6th Two-Day Meeting on Propulsion Simulations using OpenFOAM technology

Accelerating CFD simulations of reactive flows through Cell Agglomeration and Adaptive Chemistry techniques

Alberto Cuoci

Chemical Reaction Engineering
and Chemical Kinetics

Department of Chemistry, Materials,
and Chemical Engineering “G. Natta”

Combustion and detailed kinetics

Real fuels and surrogates

synergistic effects among the different components

Biofuels

bioalcohols, biodiesel, green diesel, bioethers

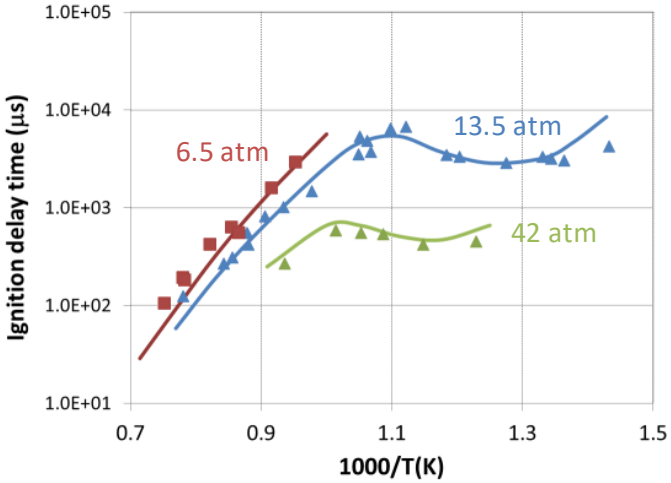
Pollutant emissions

NOx, SOx, PAHs, soot

Complex phenomena

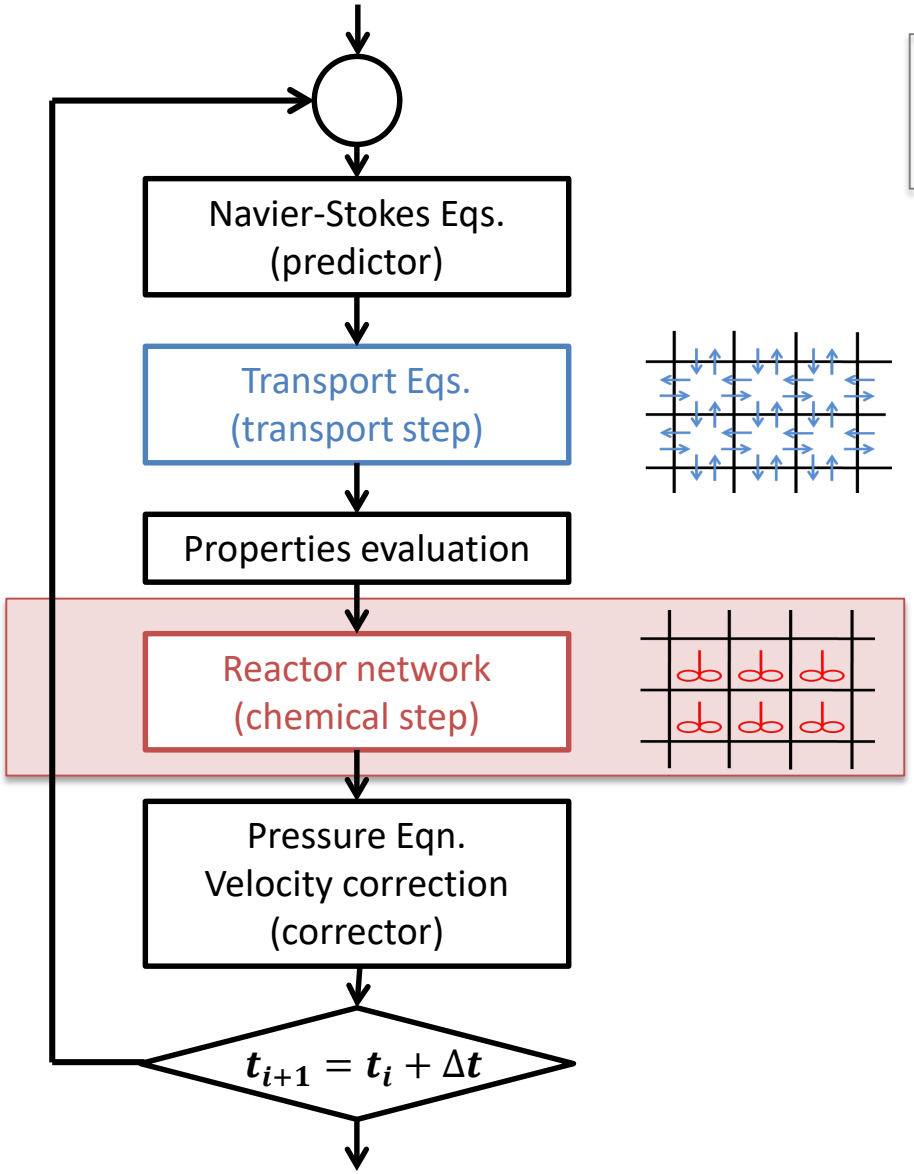
Chemical instabilities, NTC, etc.

Negative temperature Coefficients (NTC)



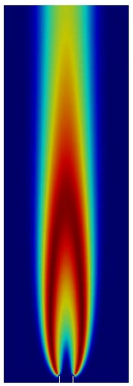
Experimental data from:
Ciezki H.K. and Adomeit G., *Shock-tube investigation of self-ignition of n-heptane-air mixtures under engine relevant conditions*, Combustion and Flame 93 p. 421–433 (1993)

Operator splitting: transport vs chemistry

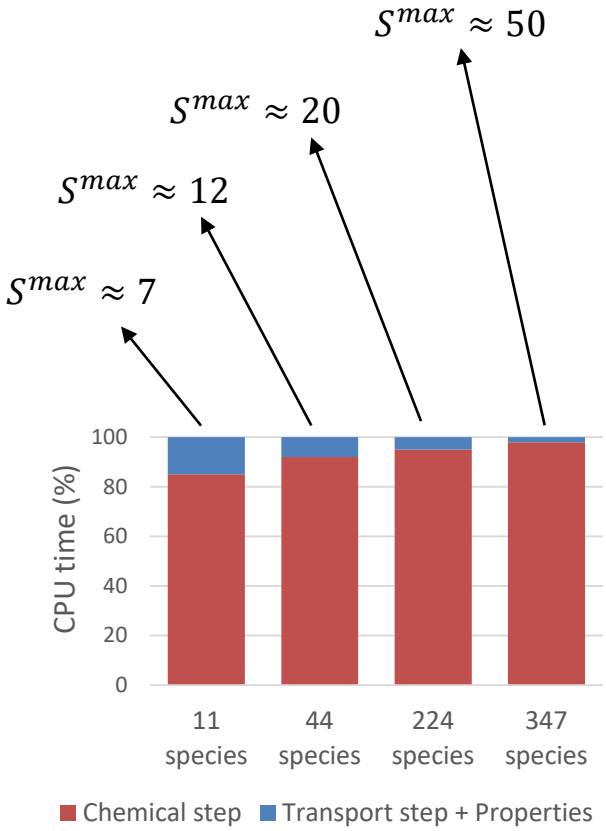


Maximum theoretical speed-up:

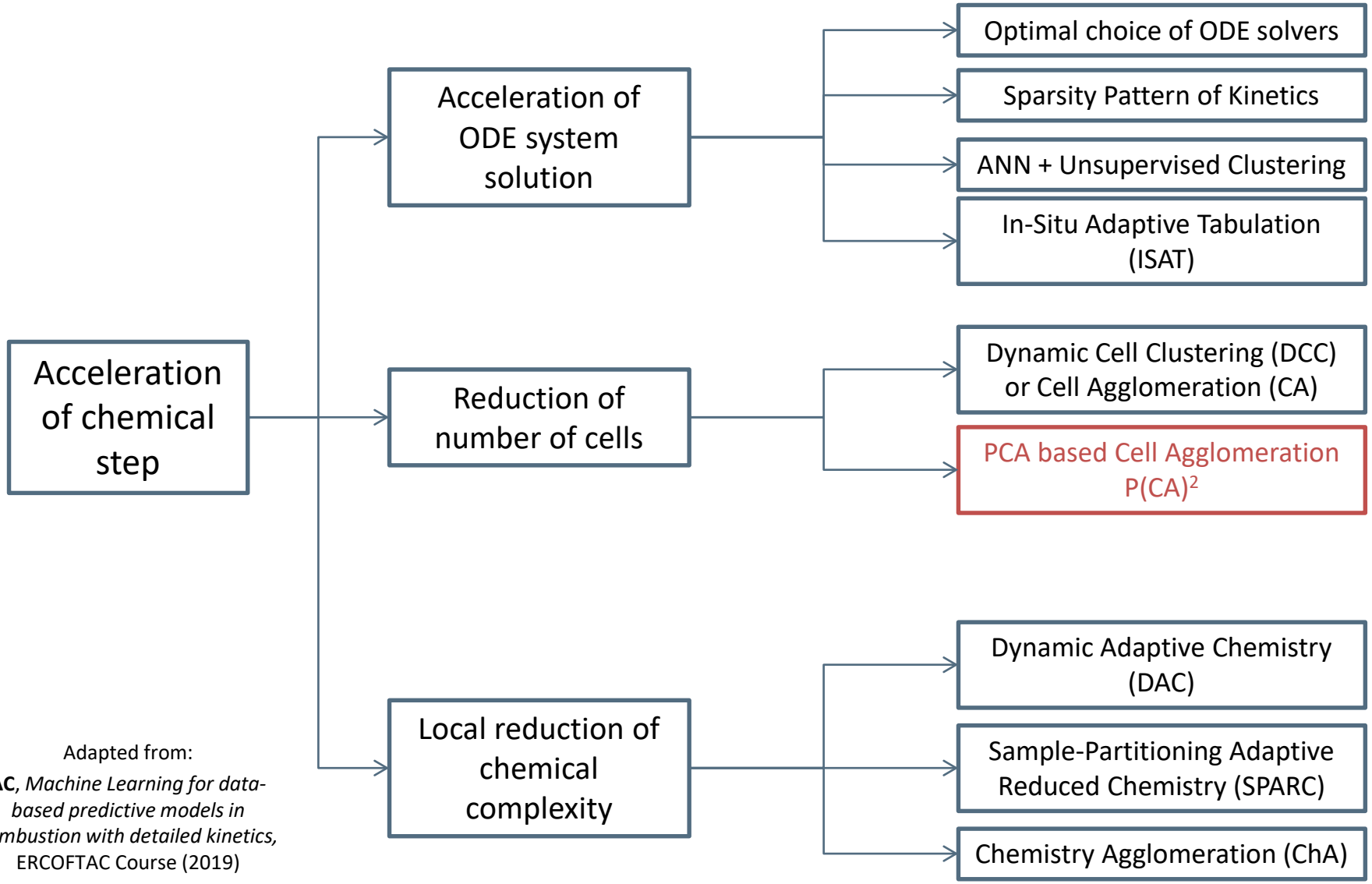
$$S^{max} = \frac{1}{1 - C_{chem}}$$



Pulsating laminar coflow flame



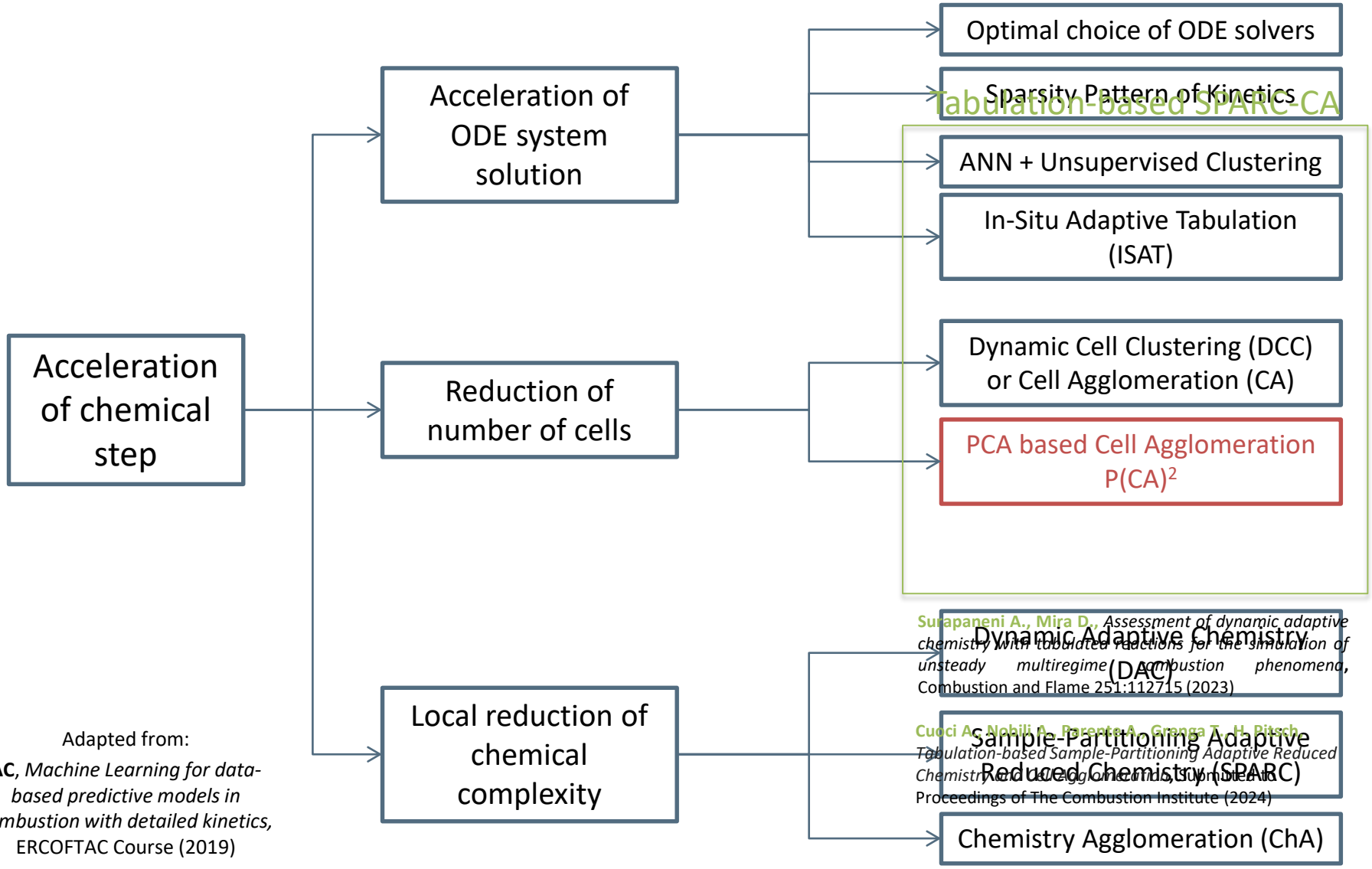
Acceleration of chemical step (I)



Adapted from:

AC, *Machine Learning for data-based predictive models in combustion with detailed kinetics,* ERCOFTAC Course (2019)

Acceleration of chemical step (II)



Adapted from:

AC, *Machine Learning for data-based predictive models in combustion with detailed kinetics*, ERCOFTAC Course (2019)

Surapaneni A., Mira D., *Assessment of dynamic adaptive chemistry with tabulated reactions for the simulation of unsteady multiregime combustion phenomena*, Combustion and Flame 251:112715 (2023)

Cuoci A., Nobili A., Parente A., Granga T., H. Pitsch, *Tabulation-based Sample-Partitioning Adaptive Reduced Chemistry Approach Coupled with CFD*, Submitted to Proceedings of The Combustion Institute (2024)

Outline

1. P(CA)^2: PCA-based Cell Agglomeration P(CA)^2

- Dynamic Cell Agglomeration and PCA
- Pulsating laminar coflow flame

2. Tabulation-based SPARC-CA

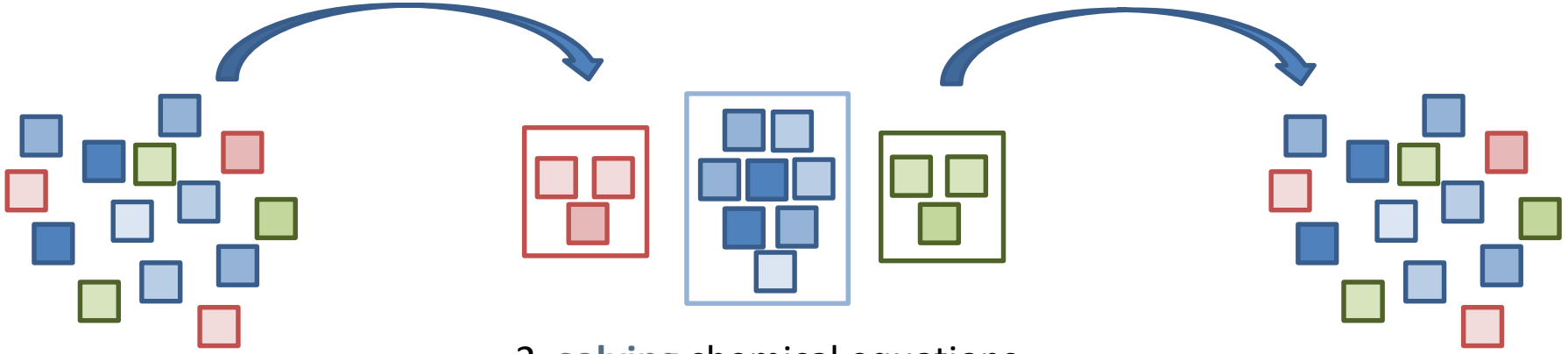
- Temporally-evolving planar jet-flame
- 2D turbulent non-premixed flame including soot chemistry

Dynamic Cell Agglomeration (DCA)

Dynamic Cell Agglomeration (DCA) dynamically agglomerates regions of the domain that have **similar thermochemical conditions**.

1. **clustering** similar cells into clusters

3. **mapping** the cluster-averaged solution back to the individual cells



2. **solving** chemical equations based on cluster averaged state variables

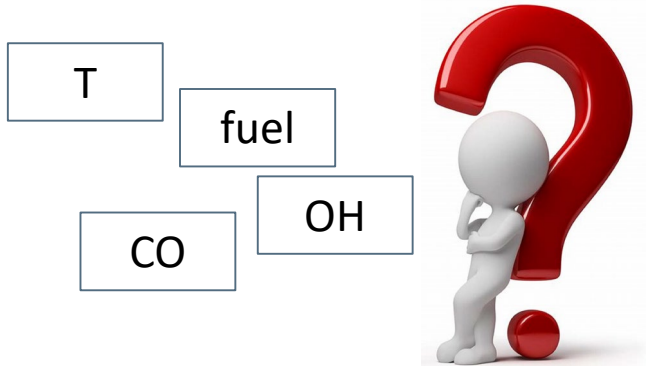
Liang et al., Combustion Science and Technology 181(11), p.1345-1371 (2009)

Clustering: selection of relevant *features*

How to define/identify **similar thermochemical conditions**?

Selection of ***features***

A natural choice is **temperature** and a limited number of **key-species**



Problems!

1. most abundant species are **not always the optimal choice**
2. **slowly-forming pollutants** (such as NOx or soot) make the selection of proper features more complex
3. it is difficult to identify **a priori** the optimal subset of species

Dynamic identification of features: PCA

PCA (Principal Component Analysis) to dynamically identify the optimal set of relevant features, evolving in time, following the evolution of combustion process

Current complete **thermochemical state**

$$\mathbf{X} = \begin{bmatrix} T_1 & Y_{1,1} & \dots & Y_{1,NS} \\ T_2 & Y_{2,1} & \dots & Y_{2,NS} \\ \dots & \dots & \dots & \dots \\ T_N & Y_{N,1} & \dots & Y_{N,NS} \end{bmatrix}$$

normalization

PCA

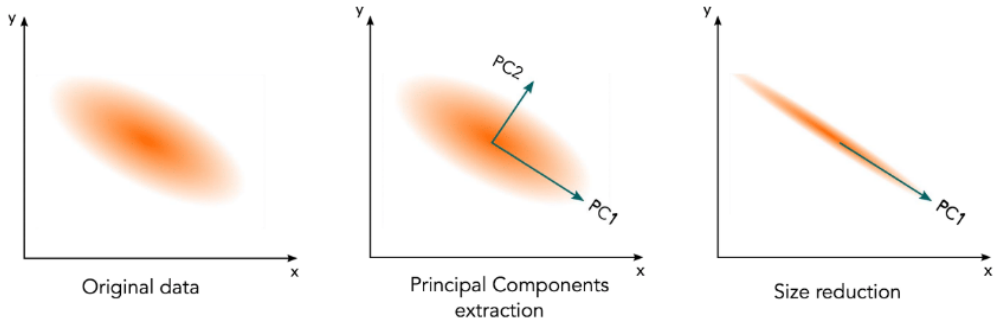
Principal Components

eigenvectors obtained from the decomposition of the covariance matrix

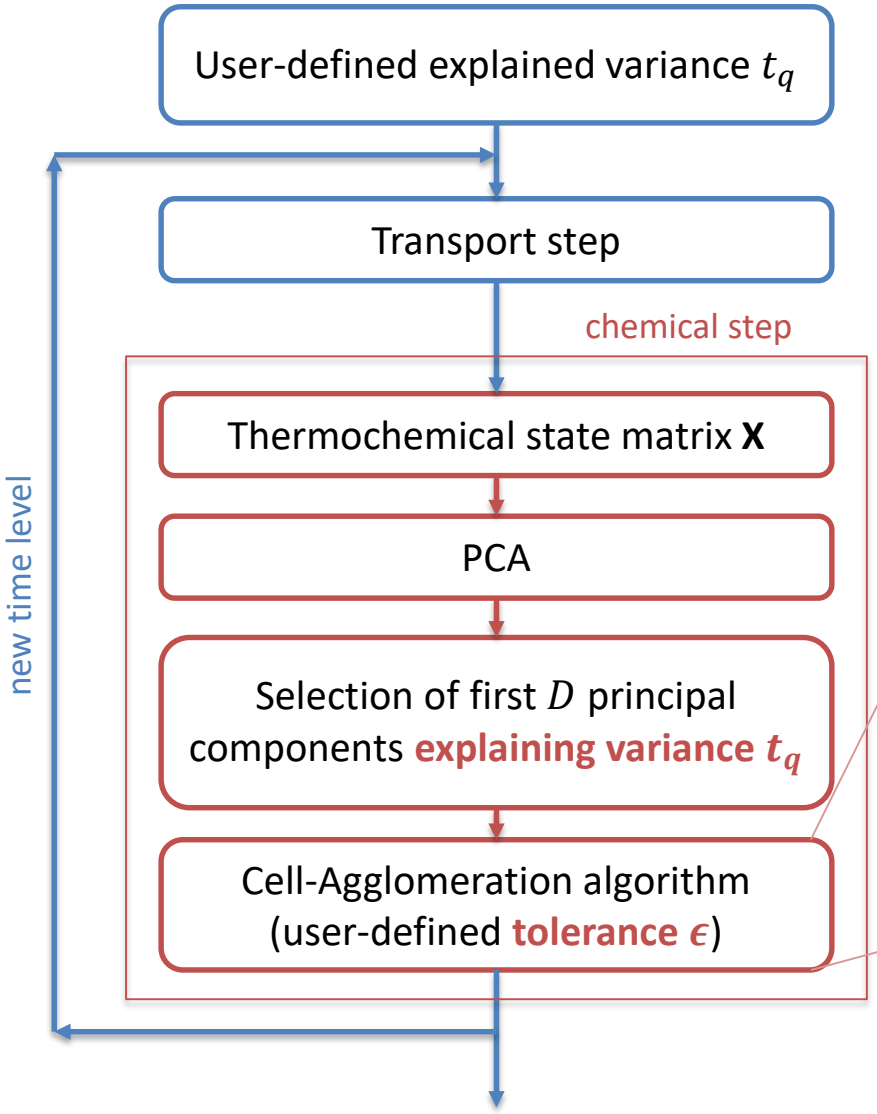
$Y_{i,j}$ =mass fraction of species j in cell i

Input data matrix:
N observations of $NS + 1$ variables

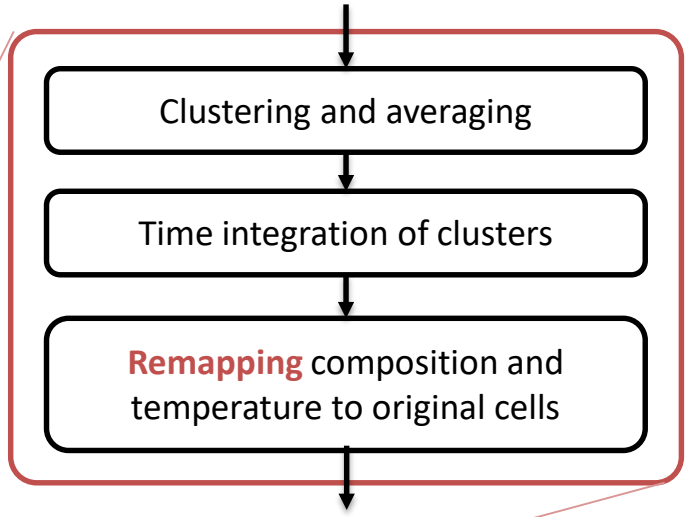
N = number of cells
NS = number of species



P(CA)²: PCA-based Cell Agglomeration



By fixing t_q, the number D of principal components to be used is **automatically determined**.



F. Perini, R.D. Reitz, *Computationally efficient dimension reduction of combustion chemistry via Principal Components Analysis based domain partitioning*, Frontiers in Computational Physics: Energy Sciences Zurich, Switzerland June 5, 2015

Pulsating laminar coflow flame

ISF F3 flames

Internal diameter: 4 mm
Velocities: 35 cm/s
Fuel composition: 80% C2H4 + 20% N2

Artificially imposed sinusoidal fluctuations of fuel stream velocity

Amplitude: 90%, Frequency: 10 Hz

Kinetic mechanism

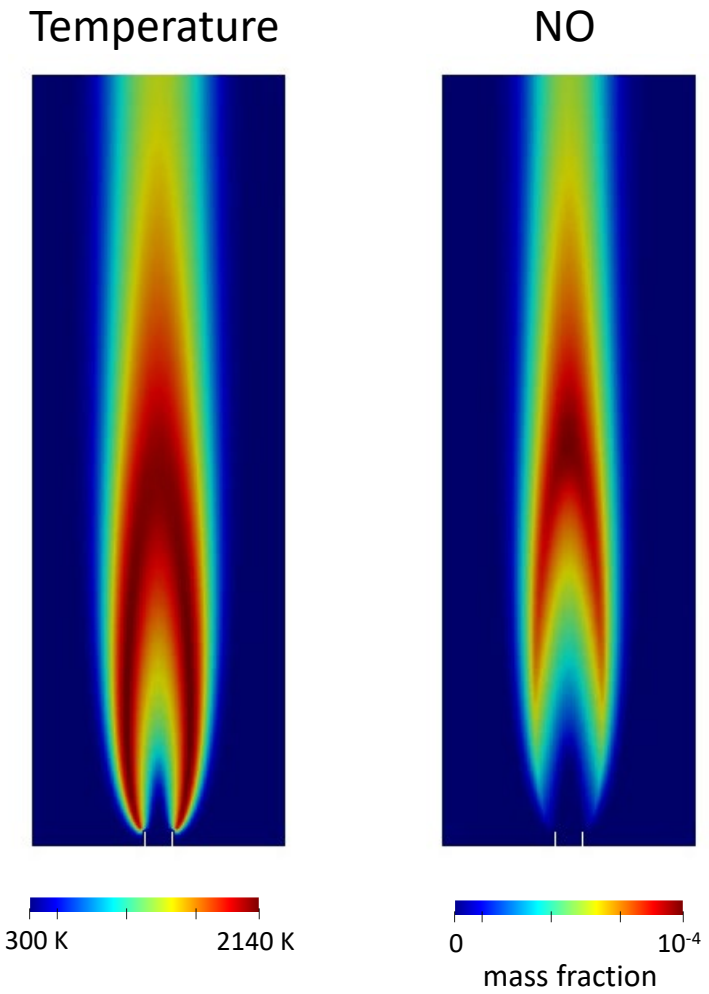
224 species and 5980 reactions
NOx chemistry included
https://creckmodeling.chem.polimi.it

Computational domain

2D region (55 x 120 mm)
~25,000 cells

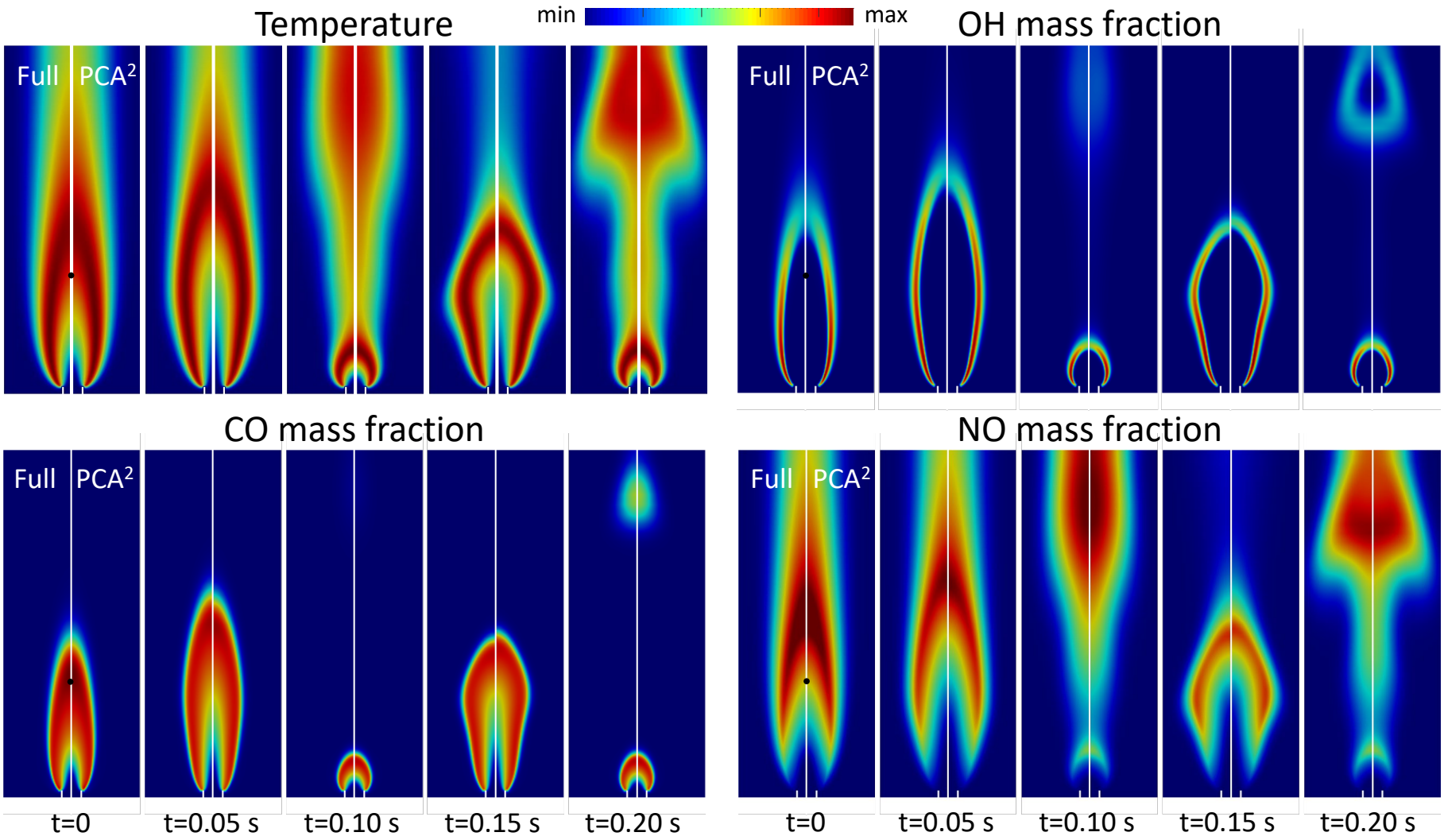
Solver

laminarSMOKE++ (based on OpenFOAM 10)
https://github.com/acuoci/laminarSMOKE



Smooke M.D., Long M.B., Connelly B.C., Colket M.B., Hall R.J., Combustion and Flame, 143(4), p. 613-628 (2005)

Example: $t_q = 50\%$ and $\epsilon = 0.010$

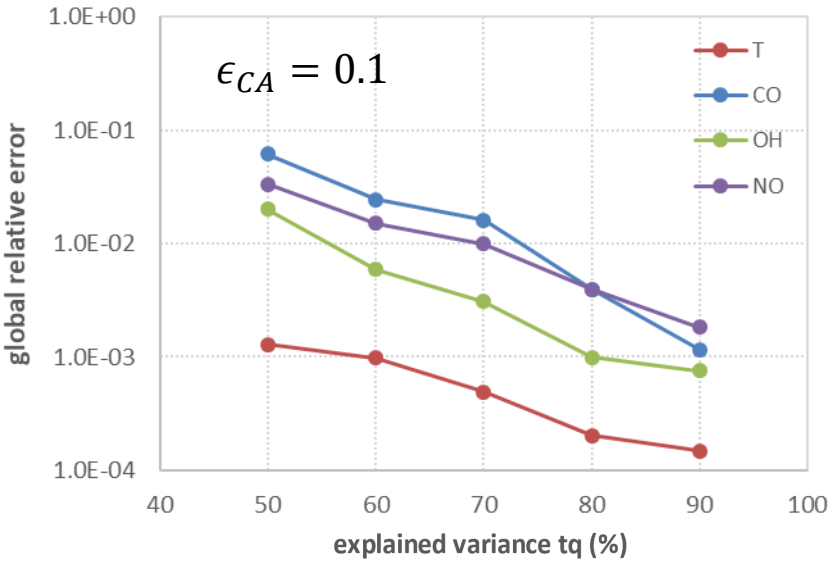


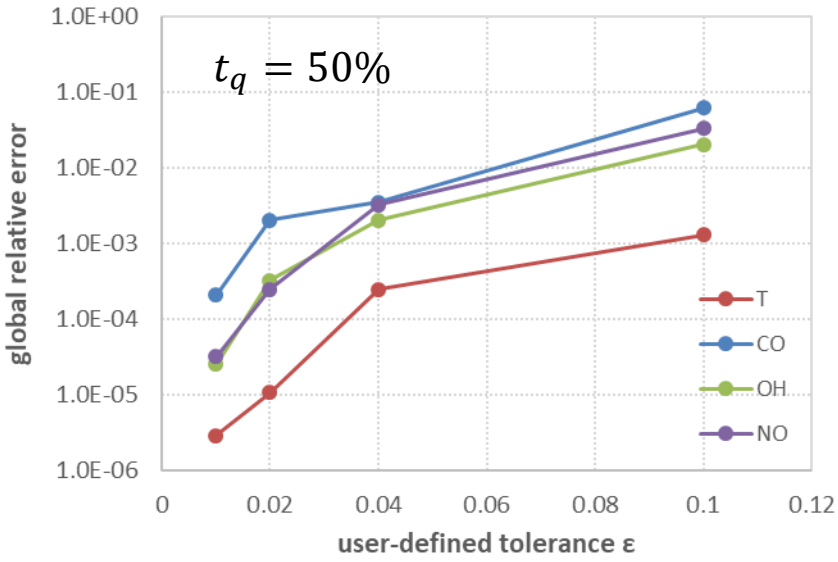
https://www.kaggle.com/datasets/albertocuoci/laminar-coflow-flame-isf-f3a-pulsating

Global relative error

User-defined parameters

1) Explained level of variance: t_q
2) CA (Cell Agglomeration) tolerance: ϵ_{CA}

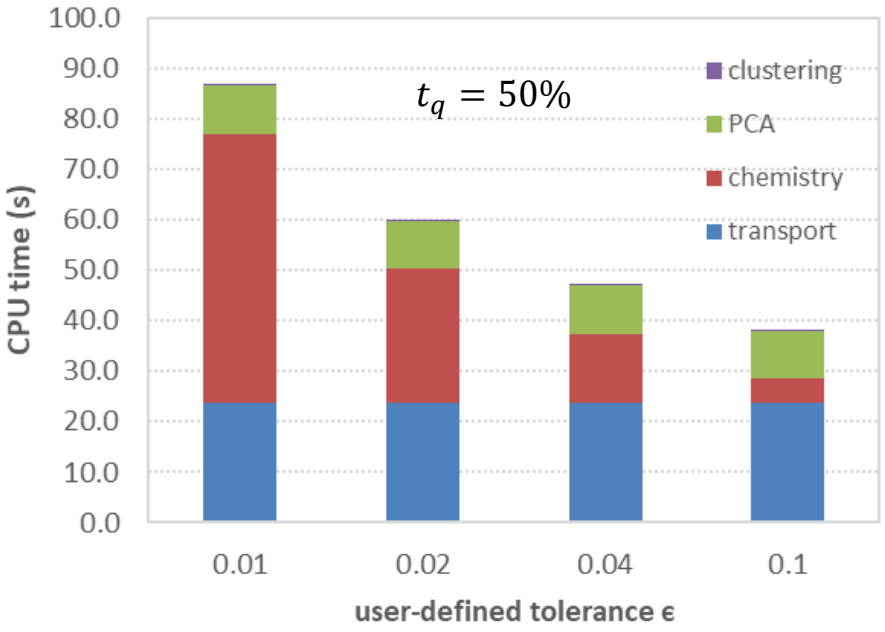


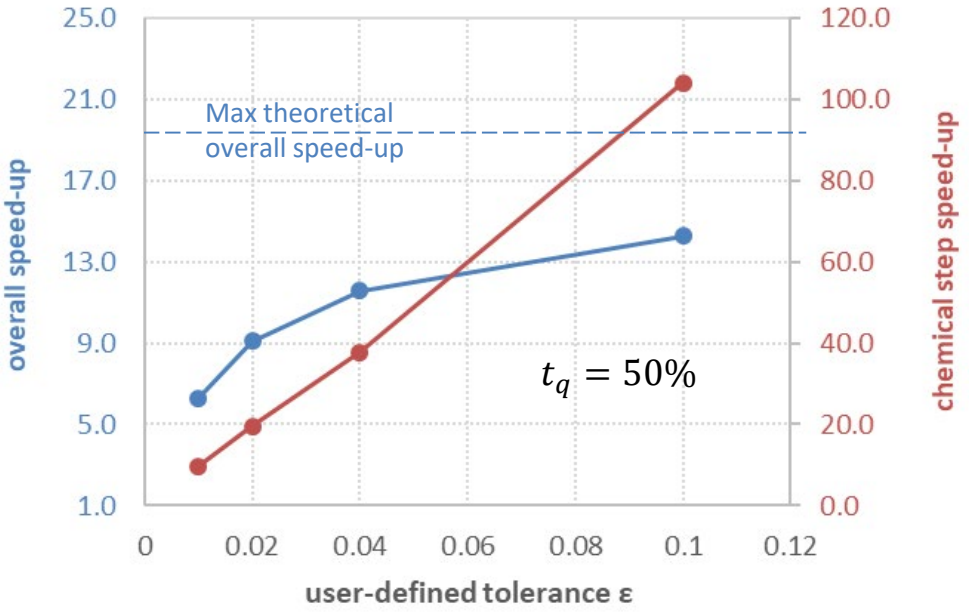


Computational performances

CRECK PAH mechanism (224 species)

Chemistry CPU time: ~95%





Outline

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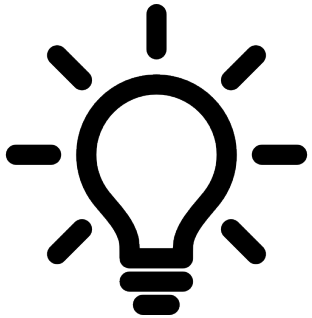
SPARC: Sample-Partitioning Adaptive Reduced Chemistry

(Dynamic) Adaptive Reduced Chemistry (ARC)

The **computational overhead** needed for the on-the-fly reduction of the mechanism can be significant, strongly reducing the efficiency of DAC



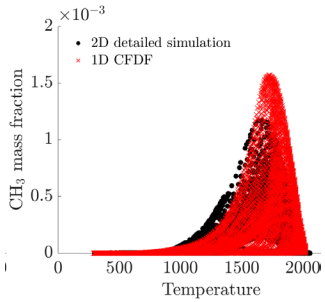
Pre-partitioning

- A **library of reduced mechanisms** is built in a pre-processing step, covering the composition space which is expected to be visited by the reactive systems of interest.
- During the CFD simulation, before carrying out the chemical step, **each cell is classified**, i.e., the reduced mechanism available in the library is identified "instantaneously" and applied

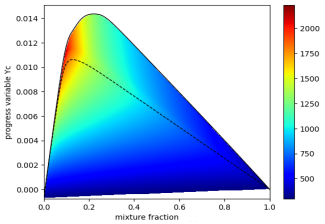
D.A. Schwer, P. Lu, and W.H. Green, Combustion and Flame, 133(4):451-465, 2003
Y. Liang, S.B. Pope, and P. Pepiot, Combustion and Flame, 162(9), 2015
D'Alessio G., Parente A., Stagni A., Cuoci A., Combustion and Flame, 211, p. 68-82, 2020

Tabulation-based SPARC-CA: Overall Methodology

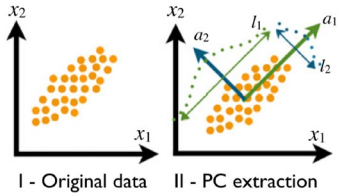
1. Pre-processing phase (SPARC)



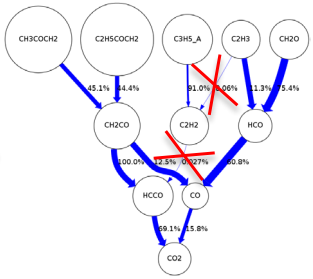
Dataset generation



Dataset re-mapping (or off-line classification)



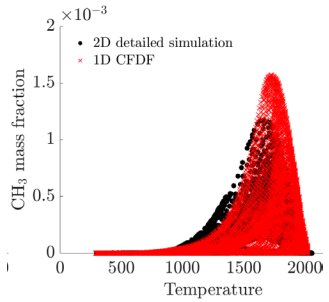
Partitioning



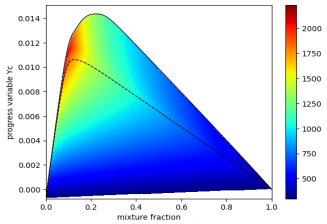
Reduced mechanisms

Tabulation-based SPARC-CA: Overall Methodology

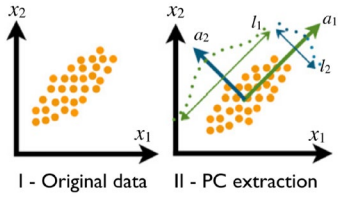
1. Pre-processing phase (SPARC)



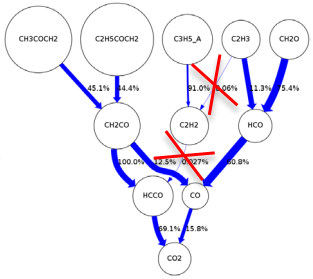
Dataset generation



Dataset re-mapping (or off-line classification)

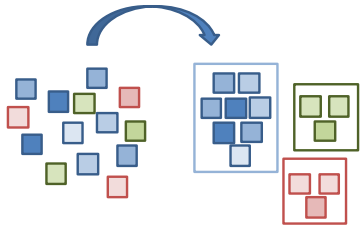


Partitioning

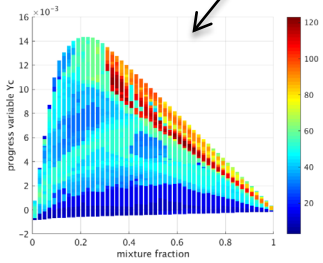


Reduced mechanisms

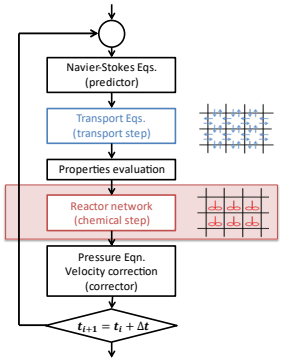
2. CFD simulation phase (CA)



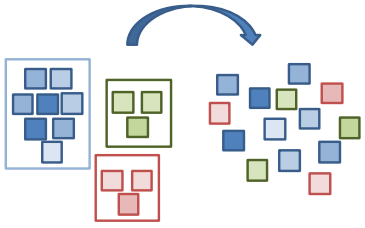
Cell agglomeration (CA)



On-the-fly classification



Numerical integration

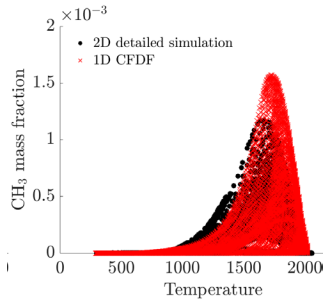


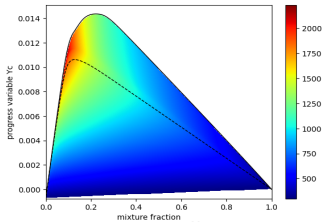
Back-mapping

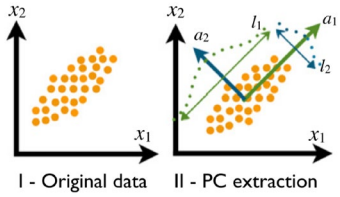
Tabulation-based SPARC-CA: Overall Methodology

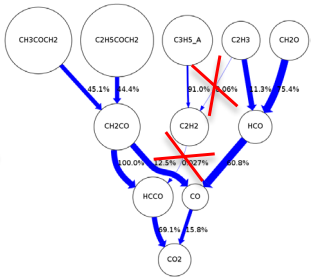
1. Pre-processing phase (SPARC)

Kinetic Reduction tolerance ϵ_{DRG}









Dataset generation

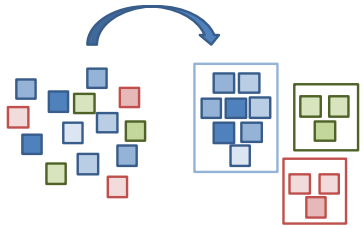
Dataset re-mapping (or off-line classification)

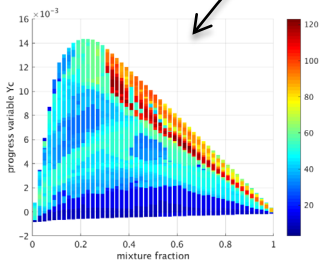
Partitioning

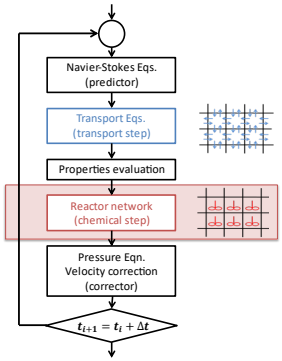
Reduced mechanisms

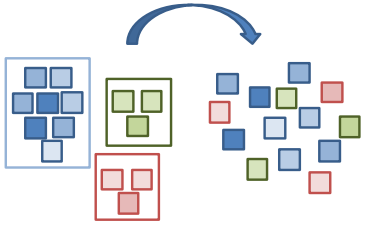
2. CFD simulation phase (CA)

Cell Agglomeration tolerance ϵ_{CA}









Cell agglomeration (CA)

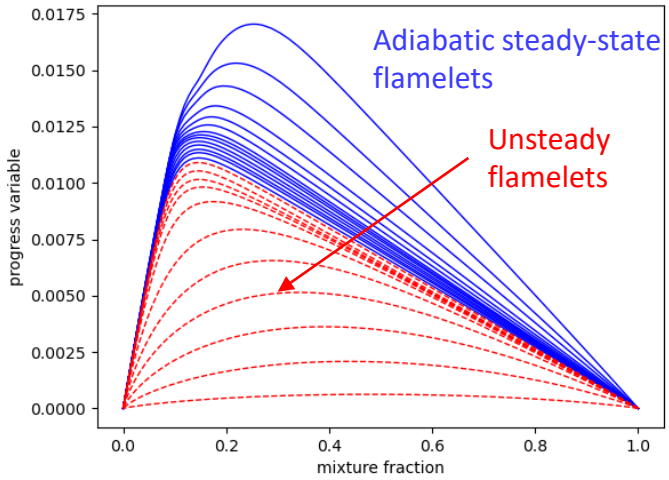
On-the-fly classification

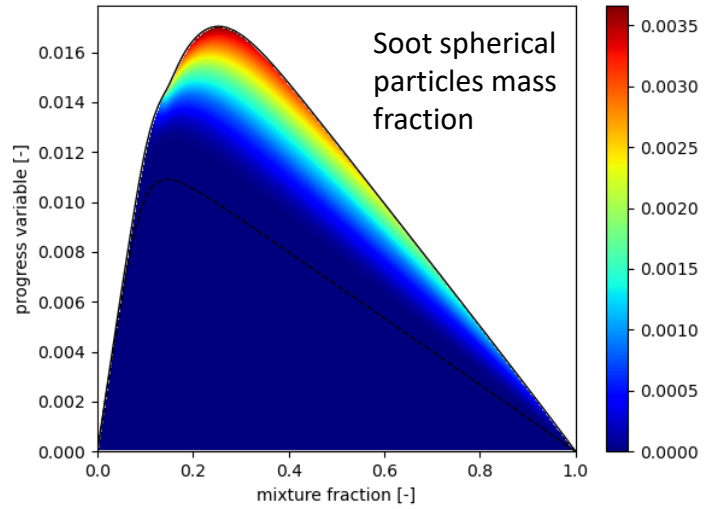
Numerical integration

Back-mapping

Example of training dataset preparation

Fuel: C2H4/N2 0.90/0.10





Dataset generation

the training dataset is constructed from steady and unsteady adiabatic diffusion flamelets

Dataset re-mapping

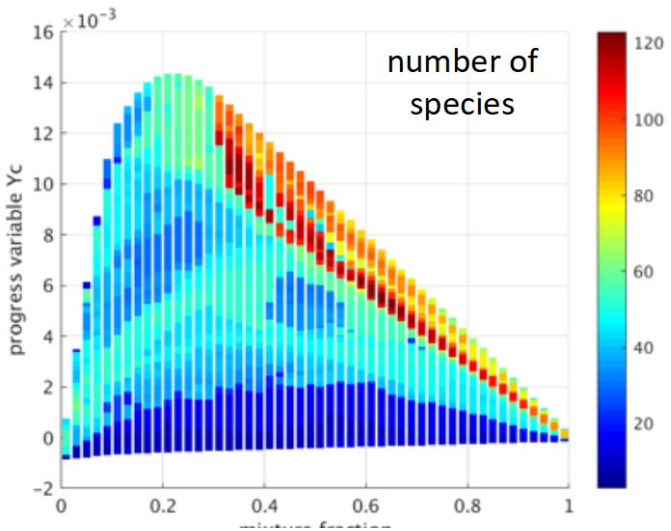
the generated database is re-mapped over two control variables, the mixture fraction ξ and the progress variable Y_C

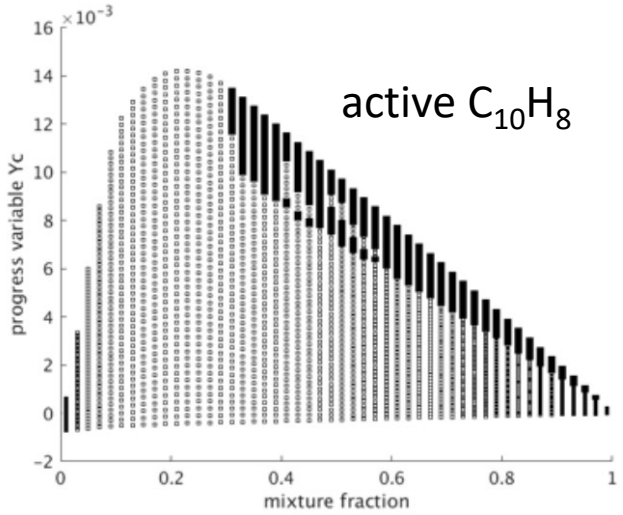
$$Y_C = \alpha_{CO2} X_{CO2} + \alpha_{H2O} X_{H2O} + \alpha_{CO} X_{CO} + \cdots$$

Example of lookup table generated using a detailed kinetic mechanism including the soot chemistry via a Discrete Sectional Method (DSM)

Reduced chemistry library

Original mechanism:
226 species, ~10,400 reactions





Partitioning

A clustering algorithm in the $\xi - Y_C$ space is adopted to identify continuous regions (i.e., clusters) having similar kinetic behavior

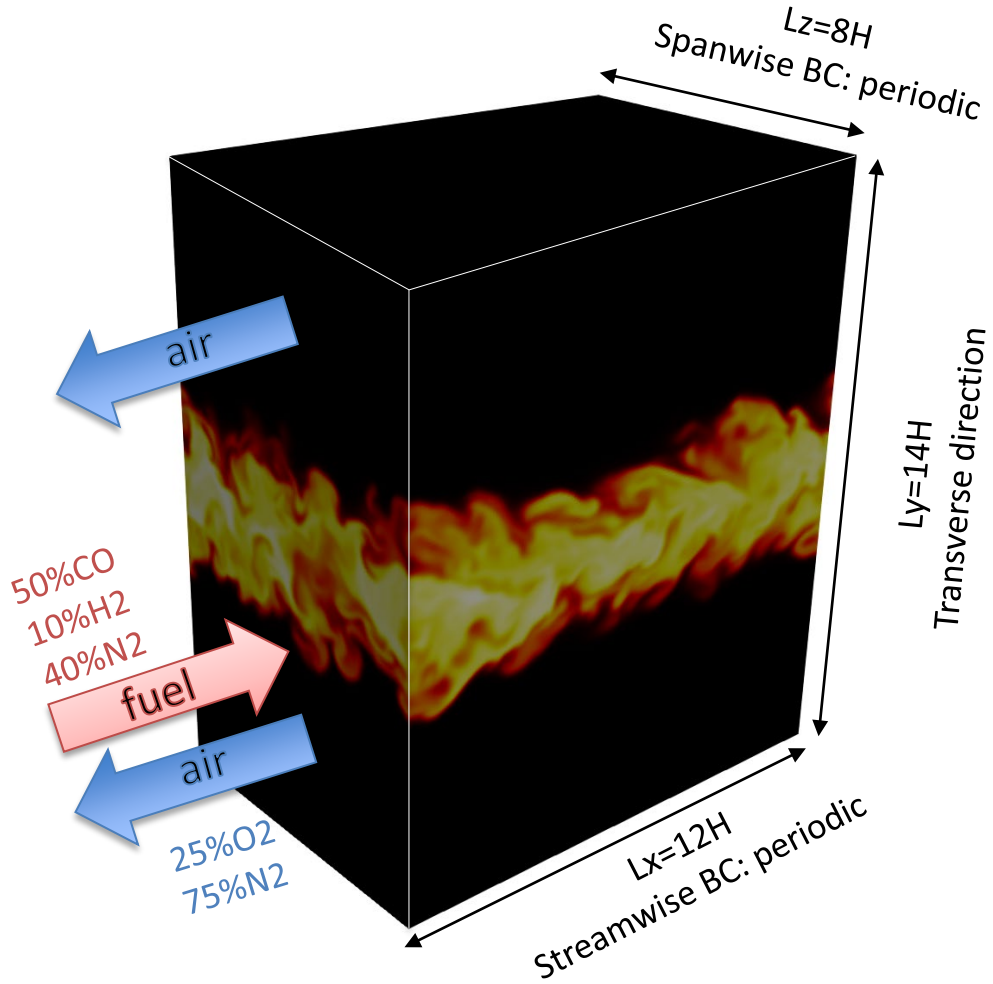
Surapaneni A., Mira D., Combustion and Flame 251:112715 (2023)

Generation of reduced mechanisms

For each cluster of the dataset, a reduced mechanism is generated via the Directed Relation Graph (DRG) method

P. Pepiot-Desjardins, H. Pitsch, Combustion Theory and Modelling 12, 1089-1108 (2008)

Temporally-evolving planar jet-flame



H = 1.37 mm
Re = 9079
tj = 4.96 µs

U = 276.4 m/s
Da = 0.011
Ma = 0.30

2D Mesh
Δx = 30 µm or 45 µm
Mesh: 548x640 or 365x426
Cells: ~350k or ~156k

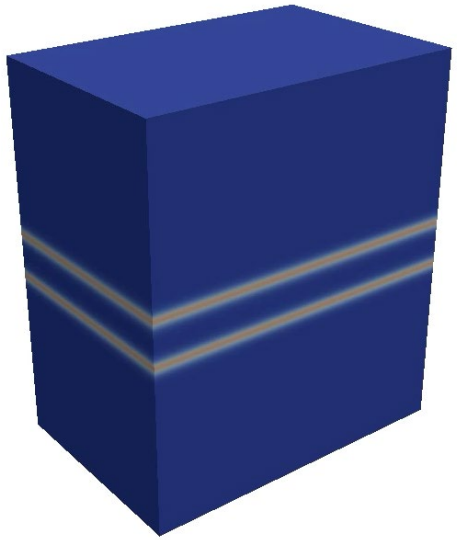
Quasi-DNS (3D)
Δx = 90 µm
Mesh: 182 x 214 x 122
Cells: ~4.75M

Kinetic mechanisms
Detailed H2/CO + NOx mechanism by **CRECK:**
57 species and 385 reactions
https://creckmodeling.chem.polimi.it

Solver
laminarSMOKE++ (based on OF-10)
Time discretization: 2nd order backward Euler
Space discretization: OF *cubic* scheme

Hawkes et al., Scalar mixing in direct numerical simulations of temporally evolving plane jet flames with skeletal CO/H2 kinetics, Proceedings of the Combustion Insitute, 31, p. 1633-1640 (2007)

Global relative error

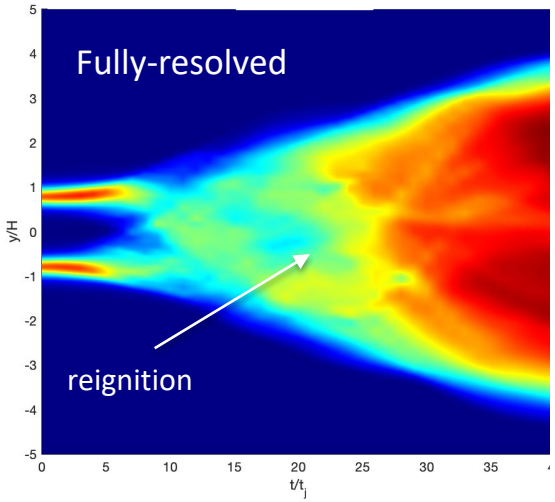


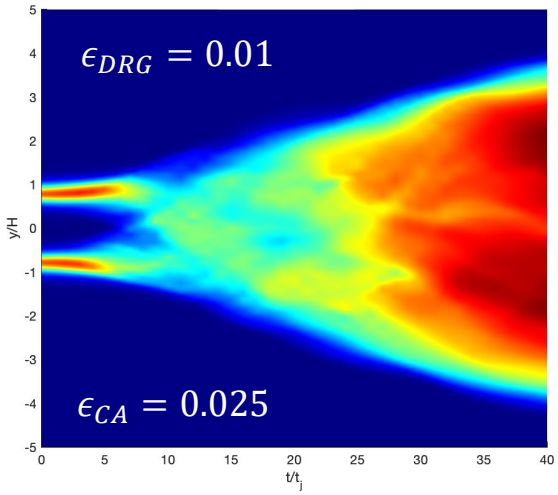
Relevant fields (temperature and mass fractions of species) are **spatially-averaged** over x-z planes

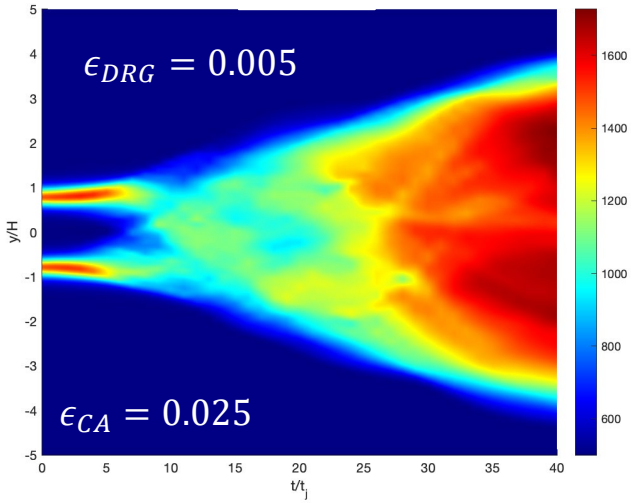
$$\varepsilon = \frac{1}{N_Y N_T} \sum_{k=1}^{N_T} \sum_{i=1}^{N_Y} \frac{\left|\psi_{k,i}^{CA} - \psi_{k,i}\right|}{\psi_{max}}$$

$\psi_{k,i}$ spatially-averaged fully-resolved solution at y_i at time k

$\psi_{k,i}^{CA}$ spatially averaged CA-based solution at y_i at time k



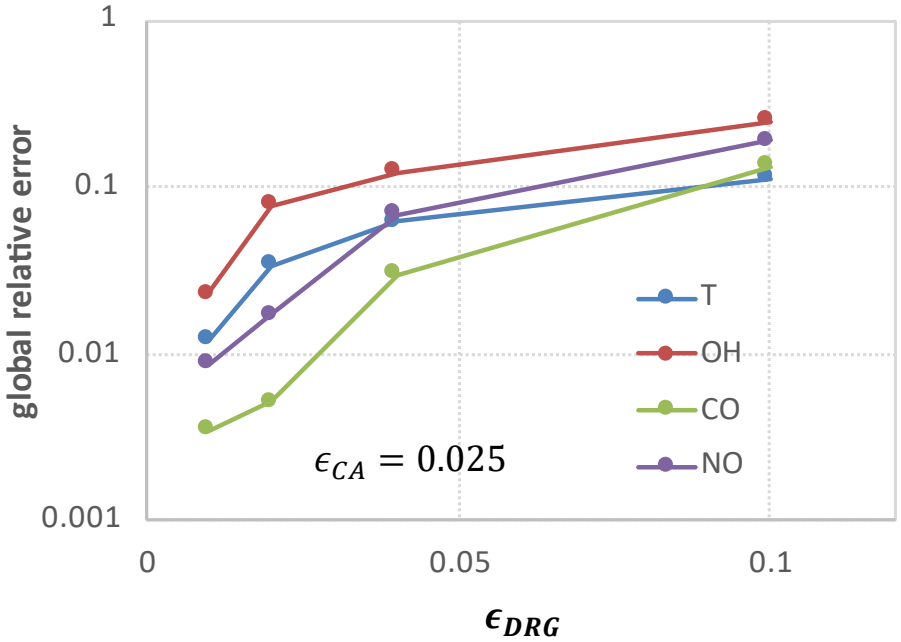


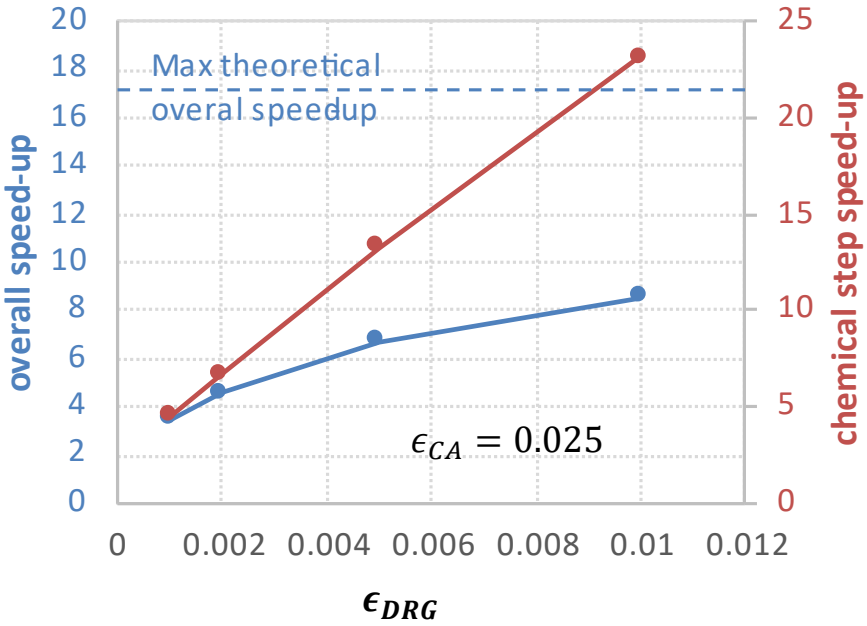


Computational performances

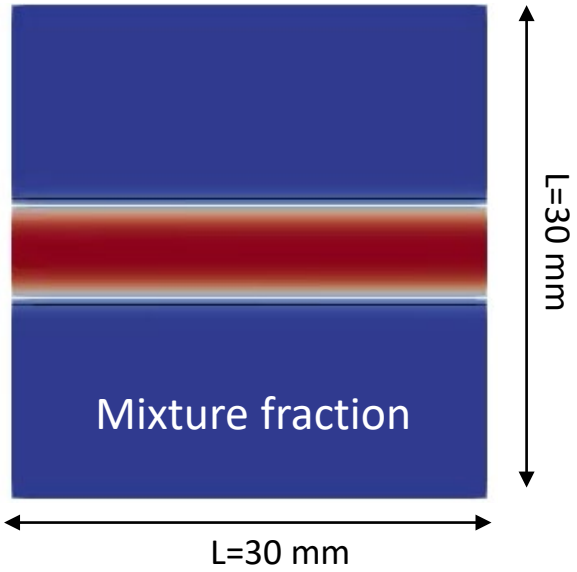
CRECK2003-NOX mechanism (57 species)

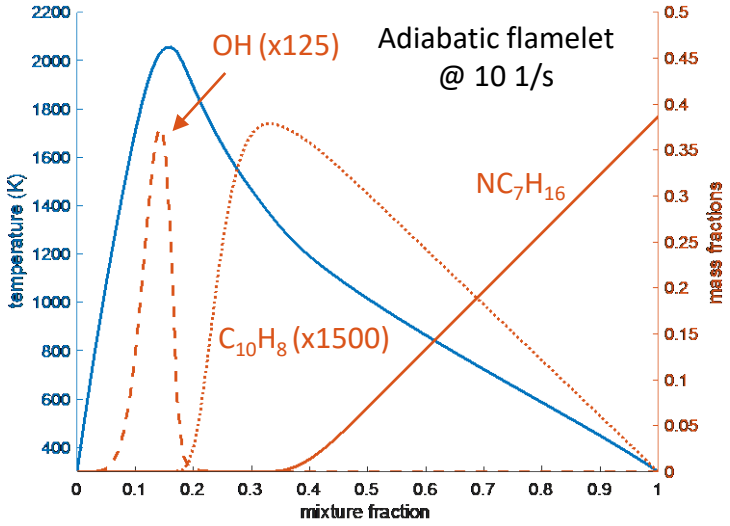
Chemistry CPU time: 93%





2D turbulent non-premixed flame





Quasi-DNS (2D Mesh)

Δx = 75 µm
Mesh: 400 x 400
Cells: 160k
Simulation time: 30 ms (max Courant number: 0.2)
Boundary conditions: periodic

Kinetic mechanism

CRECK HT-PRF + Soot **(Discrete Sectional Method)**:
226 (pseudo-)species, ~10,400 reactions

Numerical details

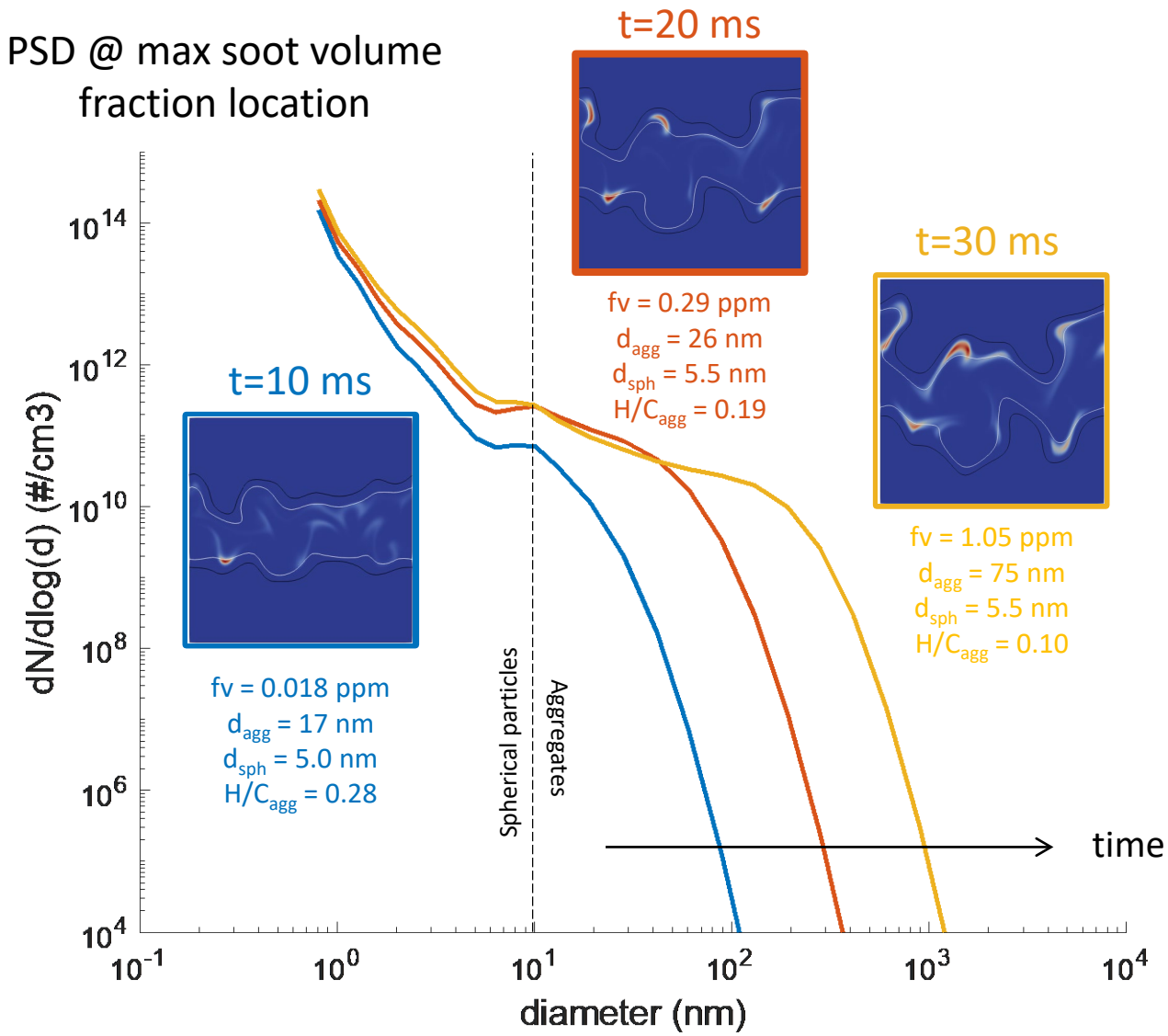
Solver: laminarSMOKE++ (based on OF-10)
Time discretization: 2nd order backward Euler
Space discretization: OF *cubic* scheme

Operating conditions

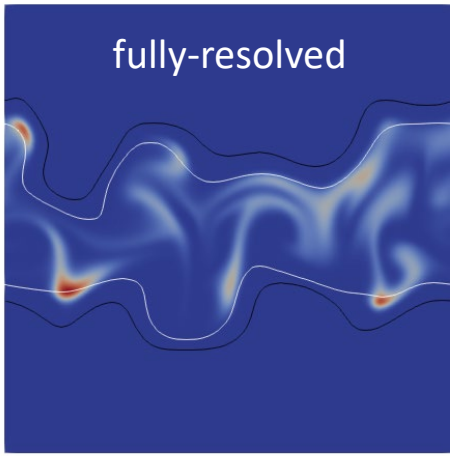
Fuel: 84.4% NC7H16 + 15.6% N2
Oxidizer: 21% O2 + 79% N2
Initial temperature: 300 K
Initial pressure: 1 atm

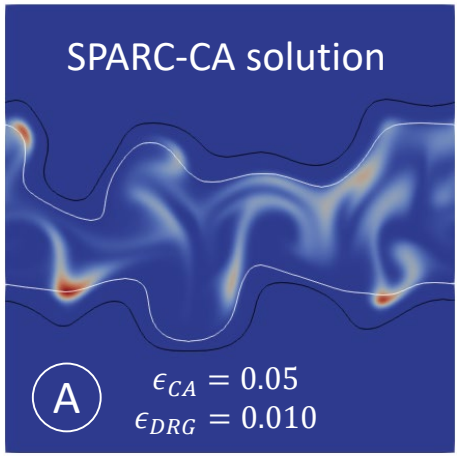
Bisetti et al., On the formation and early evolution of soot in turbulent nonpremixed flames, Combustion and Flame, 159, p. 317-335 (2012)

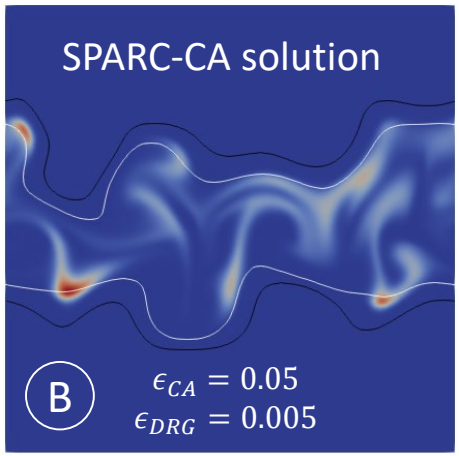
Particle Size Distribution (PSD) of soot



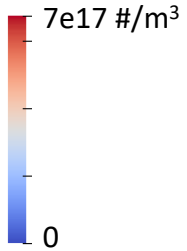
Computational performances

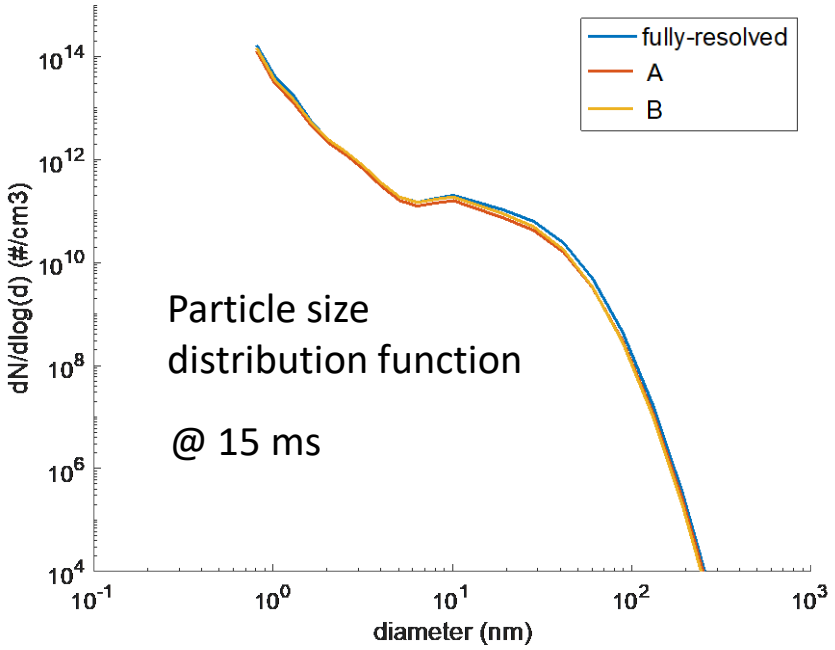


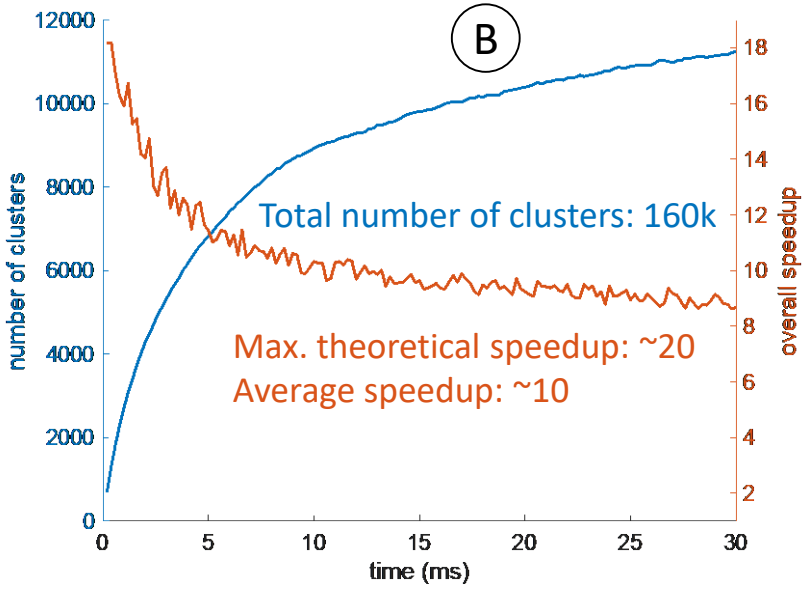




Soot particle number density @ 15 ms





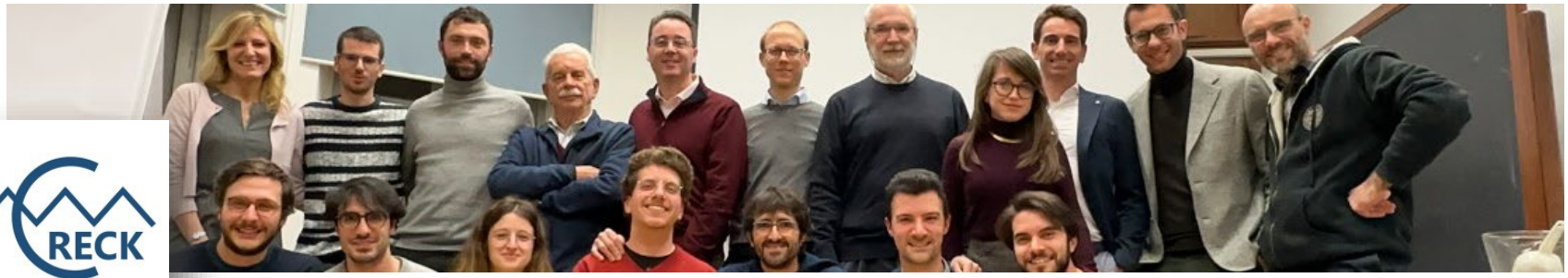


Summary

1. **Reducing the number of cells: P(CA)^2**
   - Combination of Cell Agglomeration and PCA
   - Optimal/automatic choice of features for cell agglomeration

2. **… and reducing the kinetic complexity: Tabulation-based SPARC-CA**
   - Combination of Adaptive Reduced Chemistry (ARC) and Cell-Agglomeration
   - Chemical reduction as a preprocessing step

Acknowledgements



http://creckmodeling.chem.polimi.it

Heinz Pitsch

Alessandro Parente

Giuseppe D'Alessio

Temistocle Grenga

Alexander von Humboldt Stiftung/Foundation

Part of this work was supported by the **Alexander von Humboldt Foundation**

Thank you!

… and see you in Milan in July 2024!

http://www.combustionsymposia.org/2024/

Backup slides

Thank you!

CRECK Modeling Group
Department of Chemistry, Materials and Chemical Engineering “G. Natta”
creckmodeling.chem.polimi.it

Follow us on Social Media
@CreckModeling

… and see you in Milan in 2024!

http://www.combustionsymposia.org/2024/

Available frameworks and codes @ CRECK Lab

OpenSMOKE++

https://www.opensmokepp.polimi.it

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

- **Ideal reactors** (batch, PFR, CSTR, shock-tubes, RCM)
- **Laminar 1D flames** (burner stabilized, freely propagating, counter-flow flames)
- Isolated fuel droplets
- Steady-state laminar flamelets
- Heterogeneous catalytic ideal reactors (batch, PFR, CSTR)

Cuoci A. et al., Computer Physics Communications, 192, pp. 237-264, DOI: 10.1016/j.cpc.2015.02.014

Cuoci A. et al. (2013) Combustion and Flame, 160 (5), pp. 870-886, DOI: 10.1016/j.combustflame.2013.01.011

OpenFOAM-based Codes

laminarSMOKE++

- CFD of laminar reacting flows (coflow flames, burner stabilized stagnation flames, …)

flameletSMOKE++

- Turbulent flames based on the steady-state laminar flamelet

edcSMOKE++

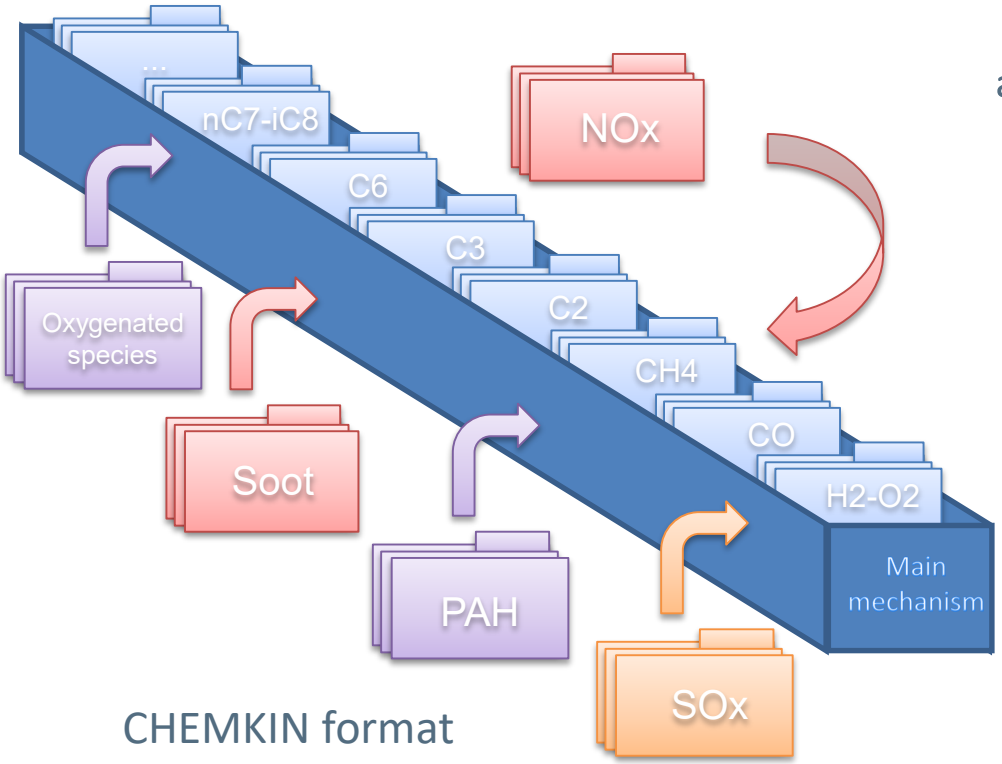
- Turbulent flames based on the Eddy Dissipation Concept (EDC) model

catalyticFOAM*

- Simulation of catalytic heterogeneous (gas/solid) reactors

* In cooperation with M. Maestri (POLIMI)

CRECK Detailed Mechanisms



CHEMKIN format

Kinetic mechanism of **pyrolysis, oxidation and combustion** of small (C1-C3) and large hydrocarbons up to Diesel and jet fuels (C16) as well as several pollutants

Hierarchy

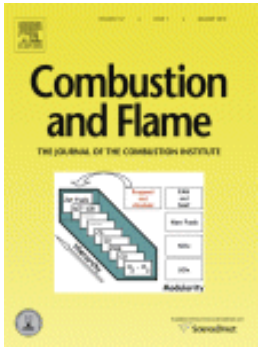
Modularity

Generality

~ 600 chemical species

~ 20,000 reactions

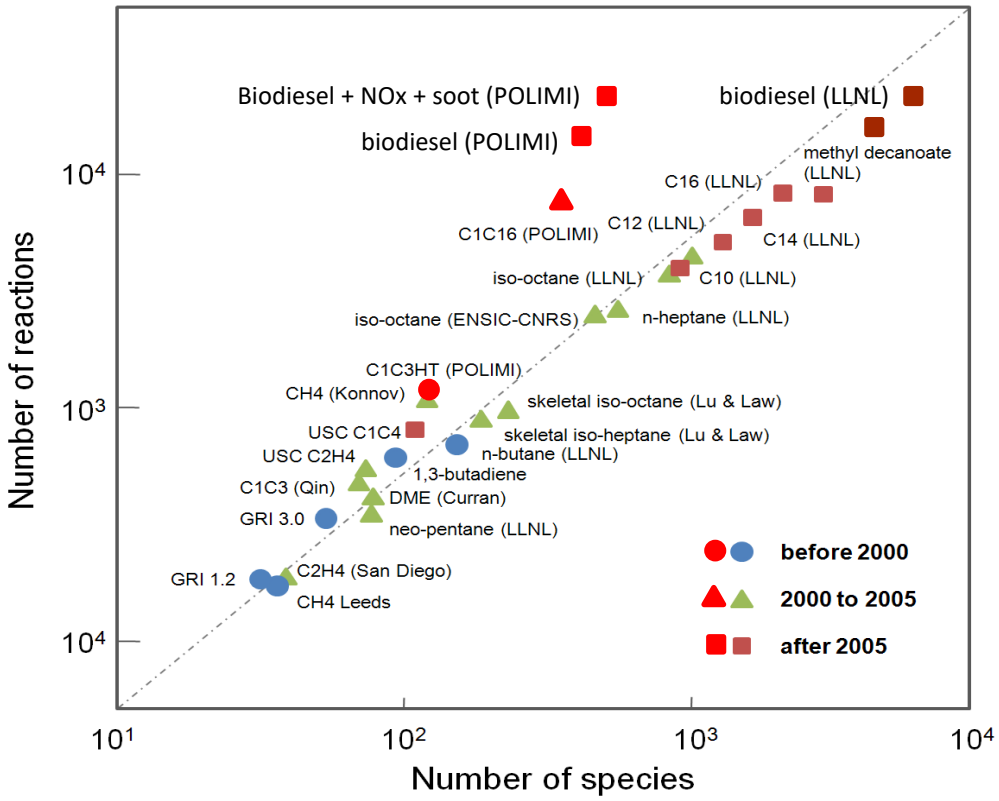
http://creckmodeling.chem.polimi.it



Frassoldati, A. et al., Combustion and Flame 157(2010), pp. 2-16 [Link]

Ranzi, E. at al., Progress in Energy and Combustion Science 38 (2012), pp. 468-501 [Link]

Detailed kinetic mechanisms



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)

need of **numerical techniques** and **computational tools** to make:

- the use of large kinetic mechanisms computationally efficient
- their **integration** in new and/or existing numerical codes as smooth as possible

Detailed chemistry and CFD: challenges

1. Number of equations

Detailed kinetic mechanisms may involve dozens or **hundreds** of chemical species

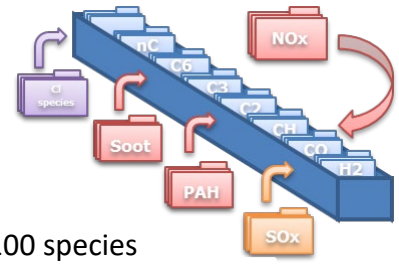
2. Non-linearity and coupling

The transport equations of species and energy are very **non-linear and strongly coupled**

3. Stiffness

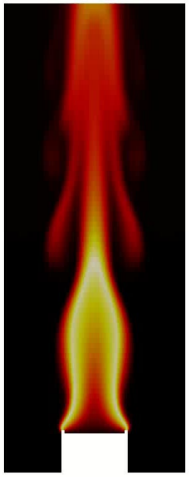
The **characteristic times** of species involved in a kinetic scheme can differ by several order of magnitudes

Detailed kinetic mechanisms

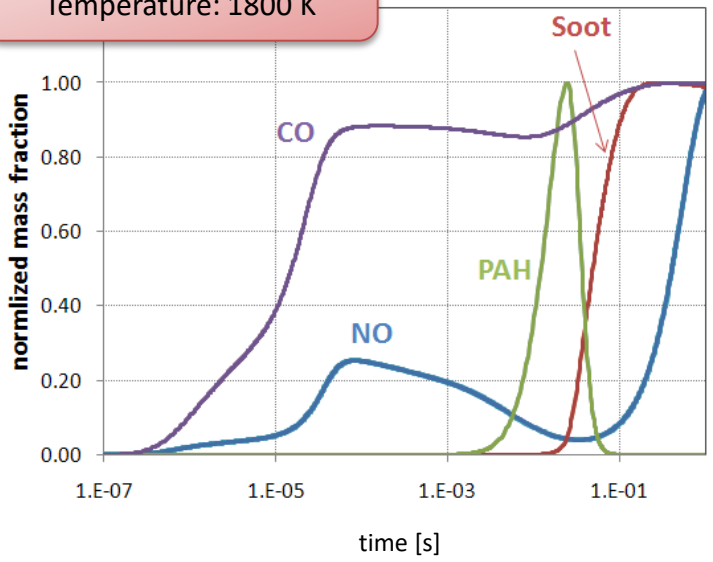


~ 100 species
~ 1,000 reactions

Unsteady flame



Inlet mixture: C_3H_8 + Air
Temperature: 1800 K



Implicit treatment of chemistry via operator-splitting

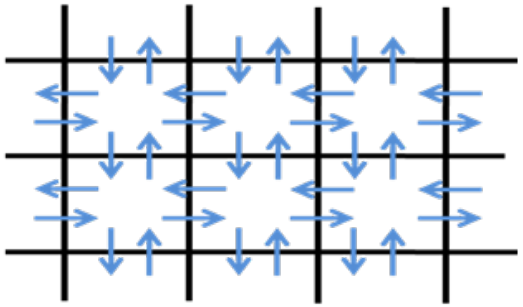
$$\frac{d\mathbf{Y}}{dt} = \mathbf{T} + \mathbf{S}$$

Transport (convection + diffusion)

Chemistry (reactions)

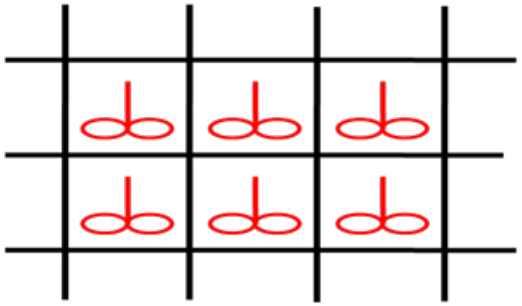
$$\begin{cases} \Delta\mathbf{Y}_1^n = \Delta t\mathbf{T}^n \\ \Delta\mathbf{Y}_2^n = \Delta t\mathbf{S}^n \end{cases}$$

Transport step (Δt)



$$\frac{d\mathbf{Y}}{dt} = \mathbf{T}$$

Chemical step (Δt)



$$\frac{d\mathbf{Y}}{dt} = \mathbf{T}$$

Strang G., *On the construction and comparison of difference schemes.* SIAM Journal of Numerical Analysis, 5, p. 506-517 (1968)

Ren Z., Pope S.B., *Second-order splitting schemes for a class of reactive systems.* Journal of Computational Physics, 227 p. 8165-8176 (2008)

Advertisement

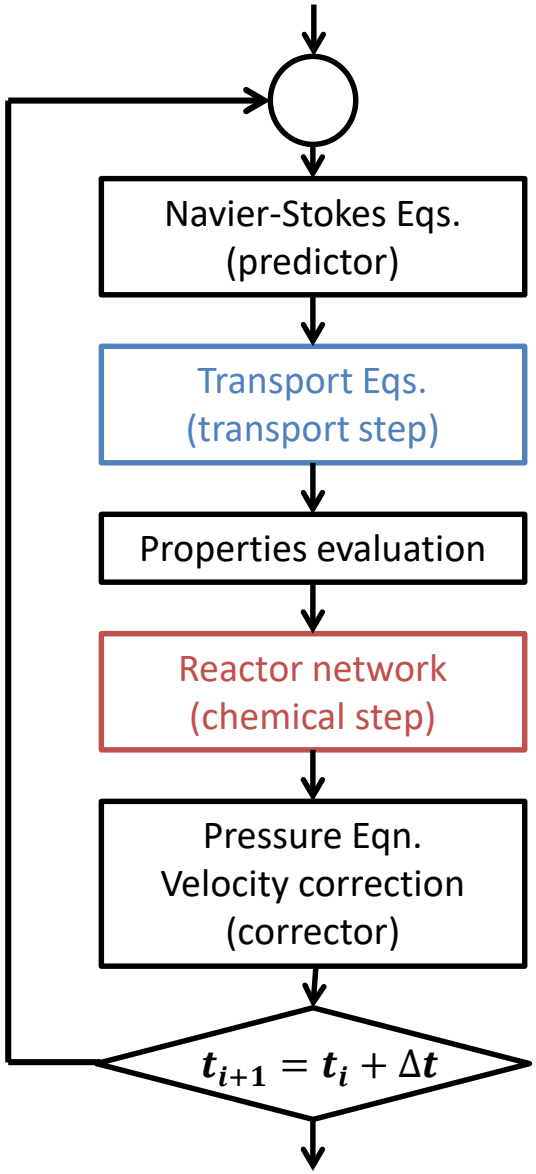
The CRECK Modeling Lab is recruiting PhD Students and Postdocs

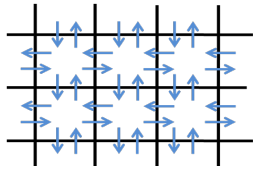
- Numerical modeling of **reactive flows** with detailed kinetics
- Development of **detailed kinetic mechanisms** for pyrolysis, oxidation and combustion of gaseous fuels
- Theoretical calculation of **rate constants** in gas-phase and heterogeneous phase
- Modeling of volatilization, gasification and combustion of **biomasses**
- Modeling of thermal conversion (gasification/pyrolysis) of **plastics**
- CFD and compartment-based modeling of **bioreactors**

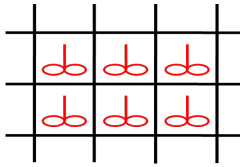
We are open to possible collaborations on the same topics!

http://creckmodeling.chem.polimi.it

Implicit treatment of chemistry (II)







Chemical Step = **independent ODE systems** with IC

Implicit ODE solvers are mandatory!

Implicit ODE solvers are **computationally very expensive**

The cost increases more than linearly with the number of species N_S:

$$cost \sim N_S^{2 \div 3}$$

Need of acceleration techniques for speeding-up the chemical step

Cuoci, A., Frassoldati, A., Faravelli, T., Ranzi, E., *Numerical modeling of laminar flames with detailed kinetics based on the operator-splitting method* (2013) Energy and Fuels, 27 (12), pp. 7730-7753

Stiff ODE solvers in OpenFOAM

For each solver, a C++ interface in OpenFOAM was created

1. Creating ODE System objects

```
ODESystem_BatchReactor_DVODE *odeSystemObject;
odeSystemObject = ODESystem_BatchReactor_DVODE::GetInstance();
```

2. Creating ODE System Solver

```
OpenSMOKE_DVODE<ODESystem_BatchReactor_DVODE>    ode(odeSystemObject);
```

3. Setting numerical parameters

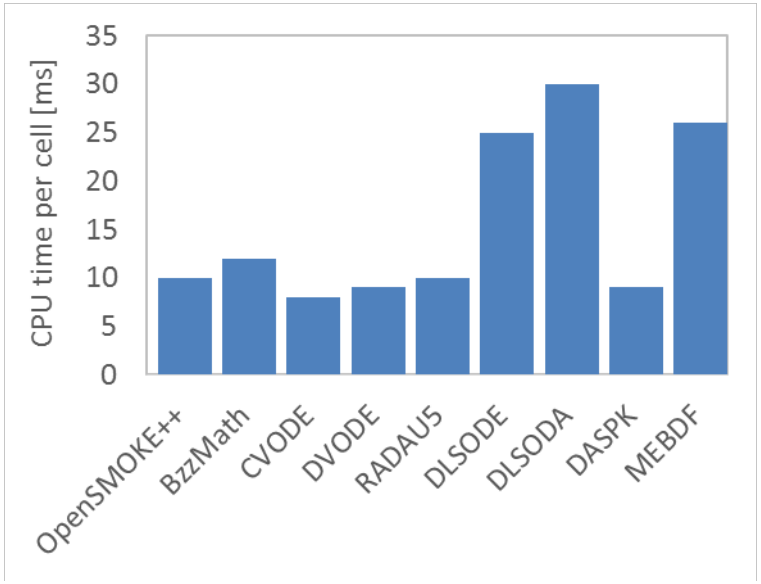
```
ode.SetMaximumNumberOfSteps(100000);
ode.SetAnalyticalJacobian(false);
ode.SetAbsoluteTolerance(aTol);
ode.SetRelativeTolerance(rTol);
```

4. Looping on computational cell

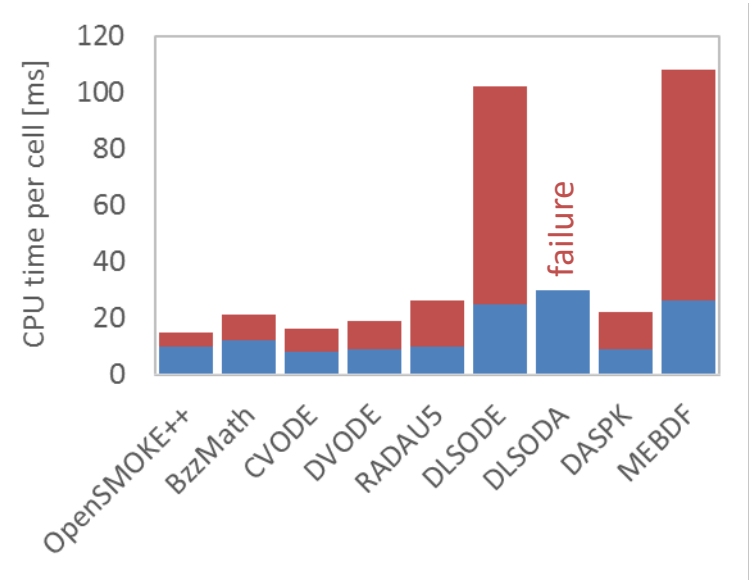
```
ode.SetInitialValues(t0,Y0);
ode.Solve(tf);
ode.Solution(yF);
```

Performance of stiff ODE solvers (II)

Homogeneous mechanism
105 species, 1700 reactions



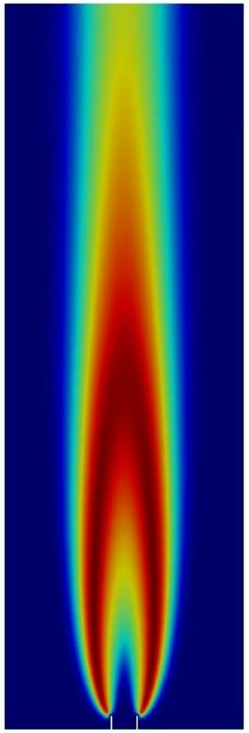
Addition of a heterogeneous mechanism
12 species, 38 reactions



Micro-kinetic mechanisms for heterogeneous reactions are usually very non-linear because the activation energy may depend on the coverage (i.e., the composition on the catalytic wall)

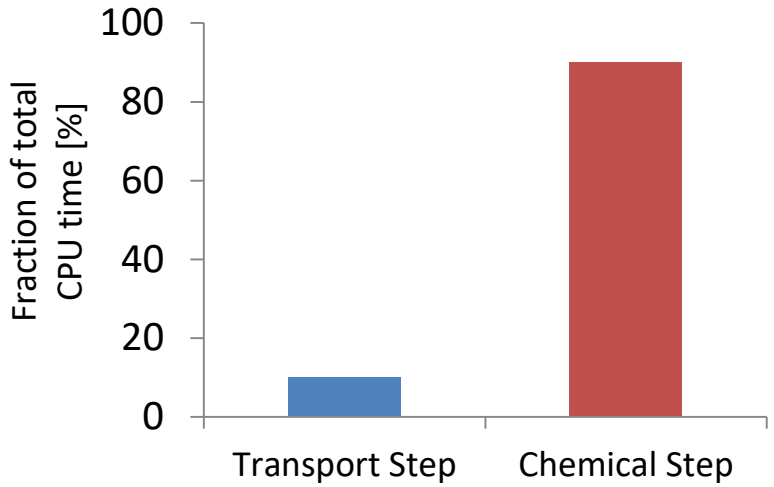
$$r_j = A_j \cdot T^{\beta_j} \cdot \exp\left(-\frac{E_{att,j}(\theta_i)}{RT}\right) \prod_{i=1}^{NC} (c_i)^{\nu_{ij}}$$

Stiff ODE solvers for chemistry



Pulsating laminar coflow flame

Imposed sinusoidal fluctuations of fuel stream velocity
Amplitude: 90%
Frequency: 10 Hz

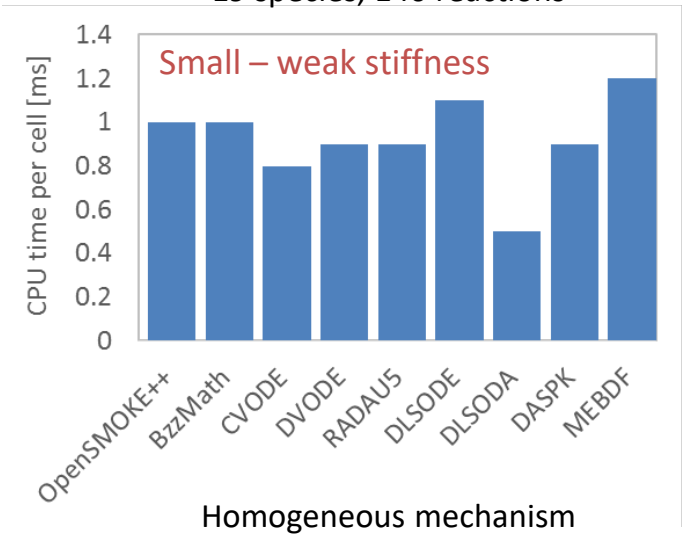


Most of the CPU Time (>90%) is spent for the numerical integration of the ODE systems corresponding to the chemical step

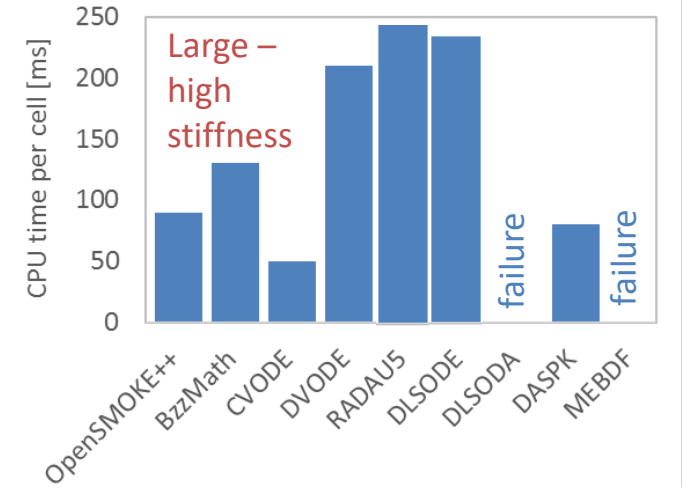
	Language	Code available	License
OpenSMOKE++	C++	Yes	Academic use only
BzzMath	C++	No	Academic use only
DVODE	FORTRAN	Yes	Free
CVODE	C	Yes	Free
DLSODE	FORTRAN	Yes	Free
DLSODA	FORTRAN	Yes	Free
RADAU5	FORTRAN	Yes	Free
DASPK	FORTRAN	Yes	Free
MEBDF	FORTRAN	Yes	Free

Performance of stiff ODE solvers

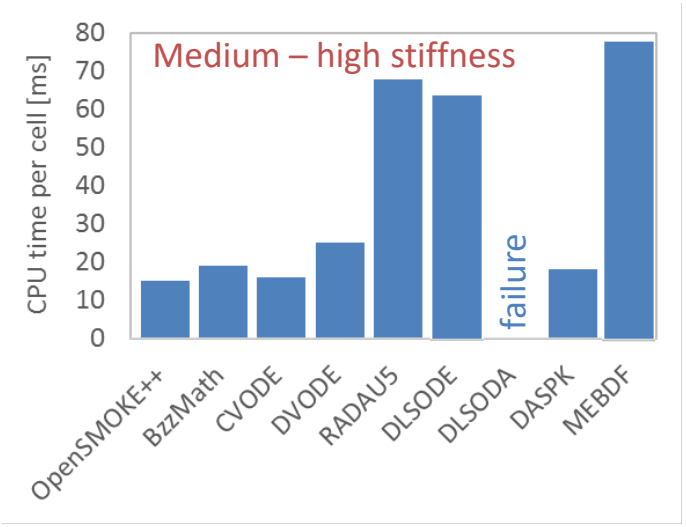
Homogeneous mechanism
19 species, 140 reactions



Homogeneous mechanism
680 species, 2400 reactions



Homogeneous mechanism
156 species, 5400 reactions



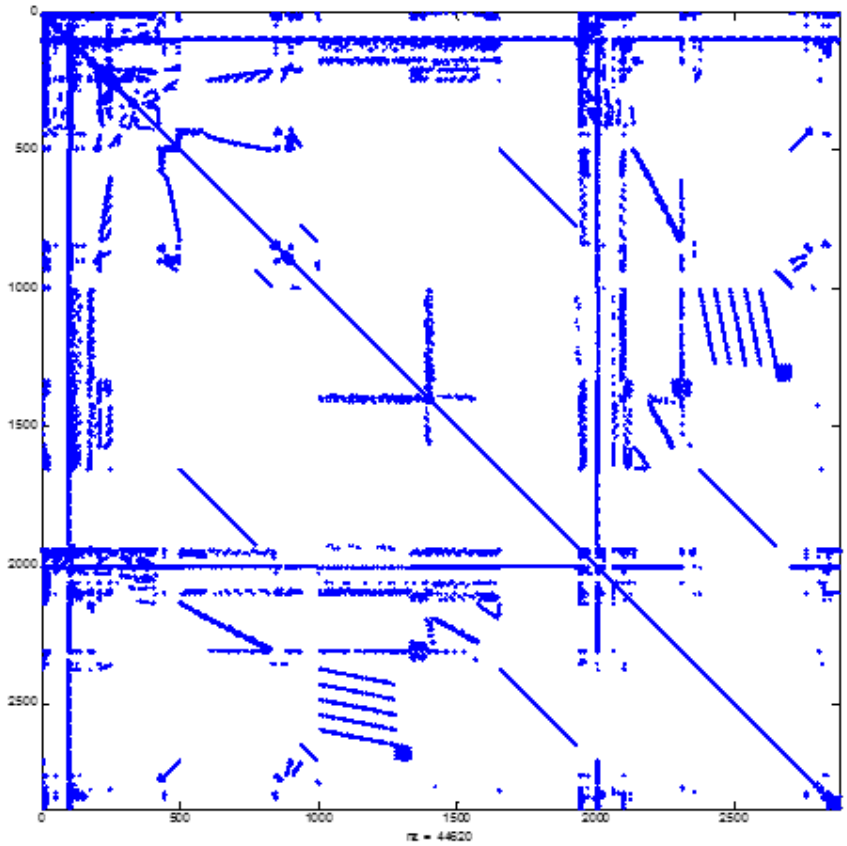
The best ODE solver depends on the features of the kinetic mechanism adopted:

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

Cuoci A. et al., *OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms* (2015) Computer Physics Communications, 192, pp. 237-264

Sparse linear solvers for detailed chemistry (I)

Jacobian sparsity pattern



LLNL methyl-decanoate
Species: 2878
Reactions: 8555
Non-zero elements: 44620 / 8M (0.50%)

Stiff ODE system

$$\frac{dY_j}{dt} = S_j$$

Jacobian matrix

$$J_{ij} = \frac{dS_i}{dY_j}$$

Implicit methods

OpenSMOKE++ ODE solver was extended to sparse systems

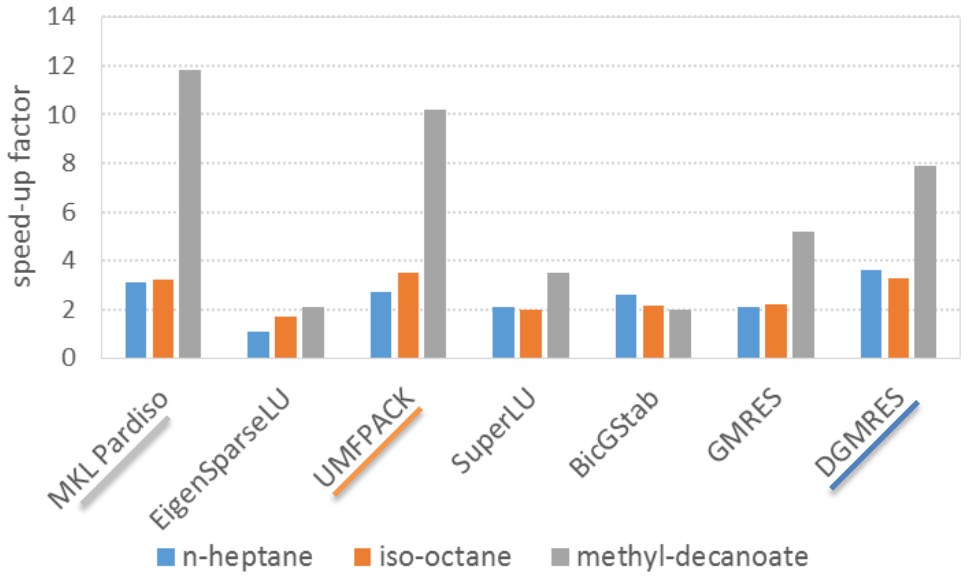
- EigenSparseLU
- MKL Pardiso
- UMFPACK
- SuperLU (serial)

Direct solvers

- BiCGStab
- GMRES
- DGMRES

Iteratives solvers

Sparse linear solvers for detailed chemistry (III)

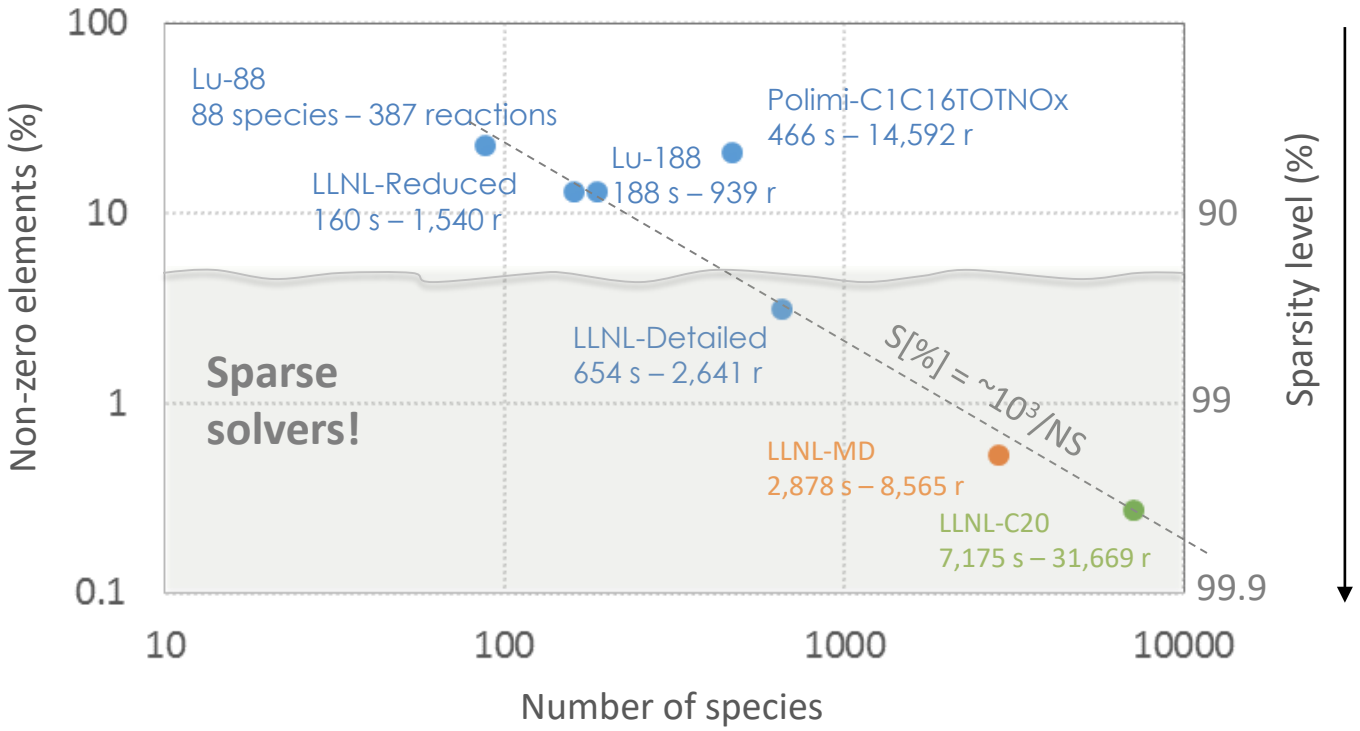


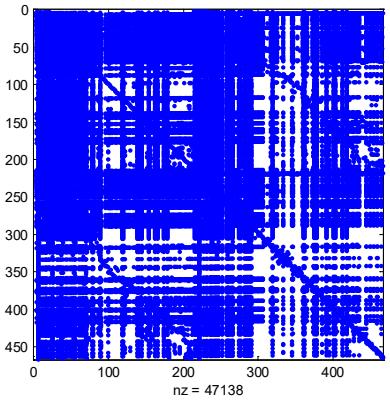
Speed-up factors of sparse linear solvers with respect to the OpenSMOKE++ dense solver

	n-heptane	Iso-octane	Methyl-decanoate
Species	658	878	2878
Reactions	2827	3769	8555
Non-zero elements	13151	18,471	44,620
% sparsity	97%	97.7%	99.5%

The larger the sparsity of a kinetic mechanism, the larger the speed-up factor in using a sparse linear solver

Sparse linear solvers for detailed chemistry (II)





Polimi-C1C16TOTNOx
466 species
14,592 reactions
Sparsity = 79%

- The sparsity level of a mechanism is also a function of the technique adopted for its development
- Adoption of sparse algorithms is convenient only if the sparsity is sufficiently high **(>95%)**

Analysis of computational costs

The cost for a chemical step in a CFD simulation carried out on a grid with N cells is:

$$C_{chem} \sim N \times N_S^{\alpha} \qquad \text{with } \alpha = 2 \div 3$$

Under the assumption that $N \gg N_S$, it is possible to demonstrate that the cost of PCA scales as:

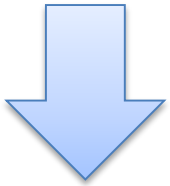
$$C_{PCA} \sim N \times N_S^2$$

Thus, **the relative cost of PCA with respect to the chemical step does not increase with the size of the mesh** and it is expected to slightly decrease with the number of species:

$$\frac{C_{PCA}}{C_{chem}} \sim \frac{1}{N_S^{\alpha-2}}$$

Dynamic Cell Agglomeration (DCA)

On which basis can reacting cells be regarded as similar or different?



Clustering algorithms

The grouping of computational cells, in the calculation domain, into clusters is achieved by using **clustering algorithms** which identify cells that have similar thermochemical states.

How to conservatively redistribute the species among the cells, after integration?

Liang L., Stevens J. G., Farrell J.T., *A Dynamic Multi-Zone Partitioning Scheme for Solving Detailed Chemical Kinetics in Reactive Flow Computations*, Combustion Science and Technology 181(11), p.1345-1371 (2009)

G.M. Goldin, Z. Ren, S. Zahirovic, *A cell agglomeration algorithm for accelerating detailed chemistry in CDF*, Combust. Theory Model., 13, pp. 721–739 (2009)

Conservative remapping procedure

A simple, weighted remapping of the species mass fractions changes from the cluster is not able to ensure mass conservation and it would gradually deteriorate the solution.

Mass fraction change in cluster k (over time step $\Delta t = t^{n+1} - t^n$)

$$\Delta Y_{k,j} = Y_{k,j}^{n+1} - Y_{k,j}^{n}$$

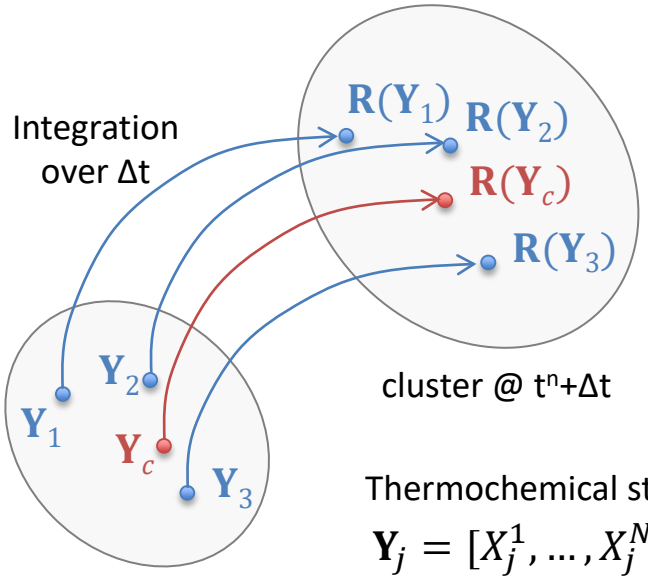
Change of species partial density to be mapped back to the original cells i

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n} + \begin{cases} \Delta Y_{k,j}\ \rho_i^n & if\ \ \Delta Y_{k,j} \geq 0 \\ \Delta Y_{k,j}\ \rho_k^n \dfrac{\rho_{i,j}^n}{\rho_{k,j}^n} & if\ \ \Delta Y_{k,j} < 0 \end{cases}$$

The cells' temperatures are estimated from the updated mixture sensible enthalpy.

Liang L., Stevens J. G., Farrell J.T., *A Dynamic Multi-Zone Partitioning Scheme for Solving Detailed Chemical Kinetics in Reactive Flow Computations*, Combustion Science and Technology 181(11), p.1345-1371 (2009)

Linearized solution remapping (I)



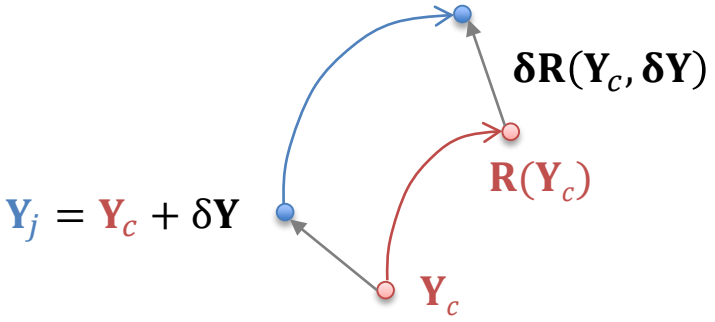
Chemical step: ODE integration

$$\mathbf{R}(\mathbf{Y}_j) = \int_{t^n}^{t^n+\Delta t} \mathbf{f}(\mathbf{Y}_j, \mathbf{Y}, t)\,dt$$

Thermochemical state of cell j

$$\mathbf{Y}_j = [X_j^1, \ldots, X_j^{NS}, T_j]$$

$$\mathbf{R}(\mathbf{Y}_j) = \mathbf{R}(\mathbf{Y}_c) + \boldsymbol{\delta}\mathbf{R}(\mathbf{Y}_c, \boldsymbol{\delta}\mathbf{Y})$$



If $\boldsymbol{\delta}\mathbf{Y}$ is small enough:

$$\mathbf{R}(\mathbf{Y}_j) \approx \mathbf{R}(\mathbf{Y}_c) + \left.\frac{\partial R^i}{\partial Y^k}\right|_{\mathbf{Y}_c} \boldsymbol{\delta}\mathbf{Y} = \mathbf{R}(\mathbf{Y}_c) + \mathbf{S}\cdot\boldsymbol{\delta}\mathbf{Y}$$

Matrix of linearized mapping gradients $S_{ik} = \left.\frac{\partial R_i}{\partial Y^k}\right|_{\mathbf{Y}_c}$

Pope S.B., "Combustion Theory and Modelling, 1 (1997) 41-63

Linearized solution remapping (II)

$$\mathbf{R}(\mathbf{Y}_j) \approx \mathbf{R}(\mathbf{Y}_c) + \left.\frac{\partial R^i}{\partial Y^k}\right|_{\mathbf{Y}_c} \boldsymbol{\delta}\mathbf{Y} = \mathbf{R}(\mathbf{Y}_c) + \mathbf{S} \cdot \boldsymbol{\delta}\mathbf{Y}$$

F. Perini, R.D. Reitz, Frontiers in Computational Physics: Energy Sciences Zurich, Switzerland June 5, 2015

The linear mapping gradients are the **first-order sensitivities** of the ODE system w.r.t. the initial conditions evaluated at the final integration time:

$$\begin{cases} \dfrac{d\mathbf{S}}{dt} = \mathbf{J}(t, \mathbf{Y}) \cdot \mathbf{S}(t, \mathbf{Y}) \\ \mathbf{S}(t, \mathbf{Y}_c) = \mathbf{I} \end{cases}$$

- Dense, stiff ODE system with N_S^2 equations
- Computationally too expensive to be solved on-the-fly

Linearized solution mapping in the PC space (i.e., reduced sensitivity system):

$$\mathbf{R}(\mathbf{p}_j) \approx \mathbf{R}(\mathbf{p}_c) + \left.\frac{\partial R^i}{\partial p^k}\right|_{\mathbf{p}_c} \boldsymbol{\delta}\boldsymbol{p} = \mathbf{R}(p_c) + \tilde{\mathbf{S}} \cdot \boldsymbol{\delta}\mathbf{p}$$

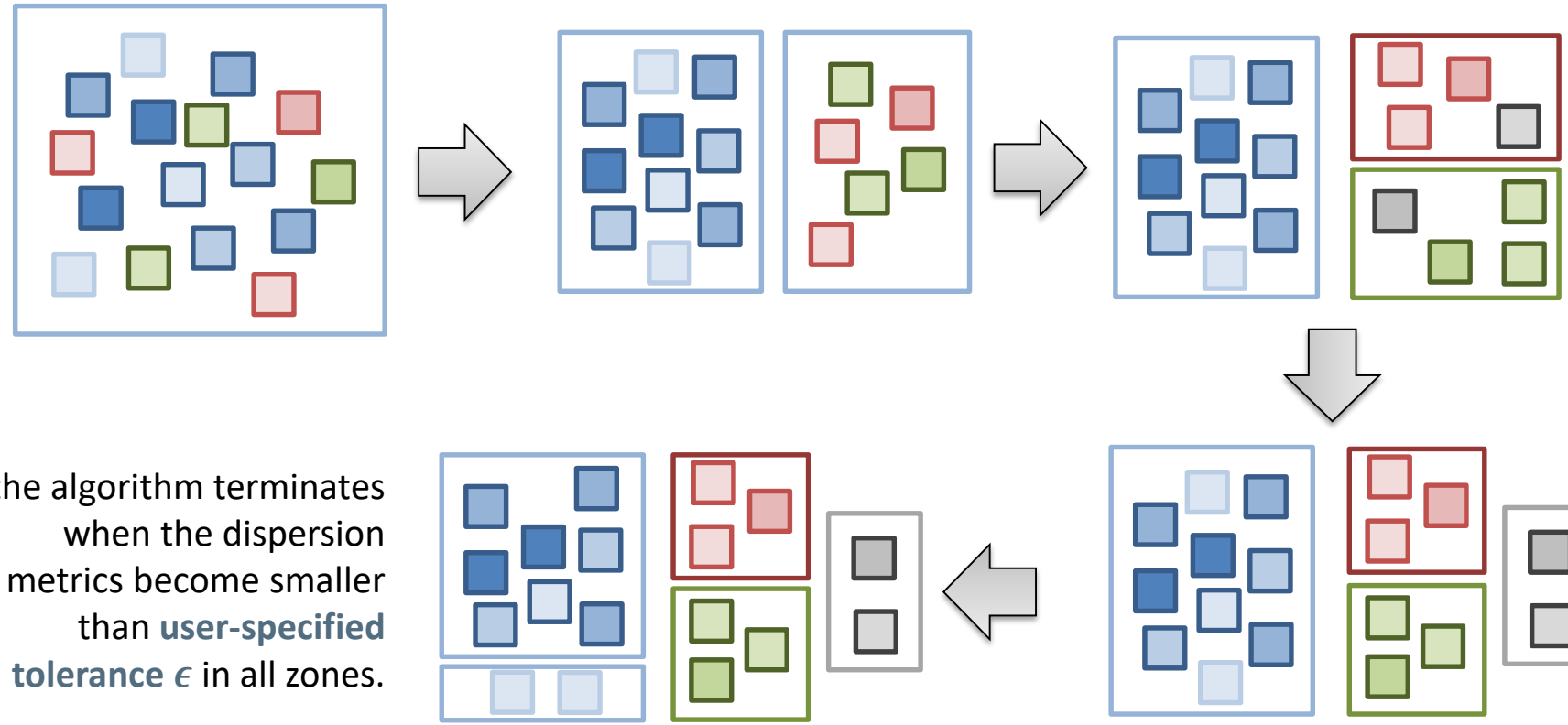
Matrix of linearized mapping gradients $\tilde{S}_{ik} = \left.\dfrac{\partial R_i}{\partial p^k}\right|_{\mathbf{p}_c}$ only N_{PC}^2 elements

Dynamic Multi-Zone (DMZ) clustering

As opposed to static algorithms such as a basic k-means algorithm, the DMZ algorithm (Liang 2009) does not require the *a priori* specification of the number of zones.

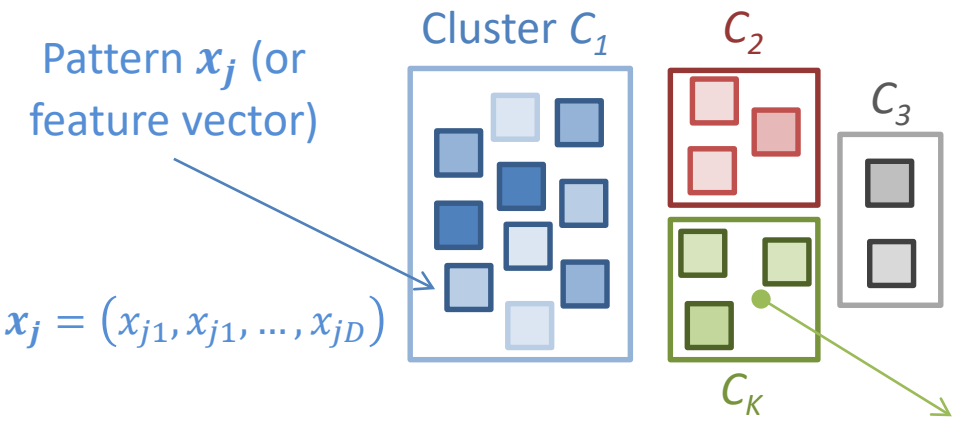
the algorithm starts by initializing all the cells as 1 big zone

the number of zones evolves as bigger zones are split into smaller ones via a **bisection-splitting** algorithm



the algorithm terminates when the dispersion metrics become smaller than **user-specified tolerance ϵ** in all zones.

Dynamic Multi-Zone (DMZ) partitioning (I)



D is the number of **features (i.e principal components)** on which the clustering is applied

n_k is the number of patterns in cluster k

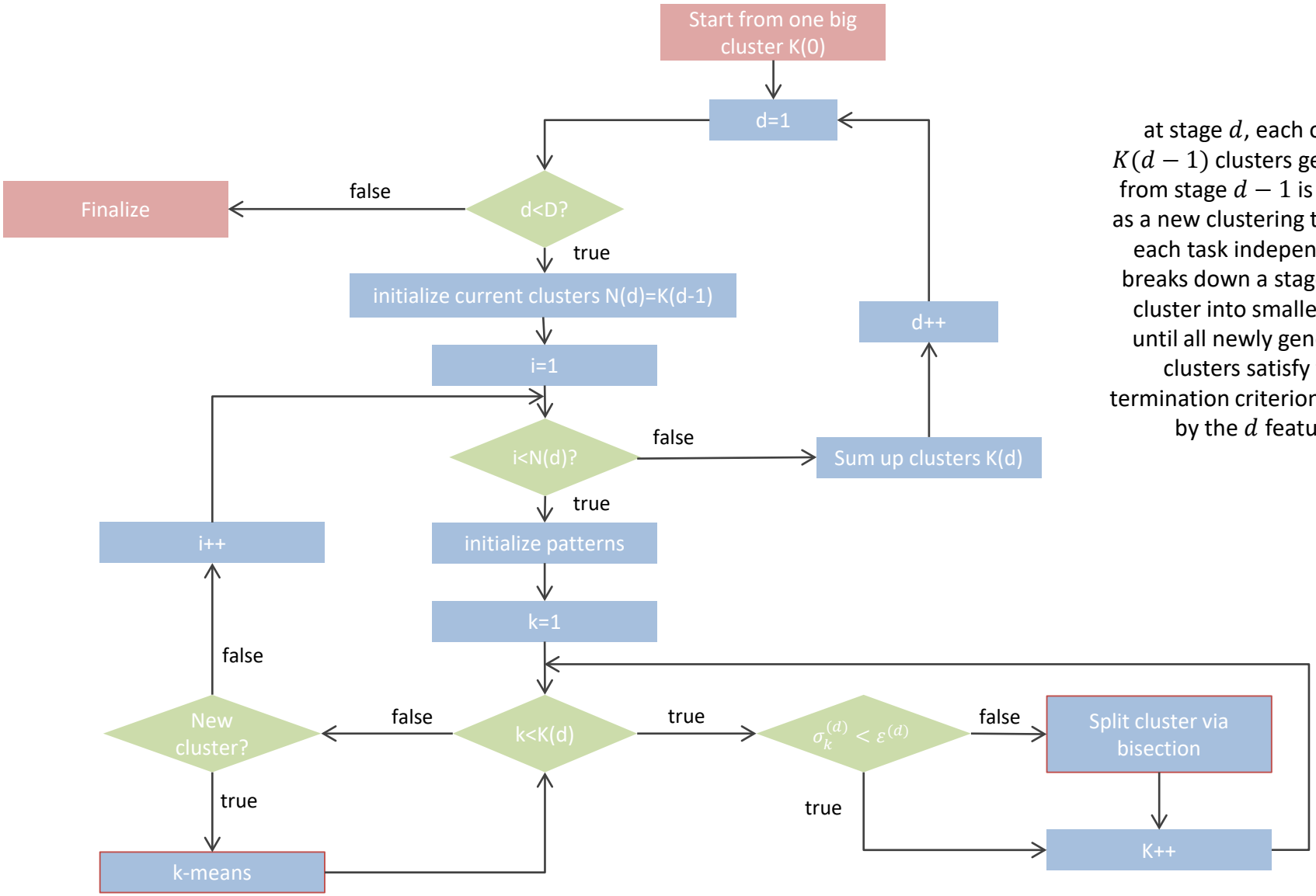
Distance between the d^{th} feature $\quad dist^{(d)}\left(x_i^{(d)}, x_i^{(d)}\right) = \left|x_i^{(d)} - x_i^{(d)}\right|$

Dispersion of feature d in cluster C_K $\quad \sigma_k^{(d)} = max\left\{dist^{(d)}\left(x_i^{(d)}, x_i^{(d)}\right)\right\}$

Clustering in each dimension d is terminated when the dispersion becomes smaller than the user-specified tolerance $\epsilon^{(d)}$ in all clusters and **in all dimensions**:

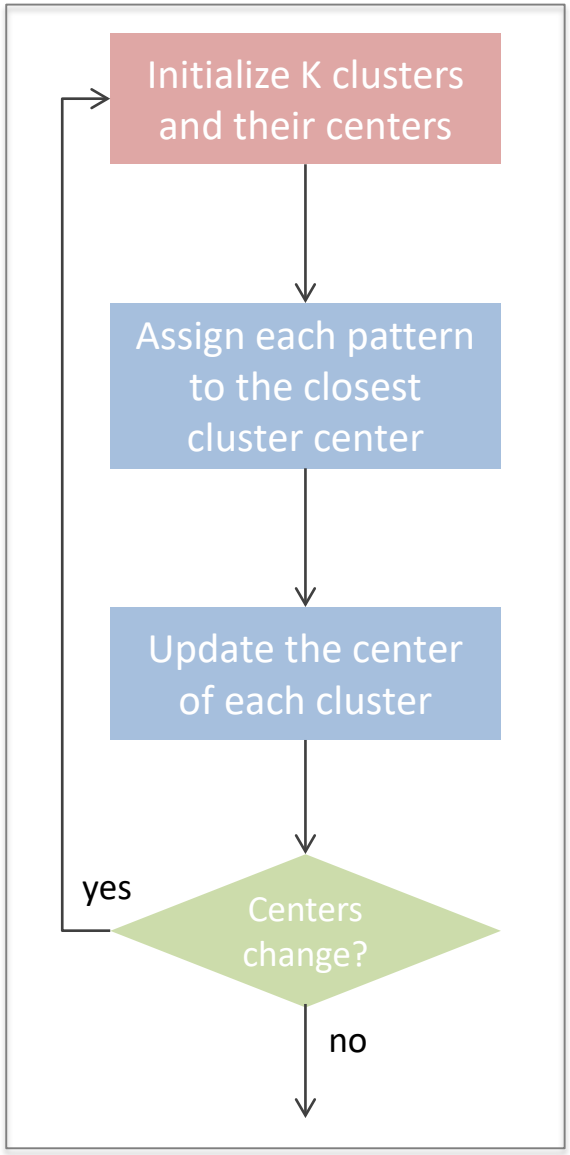
$$\sigma_k^{(d)} < \epsilon^{(d)}$$

Dynamic Multi-Zone (DMZ) partitioning (II)



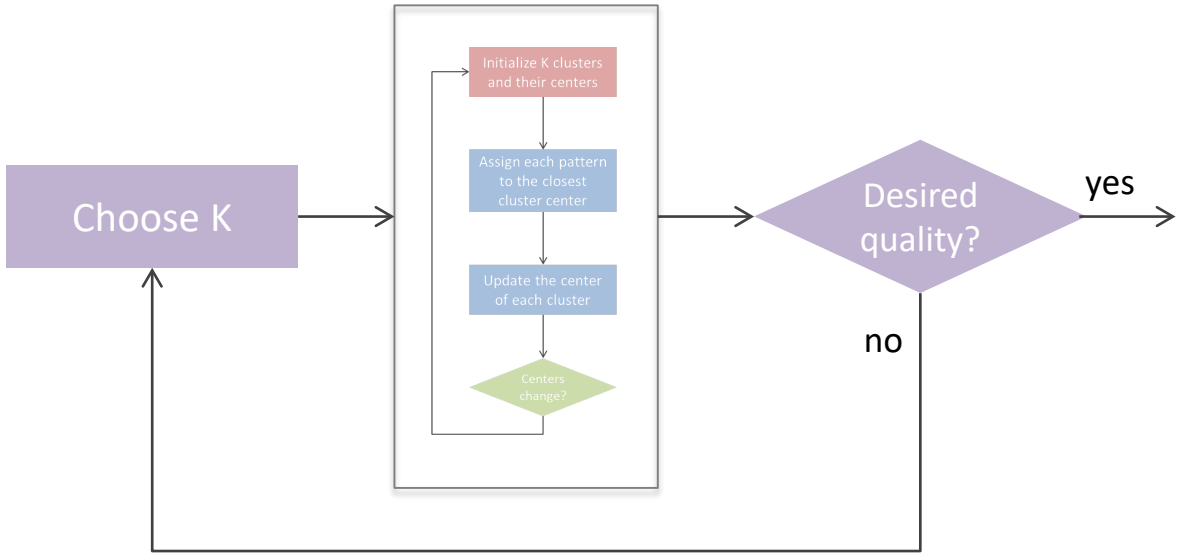
at stage d, each of the $K(d-1)$ clusters generated from stage $d-1$ is treated as a new clustering task, and each task independently breaks down a stage $d-1$ cluster into smaller ones until all newly generated clusters satisfy the termination criterion defined by the d feature

Unsupervised classification: k-means



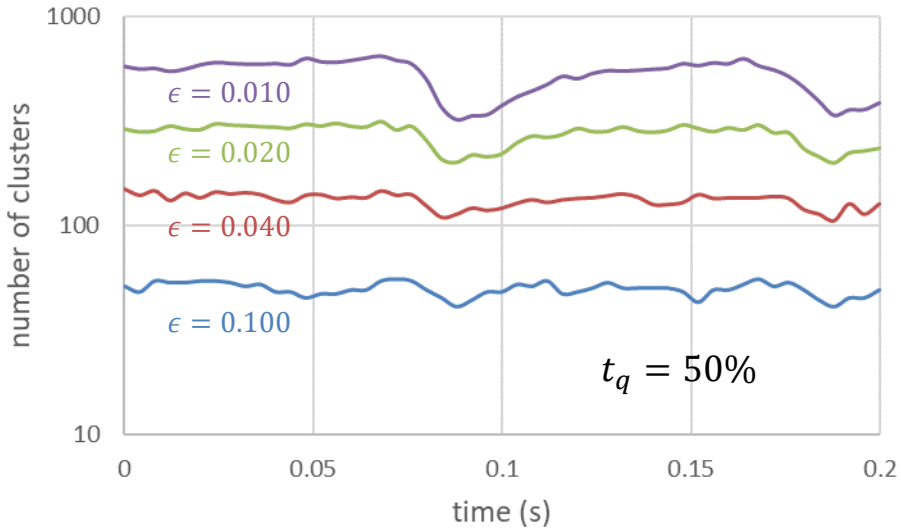
One of the major problems of data clustering via k-means is represented by the estimation of the optimal number of clusters K

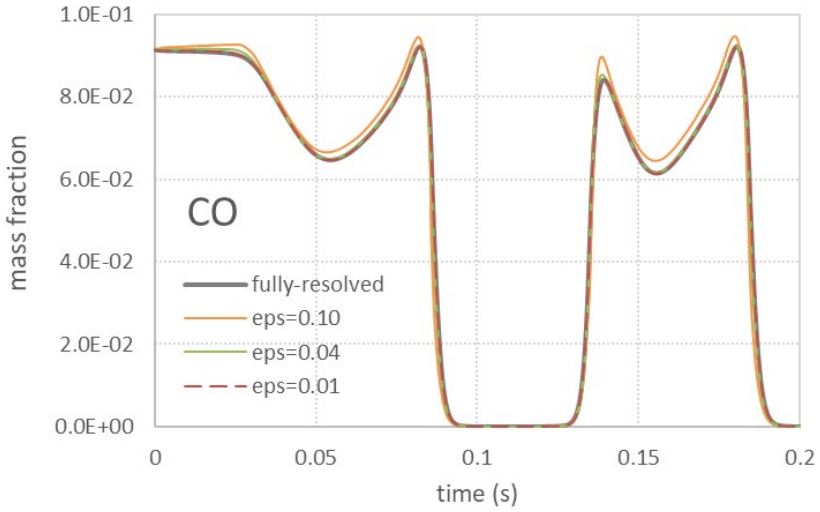
Typically, the k-means clustering algorithm is repeated at increasing number of partition clusters K, and that is stopped after that the desired partition quality has been reached. This process of course is very computationally expensive

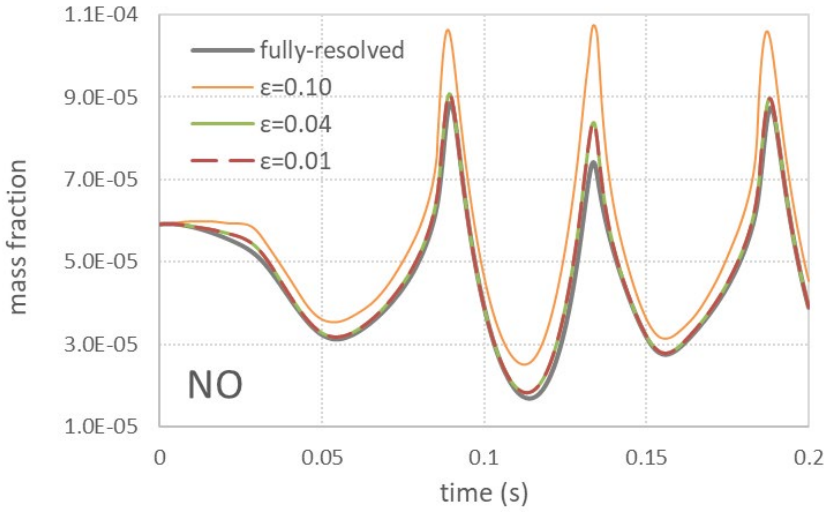


Impact of user-defined tolerance ϵ

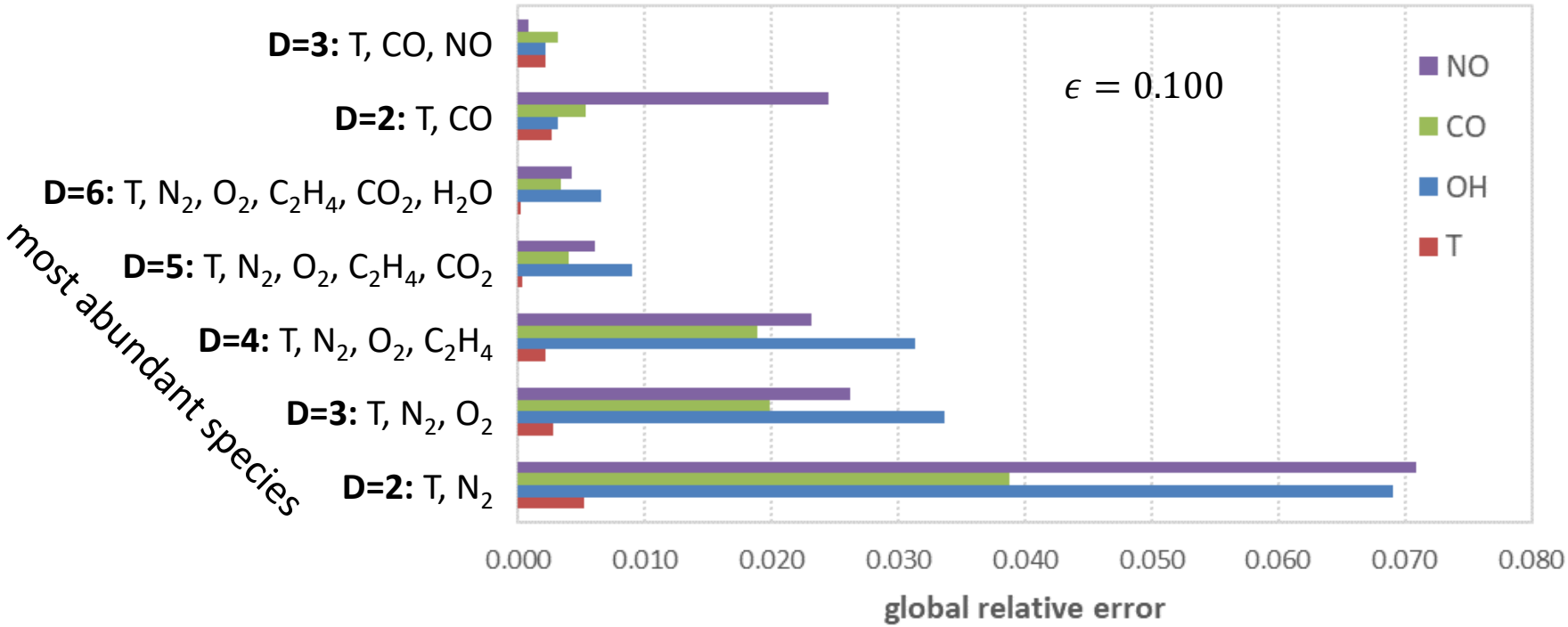
Number of clusters as a function of the user-defined clustering tolerance ϵ





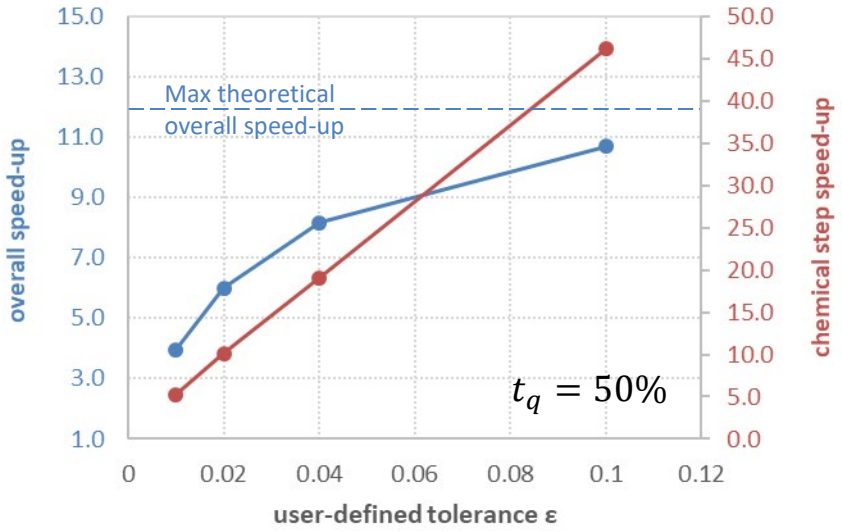


Conventional Cell Agglomeration

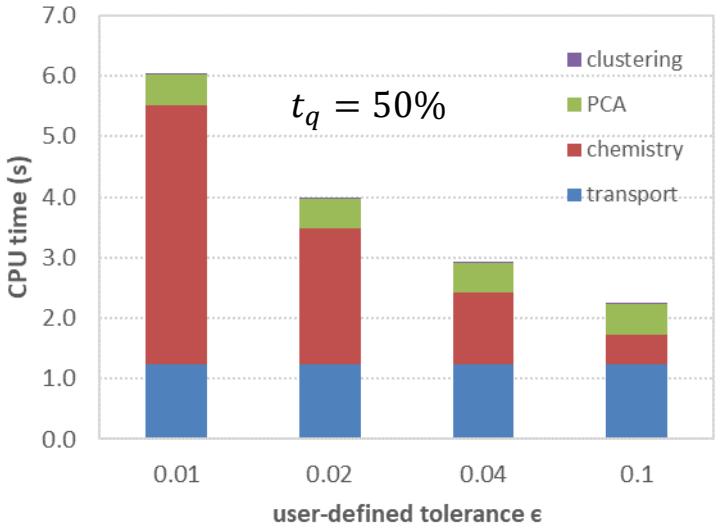


- the results are very sensitive to the choice of the $D - 1$ species
- the overall error is systematically larger than the corresponding P(CA)^2 simulation carried out with the same values of D and ϵ

Computational performances (I)

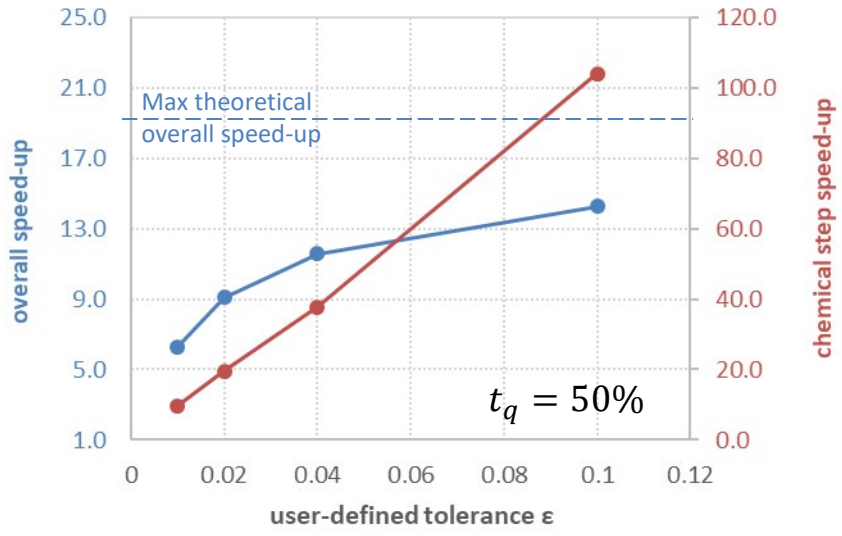


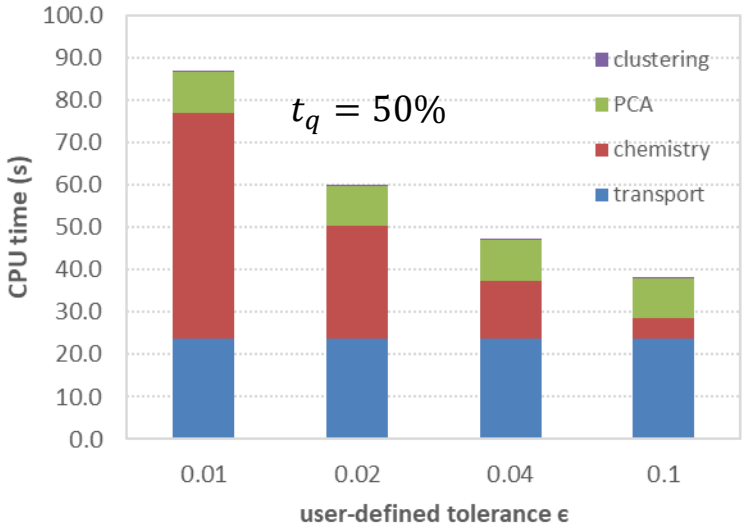
- As expected, the overall computational cost of the CA-based simulation decreases monotonically with increasing tolerances.
- The saving in CPU time impacts the chemical step only



- The PCA computational time does not depend on the clustering parameters t_q and ϵ
- The clustering time is negligible

Computational Performances





Kinetic mechanism

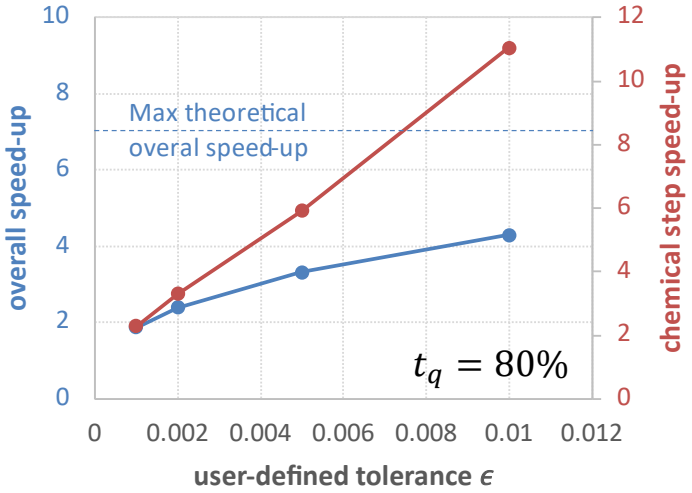
224 species and 5939 reactions
PAH chemistry included
(up 2 aromatic rings)

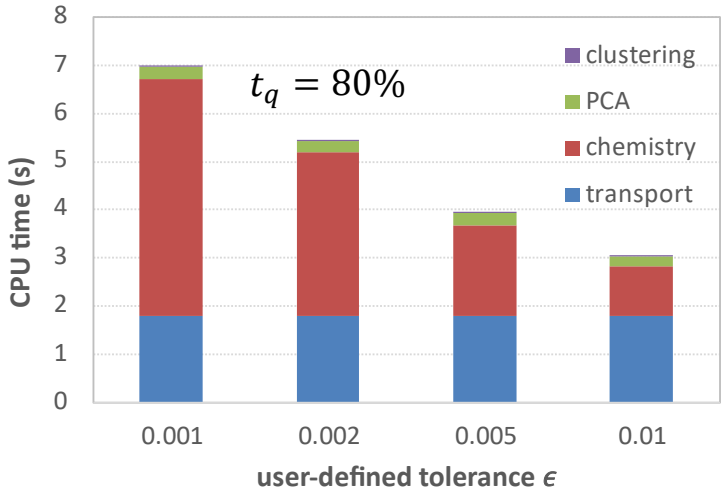
- By increasing t_q and/or decreasing the tolerance ε, the accuracy of the CA-based simulation increases monotonically
- Also in this case, the cost associated with the clustering algorithm is negligible, despite the higher number of species.
- As expected, the cost of the PCA step (~10 s) increases in terms of absolute values, but it is still only ~2% of the computational time of the original chemical step (~520 s).

Analysis of computational time

Hawkes (2007) mechanism (11 species)

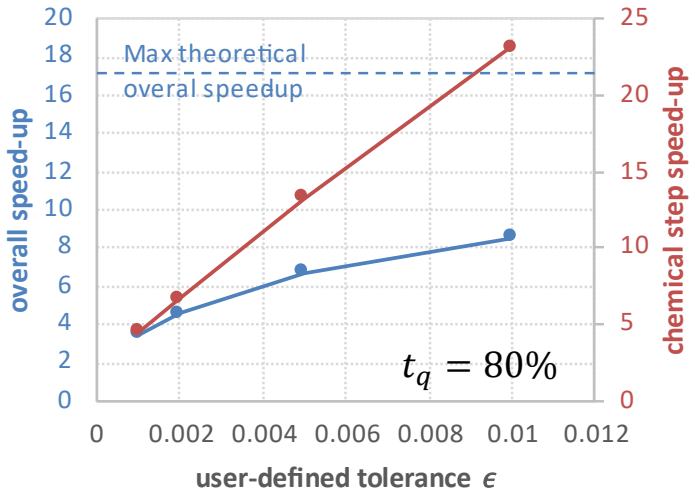
Chemistry CPU time: 86%

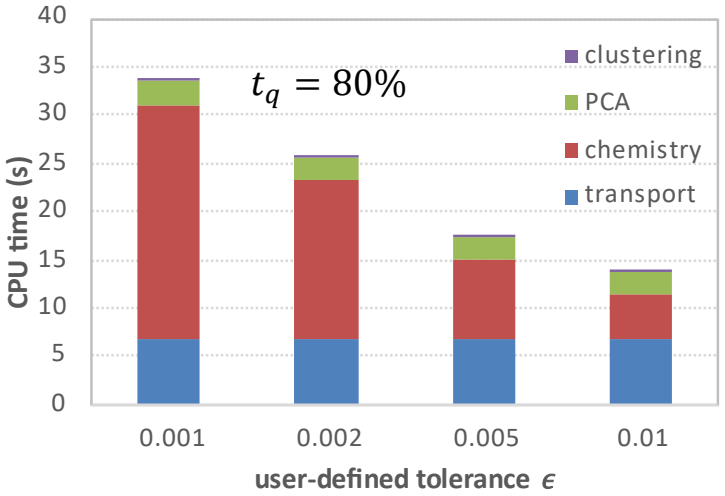




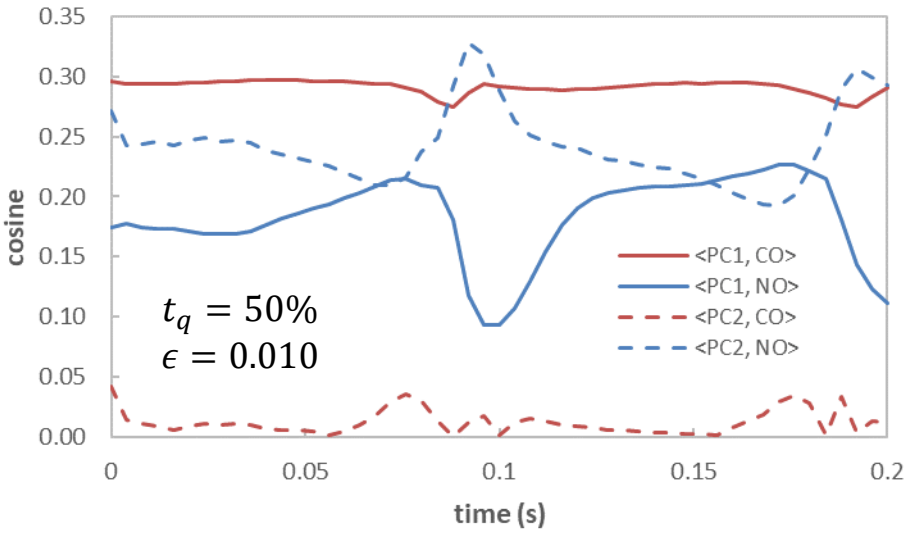
CRECK2003NOX mechanism (57 species)

Chemistry CPU time: 95%



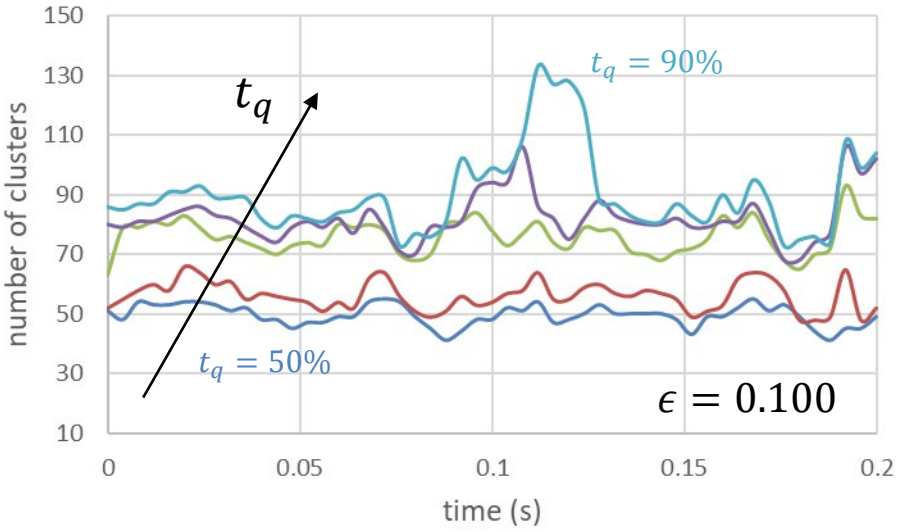


Impact of user-defined explained variance t_q

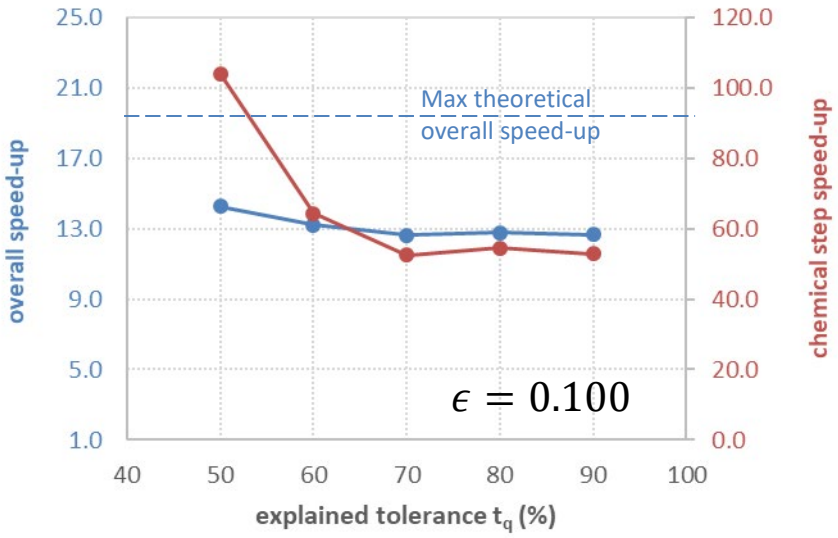


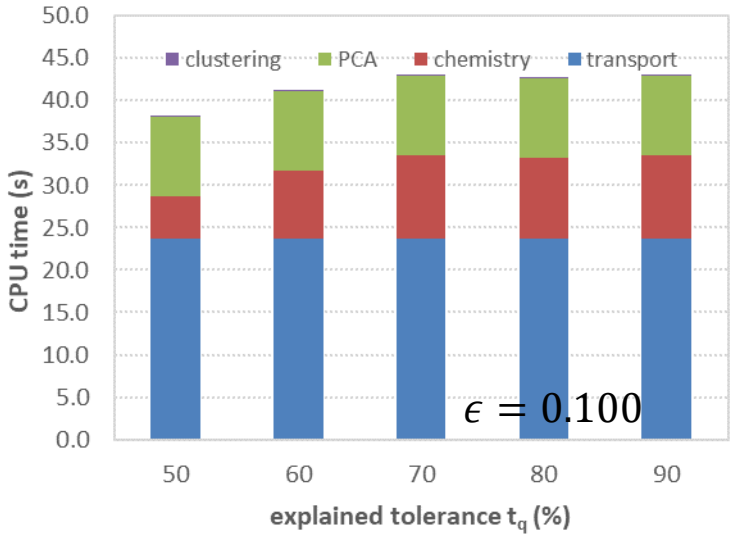
Temporal evolution of cosine values of the angles between the first 2 principal axes and species CO and NO

Number of clusters as a function of the user-defined explained variance t_q



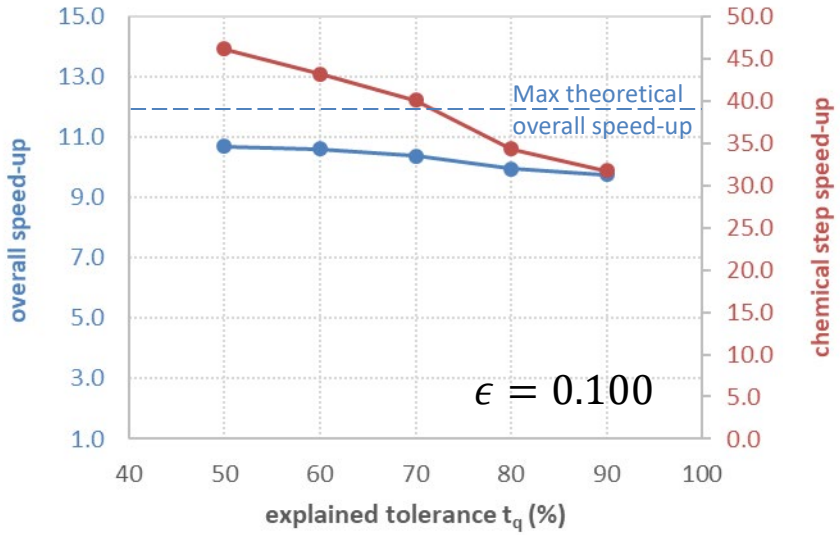
Computational times: impact of t_q



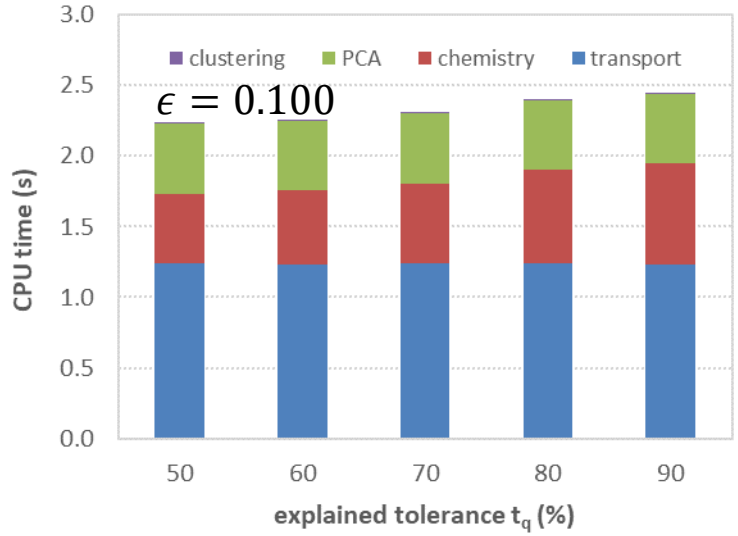


- By increasing the number of features D and/or decreasing the tolerance ε, the accuracy of the CA-based simulation increases monotonically
- Also in this case, the cost associated with the clustering algorithm is negligible, despite the higher number of species.
- As expected, the cost of the PCA step (~10 s) increases in terms of absolute values, but it is still only ~2% of the computational time of the original chemical step (~520 s).

Computational times: impact of t_q



- As expected, the overall computational cost of the CA-based simulation decreases monotonically with increasing tolerances.
- The saving in CPU time impacts the chemical step only



- The PCA computational time does not depend on the clustering parameters t_q and ϵ
- The clustering time weakly increases with the increasing number of features, but it is basically negligible

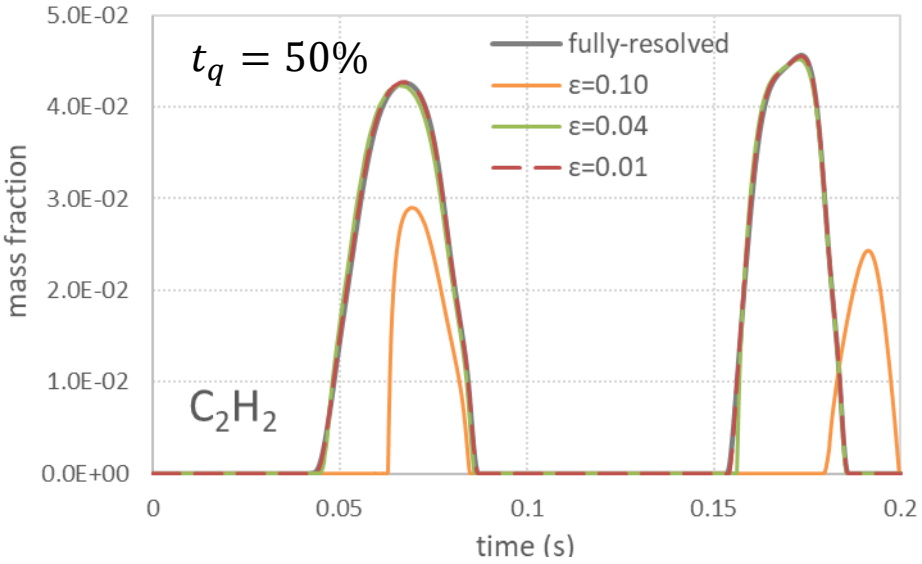
Detailed mechanism including PAHs

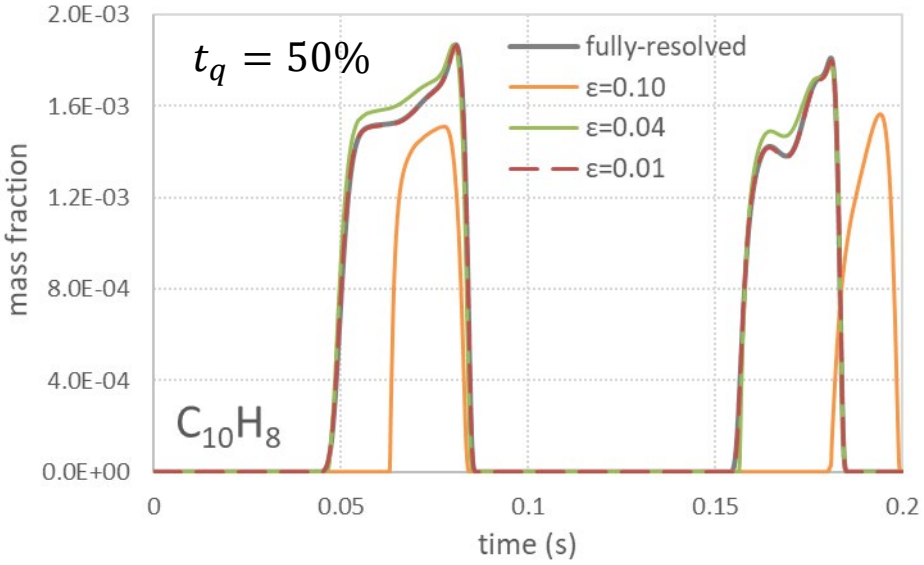
ISF F3 flames
Internal diameter: 4 mm
Velocities: 35 cm/s
Fuel composition: 80% C2H4 + 20% N2

Artificially imposed sinusoidal fluctuations of fuel stream velocity
Amplitude: 90%
Frequency: 10 Hz

Kinetic mechanism
224 species and 5939 reactions
PAH chemistry included
(up 2 aromatic rings)

Computational domain
2D region (55 x 120 mm)
~25,000 cells





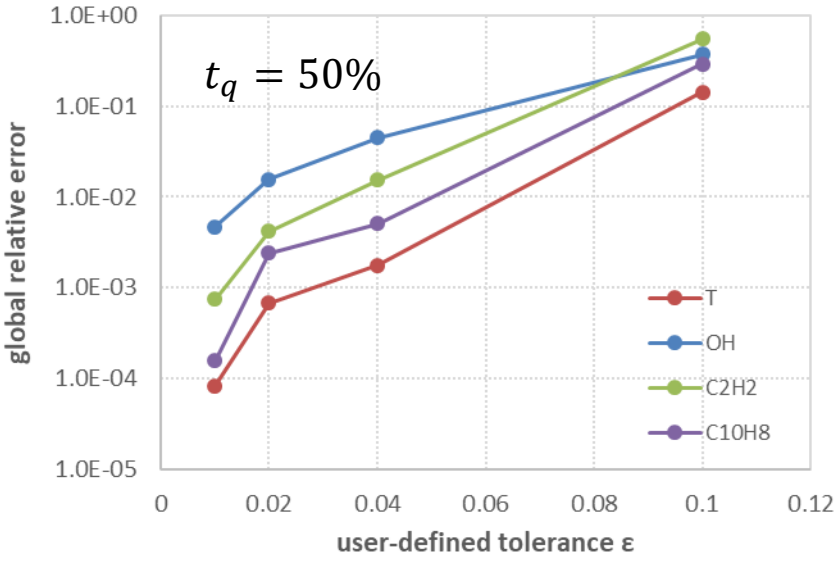
Global relative error

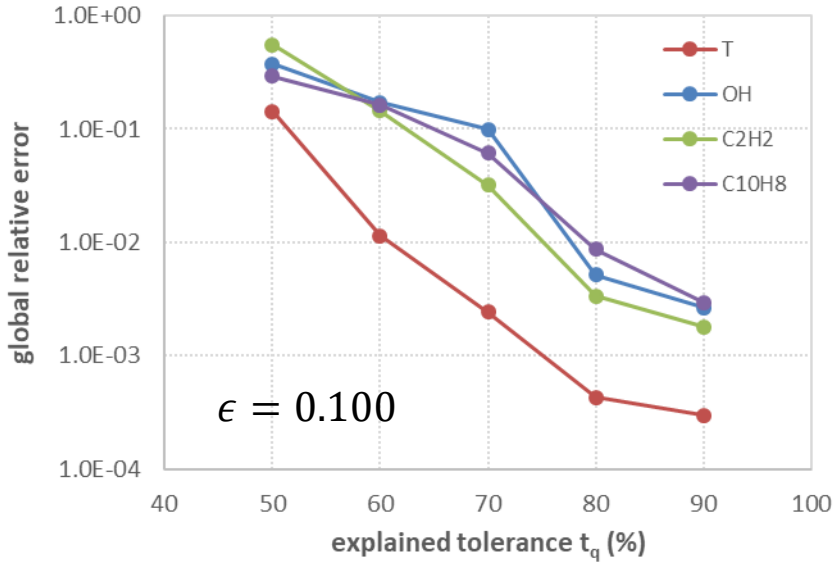
Global relative error

$$\varepsilon = \frac{1}{N_C N_T} \sum_{k=1}^{N_T} \sum_{i=1}^{N_C} \frac{\left|\psi_{k,i}^{CA} - \psi_{k,i}\right|}{\psi_{max}}$$

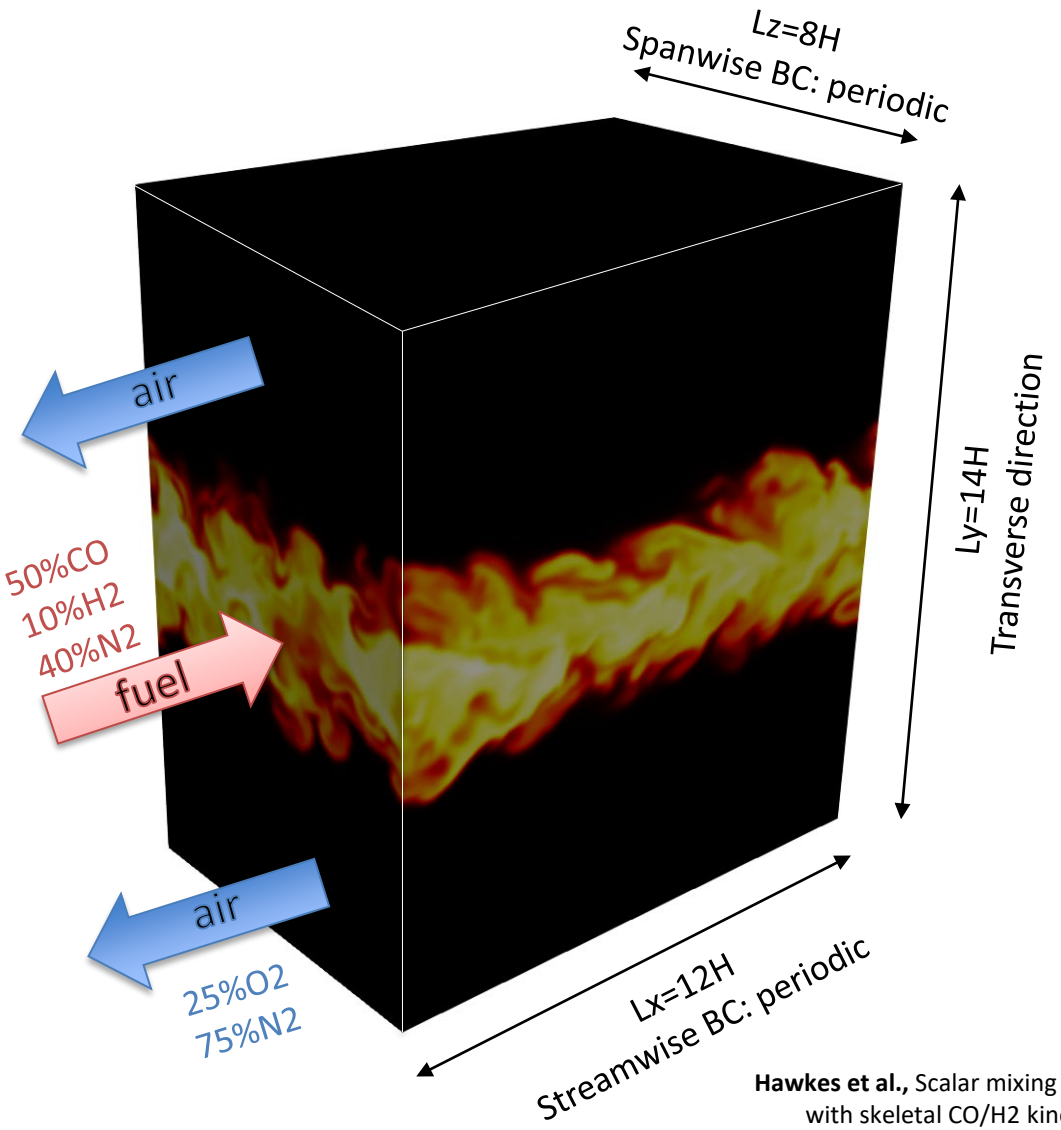
$\psi_{k,i}$ fully-resolved solution in cell i at time k

$\psi_{k,i}^{CA}$ CA-based solution in cell i at time k





Temporally-evolving planar jet-flame



Flame H

H = 1.37 mm
Re = 9079
tj = 4.96 µs
U = 276.4 m/s
Da = 0.011
Ma = 0.30

Quasi-DNS

Δx = 45 µm
Mesh: 365 x 426 x 243
Cells: ~37.8M

Solver

laminarSMOKE++ (based on OF-9)
https://github.com/acuoci/laminarSMOKE
Time discretization: implicit 2nd order backward Euler
Space discretization: OF *cubic* scheme

Hawkes et al., Scalar mixing in direct numerical simulations of temporally evolving plane jet flames with skeletal CO/H2 kinetics, Proceedings of the Combustion Insitute, 31, p. 1633-1640 (2007)

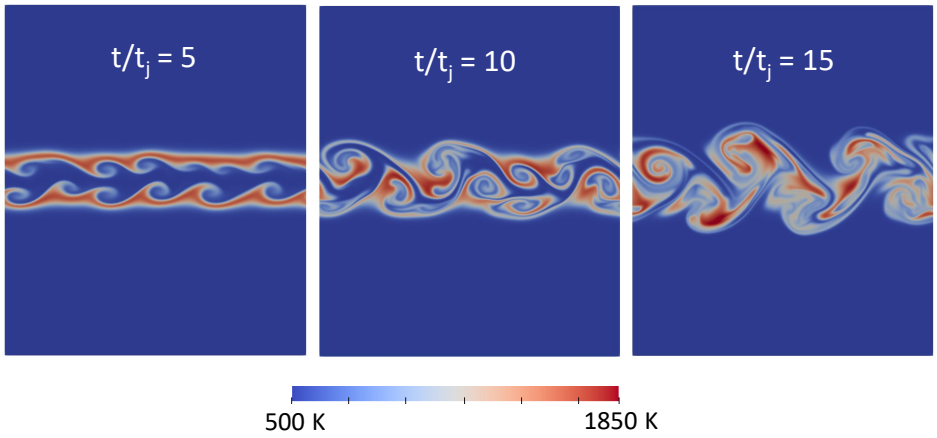
Sensitivity analyses: 2D simulations

Sensitivity analysis to PCA[2] parameters were carried out on 2D cases
- explained variance
- clustering tolerances

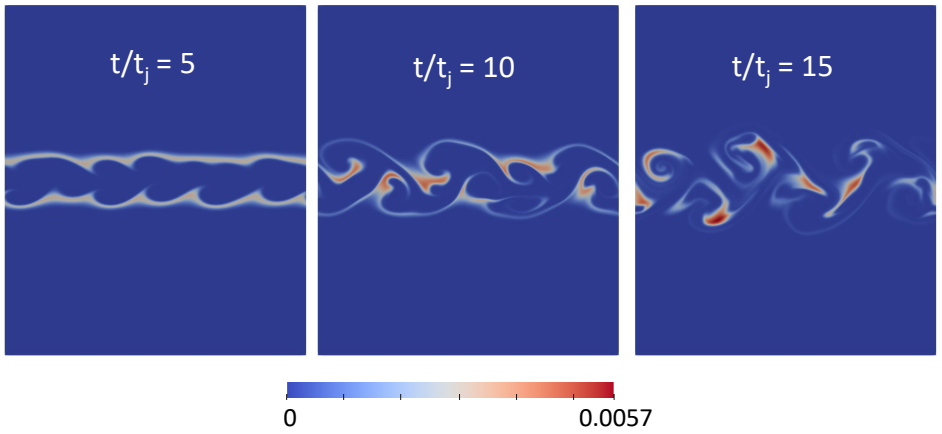
2D Mesh
Δx = 30 µm or 45 µm
Mesh: 548x640 or 365x426
Cells: ~350k or ~156k

Kinetic mechanisms
- Skeletal H2/CO mechanism by **Hawkes** et al. (2007): 11 species and 21 reactions
- Detailed H2/CO + NOx mechanism by **CRECK** Modeling Lab: 57 species and 385 reactions

Temperature



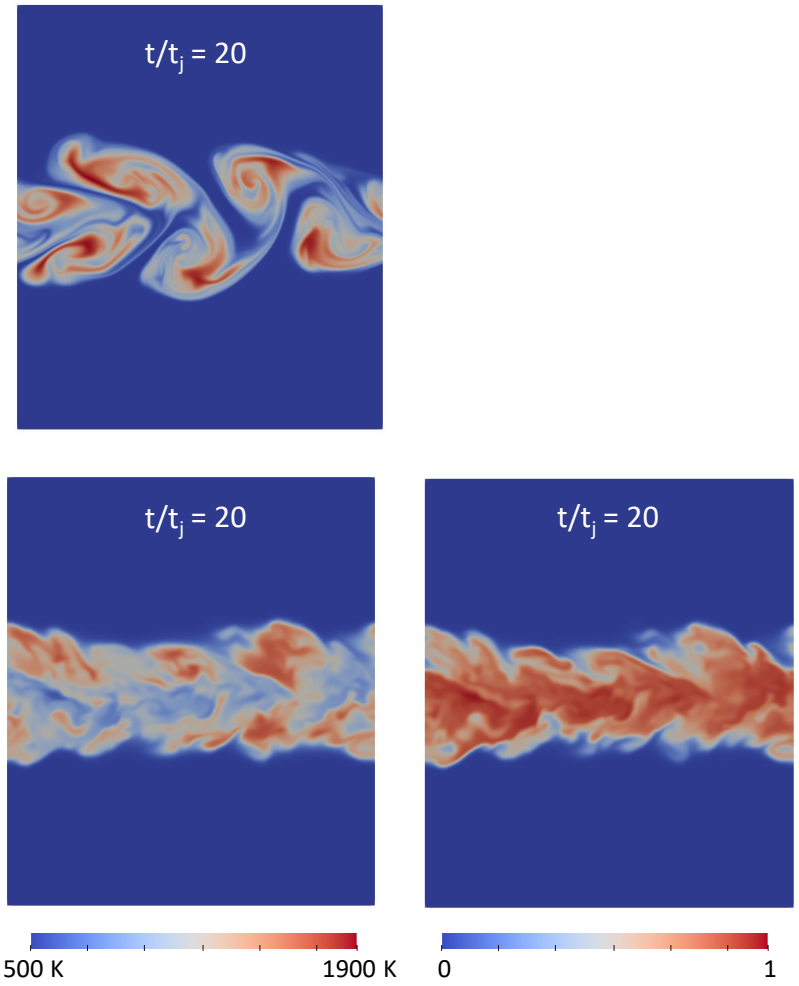
OH mass fraction



Comparison 2D vs 3D

temperature

mixture fraction



Stanley et al. (1998)

2D and 3D flows are **qualitatively very different**

- 2D jets are dominated by a large vortex dipole instability, which does not occur in 3D
- in 2D, large coherent structures
- in 2D, over-prediction of extinguished states
- in 3D, more small-scale structures
- In 3D, high-dissipation structures are more transient

Principal Component Analysis

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1Q} \\ x_{21} & x_{22} & \dots & x_{2Q} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nQ} \end{bmatrix} = \begin{bmatrix} T^1 & Y_1^1 & \dots & Y_p^1 \\ T^2 & Y_1^2 & \dots & Y_p^2 \\ \vdots & \vdots & \ddots & \vdots \\ T^n & Y_1^n & \dots & Y_p^n \end{bmatrix}$$

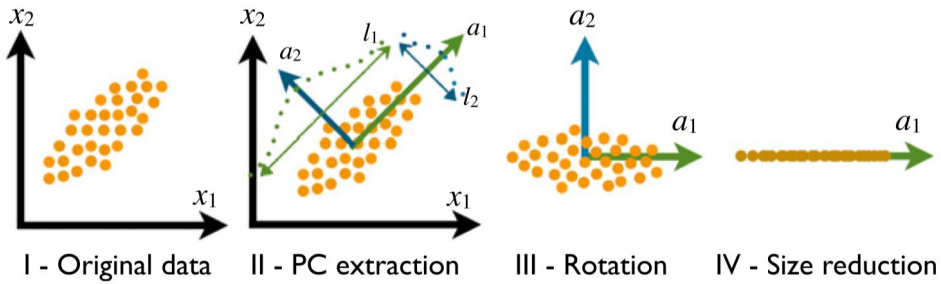
Instantaneous snapshot

State variable

Rows represent observations and columns correspond to the problem variables (T, and species mass fraction).

Covariance matrix

$$\mathbf{S} = \mathbf{X}^\mathbf{T}\mathbf{X} \longrightarrow \mathbf{S} = \mathbf{ALA}^\mathbf{T}$$



PC (Principal Components): eigenvectors of S, i.e. the columns of A

Eigenvalues: i.e. the diagonal of the L matrix, the portion of variance they account for.

Local PCA

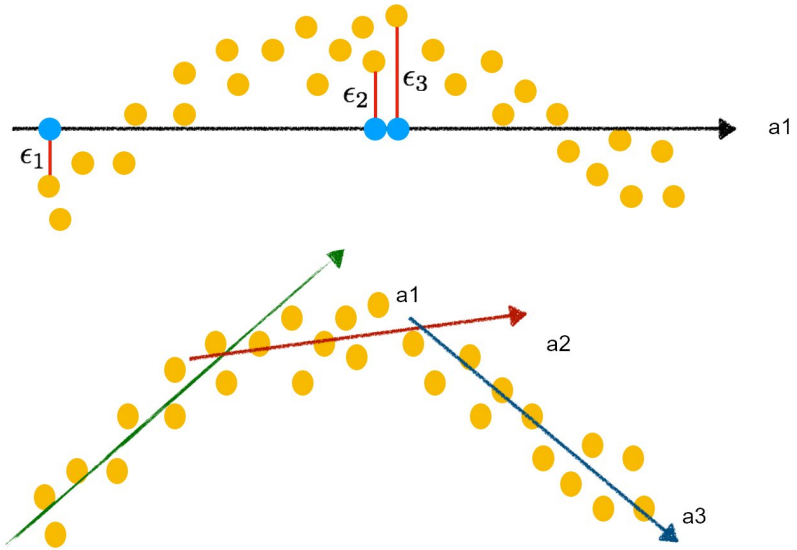
Problem

Because PCA is a linear combination of basis function, for **highly non-linear systems** such as combustion applications, a large number of PCs is required to describe the problem properly.

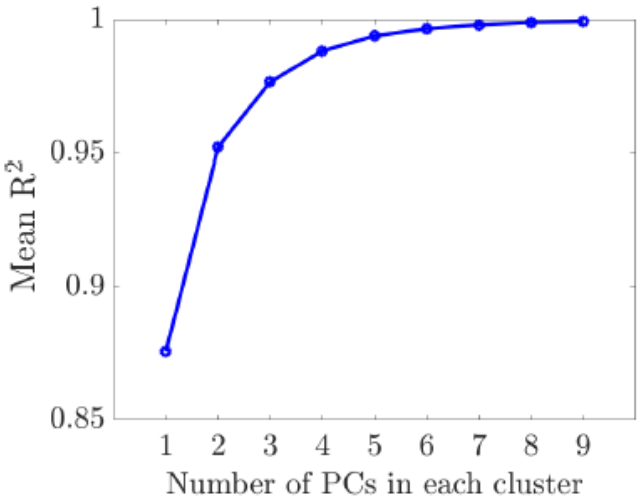
Solution

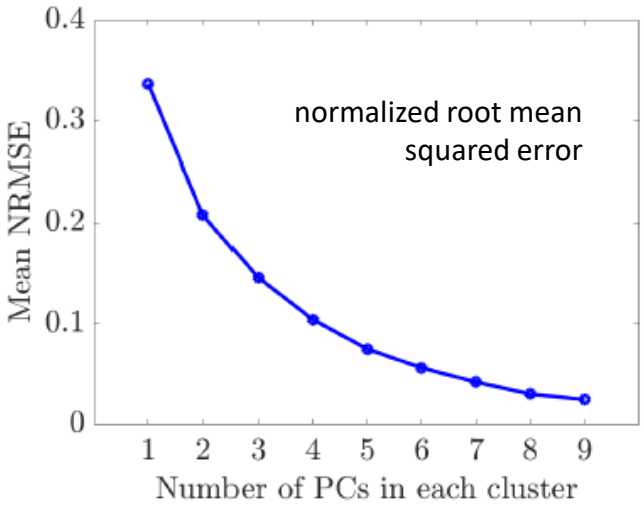
With a **local formulation of PCA (LPCA)** we overcome this problem.

The LPCA finds clusters of data which are characterized by similar properties, In each cluster PCA is performed, and a set of local PCs is found



Partitioning via LPCA and k-means





1. Initialization

The initial clusters centroids are chosen from a **k-means solution**. The eigenvector matrix in each cluster is initialized as the identity matrix.

2. Partition

Each observation is assigned to a cluster by means of the calculation of a reconstruction error.

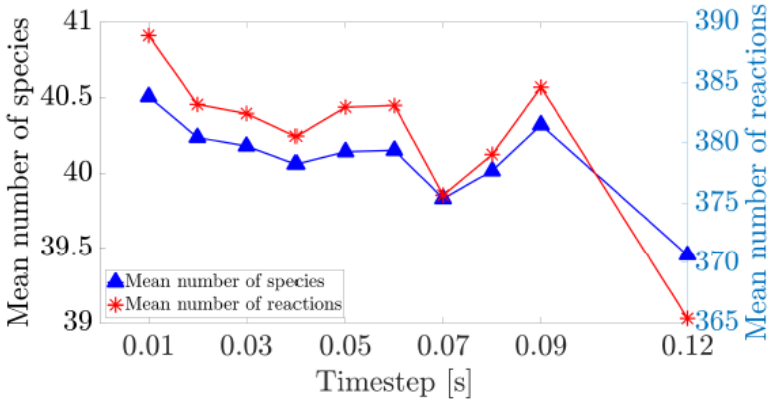
3. Update

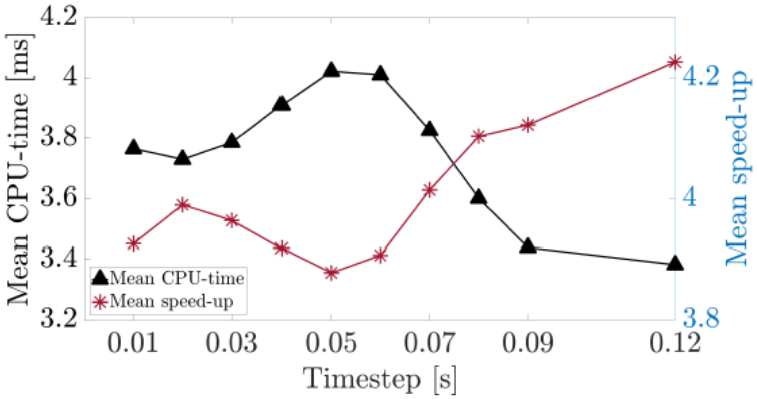
The cluster centroids are updated on the basis of the partitioning carried out at step 2.

4. Local-PCA

LPCA is performed in each cluster found at step 2.

Unsteady flame: new conditions (II)





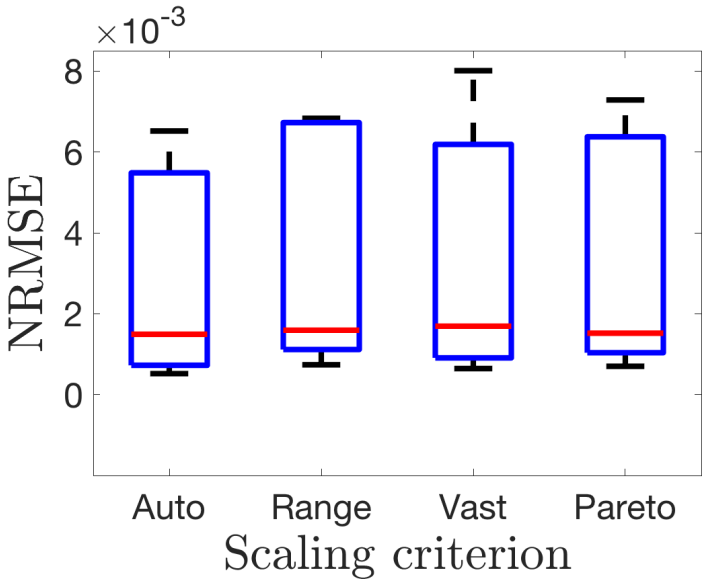
The average number of active species and reactions change in time because of the flame evolution

The active species and active reactions are strictly correlated

The CPU time is strongly dependent on the number of species

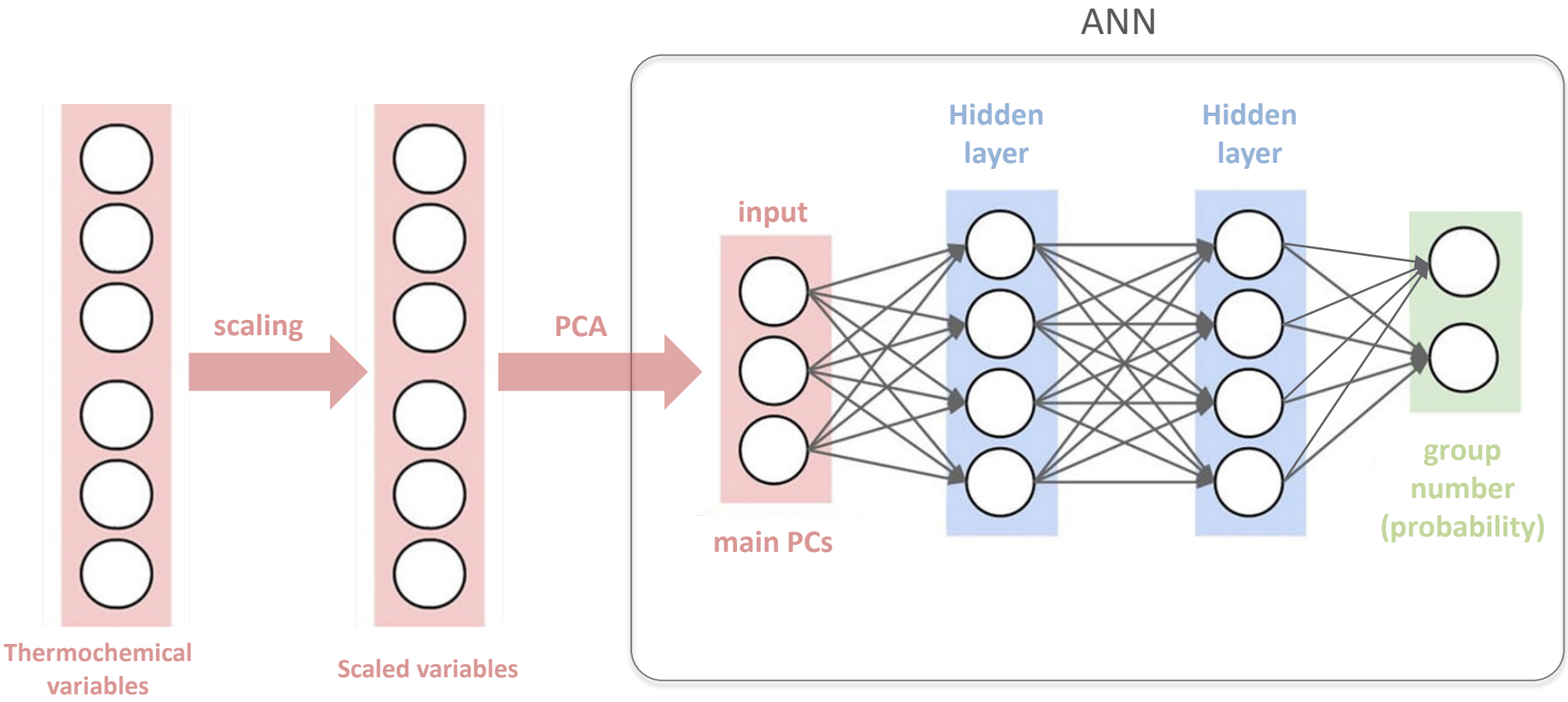
Scaling criterion of training data

The scaling criterion has a reduced effect on the chemical reduction and consequently on the adaptive simulation accuracy



ε_{DRGEP}	n_{sp}^{mean}	n_{sp}^{max}	λ_{mean}
AUTO	43	50	0.071
PARETO	41	51	0.070
VAST	43	52	0.074
RANGE	40	48	0.074

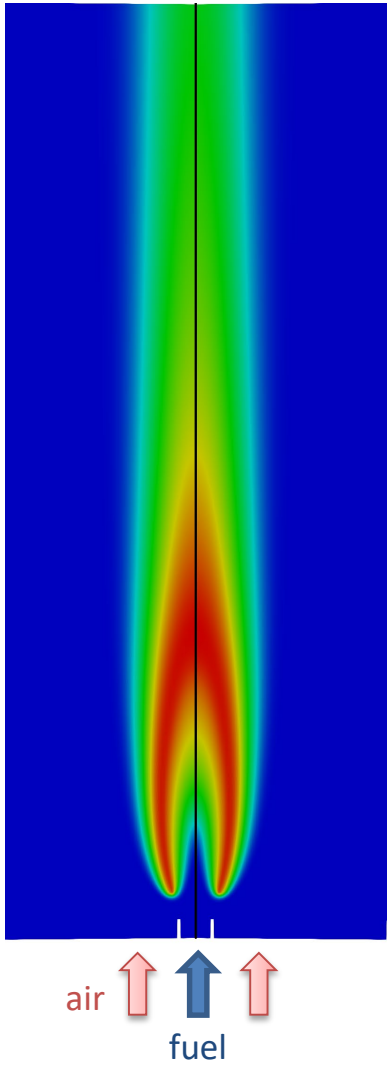
On-the-fly classification via ANN (II)



The ANN solves a **multi-class classification** problem

D'Alessio G., Cuoci A., Parente A., *Feature extraction and artificial neural networks for the on-the-fly classification of high-dimensional thermochemical spaces in adaptive-chemistry simulations*, Data-Centric Engineering (2020)

A test case: steady-state laminar coflow flame



Fuel stream

Composition:34% C_2H_4, 66% N_2

Velocity: 35 cm/s (parabolic)

Oxidizer stream

Composition: 21% O_2, 79% N_2

Velocity: 35 cm/s (flat)

Geometry

Fuel nozzle diameter: 4 mm

Thickness: 0.38 mm

Coflow diameter: 50 mm

R.K. Mohammed, et al., *Computational and experimental study of a forced, time-varying, axisymmetric, laminar diffusion flame*, Symposium (International) on Combustion, 27(1):693-702, 1998.

Numerical simulation

Axisymmetric 2D Mesh

Domain: 54 x 120 mm

Cells: ~25,000

Kinetic mechanism

POLIMI_C1C3_HT_1412

84 species and 1698 reactions

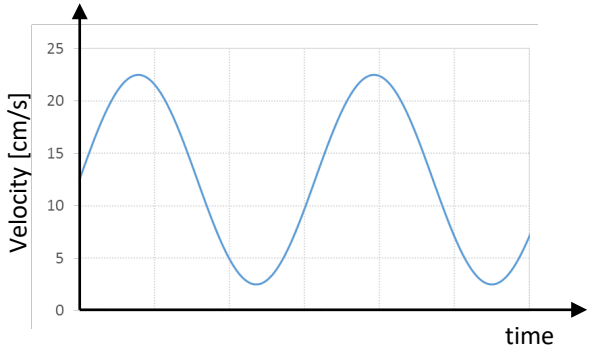
CFD code

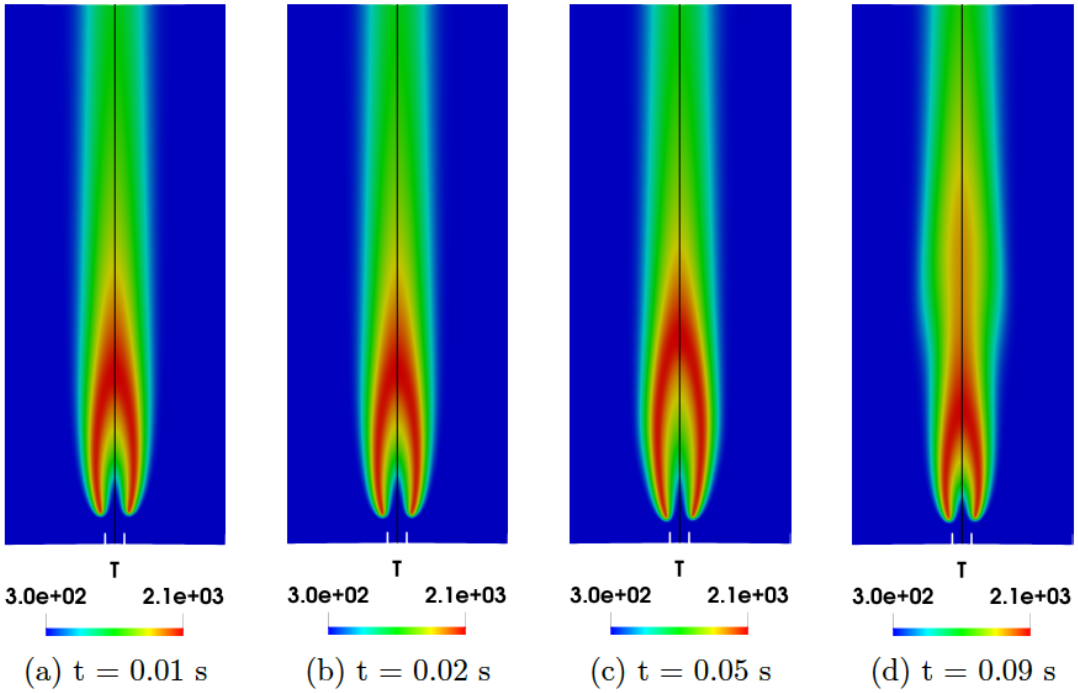
`laminarSMOKE` (based on the operator splitting approach)

Generation of training dataset

The dataset was created by introducing a perturbation in the fuel inlet velocity, according to a sinusoidal function with prescribed amplitude A and frequency f

$$v_{fuel}(t) = v_{fuel}^{ss}[1 + A\ sin(2\pi f t)]$$





(a) t = 0.01 s (b) t = 0.02 s (c) t = 0.05 s (d) t = 0.09 s

Dataset: f10A25

A dataset with ~130,000 observations was created by imposing a frequency of 10 Hz and an amplitude of 0.25

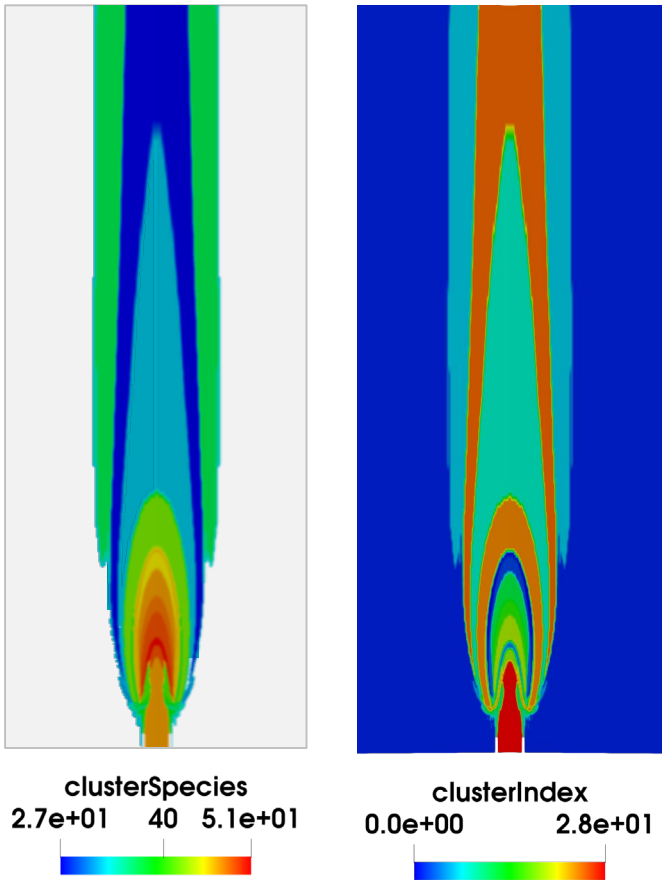
https://www.kaggle.com/datasets/albertocuoci/laminar-coflow-flame-drm19-ch4n2-6535

Reduction of kinetics: DRG-EP

DRG-EP is applied in each cluster to generate the reduced mechanisms.

- For each sample point a reduced mechanism was generated. A single reduced mechanism for each cluster was created as the union of species and reactions corresponding to the individual reduced mechanisms of each sample point for that cluster.

- Fuel and oxidizer were assumed as target species for DRG-EP, and several **tolerance thresholds** ε were tested (0.005 to 0.1)



P. Pepiot-Desjardins, H. Pitsch, *An efficient error-propagation-based reduction method for large chemical kinetic mechanisms*, Combustion Theory and Modelling 12 (2008) 1089–1108

A priori analysis of partitioning

ε_{DRGEP}	n_{sp}^{mean}	n_{sp}^{max}	λ_{mean}
0.030	31	38	0.080
0.020	34	42	0.079
0.010	39	44	0.075
0.005	43	50	0.071

Dissimilarity coefficient $\lambda = \frac{1}{n_{sp}} \sum_{i=1}^{n_{sp}} (1 - x_i)$ Good partitioning: $\lambda \to 0$

$$x_i = \frac{1}{n_{obs}} \sum_{j=1}^{n_{obs}} \delta_{ij}$$

$$\delta_{ij} = \begin{cases} 1 & \text{If species } i \text{ is included in reaction mechanism generated by observation j} \\ 0 & \text{otherwise} \end{cases}$$

A posteriori analysis of partitioning

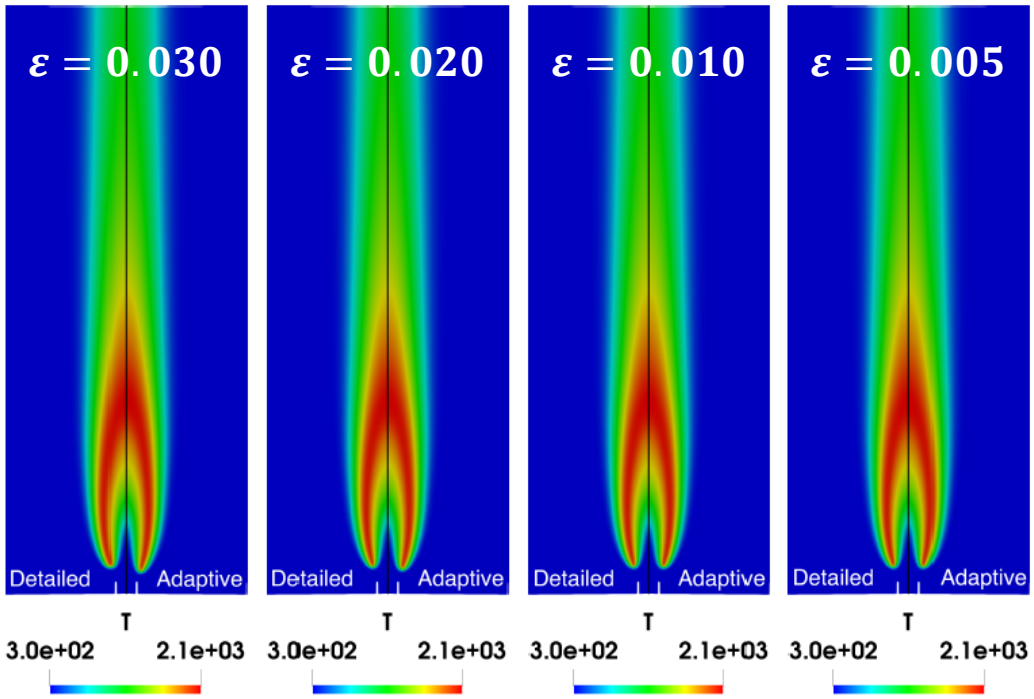
1. Steady-state flame
2. Unsteady flame: f=10Hz, A=025

Same data used for training (Testing purposes only)

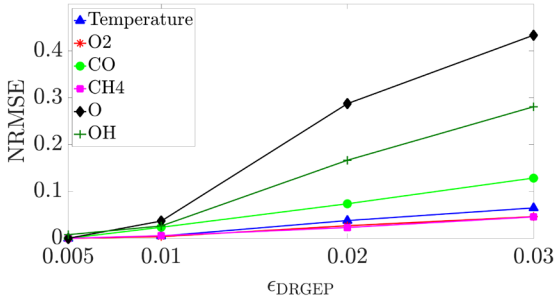
3. Unsteady flames: f=10, 40, 80 Hz, A = 0.50, 0.75, 0.90

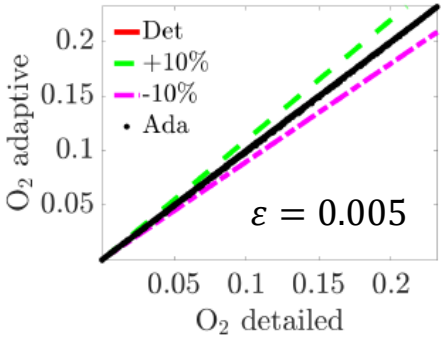
! Exploration of new conditions not included in the training dataset

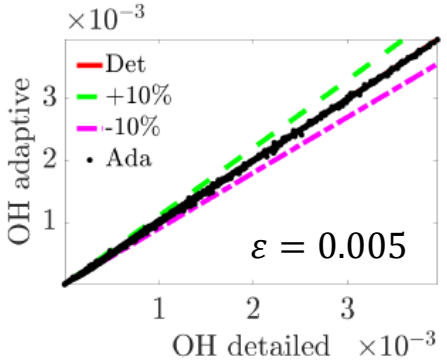
Results: steady-state flame

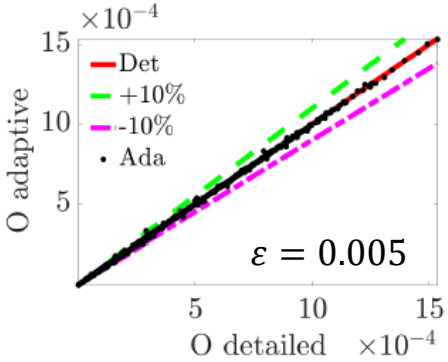


ε_{DRGEP}	Speed-up
0.030	5.4
0.020	4.9
0.010	4.6
0.005	4.0

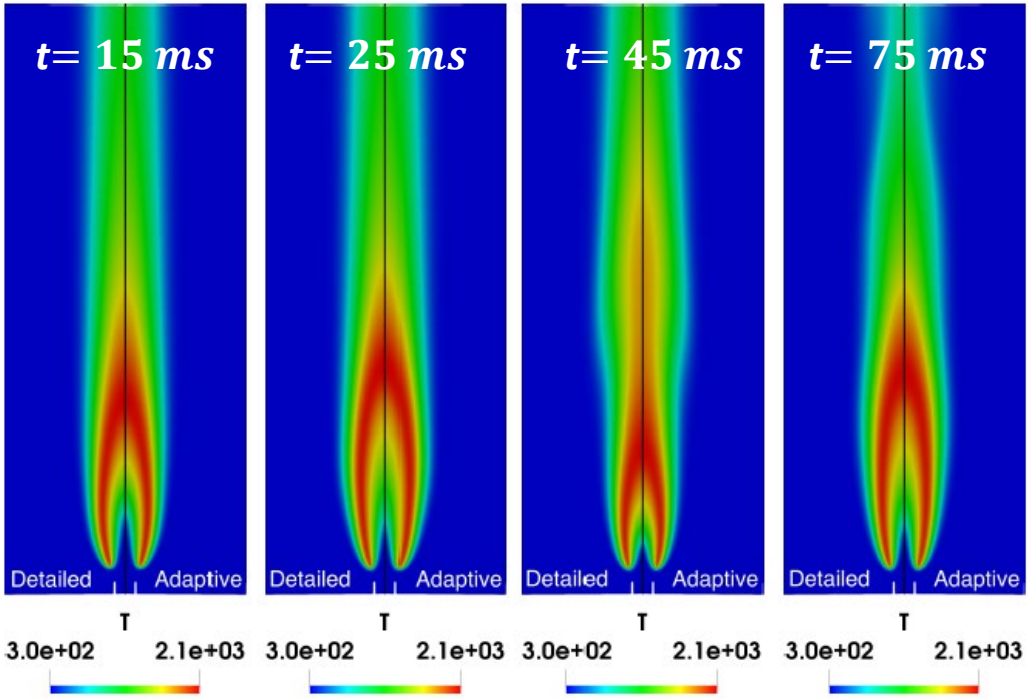


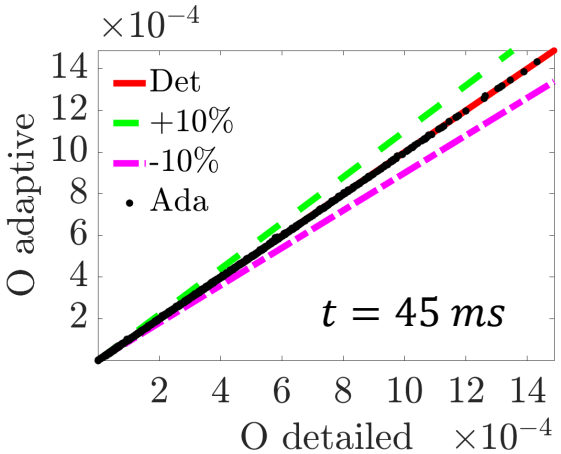


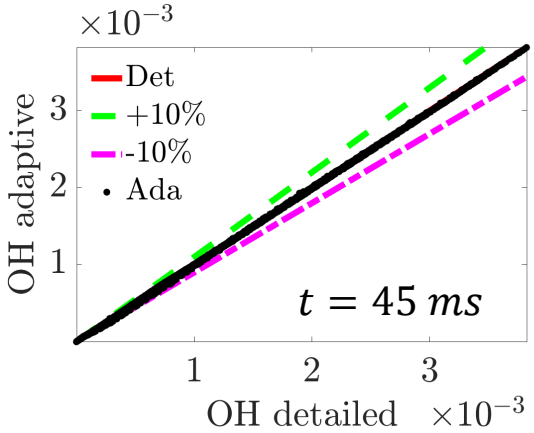




Results: unsteady flames







Same training dataset

f10A25

$\varepsilon = 0.005$

New conditions

f = 20 Hz

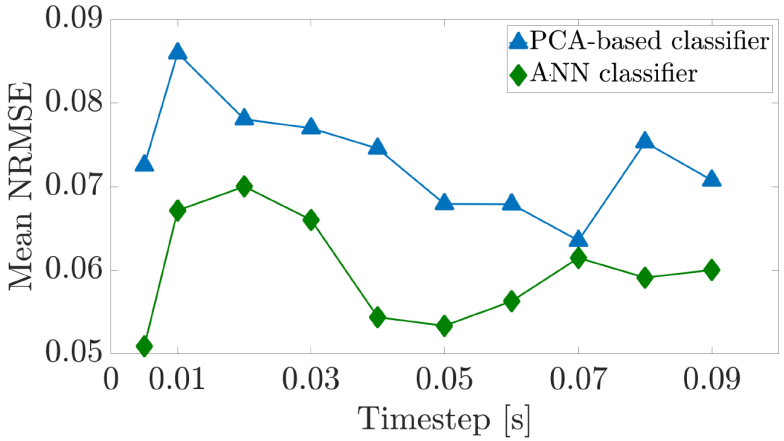
A = 0.25

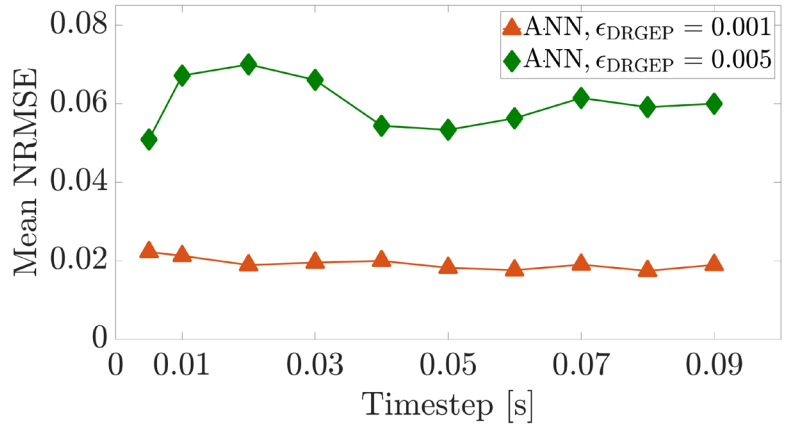
Results: average errors

- The ANN used for the classification consisted of **2 hidden layers with 200 and 400 neurons**, respectively, chosen after an optimization of the hyper-parameters to achieve a satisfactory accuracy in the class prediction.

- The activation functions chosen for the hidden layers were both **ReLU (Rectified Linear Unit)**, with a **softmax activation** for the output layer as required in case of multi-class classification tasks.

Averaged normalized root mean square error over time





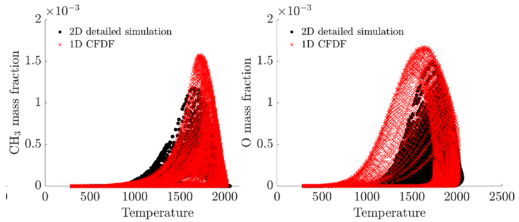
SPARC: Sample-Partitioning Adaptive Reduced Chemistry

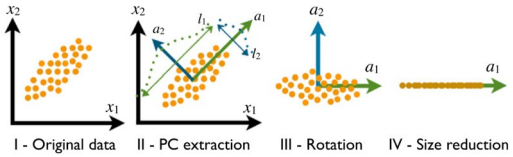
Training phase

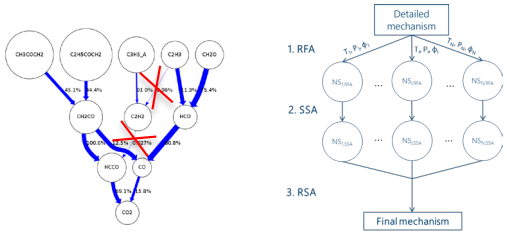
1. • Data generation
2. • Clustering based on similarity of thermochemical state
3. • Generation of reduced kinetic mechanisms via DRG-EP

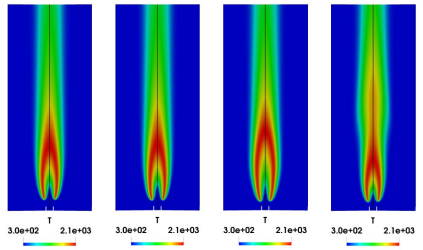
Simulation

4. • CFD simulation based on reduced mechanisms









D'Alessio G., Parente A., Stagni A., Cuoci A., *Adaptive chemistry via pre-partitioning of composition space and mechanism reduction*, Combustion and Flame, 211, p. 68-82 (2020)

SPARC: Sample-Partitioning Adaptive Reduced Chemistry

Training phase

1. • Data generation

Choice of a proper **training dataset** is the most important step!

2. • Clustering based on similarity of thermochemical state

Supervised/Unsupervised clustering

3. • Generation of reduced kinetic mechanisms via DRG-EP

Reduction is done off-line, so more advanced (expensive) techniques can be used

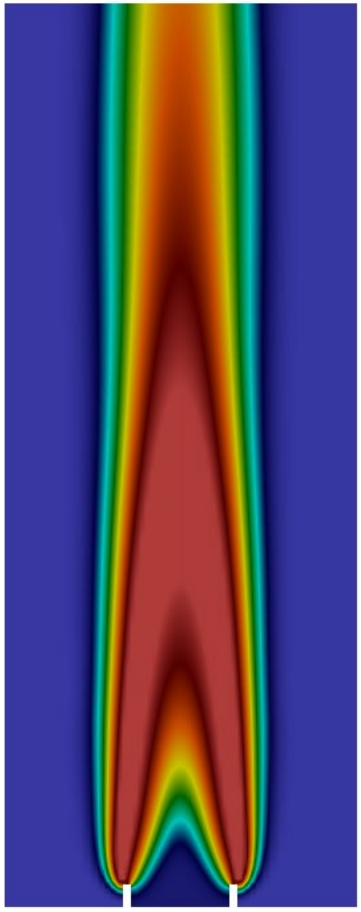
Simulation

4. • CFD simulation based on reduced mechanisms

Fast **on-the-fly classification** is required

D'Alessio G., Parente A., Stagni A., Cuoci A., *Adaptive chemistry via pre-partitioning of composition space and mechanism reduction*, Combustion and Flame, 211, p. 68-82 (2020)

A test case: $nC_7H_{16}/CH_4/N_2$ laminar flame



Fuel stream
Composition: 2.47% nC_7H_{16}, 48.7% CH_4, 48.7% N_2
Velocity: 10.12 cm/s (parabolic)

Oxidizer stream
Composition: 21% O_2, 79% N_2
Velocity: 12.32 cm/s (flat)

Geometry
Fuel nozzle diameter: 11 mm
Thickness: 0.90 mm
Coflow diameter: 50 mm

Axisymmetric 2D Mesh
Domain: 40 x 100 mm
Cells: ~10,000

Kinetic mechanism
POLIMI_PRF_PAH_HT_1412
176 species and 6067 reactions

CFD code
`laminarSMOKE` (based on the operator splitting approach)

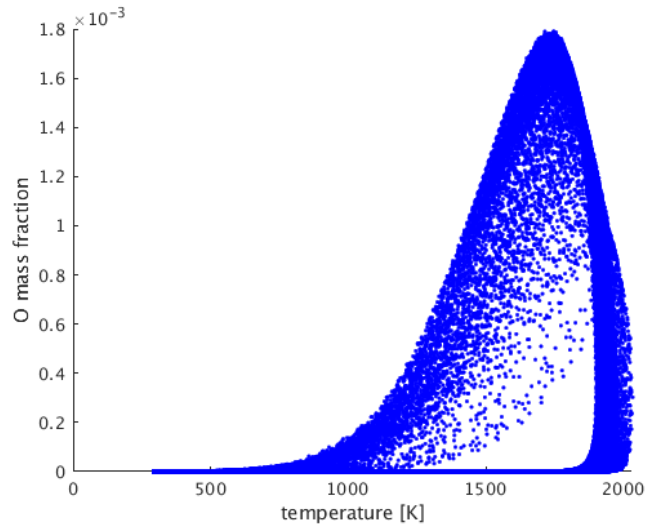
M. Kashif et al., *Sooting propensities of some gasoline surrogate fuels: Combined effects of fuel blending and air vitiation*, Combustion and Flame, 162(5):1840–1847, 2015

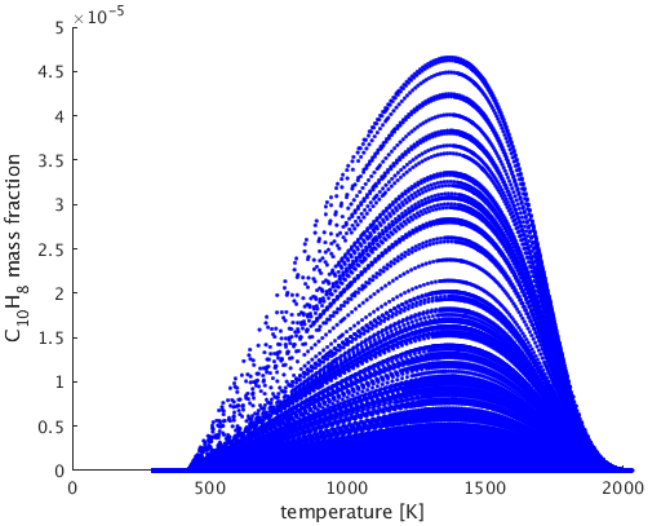
Generated of training dataset

- The generated data set must cover adequately the composition space that is expected to be visited during the simulation of the system under investigation

- The samples were generated by means of **1D counterflow diffusion flames (CFDF)**, adopting a wide range of strain rates randomly chosen from 15 to 1000 1/s (i.e., from **thermodynamic equilibrium to extinction)**

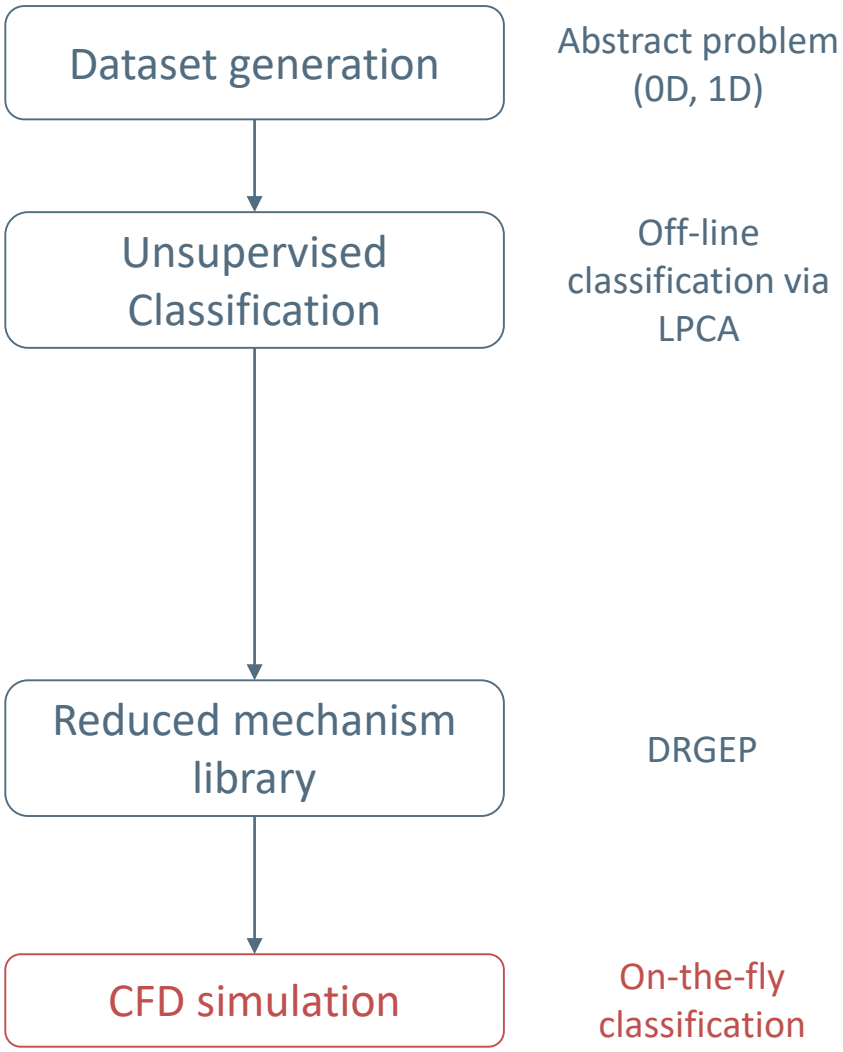
- The resulting data set consists of about 220,000 observations, corresponding to ~100 different CFDF flames.





On-the-fly classification via ANN

- If the chemical mechanism consists of a large number of species, the classification can be a difficult task to accomplish since the **use of distances in high-dimensional spaces can sometimes lead to poor results** (Aggarwal, 2001)
- **ANN** represent a valid alternative to improve the classification efficiency, as they do not rely on the use of the metrics in high-dimensional spaces



D'Alessio G., Cuoci A., Parente A., *Feature extraction and artificial neural networks for the on-the-fly classification of high-dimensional thermochemical spaces in adaptive-chemistry simulations*, Data-Centric Engineering (2020)

On-the-fly classification via ANN

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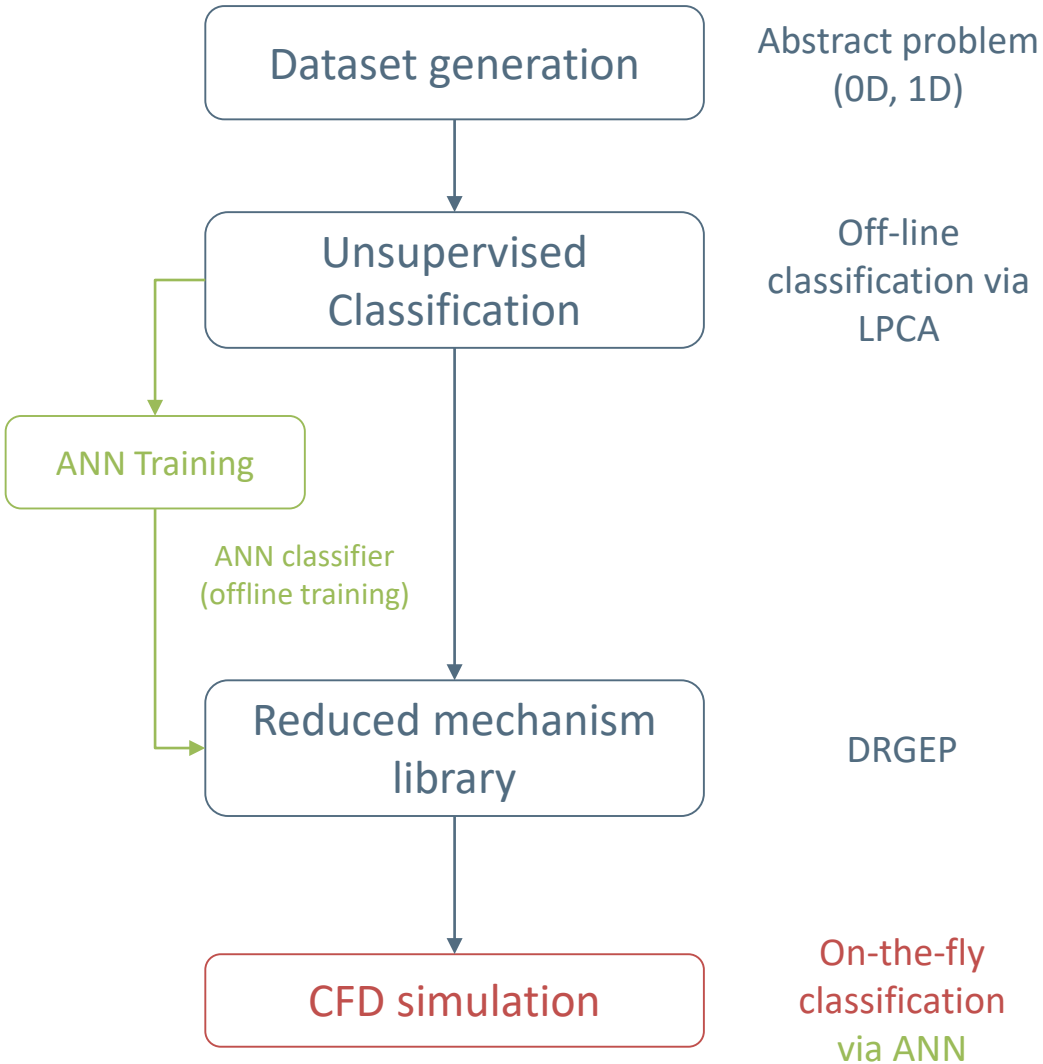

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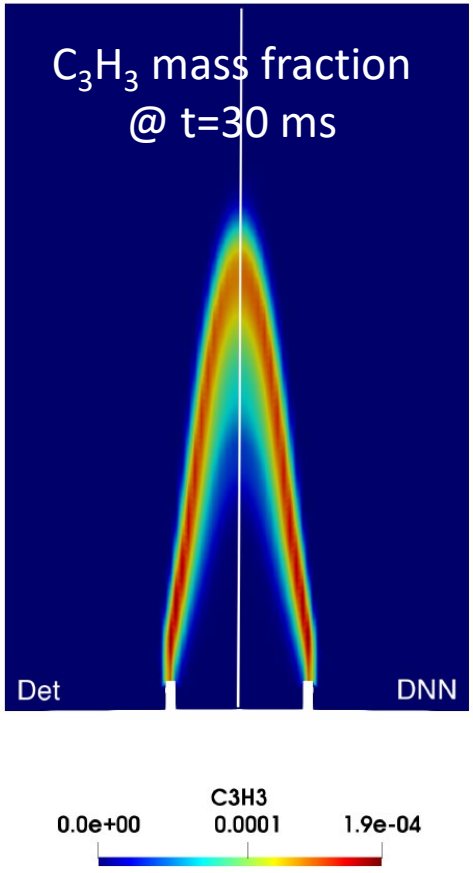
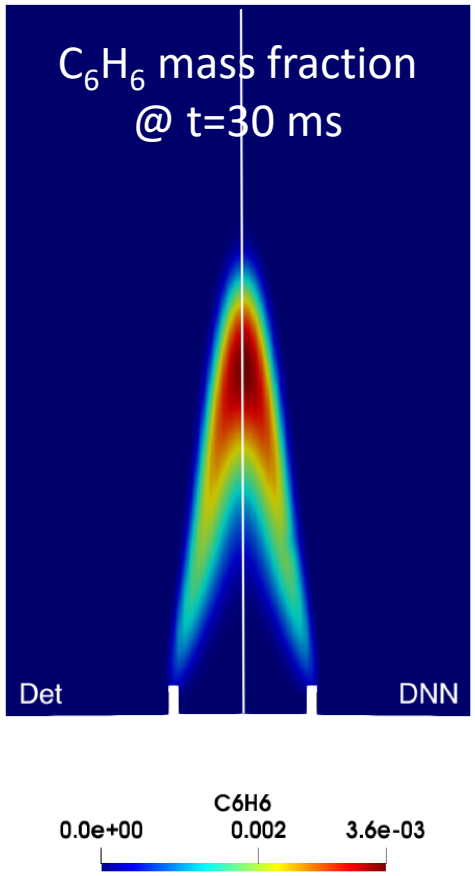
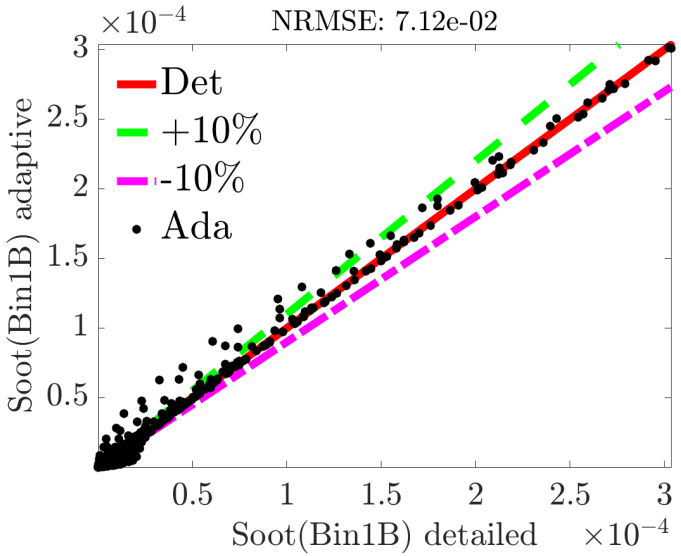
Results: comparison with full-chemistry



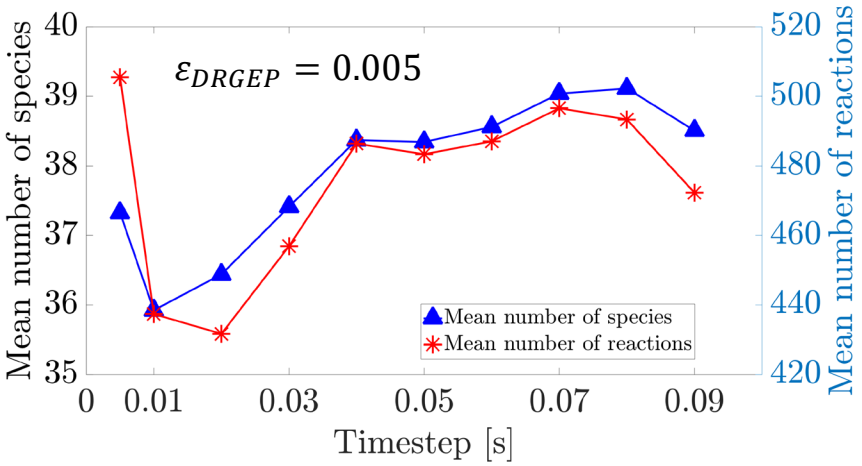




BIN1B (C_{20}) is the heaviest species in the mechanism, and it is a soot precursor

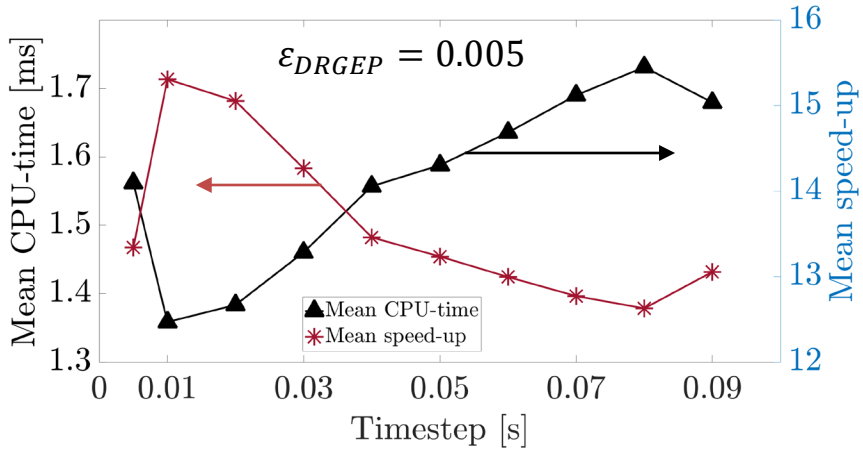
A satisfactory level of agreement is observed not only for main species, but also for radicals (such as propargyl) and heavy species (such as benzene and soot precursors).

Results: speed-up



The reduction in terms of number of species is remarkable (about 50%).

A stronger reduction in the number of active reactions is evident: less than 10% of the original reactions are retained.



The **speedup factor** changes in time because the number of species and reactions can also change in time depending on the local flame chemistry

Numerical solution