DATA-DRIVEN, PHYSICS-INFORMED SIMULATION OF TURBULENT REACTING FLOWS:

current state, challenges and perspectives

Alessandro Parente, Axel Coussement, Giuseppe D'Alessio, Kamila Zdybał, Rafi Malik

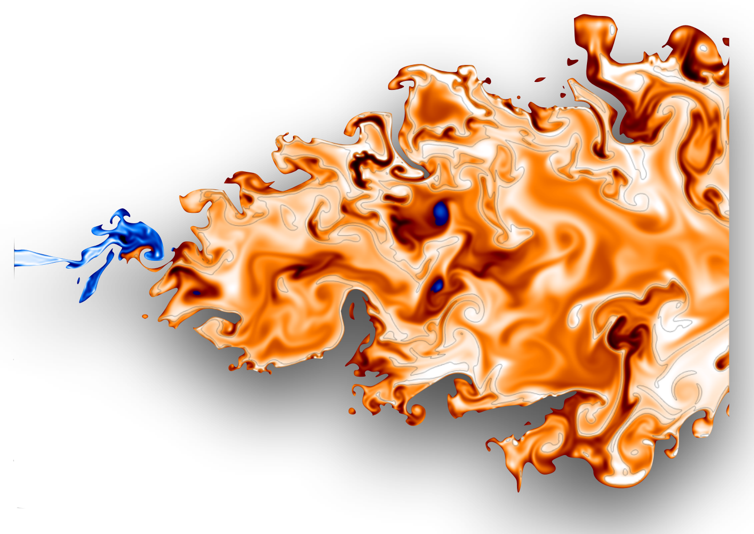
ERCOFTAC Autumn Festival 2023

Science has entered a *fourth paradigm*, based on the availability of massive data and new analytics

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v})$$

$$\frac{\partial \rho_i}{\partial t} = -\nabla \cdot (\rho_i \mathbf{v}) - \nabla \cdot \mathbf{J}_i + \omega_i$$

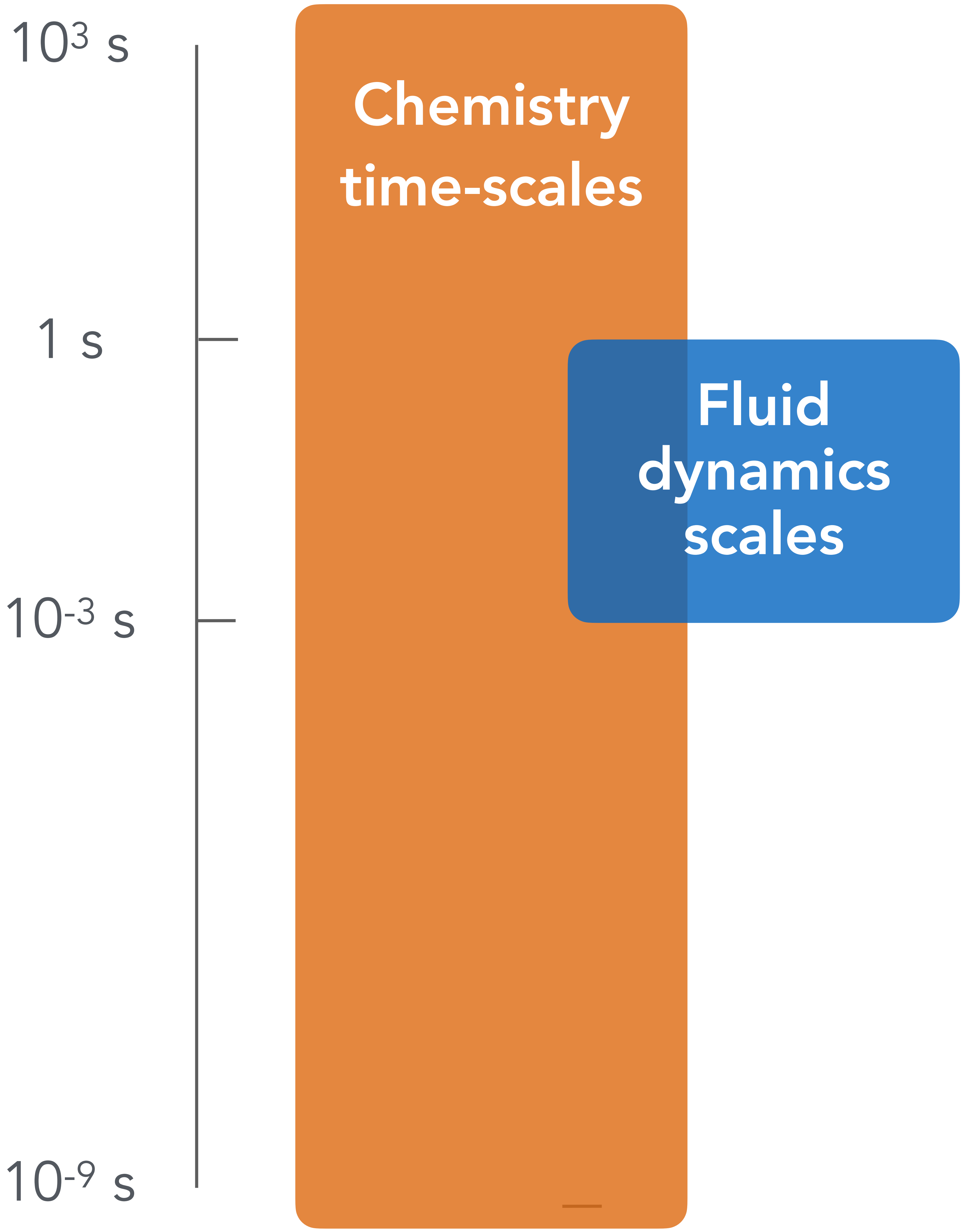
$$\frac{\partial \rho \mathbf{v}}{\partial t} = -\nabla \cdot (\rho \mathbf{v}\mathbf{v}) - \nabla \cdot \mathbf{T} - \nabla p + \sum_{i=1}^{n_s} \rho_i \mathbf{f}_i$$



Renaissance — Computers — Big data — **Now**

Experimental science	**Theoretical science**	**Computational science**	**Data-intensive science**
Empiricism: observation of natural phenomena	*Theories, modelling and generalisation*	*Simulations and high-performance computing*	*Reconciliation of theory, experiments & simulations*

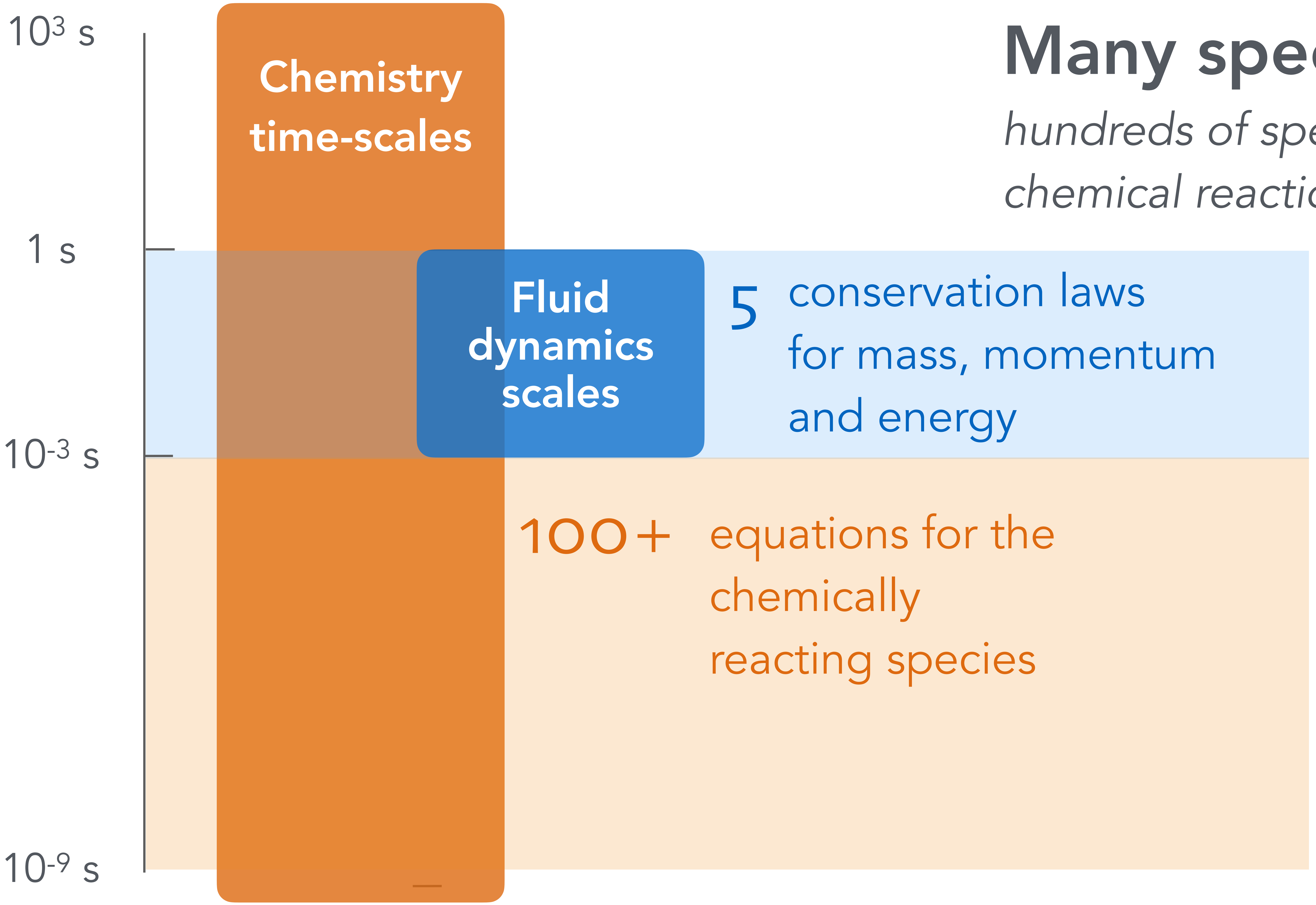
Grand challenges in turbulent reacting flows



Small scales

Chemical time scales span 12 decades and can strongly overlap with fluid dynamic ones

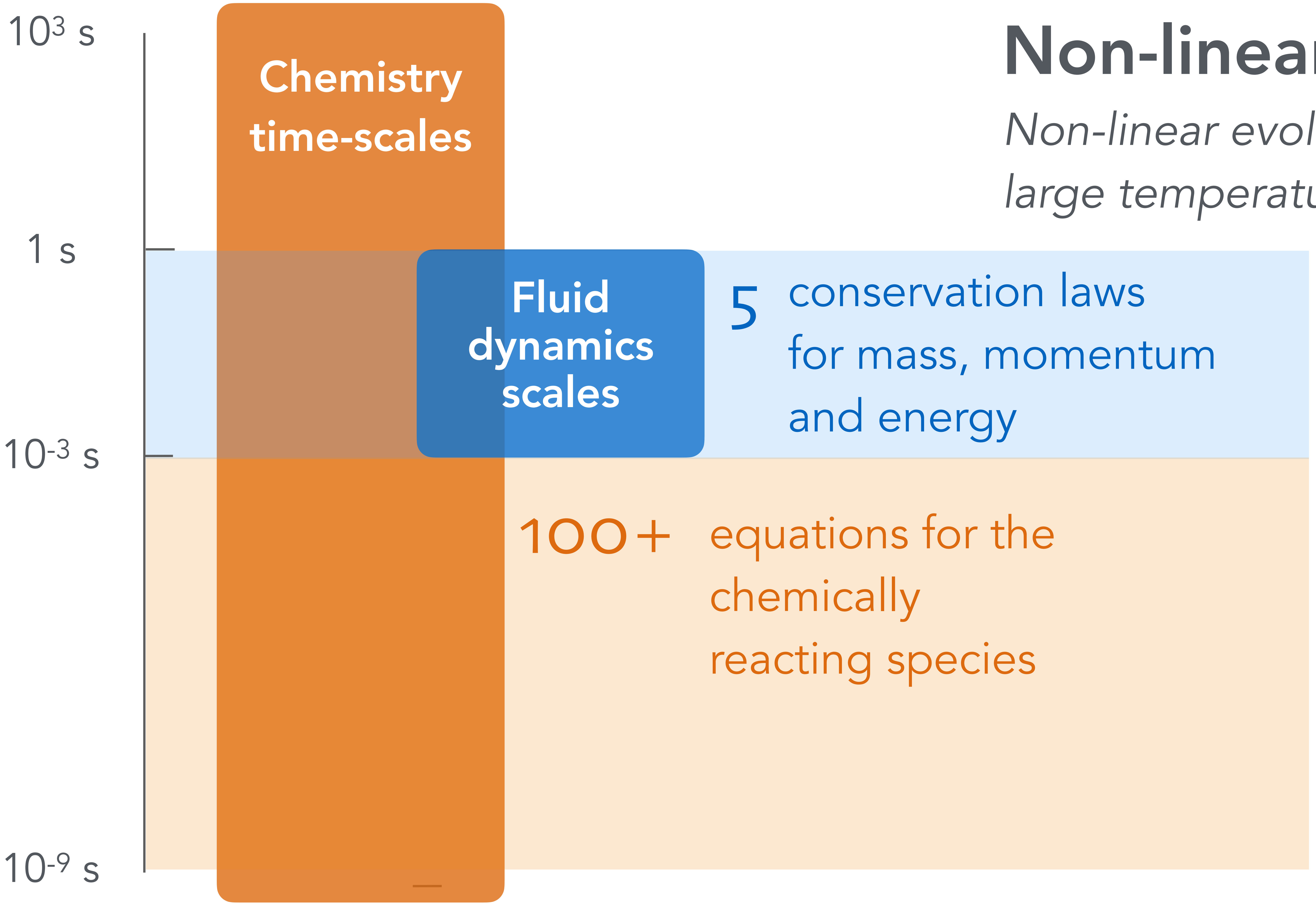
Grand challenges in turbulent reacting flows



Many species

hundreds of species tightly coupled via thousands chemical reactions

Grand challenges in turbulent reacting flows



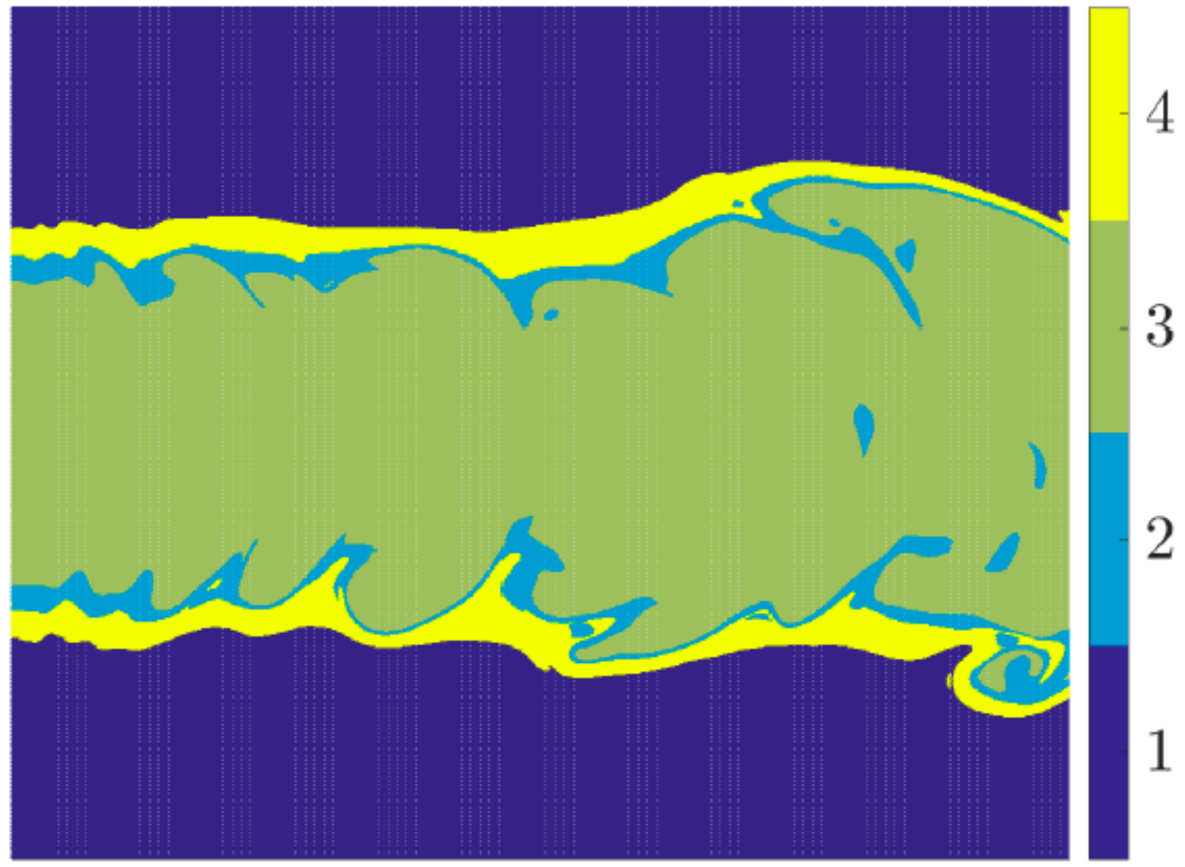
Non-linear interactions

Non-linear evolution of the chemical state-space and large temperature fluctuations

$$k_{f,j} = A_{f,j} T^{\beta_{f,j}} exp\left(-\frac{E_{f,j}}{RT}\right)$$

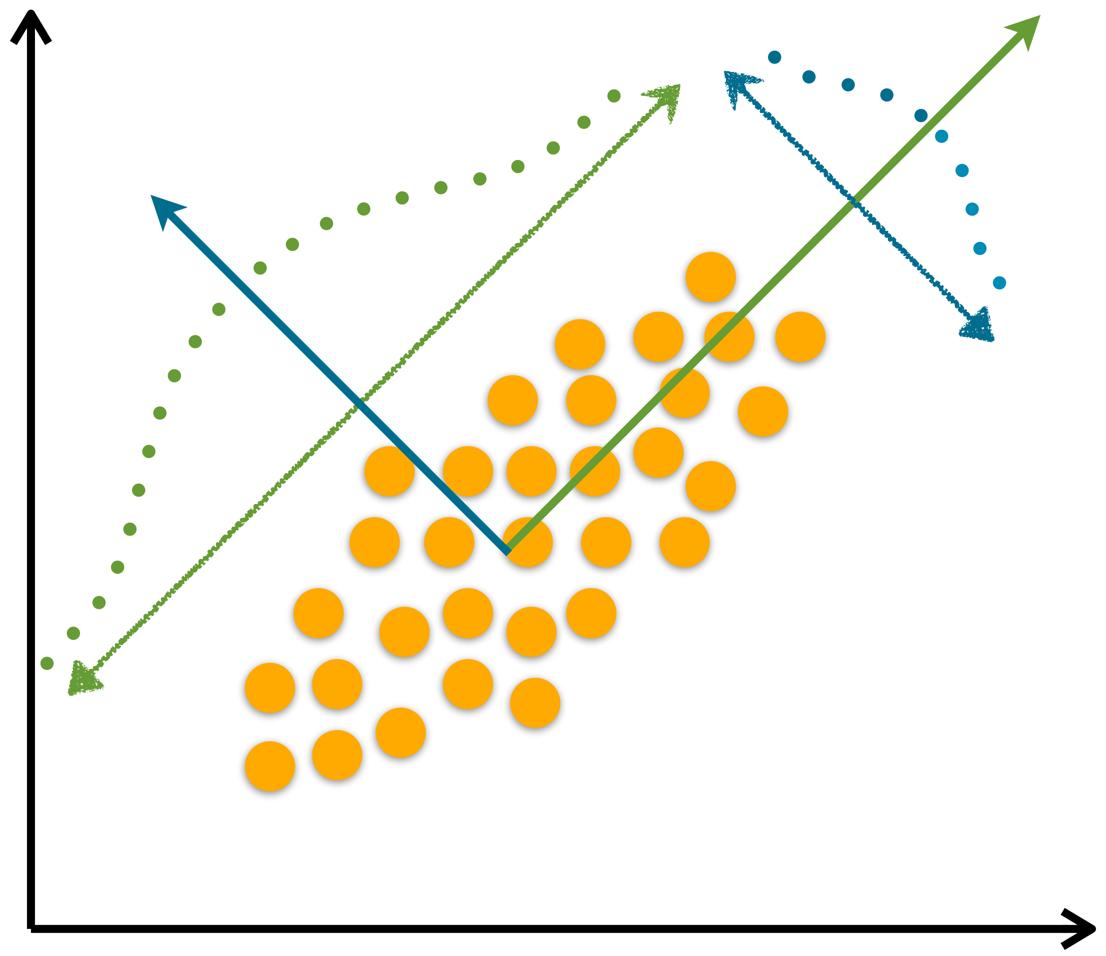
Machine learning for combustion

Feature extraction



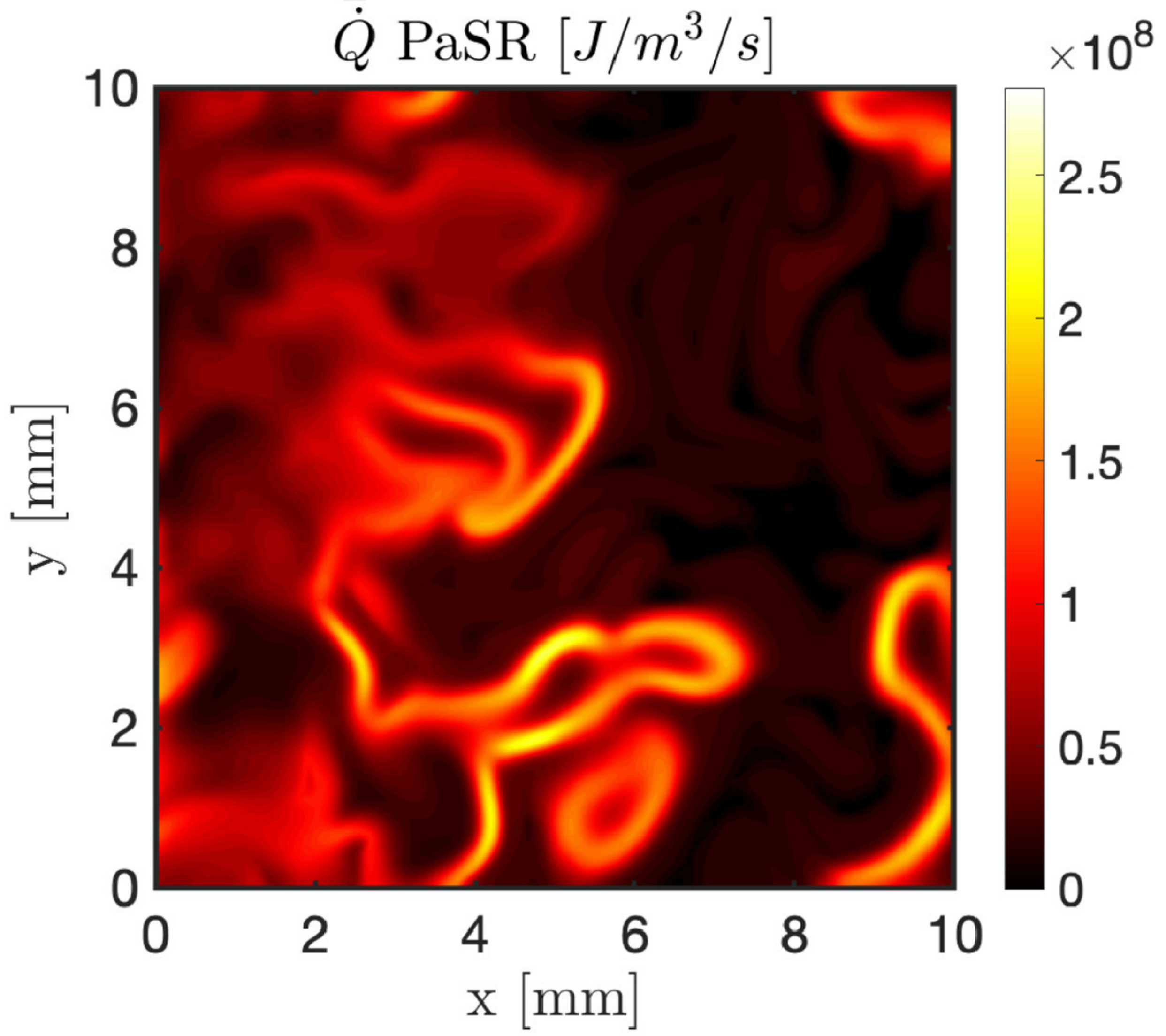
Improving knowledge and description of turbulent reacting flows

Dimensionality reduction



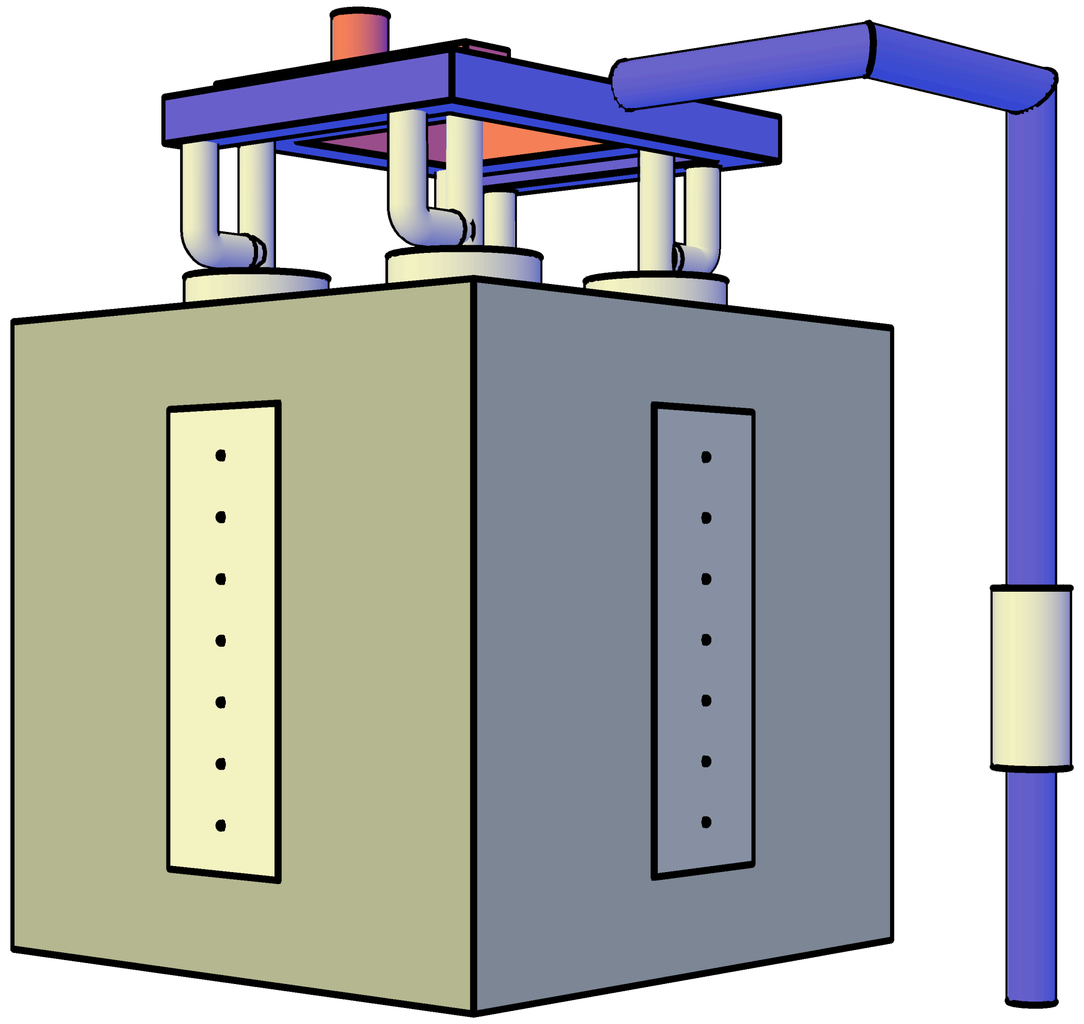
Reducing the cost of large-scale combustion simulations

Data-enhanced models and closures



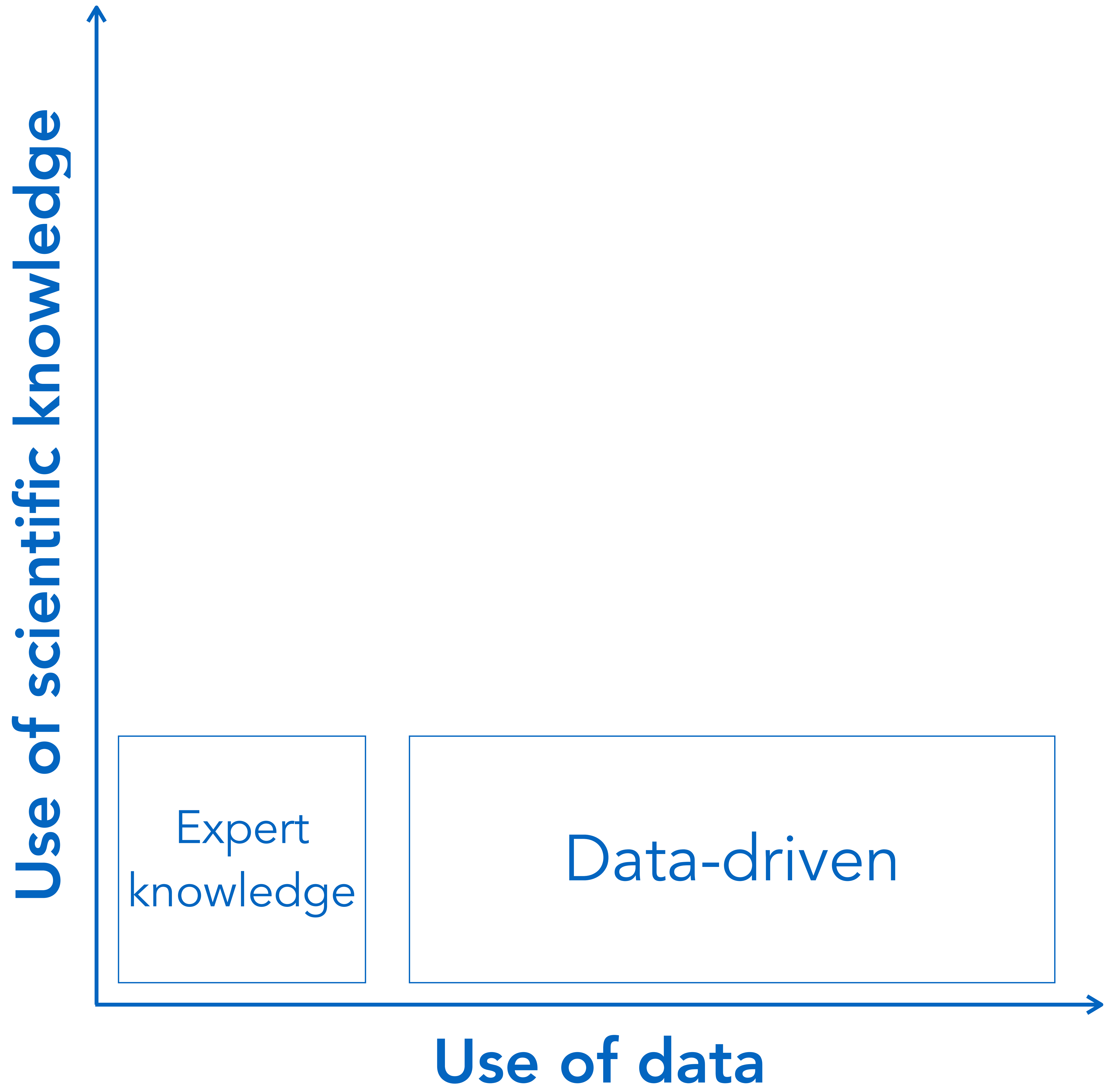
Adaptive combustion closures and chemistry models

Reduced-order models and digital twins



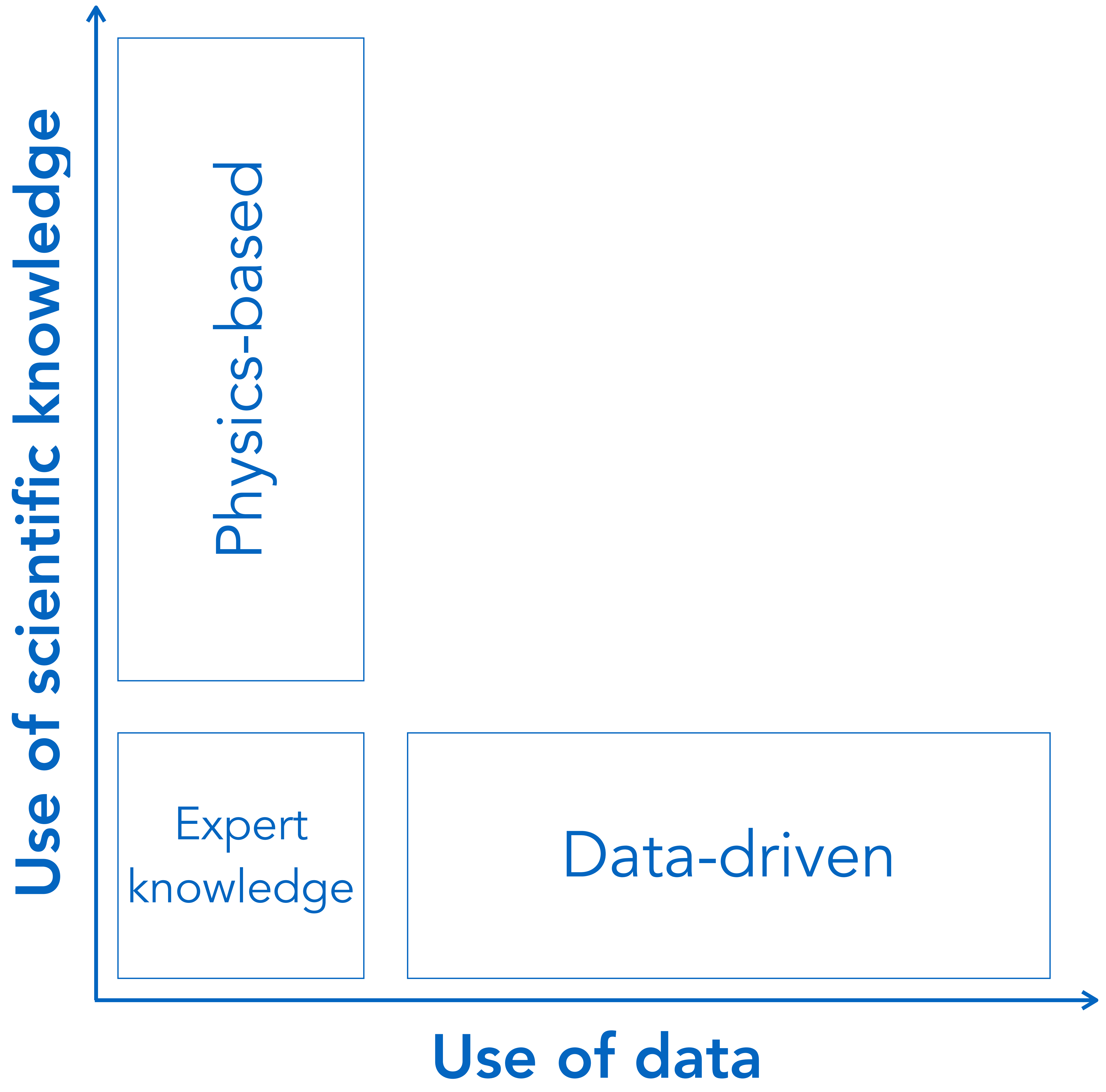
Retrofitting, optimising, troubleshooting, sensing and new design

Physics-based, data-driven approaches



"Without data you're just another person with an opinion" - W. Edwards Deming

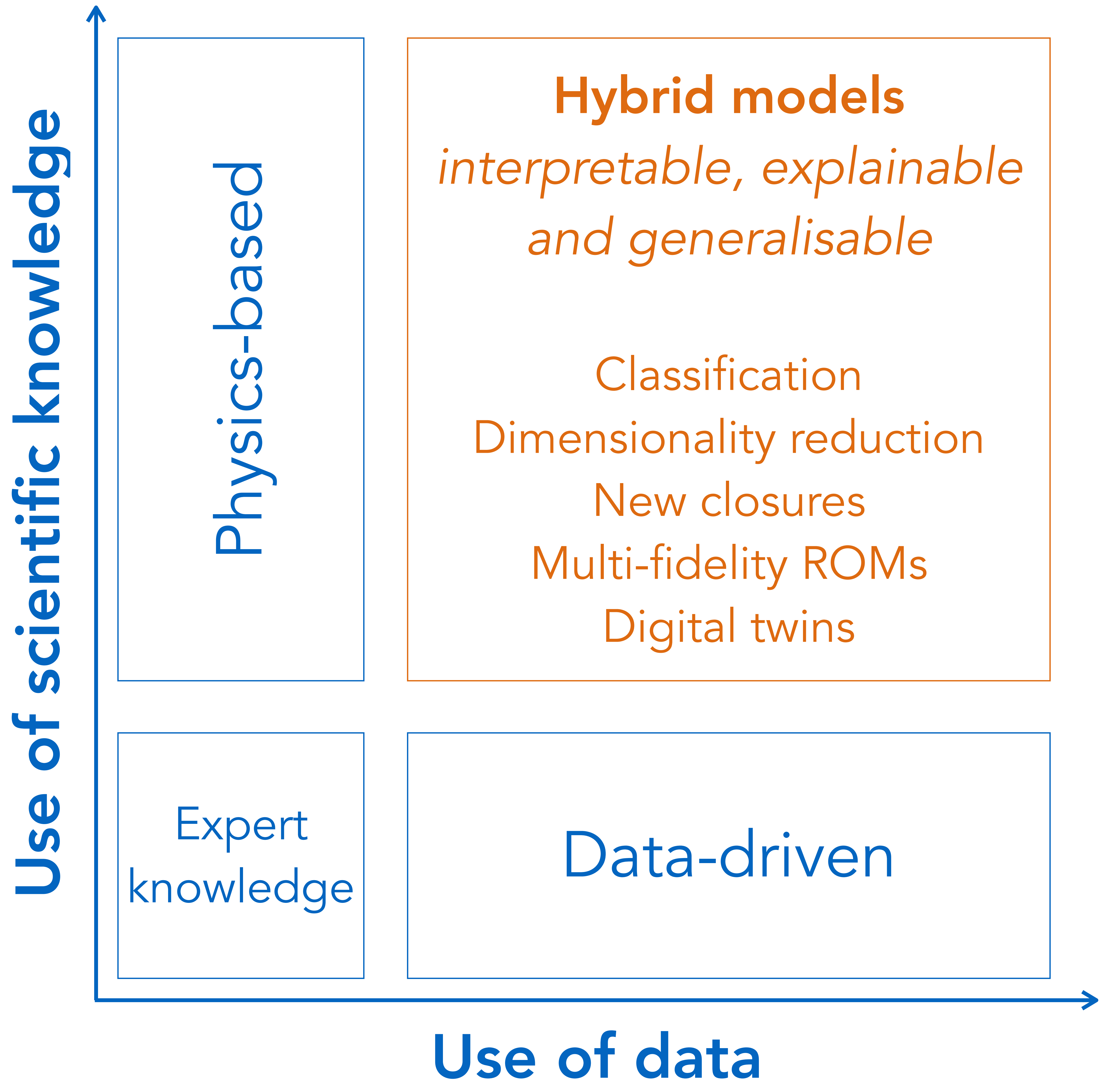
Physics-based, data-driven approaches



"Without data you're just another person with an opinion" - W. Edwards Deming

"Without physical knowledge, you're just another person with an opinion or data" - unknown

Physics-based, data-driven approaches



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Data-driven modelling for dimensionality reduction

State-space methods

Equilibrium, Steady Laminar Flamelets (SLFM)
Flamelet Prolongation of the ILDM (FPI) /
Flamelet generated Manifold (FGM)

Parameterization of the chemical state-space based on optimal reaction variables

Rate-based methods

Intrinsic Low-Dimensional Manifolds (ILDM),
Computational Singular Perturbation (CSP),
Directed-Relation Graph (DRG) …

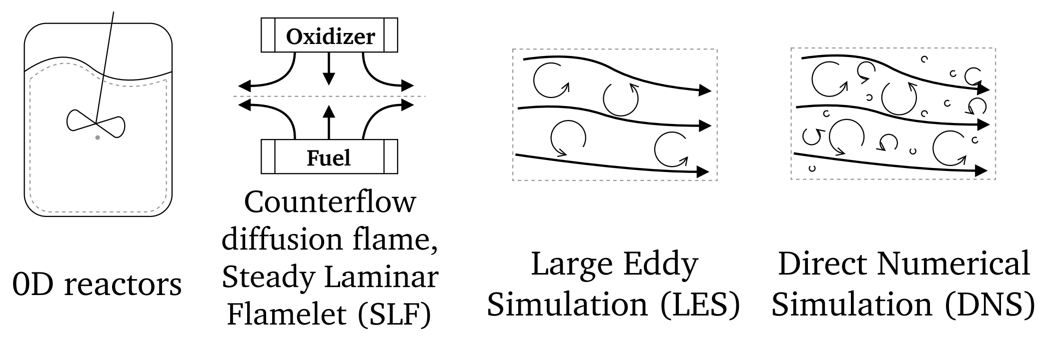
Reduction of the number of species and reactions involved in the kinetic mechanism

Data-driven modelling for dimensionality reduction

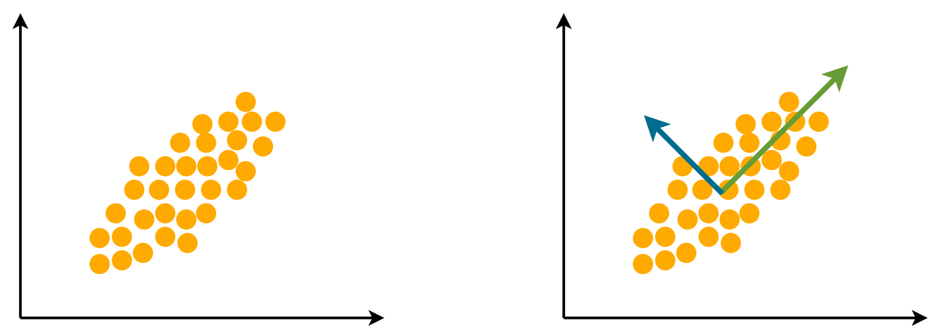
State-space methods

Transport of Principal Components

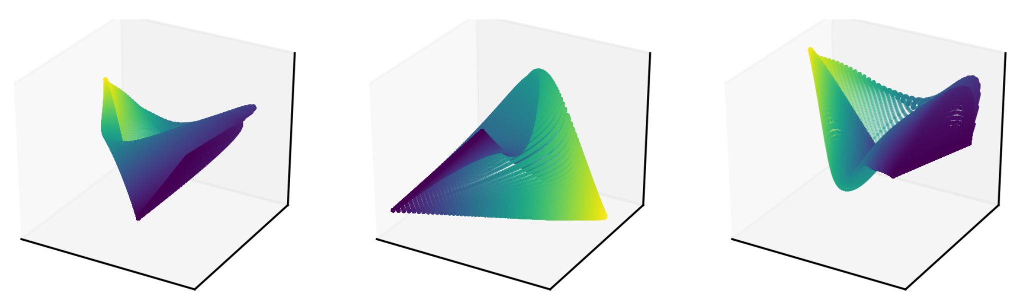
1. Training



2. Dimensionality reduction



3. Parameterisation

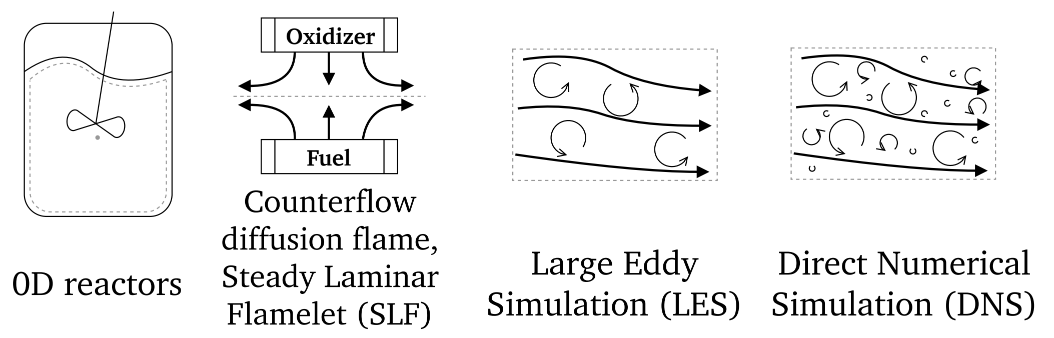


M. R. Malik, P. Obando Vega, A. Coussement, A. Parente, Proceedings of the Combustion Institute, 2020.

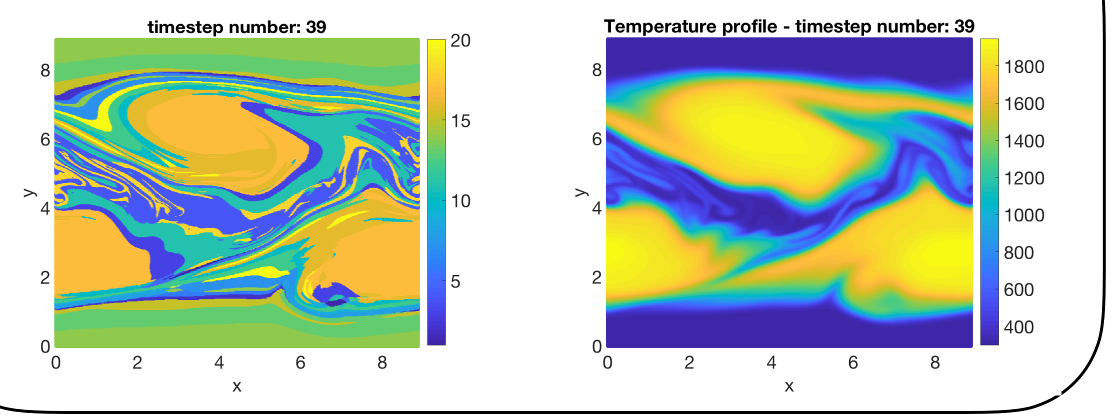
Rate-based methods

Pre-partitioned adaptive chemistry

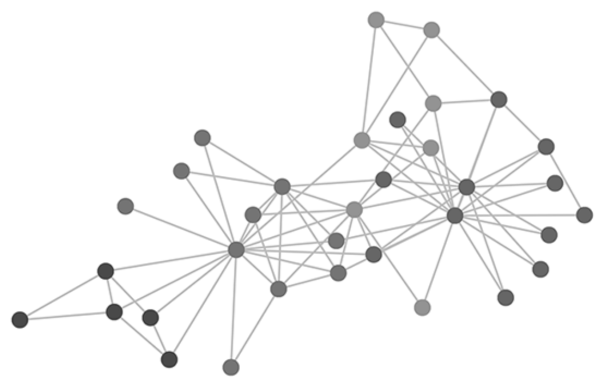
1. Training



2. Classification



3. Mechanism reduction



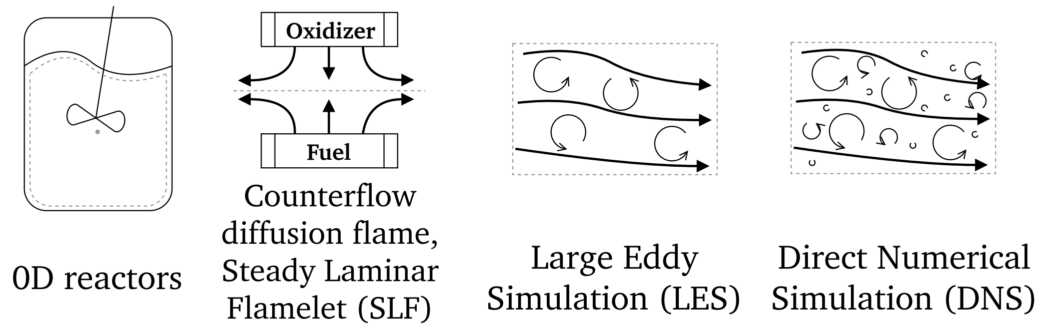
G. D'Alessio, A. Parente, A. Stagni, A. Cuoci, Combustion and Flame, 211, 2020, 68-82

Data-driven modelling for dimensionality reduction

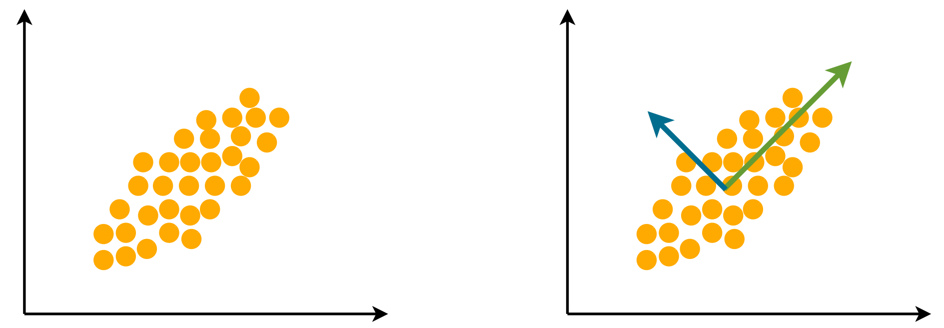
State-space methods

Transport of Principal Components

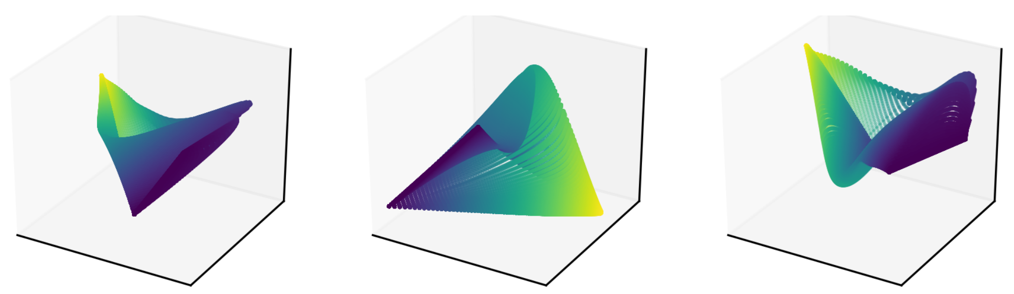
1. Training



2. Dimensionality reduction



3. Parameterisation



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Proceedings of the Combustion Institute, 2020.

Rate-based methods

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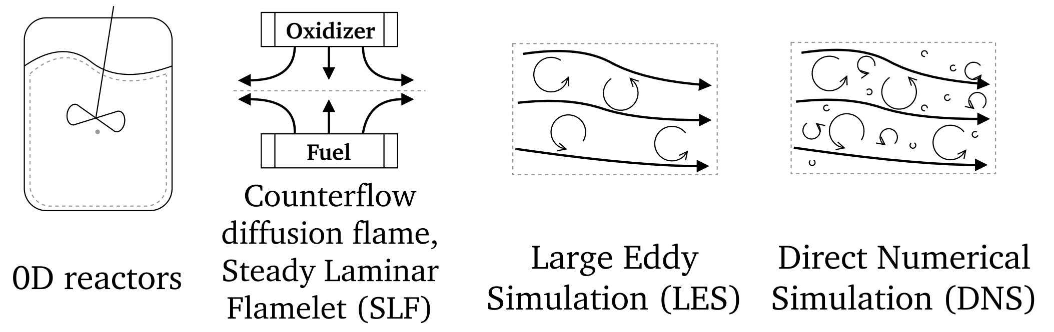

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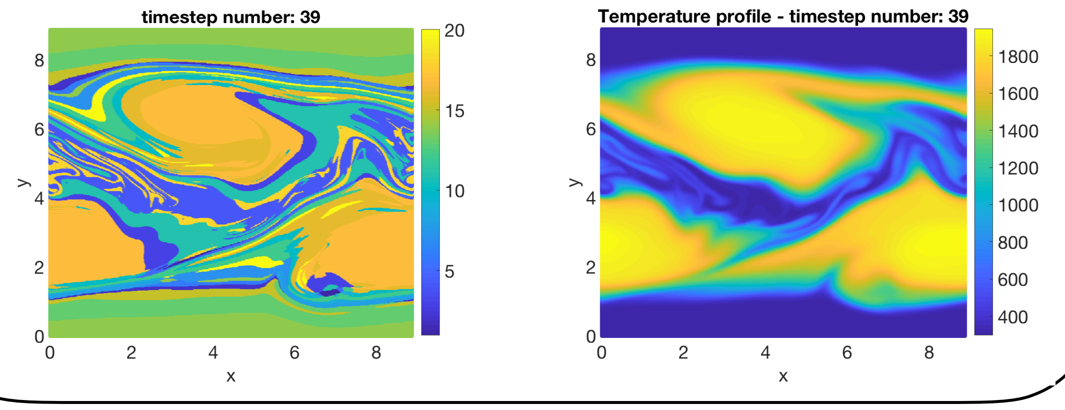

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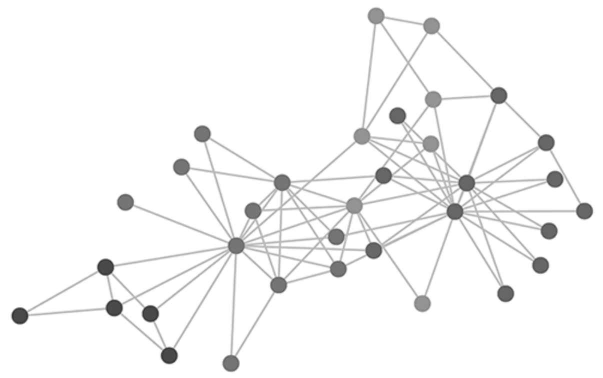
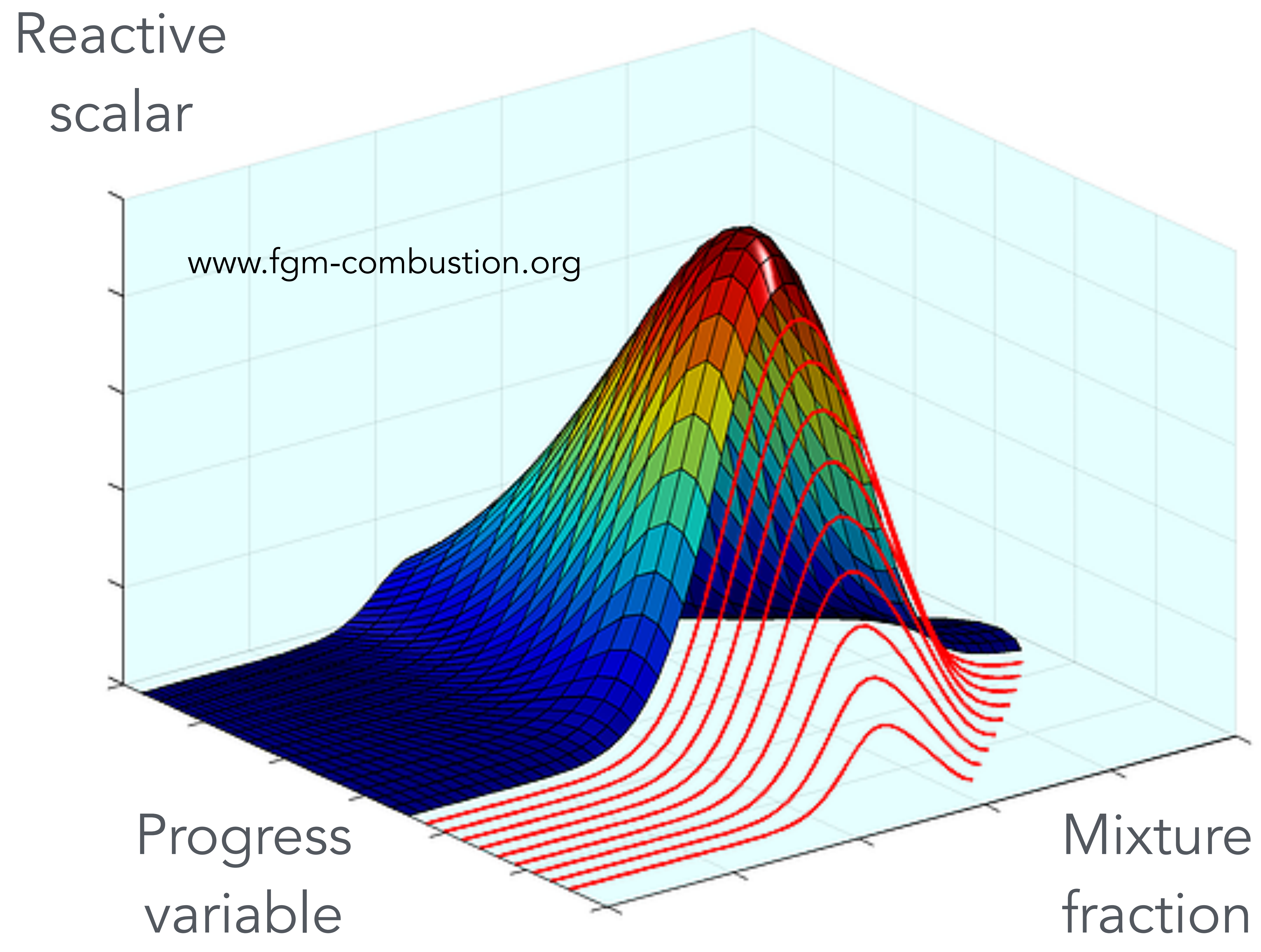


G. D'Alessio, A. Parente, A. Stagni, A. Cuoci,
Combustion and Flame, 211, 2020, 68-82

Reactive scalars are correlated in state-space: how can we best parameterise the manifolds?



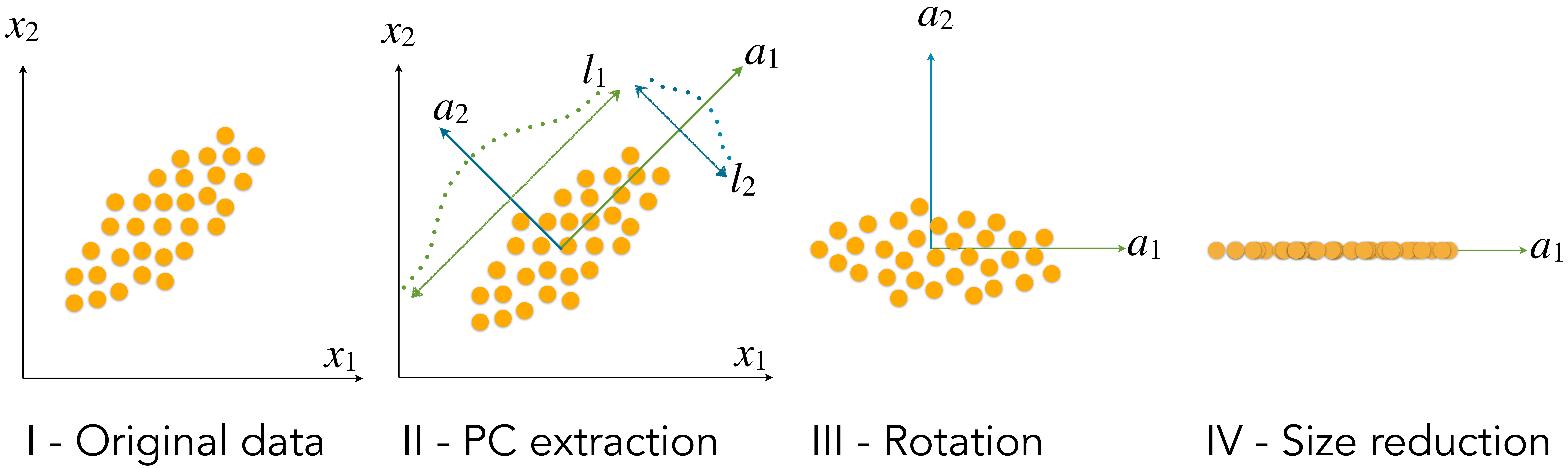
(Linear) modal decomposition methods such as Principal Component Analysis provide a parameterisation that can be used to derive transport models for combustion simulations

PCA can be used to generalise the selection of "optimal progress variables" in state-space methods

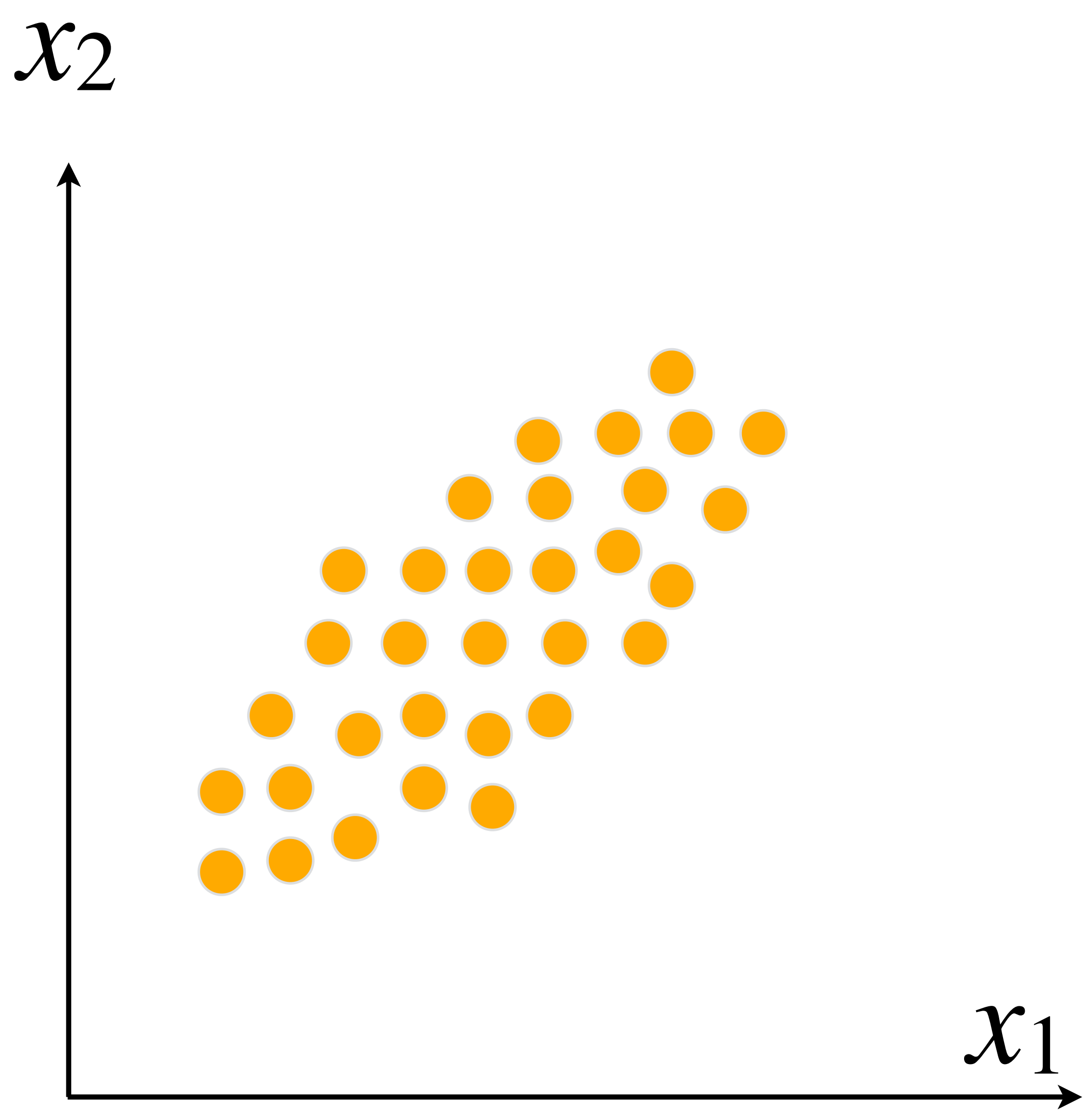
Principal Component Analysis is the simplest data mining approach for combustion data

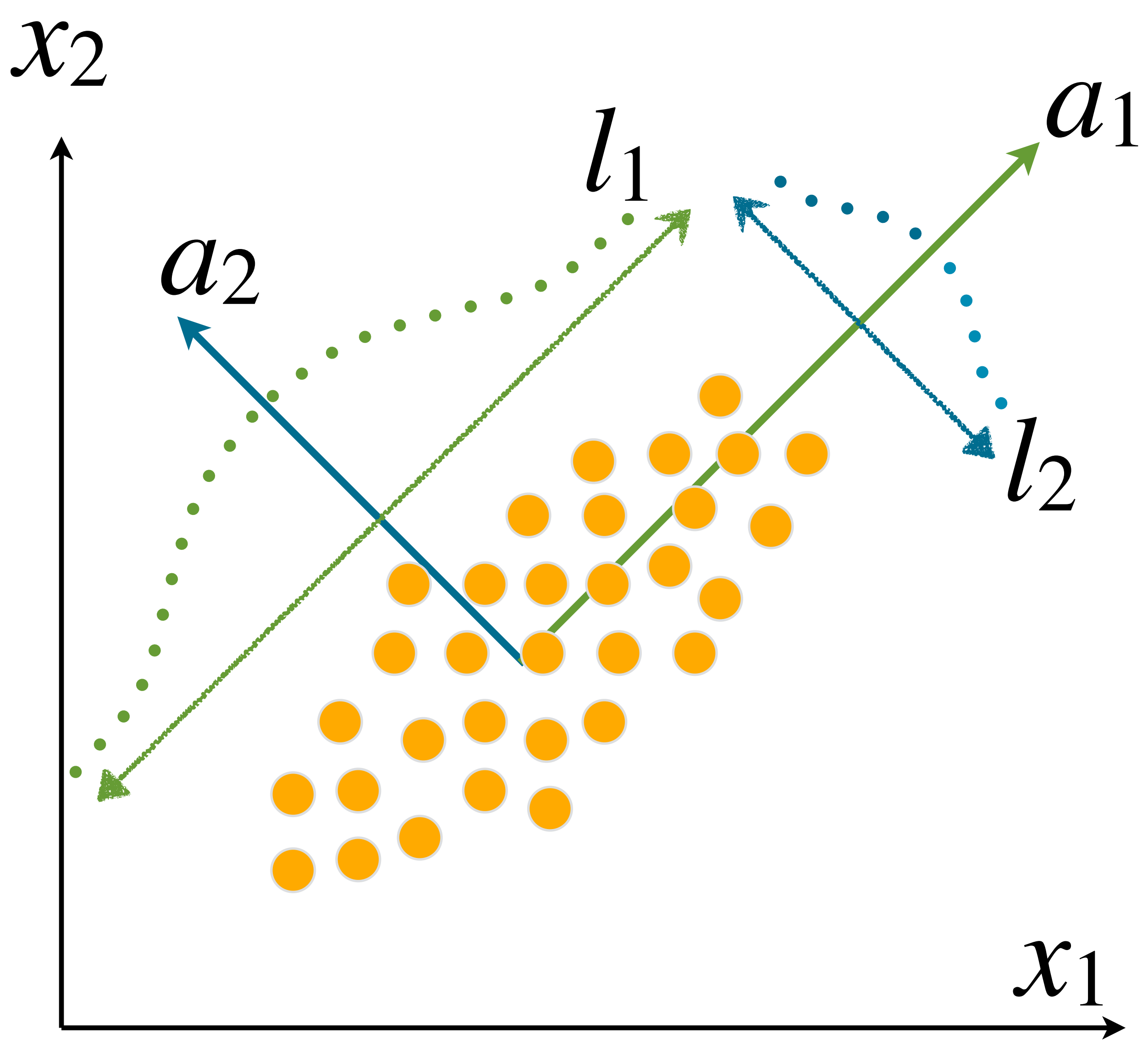
$$\mathbf{X} = \begin{array}{cc} & \text{State variables} \\ \text{Observations} & \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1Q} \\ x_{21} & x_{22} & \dots & x_{2Q} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nQ} \end{bmatrix} \end{array} = \begin{bmatrix} T^1 & Y_1^1 & \dots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

PCA is an eigenvalue/eigenvector problem applied to the covariance matrix of the data set, **S**



A new coordinate system is identified in the direction of maximum variance





$$\mathbf{S} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X} = \mathbf{ALA}^T$$

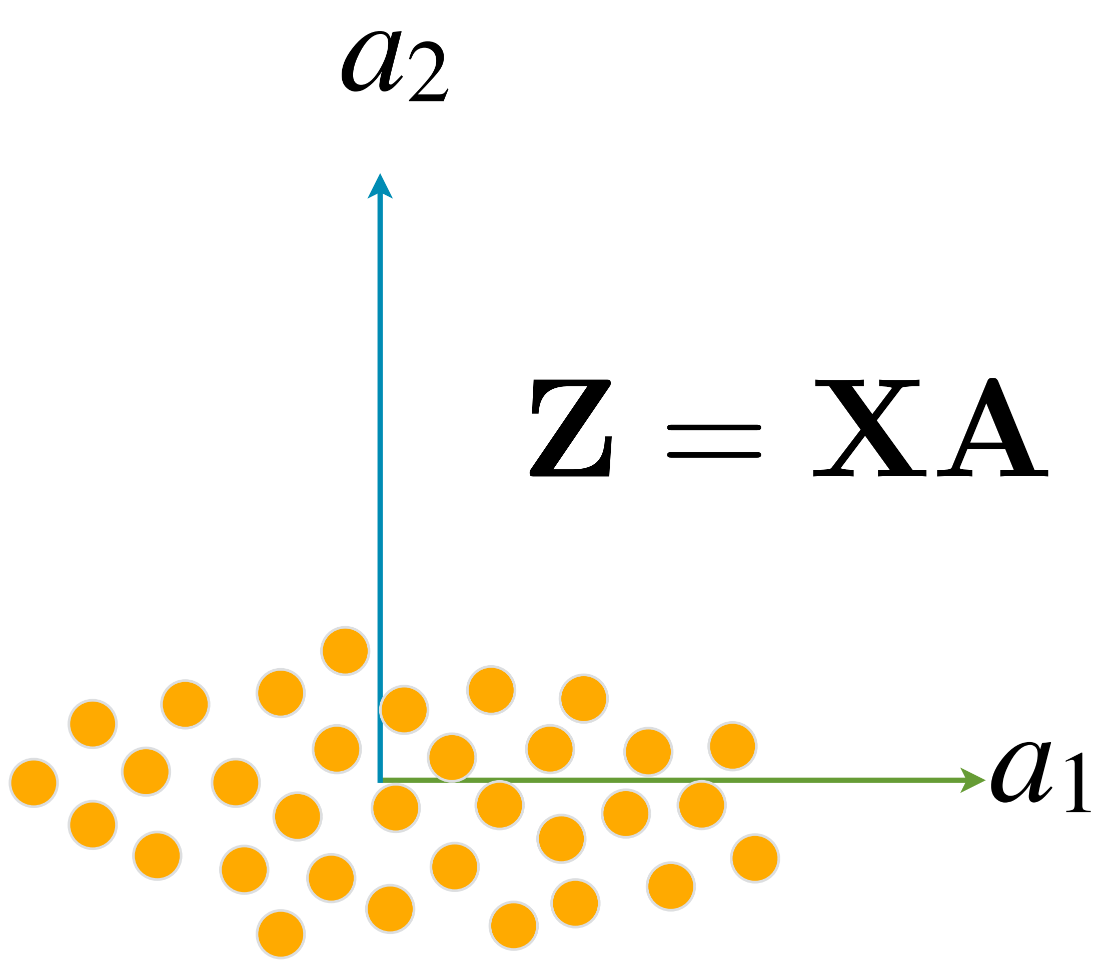
$$l_1 > l_2 > \ldots > l_p$$

$$\mathbf{a}_i \cdot \mathbf{a}_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

$$\begin{bmatrix} x_{11} & \ldots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \ldots & x_{np} \end{bmatrix}$$

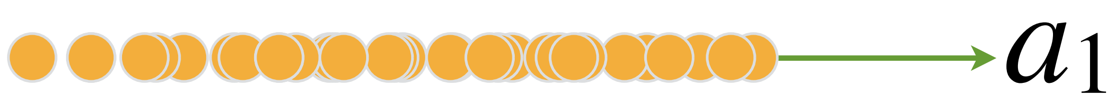
$$\begin{bmatrix} a_{11} & \ldots & a_{1p} \\ \vdots & \ddots & \vdots \\ a_{p1} & \ldots & a_{pp} \end{bmatrix} \begin{bmatrix} l_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & l_p \end{bmatrix} \begin{bmatrix} a_{11} & \ldots & a_{p1} \\ \vdots & \ddots & \vdots \\ a_{1p} & \ldots & a_{pp} \end{bmatrix}$$

Keeping only the most energetic directions, the original dimensionality can be reduced



$$\mathbf{Z} = \mathbf{X}\mathbf{A} \xrightarrow{\mathbf{A}^{-1} = \mathbf{A}^T} \mathbf{X} = \mathbf{Z}\mathbf{A}^T$$

$$\mathbf{Z}_q = \mathbf{X}\mathbf{A}_q \rightarrow \widetilde{\mathbf{X}} = \mathbf{Z}_q\mathbf{A}_q^T$$

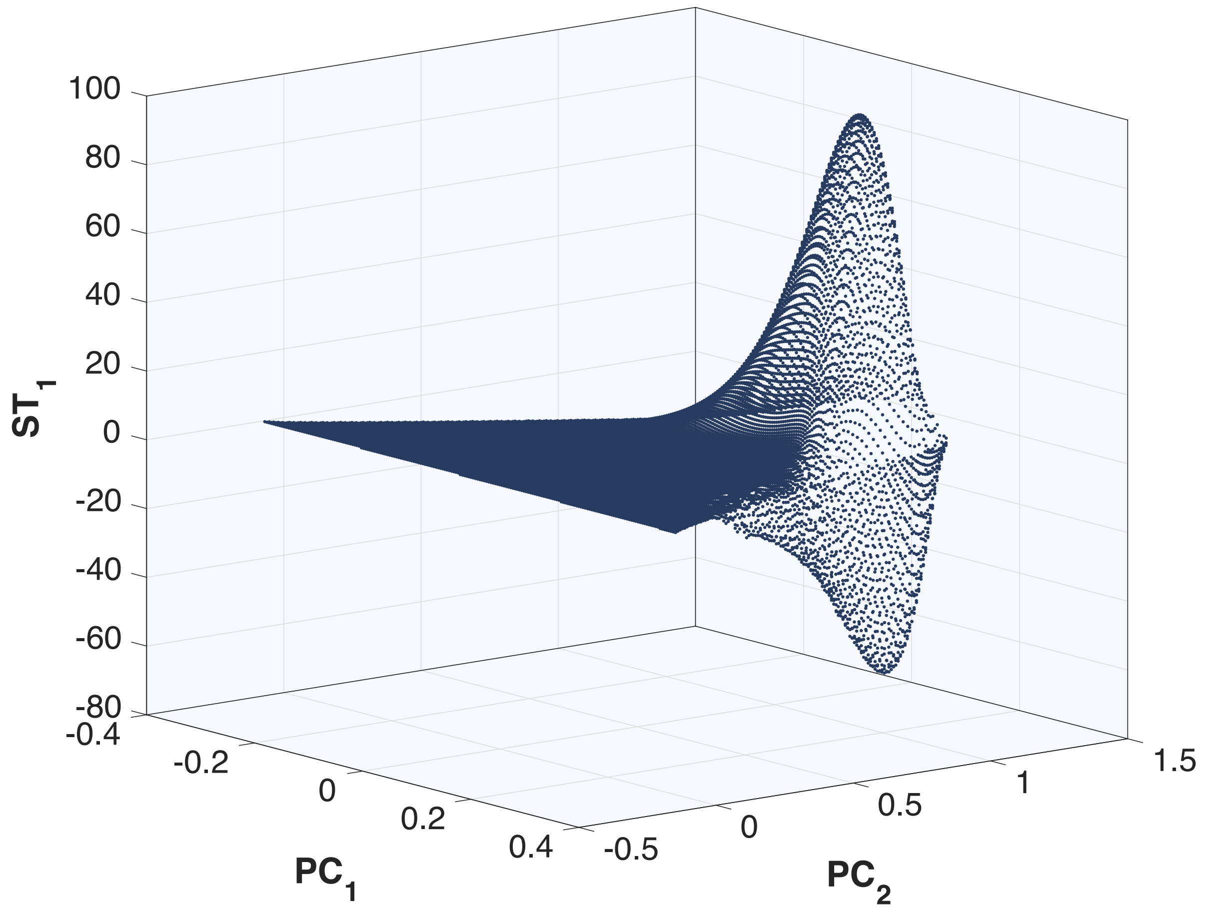


$$\begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1p} \\ \vdots & \ddots & \vdots \\ a_{p1} & \cdots & a_{pp} \end{bmatrix}$$

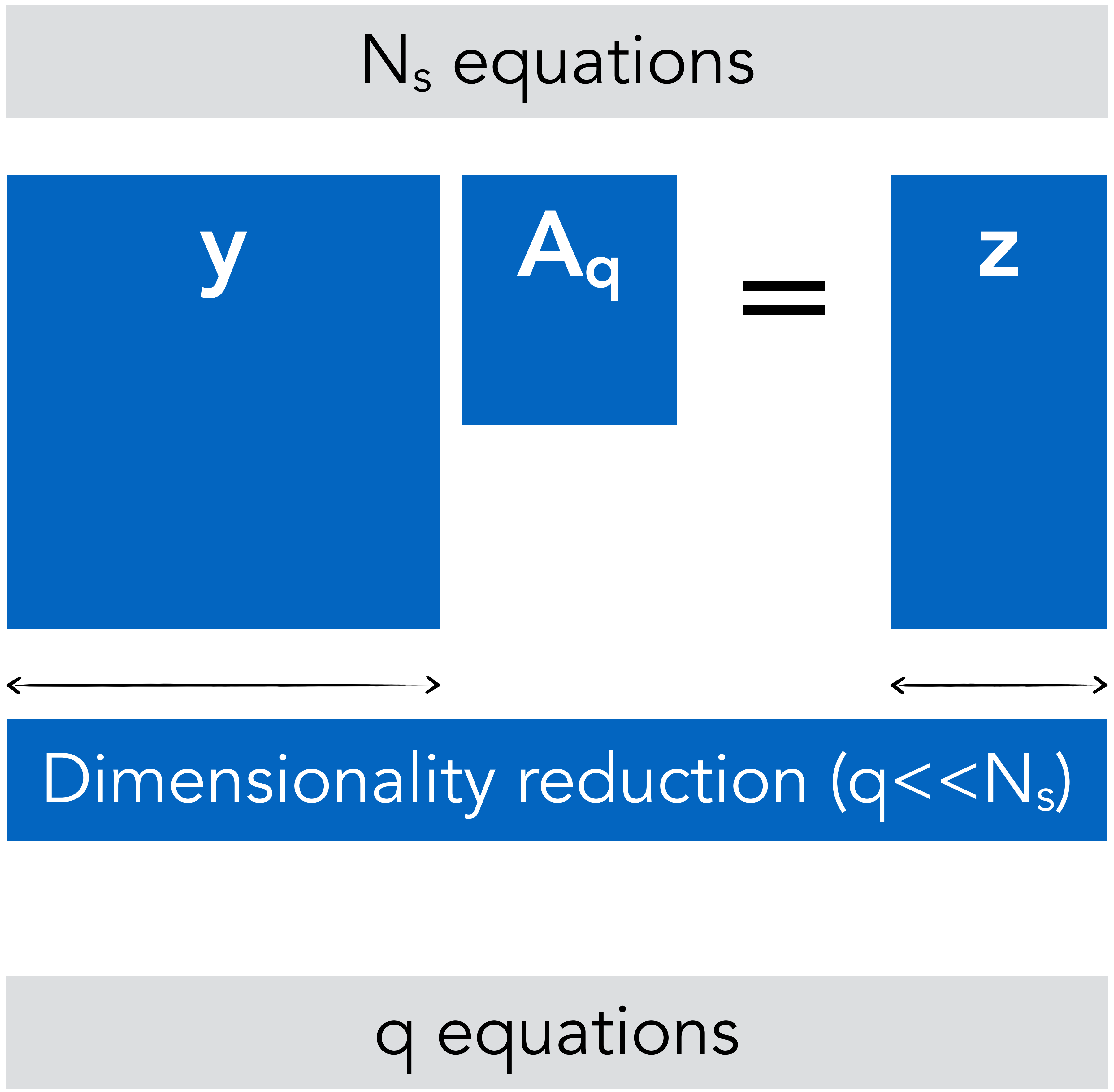
$$\begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1q} \\ \vdots & \ddots & \vdots \\ a_{p1} & \cdots & a_{pq} \end{bmatrix}$$

PCA encodes the state space into a low-dimensional manifold using features for which transport equations can be solved

$$\rho \frac{\mathrm{D}(\mathbf{y})}{\mathrm{D}t} = -\nabla \cdot (\mathbf{j_y}) + (s_\mathbf{y})$$



$$\mathbf{Z} = \mathbf{Y}\mathbf{A_q}$$



$$\rho \frac{\mathrm{D}(\mathbf{z})}{\mathrm{D}t} = -\nabla \cdot (\mathbf{j_z}) + (s_\mathbf{z})$$

J. Sutherland and A. Parente, *Proc. Combust. Inst.* **32** (2009) 1563-1570.

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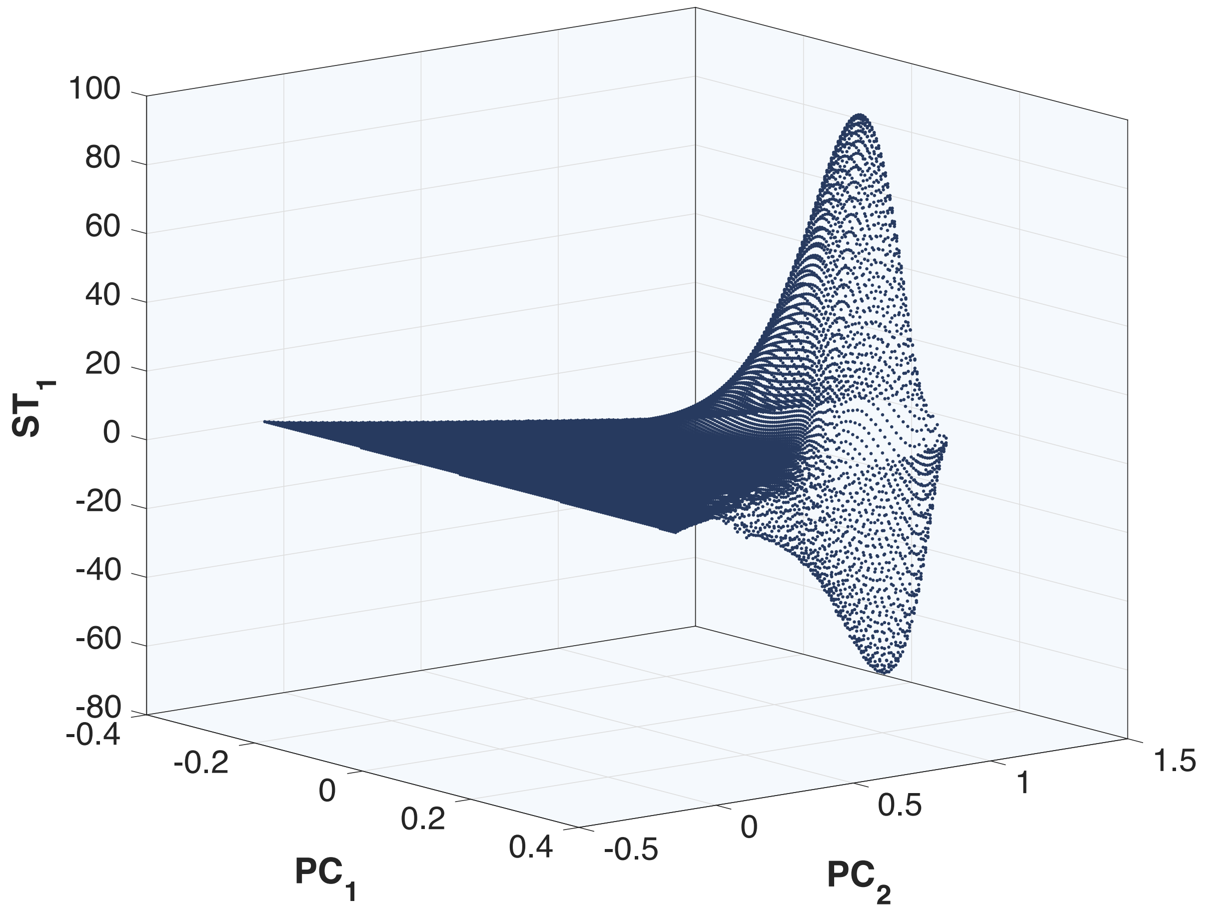

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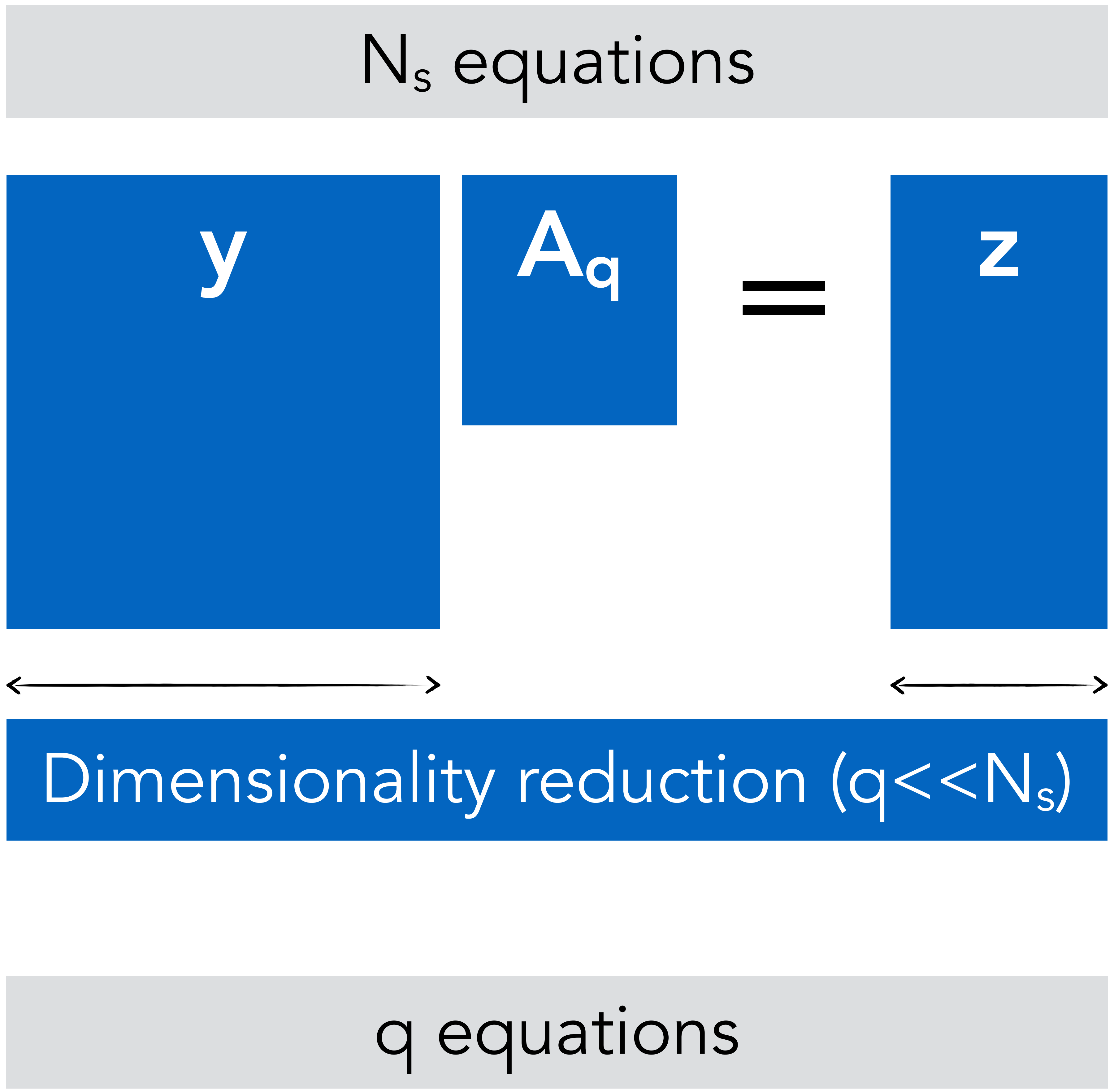


J. Sutherland and A. Parente, *Proc. Combust. Inst.* **32** (2009) 1563-1570.

The direct reconstruction of the chemical source terms from the reconstructed state space is affected by non-linear error propagation

$$\mathbf{Z}_q$$

$$\downarrow$$

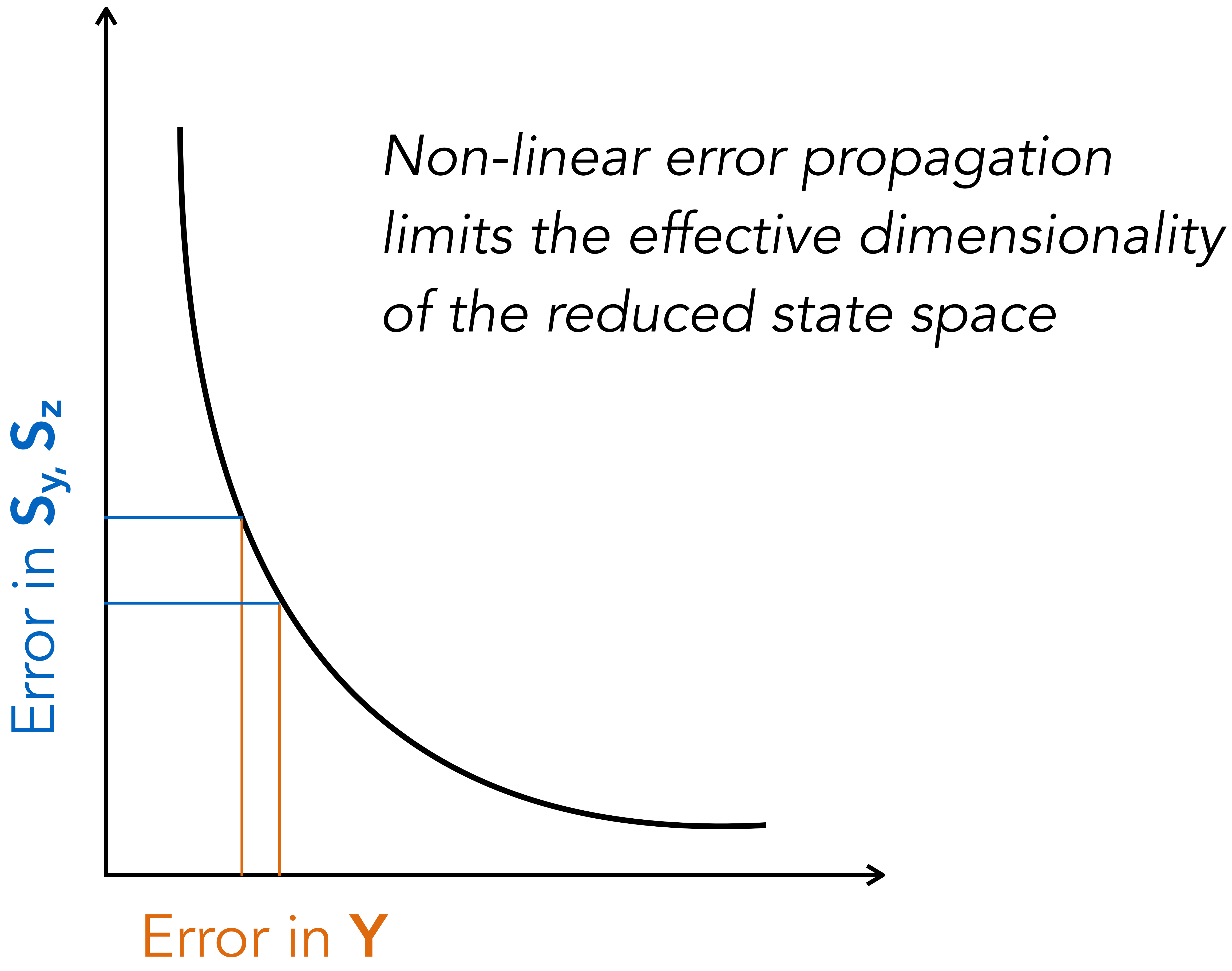
$$\widetilde{\mathbf{Y}}_q$$

$$\downarrow$$

$$\widetilde{\mathbf{S}}_y$$

$$\downarrow$$

$$\widetilde{\mathbf{S}}_z = \widetilde{\mathbf{S}}_y \mathbf{A}_q \mathbf{D}^{-1}$$

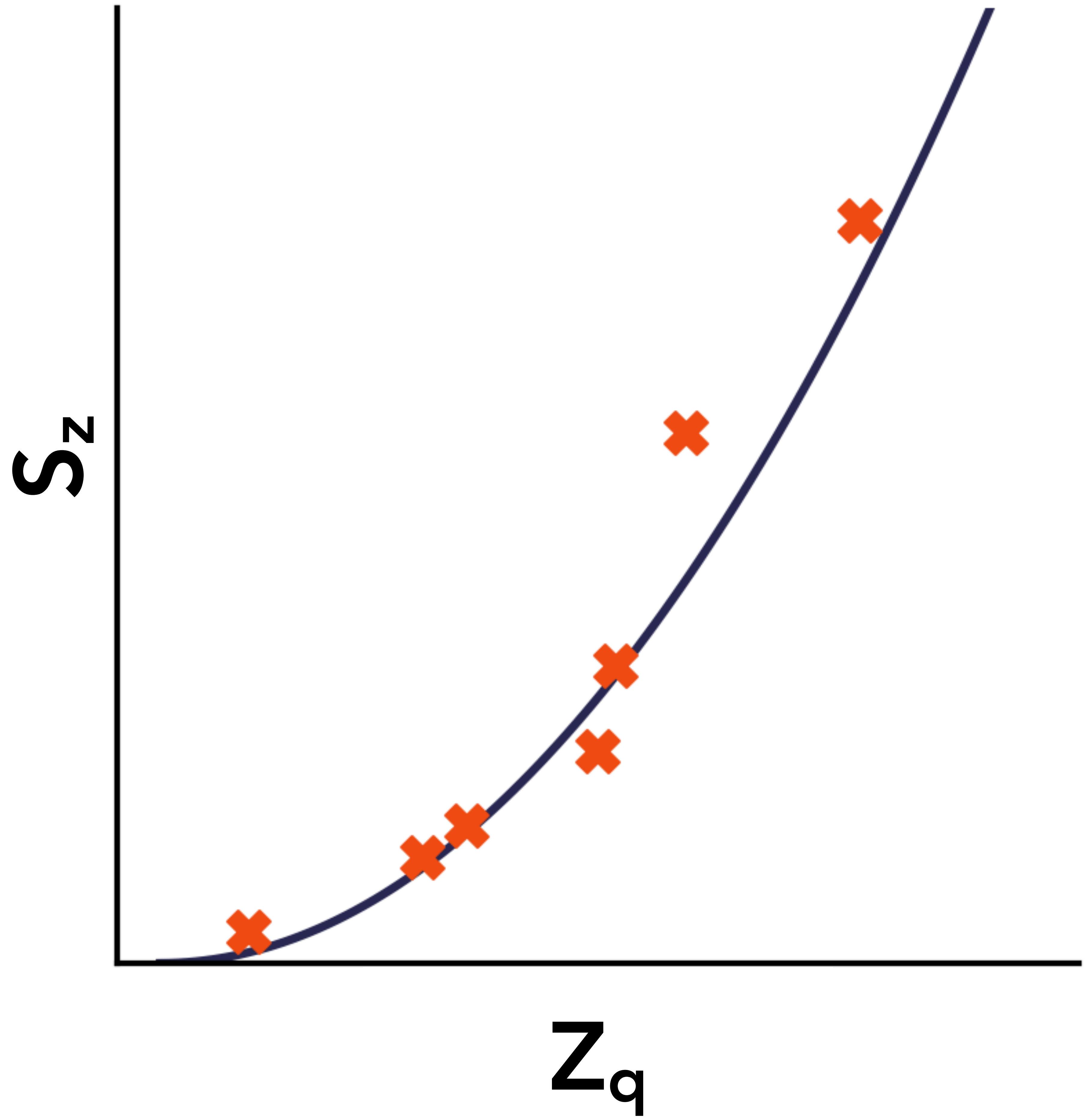


A non-linear mapping (regression) can be used to encode the non-linear relationship between state-space and sources

$$\mathbf{Z}_q$$

$$\downarrow$$

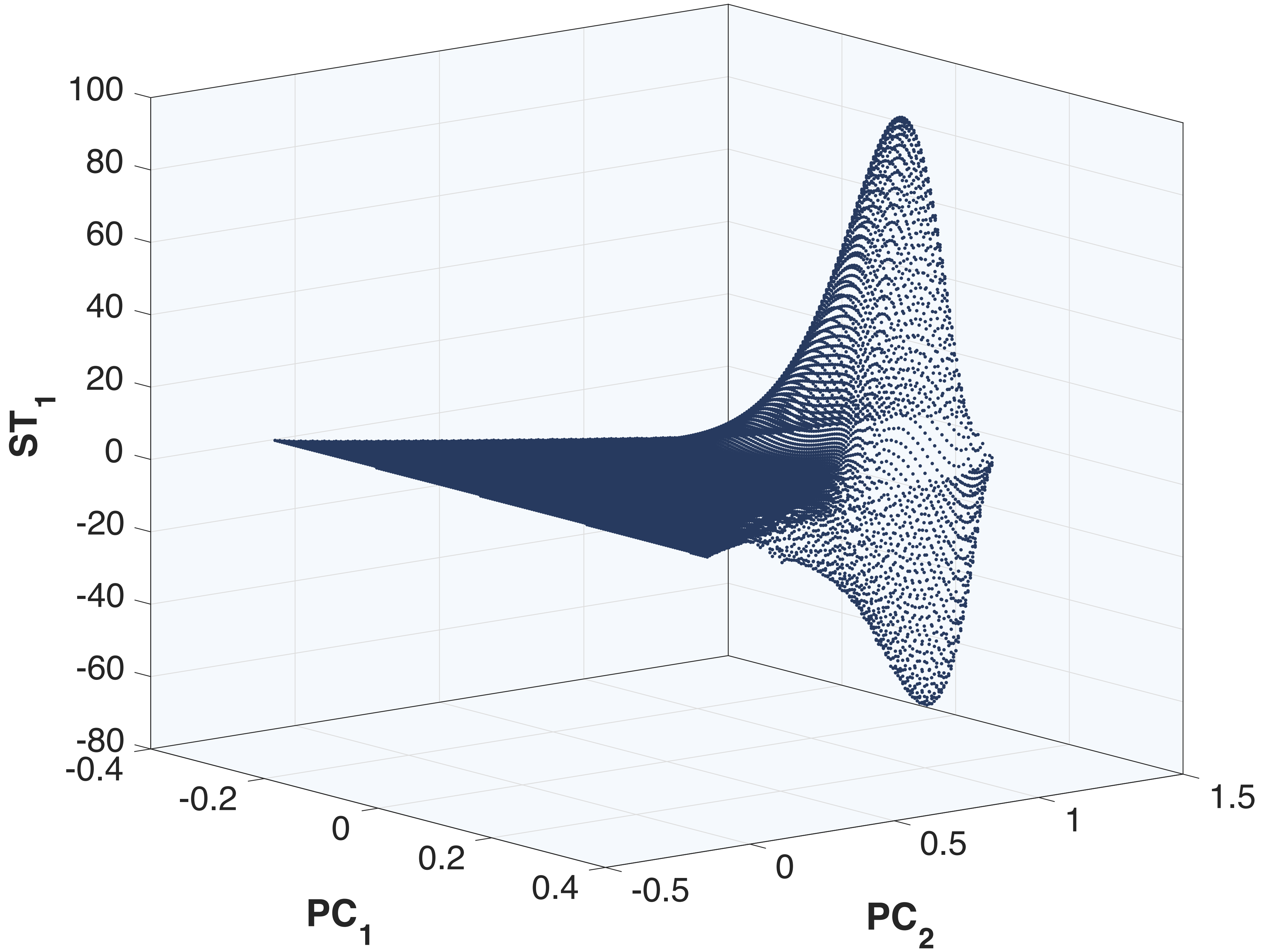
$$\widetilde{\mathbf{S}}_z = f\left(\mathbf{Z}_q\right)$$



PC source term mapping using supervised non-linear regression algorithms

MARS - Multi-Adaptive Regression Splines

A. Biglari, J.C. Sutherland, *Combust Flame* **159** (2012) 1960-1970.
Y. Yang, S.B. Pope, J.H. Chen, *Combust Flame* **160** (2014) 1967-1980.



ANN - Artificial Neural Networks

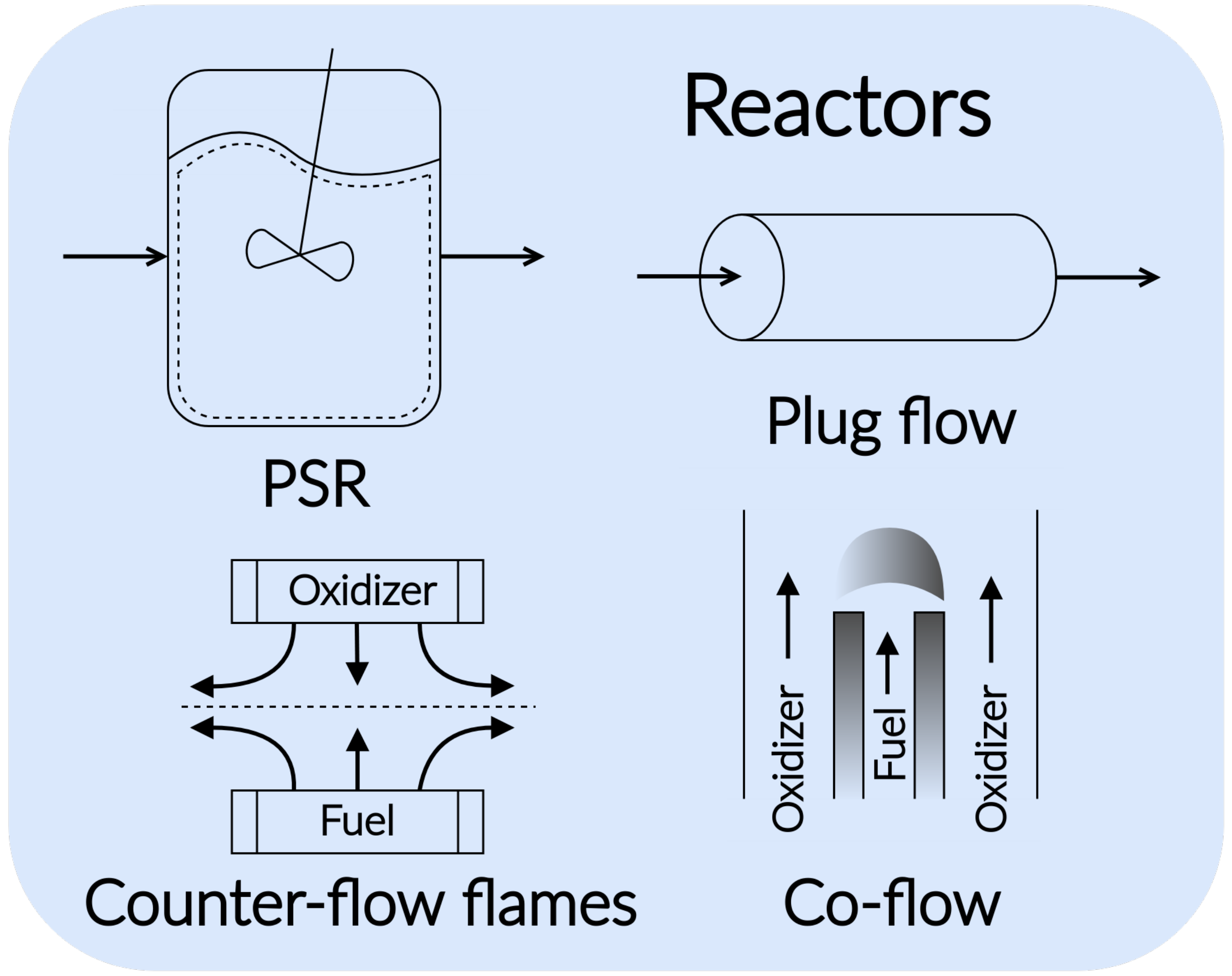
H. Mirgolbabaei, T. Echekki, *Combust Flame* **160** (2013) 898-908.
H. Mirgolbabaei, T. Echekki, *Combust Flame* **162** (2015) 1919-1933.

GPR - Gaussian Process Regression

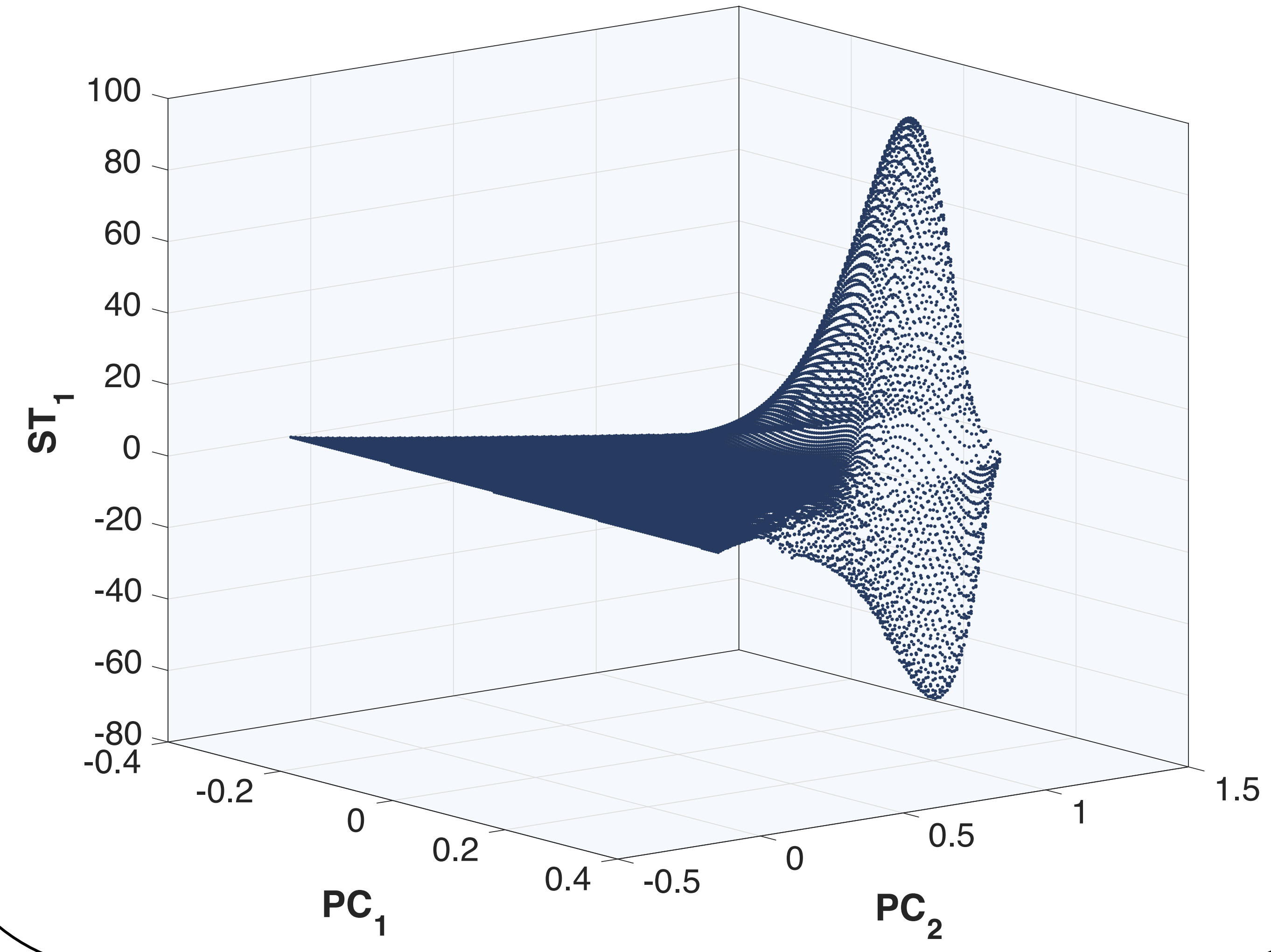
B.J. Isaac, J.N. Thornock, J.C. Sutherland, P.J. Smith, A. Parente, *Combust Flame* **162** (2015) 2592–2601.
M.R. Malik, B.J. Isaac, A. Coussement, P.J. Smith, A. Parente, *Combust Flame* **187** (2018) 30-41.

Applications of the PCA-GPR framework

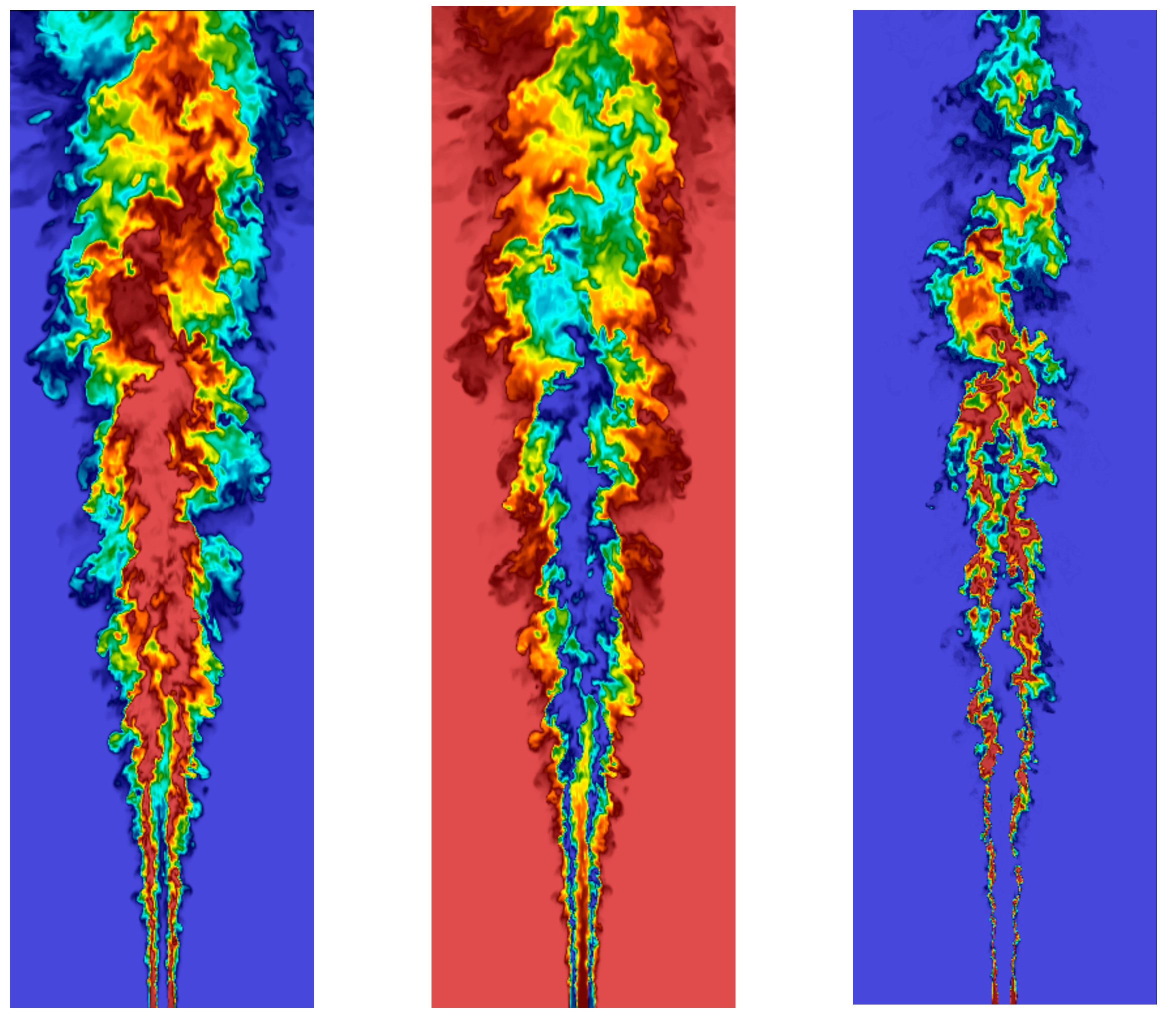
1. Training data



2. Parameterisation by PCA-GPR/ANN/…



3. Multi-scale simulations



Applications of the PCA-GPR framework

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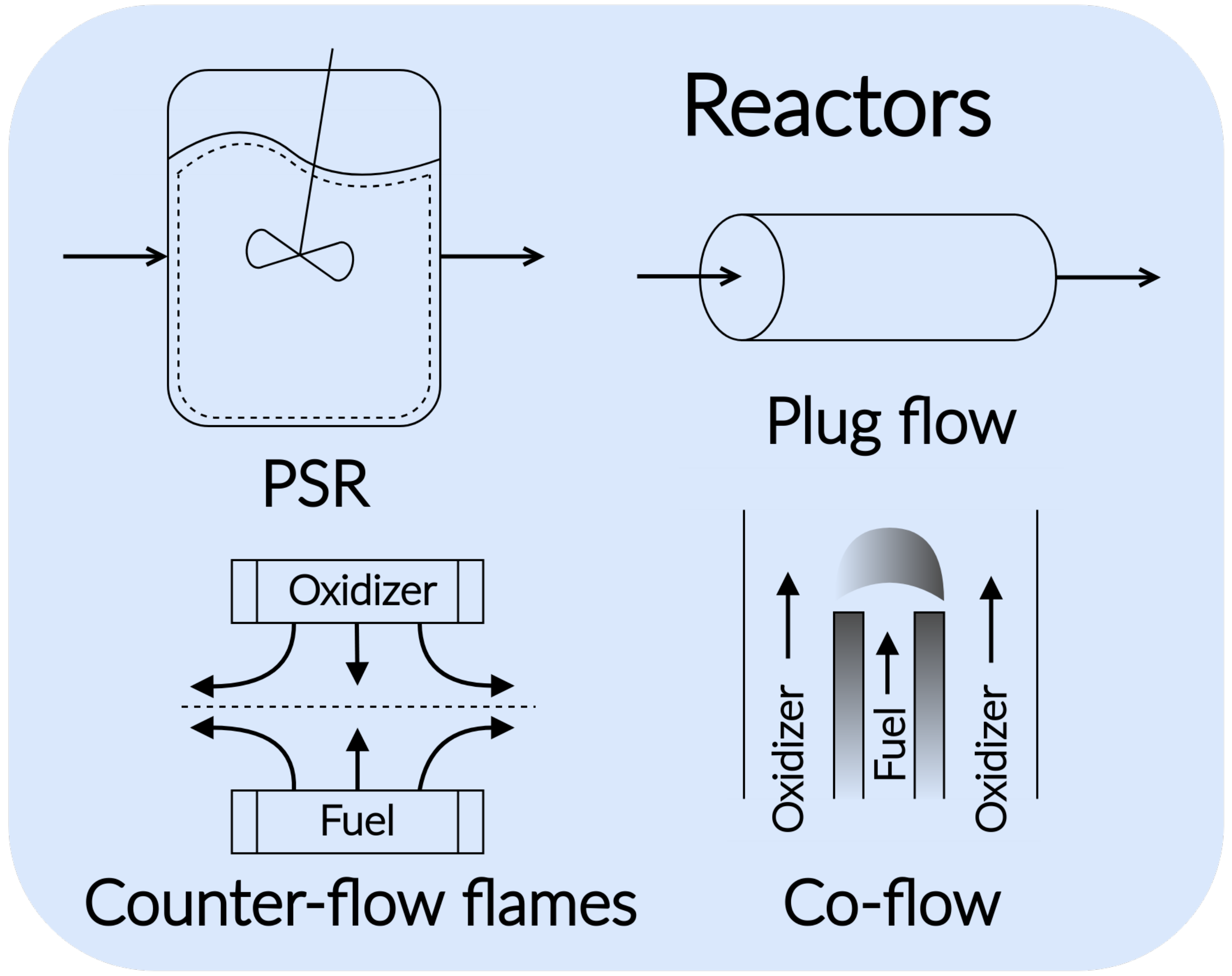
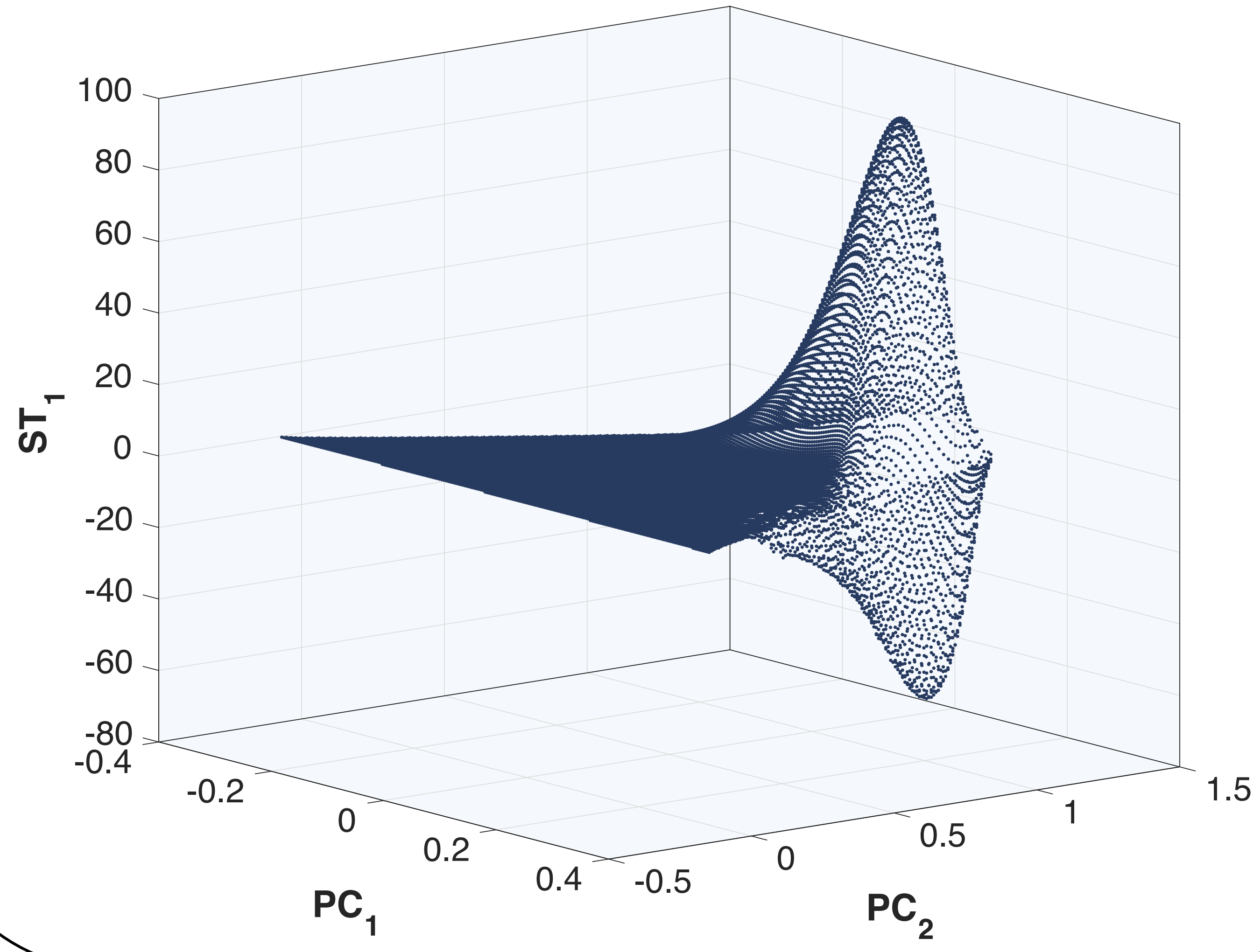


Cheap function evaluations

2. Parameterisation by PCA-GPR/ANN/…



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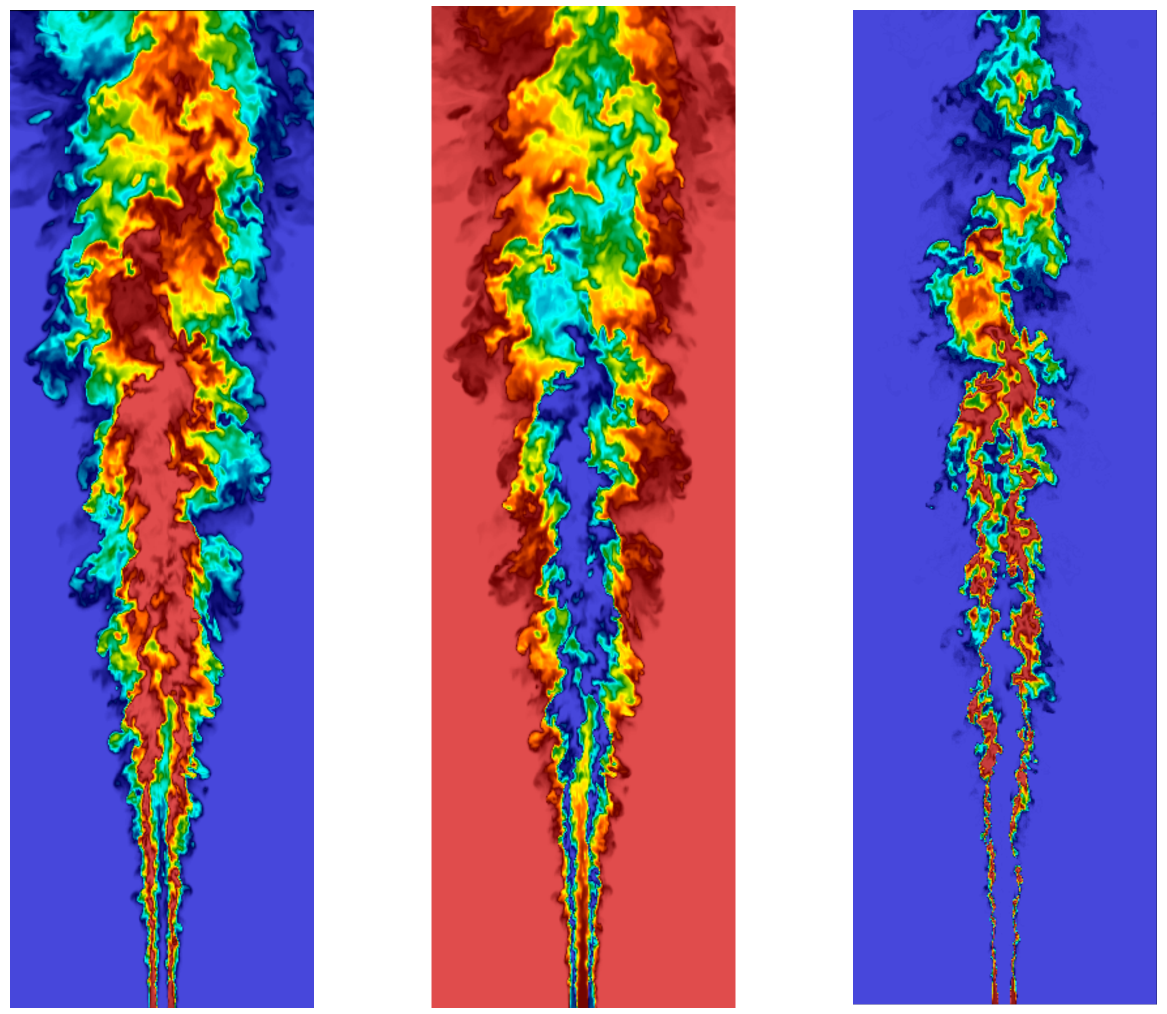
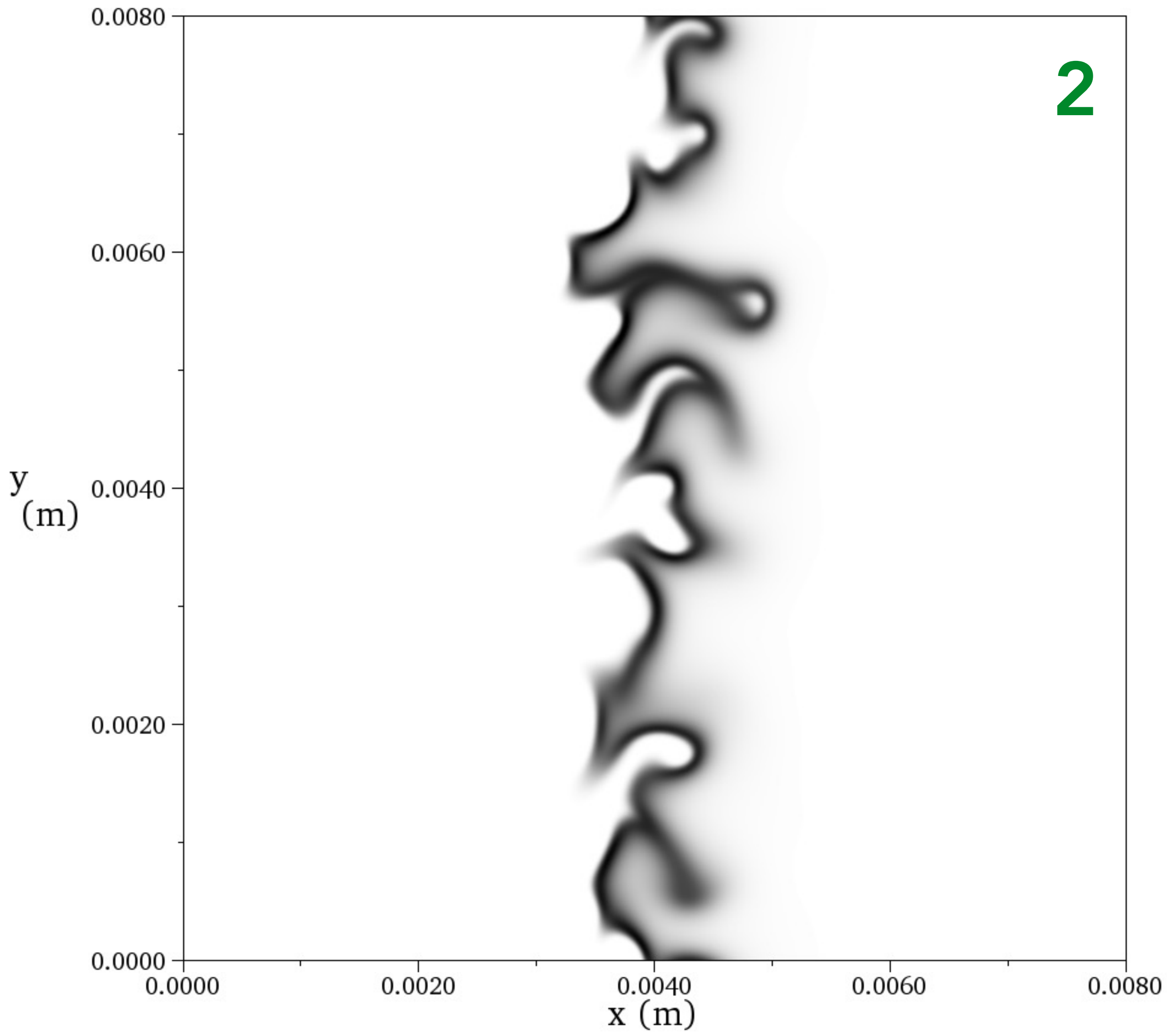
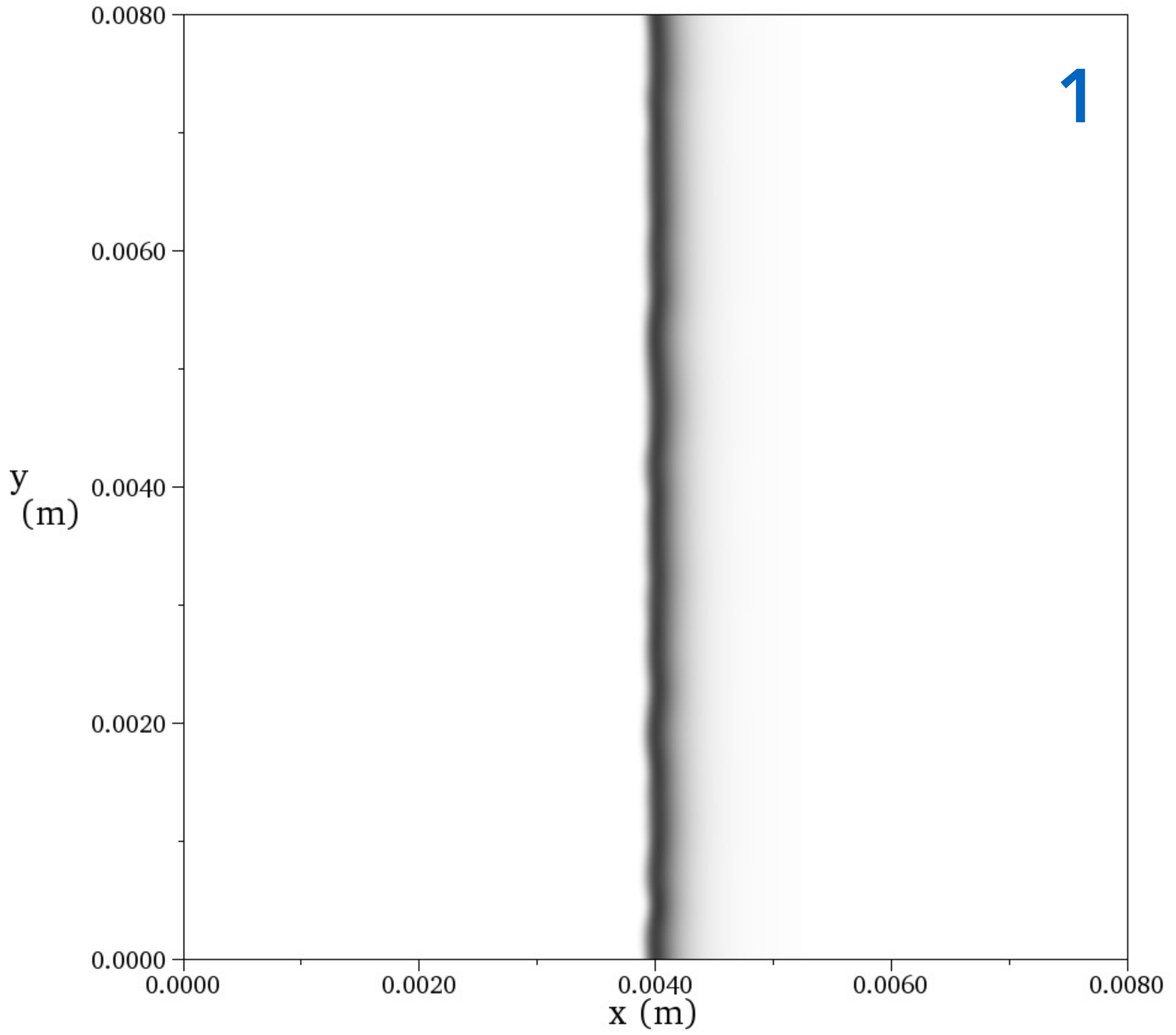


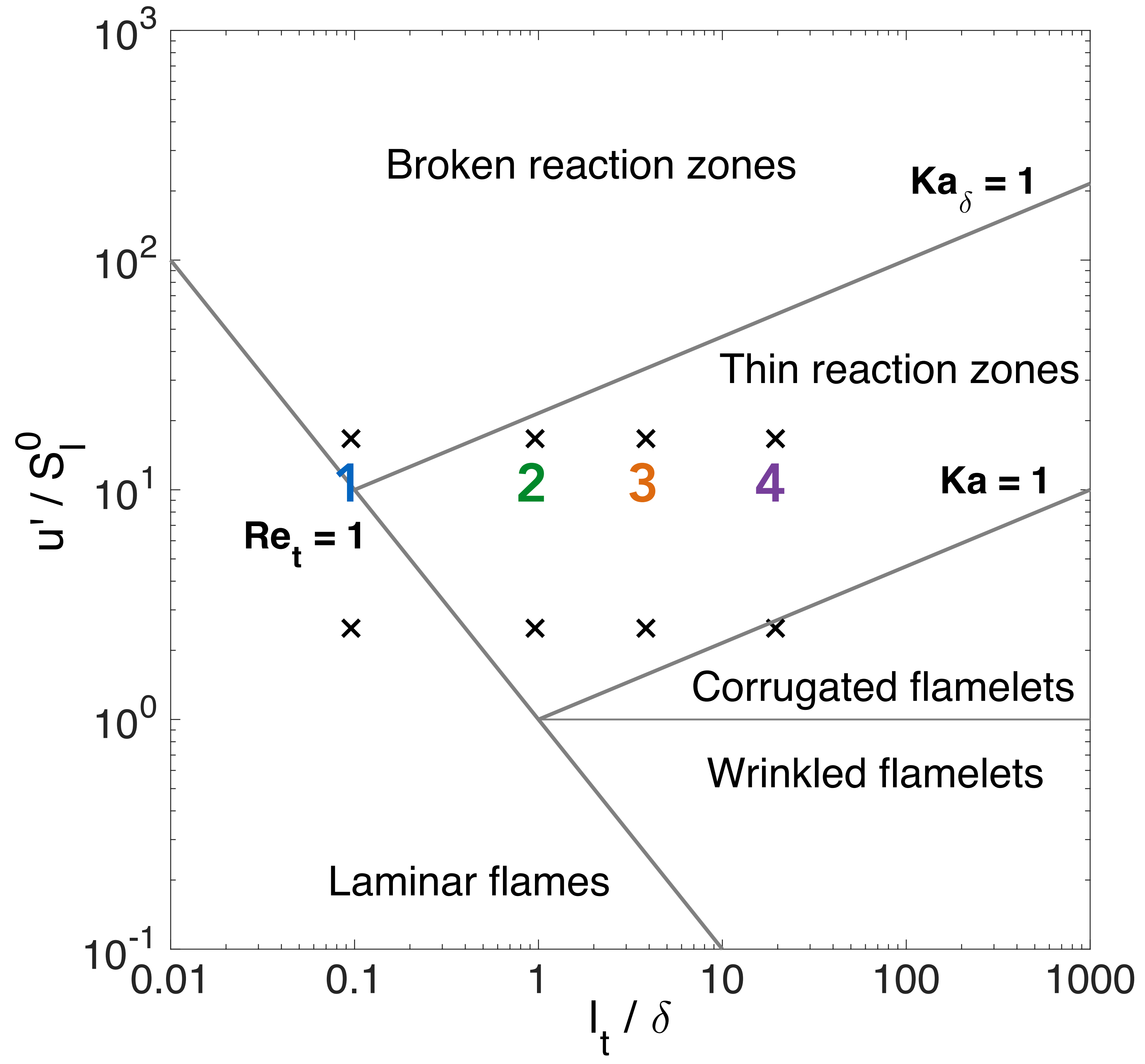
Expensive function evaluations

PCA models from simple reactors can be used on complex configurations

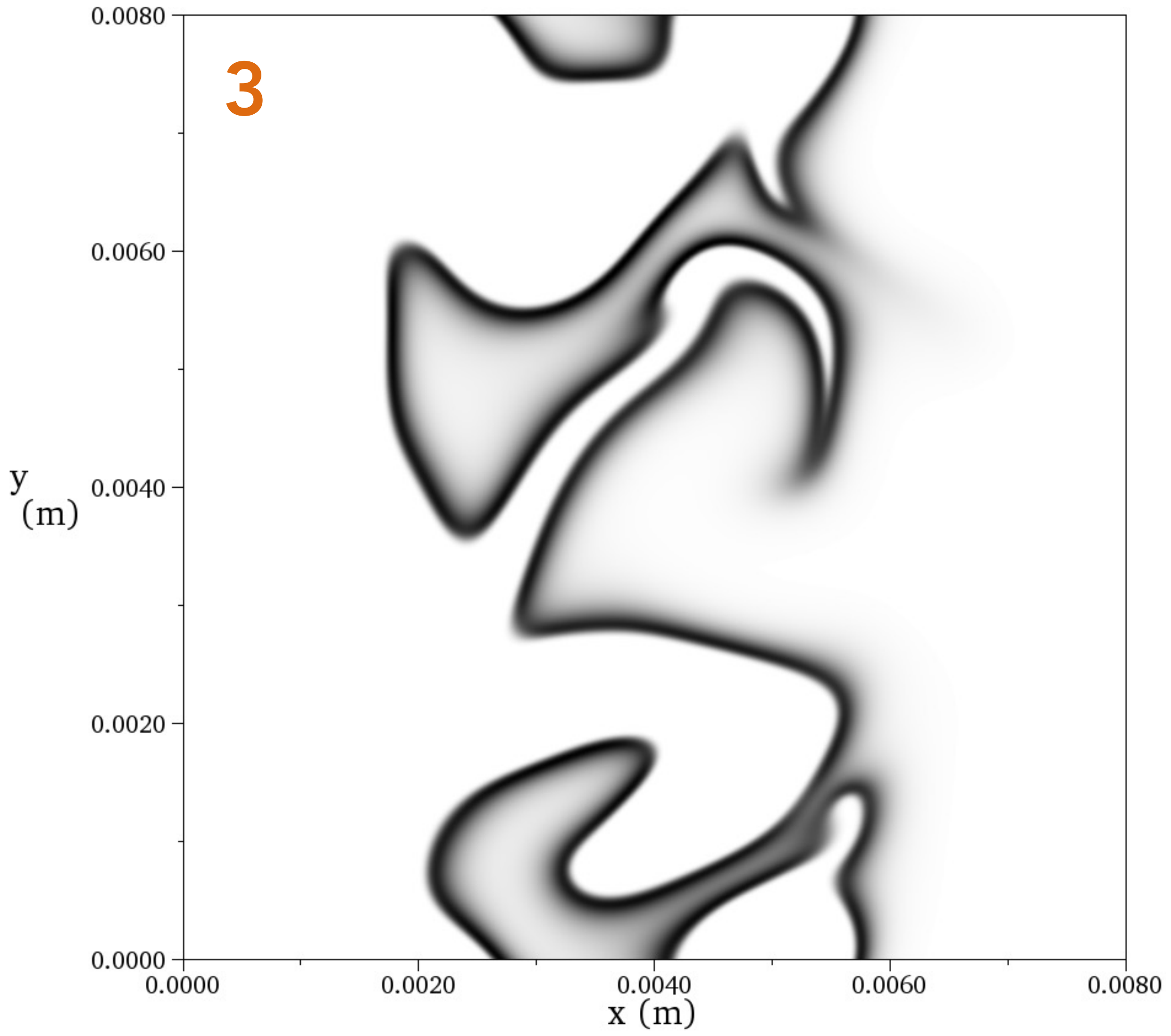
PC-transport model trained on a single laminar flame and used to predict eight syngas, turbulent premixed flames

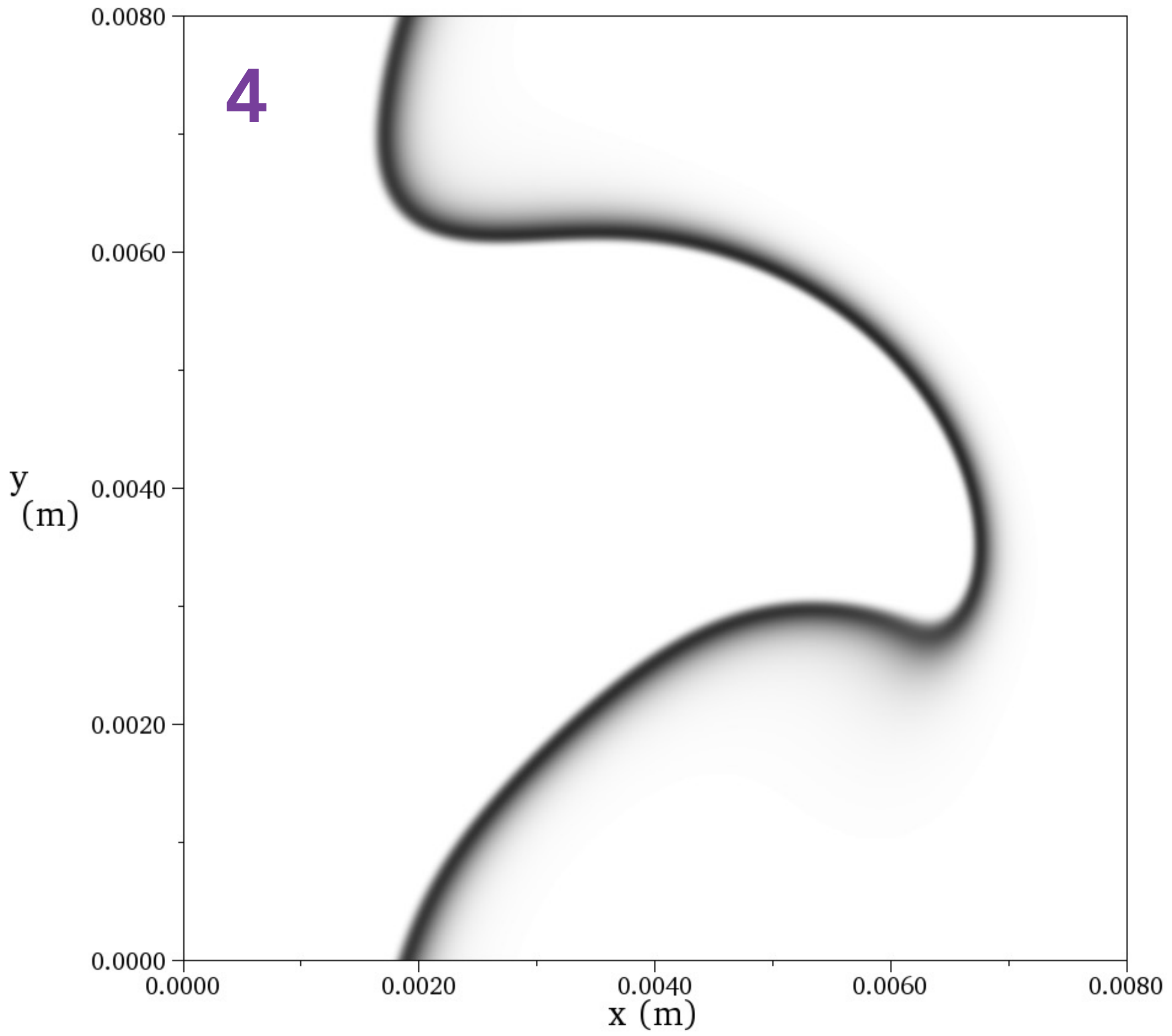




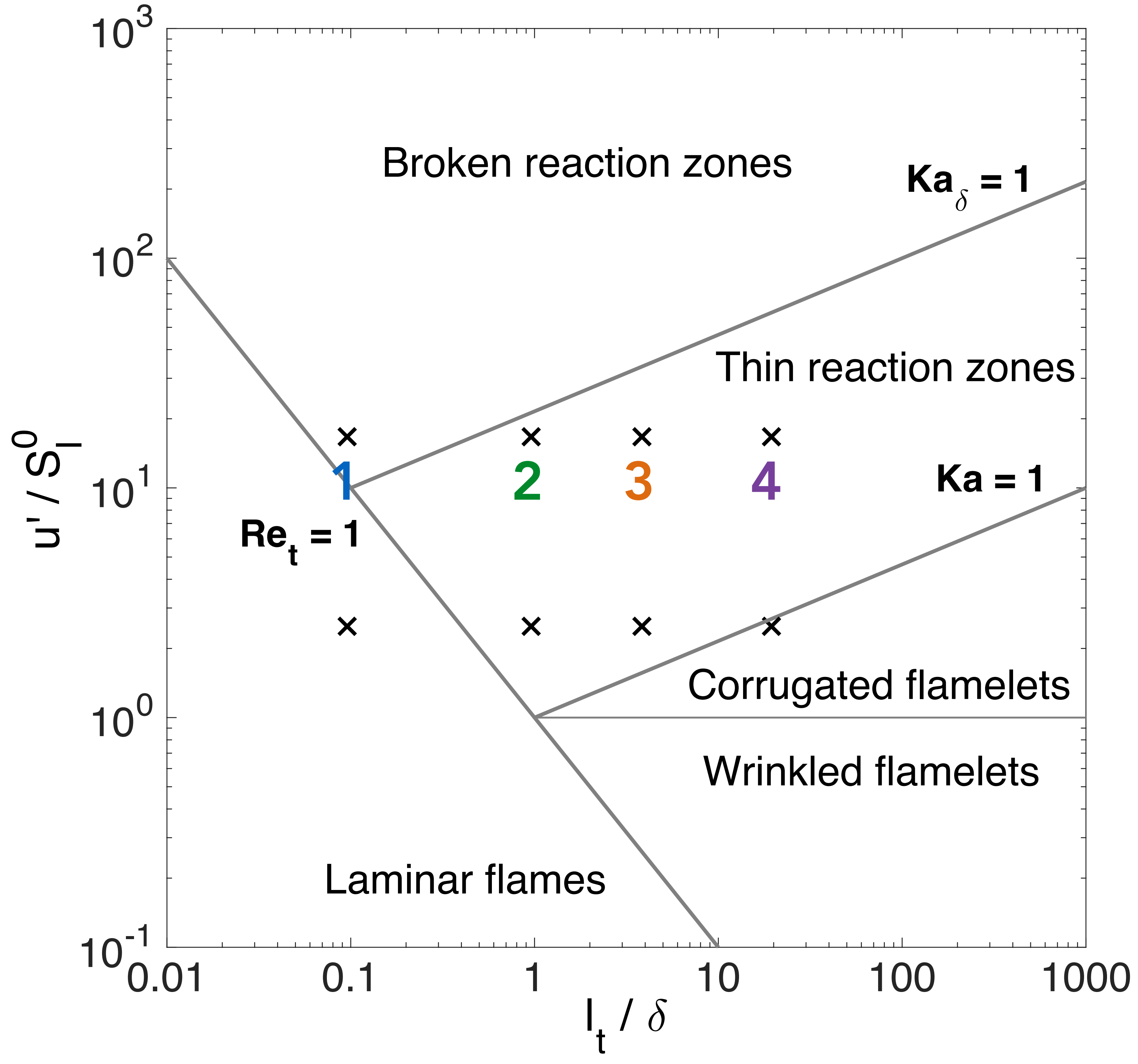


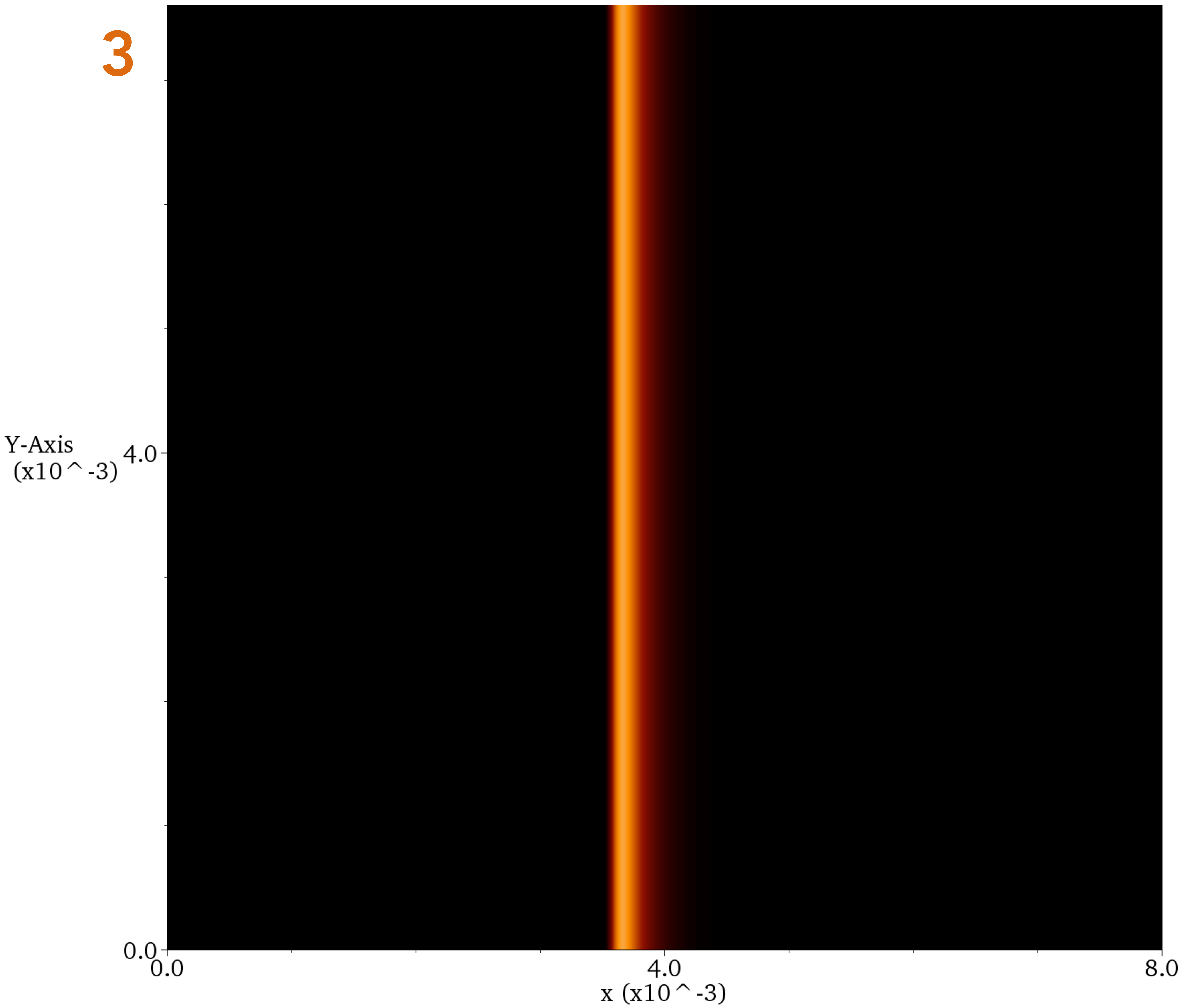
A. Coussement, B. Isaac, O. Gicquel and A. Parente, *Combust Flame* 168 (2016) 83–97.





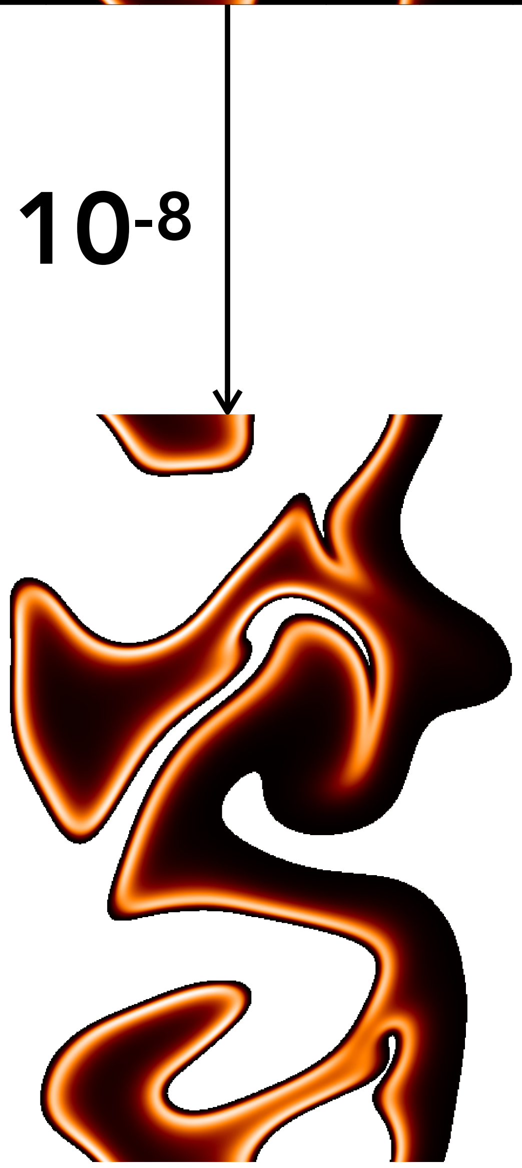
PCA models from simple reactors can be used on complex configurations



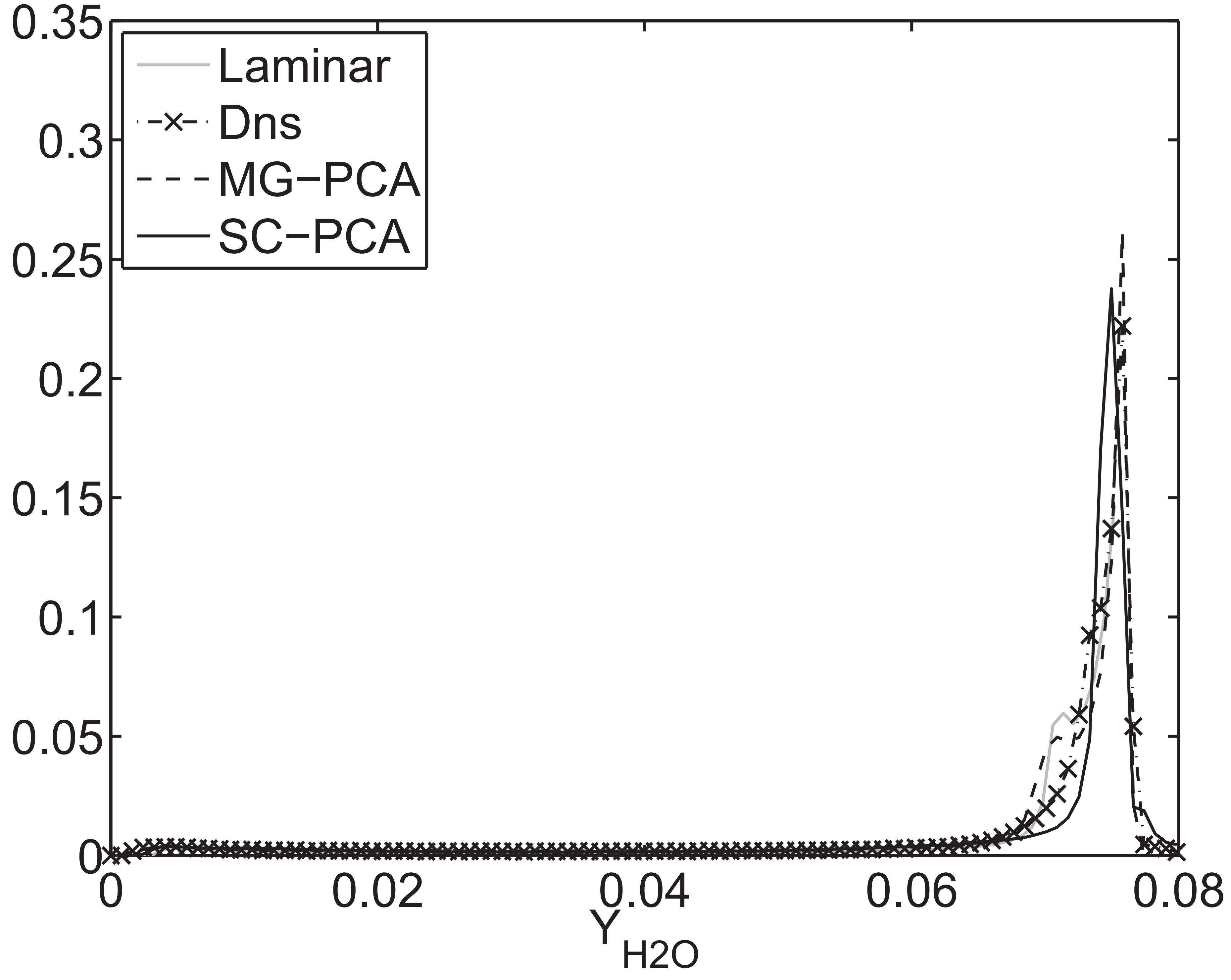


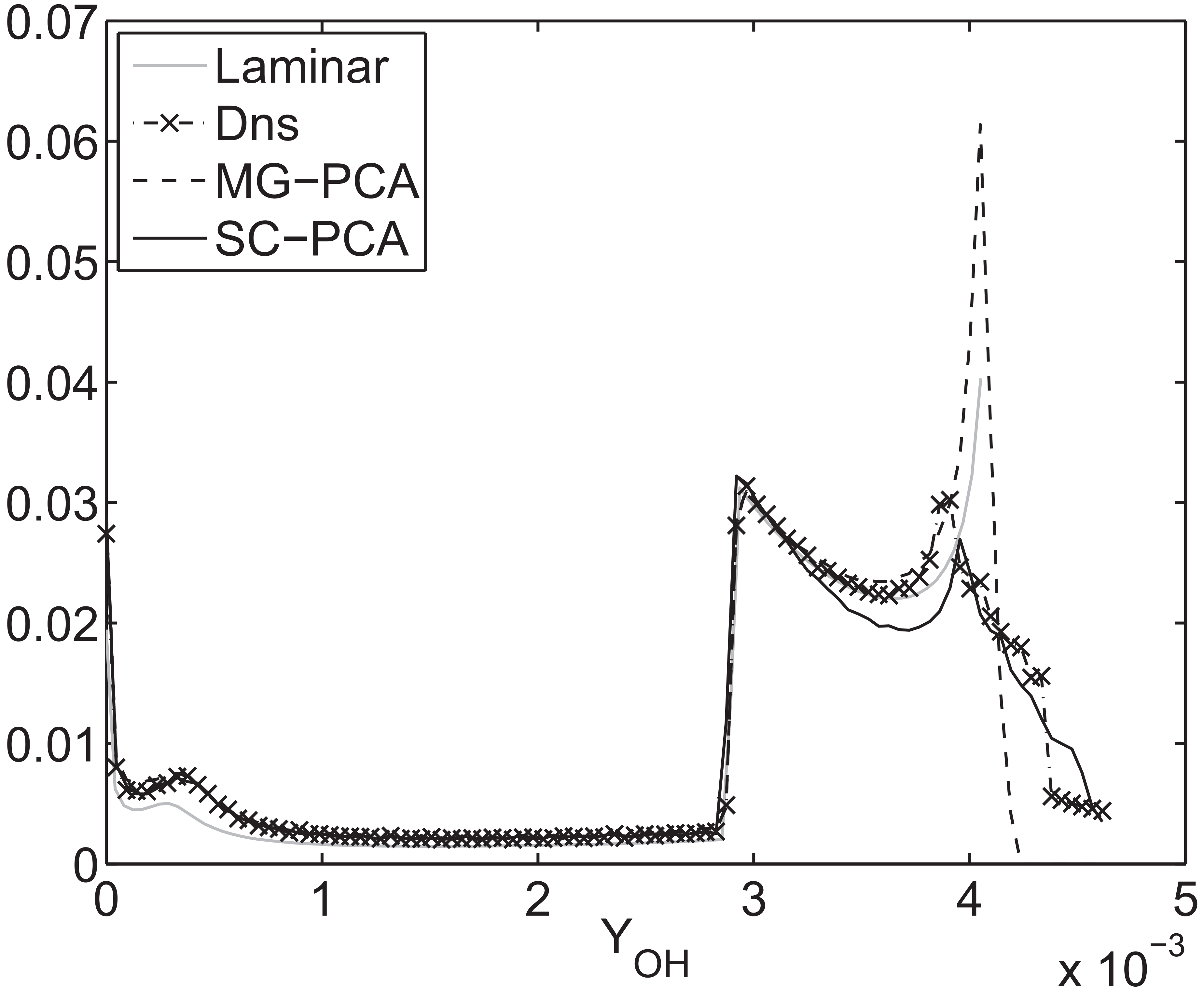
PCA models from simple reactors can be used on complex configurations

$Y_{HCO} > 10^{-8}$



Conditional PDF for selected species, for a case in the *thin reaction zones*





A. Coussement, B. Isaac, O. Gicquel and A. Parente, *Combust Flame* 168 (2016) 83–97.

PC-transport (PCA-GPR) simulation of Flames D and F

Training data

Database of laminar counter-diffusion flames

Fuel stream: 25% CH_4, 75% air (by vol)

Unsteady simulations with sinusoidal strain rate

80,000 observations per variable

3D simulation using OpenFOAM

Domain

0.6m x 0.3m x 0.3m, conical mesh, 3.2M cells, resolution: d/8=0.45mm

Settings

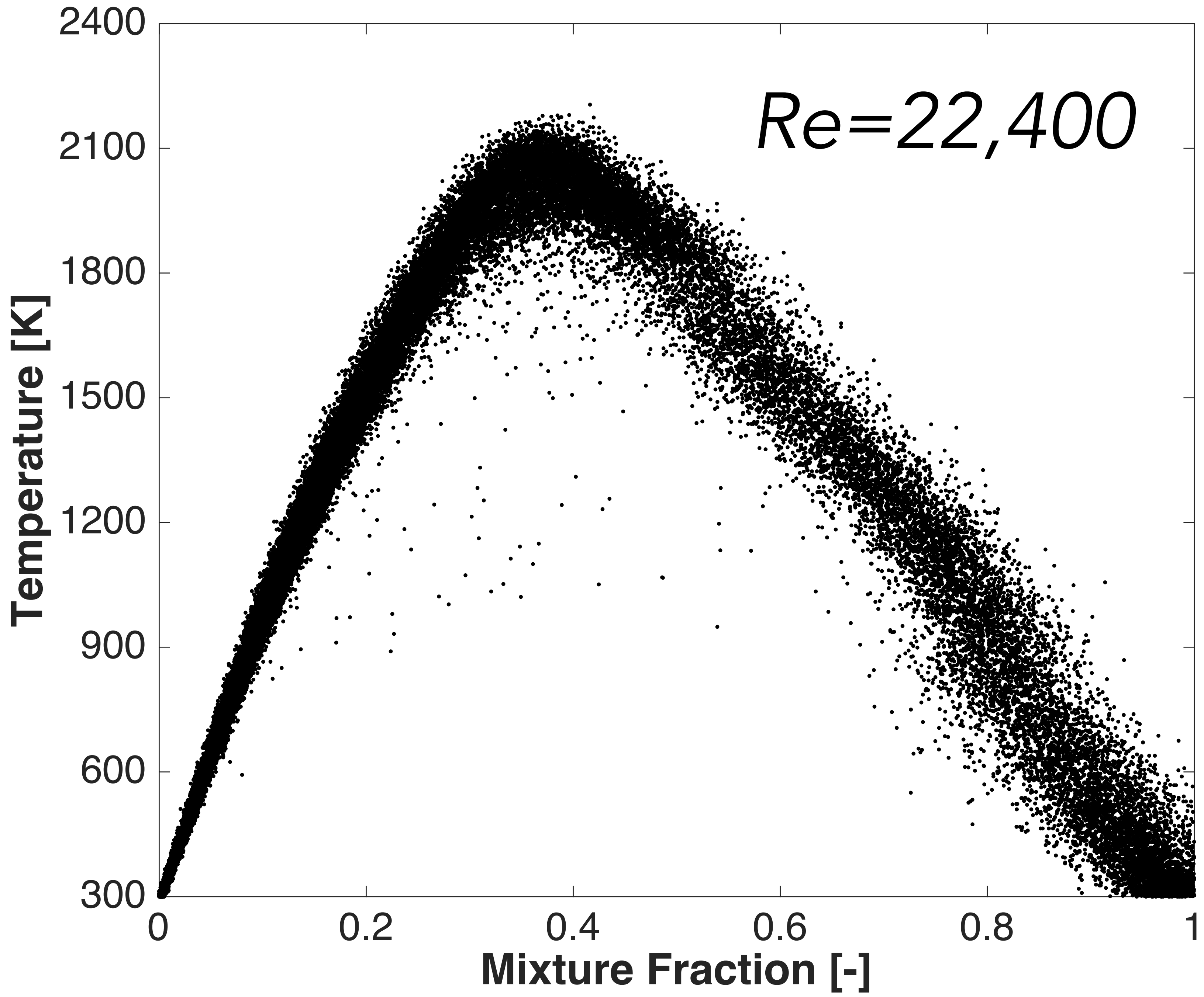
Turbulence generator: Digital Filter (Klein, 2003)

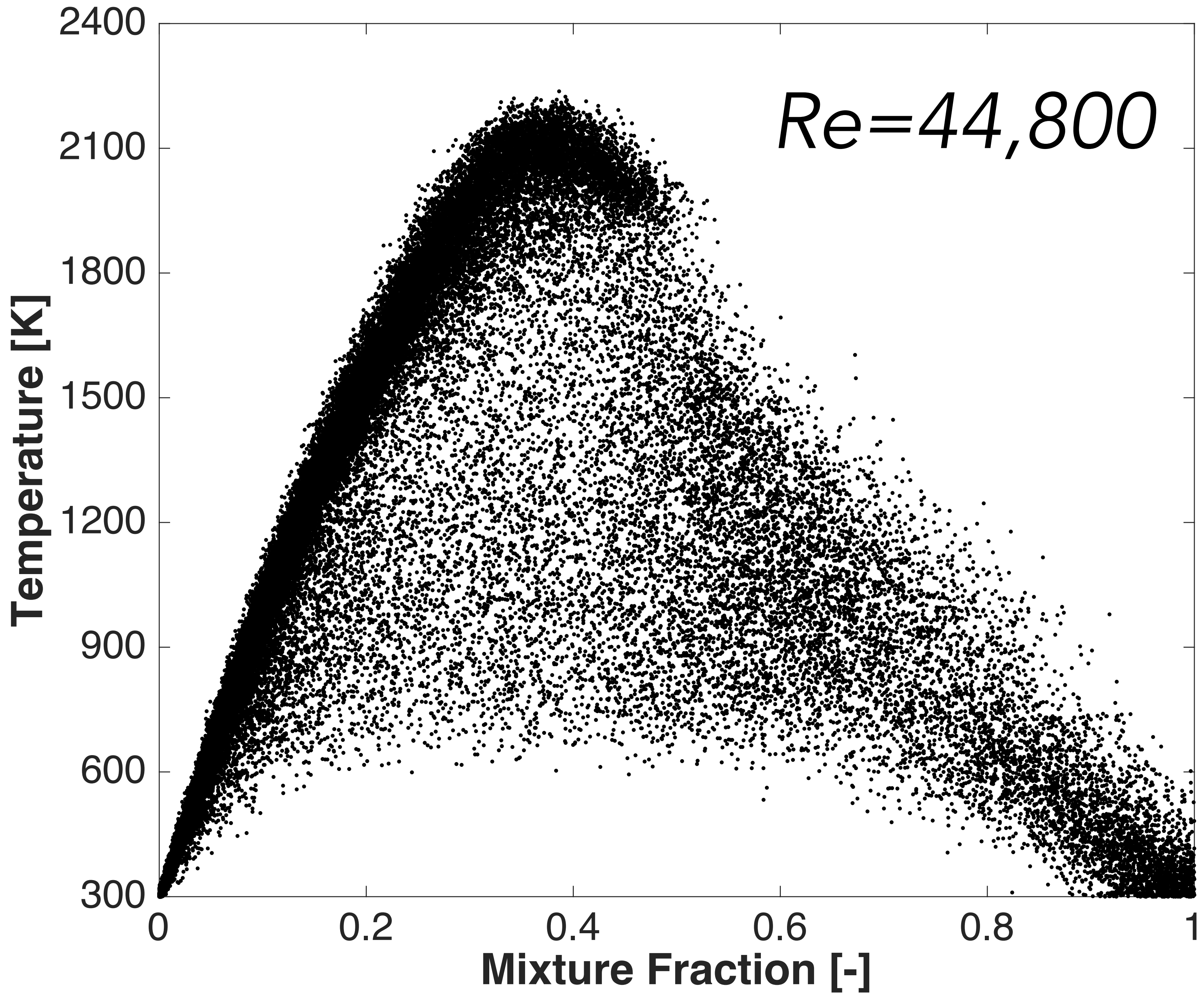
2^{nd} order in time, 2^{nd} order space, WALE model

2 transported variables: Z_1 and Z_2 (negligible effect of sub grid closure)

M. R. Malik, P. Obando Vega, A. Coussement, A. Parente, Proc Comb Inst 38 (2021) 2635-2643.

Complexity increases when going from flame D to flame F



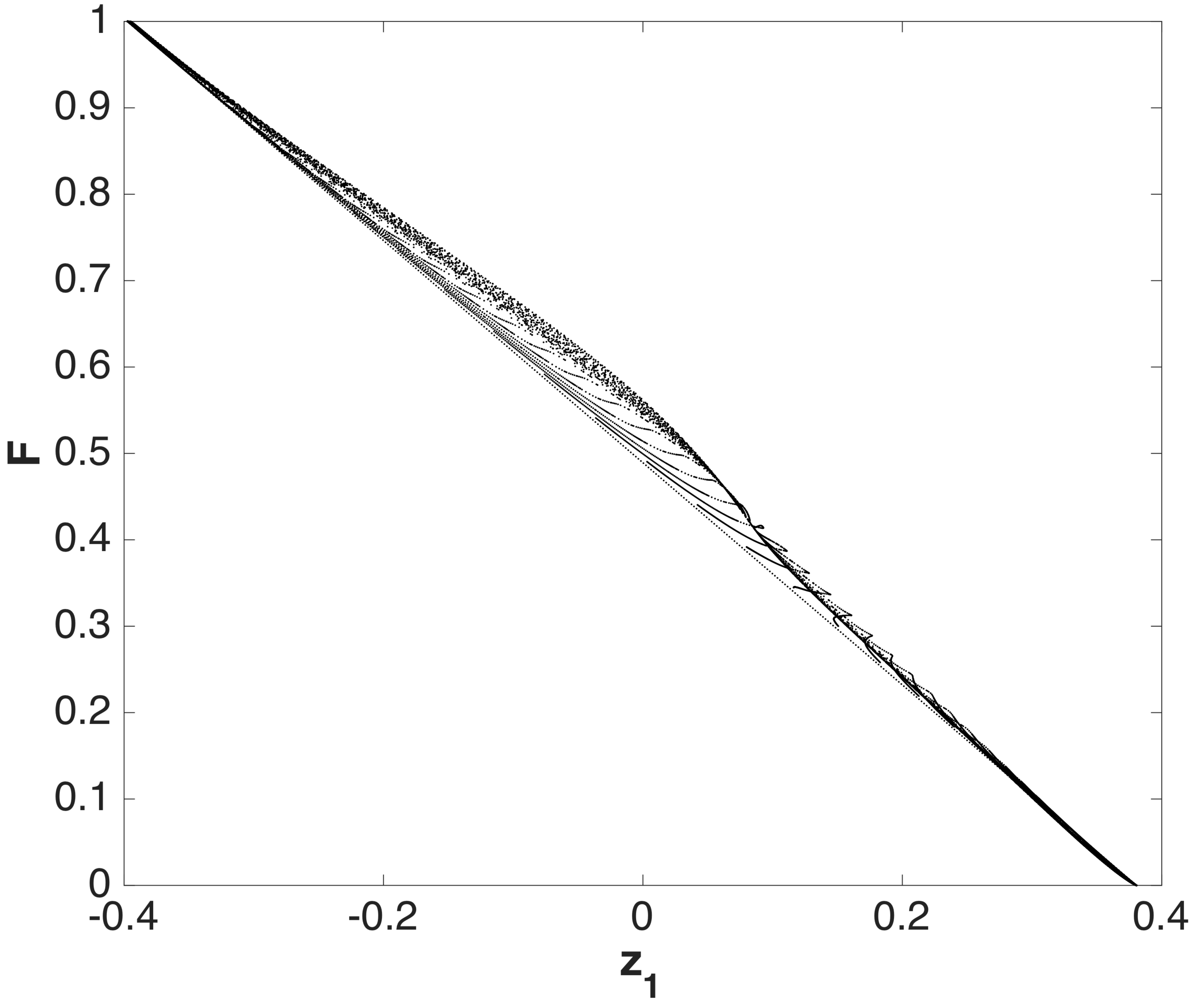


same system, different Reynolds number, Z captures most non-linearity

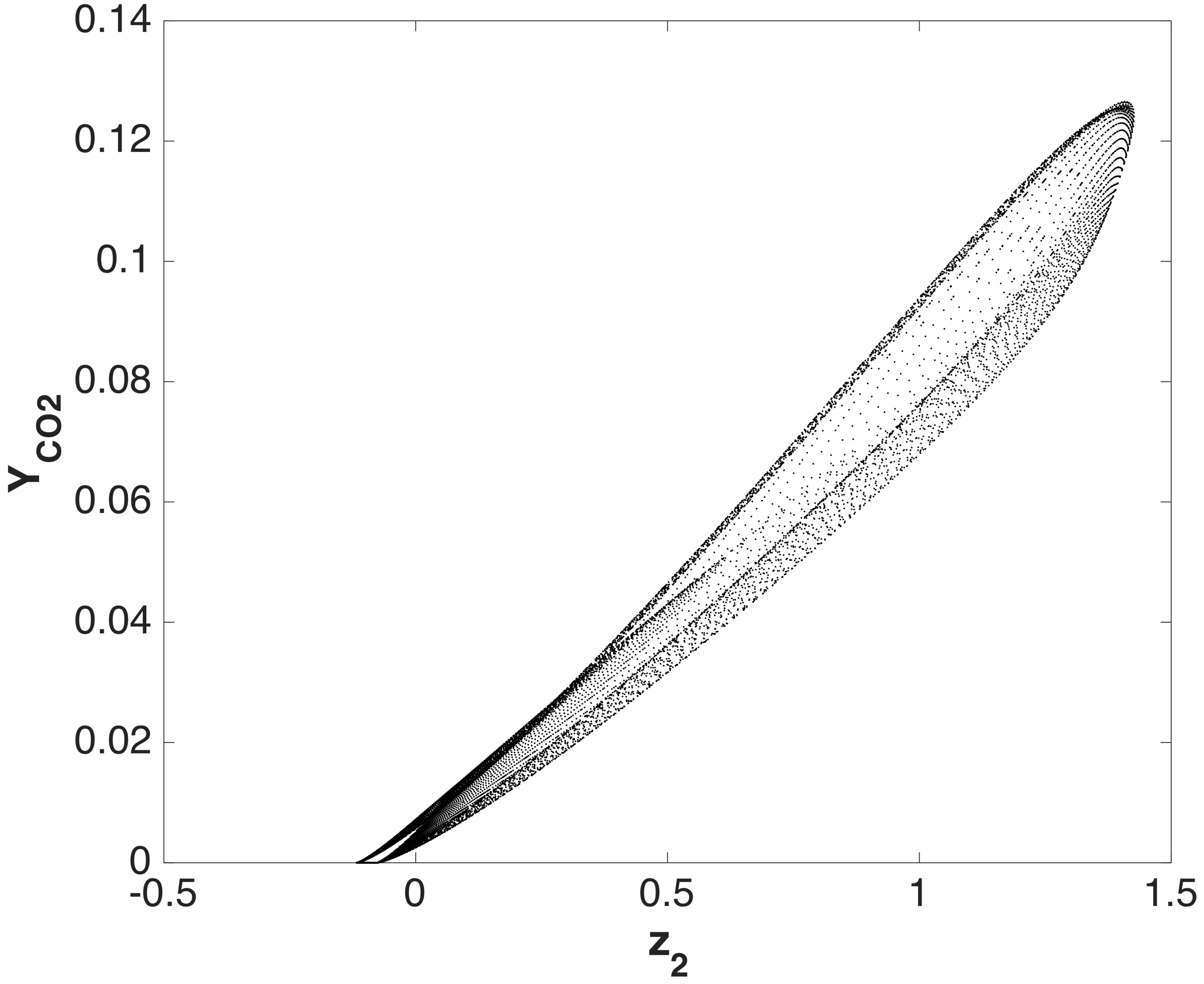
$$f = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}}$$

The PCs can be associated to physically interpretable variables

PC_1: mixture fraction



PC_2: progress of reaction



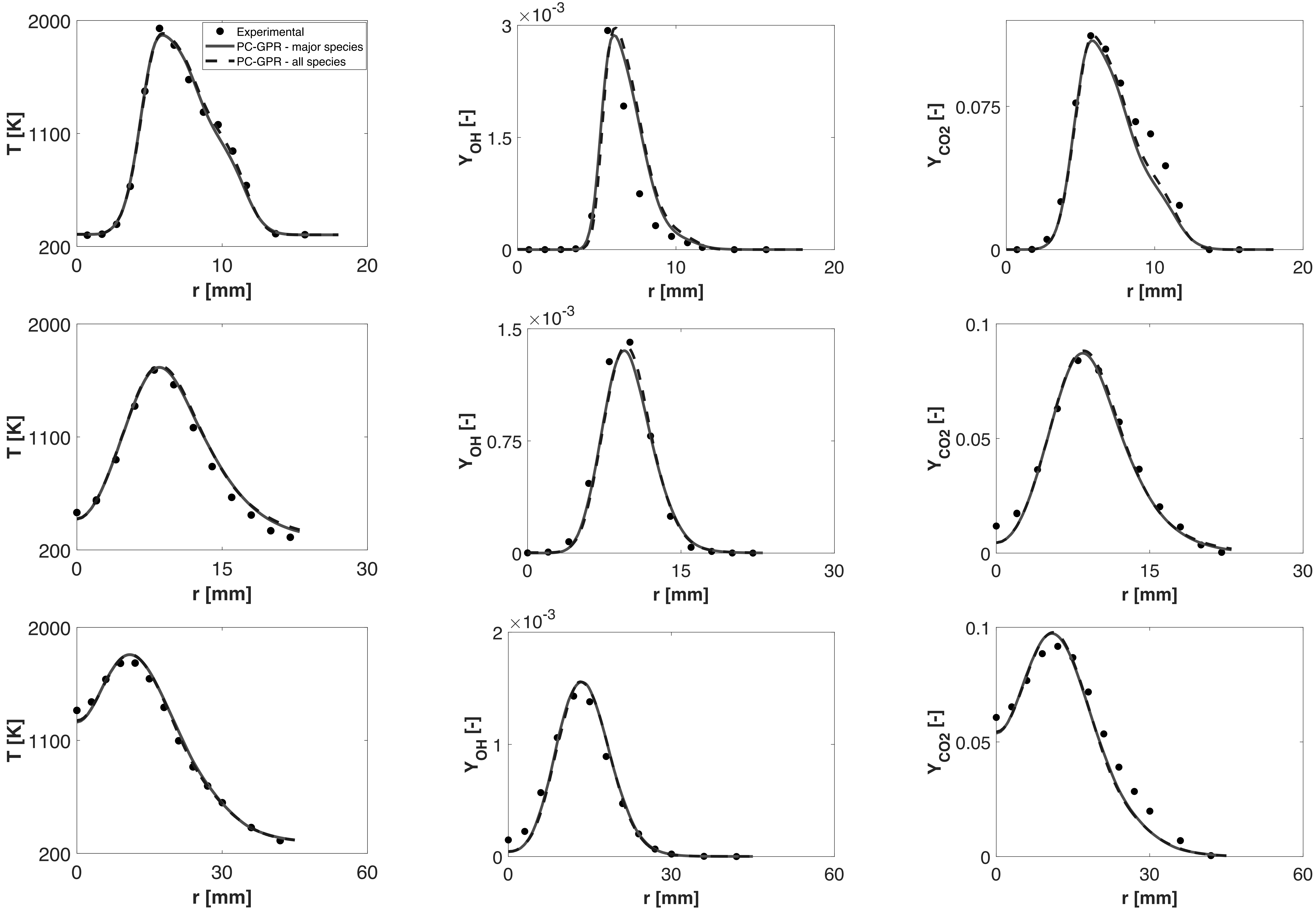
PCA finds the optimal parameterisation with no supervision: generalisation of tabulation methods

Flame D

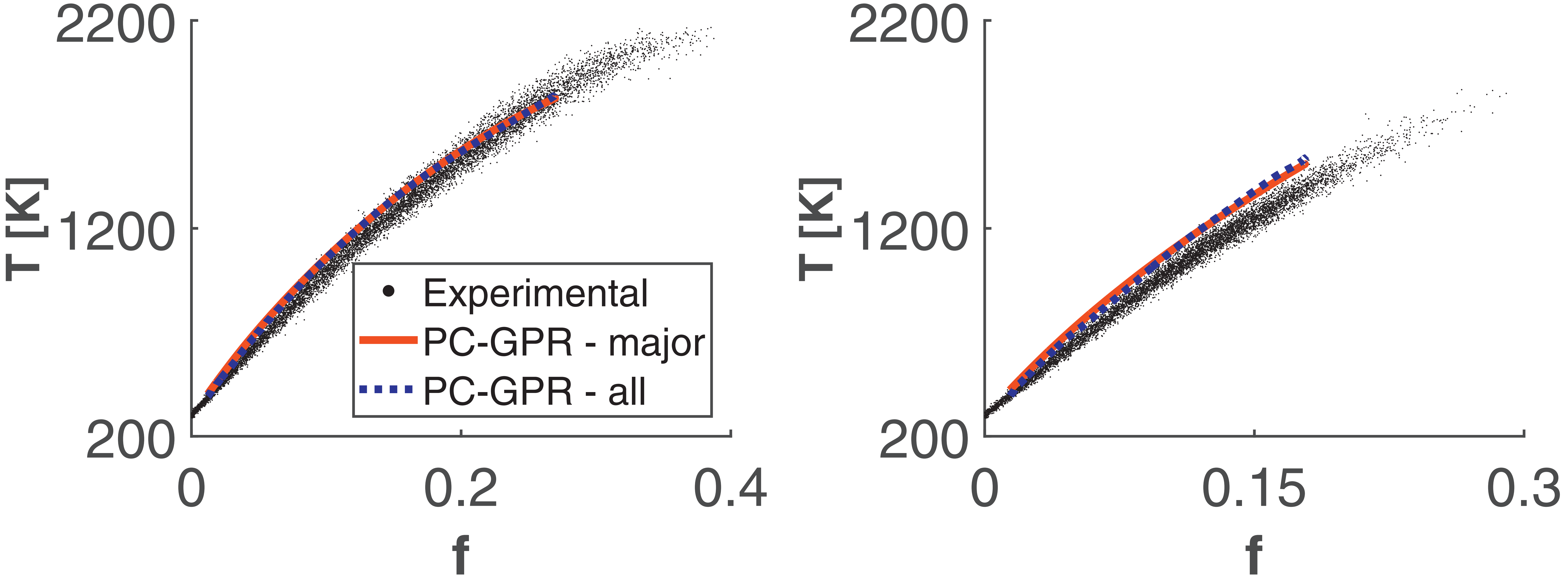
x/D=3

x/D=15

x/D=30

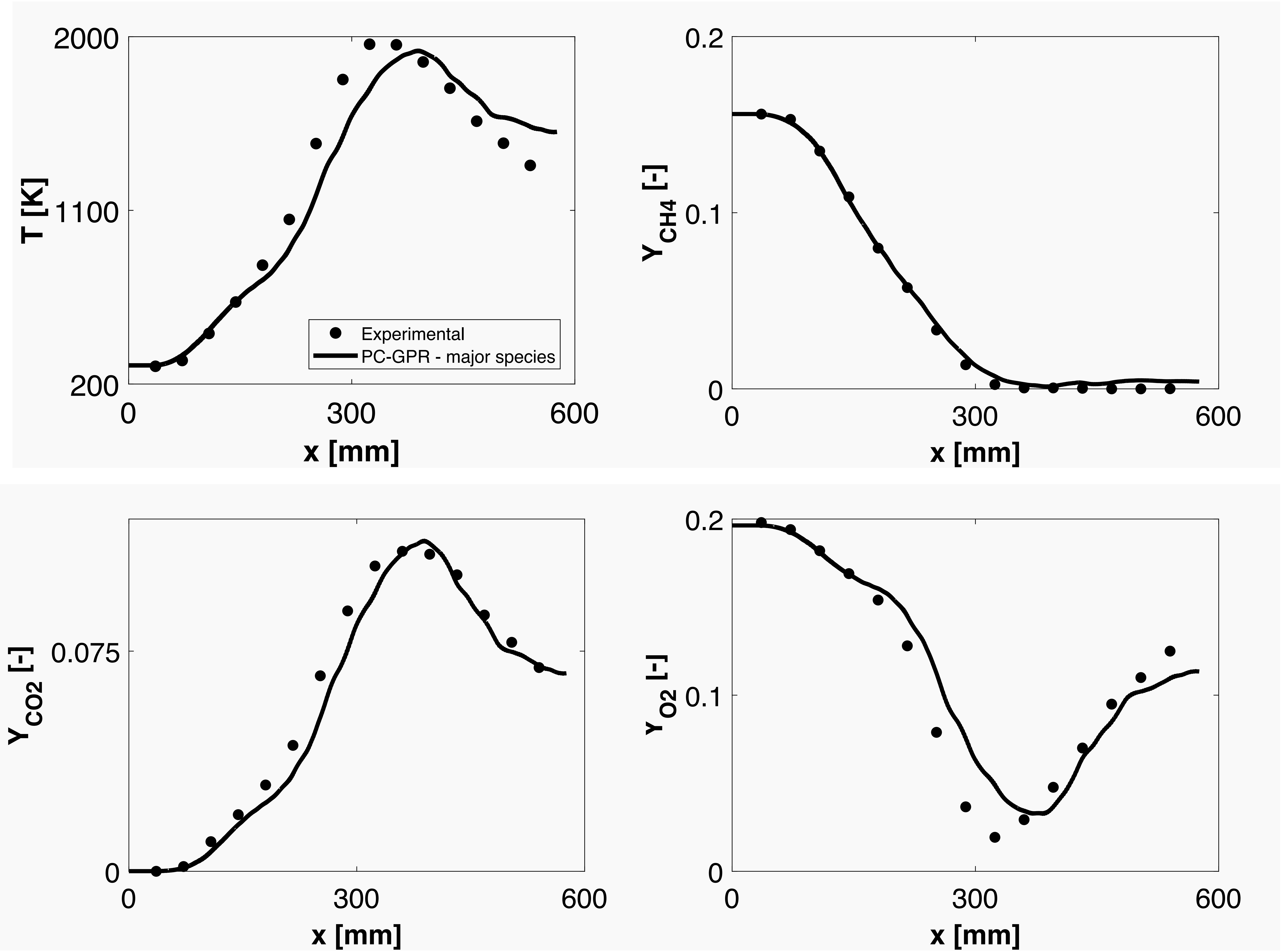


Flame D - conditional averages



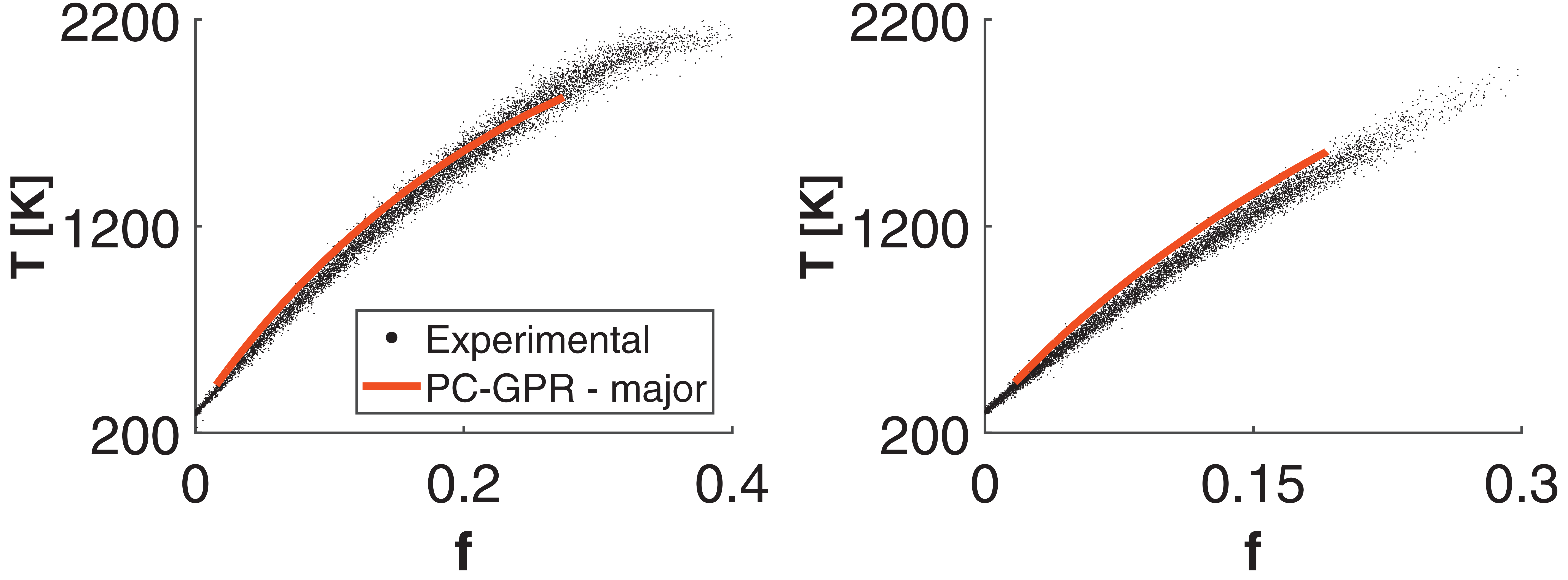
(a) $x/D = 60$ (b) $x/D = 75$

Flame F

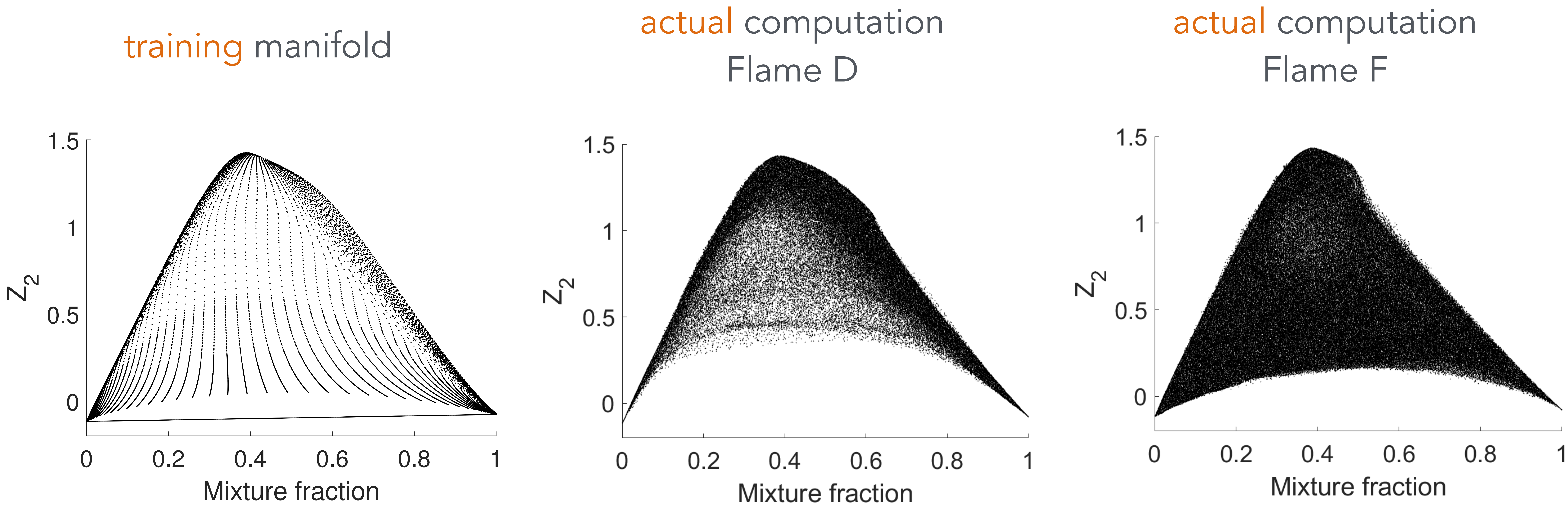


2000
1100
200
T [K]
0
300
600
x [mm]
Experimental
PC-GPR - major species
0.2
0.1
0
Y_{CH4} [-]
0
300
600
x [mm]
0.075
0
Y_{CO2} [-]
0
300
600
x [mm]
0.2
0.1
0
Y_{O2} [-]
0
300
600
x [mm]

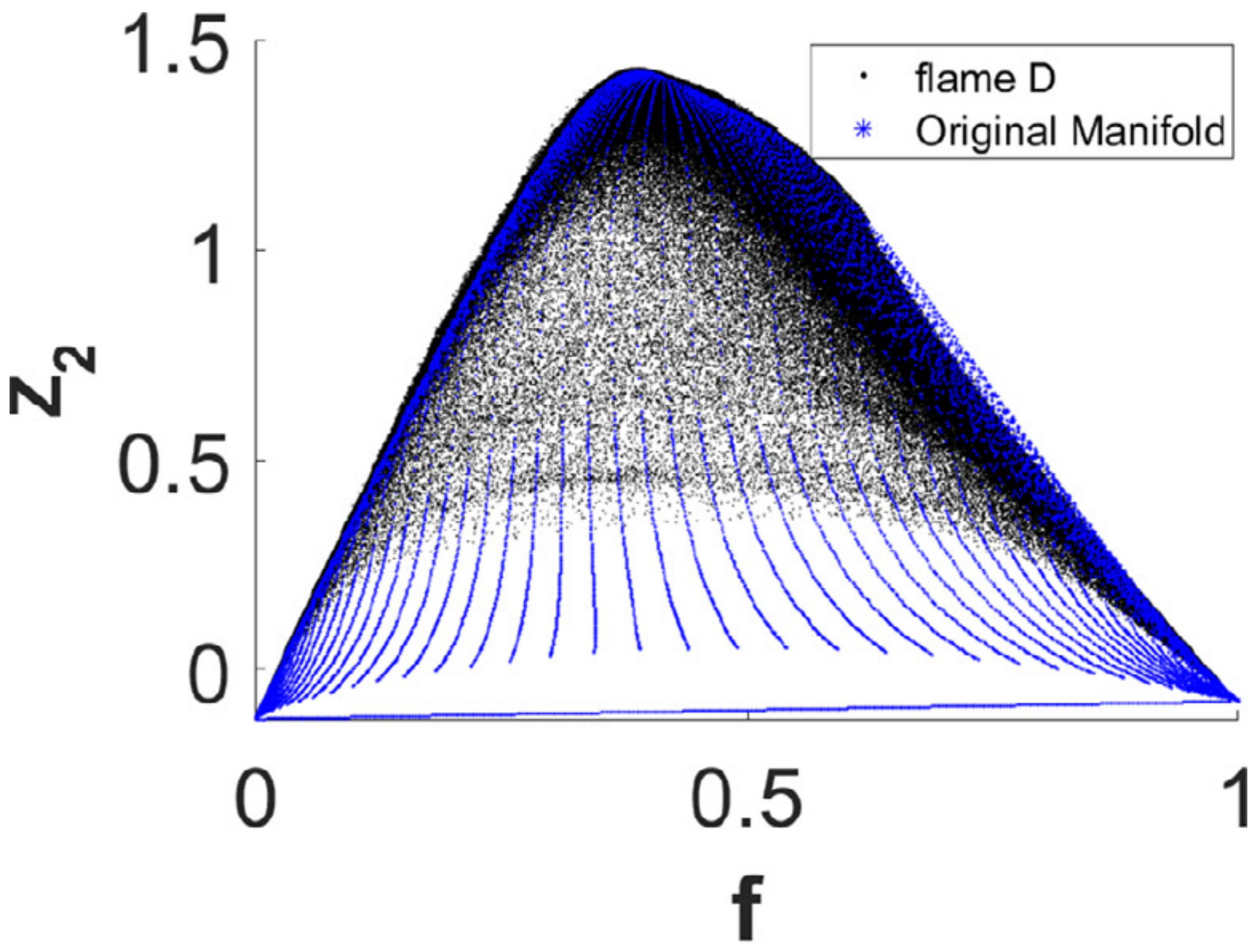
Flame F - conditional averages



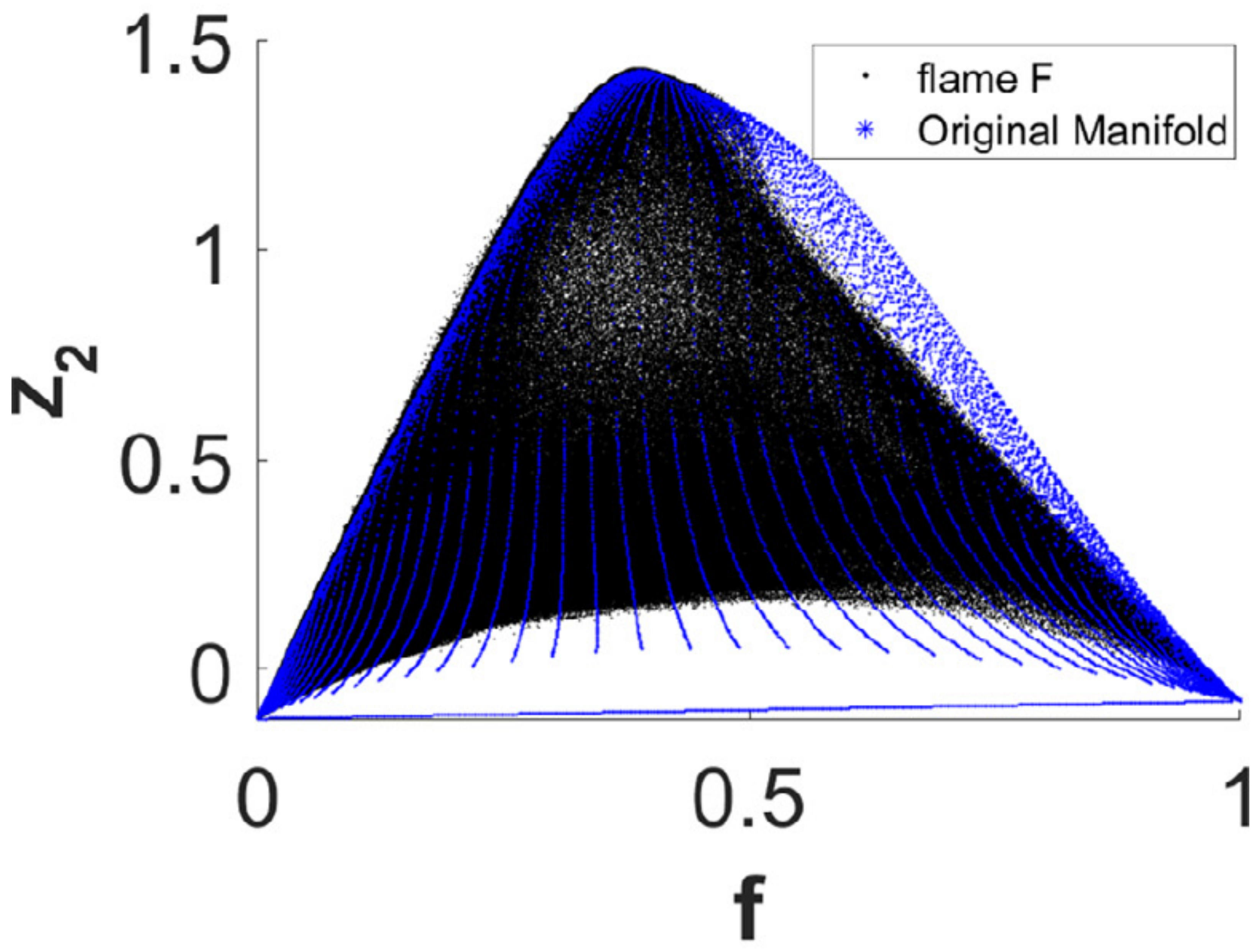
Bounds, training manifolds and actual computation



Bounds, training manifolds and actual computation



(a) flame D vs original manifold



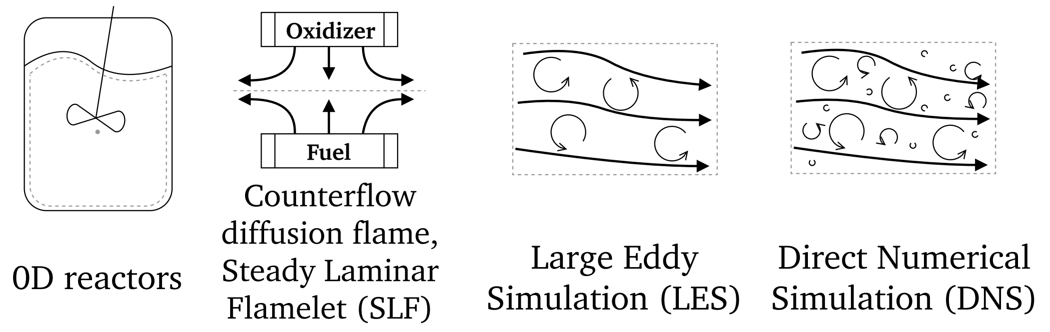
(b) flame F vs original manifold

Data-driven modelling for dimensionality reduction

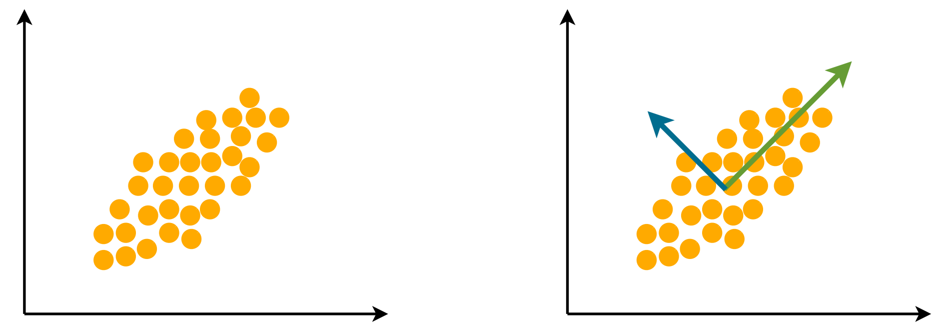
State-space methods

Transport of Principal Components

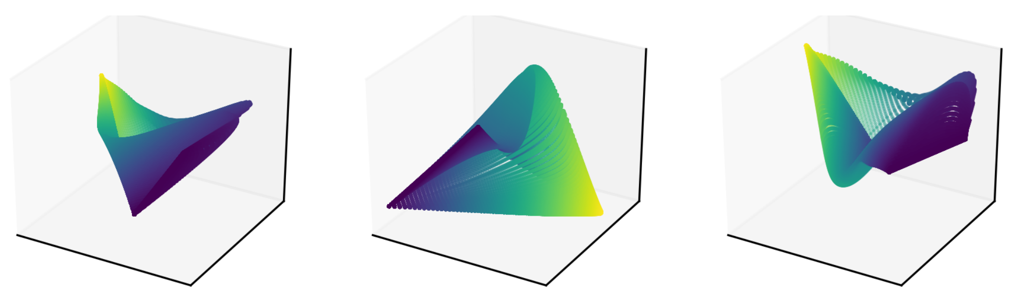
1. Training



2. Dimensionality reduction



3. Parameterisation

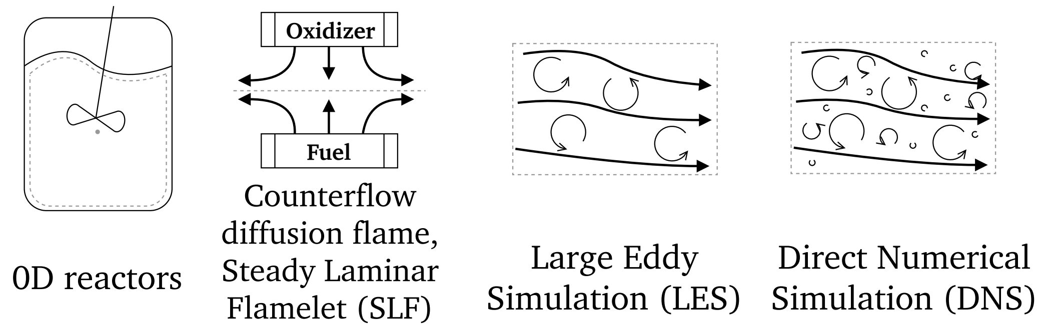


M. R. Malik, P. Obando Vega, A. Coussement, A. Parente,
Proceedings of the Combustion Institute, 2020.

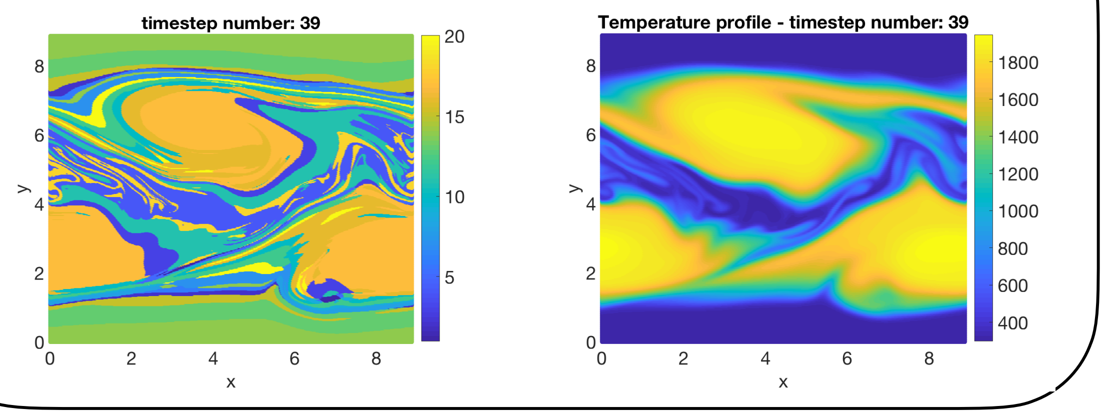
Rate-based methods

Pre-partitioned adaptive chemistry

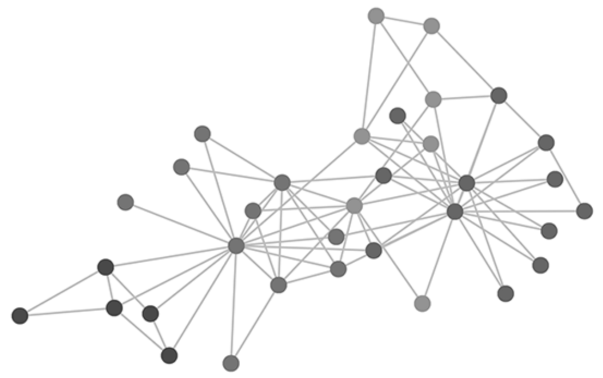
1. Training



2. Classification



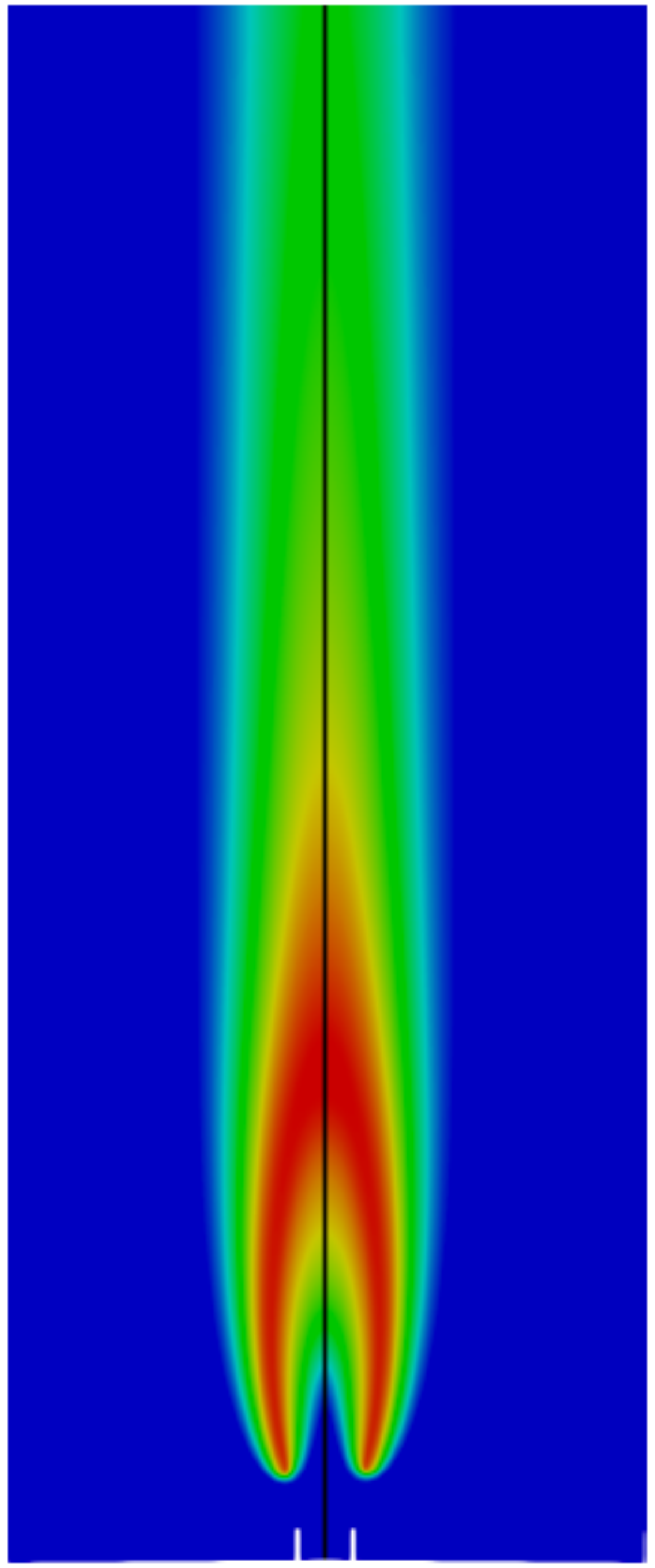
3. Mechanism reduction



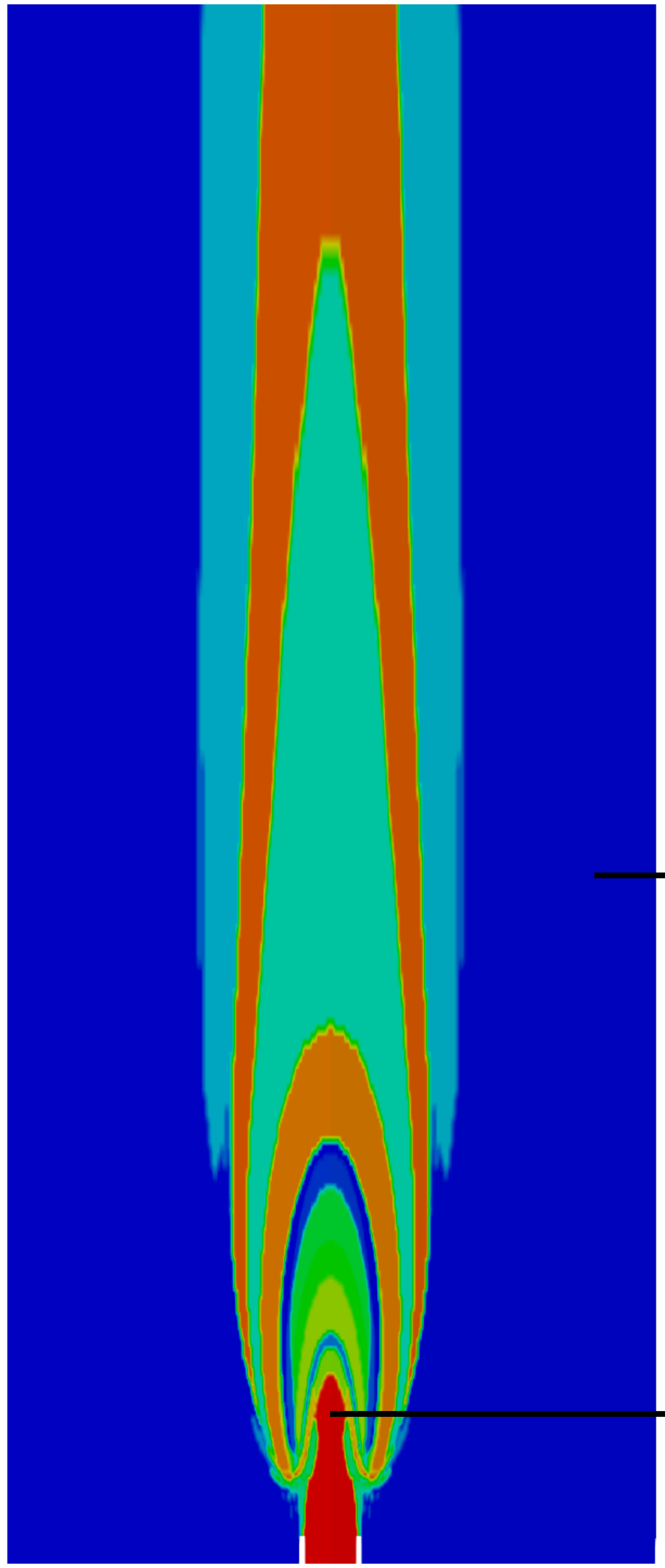
G. D'Alessio, A. Parente, A. Stagni, A. Cuoci,
Combustion and Flame, 211, 2020, 68-82

Sample-Partitioning Adaptive Reduced Chemistry

Classification of state-space and locally optimal chemical mechanisms



classification →



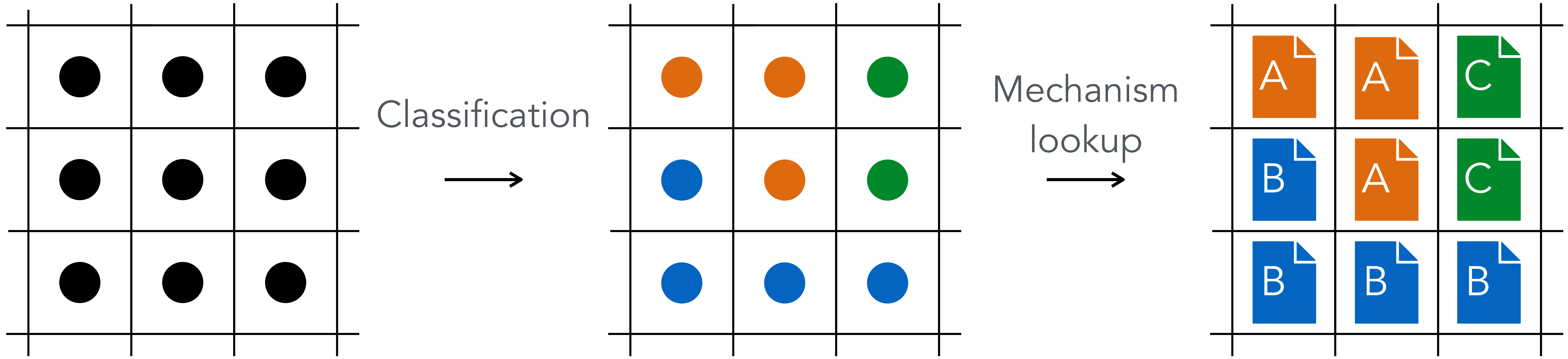
Here I need only 2 species (O_2 and N_2)

Here I need all species

Sample-Partitioning Adaptive Reduced Chemistry

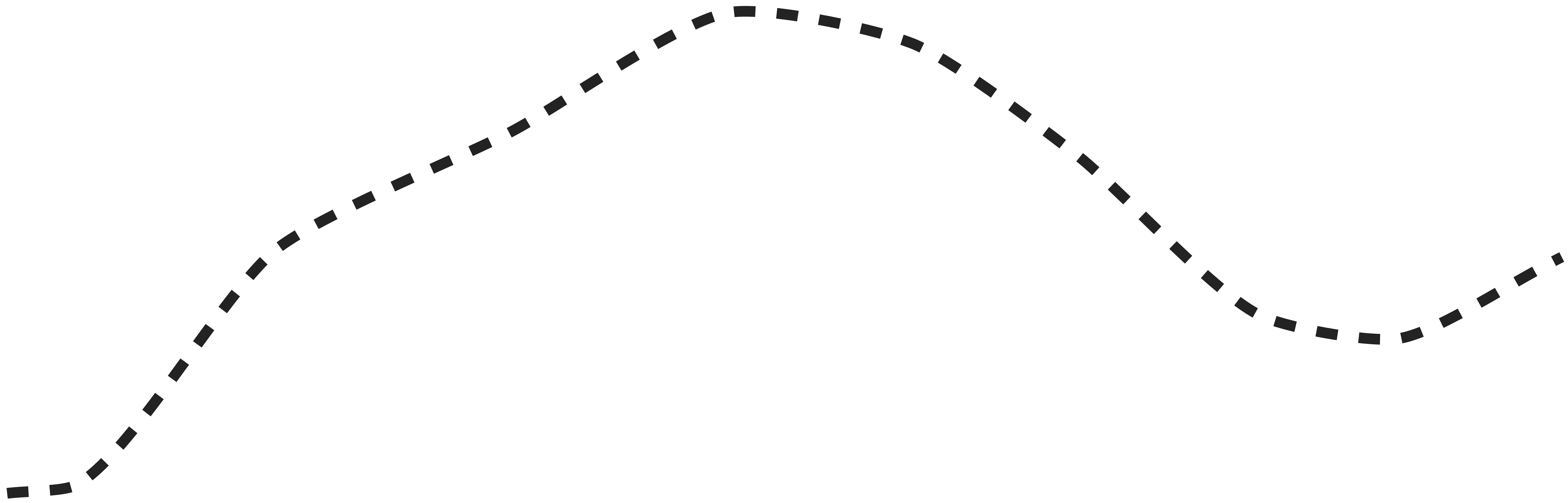
Preprocessing

Run time

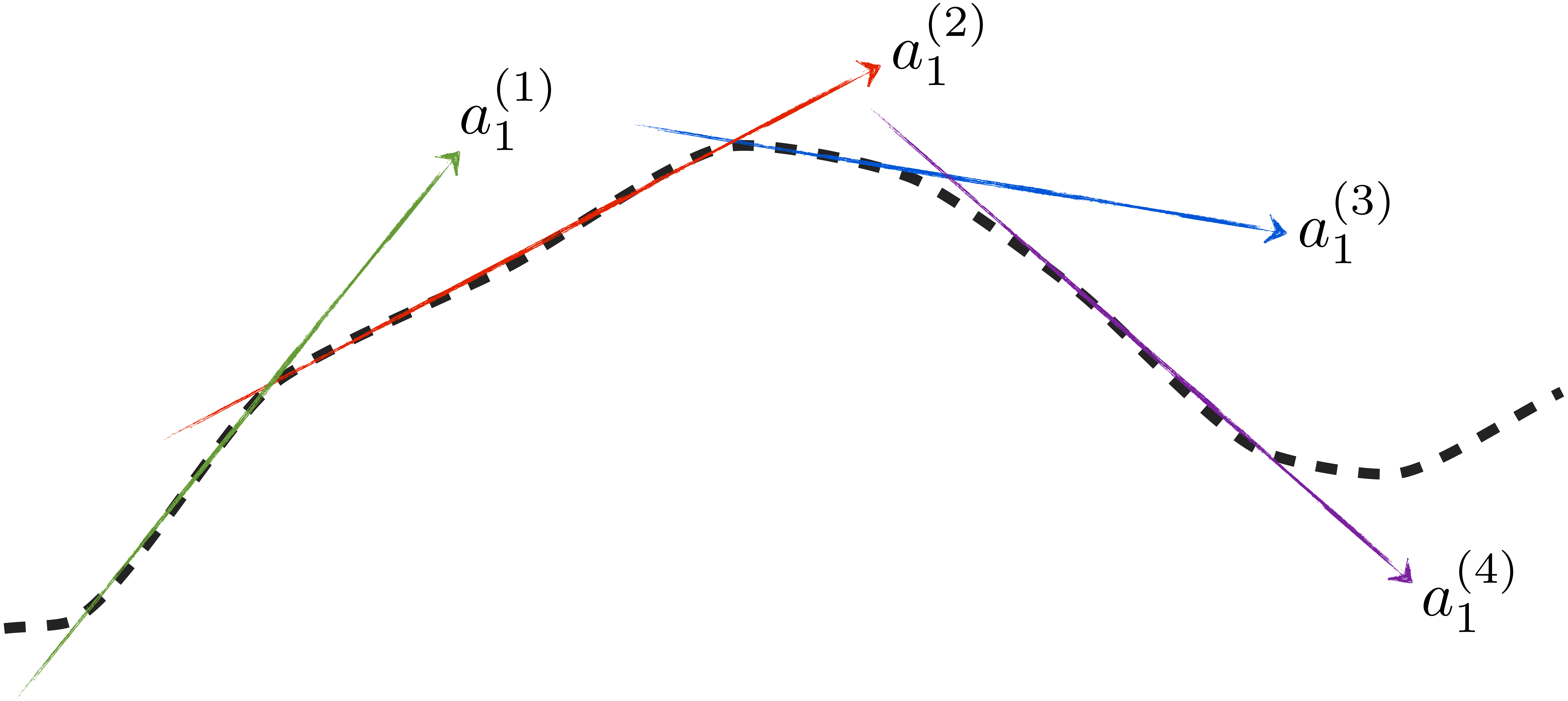


105

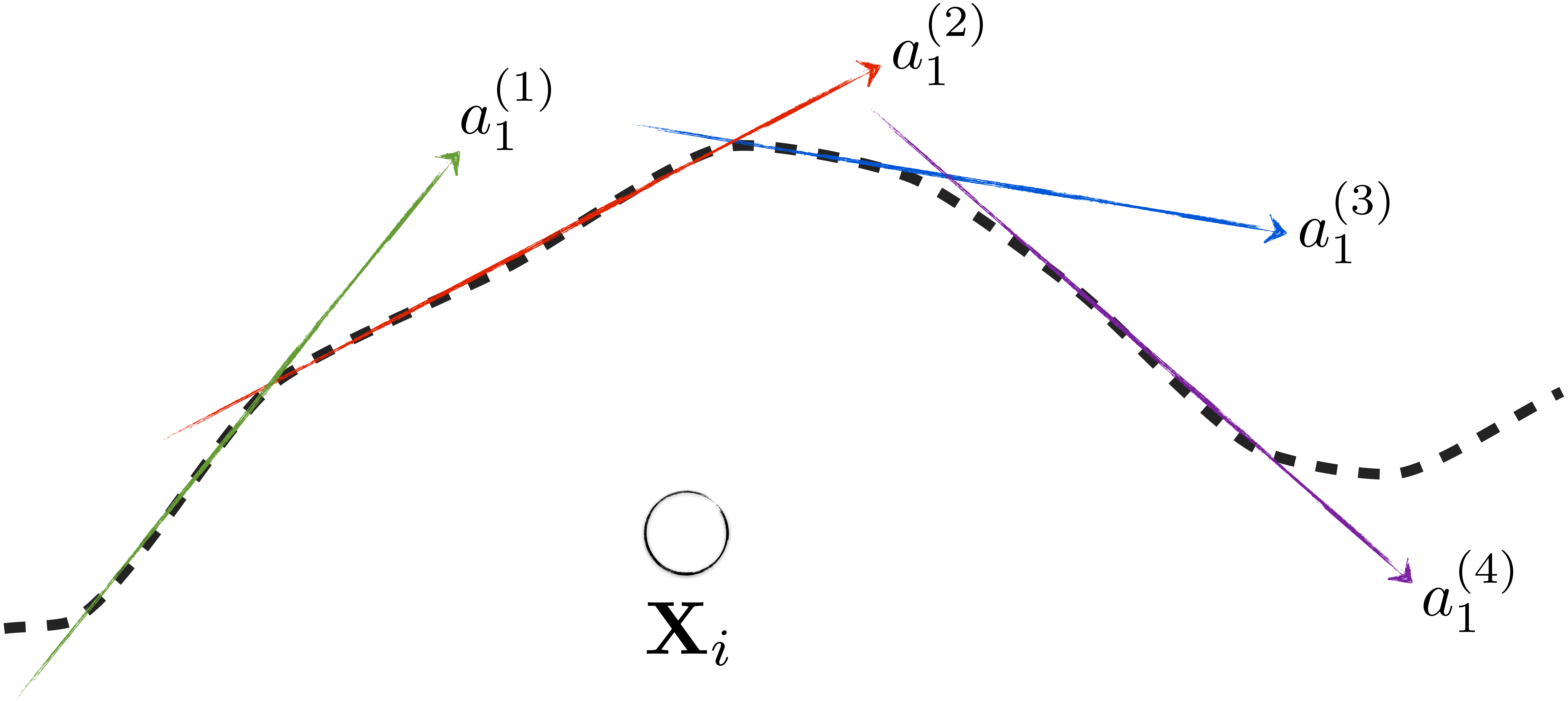
Our clustering approach relies on local PCA



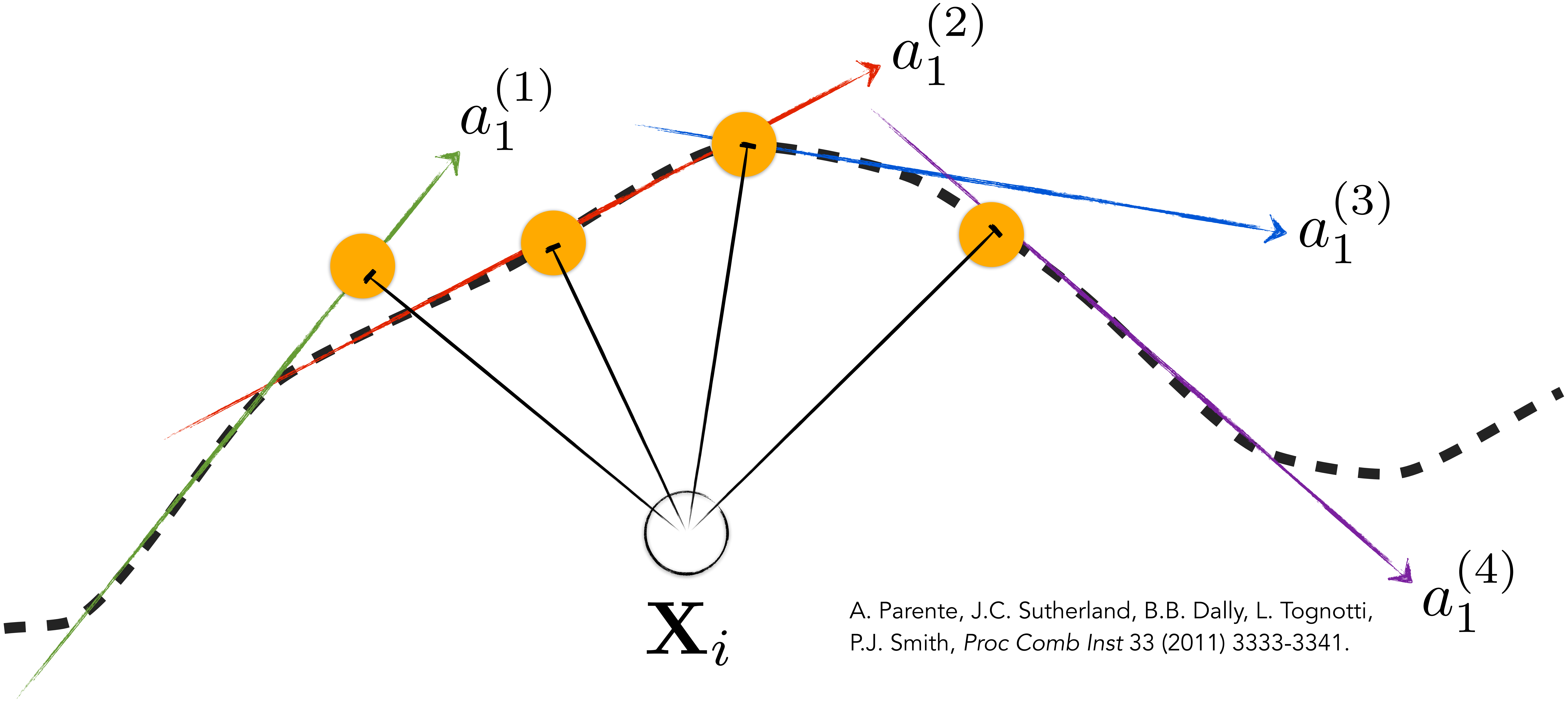
Our Local PCA approach combines dimensionality reduction and vector quantisation in a single step



A multi-dimensional point is assigned to the cluster ensuring the lowest low-dimensional reconstruction



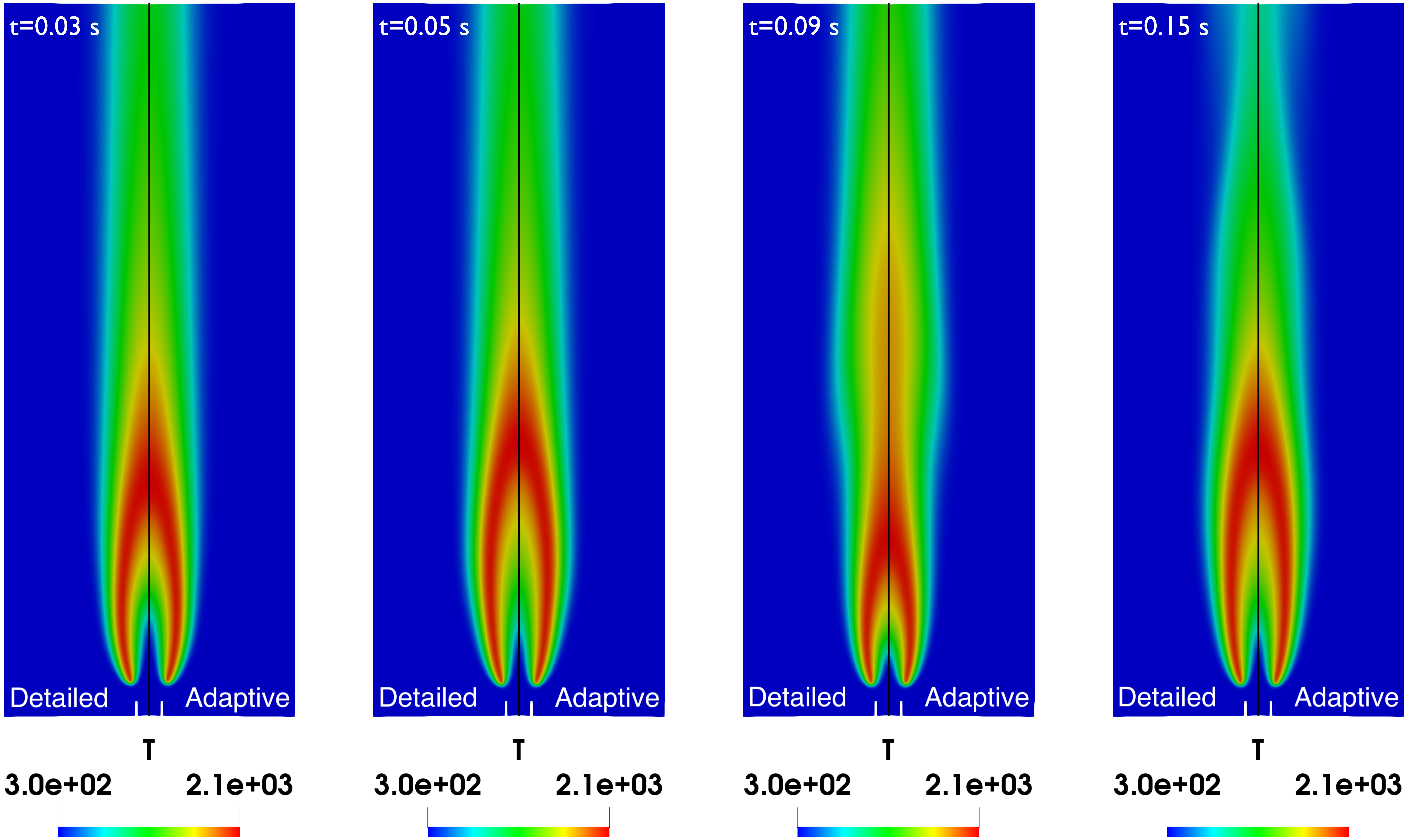
The approach is iterative and requires the specification of a hyper parameter, the number of clusters



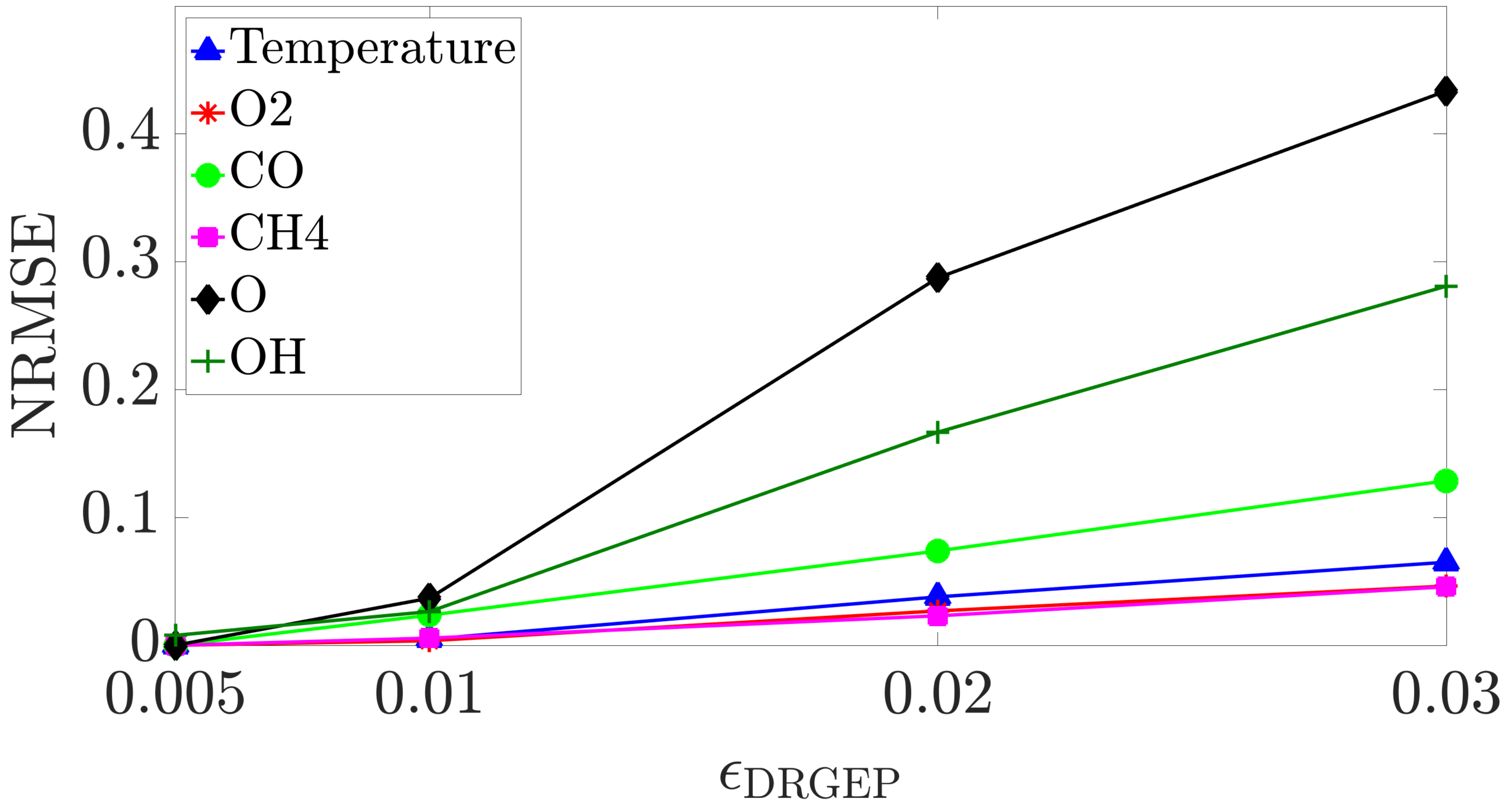
A. Parente, J.C. Sutherland, B.B. Dally, L. Tognotti, P.J. Smith, *Proc Comb Inst* 33 (2011) 3333-3341.

Application to an unsteady co-flow methane flame

(ε_{DRGEP}=0.005)

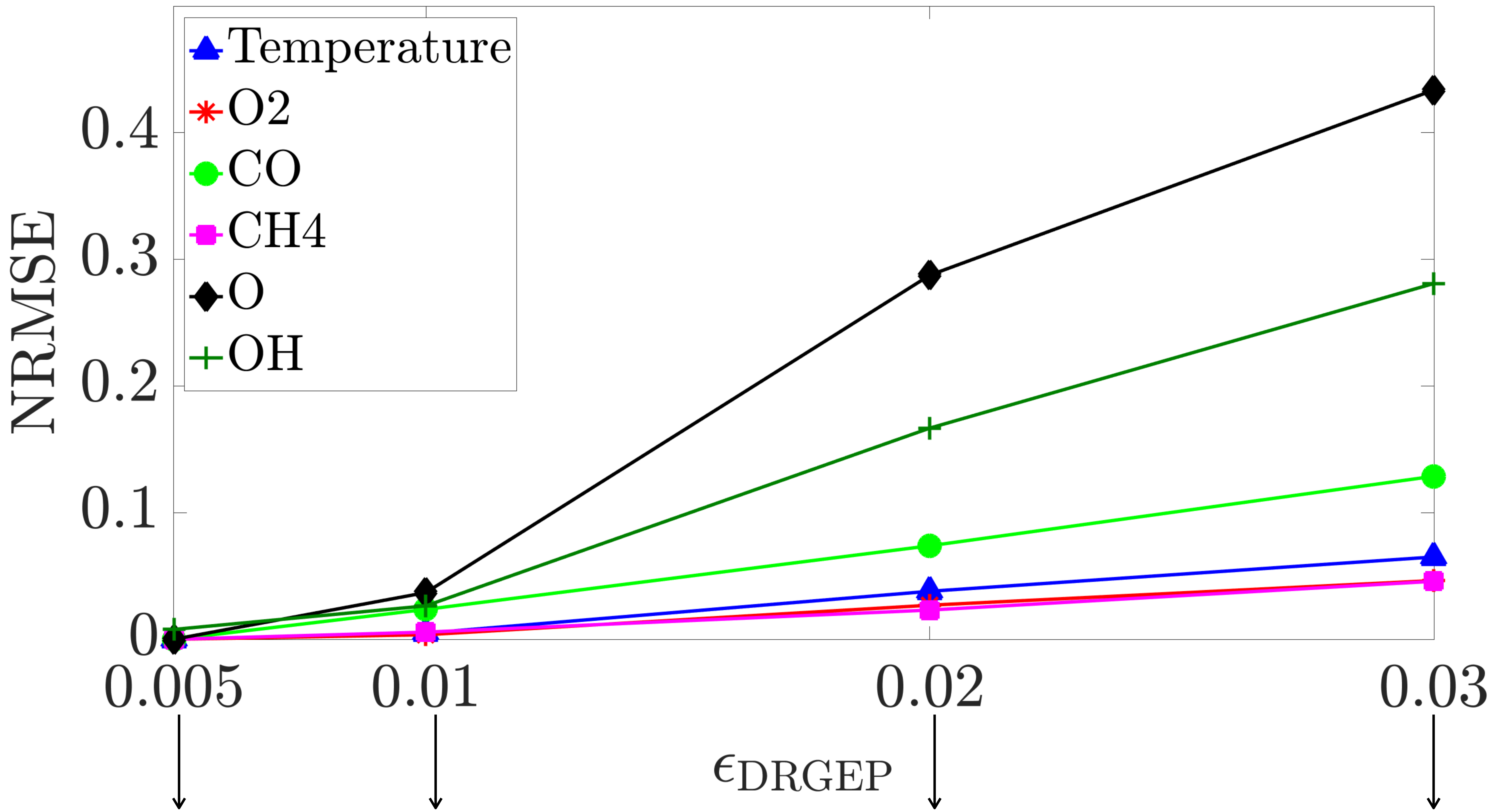


Relation between the error and the DRGEP threshold



G. D'Alessio, A. Stagni, A. Parente, A. Cuoci, *Combust Flame* 211 (2020) 68-82

Relation between the error and the DRGEP threshold



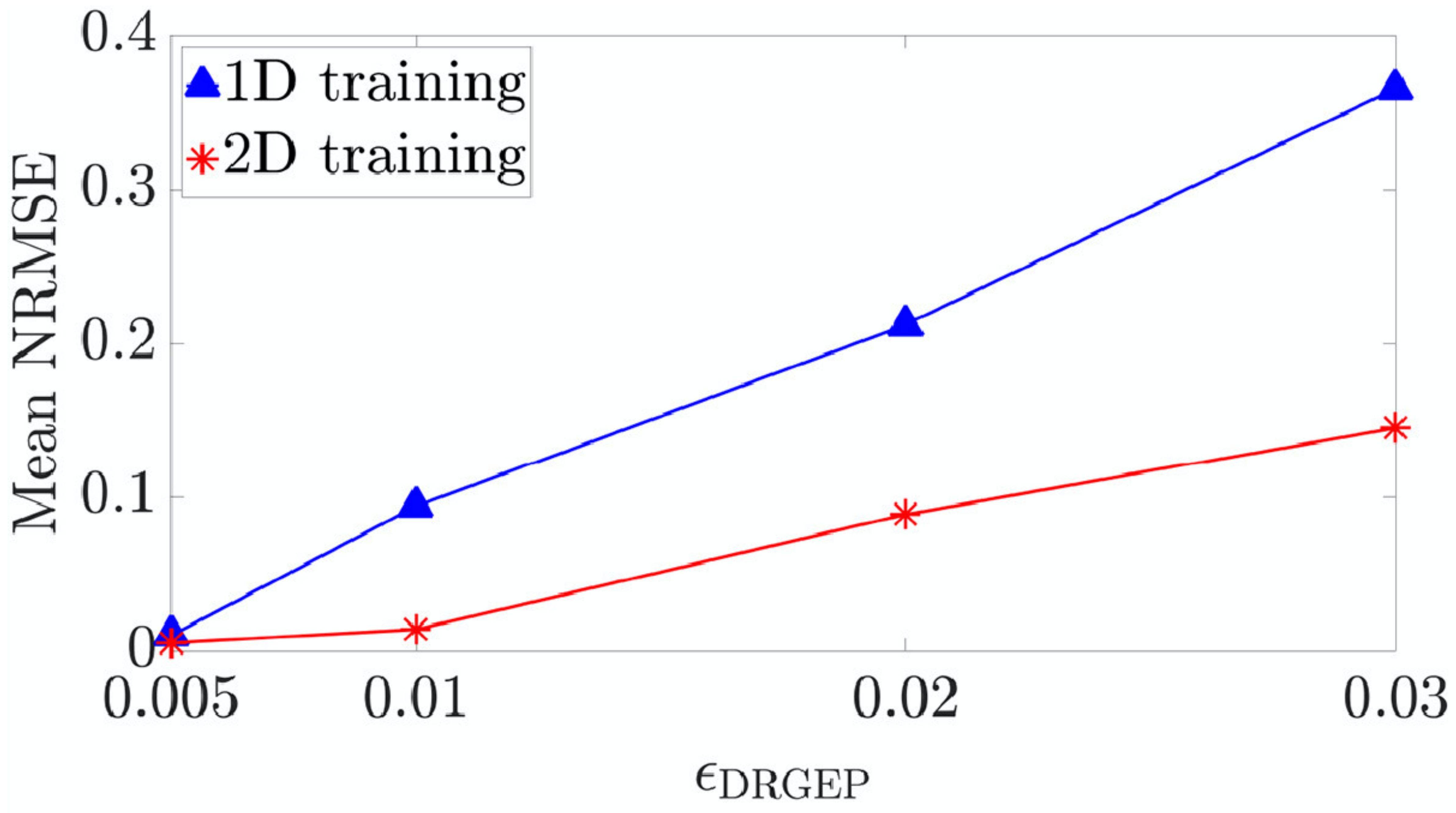
Speed up ~4 ~4.6 ~4.9 ~5.4

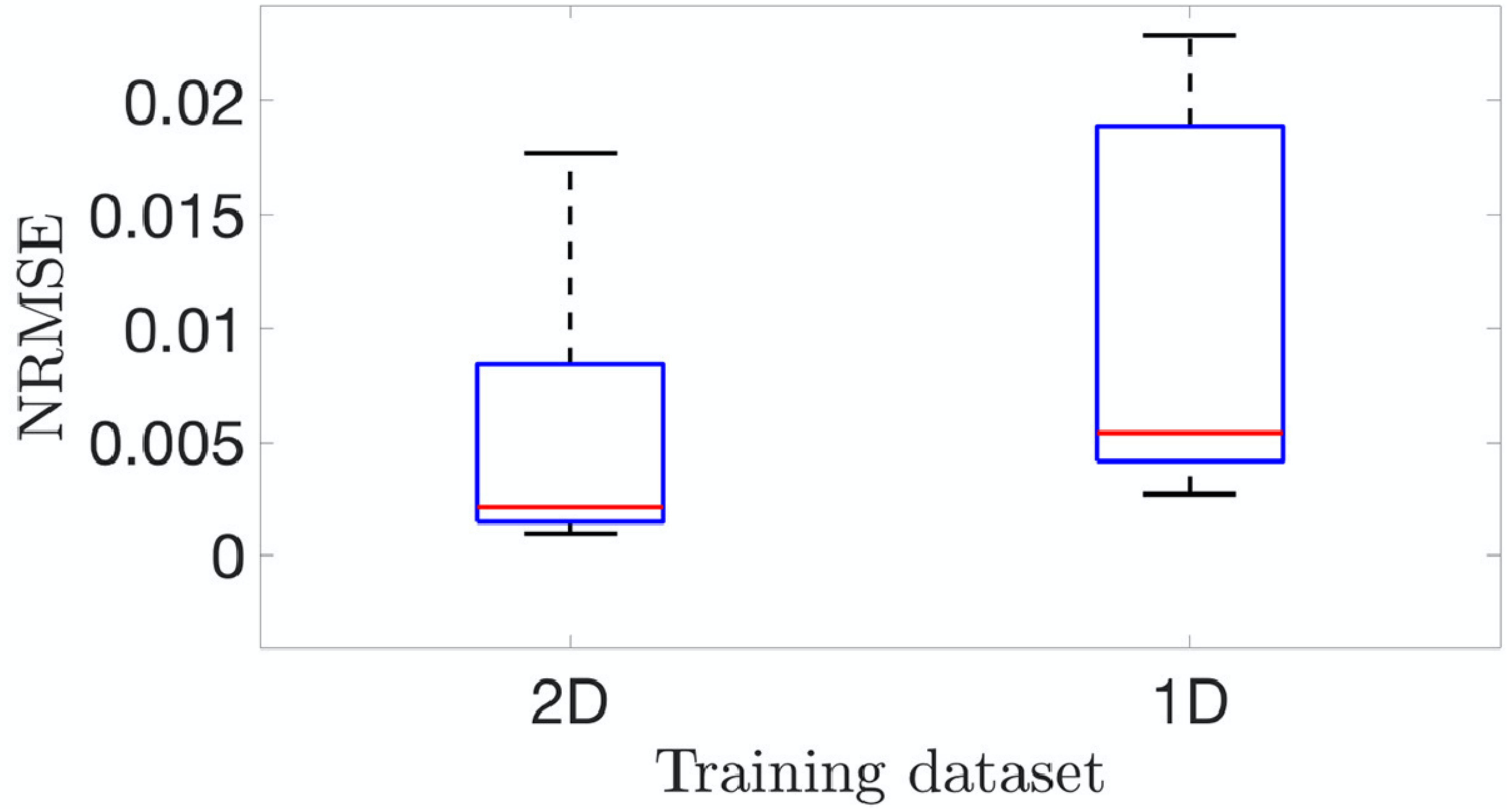
Mechanism size:

~100 species

G. D'Alessio, A. Stagni, A. Parente, A. Cuoci, *Combust Flame* 211 (2020) 68-82

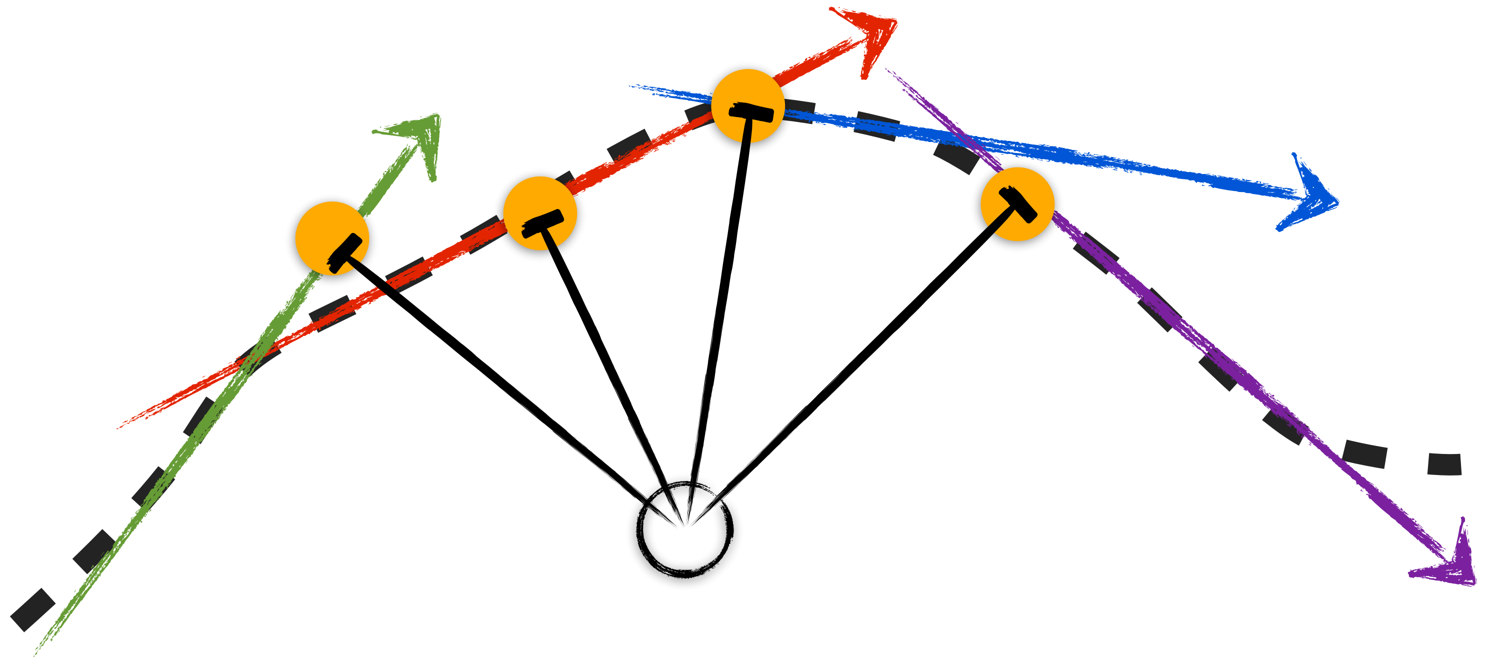
Impact of the training dataset



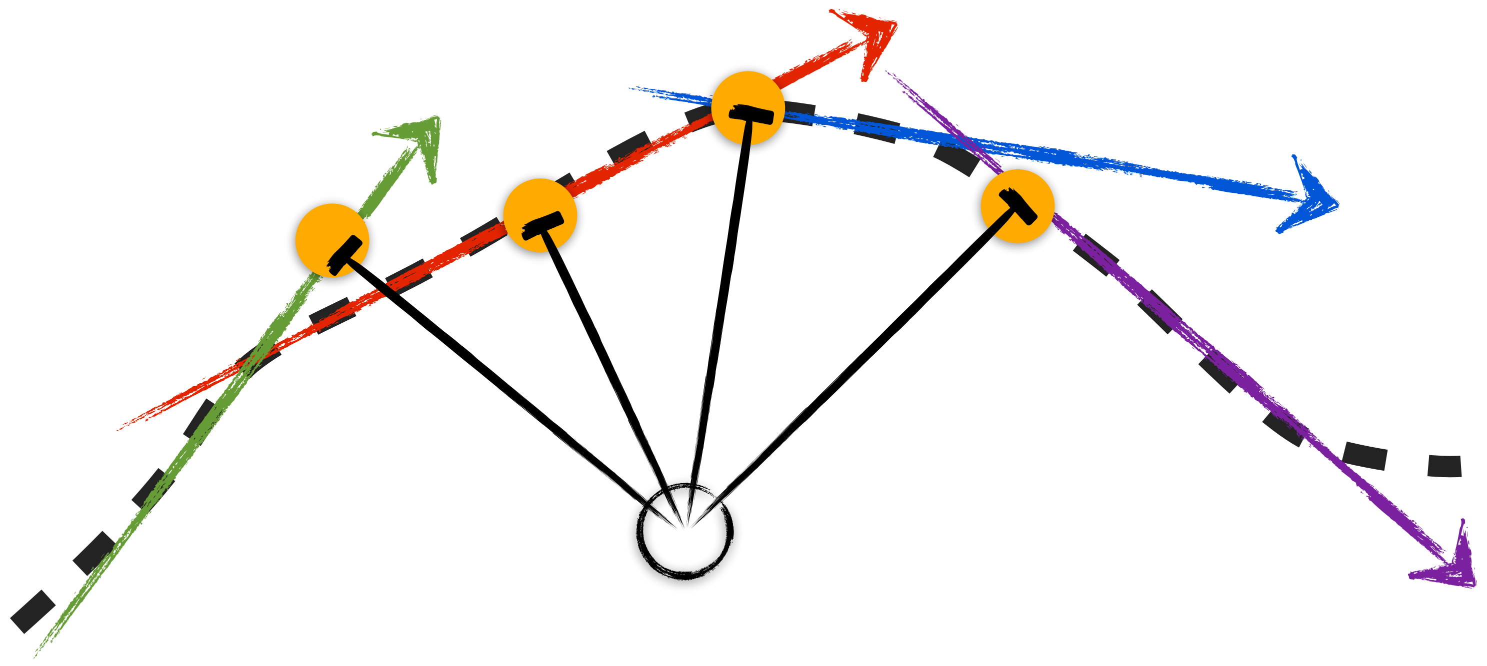


Extension to transportation fuels: accuracy of on-the-fly classification

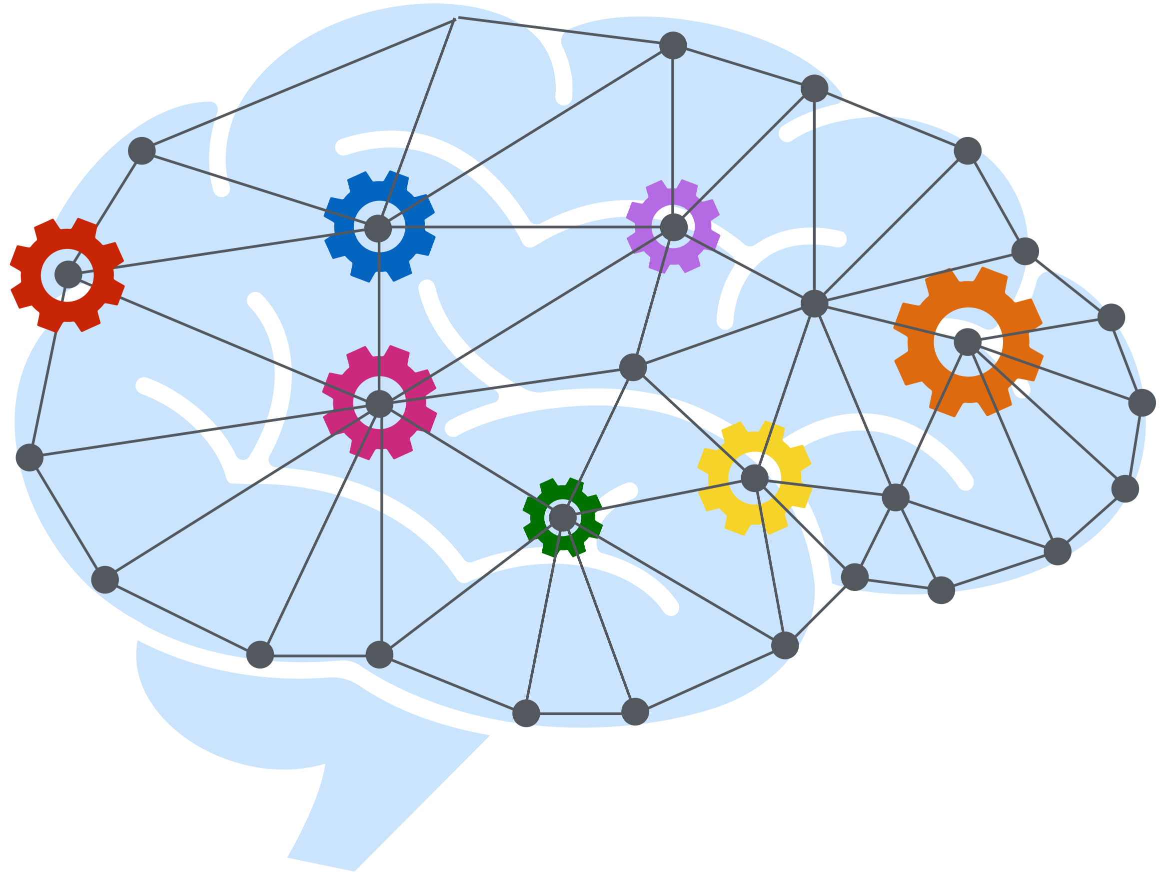
LPCA for training data and *on-the-fly* classification



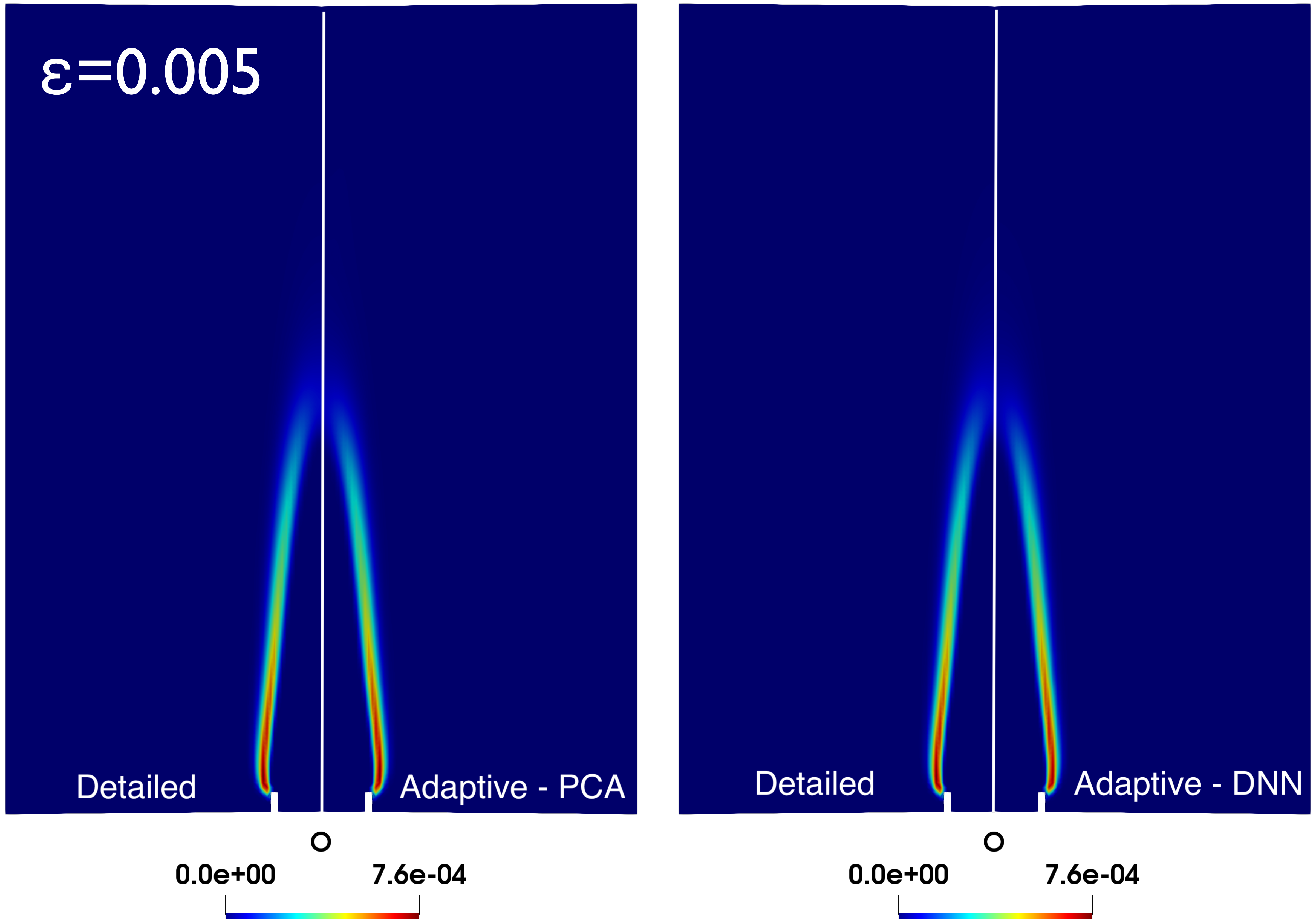
LPCA for training data classification

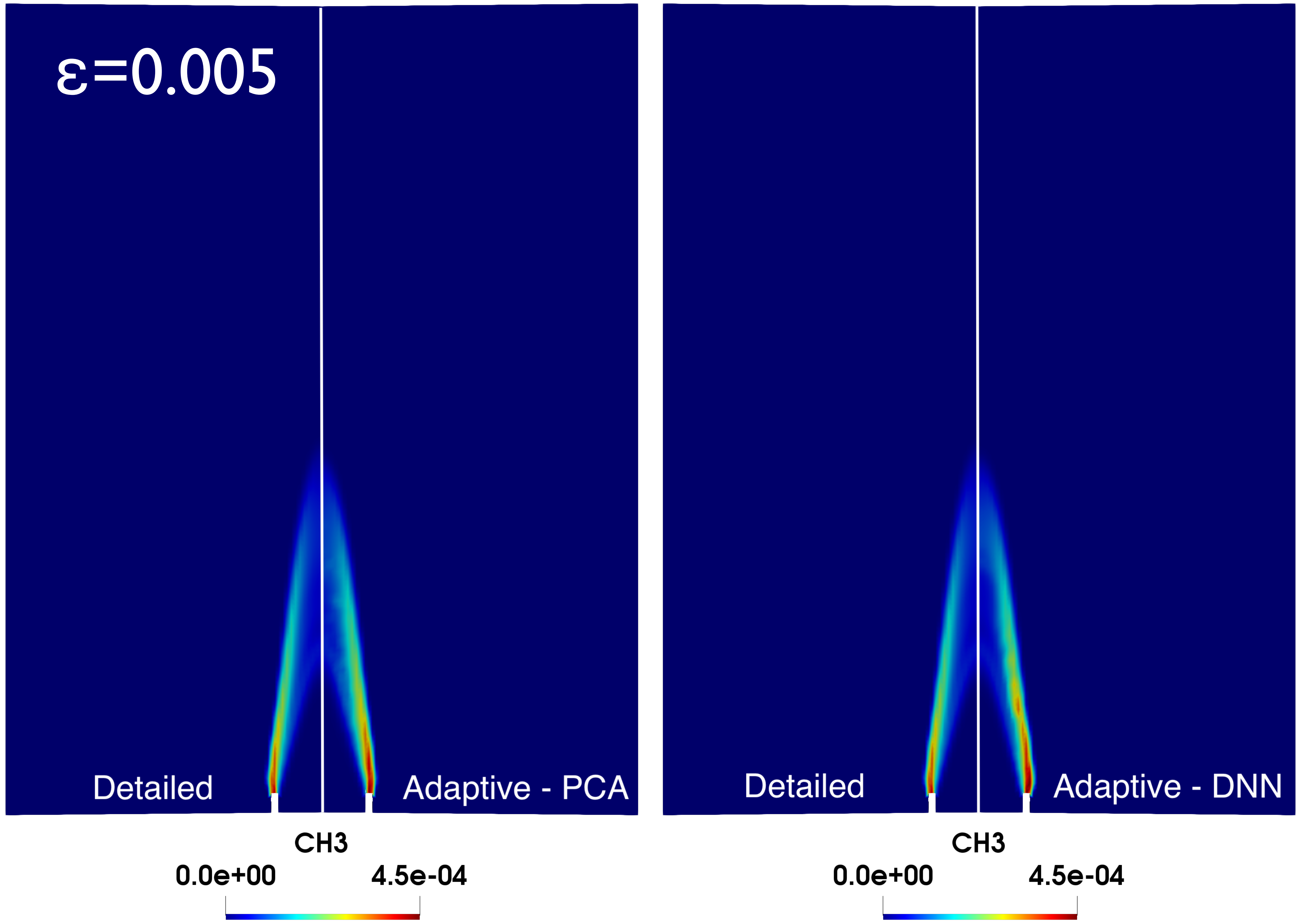


Deep learning for the *on-the-fly* classification

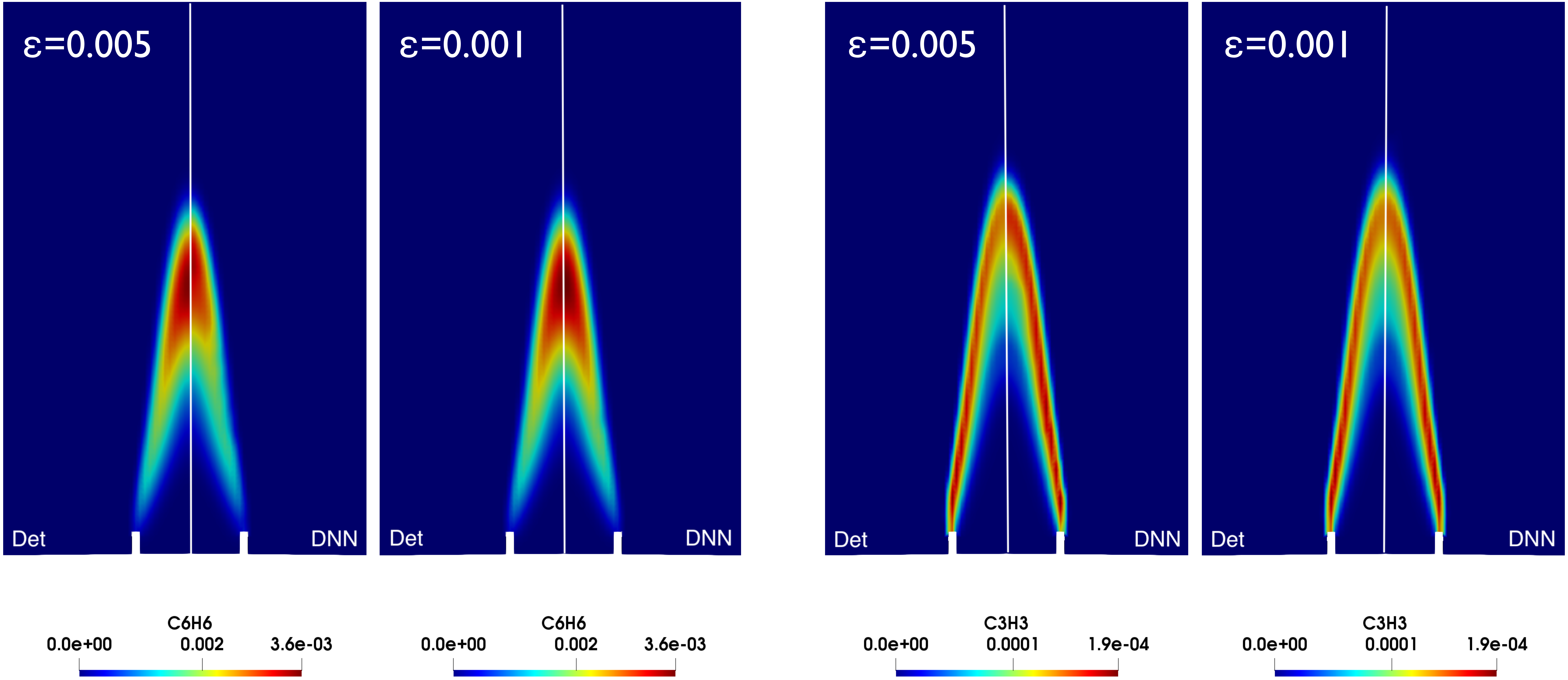


Application to an unsteady co-flow n-heptane flame

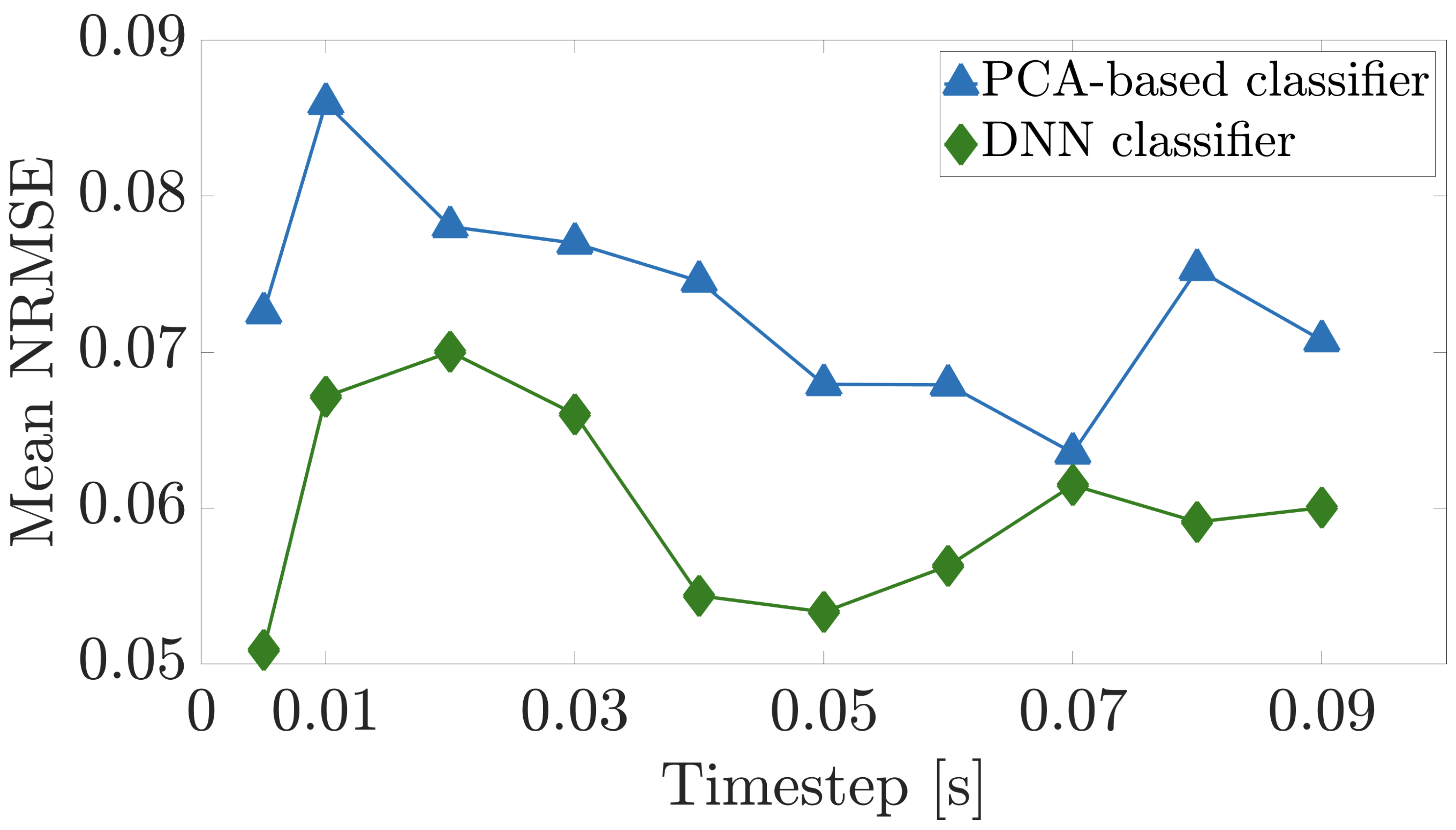


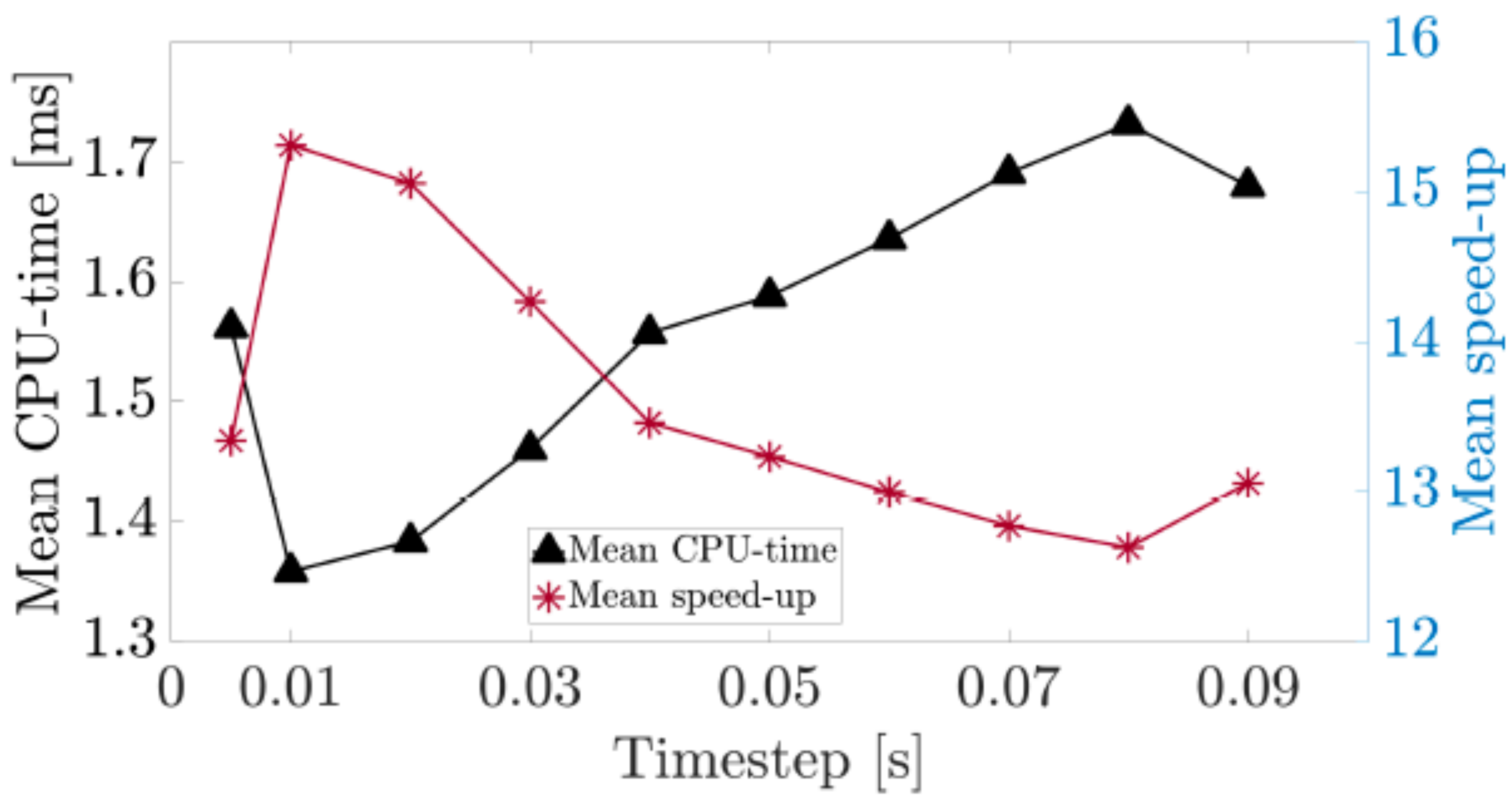


Prediction of soot precursors



Extension to transportation fuels: unsteady co-flow n-heptane flame



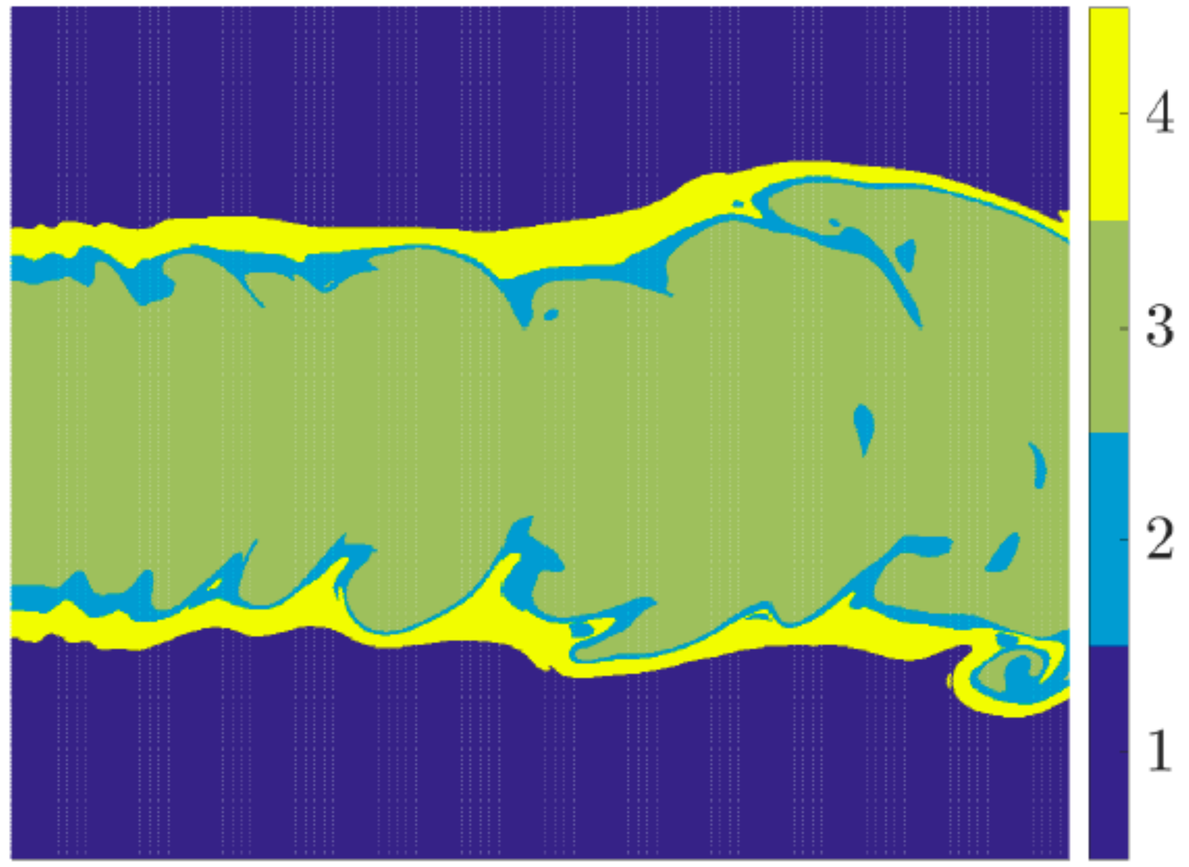


Mechanism size:

172 species and 6,067 reactions

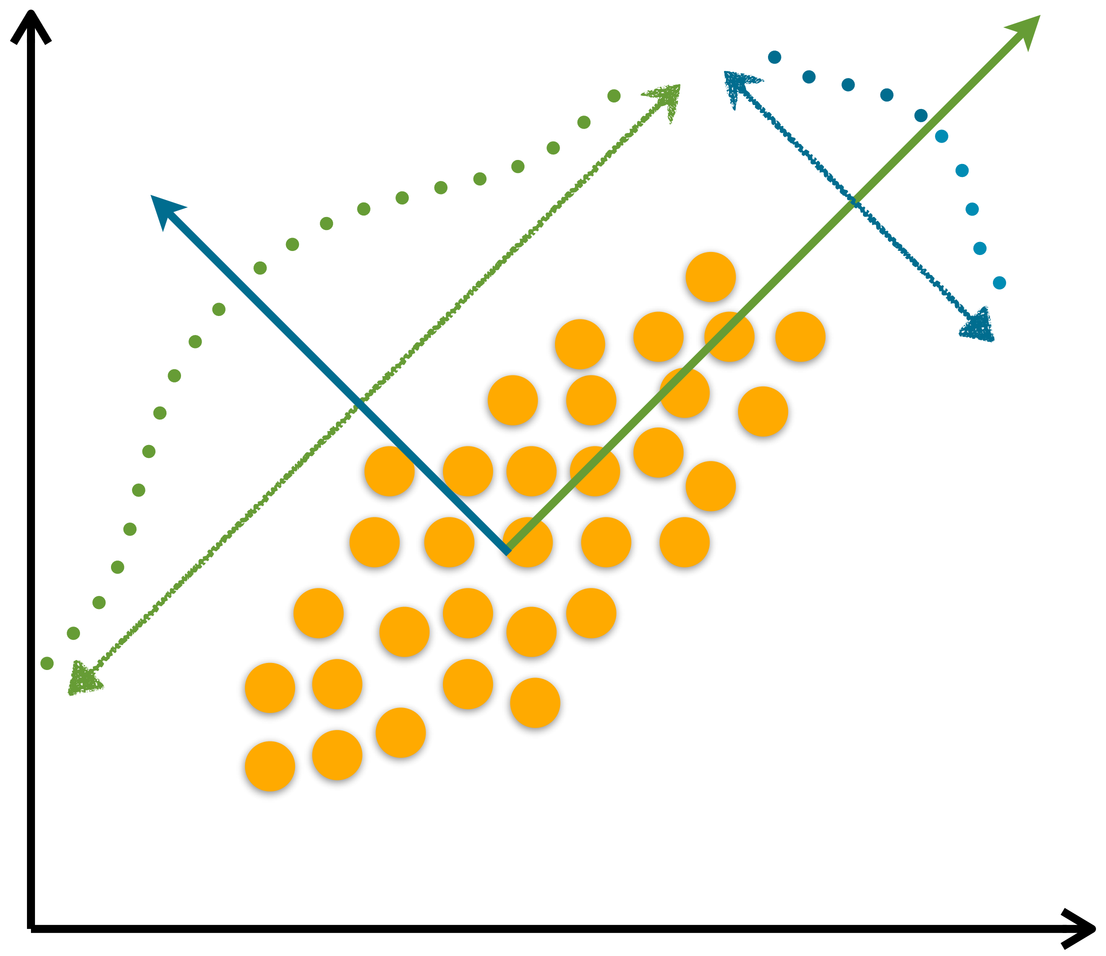
Machine learning for combustion

Feature extraction



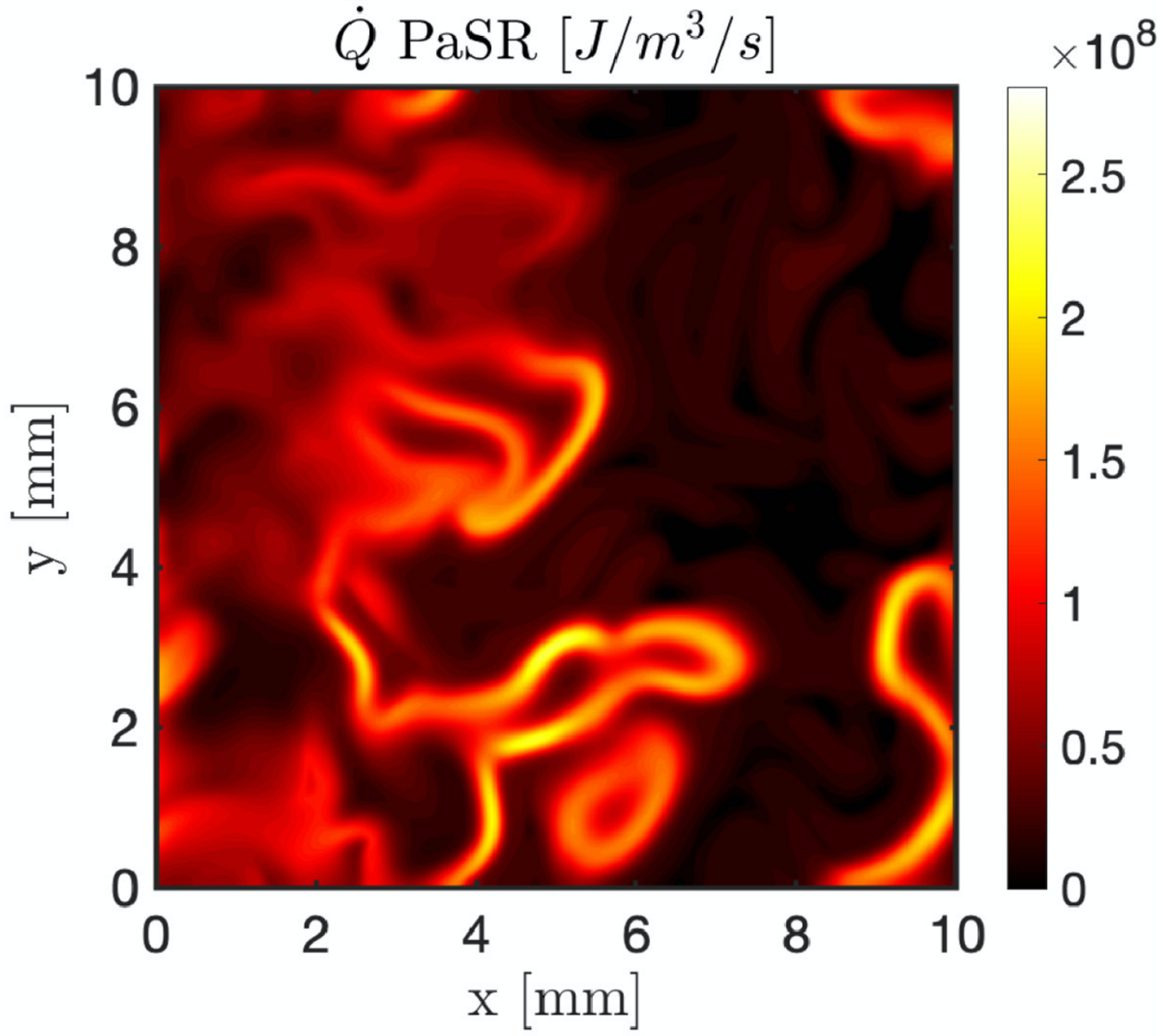
Improving knowledge and description of turbulent reacting flows

Dimensionality reduction



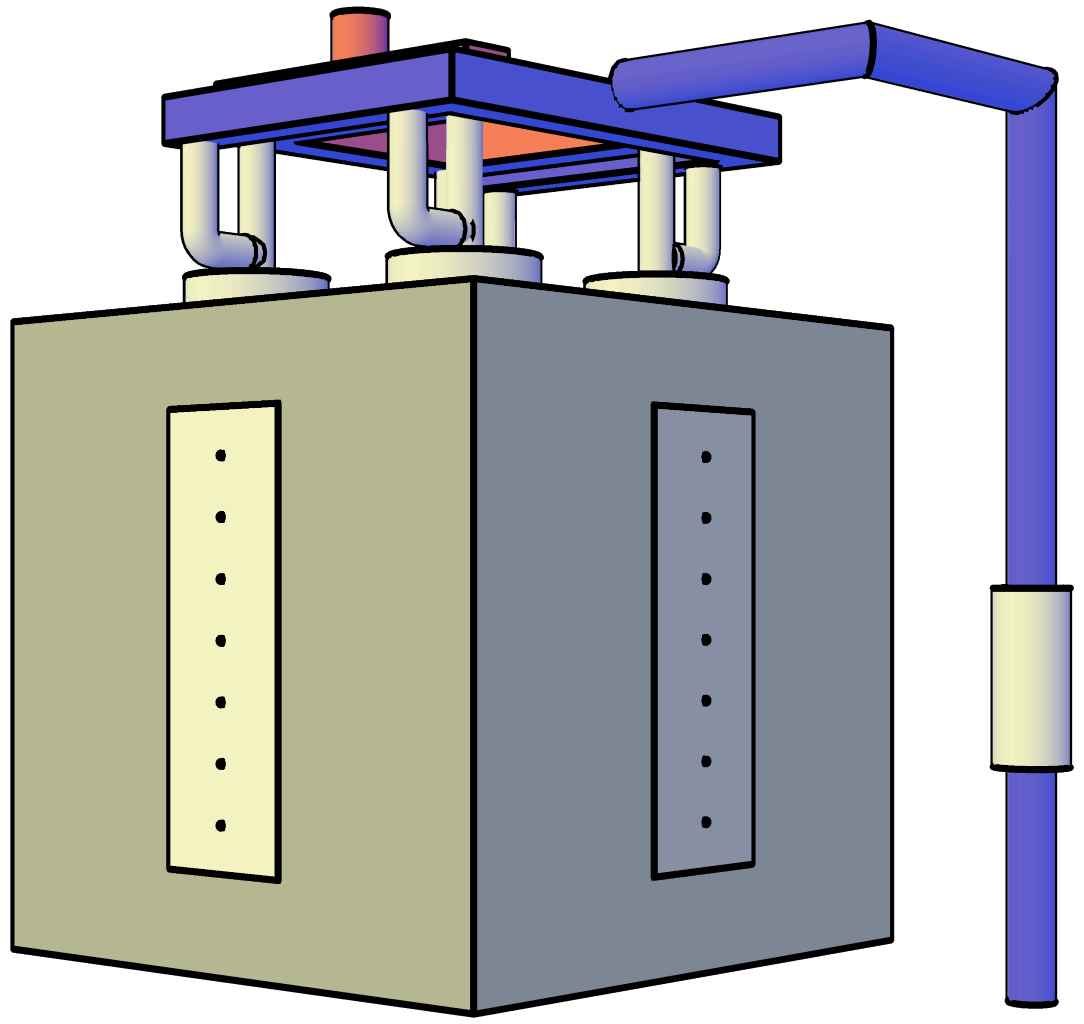
Reducing the cost of large-scale combustion simulations

Data-enhanced models and closures

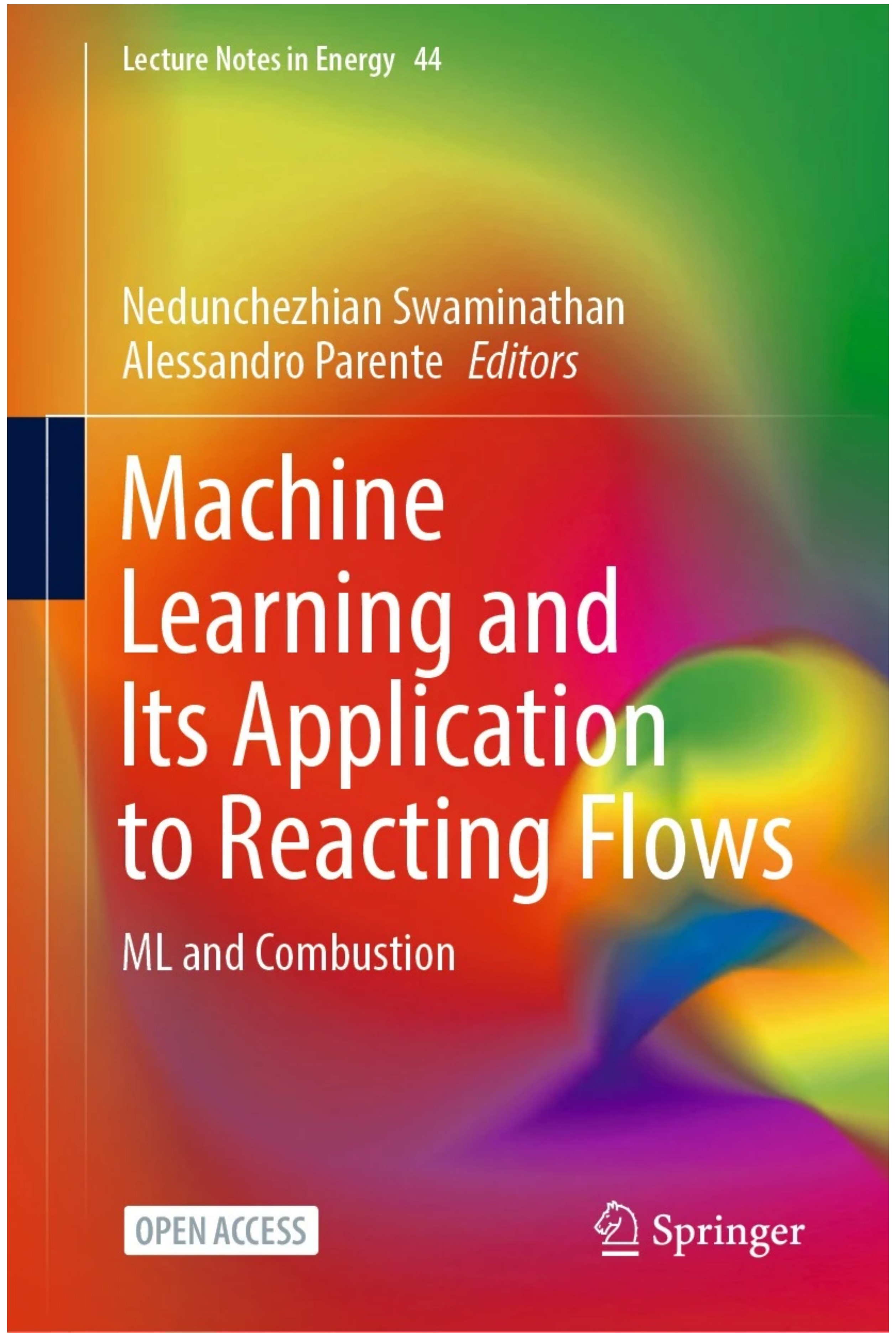


Developing adaptive combustion closures and chemistry models

Reduced-order models and digital twins



Retrofitting, optimising, troubleshooting, sensing and design



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Reduced-Order Modeling of Reacting Flows Using Data-Driven Approaches

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Cyber-Physical systems and digital twins for the decarbonisation of energy-intensive industries

Acknowledgements

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