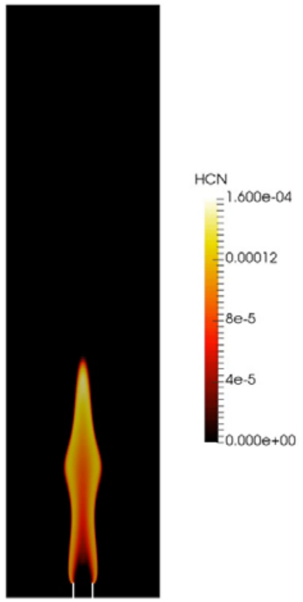
2D computational domain: 75 x 300 mm^2
Number of cells: 58,000
Spatial discretization: 2nd order centered
Time integration: Cranck-Nicolson
ODE solver: OpenSMOKE++
Absolute tolerance: 1e-12
Relative tolerance: 1e-7
Linear solver: Sparse, MKL Pardiso

Kinetic mechanism: POLIMI_2015
Soot model: discrete sectional method
Number of species: 210
Number of reactions: 10,800



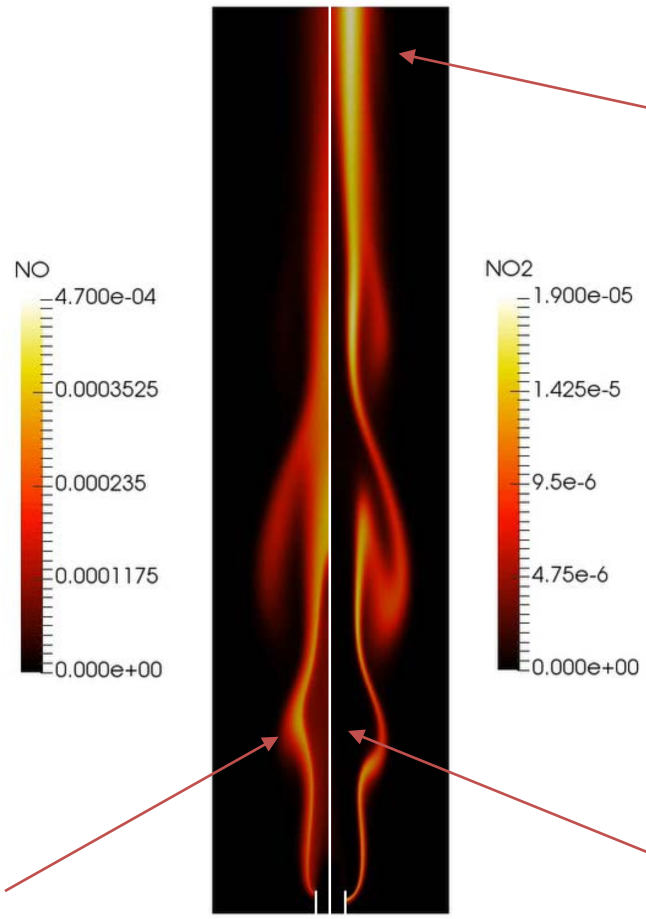


Naturally flickering flame (IV)



NO is converted to HCN in the very rich region of the flame

NOx (nitrogen oxides) mass fractions



NO to NO2 conversion is kinetically controlled (slow reaction):
$NO+HO_2=NO_2+OH$

NO2 is more stable than NO at low temperature (< 900K)

NO formation mainly occurs along the flame front (high temperatures are required)

No NO2 in the rich region, because of reaction with H radical:
$NO_2+H=NO+OH$

Outline

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   3. The OpenSMOKE++ Suite
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2. **Training**
   1. **Introduction (environment preparation, organization, …)**
   2. Preprocessing of thermodynamics, transport and kinetics
   3. OpenSMOKE++ Maps for thermodynamics, transport and kinetics
   4. OpenSMOKE++ for modeling a batch reactor
   5. A multidimensional laminar solver for reacting flows

Download the training session material

The source code adopted in this Training Session can be downloaded from the GitHub repository available at the following address:

https://github.com/acuoci/OpenFOAMTrainingCombustion

You can download the corresponding zip file:

```
https://github.com/acuoci/OpenFOAMTrainingCombustion/archive/master.zip
```

or clone the repository:

```
git clone https://github.com/acuoci/OpenFOAMTrainingCombustion.git
```

Preparation of your environment

The `OpenSMOKE++` libraries rely some third-party libraries for some important tasks:

- `Eigen++` (for linear algebra operations)
- `RapidXML` (for XML file management)
- `Boost C++` (for string manipulation, file system operations, etc.)

The `Eigen++` and `RapidXML` libraries do not require precompilation, since they are entirely based on header files and they are provided together with the `OpenSMOKE++` libraries. The `Boost C++` libraries are not provided with `OpenSMOKE++`. Usually they are already available in your Linux distribution. If not, you need to install them. For Ubuntu and SuSE distribution you can use the following commands:

Ubuntu (versions 14.04 or above)

```
sudo apt-get install libboost-all-dev
```

SuSE (OpenSuSE/SLES v12 or above, or Tumbleweed)

```
sudo zypper install boost-devel
```

Compiling Boost C++ from source code

If you cannot install the `Boost C++` libraries using the commands reported in the previous slide, You need to download the source code and compile it:

1. Download the source code from:
   https://dl.bintray.com/boostorg/release/1.64.0/source/

2. Follow the compilation and installation instructions reported at:
   http://www.boost.org/doc/libs/1_64_0/more/getting_started/unix-variants.html

After compilation and installation, set the environment variable pointing at the location where the compiled `Boost C++` libraries have been installed (i.e. the folder containing the `include` and `lib` subfolders):

bash or ksh

```
export BOOST4OPENSMOKEPP=/path/to/boost
```

tcsh or csh

```
setenv BOOST4OPENSMOKEPP /path/to/boost
```

Checking if your environment is OK

In order to check if the environment is OK, we compile and run a simple application based on `OpenSMOKE++` and `OpenFOAM`.

1. Go to the `Training/TestEnvironment` folder
2. Compile the source code by typing: `wmake`
3. If compilation successfully completed, run the solver by typing: `testEnvironment`

If everything was done properly, you should have the following output on the screen:

```
...
Selecting ODE solver seulex
0.000000e+00
1.000000e-06
2.000000e-06
3.000000e-06
4.000000e-06
5.000000e-06
6.000000e-06
7.000000e-06
8.000000e-06
9.000000e-06
```

Organization

`OpenFOAMTrainingCombustion`

- `Docs`
- `KineticMechanisms`
- `Libraries`
- `PreProcessing`
- `Training`

`Docs`
Documentation files (including this presentation)

`KineticMechanisms`
Collection of several detailed kinetic mechanisms in CHEMKIN format (thermodynamics, transport and kinetic files) adopted for running the simulations

`Libraries`
Source code of required libraries (`OpenSMOKE++`, `Eigen++`, `RapidXML`)

`PreProcessing`
Folder where pre-processing of kinetic mechanisms is carried out

`Training`
Source code of examples adopted in the current training session

KineticMechanisms folder

Global_H2_1step/Global_CH4_1step
Global 1-step mechanisms for hydrogen or methane combustion. Useful only for first-guess solutions. Here adopted only because their reduced computational time.

POLIMI_H2_1412
Detailed mechanism for hydrogen combustion: 9 species, 20 reactions

POLIMI_H2CO_1412
Detailed mechanism for syngas (H2+CO) combustion: 14 species, 33 reactions

POLIMI_H2CO_NOX_1412
Detailed mechanism for syngas (H2+CO) combustion with NOX (nitrogen oxides) chemistry (thermal, prompt, NNH, ...): 32 species, 173 reactions

POLIMI_CH4_Pyrolysis
Detailed mechanism for methane pyrolysis: 28 species, 157 reactions

GRI30noNOX
Detailed mechanism for methane combustion without NOX: 36 species, 219 reactions

GRI30
Detailed mechanism for methane combustion with NOX: 53 species, 325 reactions

Libraries folder

OpenSMOKEpp

This is the latest version of OpenSMOKE++ library. It is entirely based on header files, which means that no compilation is required.

eigen-3.3.3

Eigen is a C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms. It is entirely based on header files, which means that no compilation is required. New versions can be downloaded from:
http://eigen.tuxfamily.org/index.php?title=Main_Page

Rapidxml-1.13

RapidXML is a very fast XML parser, user-friendly and very portable, since entirely based on header files. New versions can be downloaded from:
http://rapidxml.sourceforge.net/index.htm

Training folder

TestEnvironment
Source code for testing the OpenFOAM/OpenSMOKE++ environment

OpenSMOKEpp_CHEMKIN_PreProcessor
Source code for OpenSMOKE++ kinetic preprocessor

Maps
Source code showing how to use the OpenSMOKE++ Maps for thermodynamics, transport properties, and detailed kinetics

BatchReactor
Source code showing how to implement a batch reactor solver coupling OpenSMOKE++ with OpenFOAM

Solvers
Source code for multidimensional solvers for laminar reacting flows with detailed kinetic mechanisms (steady-state and unsteady) based on OpenFOAM and coupled with OpenSMOKE++

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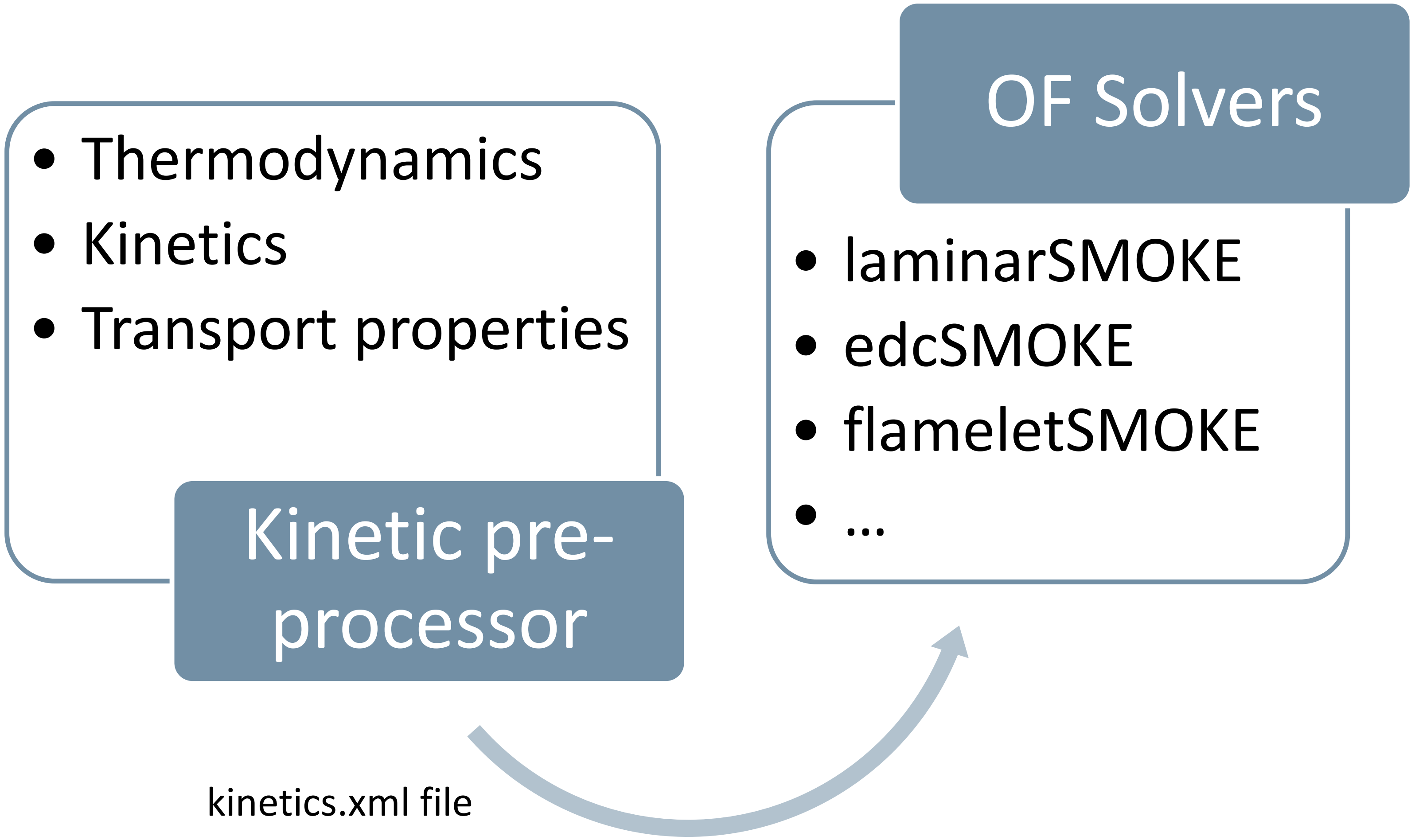
Preprocessing of CHEMKIN mechanisms



Compiling the CHEMKIN PreProcessor

The `OpenSMOKEpp_CHEMKIN_PreProcessor` is a utility to pre-process thermodynamics, transport properties and chemical reactions available in `CHEMKIN` format.

1. The source code is available in the `Training/OpenSMOKEpp_CHEMKIN_PreProcessor` folder
2. Open the `Training/OpenSMOKEpp_CHEMKIN_PreProcessor` folder
3. Type `wmake`

Running the CHEMKIN PreProcessor (I)

In order to preprocess a kinetic mechanism, three files are needed (the names are arbitrary):

1. `Thermo.CKT` (thermodynamic properties)
2. `Transport.TRC` (transport properties)
3. `Kinetics.CKI` (reactions)

Examples of kinetic mechanisms are available in the `KineticMechanisms` folder

The CRECK Modeling group at Politecnico di Milano provides detailed kinetic mechanisms describing pyrolysis, combustion, and oxidation of several fuels (hydrogen, methane, propane, PRF, diesels, jet-fuels, biofuels, etc.): http://creckmodeling.chem.polimi.it/

A **User's Guide** explaining the features and the complete list of options of OpenSMOKE++ Kinetic PreProcessor is available in the `Docs` folder (`CHEMKIN_PrePreprocessor.pdf` file).

Running the CHEMKIN PreProcessor (II)

As a first example, the `POLIMI_H2_1412` kinetic mechanism will be pre-processed.

The required files (trhermodynamics, transport, and kinetics) are available in the `KineticMechanisms/POLIMI_H2_1412` folder, but we recommend to preprocess kinetic mechanisms from a different folder. In this training session, we will use the PreProcessing folder for preprocessing activities.

1. Go to the `PreProcessing/POLIMI_H2_1412` folder
2. Run the `OpenSMOKEpp_CHEMKIN_PreProcessor :`
   ```
   OpenSMOKEpp_CHEMKIN_PreProcessor --input input.dic
   ```
3. Results are available in the `kinetics-POLIMI_H2_1412` folder

Running the CHEMKIN PreProcessor (III)

The `input.dic` file (the name is arbitrary) is a text file in which the user specifies the paths to the three files containing thermodynamics, transport properties and chemical reactions

```
Dictionary CHEMKIN_PreProcessor
{
      @Thermodynamics  POLIMI_TOT_NOX_1412.CKT;
      @Transport       POLIMI_TOT_NOX_1412.TRC;
      @Kinetics        POLIMI_H2_1412.CKI;

      @Output          kinetics-POLIMI_H2_1412;
}
```

`input.dic`

Analysis of thermodynamic properties (I)

It is important to check the consistency of thermodynamic data:

- continuity of thermodynamic functions
- continuity of first-order derivative (recommended)
- monotonic behavior of thermodynamic functions

```
Dictionary CHEMKIN_PreProcessor
{
      @Thermodynamics          POLIMI_TOT_NOX_1412.CKT;
      @Transport               POLIMI_TOT_NOX_1412.TRC;
      @Kinetics                POLIMI_H2_1412.CKI;
      @CheckThermodynamics     true;

      @Output            kinetics-POLIMI_H2_1412;
}
```

input.dic

Analysis of thermodynamic properties (II)

```
==========================================================
    Status  of  specific   heat
----------------------------------------------------------
Name    Tl  Tm      Th       Cp/R(-)     Cp/R(+)       e(%)
==========================================================
H2      200 750     3500    3.55E+00    3.55E+00    1.37E-07
O2      200 760     3500    4.02E+00    4.02E+00    2.84E-07
H2O     200 1590    3500    5.77E+00    5.77E+00    1.07E-07
H2O2    200 1180    3500    7.99E+00    7.99E+00    3.25E-08
O       200 950     3500    2.52E+00    2.52E+00    3.17E-08
H       200 1490    3500    2.50E+00    2.50E+00    1.71E-10
OH      200 880     3500    3.65E+00    3.65E+00    5.68E-08
HO2     200 1540    3500    6.32E+00    6.32E+00    1.77E-07
N2      200 1050    3500    3.96E+00    3.96E+00    1.80E-07
```

ThermodynamicsStatus.out

Analysis of thermodynamic properties (III)

```
==================================================
Anomalous behaviour of thermodynamic properties
==================================================
HT Cp for O in [950.00-3500.00] has local maxima at: 1926.35
LT Cp for H in [200.00-1490.00] has local maxima at: 605.76 1321.10
HT Cp for H in [1490.00-3500.00] has local maxima at: 2287.83 3148.97
LT Cp for N2 in [200.00-1050.00] has local maxima at: 330.66
```

ThermodynamicsStatus.out

Rewriting the thermodynamic properties (I)

When the `@CheckThermodynamics` option is turned on, the thermodynamic properties are corrected in order to ensure the continuity up to the 3rd order derivative and rewritten in new file

thermo.CHEMKIN.CKT

```
! This thermodynamic database was obtained by fitting the thermodynamic
! Properties extracted from the following file: POLIMI_TOT_NOX_1412.CKT
! The thermodynamic properties are fitted in order to preserve not only the
! continuity of each function at the intermediate temperature, but also the
! Continuity of the derivatives, from the 1st to the 3rd order. The intermediate
! temperatures are chosen in order to minimize the fitting error.

THERMO ALL
270.   1000.   3500.
H2                       H   2                G    200.00   3500.00  750.00      1
 3.73110903e+00-8.86706232e-04 1.12286898e-06-3.74349785e-10 4.17963677e-14    2
-1.08851547e+03-5.35285859e+00 3.08866002e+00 2.53968851e-03-5.72992050e-06    3
 5.71701864e-09-1.98865977e-12-9.92148123e+02-2.43823453e+00                   4
O2                       O   2                G    200.00   3500.00  760.00      1
 2.81750647e+00 2.49838007e-03-1.52493520e-06 4.50547600e-10-4.87702781e-14    2
-9.31713391e+02 7.94729339e+00 3.46035082e+00-8.85011230e-04 5.15281079e-06    3
-5.40712432e-09 1.87809548e-12-1.02942573e+03 5.02236119e+00                   4
```

Rewriting the thermodynamic properties (II)

In addition, the thermodynamic properties are also re-fitted and rewritten using exactly the same intermediate temperature for every species (default 1000 K). This could be required by some old applications.

`thermo.CHEMKIN.fixedT.CKT`

```
! This thermodynamic database was obtained by fitting the thermodynamic
! Properties extracted from the following file: POLIMI_TOT_NOX_1412.CKT
! The thermodynamic properties are fitted in order to preserve not only the
! continuity of each function at the intermediate temperature, but also the
! Continuity of the derivatives, from the 1st to the 3rd order. The
! intermediate temperatures are the same for all the species.

THERMO ALL
270.   1000.   3500.
H2                      H   2               G    200.00   3500.00 1000.00      1
 3.87655112e+00-1.22795344e-03 1.39229943e-06-4.61414188e-10 5.16896624e-14    2
-1.13335667e+03-6.12445685e+00 3.23482792e+00 1.33893937e-03-2.45803978e-06    3
 2.10547862e-09-5.90033540e-13-1.00501203e+03-3.02851335e+00                   4
O2                      O   2               G    200.00   3500.00 1000.00      1
 2.67521006e+00 2.83203854e-03-1.78825691e-06 5.35610921e-10-5.84339610e-14    2
-8.87805402e+02 8.70230607e+00 3.32264375e+00 2.42303767e-04 2.09634526e-06    3
-2.05412386e-09 5.88999733e-13-1.01729214e+03 5.57881275e+00                   4
```

Analysis of transport properties (I)

Transport properties of individual species can be rewritten using a simple analytical expression based on a 3rd order polynomial function

```
Dictionary CHEMKIN_PreProcessor
{
      @Thermodynamics           POLIMI_TOT_NOX_1412.CKT;
      @Transport                POLIMI_TOT_NOX_1412.TRC;
      @Kinetics                 POLIMI_H2_1412.CKI;
      @TransportFittingCoefficients true;

      @Output            kinetics-POLIMI_H2_1412;
}
```

input.dic

Analysis of transport properties (II)

```
-----------------------------------------------------------------------------------------------
                       VISCOSITY FITTING COEFFICIENTS

             mu = exp( A + B*logT + C*(logT)^2 + D*(logT)^3 )  [kg/m/s]

  Species    A             B             C              D             mu(298K)      mu(1000K)
-----------------------------------------------------------------------------------------------


  1. H2     -1.583982e+01 8.692958e-01 -3.054617e-02  1.384164e-03  8.958993e-06  1.967286e-05
  2. O2     -1.906650e+01 2.494518e+00 -2.440586e-01  1.072526e-02  2.053924e-05  4.794243e-05
  3. H2O    -2.028994e+01 2.046198e+00 -7.669556e-02 -7.595355e-04  1.284832e-05  4.252813e-05
  4. H2O2   -1.903595e+01 2.494518e+00 -2.440586e-01  1.072526e-02  2.117638e-05  4.942964e-05
  5. O      -1.702676e+01 1.755265e+00 -1.474358e-01  6.515978e-03  2.473511e-05  5.605138e-05
  6. H      -2.213944e+01 3.389886e+00 -3.580432e-01  1.556519e-02  9.447645e-06  2.306615e-05
  7. OH     -1.699621e+01 1.755265e+00 -1.474358e-01  6.515978e-03  2.550241e-05  5.779014e-05
  8. HO2    -1.905099e+01 2.494518e+00 -2.440586e-01  1.072526e-02  2.086024e-05  4.869171e-05
  9. N2     -1.853769e+01 2.232971e+00 -2.102014e-01  9.264622e-03  1.799150e-05  4.152188e-05


 -----------------------------------------------------------------------------------------------
```

TransportProperties_Coefficients.out

Reverse reaction rates (I)

For each reversible reaction the reverse kinetic constants are estimated assuming the Arrhenius' law.

```
Dictionary CHEMKIN_PreProcessor
{
       @Thermodynamics     POLIMI_TOT_NOX_1412.CKT;
       @Transport          POLIMI_TOT_NOX_1412.TRC;
       @Kinetics           POLIMI_H2_1412.CKI;
       @ReverseFitting     true;

       @Output             kinetics-POLIMI_H2_1412;
}
```

input.dic

Reverse reaction rates (II)

The kinetic parameters of the reverse reactions are then written on the `Reaction_FittedKinetics.out` file.

```
==========================================================================
    Reaction           A            Beta            E          Reaction
     index       [kmol,m3,s]                     [cal/mol]
 =========================================================================
 8               1.2072e+10    -1.327         -7393.17     H2+M=2H+M
 9               9.8066e+07    -0.922         -3665.47     O2+M=2O+M
 1               2.9746e+09     0.183           -92.14     O2+H=O+OH
 15              6.4850e+06     1.060          4188.86     H2O+H=H2+OH
 2               2.2959e+10    -0.022          8594.16     H2+O=H+OH
 7               4.9835e+02     2.362         14106.98     2OH=H2O+O
 17              1.0893e+08     0.690         23969.46     H2O2+H=H2+HO2
 5               1.0054e+08     0.677         38520.04     H+HO2=2OH
 12              2.8566e+11    -0.374         38723.57     2HO2=O2+H2O2
 3               2.9177e+16    -1.779         48821.40     O2+H(+M)=HO2(+M)
 13              2.9572e+23    -3.406         50244.70     2OH(+M)=H2O2(+M)
 6               4.2181e+09     0.294         53337.18     O+HO2=O2+OH
 ...
```

Reaction tables (I)

For each reaction it is possible to write details about the reaction rate, the reaction enthalpy and entropy, equilibrium constant, etc.

```
Dictionary CHEMKIN_PreProcessor
{
        @Thermodynamics     POLIMI_TOT_NOX_1412.CKT;
        @Transport          POLIMI_TOT_NOX_1412.TRC;
        @Kinetics           POLIMI_H2_1412.CKI;
        @ReactionTables     true;

        @Output             kinetics-POLIMI_H2_1412;
}
```

input.dic

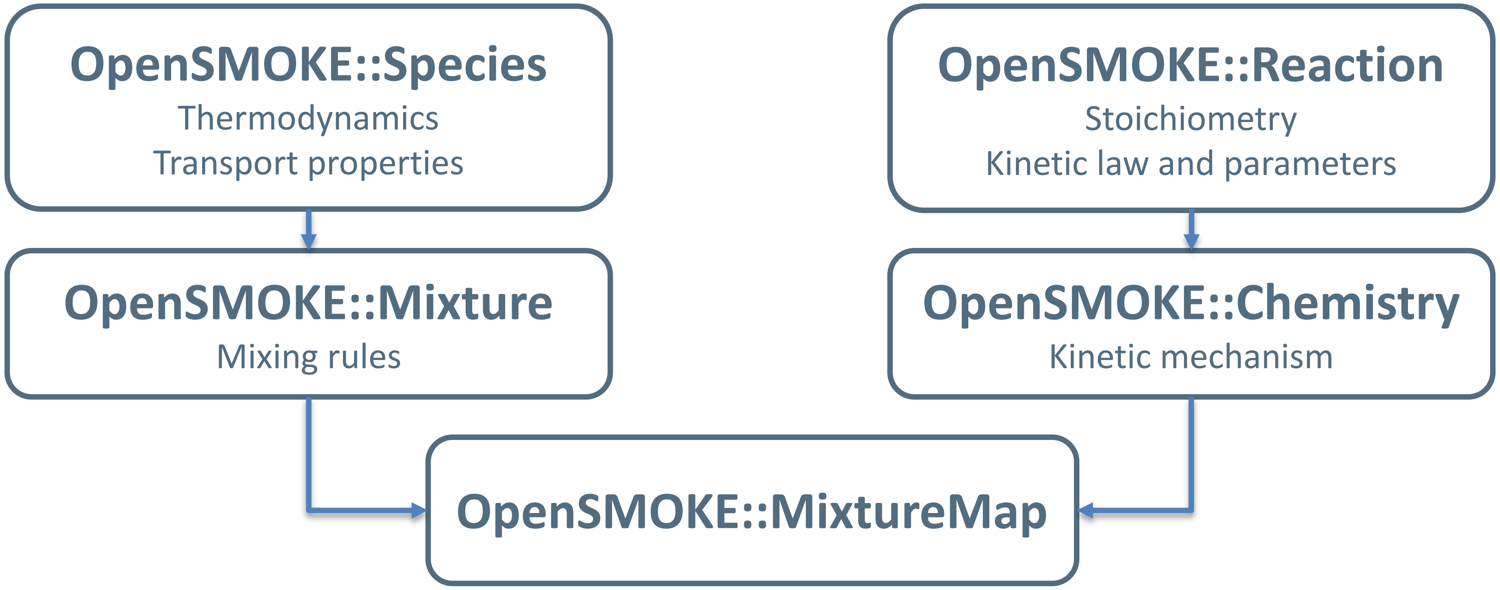
Reaction tables (II)

The reaction tables are then written on the `Reaction_FittedKinetics.out` file.

```
==========================================================================
 KINETIC DATA - REACTION  1 Simple
  O2 + H  = O + OH
==========================================================================
 Change in moles in the reaction = 0.000
 Reaction order (forward)  = 2.000
 Reaction order (backward) = 2.000
 k = 9.600000e+11 T^-0.200 exp(-6.956615e+07/RT)  [m3/kmol/s] and [J/kmol]
 k = 9.600000e+14 T^-0.200 exp(-16625.00/RT)  [cm3/mol/s] and [cal/mol]
 Reverse reaction units: [m3/kmol/s] or [cm3/mol/s]
 -------------------------------------------------------------------------
    Temp.   kF             Keq         kR             DG           DH
    [K]     [kmol,m3,s]   [-]         [kmol,m3,s]  [kcal/mol]   [kcal/mol]
 -------------------------------------------------------------------------
    300     2.369e-01     2.418e-11  9.796e+09    14.572        16.375
    1000    5.605e+07     5.119e-03  1.095e+10    10.481        16.011
    1500    8.406e+08     7.248e-02  1.160e+10    7.822         15.521
    2000    3.201e+09     2.620e-01  1.222e+10    5.324         15.086
    2500    7.067e+09     5.547e-01  1.274e+10    2.928         14.700
 -------------------------------------------------------------------------
```

Outline

OpenSMOKE++ Maps



```
OpenSMOKE::MixtureMap *map = new OpenSMOKE::MixtureMap(fileName);

map->updateStatus(T,P,y);             // update status
R = map->formationRates();            // formation rates
r = map->reactionRates();             // reaction rates
J = map->Jacobian();                  // Jacobian matrix
ropa = map->ROPA();                   // Rate of Production Analysis
```

OpenSMOKE++ Maps (II)

`OpenSMOKE++` is based on the concept of `Maps`, i.e. classes containing the data (imported from the xml files resulting from the preprocessing operations) and the functions to manage thermodynamic and transport properties and chemical reactions.

In particular in this training session we will focus the attention on maps based on the CHEMKIN standard:

- `OpenSMOKE::ThermodynamicsMap_CHEMKIN`
- `OpenSMOKE::TransportPropertiesMap`
- `OpenSMOKE::KineticsMap_CHEMKIN`

The source code is available in the `Training/Maps` folder:

`Training/Maps`

- `01-thermodynamics`
- `02-transport`
- `03-kinetics`

Including OpenSMOKE++ definitions

1. Go to the `Training/Maps/01-thermodynamics/` folder
2. Open the `trainingMapsThermodynamics.C` file

In order to use the `OpenSMOKE++ Maps` (thermodynamics, transport and kinetics), proper definitions must be included

```
// OpenSMOKE++ Definitions
#include "OpenSMOKEpp"

// CHEMKIN maps
#include "maps/Maps_CHEMKIN"
```

Importing the thermodynamic map

```
// OpenSMOKE++ Thermodynamic Map
OpenSMOKE::ThermodynamicsMap_CHEMKIN* thermoMap;

// Import map from preprocessed XML file
{
    boost::filesystem::path file_path =
                          "kinetics-POLIMI_H2_1412/kinetics.xml";

    // Open XML file containing the thermodynamic data
    rapidxml::xml_document<> doc;
    std::vector<char> xml_string;
    OpenSMOKE::OpenInputFileXML(doc, xml_string, file_path);

    // Import
    thermoMap = new OpenSMOKE::ThermodynamicsMap_CHEMKIN(doc);
}
```

Basic public functions

```
// Number of species
thermoMap->NumberOfSpecies();

// List of species
for (unsigned int i=0;i<thermoMap->NumberOfSpecies();i++)
    thermoMap->NamesOfSpecies()[i];

// Molecular weights [kg/kmol]
for (unsigned int i=0;i<thermoMap->NumberOfSpecies();i++)
    thermoMap->MW(i);
```

The complete list of public functions for `ThermodynamicsMap_CHEMKIN` class is available here:

`Libraries/OpenSMOKEpp/maps/ThermodynamicsMap_CHEMKIN.h`

Mixture averaged properties

```
// Set thermodynamic map
thermoMap->SetTemperature(T);
thermoMap->SetPressure(P);

// Molecular weight (in kg/kmol)
const double mw = thermoMap->MolecularWeight_From_MoleFractions(x.data());

// Constant pressure specific heat (in J/kmol/K)
const double cp = thermoMap->cpMolar_Mixture_From_MoleFractions(x.data());

// Enthalpy (in J/kmol)
const double h = thermoMap->hMolar_Mixture_From_MoleFractions(x.data());

// Entropy (in J/kmol/K)
const double s = thermoMap->sMolar_Mixture_From_MoleFractions(x.data());

// Internal energy (in J/kmol)
const double u = thermoMap->uMolar_Mixture_From_MoleFractions(x.data());

// Gibb's free energy (in J/kmol)
const double g = thermoMap->gMolar_Mixture_From_MoleFractions(x.data());

// Helmotz's free energy (in J/kmol)
const double a = thermoMap->aMolar_Mixture_From_MoleFractions(x.data());
```

Species properties

```
// Constant pressure specific heat (in J/kmol/K)
Eigen::VectorXd cp_species(thermoMap->NumberOfSpecies());
thermoMap->cpMolar_Species(cp_species.data());

// Enthalpy (in J/kmol)
Eigen::VectorXd h_species(thermoMap->NumberOfSpecies());
thermoMap->hMolar_Species(h_species.data());

// Entropy (in J/kmol/K)
Eigen::VectorXd s_species(thermoMap->NumberOfSpecies());
thermoMap->sMolar_Species(s_species.data());

// Internal energy (in J/kmol)
Eigen::VectorXd u_species(thermoMap->NumberOfSpecies());
thermoMap->uMolar_Species(u_species.data());

// Gibb's free energy (in J/kmol)
Eigen::VectorXd g_species(thermoMap->NumberOfSpecies());
thermoMap->gMolar_Species(g_species.data());

// Helmotz's free energy (in J/kmol)
Eigen::VectorXd a_species(thermoMap->NumberOfSpecies());
thermoMap->aMolar_Species(a_species.data());
```

Temperature from enthalpy

```
// Enthalpy (in J/kmol)
double h = 1e6;

// Temperature from enthalpy
const double Tguess = 300.;
const double T = thermoMap->GetTemperatureFromEnthalpyAndMoleFractions
                                  (h, P, x.data(), Tguess);
```

Using different types of vectors

```
{
    // STL vectors (from 0 to N-1)
    std::vector<double> x(thermoMap->NumberOfSpecies());

    // Molecular weight (in kg/kmol)
    const double mw = thermoMap->MolecularWeight_From_MoleFractions(x.data());
}

{
    // Native OpenSMOKE++ Vectors (from 1 to N)
    OpenSMOKE::OpenSMOKEVectorDouble x(thermoMap->NumberOfSpecies());

    // Molecular weight (in kg/kmol)
    const double mw =
            thermoMap->MolecularWeight_From_MoleFractions(x.GetHandle());
}

{
    // Eigen C++ vectors (from 0 to N-1)
    Eigen::VectorXd x(thermoMap->NumberOfSpecies());

    // Molecular weight (in kg/kmol)
    const double mw = thermoMap->MolecularWeight_From_MoleFractions(x.data());
}
```

Importing the transport map

```
// OpenSMOKE++ Maps
OpenSMOKE::ThermodynamicsMap_CHEMKIN*       thermoMap;
OpenSMOKE::TransportPropertiesMap_CHEMKIN*  tranMap;

// Import map from preprocessed XML file
{
    boost::filesystem::path file_path =
                        "kinetics-POLIMI_H2_1412/kinetics.xml";

    // Open XML file containing the thermodynamic data
    rapidxml::xml_document<> doc;
    std::vector<char> xml_string;
    OpenSMOKE::OpenInputFileXML(doc, xml_string, file_path);

    // Import
    thermoMap = new OpenSMOKE::ThermodynamicsMap_CHEMKIN(doc);
    tranMap = new OpenSMOKE::TransportPropertiesMap_CHEMKIN(doc);
}
```

The complete list of public functions is available here:
`Libraries/OpenSMOKEpp/maps/TransportPropertiesMap.h`

Mixture averaged transport properties

```
// Set maps
tranMap->SetTemperature(T);
tranMap->SetPressure(P);


// Dynamic viscosity (in kg/m/s)
const double eta = tranMap->DynamicViscosity(x.data());

// Thermal conductivity (in W/m/K)
const double lambda = tranMap->ThermalConductivity(x.data());

// Planck mean absorption coefficient (in 1/m)
const double kPlanck = tranMap->kPlanckMix(x.data());
```

Diffusion coefficients

```
// Molecular diffusion coefficients (in m2/s)
Eigen::VectorXd GammaMix(thermoMap->NumberOfSpecies());
tranMap->MassDiffusionCoefficients(GammaMix.data(), x.data());

// Thermal diffusion ratios (i.e. Soret effect)
Eigen::VectorXd TetaMix(thermoMap->NumberOfSpecies());
tranMap->ThermalDiffusionRatios(TetaMix.data(), x.data());

// Thermal diffusion coefficients (i.e. Soret effect) (in m2/s)
Eigen::VectorXd GammaSoretMix(thermoMap->NumberOfSpecies());
for (unsigned int i=0;i<thermoMap->NumberOfSpecies();i++)
    GammaSoretMix(i) = GammaMix(i)*TetaMix(i)*thermoMap->MW(i)/mw;
```

Importing the kinetic map

```
// OpenSMOKE++ Maps
OpenSMOKE::ThermodynamicsMap_CHEMKIN*   thermoMap;
OpenSMOKE::KineticsMap_CHEMKIN*         kineticsMap;

// Import map from preprocessed XML file
{
    boost::filesystem::path file_path =
                        "kinetics-POLIMI_H2_1412/kinetics.xml";

    // Open XML file containing the thermodynamic data
    rapidxml::xml_document<> doc;
    std::vector<char> xml_string;
    OpenSMOKE::OpenInputFileXML(doc, xml_string, file_path);

    // Import
    thermoMap = new OpenSMOKE::ThermodynamicsMap_CHEMKIN(doc);
    kineticsMap = new OpenSMOKE::KineticsMap_CHEMKIN(*thermoMap, doc);
}
```

The complete list of public functions is available here:
`Libraries/OpenSMOKEpp/maps/TransportPropertiesMap.h`

Reaction rates (net, forward, backward)

```
// Set maps
thermoMap->SetTemperature(T);
thermoMap->SetPressure(P);
kineticsMap->SetTemperature(T);
kineticsMap->SetPressure(P);

// Concentrations (in kmol/m3)
const double cTot = P/(PhysicalConstants::R_J_kmol*T);
Eigen::VectorXd c(thermoMap->NumberOfSpecies());
c = cTot*x;

// Reaction rates (in kmol/m3/s)
Eigen::VectorXd r(kineticsMap->NumberOfReactions());
kineticsMap->ReactionRates(c.data());
kineticsMap->GetReactionRates(r.data());

// Forward and backward reaction rates (in kmol/m3/s)
Eigen::VectorXd rf(kineticsMap->NumberOfReactions());
kineticsMap->GetForwardReactionRates(rf.data());
Eigen::VectorXd rb(kineticsMap->NumberOfReactions());
kineticsMap->GetBackwardReactionRates(rb.data());
```

Formation rates (net, production, destruction)

```
// Formation rates (in kmol/m3/s)
Eigen::VectorXd R(thermoMap->NumberOfSpecies());
kineticsMap->FormationRates(R.data());


// Production and destruction rates (in kmol/m3/s)
Eigen::VectorXd RP(thermoMap->NumberOfSpecies());
Eigen::VectorXd RD(thermoMap->NumberOfSpecies());
kineticsMap->ProductionAndDestructionRates(RP.data(), RD.data());


// Heat release (in J/m3/s)
const double Q = kineticsMap->HeatRelease(R.data());
```

Derivatives of formation rates

```
// Derivative of formation rates with respect to conc. (in 1/s)
const int NC = thermoMap->NumberOfSpecies();
Eigen::MatrixXd dR_over_dC(NC, NC);
kineticsMap->DerivativesOfFormationRates(c.data(), &dR_over_dC);
```

Outline

Isothermal, constant volume batch reactor (I)

We want to write a solver for a single **isothermal, constant volume batch reactor**, by combining `OpenSMOKE++` with `OpenFOAM`

Governing equations

$$\begin{cases} \dfrac{dN_i}{dt} = R_i V \\ N_i(t=0) = N_i^0 \end{cases}$$

N_i: number of moles of species i
R_i: formation rate of species i
V: reactor volume

Since the reactor volume is constant, the ODE system reported above can be rewritten in terms of concentrations (N_i=$C_i V$)

$$\begin{cases} \dfrac{dC_i}{dt} = R_i \\ C_i(t=0) = C_i^0 \end{cases}$$

Governing equations for a constant volume batch reactor

Isothermal, constant volume batch reactor (II)

Unless reactions occur without change of moles, total concentration of species and pressure changes in time. This can be described through the equation of state of ideal gases:

$$P = \frac{nRT}{V} = C_{tot}RT = RT\sum_{i=1}^{N} C_i$$

Or equivalently, in a differential form:

$$\begin{cases} \dfrac{dP}{dt} = RT\sum_{i=1}^{N}\dfrac{dC_i}{dt} = RT\sum_{i=1}^{N} R_i \\ P(t=0) = P_0 \end{cases}$$

Isothermal, constant volume batch reactor (III)

Thus, the isothermal, constant volume batch reactor is described by a system of non-linear ODEs with initial conditions + an algebraic (explicit) equation for pressure:

$$\begin{cases} \dfrac{dC_i}{dt} = R_i \\ C_i(t=0) = C_i^0 \end{cases} \quad + \quad P(t) = RT\sum_{i=1}^{N} C_i(t)$$

OpenFOAM

solution of ODE system by using the `ODESolver` and `ODESystem` classes

OpenSMOKE++

Thermodynamic and kinetic maps for calculating the formation rates for arbitrarily complex kinetic mechanism

Basic structure

1. Definition of a class corresponding to the equations describing the batch reactor (derived from `ODESystem` and based on `OpenSMOKE++ Maps`)

```
class batchIsothermalOdeSystem : public ODESystem
```

2. Creation of a `batchIsothermalOdeSystem` object

```
batchIsothermalOdeSystem batch(thermoMap, kineticsMap, T);
```

3. Creation of a `ODESolver` object

```
autoPtr<ODESolver> odeSolver = ODESolver::New(batch, dict);
```

4. Numerical solution of ODE system

```
odeSolver->solve(tStart, tStart + dt, cStart, dtStart);
```

ODESystem for isothermal batch reactor (I)

```
class batchIsothermalOdeSystem : public ODESystem
{

public:

    batchIsothermalOdeSystem(OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap,
                OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap, const double T);

    label nEqns() const;

    void derivatives( const scalar t, const scalarField& c, scalarField& dcdt )
    const;

    void jacobian( const scalar t, const scalarField& c, scalarField& dfdt,
    scalarSquareMatrix& dfdc ) const;

private:

    OpenSMOKE::ThermodynamicsMap_CHEMKIN&  thermoMap_;
    OpenSMOKE::KineticsMap_CHEMKIN&        kineticsMap_;

    double T_;
};
```

Equations (isothermal conditions)

```
void batchIsothermalOdeSystem::derivatives
    ( const scalar t, const scalarField& c, scalarField& dcdt ) const
{
    // Calculate pressure
    const double cTot = std::accumulate(c.begin(), c.end(), 0.);
    const double P = cTot*(PhysicalConstants::R_J_kmol*T_);

    // Set maps
    thermoMap_.SetTemperature(T_);
    thermoMap_.SetPressure(P);
    kineticsMap_.SetTemperature(T_);
    kineticsMap_.SetPressure(P);

    // Calculates kinetics
    Eigen::VectorXd R(thermoMap_.NumberOfSpecies());
    kineticsMap_.ReactionRates(c.cdata());
    kineticsMap_.FormationRates(R.data());

    // Species equations
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        dcdt[i] = R(i);
}
```

Jacobian matrix (isothermal conditions)

```
void batchIsothermalOdeSystem::jacobian( const scalar t, const scalarField& 
c, scalarField& dfdt, scalarSquareMatrix& dfdc ) const
{
    // Calculate pressure
    const double cTot = std::accumulate(c.begin(), c.end(), 0.);
    const double P = cTot*(PhysicalConstants::R_J_kmol*T_);

    // Set maps
    thermoMap_.SetTemperature(T_);
    thermoMap_.SetPressure(P);
    kineticsMap_.SetTemperature(T_);
    kineticsMap_.SetPressure(P);

    // Derivative of formation rates with respect to conc (in 1/s)
    Eigen::MatrixXd dR_over_dC(NC, NC);
    kineticsMap_.DerivativesOfFormationRates(c.cdata(), &dR_over_dC);

    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        for (unsigned int j=0;j<thermoMap_.NumberOfSpecies();j++)
            dfdc[i][j] = dR_over_dC(i,j);
}
```

Creating the ODE solver

```
// Create the ODE system as object of type batchOdeSystem
batchIsothermalOdeSystem batch(thermoMap, kineticsMap, T);

// Create dictionary and add the odeSolver name (from command line)
dictionary dict;
dict.add("solver", args[1]);

// Create the selected ODE system solver
autoPtr<ODESolver> odeSolver = ODESolver::New(batch, dict);
```

Solving the ODE system

```
// Integration loop
for (label i=0; i<n; i++)
{
    batch.derivatives(tStart, c, dc);
    odeSolver->solve(tStart, tStart + dt, c, dtStart);
    tStart += dt;

    // Reconstruct pressure
    const double cTot = std::accumulate(c.begin(), c.end(), 0.);
    P = cTot*(PhysicalConstants::R_J_kmol*T);
}
```

Compiling and running the batch reactor

Compilation

1. Go to the `Training/BatchReactor/01-isothermal/` folder
2. Type `wmake`

Execution

1. Type `batchReactorIsothermal <ODESolver>`
2. Look at the solution in the `Solution.out` file

A stiff ODE solver (such as `seulex` or `SIBS`) is recommended, even if the kinetic mechanism is small:

```
batchReactorIsothermal seulex
```

```
<ODESolver> options
Euler
EulerSI
RKCK45
RKDP45
RKF45
Rosenbrock12
Rosenbrock23
Rosenbrock34
SIBS
Trapezoid
rodas23
rodas34
seulex
```

Example: syngas

Initial conditions

$T = 1000K$

$P = 101325\ Pa$

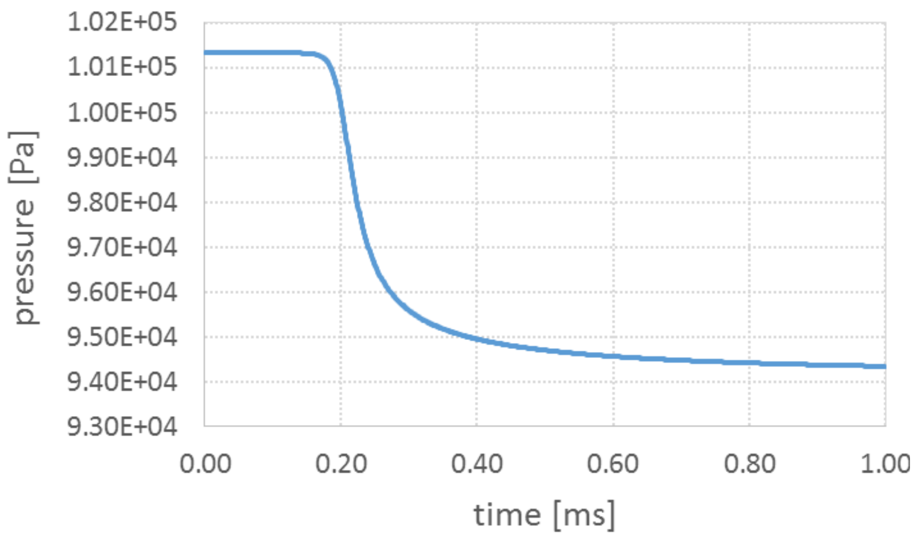
11% H2 + 11% CO + 17% O2 + 61% N2

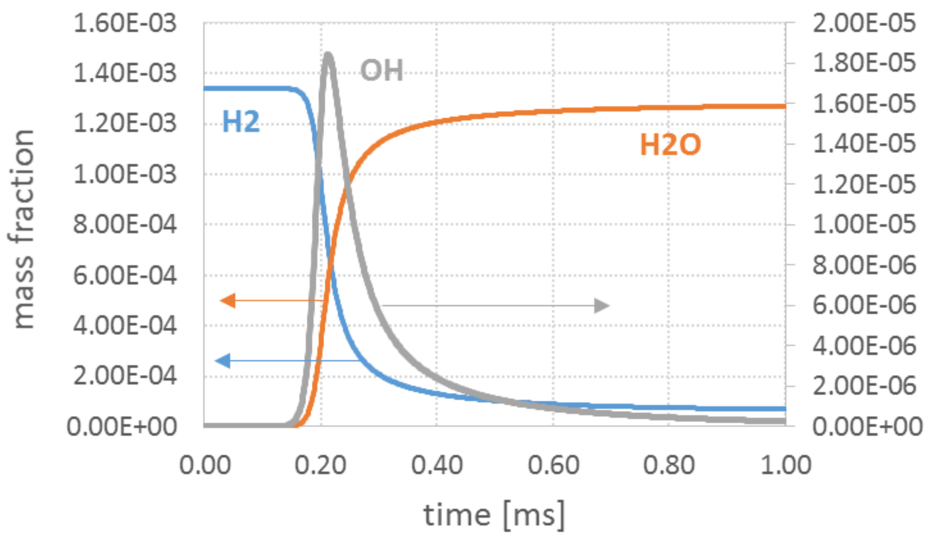
Kinetic mechanism

POLIMI_H2CO_1412

Species: 14

Reactions: 33





Example: methane

Initial conditions

$T = 1200K$

$P = 101325\ Pa$

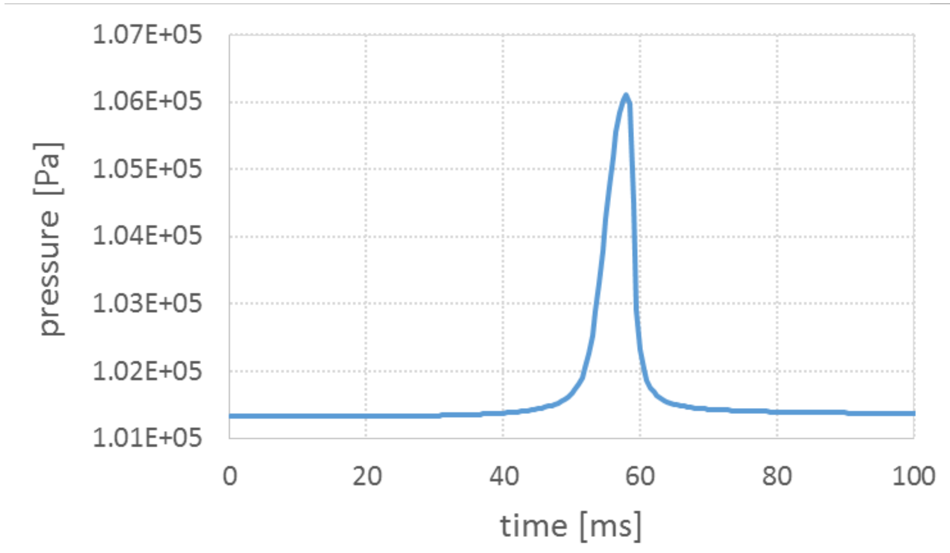
9.5% CH_4 + 19% O_2 + 71.5% N_2

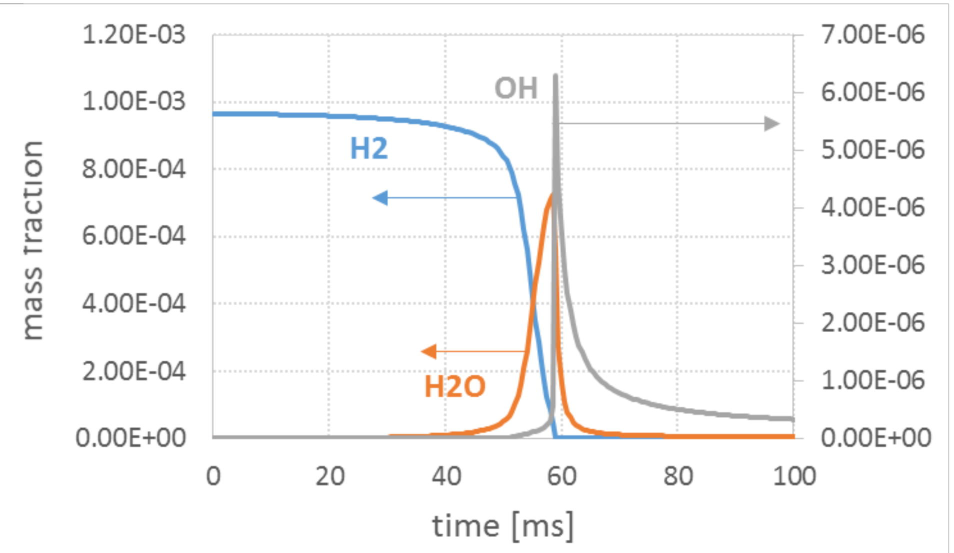
Kinetic mechanism

GRI30

Species: 53

Reactions: 325





Adiabatic, constant volume batch reactor

In case of **adiabatic, constant volume batch reactor**, the equations governing the evolution of concentrations of species and pressure are the same we already developed in isothermal conditions:

$$\begin{cases} \dfrac{dC_i}{dt} = R_i \\ C_i(t=0) = C_i^0 \end{cases} \quad + \quad P(t) = RT(t)\sum_{i=1}^{N} C_i(t)$$

The difference is now that temperature changes in time. Instead of writing an additional differential equation describing the evolution of temperature, we can, equivalently, impose that the total internal energy is constant (definition of adiabatic reactor):

$$U(t) = U_0$$

From the internal energy we can estimate the enthalpy and then, from pressure and composition we can always calculate the temperature (see the `GetTemperatureFromEnthalpyAndMoleFractions` function)

Equations (adiabatic conditions) (I)

```
void batchAdiabaticOdeSystem::derivatives
    ( const scalar t, const scalarField& cc, scalarField& dcdt ) const
{
    // Reconstruct concentrations and mole fractions
    Eigen::VectorXd c(thermoMap_.NumberOfSpecies());
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        c(i) = std::max(cc[i],0.);
    Eigen::VectorXd x(thermoMap_.NumberOfSpecies());
    const double cTot = c.sum();
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        x(i) = c[i]/cTot;
    const double mw = thermoMap_.MolecularWeight_From_MoleFractions(x.data());

    ...
}
```

It is extremely important to clean the current concentrations, by removing negative values

Equations (adiabatic conditions) (II)

```
void batchAdiabaticOdeSystem::derivatives
    ( const scalar t, const scalarField& cc, scalarField& dcdt ) const
{
    ...

    // Calculate temperature and pressure (by successive substitutions)
    double P = PInitial_;
    double T = TInitial_;
    for(int i=0;i<maxIterations_;i++)
    {
        const double Pold = P;
        const double H = U_+P/(cTot*mw);
        T = thermoMap_.GetTemperatureFromEnthalpyAndMoleFractions
                         (H*mw, P, x.data(), T);
        P = cTot*(PhysicalConstants::R_J_kmol*T);
        if (std::fabs(P-Pold)/P<1e-4) break;
    }

    ...
}
```

Internal energy is constant (by definition of adiabatic constant volume batch reactor). In order to get the temperature, an **iterative procedure** is needed, since the reactor pressure is unknown

Equations (adiabatic conditions) (III)

```
void batchAdiabaticOdeSystem::derivatives
     ( const scalar t, const scalarField& cc, scalarField& dcdt ) const
{
     ...

     // Set maps
     thermoMap_.SetTemperature(T);
     thermoMap_.SetPressure(P);
     kineticsMap_.SetTemperature(T);
     kineticsMap_.SetPressure(P);

     // Calculates kinetics
     Eigen::VectorXd R(thermoMap_.NumberOfSpecies());
     kineticsMap_.ReactionRates(c.data());
     kineticsMap_.FormationRates(R.data());

     // Species equations
     for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
          dcdt[i] = R(i);
}
```

Jacobian matrix (adiabatic conditions)

```
void batchAdiabaticOdeSystem::jacobian( const scalar t, const scalarField& c,
scalarField& dfdt, scalarSquareMatrix& dfdc ) const
{
     // Reconstruct concentrations and mole fractions
     [Same code: derivatives]

     // Calculate temperature and pressure (by successive substitutions)
     [Same code: derivatives]

     // Set maps
     thermoMap_.SetTemperature(T);
     thermoMap_.SetPressure(P);
     kineticsMap_.SetTemperature(T);
     kineticsMap_.SetPressure(P);

     // Derivative of formation rates with respect to conc, (in 1/s)
     Eigen::MatrixXd dR_over_dC(NC, NC);
     kineticsMap_.DerivativesOfFormationRates(c.data(), &dR_over_dC);

     for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
          for (unsigned int j=0;j<thermoMap_.NumberOfSpecies();j++)
               dfdc[i][j] = dR_over_dC(i,j);
}
```

Compiling and running the batch reactor

Compilation

1. Go to the `Training/BatchReactor/02-adiabatic/` folder
2. Type `wmake`

Execution

1. Type `batchReactorAdiabatic <ODESolver>`
2. Look at the solution in the `Solution.out` file

A stiff ODE solver (such as `seulex` or `SIBS`) is recommended, even if the kinetic mechanism is small:

```
batchReactorAdiabatic seulex
```

```
<ODESolver> options
Euler
EulerSI
RKCK45
RKDP45
RKF45
Rosenbrock12
Rosenbrock23
Rosenbrock34
SIBS
Trapezoid
rodas23
rodas34
seulex
```

Example: syngas

Initial conditions

$T = 1000K$

$P = 101325\ Pa$

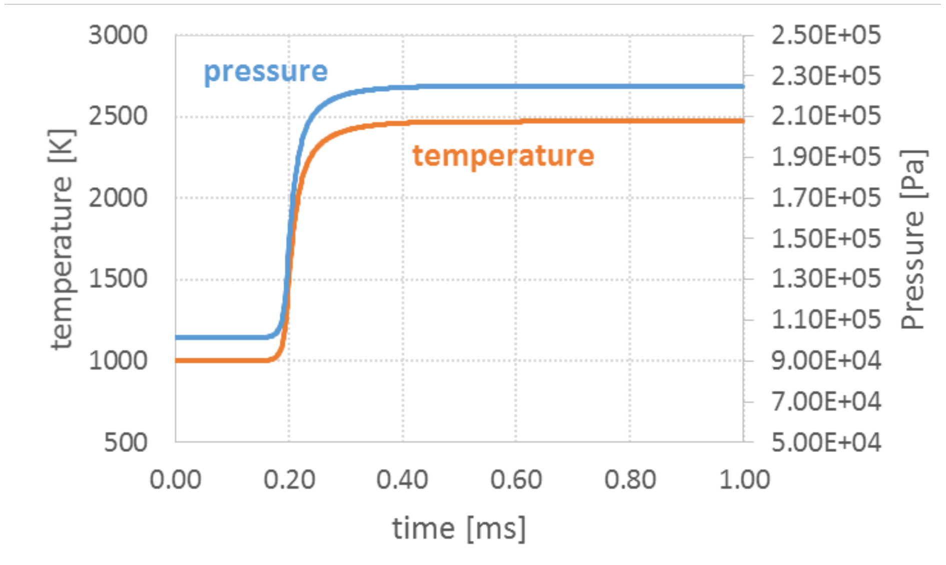
11% H2 + 11% CO + 17% O2 + 61% N2

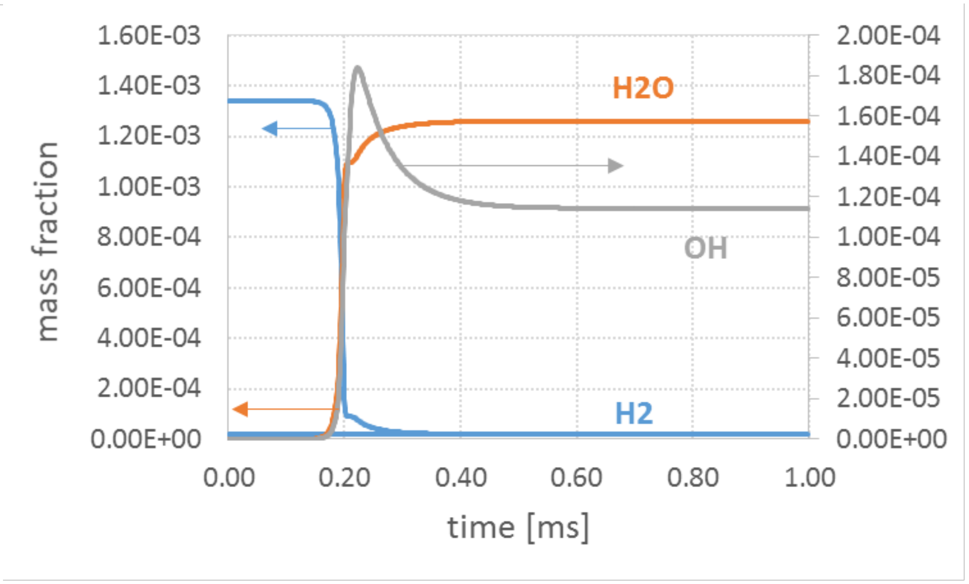
Kinetic mechanism

POLIMI_H2CO_1412

Species: 14

Reactions: 33





Example: methane

Initial conditions

$T = 1400K$

$P = 101325\ Pa$

9.5% CH4 + 19% O2 + 71.5% N2

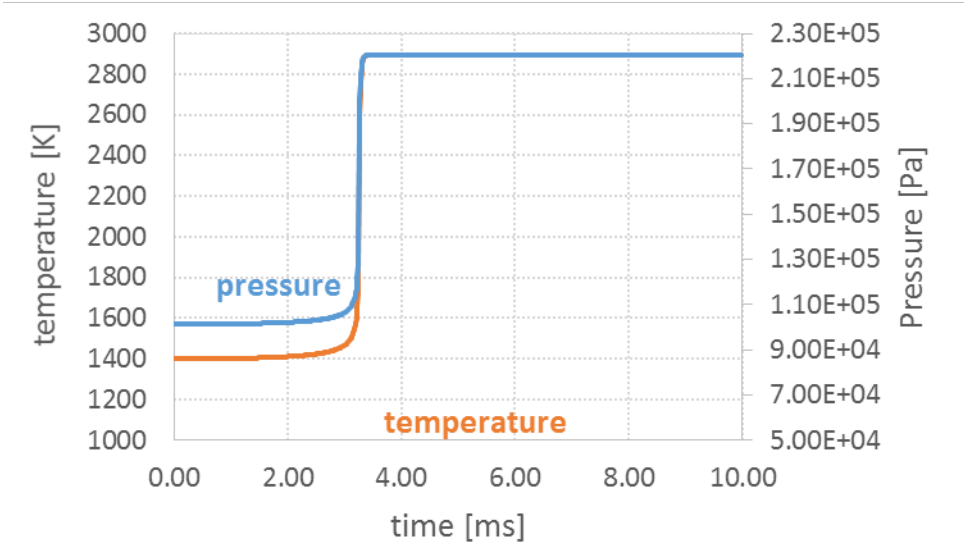
t=0.01 s

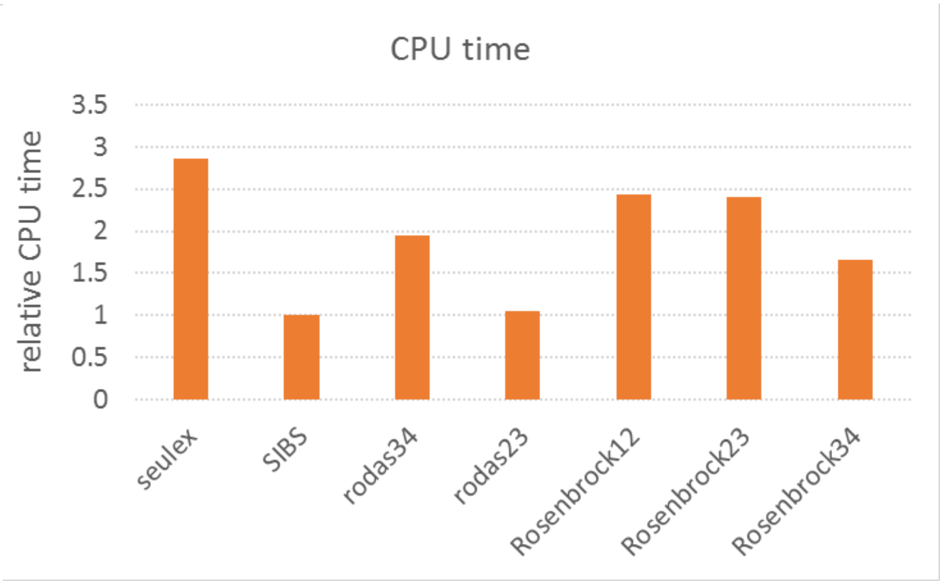
Kinetic mechanism

GRI30 (without NOX)

Species: 36

Reactions: 219





Outline

Introduction

We want to build a couple of solvers (steady-state and unsteady) for homogeneous laminar reacting flows described by arbitrarily complex kinetic mechanisms

OpenFOAM

Input/Output, mesh, spatial and temporal discretization of transport equations, solution of linear systems, solution of ODE systems

OpenSMOKE++

Thermodynamic and transport properties, chemical reactions

Outline

1. **Unsteady solver based on the operator splitting algorithm**
    1. Introduction and theory
    2. Implementation
    3. Examples

2. **Steady state solver based on the linearization of source terms**
    1. Introduction and theory
    2. Implementation
    3. Examples

Outline

Unsteady solver: equations

Continuity equation	$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{v}) = 0$
Momentum equations	$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla(\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \boldsymbol{\tau} + \rho \boldsymbol{g}$
Energy equation	$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \boldsymbol{v} \nabla T = \lambda \nabla^2 T + Q_R$
Species equations	$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho \boldsymbol{v} Y_k) = \nabla(\rho \Gamma_k \nabla Y_k) + R_k \qquad k = 1, \dots, N$

Simplifying hypotheses
- No radiative heat transfer
- No enthalpy fluxes due to preferential mass diffusion
- No thermodiffusion (Soret effect)
- No correction velocity on mass diffusion fluxes

Unsteady solver: algorithm

Continuity equation $$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{v}) = 0$$

Momentum equations $$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla(\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \boldsymbol{\tau} + \rho \boldsymbol{g}$$

PIMPLE Algorithm

Energy equation $$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \boldsymbol{v} \nabla T = \lambda \nabla^2 T + Q_R$$

Strongly non linear terms

Species equations $$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho \boldsymbol{v} Y_k) = \nabla(\rho \Gamma_k \nabla Y_k) + R_k \qquad k = 1, \dots, N$$

Operator-splitting approach

Operator-splitting (I)

Energy equation $$\rho C_P \frac{\partial T}{\partial t} = -\rho C_P \boldsymbol{v} \nabla T + \lambda \nabla^2 T + Q_R$$

Species equations $$\frac{\partial}{\partial t}(\rho Y_k) = -\nabla(\rho \boldsymbol{v} Y_k) + \nabla(\rho \Gamma_k \nabla Y_k) + R_k \qquad k = 1, \dots, N$$

T = transport processes (convection and diffusion), **weakly non linear**, non-local

S = non linear, stiff processes (homogeneous reactions), **local**

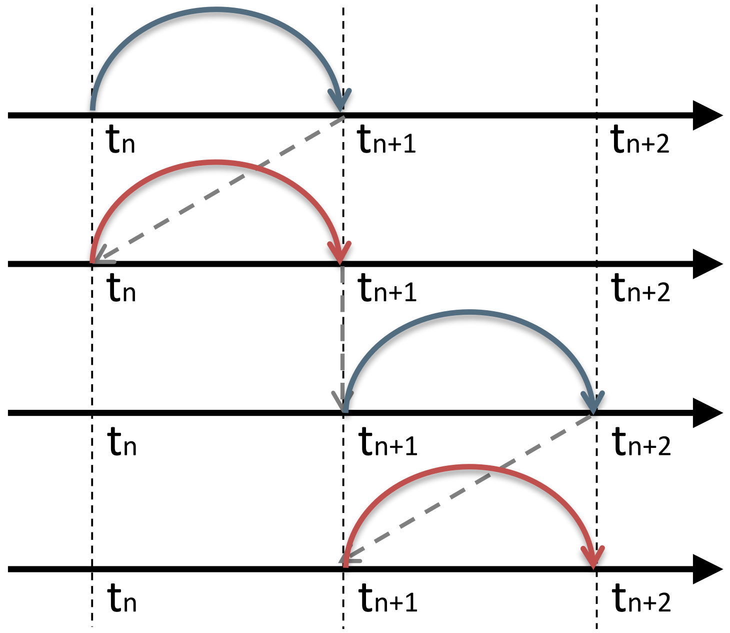
Energy equation $$\rho C_P \frac{\partial T}{\partial t} = T_T + S_T$$

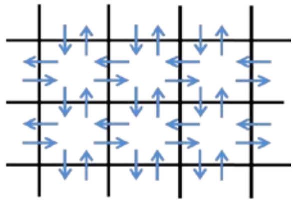
Species equations $$\frac{\partial}{\partial t}(\rho Y_k) = T_k + S_k \qquad k = 1, \dots, N$$

Operator-splitting (II)

Non linear transport equations for species and energy

$$\frac{\partial \varphi}{\partial t} = T + S$$

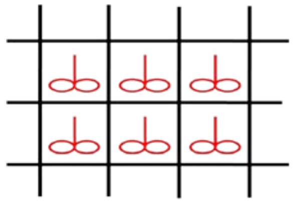




$$\frac{\partial \varphi}{\partial t} = T$$

Transport

Chemistry



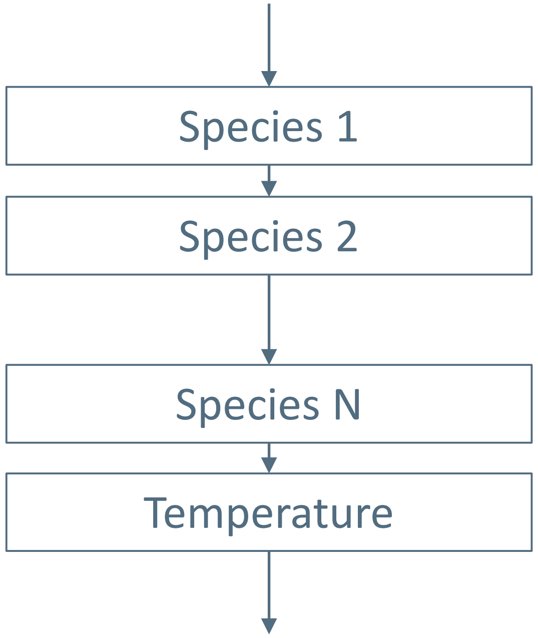
$$\frac{\partial \varphi}{\partial t} = S$$

Transport step

Species equations $$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho \boldsymbol{v} Y_k) = \nabla(\rho \Gamma_k \nabla Y_k) \qquad k = 1, \dots, N$$

Energy equation $$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \boldsymbol{v} \nabla T = \lambda \nabla^2 T$$

- The equations are weakly non linear
- The only source of non-linearity is represented by transport and thermodynamic properties, which are function of temperature and composition
- A segregated approach is in general feasible



Chemical step

Species equations $$\frac{\partial}{\partial t}(\rho Y_k) = R_k \qquad k = 1, \dots, N$$

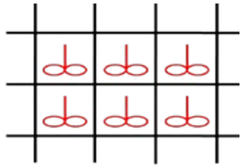
Energy equation $$\rho C_P \frac{\partial T}{\partial t} = Q_R$$

These equations are **LOCAL**, i.e. no spatial discretization operators are present

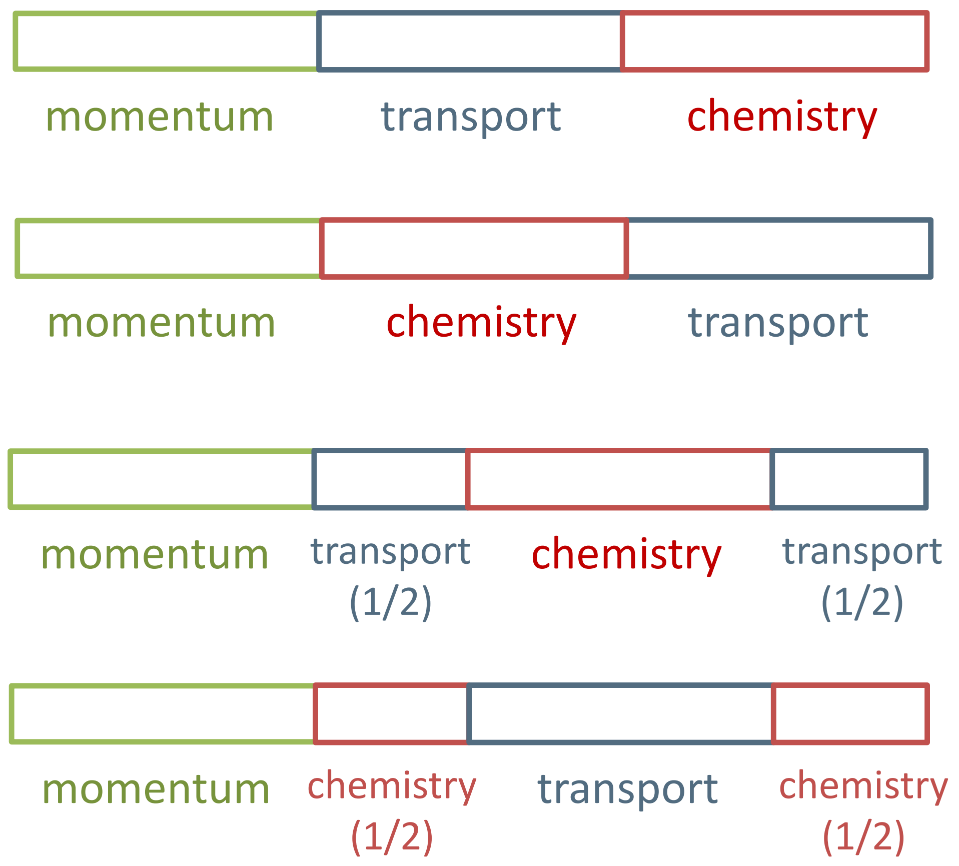
- Since there are no transport, the total mass remains constant
- The volume of a cell is constant in time
- Thus, the density is constant during the chemical step

Chemical step equations $$\begin{cases} \dfrac{\partial Y_k}{\partial t} = \dfrac{R_k}{\rho} & k = 1, \dots, N \\ \dfrac{\partial T}{\partial t} = \dfrac{Q_R}{\rho C_P} \end{cases}$$

Each cell behaves like a batch reactor



Operator splitting: many alternatives



1st order operator splitting
(this training session)

1st order operator splitting
(alternative version)

2nd order operator splitting
Strang method

2nd order operator splitting
Strang method

Sportisse B., *An Analysis of Operator Splitting Techniques in the Stiff Case*,
Journal of Computational Physics, 161(1), p. 140-168 (2000)

Consistent operator splitting

If the operator-splitting technique is used for approaching steady-state solutions (i.e. the unsteady solver is actually adopted for solving a steady state problem, through integration over a sufficiently long time), it is more accurate to use a consistent formulation:

$$\frac{\partial \varphi}{\partial t} = T + S \quad \Longrightarrow \quad \begin{cases} \dfrac{\partial \varphi}{\partial t} = T - T_{old} & \text{Transport step} \\[2ex] \dfrac{\partial \varphi}{\partial t} = S + T_{old} & \text{Chemical step} \end{cases}$$

Because the transport term was incorporated into the chemical integration, now the RHS remains consistent with the original discretized equations, and the splitting error is minimized.

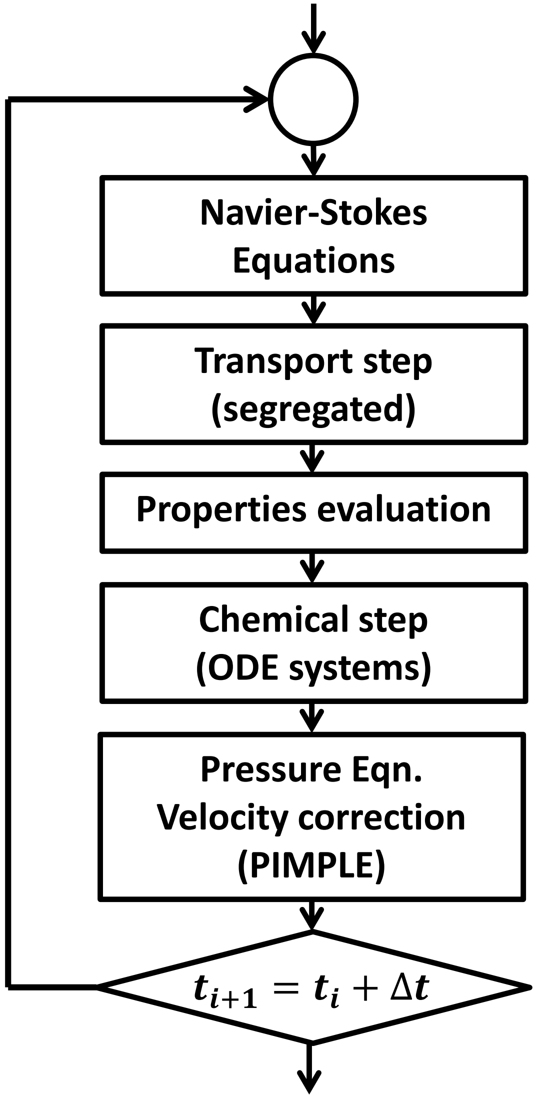
D.A. Schwer, P. Lu,W.H. Green Jr., V. Semiao, *A consistent-splitting approach to computing stiff steady-state reacting flows with adaptive chemistry*, Combustion Theory and Modelling, 7, p. 383-399 (2003)

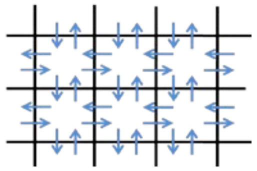
Outline

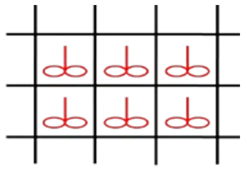
1. **Unsteady solver based on the operator splitting algorithm**
    1. Introduction and theory
    2. **Implementation**
    3. Examples

2. **Steady state solver based on the linearization of source terms**
    1. Introduction and theory
    2. Implementation
    3. Examples

Unsteady solver (I)


Navier-Stokes Equations
Transport step (segregated)
Properties evaluation
Chemical step (ODE systems)
Pressure Eqn. Velocity correction (PIMPLE)
$t_{i+1} = t_i + \Delta t$





$$\frac{\partial \varphi}{\partial t} = T(\varphi) + S(\varphi)$$

φ: Dependent variables (Y_k and T)
$T(\varphi)$ is the rate of change of φ due to transport
$S(\varphi)$ is the rate of change of φ due to reactions

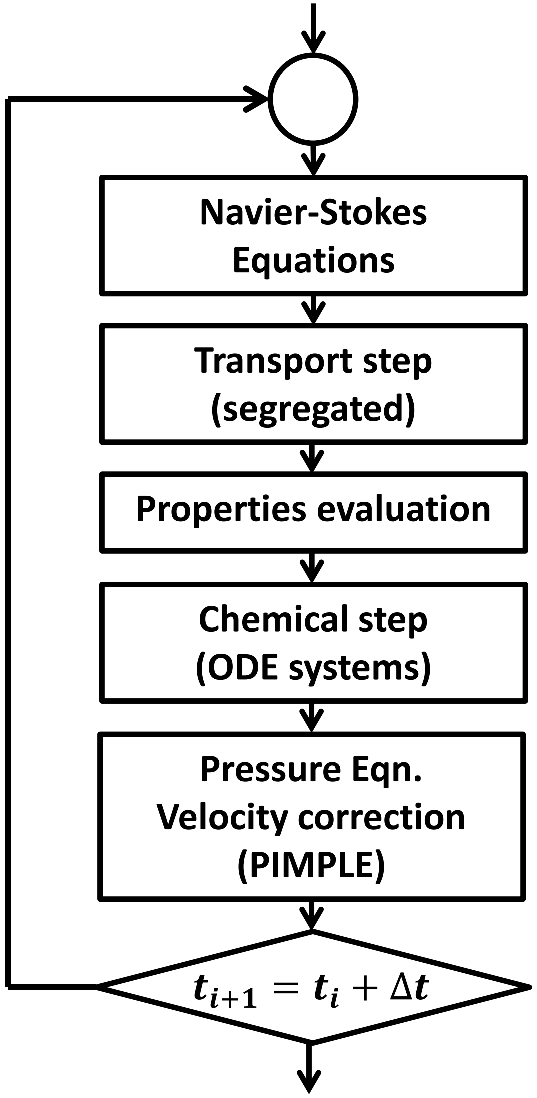
Sub-step 1. The transport terms (convection and diffusion) are integrated over Δt by solving:

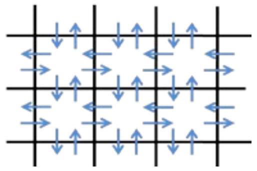
$$\frac{\partial \varphi^{(a)}}{\partial t} = T\left(\varphi^{(a)}\right)$$

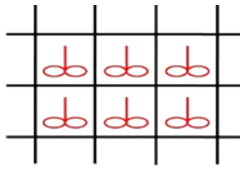
Sub-step 2. The reaction terms are integrated over Δt through the solution of N_{cells} independent stiff ODE systems:

$$\frac{\partial \varphi^{(b)}}{\partial t} = S\left(\varphi^{(b)}\right)$$

Unsteady solver (II)


Navier-Stokes Equations
Transport step (segregated)
Properties evaluation
Chemical step (ODE systems)
Pressure Eqn. Velocity correction (PIMPLE)
$t_{i+1} = t_i + \Delta t$





```
while (pimple.loop())
{
    // Transport
    #include "UEqn.H"
    #include "YEqn.H"
    #include "TEqn.H"

    // Chemistry
    #include "chemistry.H"

    // Update transport properties
    #include "transportProperties.H"

    // Pressure corrector loop
    while (pimple.correct())
    {
        if (pimple.consistent())
            #include "pcEqn.H"
        else
            #include "pEqn.H"
    }
}
```

Unsteady solver initialization

```
int main(int argc, char *argv[])
{
    // OpenFOAM stuff
    #include "setRootCase.H"
    #include "createTime.H"
    #include "createMesh.H"
    #include "createControl.H"
    #include "createTimeControls.H"
    #include "initContinuityErrs.H"
    #include "createMRF.H"
    #include "createFvOptions.H“
    #include "createBasicFields.H"

    // OpenSMOKE++
    #include "createChemicalFields.H"
    #include "transportProperties.H"

    // OpenFOAM stuff
    #include "createAdditionalFields.H"
    #include "compressibleCourantNo.H"
    #include "setInitialDeltaT.H“
    ...
```

Importing OpenSMOKE++ Maps

```
const dictionary& kineticsDictionary = solverOptions.subDict("Kinetics");
Foam::string kinetics_folder = kineticsDictionary.lookup("folder");

// Open XML file containing the thermodynamic data
rapidxml::xml_document<> doc;
std::vector<char> xml_string;
OpenSMOKE::OpenInputFileXML(doc, xml_string, kinetics_folder + "/kinetics.xml");

OpenSMOKE::ThermodynamicsMap_CHEMKIN       thermoMap(doc);
OpenSMOKE::KineticsMap_CHEMKIN             kineticsMap(thermoMap, doc);
OpenSMOKE::TransportPropertiesMap_CHEMKIN  transportMap(doc);

// Inert species
word inertSpecies(kineticsDictionary.lookup("inertSpecies"));
label inertIndex = thermoMap.IndexOfSpecies(inertSpecies)-1;

// ODE solver
word odeSolver(kineticsDictionary.lookup("ODESolver"));
```

Transport properties

```
forAll(TC, celli)
{
    // Set maps
    thermoMap.SetPressure(pC[celli]);
    thermoMap.SetTemperature(TC[celli]);
    transportMap.SetPressure(pC[celli]);
    transportMap.SetTemperature(TC[celli]);

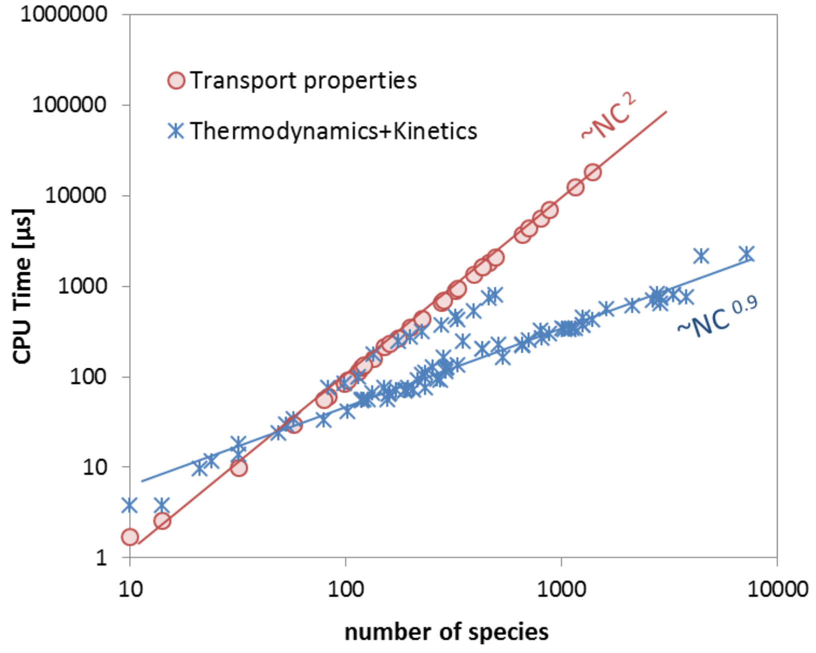
    // Constant pressure specific heat [J/kg/K]
    cpC[celli] = thermoMap.cpMolar_Mixture_From_MoleFractions(x.data())/mw;

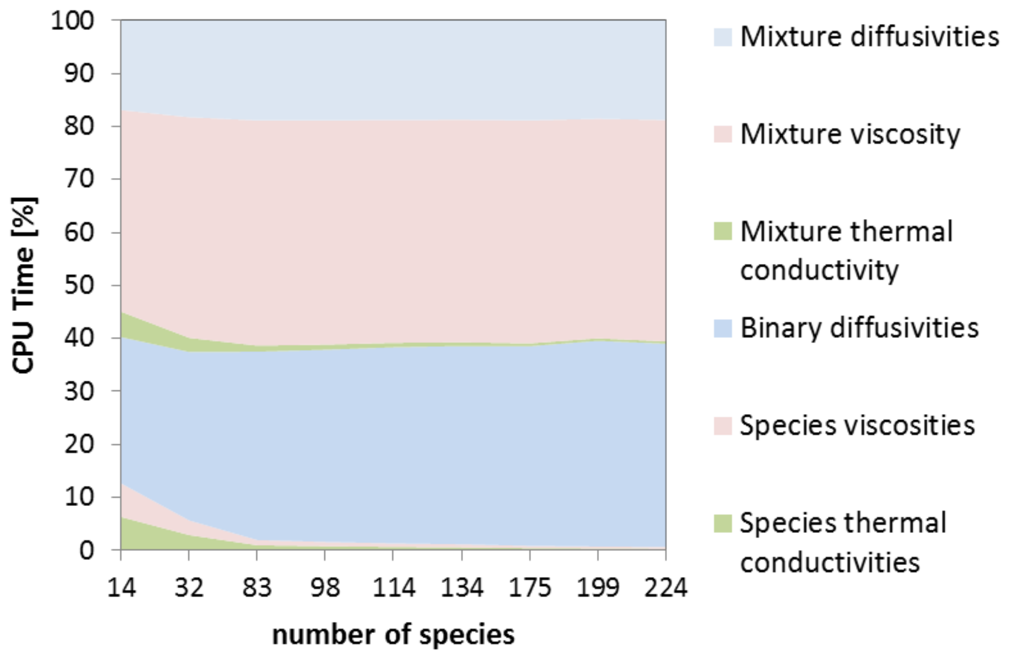
    // Dynamic viscosity [kg/m/s]
    etaCells[celli] = transportMap.DynamicViscosity(x.data());

    // Thermal conductivity [W/m/K]
    lambdaCells[celli] = transportMap.ThermalConductivity(x.data());

    // Diffusion coefficients [m2/s]
    transportMap.MassDiffusionCoefficients(GammaMixVector.data(), x.data());
    for(int i=0;i<thermoMap.NumberOfSpecies();i++)
        GammaMix[i].ref()[celli] = GammaMixVector(i);
}
```

Computational cost of transport properties





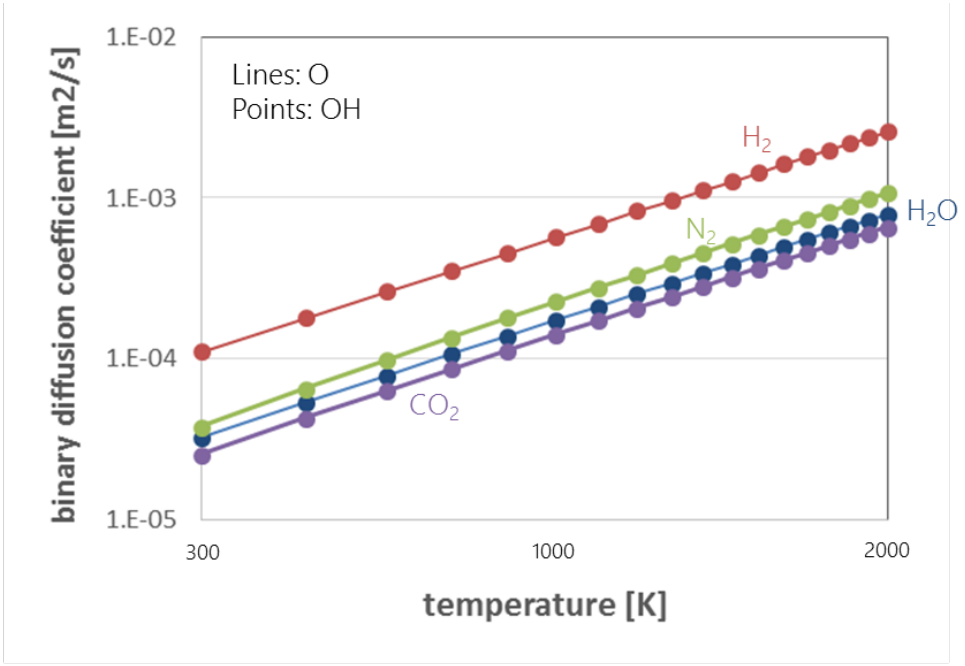
- The cost of evaluation of transport properties (in particular diffusion) increases **quadratically** with the number of species
- For large mechanisms (>100 species) the computational cost of transport properties is not negligible
- In fully-coupled methods proper techniques must be applied to **reduce the computational cost of transport properties**

Species bundling

Many species possess similar diffusivities because of similar molecular properties (molecular weight, structure, collision cross section, etc.)

Such species are expected to behave similarly in terms of diffusive transport

Species with similar diffusivities can be bundled in a same group with a representative species



The diffusivities of O and OH with other species are almost identical

Lu, Law, *Diffusion coefficient reduction through species bundling*, Combustion and Flame, 148, p. 117-126 (2007)

Species bundling in OpenSMOKE++

Step 1: pre-processing with species bundling

```
Dictionary CHEMKIN_PreProcessor
{
        @Thermodynamics     POLIMI_TOT_NOX_1412.CKT;
        @Transport          POLIMI_TOT_NOX_1412.TRC;
        @Kinetics           POLIMI_PRF_PAH_HT_1412.CKI;
        @SpeciesBundling    true;
        @Output             kinetics-POLIMI_PRF_PAH_HT_1412;
}
```

Step 2: importing the transport map with species bundling

```
tranMap = new OpenSMOKE::TransportPropertiesMap_CHEMKIN(doc);
tranMap->ImportSpeciesBundlingFromXMLFile(doc, bundling_eps);
```

Step 3: evaluation of diffusion coefficients through species bundling

```
tranMap.MassDiffusionCoefficients(GammaMixVector.data(), x.data(), true);
for(int i=0;i<thermoMap.NumberOfSpecies();i++)
        GammaMix[i].ref()[celli] = GammaMixVector(i);
```

chemistry.H (I)

- Each cell behaves like a constant volume batch reactor, which is described by a set of ODE with initial conditions

- There is no need to create a `ODESystem` object and a `ODESolver` object for each cell. We can reuse the same for all the cells

```
// Create dictionary and add the odeSolver name
dictionary dict;
dict.add("solver", odeSolver);

// Create the ODE system as object of type batchOdeSystem
batchAdiabaticOdeSystem batch(thermoMap, kineticsMap);

// Create the selected ODE system solver
autoPtr<ODESolver> odeSolver = ODESolver::New(batch, dict);
```

chemistry.H (II)

We imagine that enthalpy is kept constant during the chemical step

```
forAll(TC, celli)
{
     ...
     // Enthalpy
     thermoMap.SetTemperature(TC[celli]); thermoMap.SetPressure(pC[celli]);
     const double H = thermoMap.hMolar_Mixture_From_MoleFractions(x.data())/mw;
     batch.setEnthalpy(H);

     // Solve ODE system
     batch.setTemperature(TC[celli]); batch.setPressure(pC[celli]);
     batch.derivatives(tStart, c, dcStart);
     odeSolver->solve(tStart, tEnd, c, dtStart);

     // From concentrations to mass fractions
     cTot = std::accumulate(c.begin(), c.end(), 0.);
     for(unsigned int i=0;i<NC;i++) x(i) = c[i]/cTot;
     thermoMap.MassFractions_From_MoleFractions(x.data(), mw, y.data());
     for(unsigned int i=0;i<NC;i++)
          Y[i].ref()[celli] = massFractions(i);

     // Temperature
     TC[celli] = thermoMap.GetTemperatureFromEnthalpyAndMoleFractions
                    (H*mw, pC[celli], x.data(), TC[celli]);

}
```

Batch reactor (adiabatic) (I)

```
void batchAdiabaticOdeSystem::derivatives( const scalar t, const
                          scalarField& cc, scalarField& dcdt ) const
{
    // Reconstruct concentrations and mole fractions
    Eigen::VectorXd c(thermoMap_.NumberOfSpecies());
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        c(i) = std::max(cc[i],0.);

    Eigen::VectorXd x(thermoMap_.NumberOfSpecies());
    const double cTot = c.sum();
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        x(i) = c[i]/cTot;
    const double mw = thermoMap_.MolecularWeight_From_MoleFractions(x.data());

    // Calculate temperature (pressure is assumed constant)
    const double T_ = thermoMap_.GetTemperatureFromEnthalpyAndMoleFractions
                     (Hfixed_*mw, P0_, x.data(), TStart_);

    ...
}
```

Batch reactor (adiabatic)

```
void batchAdiabaticOdeSystem::derivatives( const scalar t, const
                          scalarField& cc, scalarField& dcdt ) const
{
    ...

    // Calculates thermodynamic properties
    thermoMap_.SetTemperature(T_);
    thermoMap_.SetPressure(P0_);

    // Calculates kinetics
    Eigen::VectorXd R(thermoMap_.NumberOfSpecies());
    kineticsMap_.SetTemperature(T_);
    kineticsMap_.SetPressure(P0_);
    kineticsMap_.ReactionRates(c.data());
    kineticsMap_.FormationRates(R.data());

    // Species equations
    for (unsigned int i=0;i<thermoMap_.NumberOfSpecies();i++)
        dcdt[i] = R(i);
}
```

Compiling the unsteady solver

Compilation

1. Go to the `Training/Solvers/laminarSolverUnsteady/src folder`
2. Type `wmake`

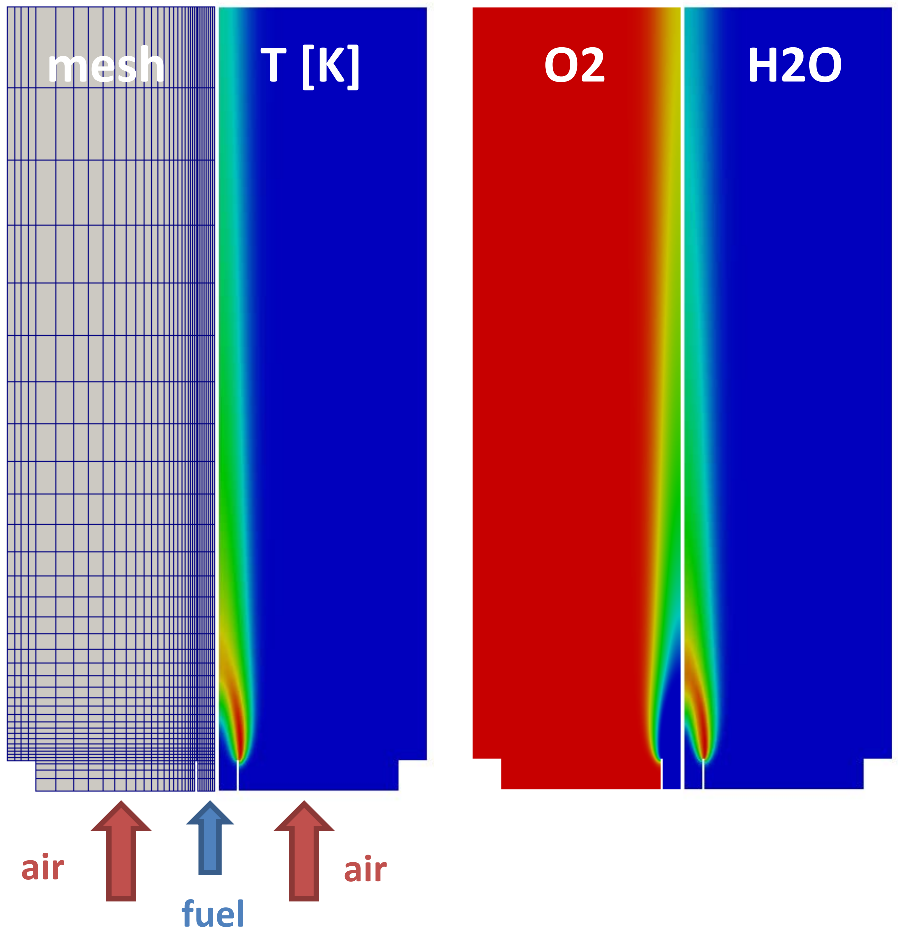
Example of a coflow flame

1. Go to the following folder:
   `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/01-global-1step`
2. Type `blockMesh`
3. Type `laminarSolverUnsteady`

Outline

Example: laminar coflow flame

V. V. Toro, A. V. Mokhov, H. B. Levinsky, M. D. Smooke, Proceedings of the Combustion Institute, 30 (2005), 485-492

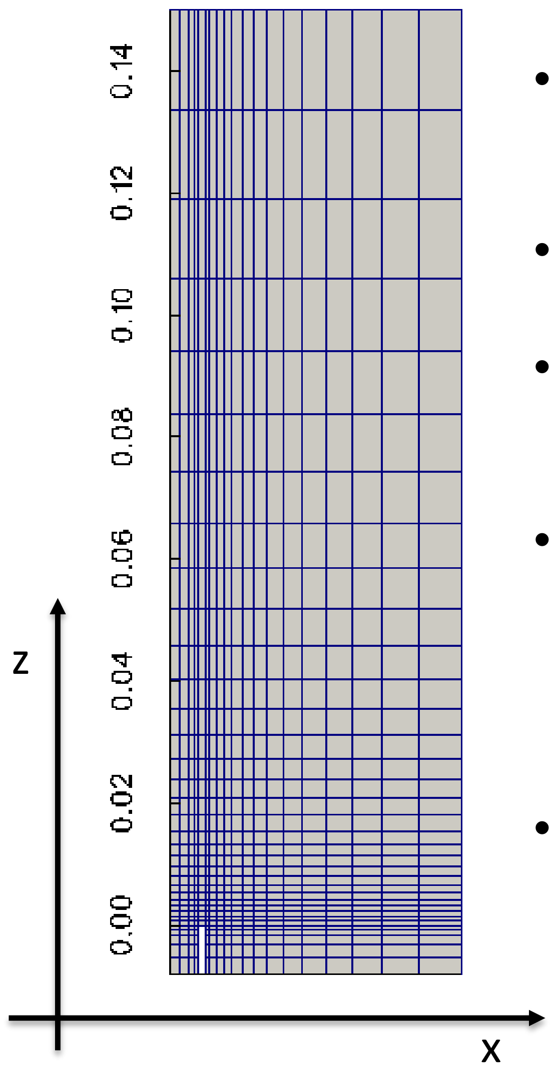


The fuel stream **(50% H_2 and 50% N_2 by volume)** is injected at ambient temperature through a circular nozzle (**i.d. 9 mm**), surrounded by an air-coflow annulus (**i.d. 95 mm**).

The fuel and coflow inlet velocities are assumed equal to **50 cm/s (Flame F3)**.

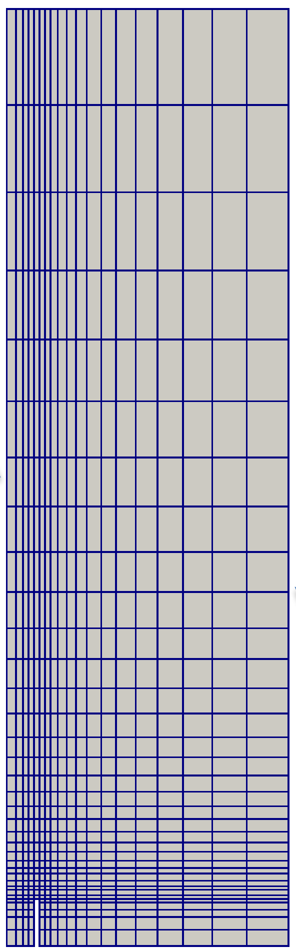
A **2D rectangular domain** meshed with a structured grid is considered.

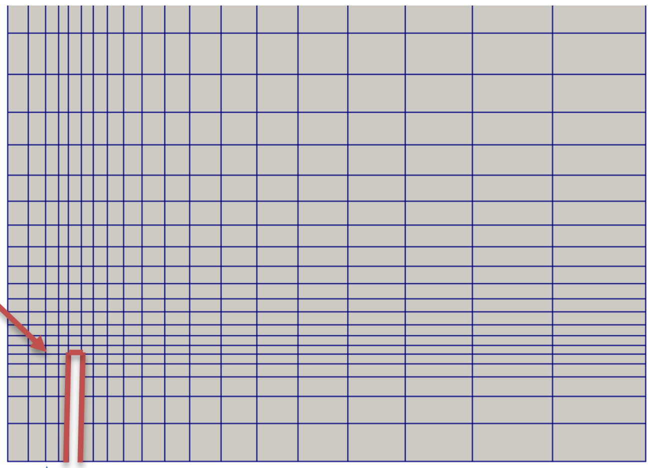
Computational mesh



- A axisymmetric mesh is chosen, due to the cylindrical symmetry of the system
- The mesh is built using the `blockMeshDict`
- The length is 150 mm (z direction) and the width is 47.5 mm (x direction)
- A very coarse mesh was chosen (with 35 cells along the axis and 19 cells along the radial direction) in order to reduce the computational time as much as possible during the training session
- You should not use this mesh for your production simulations because is too coarse

Boundaries





`outlet`
outlet section

`burnerwall`
burner wall

`axis`
axis of cylindrical symmetry

`inletfuel`
inlet section for fuel stream

`inletair`
inlet section for coflow stream

`leftside`
open boundary

Global kinetic mechanism

Our preliminary calculations are carried out using a global 1 step mechanism, available in the `PreProcessing/Global_H2_1step folder`

```
ELEMENTS
H O N
END

SPECIES
H2 O2 H2O N2
END

REACTIONS
H2 + 0.5O2 => H2O  1e14 0 20000
FORD / O2 1.00 /
END
```

Warning!
This global 1-step mechanism is used in the training session simply to reduce the computational time. Do not use it for your production simulations

The kinetic mechanism has to be pre-processed (see previous sections) using the `OpenSMOKEpp_CHEMKIN_PreProcessor`

1. Go to the `PreProcessing/Global_H2_1step` folder
2. Type `OpenSMOKEpp_CHEMKIN_PreProcessor --input input.dic`

Setup the case

The kinetic mechanism to be used is specified in the `constant/solverOptions` file

```
Kinetics
{
    folder              "../../../../../../PreProcessing/Global_H2_1step/";
    inertSpecies        N2;
    ODESolver           seulex;
}
```

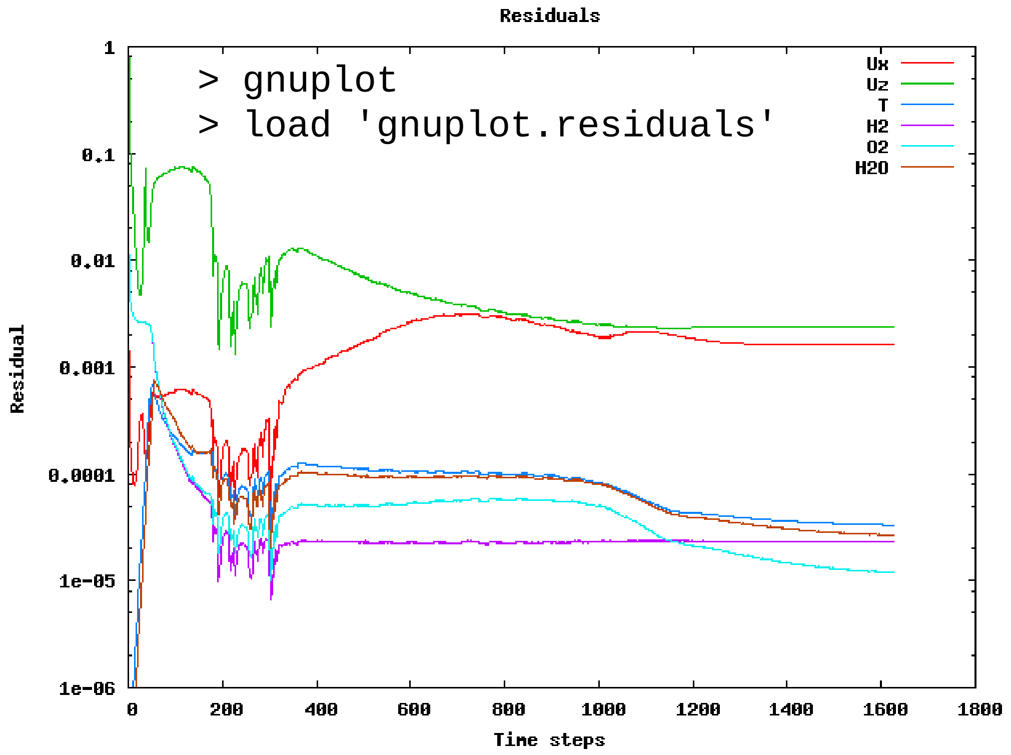
Since both the fuel and oxidizer streams are fed at ambient temperature, it is necessary to introduce a **spark** in order to ignite the mixture.

```
Spark
{
    spark           on;
    position        (5.95e-3  0.0 1.5e-3);
    time            0.;
    temperature     2200;
    duration        0.025;
    diameter        1.5e-3;
}
```

In our solver the spark is nothing but a (circular) region in which the temperature is kept fixed at a high value for a certain amount of time

Running the case

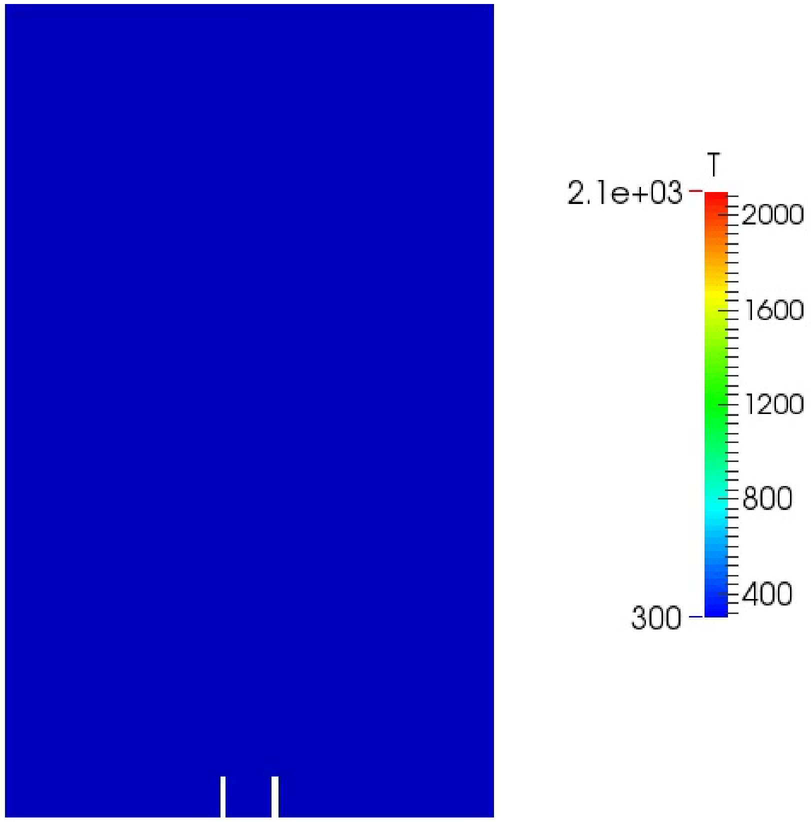
1. Go to the following folder:
   `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/01-global-1step`
2. Type `blockMesh`
3. Type `laminarSolverUnsteady > log &`
4. The simulation takes about 5 min on a single core



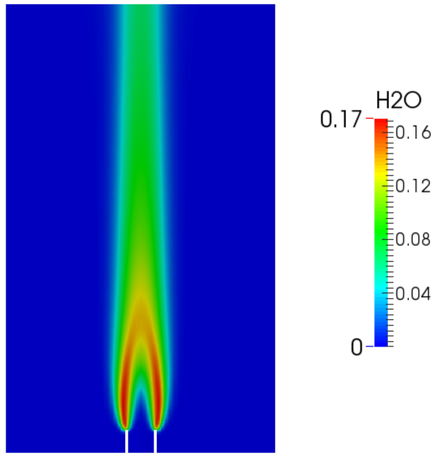
```
> gnuplot
> load 'gnuplot.residuals'
```

Results

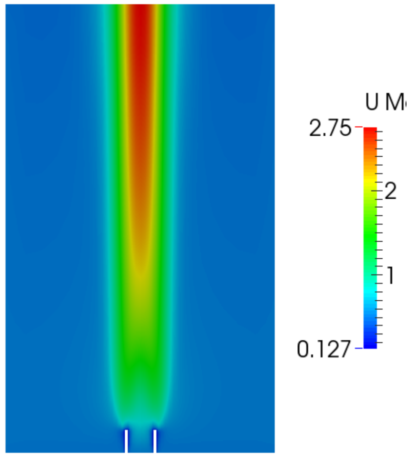
Temperature field
(evolution from 0 to 0.25 s)



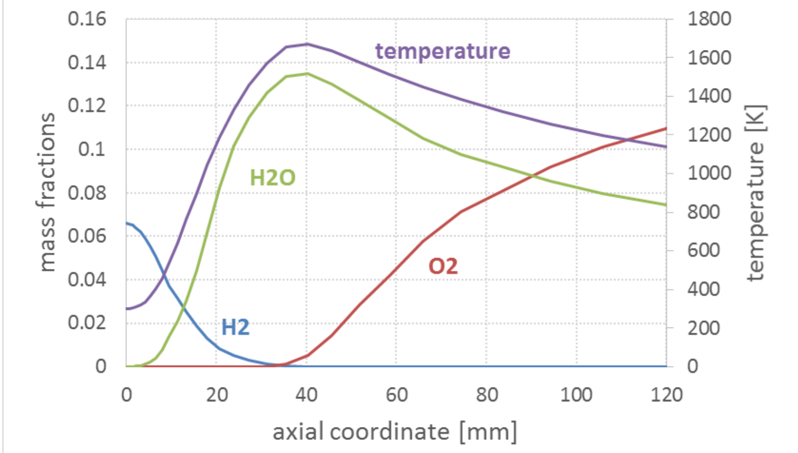
H2O mass fraction



U magnitude



```
> postProcess -func sample
```



Refining the solution using a detailed mech

Mechanism preprocessing

We want now refine the solution by using the detailed kinetic mechanism contained in the `PreProcessing/POLIMI_H2_1412`:

1. Go to the `PreProcessing/POLIMI_H2_1412` folder
2. Type `OpenSMOKEpp_CHEMKIN_PreProcessor --input input.dic`

Restarting from previous solution

We restart from the last solution (0.25 s) corresponding to the global, 1-step mechanism

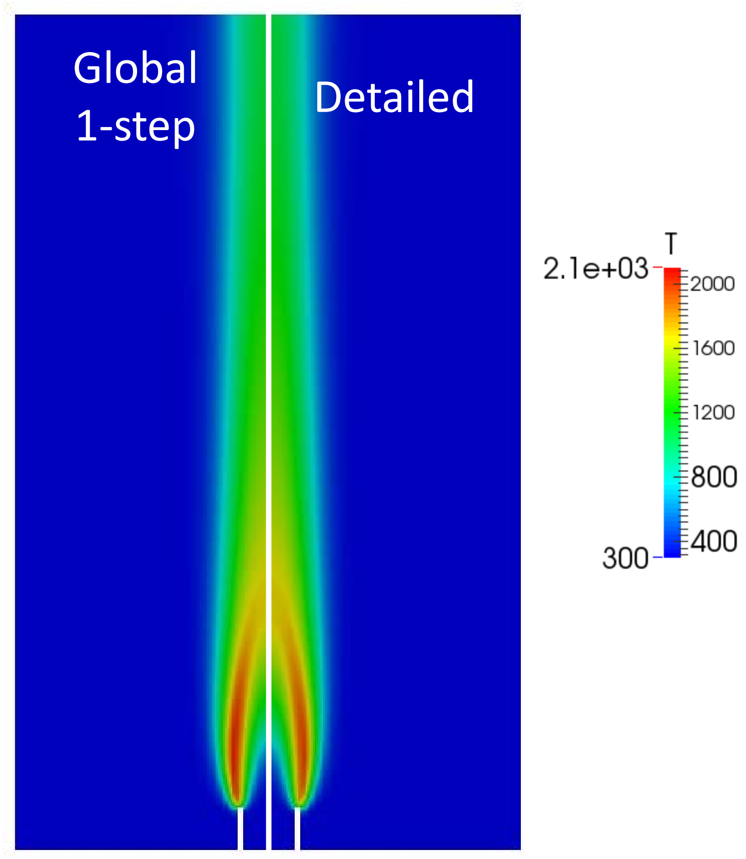
1. Go to the following folder: `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/02-detailed-polimi`
2. Copy the last solution:

```
cp -r ../01-global-1step/0.25/ .
cp ../01-global-1step/0/Ydefault 0.25/
rm –r 0.25/uniform
```

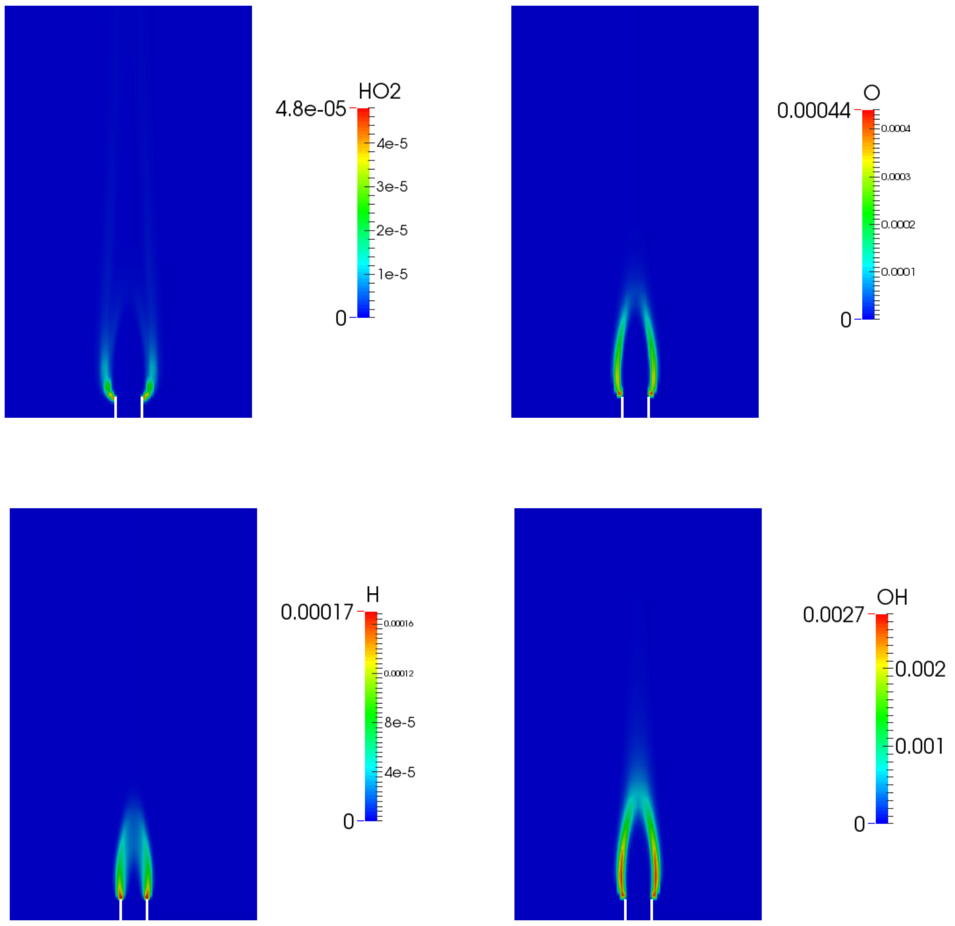
Running the simulation

1. Go to the following folder:
   `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/02-detailed-polimi`
2. Type `blockMesh`
3. Type `laminarSolverUnsteady > log &`
4. The simulation takes about 10 min on a single core (from 0.25 s to 0.30 s)

Results



Mass fraction of radical species



NOx predictions

Mechanism preprocessing

We want now add NOX predictions by using the detailed kinetic mechanism contained in the `PreProcessing/POLIMI_H2_NOX_1412`:

1. Go to the `PreProcessing/POLIMI_H2_NOX_1412` folder
2. Type `OpenSMOKEpp_CHEMKIN_PreProcessor --input input.dic`

Restarting from previous solution

We restart from the last solution obtained with the `POLIMI_H2_NOX_1412` mechanism

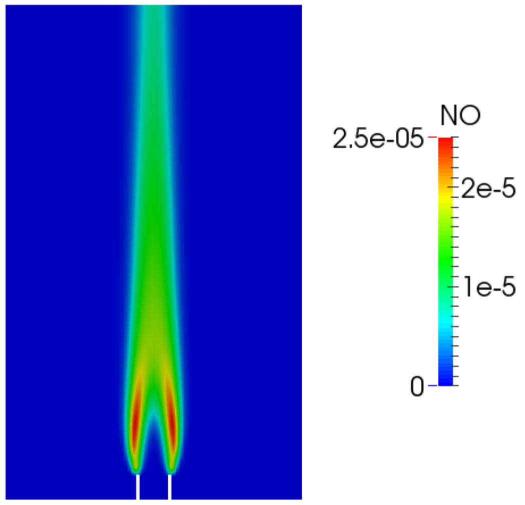
1. Go to the following folder:
   `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/03-detailed-polimi-nox`
2. Copy the last solution:

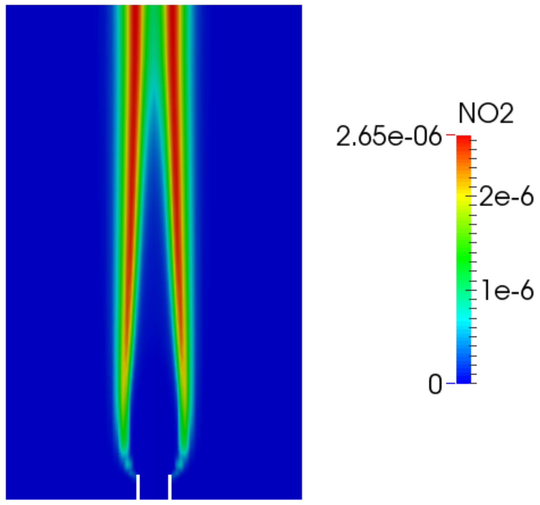
```
cp -r ../02-detailed-polimi/0.3/ .
cp ../01-global-1step/0/Ydefault 0.3/
rm –r 0.3/uniform
```

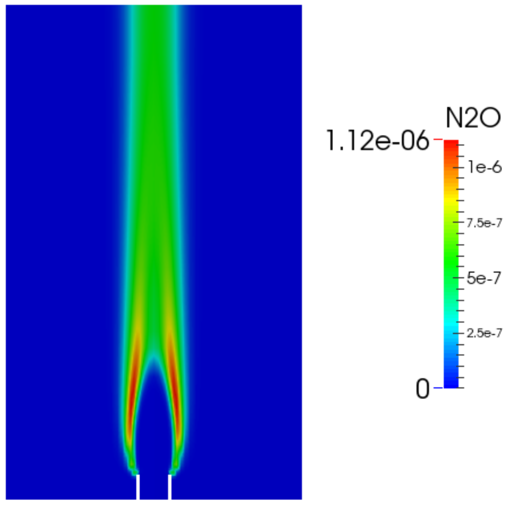
Running the simulation

1. Go to the following folder:
   `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/02-detailed-polimi-nox`
2. Type `blockMesh`
3. Type `laminarSolverUnsteady > log &`
4. The simulation takes more than 1 hour on a single core

Solutions @ 1 s

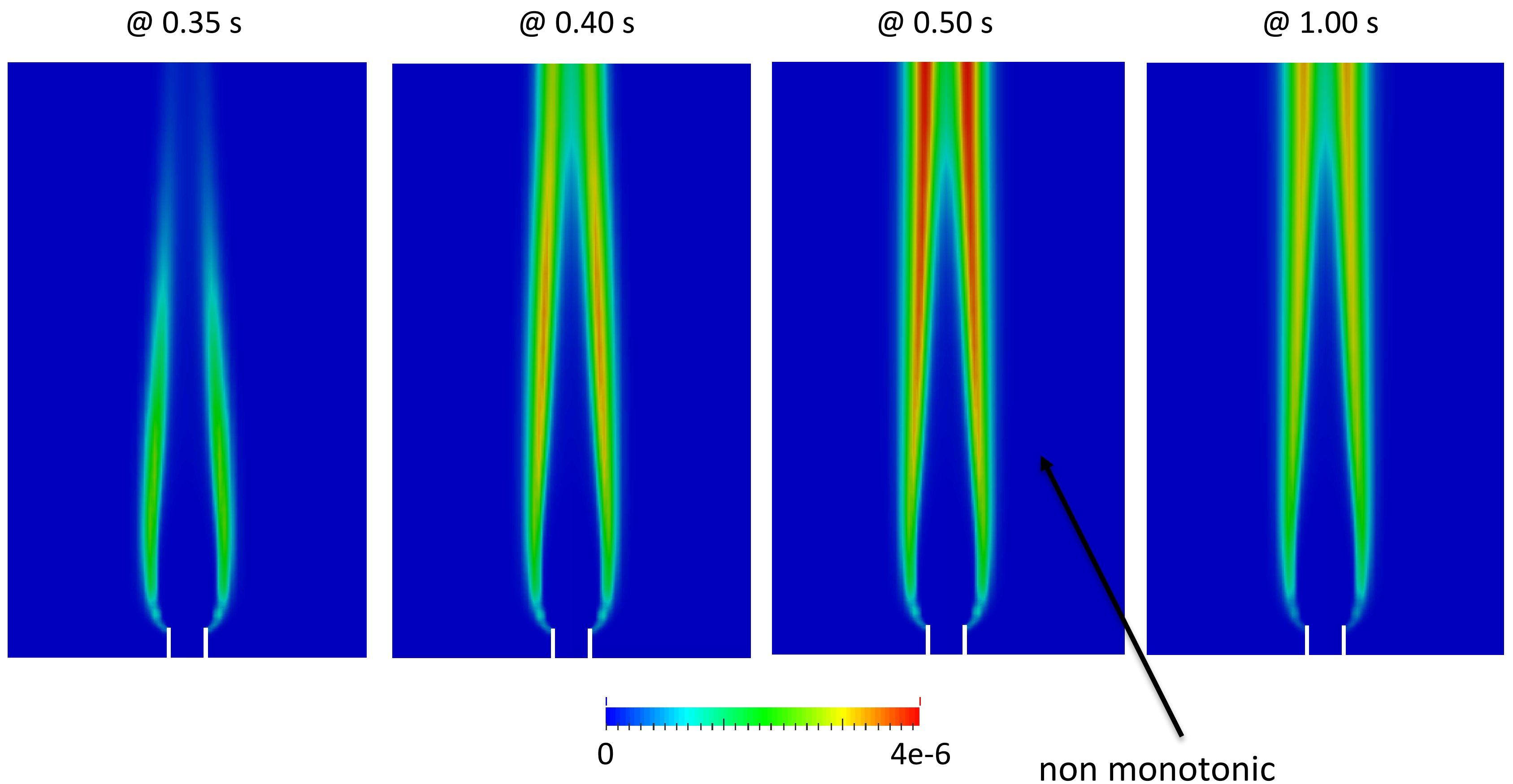






Warning: NOX chemistry is very slow!

NO2 mass fraction

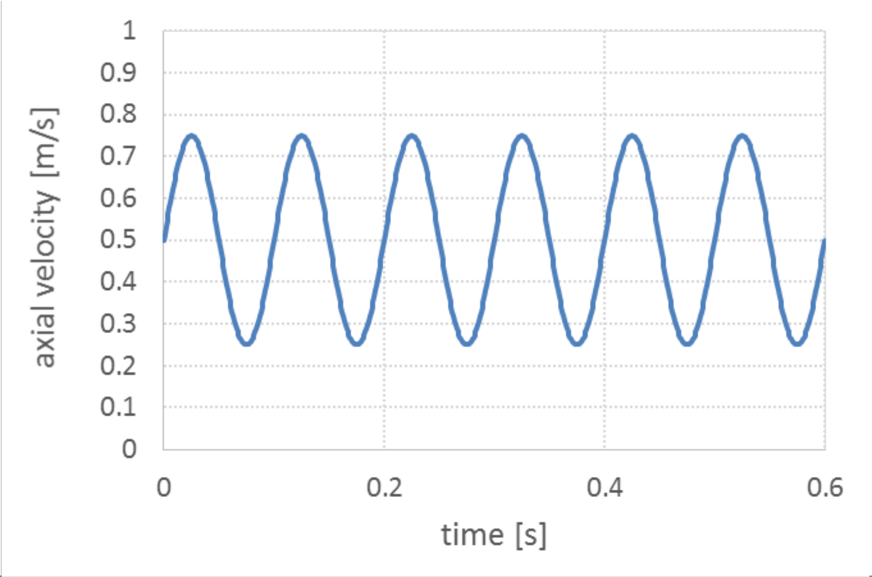


non monotonic
behavior in time!

Pulsating flame (I)

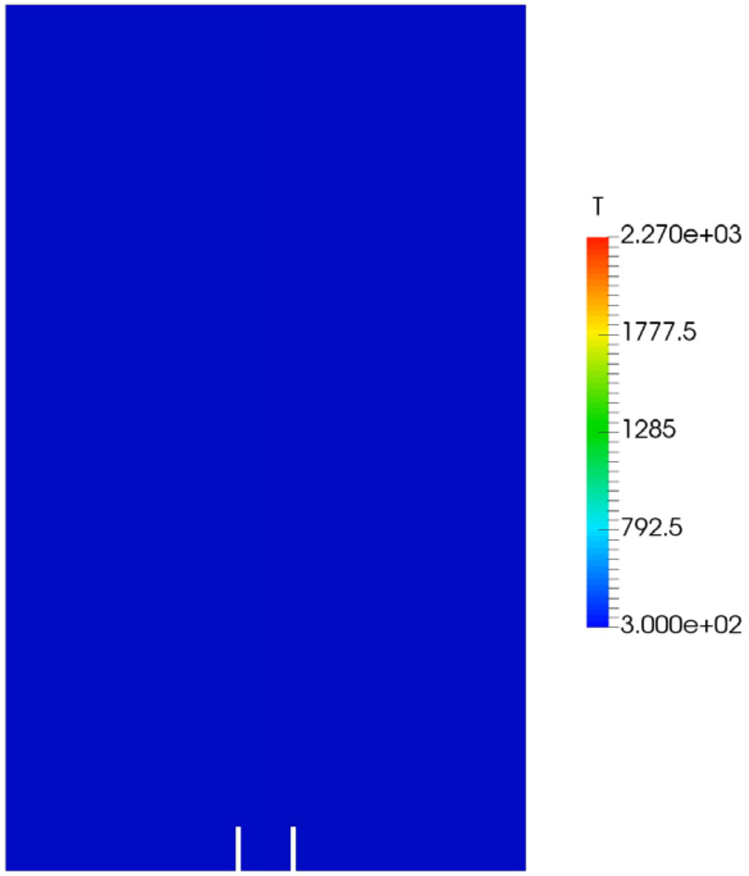
We want now to simulate the same flame under **pulsating conditions**.
A sinusoidal velocity profile is imposed to the fuel stream, with amplitude **A=50%** and frequency **f=10Hz**

```
inletfuel
{
    type          uniformFixedValue;
    uniformValue  tableFile;
    file          "$FOAM_CASE/constant/myVelocityProfile";
}
```



```
(
    ( 0      ( 0  0 0.500000000 ) )
    ( 0.001  ( 0  0 0.515697630 ) )
    ( 0.002  ( 0  0 0.531333308 ) )
    ( 0.003  ( 0  0 0.546845329 ) )
    ( 0.004  ( 0  0 0.562172472 ) )
    ( 0.005  ( 0  0 0.577254249 ) )
    ( 0.006  ( 0  0 0.592031138 ) )
    ( 0.007  ( 0  0 0.606444823 ) )
    …
)
```

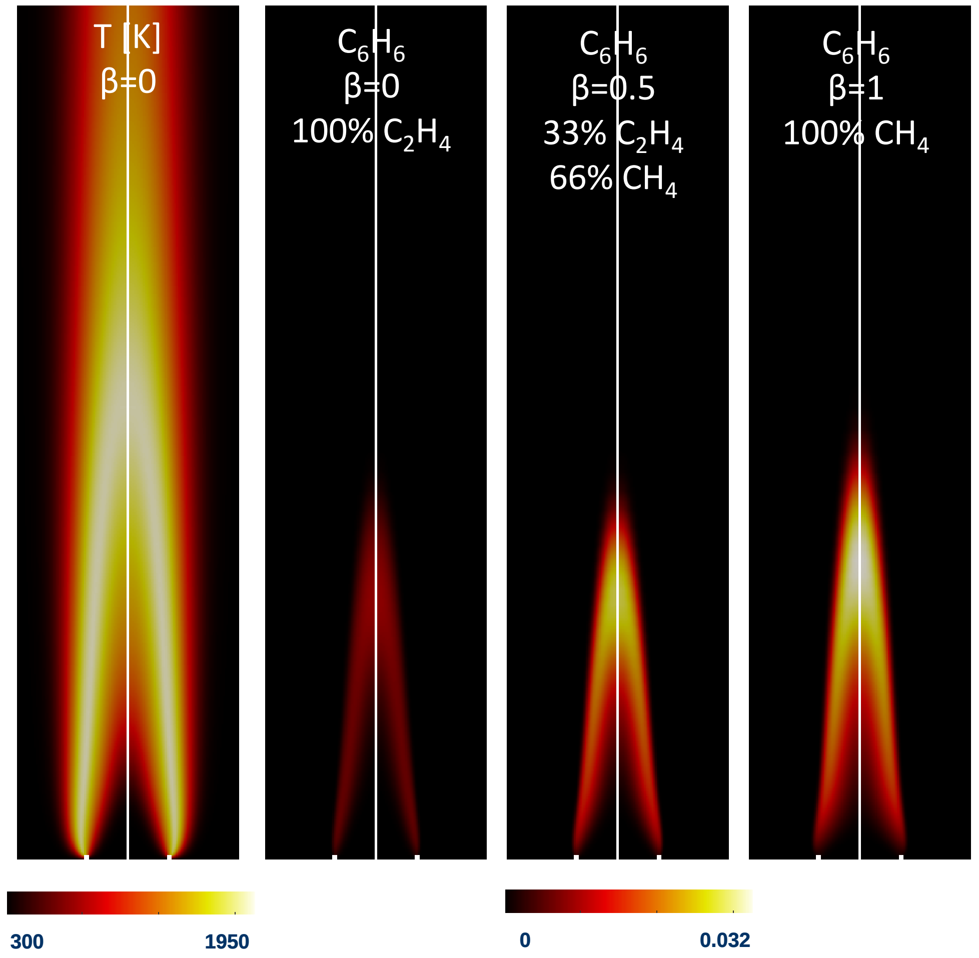
Pulsating flame (II)



In order to reduce the computational cost, the simulation is carried using the global 1-step mechanism

1. Go to the following folder: `Training/Solvers/laminarSolverUnsteady/run/coflowFlame/04-global-1step-pulsating`
2. Type `blockMesh`
3. Type `laminarSolverUnsteady > log &`
4. The whole simulation takes about 30 min on a single core. A single, complete cycle of oscillation about 15 min.

An example: $C_2H_4/CH_4/N_2$ coflow flames (I)



Cuoci A., Frassoldati A., Faravelli T., Ranzi E., Combustion and Flame, 160(5), p. 870-886 (2013)

Flame details

Fuel: CH_4/C_2H_4

Air: O_2/N_2 (23.2%, 76.8% mass)

V_{fuel}: 12.52 cm/s

V_{air}: 10.50 cm/s

Fuel nozzle diameter: 11.1 mm

Chamber diameter: 110 mm

Computational details

Domain: 2D axisymmetric (55 x 200 mm)

Computational grid: ~25,000 cells

Discretization: second order centered

Kinetic scheme

POLIMI_HT1212:

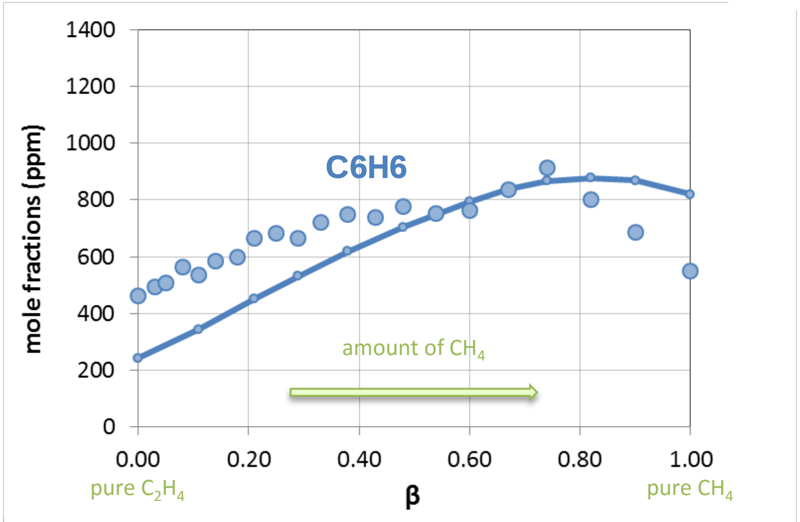
198 species, 6307 reactions

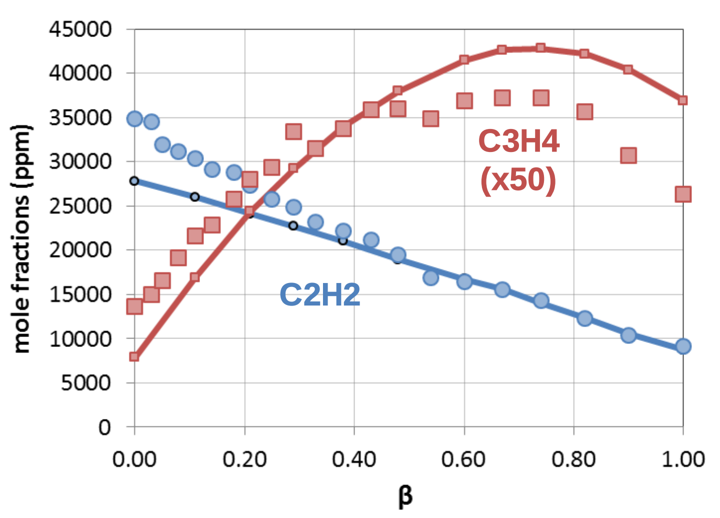
The concentrations of C_2H_4 and CH_4 are identified by the mixture parameter β:

$$\beta = \frac{X_{CH4}}{X_{CH4} + 2X_{C2H4}}$$

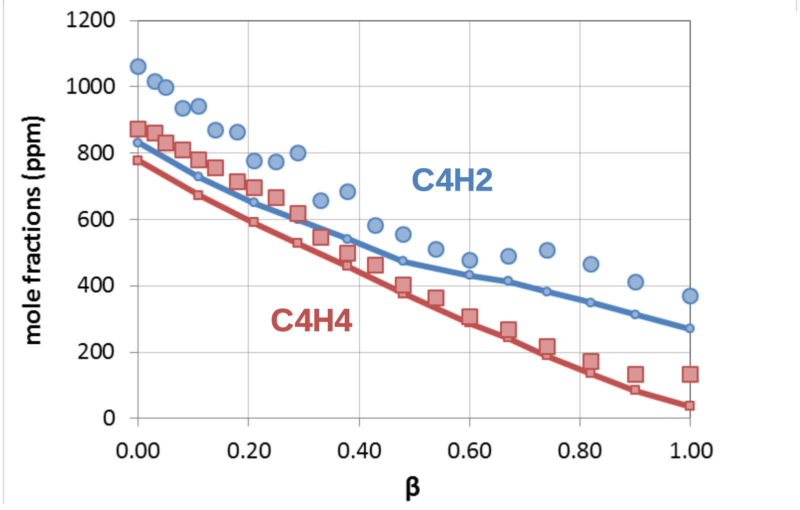
An example: $C_2H_4/CH_4/N_2$ coflow flames (II)

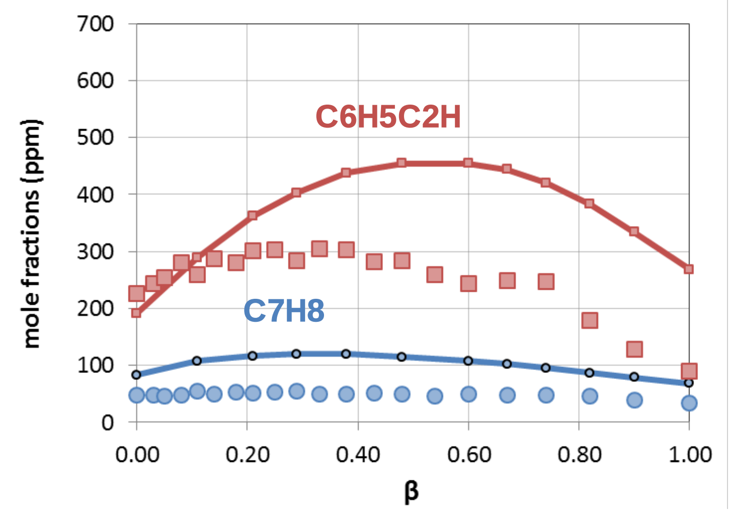
Peak values (along the center-line) of mole fractions



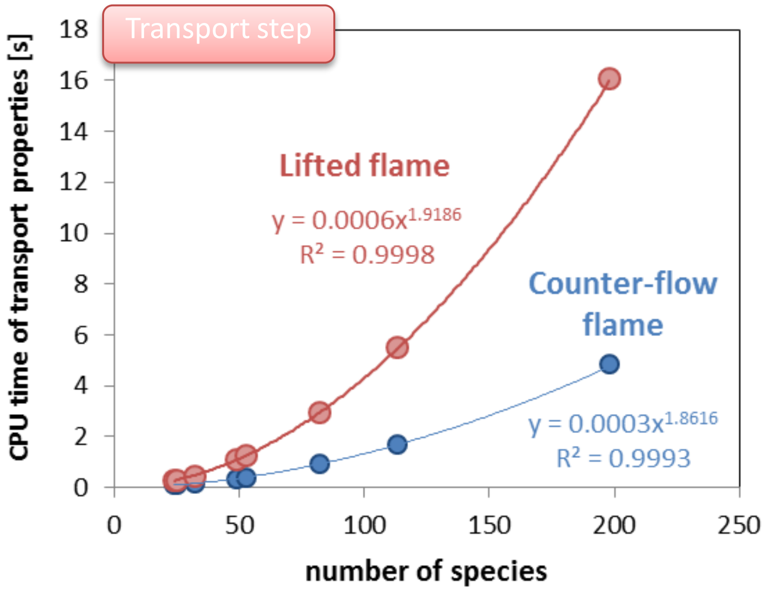


Experimental data from:
J.F. Roesler, M. Martinot, C.S. McEnally, L.D. Pfefferle, J.L. Delfau, C. Vovelle, *Combustion and Flame*, 134 (2003) 249-260.





Computational cost

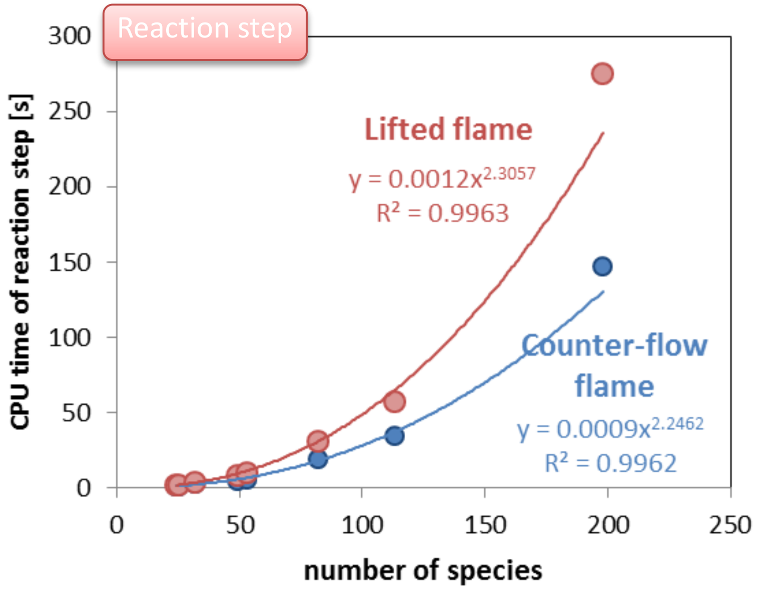


The reaction step results to be the most consuming part of the code, requiring more than **80-85% of the total computational time**.

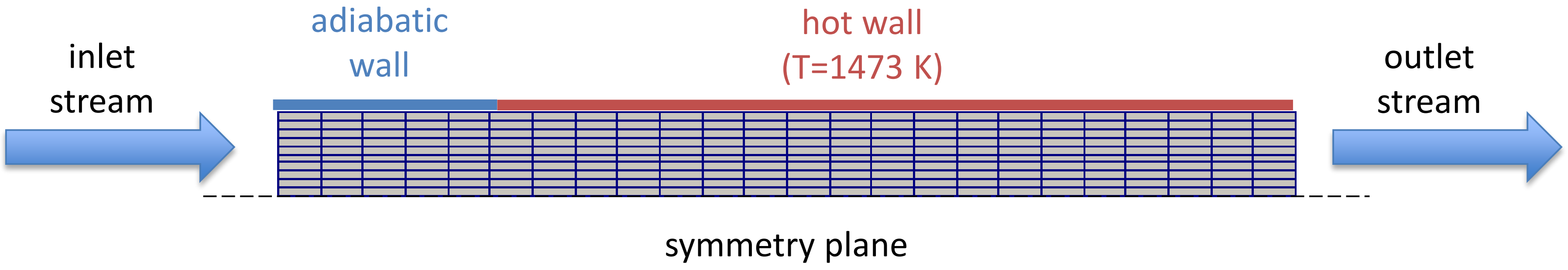
The evaluation of the transport properties and the transport step cover the 5-7% and the 10% of the total time, respectively.

The CPU time of the reaction steps **increases more than quadratically (~2.3)** with the number of species, while the transport properties with a power of ~1.8

Increasing the number of species, the relative weight of the reaction step increases.



An example: pyrolysis reactor (I)



The inlet stream is a mixture of CH4 and N2 **(70% CH4, 30% N2 by volume)** and it is fed to the reactor at temperature of 873 K and velocity (flat profile) of **20 cm/s**

The reactor is modeled as a channel, with length of 24 cm and width of 2 cm. Because of the planar symmetry along the x axis, only one half of the reactor is modeled. The adopted mesh (24 x 5) is very coarse and it is here adopted only to have small CPU times.

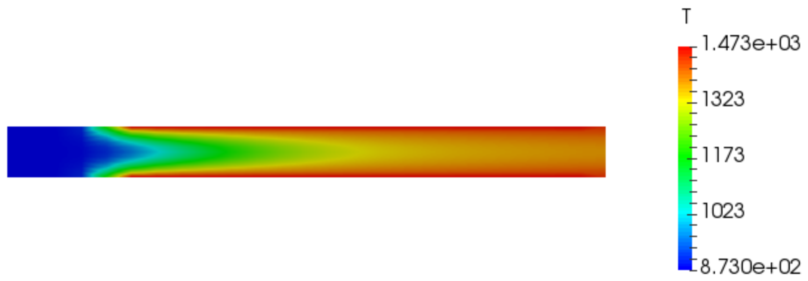
An example: pyrolysis reactor (II)

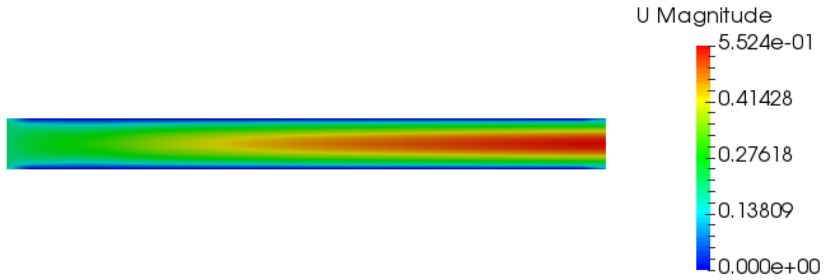
Run the simulation

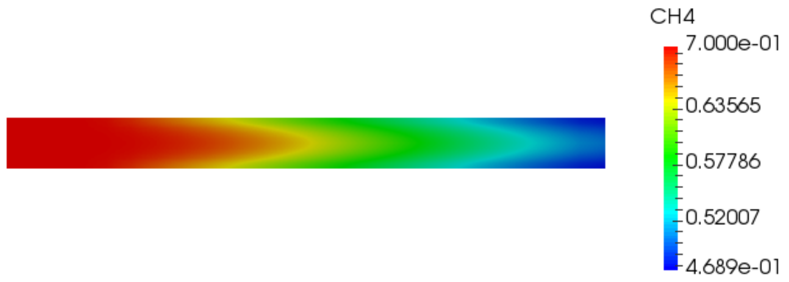
1. Go to the following folder: `Training/Solvers/laminarSolverUnsteady/run/pyrolysisReactor/01-mesh-coarse`
2. Type: `blockMesh`
3. Type: `laminarSolverUnsteady > log &`
4. The simulation takes about 5 min on a single core

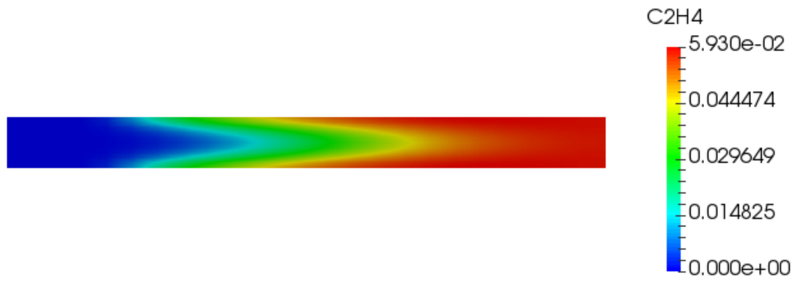
An example: pyrolysis reactor (III)

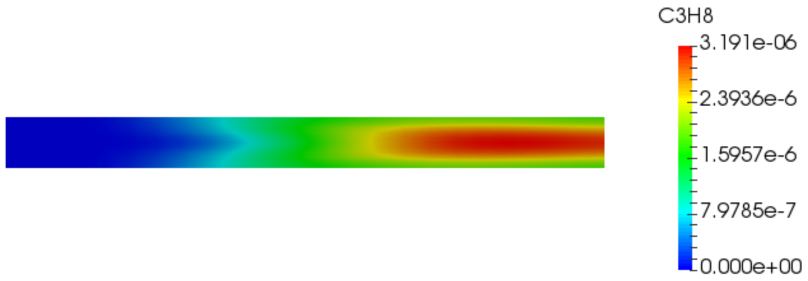
Solutions @ 2 s (steady-state)

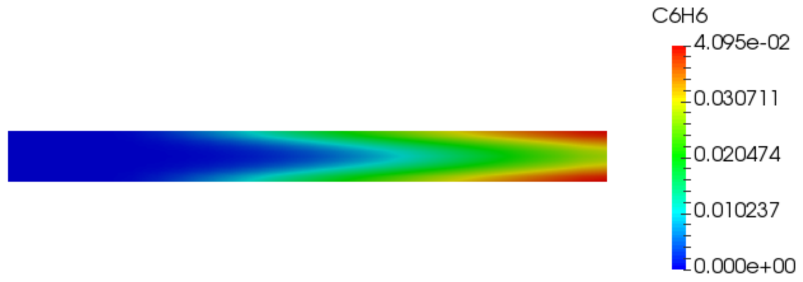








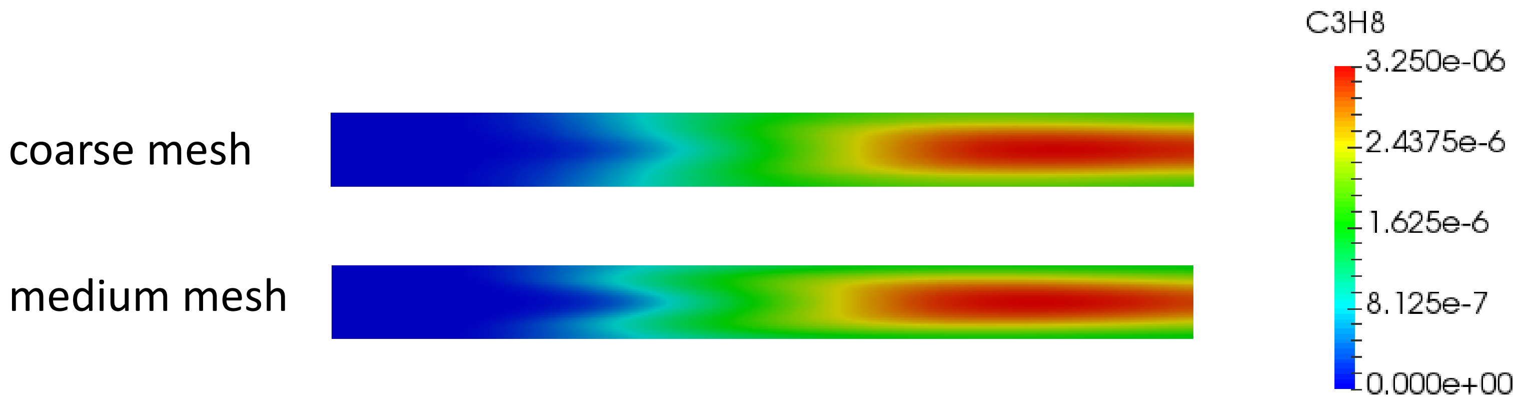




An example: pyrolysis reactor (IV)

Refine the mesh and run the simulation

1. Go to the following folder: `Training/Solvers/laminarSolverUnsteady/run/pyrolysisReactor/02-mesh-medium`
2. Type: `blockMesh`
3. Type: `mapFields ../01-mesh-coarse/ -consistent -sourceTime 2`
4. Type: `laminarSolverUnsteady > log &`
5. The simulation takes about 10 min on a single core



Outline

Steady-state solver: equations

Continuity equation	$\nabla(\rho\boldsymbol{v}) = 0$
Momentum equations	$\nabla(\rho\boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla\boldsymbol{\tau} + \rho\boldsymbol{g}$
Energy equation	$\rho C_P \boldsymbol{v}\nabla T = \lambda\nabla^2 T + Q_R$
Species equations	$\nabla(\rho\boldsymbol{v}Y_k) = \nabla(\rho\Gamma_k\nabla Y_k) + R_k \qquad k = 1, \dots, N$

Simplifying hypotheses
- No radiative heat transfer
- No enthalpy fluxes due to preferential mass diffusion
- No thermodiffusion (Soret effect)
- No correction velocity on mass diffusion fluxes

Steady-state solver: algorithm

Continuity equation	$\nabla(\rho \boldsymbol{v}) = 0$	SIMPLE Algorithm
Momentum equations	$\nabla(\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \boldsymbol{\tau} + \rho \boldsymbol{g}$	

Energy equation	$\rho C_P \boldsymbol{v} \nabla T = \lambda \nabla^2 T + Q_R$	Strongly non linear terms
Species equations	$\nabla(\rho \boldsymbol{v} Y_k) = \nabla(\rho \Gamma_k \nabla Y_k) + R_k \qquad k = 1, \dots, N$	

LINEARIZATION

Steady-state solver: chemistry (I)

$$R_k^{(n+1)} \approx R_k^{(n)} + \sum_{j=1}^{N} \left.\frac{\partial R_k}{\partial Y_j}\right|^{(n)} \left(Y_j^{(n+1)} - Y_j^{(n)}\right) = R_k^{(n)} + \sum_{j=1}^{N} J_{kj}^{(n)} \left(Y_j^{(n+1)} - Y_j^{(n)}\right)$$

Jcobian matrix $\quad J_{kj} = \dfrac{\partial R_k}{\partial Y_j}$

$$R_k^{(n+1)} \approx R_k^{(n)} + J_{kk}^{(n)} \left(Y_k^{(n+1)} - Y_k^{(n)}\right) + \sum_{\substack{j=1 \\ j\neq k}}^{N} J_{kj}^{(n)} \left(Y_j^{(n+1)} - Y_j^{(n)}\right)$$

$$R_k^{(n+1)} \approx \underbrace{\left[J_{kk}^{(n)} Y_k^{(n+1)}\right]}_{\text{implicit (linear)}} + \underbrace{\left[R_k^{(n)} - J_{kk}^{(n)} Y_k^{(n)}\right]}_{\text{explicit}} + \underbrace{\left[\sum_{\substack{j=1 \\ j\neq k}}^{N} J_{kj}^{(n)} \left(Y_j^{(n+1)} - Y_j^{(n)}\right)\right]}_{\text{off-diagonal}}$$

Steady-state solver: chemistry (II)

$$R_k^{(n+1)} \approx \left[J_{kk}^{(n)} Y_k^{(n+1)}\right] + \left[R_k^{(n)} - J_{kk}^{(n)} Y_k^{(n)}\right] + \left[\sum_{\substack{j=1 \\ j\neq k}}^{N} J_{kj}^{(n)} \left(Y_j^{(n+1)} - Y_j^{(n)}\right)\right]$$

implicit (linear) — explicit — off-diagonal

Option 1

$$R_k^{(n+1)} \approx \left[J_{kk}^{(n)} Y_k^{(n+1)}\right] + \left[R_k^{(n)} - J_{kk}^{(n)} Y_k^{(n)}\right]$$

Option 2

$$R_k^{(n+1)} \approx \left[J_{kk}^{(n)} Y_k^{(n+1)}\right] + \left[R_k^{(n)} - J_{kk}^{(n)} Y_k^{(n)}\right] + \left[\sum_{\substack{j=1 \\ j\neq k}}^{N} J_{kj}^{(n)} \left(Y_{j,pred}^{(n+1)} - Y_j^{(n)}\right)\right]$$

Predictor-corrector approach

Steady-state solver: source terms

$$\nabla(\rho \boldsymbol{v} Y_k) - \nabla(\rho \Gamma_k \nabla Y_k) = R_k$$

$$R_k^{(n+1)} \approx \left[J_{kk}^{(n)} Y_k^{(n+1)}\right] + \left[R_k^{(n)} - J_{kk}^{(n)} Y_k^{(n)}\right]$$

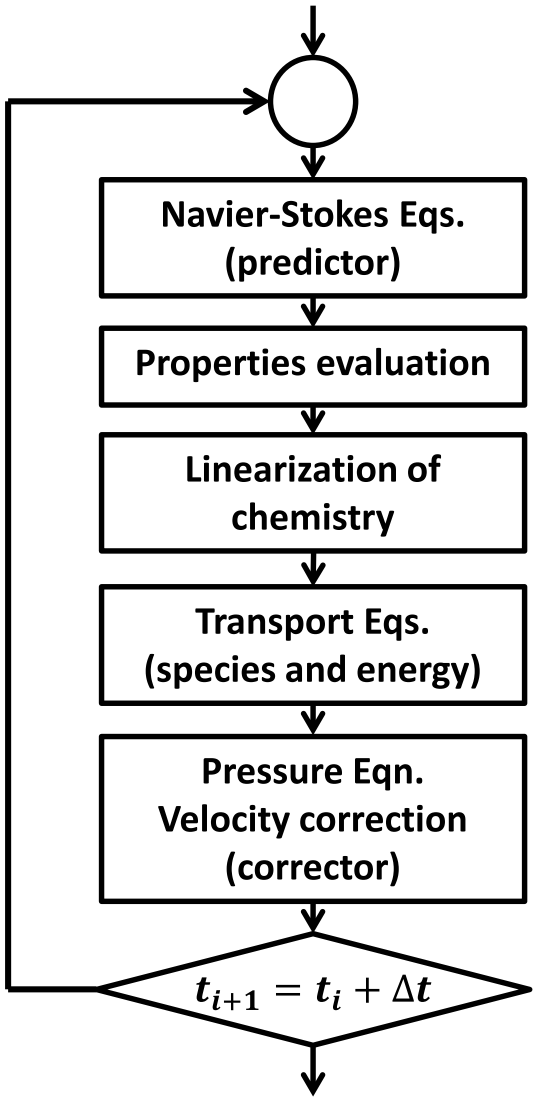
```
fvScalarMatrix YiEqn
(
       mvConvection->fvmDiv(phi, Yi)
    -  fvm::laplacian(rho*GammaMixi, Yi)
    ==
       sourceExplicit[i]
    +  fvm::Sp(sourceImplicit[i],Yi)
    +  fvOptions(rho, Yi)
);
```

Outline

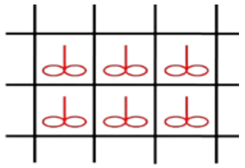
1. **Unsteady solver based on the operator splitting algorithm**
   1. Introduction and theory
   2. Implementation
   3. Examples

2. **Steady state solver based on the linearization of source terms**
   1. Introduction and theory
   2. **Implementation**
   3. Examples

Steady-state solver



Navier-Stokes Eqs. (predictor)
Properties evaluation
Linearization of chemistry
Transport Eqs. (species and energy)
Pressure Eqn. Velocity correction (corrector)
$t_{i+1} = t_i + \Delta t$



```
while (simple.loop())
{
        #include "UEqn.H"

        #include "transport.H"
        #include "chemistry.H"

        #include "YEqn.H"
        #include "TEqn.H"

        if (simple.consistent())
            #include "pcEqn.H"
        else
            #include "pEqn.H"

        runTime.write();
}
```

Steady-state solver: initialization

```
int main(int argc, char *argv[])
{
    // OpenFOAM stuff
    #include "setRootCase.H"
    #include "createTime.H"
    #include "createMesh.H"
    #include "createControl.H"
    #include "readGravitationalAcceleration.H“
    #include "createBasicFields.H"

    // OpenSMOKE++
    #include "createChemicalFields.H"
    #include "createSourceFields.H"
    #include "transportProperties.H"
    #include "createAdditionalFields.H"

    // Linear model for reacting source term
    linearModelChemistry chemistry(thermoMap, kineticsMap);

    ...
```

Fields for source terms: implicit

```
for (int i=0;i<thermoMap.NumberOfSpecies();i++)
{
    sourceImplicit.set
    (
        i,
        new volScalarField
        (
            IOobject
            (
                "SI_" + thermoMap.NamesOfSpecies()[i],
                mesh.time().timeName(),
                mesh,
                IOobject::NO_READ,
                IOobject::NO_WRITE
            ),
            mesh,
            dimensionedScalar("SI", dimensionSet(1, -3, -1, 0, 0), 0.0)
        )
    );
}
```

Fields for source terms: explicit

```
for (int i=0;i<thermoMap.NumberOfSpecies();i++)
{
    sourceExplicit.set
    (
        i,
        new volScalarField
        (
            IOobject
            (
                "SE_" + thermoMap.NamesOfSpecies()[i],
                mesh.time().timeName(),
                mesh,
                IOobject::NO_READ,
                IOobject::NO_WRITE
            ),
            mesh,
            dimensionedScalar("SE", dimensionSet(1, -3, -1, 0, 0), 0.0)
        )
    );
}
```

Evaluating chemical source terms

```
{
    const scalarField& TC = T.internalField();
    const scalarField& pC = p.internalField();

    Eigen::VectorXd J(NC+1), Source(NC+1), y(NC+1);

    forAll(TC, celli)
    {
        for(int i=0;i<NC;i++)
            y(i) = Y[i].internalField()[celli];
        y(NC) = TC[celli];

        chemistry.reactionSourceTerms(thermoMap, kineticsMap, y, pC[celli], Source);
        chemistry.reactionJacobian( thermoMap, kineticsMap, y, pC[celli], J );

        for(int i=0;i<NC+1;i++)
        {
            sourceImplicit[i].ref()[celli] = J(i);
            sourceExplicit[i].ref()[celli] = Source(i) - J(i)*y(i);
        }
    }
}
```

linearModelChemistry (I)

```
class linearModelChemistry
{

public:

    linearModelChemistry( OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap,
                          OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap);

    void reactionSourceTerms( OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap,
                              OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap,
                              const Eigen::VectorXd& y, const double P0,
                              Eigen::VectorXd& S);

    void reactionJacobian(    OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap,
                              OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap,
                              const Eigen::VectorXd& y, const double P0,
                              Eigen::VectorXd &J );

private:

    ...
};
```

linearModelChemistry (II)

```
void linearModelChemistry::reactionSourceTerms
(    OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap_,
     OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap_,
     const Eigen::VectorXd& y, const double P0, Eigen::VectorXd& S)
{
     ...

     // Calculates thermodynamic properties
     thermoMap_.SetTemperature(T); thermoMap_.SetPressure(P0);
     kineticsMap_.SetTemperature(T); kineticsMap_.SetPressure(P0);

     // Calculates kinetics
     kineticsMap_.KineticConstants();
     kineticsMap_.ReactionRates(c_.data());
     kineticsMap_.FormationRates(R_.data());

     // Species
     for (unsigned int i=0;i<NC_;++i)
          S(i) = R_(i)*thermoMap_.MW(i);

     // Energy
     const double QR_ = kineticsMap_.HeatRelease(R_.data());
     S(NC_) = QR_;
}
```

linearModelChemistry (III)

```
void linearModelChemistry::reactionJacobian(
    OpenSMOKE::ThermodynamicsMap_CHEMKIN& thermoMap,
    OpenSMOKE::KineticsMap_CHEMKIN& kineticsMap,
    const Eigen::VectorXd& y, const double P0, Eigen::VectorXd &J )
{
     ...

     // Call equations
     reactionSourceTerms(thermoMap, kineticsMap, y, P0, dy_original_);

     // Derivatives with respect to y(kd)
     for(int kd=0;kd<NE_;kd++)
     {
         .. .

         double dy = std::min(hJ, 1.e-3 + 1e-3*fabs(y(kd)));
         double udy = 1. / dy;
         y_plus_(kd) += dy;
        reactionSourceTerms(thermoMap, kineticsMap, y_plus_, P0, dy_plus_);

         J(kd) = (dy_plus_(kd)-dy_original_(kd)) * udy;
         y_plus_(kd) = y(kd);
     }
}
```

Numerical Jacobian: finite differences

Definition of Jacobian matrix $J_{kj} = \frac{\partial R_k}{\partial Y_j}$

Forward finite-difference $J_{kj} \approx \frac{R_k\left(Y_j + \Delta Y_j\right) - R_k\left(Y_j\right)}{\Delta Y_j}$ ΔY_j is a small increment

$\Delta Y_j = \epsilon_a + \epsilon_r \left|Y_j\right|$ where ϵ_a and ϵ_r are sufficiently small numbers

Decreasing the increment ΔY_j will reduce the truncation error. Unfortunately a smaller increment has the opposite effect on the cancellation error. Selecting the optimal step size for a certain problem is not trivial and may be computationally very expensive. A more accurate option is the following (ε is the machine precision):

$$\Delta Y_j = min\left(h, \epsilon_a + \epsilon_r \left|Y_j\right|\right) \qquad h = \varepsilon\, max\left(\left|Y_j\right|, \frac{1}{tol_{abs} + tol_{rel}\left|Y_j\right|}\right)$$

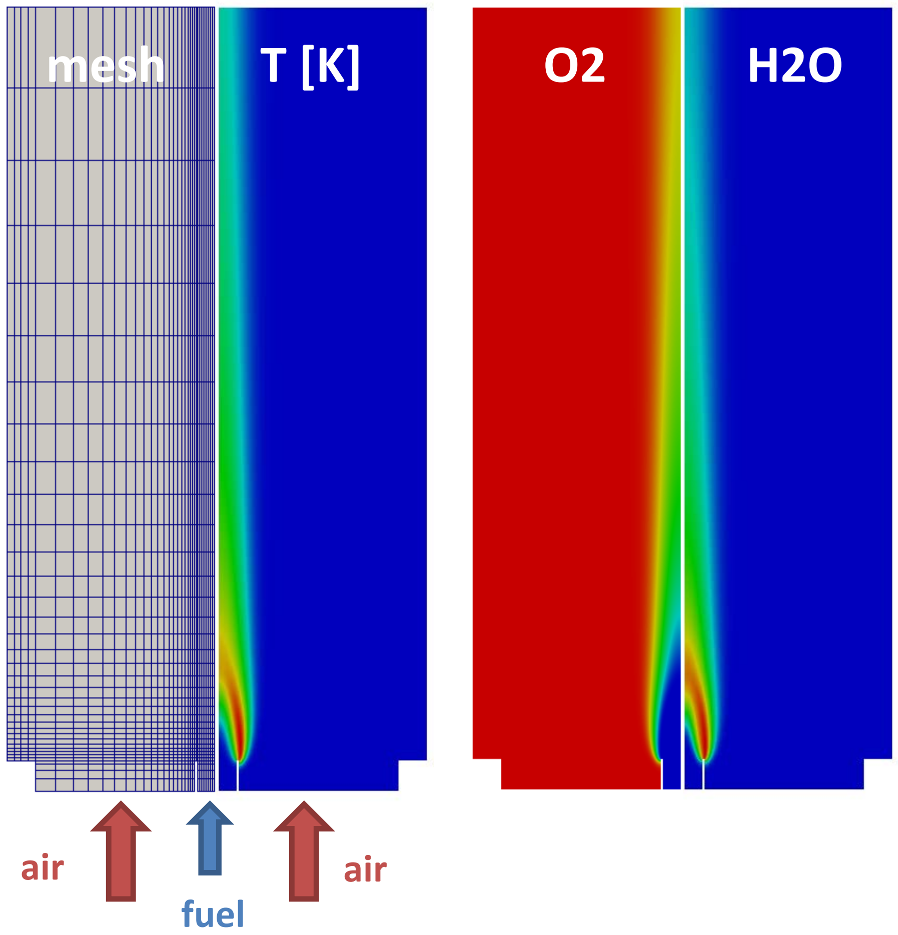
Outline

1. **Unsteady solver based on the operator splitting algorithm**
    1. Introduction and theory
    2. Implementation
    3. Examples

2. **Steady state solver based on the linearization of source terms**
    1. Introduction and theory
    2. Implementation
    3. **Examples**

Example: laminar coflow flame

V. V. Toro, A. V. Mokhov, H. B. Levinsky, M. D. Smooke, Proceedings of the Combustion Institute, 30 (2005), 485-492



The fuel stream **(50% H_2 and 50% N_2 by volume)** is injected at ambient temperature through a circular nozzle (**i.d. 9 mm**), surrounded by an air-coflow annulus (**i.d. 95 mm**).

The fuel and coflow inlet velocities are assumed equal to **50 cm/s (Flame F3)**.

A **2D rectangular domain** meshed with a structured grid is considered.

Global kinetic mechanism

Our preliminary calculations are carried out using a global 1 step mechanism, available in the `PreProcessing/Global_H2_1step folder`

```
ELEMENTS
H O N
END

SPECIES
H2 O2 H2O N2
END

REACTIONS
H2 + 0.5O2 => H2O  1e14 0 20000
FORD / O2 1.00 /
END
```

The kinetic mechanism was already pre-processed (see previous sections) using the `OpenSMOKEpp_CHEMKIN_PreProcessor`.

Setup the case

The kinetic mechanism to be used is specified in the `constant/solverOptions` file

```
Kinetics
{
    folder              "../../../../../../PreProcessing/Global_H2_1step/";
    inertSpecies        N2;
}
```

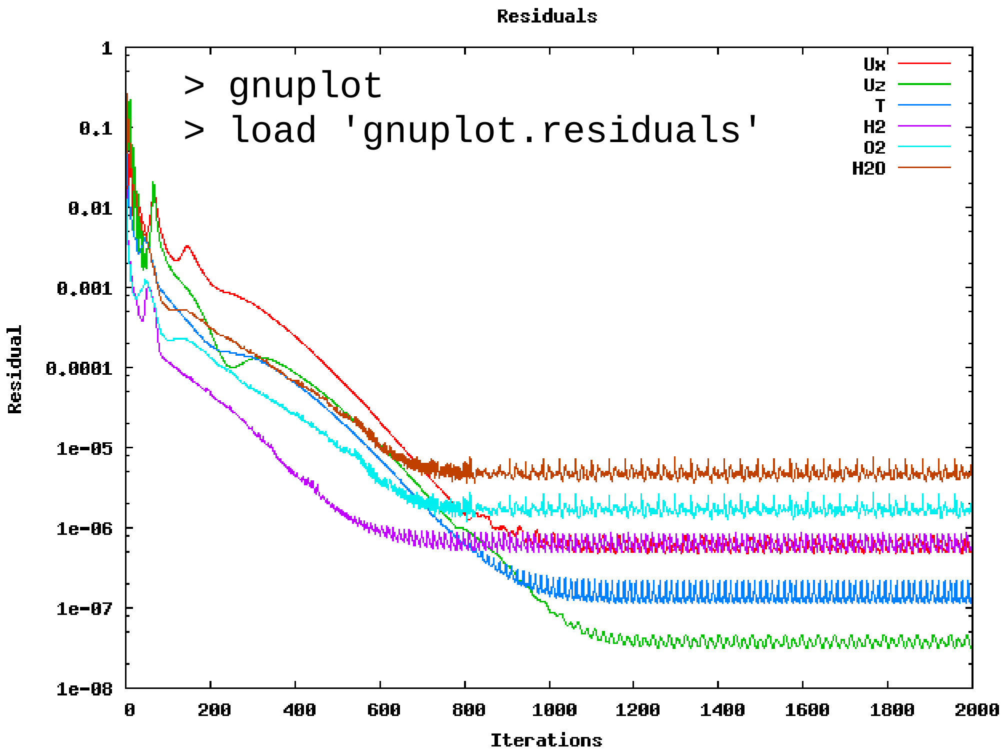
Since both the fuel and oxidizer streams are fed at ambient temperature, it is necessary to introduce a spark in order to ignite the mixture.

```
Spark
{
    spark          on;
    position       (5.95e-3  0.0 1.5e-3);
    time           0.;
    temperature    2200;
    duration       25;
    diameter       1.5e-3;
}
```

The only difference with respect to the unsteady case is the duration (which in steady state conditions means number of iterations)

Running the case

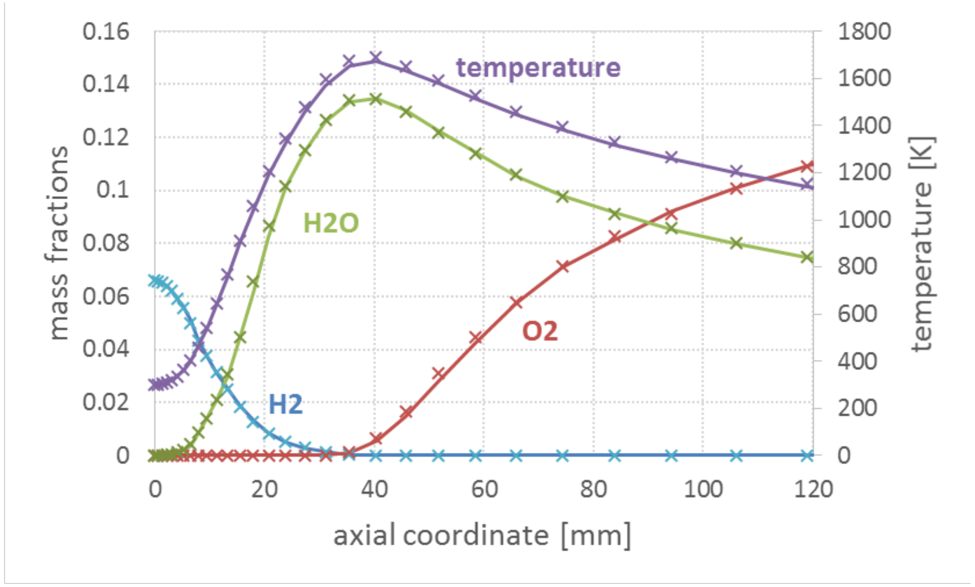
1. Go to the following folder:
   `Training/Solvers/laminarSolverSteady/run/coflowFlame/01-global-1step`
2. Type `blockMesh`
3. Type `laminarSolverSteady > log &`
4. The simulation takes less than 1 min on a single core



```
> gnuplot
> load 'gnuplot.residuals'
```

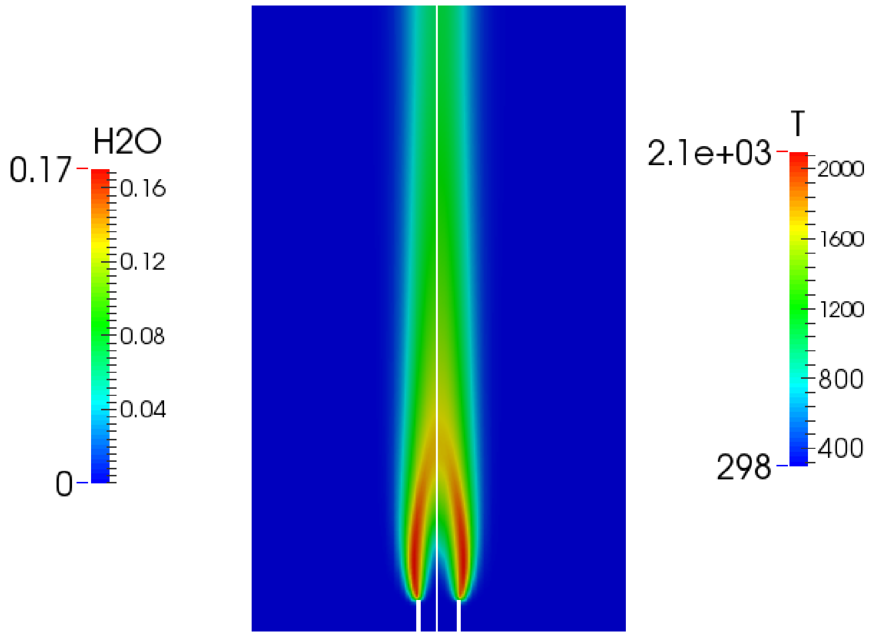
Results

Solution along the axis
Symbols: steady state solver (2000 iterations)
Lines: unsteady solver (@ 0.3 s)



```
> postProcess -func sample
```

Solution after 2000 iterations



Refining the solution using a detailed mech

Mechanism preprocessing

We want now refine the solution by using the detailed kinetic mechanism contained in the `PreProcessing/POLIMI_H2_1412`, which has been already preprocessed.

Restarting from previous solution

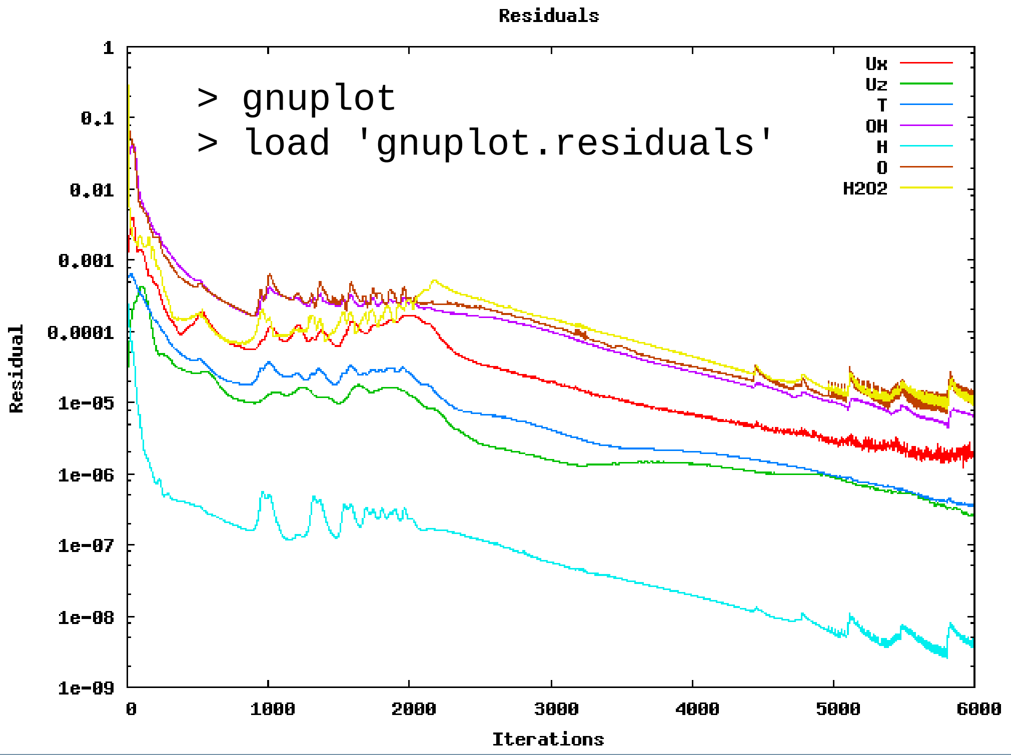
We restart from the last solution (2000 iterations) corresponding to the global, 1-step mechanism

1. Go to the following folder:
   `Training/Solvers/laminarSolverSteady/run/coflowFlame/02-detailed-polimi`
2. Copy the last solution:

```
cp -r ../01-global-1step/2000/ 0/
cp ../01-global-1step/0/Ydefault 0/
rm –r 0/uniform
```

Running the case

1. Go to the following folder:
   `Training/Solvers/laminarSolverSteady/run/coflowFlame/02-polimi-detailed`
2. Type `blockMesh`
3. Type `laminarSolverSteady > log &`
4. The simulation takes less than 5 min on a single core



```
> gnuplot
> load 'gnuplot.residuals'
```

NOx predictions

Mechanism preprocessing

We want now add NOX predictions by using the detailed kinetic mechanism contained in the `PreProcessing/POLIMI_H2_NOX_1412` (which was already preprocessed)

Restarting from previous solution

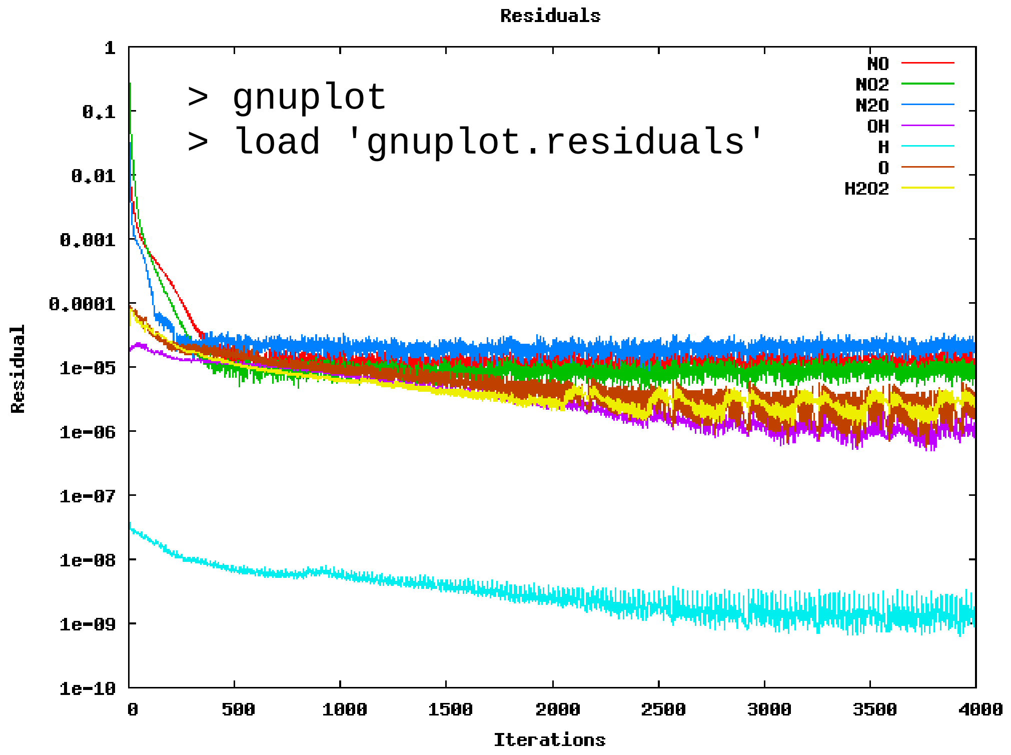
We restart from the last solution obtained with the `POLIMI_H2_NOX_1412` mechanism

1. Go to the following folder:
   `Training/Solvers/laminarSolverSteady/run/coflowFlame/03-detailed-polimi-nox`
2. Copy the last solution:

```
cp -r ../02-detailed-polimi/6000/ 0/
cp ../01-global-1step/0/Ydefault 0/
rm –r 0/uniform
```

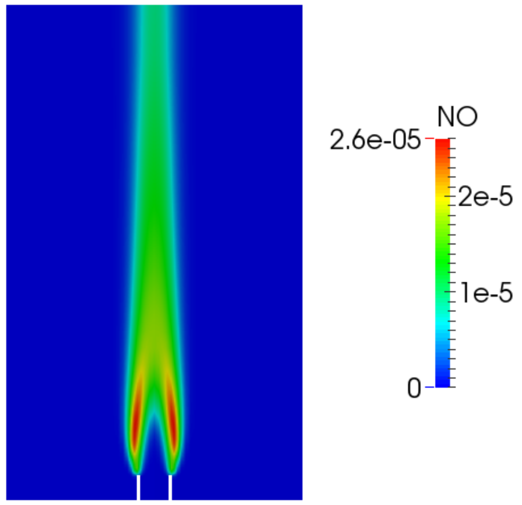
Running the case

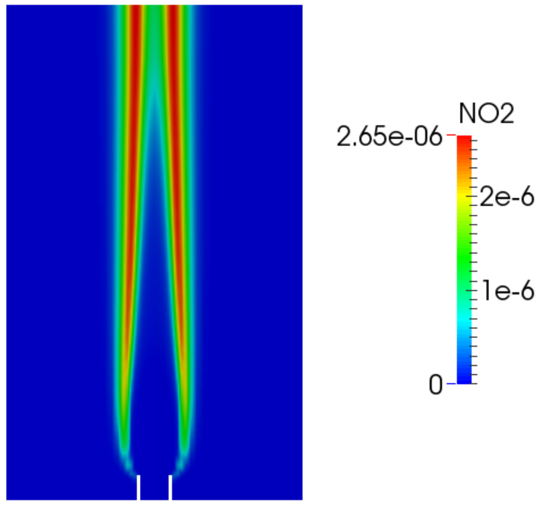
1. Go to the following folder:
   `Training/Solvers/laminarSolverSteady/run/coflowFlame/03-polimi-detailed-nox`
2. Type `blockMesh`
3. Type `laminarSolverSteady > log &`
4. The simulation takes about 5 min on a single core



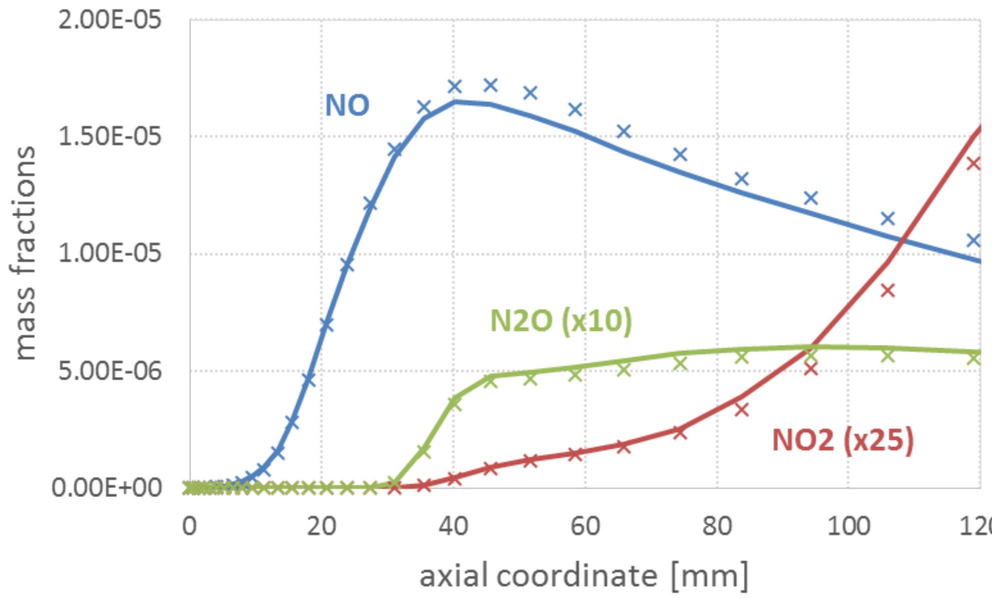
```
> gnuplot
> load 'gnuplot.residuals'
```

Results

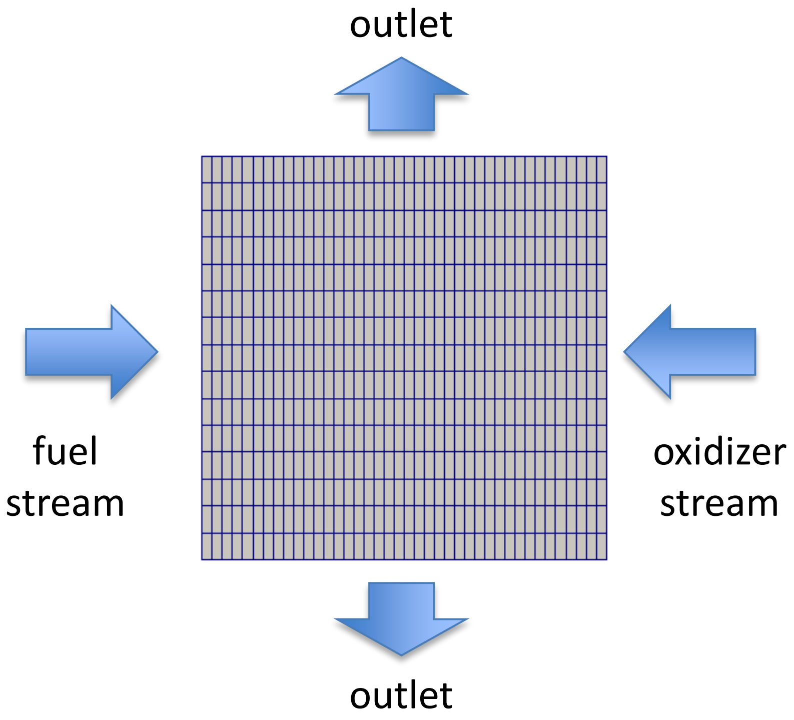




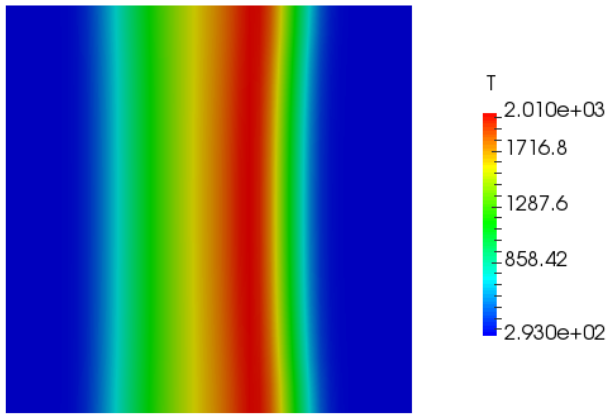
Solution along the axis
Symbols: steady state solver (5000 iterations)
Lines: unsteady solver (@ 0.5 s)



Example: 2D laminar counterflow flame (I)



Steady-state temperature field



The fuel stream **(100% CH4)** and the oxidizer stream **(21% O2, 79% N2)** are injected at ambient temperature (**293 K**) and uniform velocity (**10 cm/s**)

A **2D square domain** (2 x 2 cm) meshed with a structured grid is considered. The adopted mesh (40 x 15) is very coarse and it is here adopted only to have small CPU times.

Example: 2D laminar counterflow flame (II)

Run the simulation (global 1-step mechanism)

1. Go to the following folder: `Training/Solvers/laminarSolverSteady/run/counterFlowFlame2D/01-global-1step`
2. Type: `blockMesh`
3. Type: `laminarSolverSteady > log &`
4. The simulation takes about 5 min on a single core

Example: 2D laminar counterflow flame (III)

Refine the mechanism (GRI3.0 without NOX)

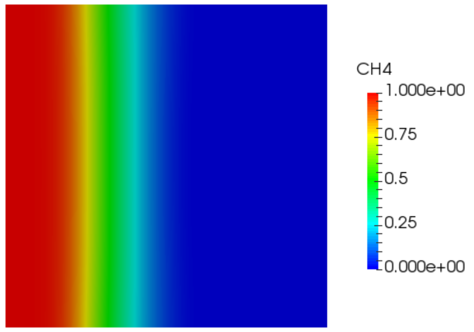
1. Go to the following folder: `Training/Solvers/laminarSolverSteady/run/counterFlowFlame2D/02-gri30-nonox`
2. Type: `blockMesh`
3. Type: `cp -r ../01-global-1step/2000/ 0/`
4. Type: `cp ../01-global-1step/0/Ydefault 0/`
5. Type: `rm –r 0/uniform`
6. Type: `laminarSolverSteady > log &`
7. The simulation takes about 10 min on a single core

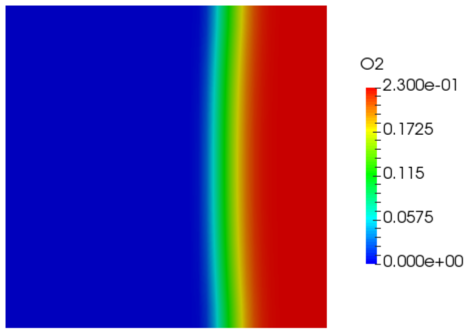
Example: 2D laminar counterflow flame (III)

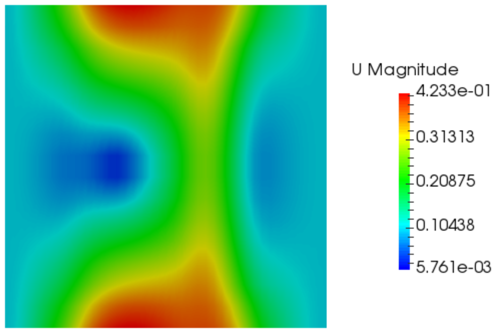
Refine the mechanism (GRI3.0, including NOX chemistry)

1. Go to the following folder: `Training/Solvers/laminarSolverSteady/run/counterFlowFlame2D/03-gri30`
2. Type: `blockMesh`
3. Type: `cp -r ../02-gri30-nonox/2000/ 0/`
4. Type: `cp ../01-global-1step/0/Ydefault 0/`
5. Type: `rm –r 0/uniform`
6. Type: `laminarSolverSteady > log &`
7. The simulation takes about 15 min on a single core

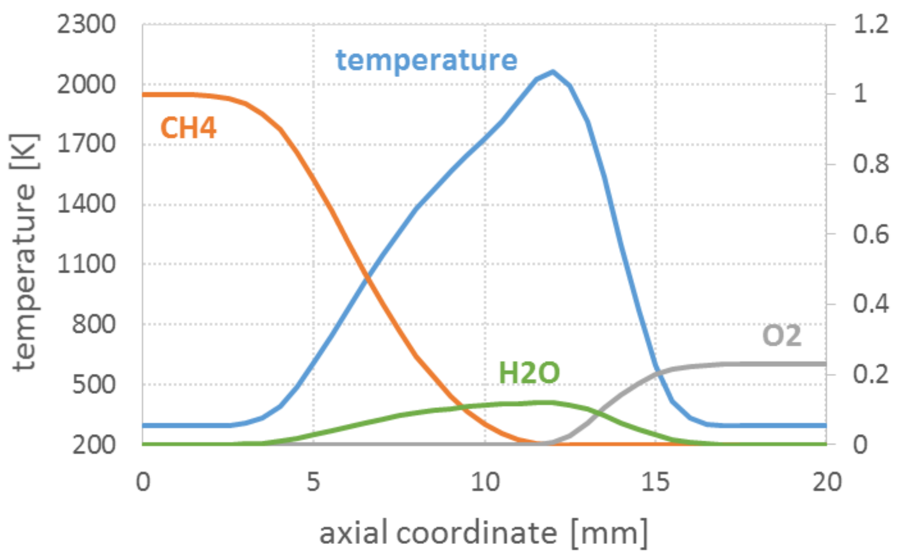
Example: 2D laminar counterflow flame (III)

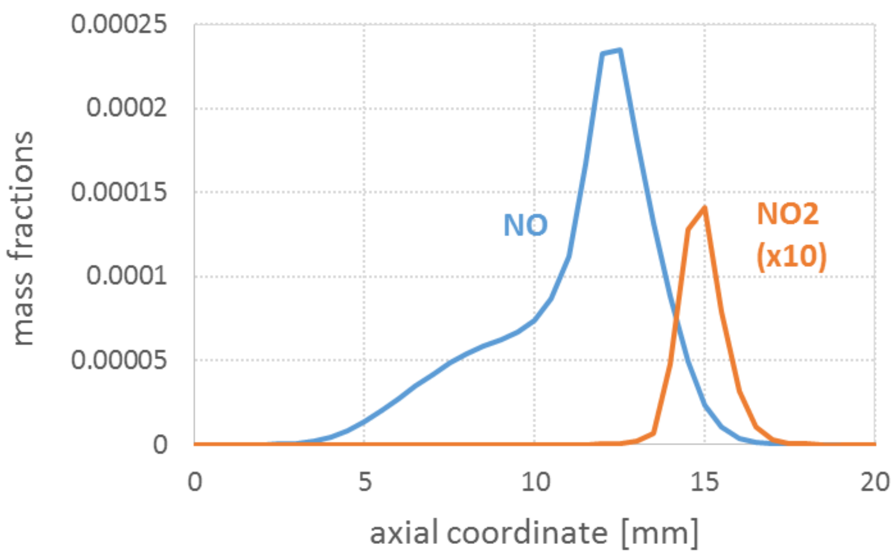






Steady-state centerline profiles





Next steps

1. **Chemical step**
   - Energy equation as differential equation
   - External ODE solvers (CVODE, DASPK, etc.)
   - Native OpenSMOKE++ solvers
   - Intel MKL® Libraries

2. **Transport step**
   - Inclusion of thermodiffusion (i.e. Soret effect)
   - Inclusion of enthalpy fluxes due to preferential mass diffusion
   - Inclusion of correction diffusion of mass diffusion fluxes

3. **Numerical Algorithm**
   - Strang splitting variants
   - Consistent operator splitting
   - Predictor/Corrector policy for steady state solver

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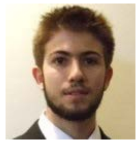
Paulo Debiagi

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OpenSMOKE++ Development

Cuoci, A., Frassoldati, A., Faravelli, T., Ranzi, E., *OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms* (2015) Computer Physics Communications, 192, pp. 237-264, DOI: 10.1016/j.cpc.2015.02.014

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