ML-aided design of chemical libraries for efficient simulations of reactive flows

Taraneh Sayadi

d'Alembert, Sorbonne University

ITV, RWTH-Aachen University

Contributors:

Clément Scherding
clement.scherding@upmc.fr
Sorbonne University

Georgios Rigas
g.rigas@imperial.ac.uk
Imperial College London

Denis Sipp
Denis.sipp@onera.fr
Onera

Peter J Schmid
peter.schmid@kaust.edu.sa
KAUST

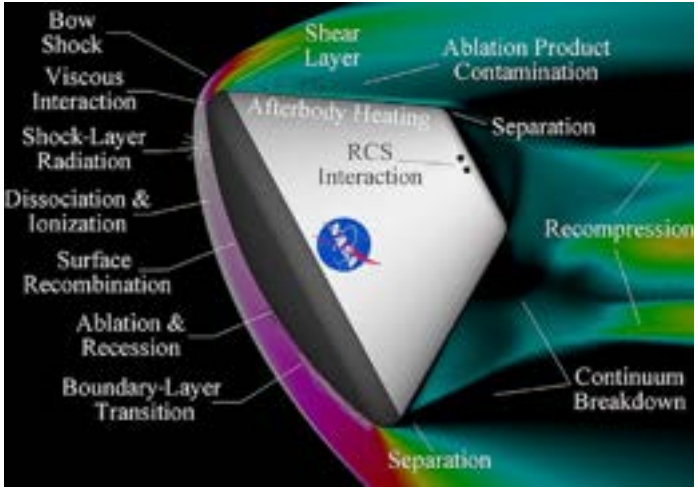
Motivation

- Hypersonic flows are relevant to a wide range of aerospace applications

- Multiple complex phenomena interacting
  - Shock waves
  - Separation
  - Transition
  - **Chemistry**

→ **Flow**

Due to high-speeds reactions are in non-equilibrium



Scanlon et al., *AIAA journal 53*(6) 2015

What is the impact of chemistry on the flow dynamics?

Physicochemical modeling of hypersonic flow

Compressible Navier-Stokes

Physicochemical modeling approaches for gases

- Thermally perfect gas (TPG)
- Finite-rate chemistry – Chemical non-equilibrium (CNEQ)
  1. Mixture composition: $S = \{O_2, N_2, NO, N, O\}$ for 5 components air mixture
  2. Species conservation equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

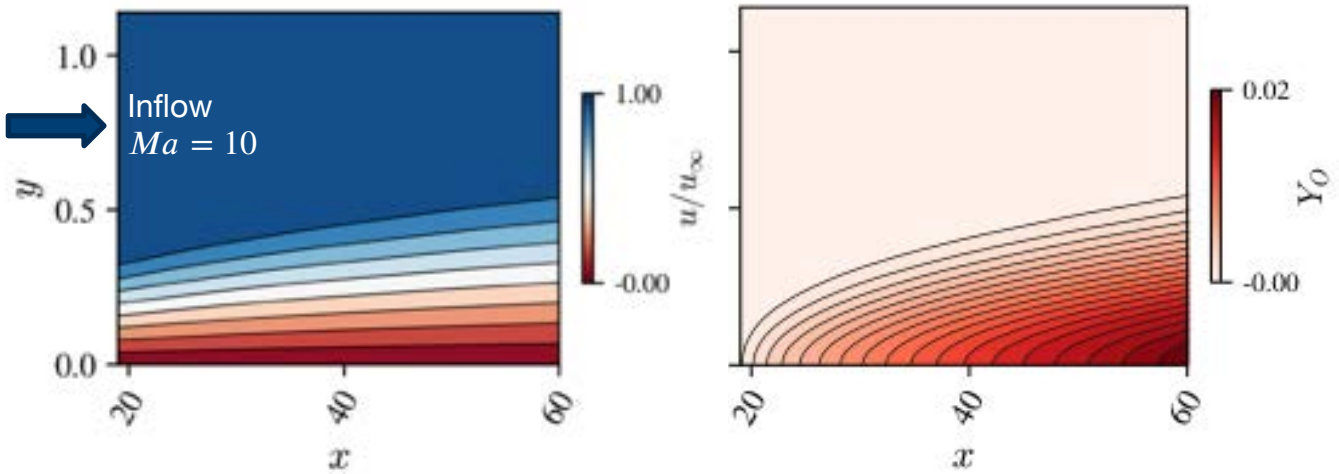
Reactions

Species diffusion

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \tau$$

$$\frac{\partial \rho e_0}{\partial t} + \nabla \cdot (\rho h_0 \mathbf{u}) = \nabla \cdot (\tau \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}$$

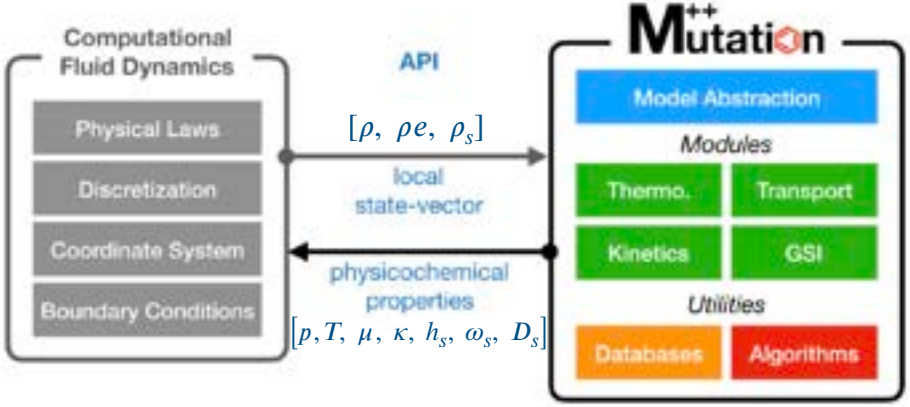
+diffusive

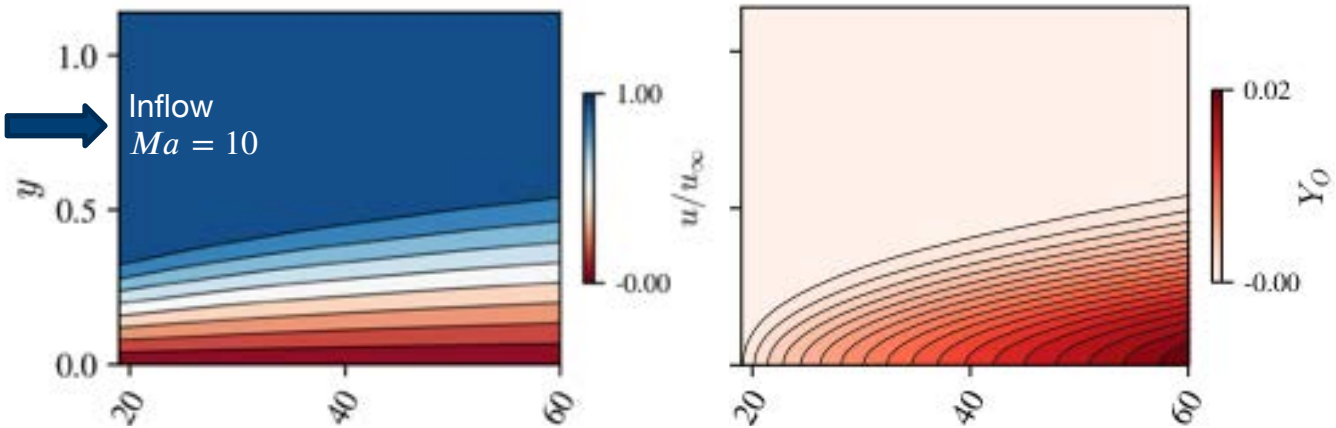


Physicochemical modeling of hypersonic flow

Thermodynamic – transport – kinetics need to be modelled accurately

→ Coupling of flow solver with Mutation⁺⁺ library [4]





- Local input/output relations
- User inputs:
  - mixture components $S = \{O_2, N_2,\ NO,\ N,\ O\}$
  - Thermodynamic model

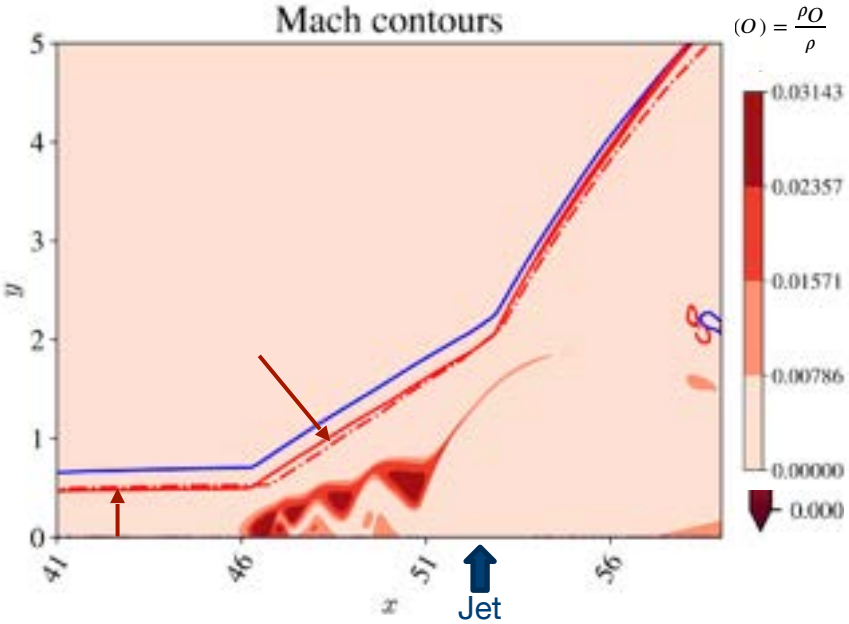
[4] - Scoggins, J. B., Leroy, V., Bellas-Chatzigeorgis, G., Dias, B., & Magin, T. E. (2020). Mutation++: Multicomponent thermodynamic and transport properties for ionized gases in C++. SoftwareX, 12, 100575.

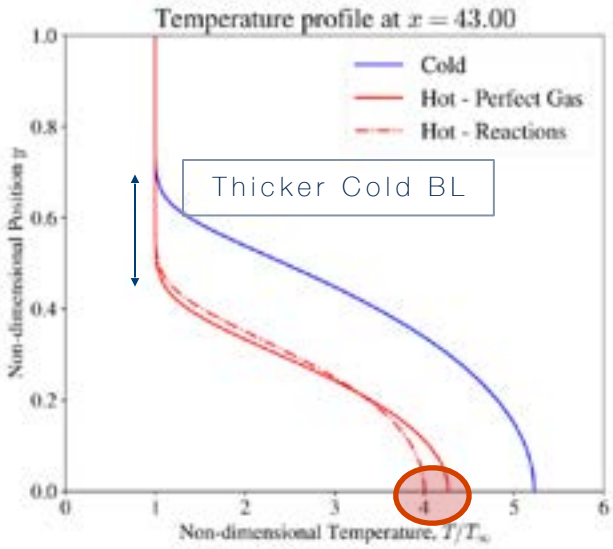
Influence of finite-rate chemistry

- 2D preliminary setup

  Sonic transverse jet $(J = 0.4)$ in $M_\infty = \frac{u_\infty}{c_\infty} = 5$ crossflow:

  - Hot : $T_\infty = 947K$
  - Cold : $T_\infty = 62.5K$





Thicker Cold BL → Higher penetration of jet

Endothermic dissociation → weaker interaction

250K difference at the wall with reactions on

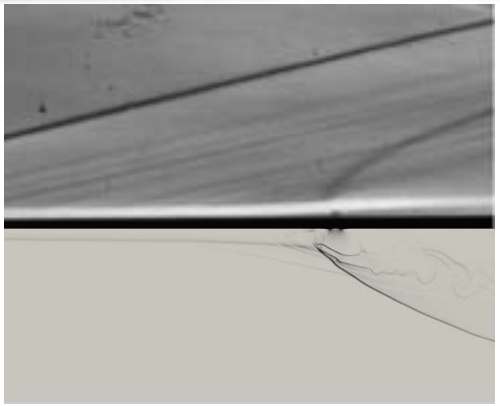
- Chemical non-equilibrium in hypersonic flows
  - Order-one influence on quantities of interests (stability, heating, transition) [1,2,3]
  - Limited experimental/numerical data

[1] - Candler, G. V. (2019). *Annual Review of Fluid Mechanics*, *51*, 379-402.
[2] – Di Renzo, M., & Urzay, J. (2021). *JFM*, *912*.
[3] – Marxen, O., Iaccarino, G., & Magin, T. E. (2014). *JFM*, *755*, 35-49.

Effects on the dynamics - 3D

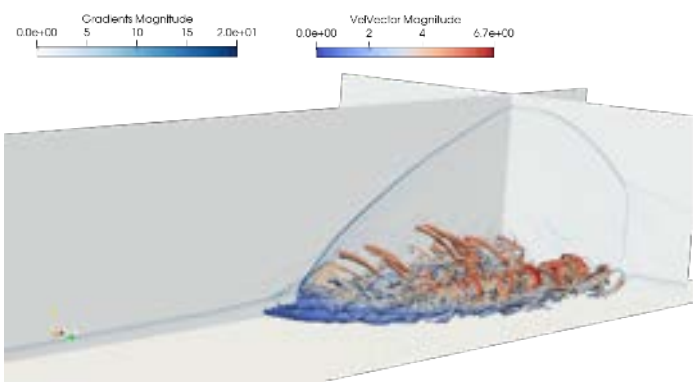
- Grid

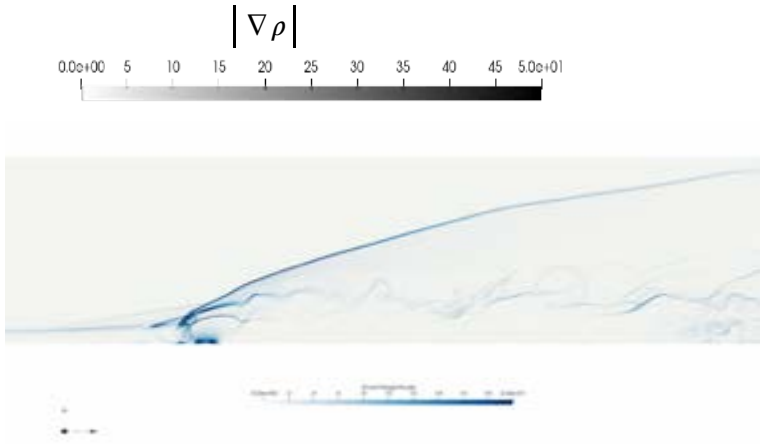
	+ units	N
X	14	2132
Y	1	697
Z	14	1024
Total	-	1.5×10^9



Experimental Schlieren [4]

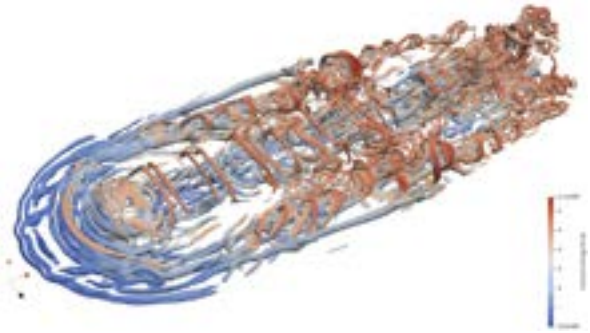
Numerical Schlieren

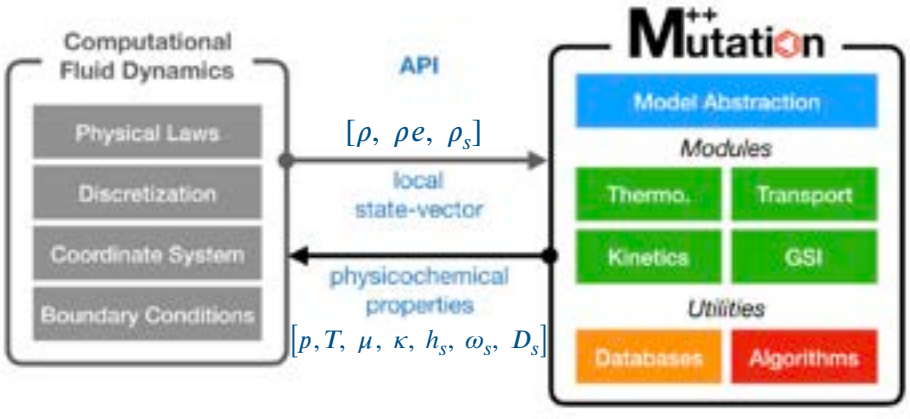


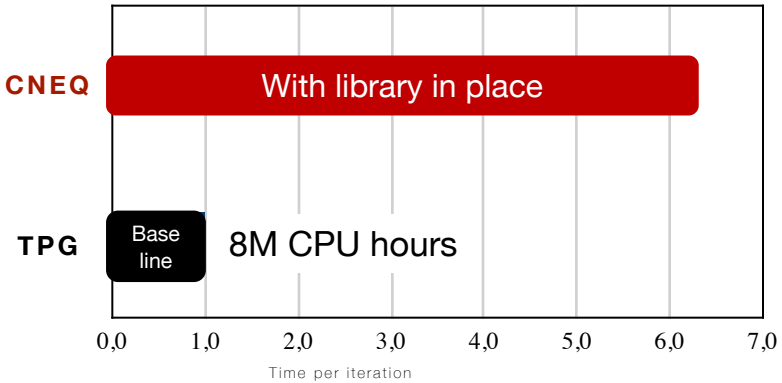


[4] – Erdem, Erinc. (2011). ACTIVE FLOW CONTROL STUDIES AT MACH 5: MEASUREMENT AND COMPUTATION. Manchester EScholar - The University of Manchester. The University of Manchester, 2011.

Challenge using thermochemical models ?







Can we extract a reduced-order thermochemical model to reduce CPU cost ?

Data-driven science (ML-driven algorithms, AI)

Governing equations

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{d\rho_s}{dt} + \nabla \cdot (\rho_s \mathbf{u}) + \nabla \cdot (\rho_s \mathbf{V}_s) = \dot{\omega}_s \quad \forall\, s$$

$$\frac{d\rho \mathbf{u}}{dt} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \tau$$

$$\frac{d\rho e_0}{dt} + \nabla \cdot (\rho h_0 \mathbf{u}) = \nabla \cdot (\tau \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}_{\text{heat}}$$

Diffusion

Reactions

Incl. diffusive

& state equations and properties

Models

Turbulence

Chemistry

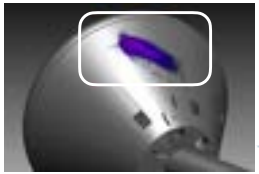
Post-analysis

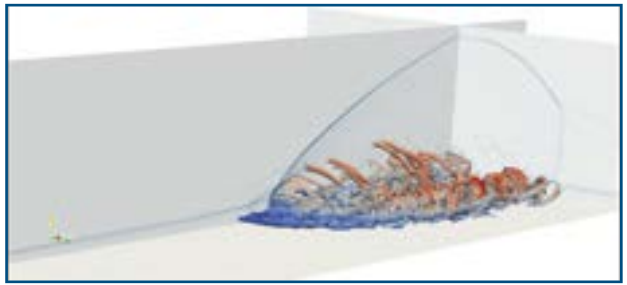
Extracting dynamics

Reduced-order Models

Control

Ivey et al. 2011





Governing equations

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{d\rho_s}{dt} + \nabla \cdot (\rho_s \mathbf{u}) + \nabla \cdot \underbrace{(\rho_s \mathbf{V}_s)}_{\text{Diffusion}} = \underbrace{\dot{\omega}_s}_{\text{Reactions}} \quad \forall\, s$$

$$\frac{d\rho \mathbf{u}}{dt} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \tau$$

$$\frac{d\rho e_0}{dt} + \nabla \cdot (\rho h_0 \mathbf{u}) = \nabla \cdot (\tau \cdot \mathbf{u}) - \nabla \cdot \underbrace{\mathbf{q}_{\text{heat}}}_{\text{Incl. diffusive}}$$

& state equations and properties

Models

Post-analysis

Control

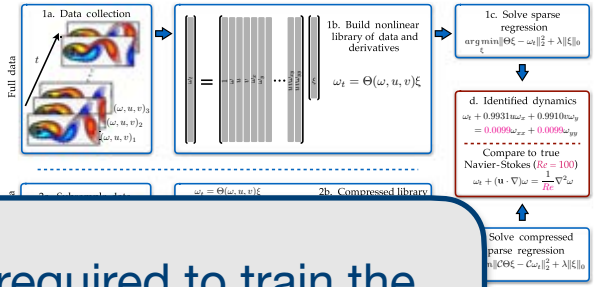
Bottleneck: large amount of data required to train the models for multi-scale multi-physics problems!

Extracting dynamics

Reduced-order Models

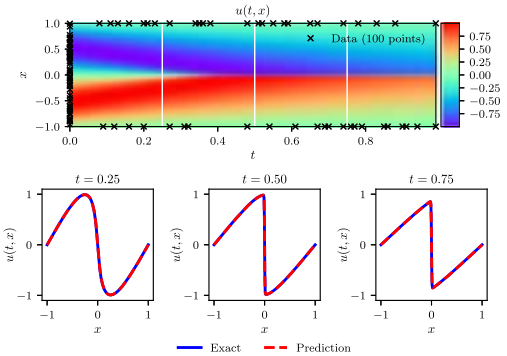
Data-driven discovery of partial differential equations

Samuel H. Rudy,[1]* Steven L. Brunton,[2] Joshua L. Proctor,[3] J. Nathan Kutz[1]

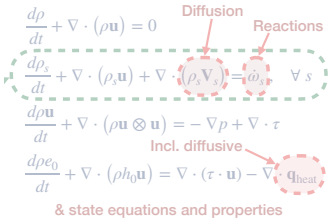


nvolving

M. Raissi[a], P. Perdikaris[b,*], G.E. Karniadakis[a]



Governing equations



Models

Improve predictability

Post-analysis

Control

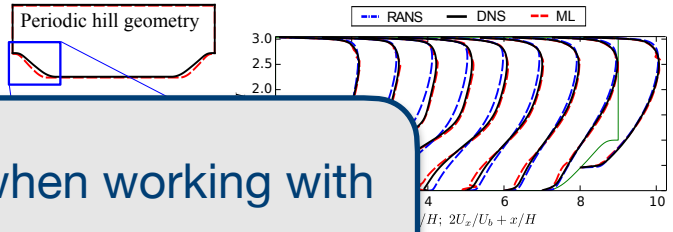
Bottleneck: Lack of generalisability when working with dynamical (time-varying) systems

Extracting dynamics

Reduced-order Models

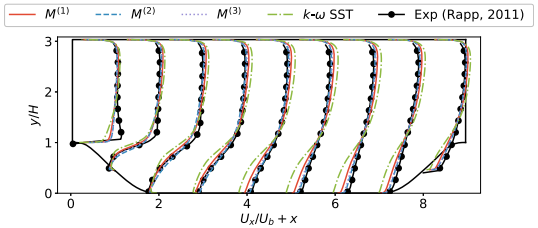
Turbulence Modeling in the Age of Data

Karthik Duraisamy[1,⋆], Gianluca Iaccarino[2,⋆], and Heng Xiao[3,⋆]

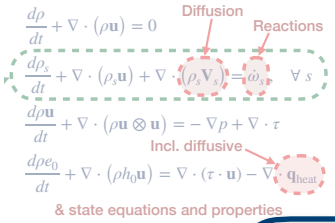


Sparse Symbolic Regression

Martin Schmelzer[1] · Richard P. Dwight[1] · Paola Cinnella[2]



Governing equations



Models

Improve Speed, while keeping accuracy

Turbulence

Chemistry

Post-analysis

Extracting dynamics

Reduced-order Models

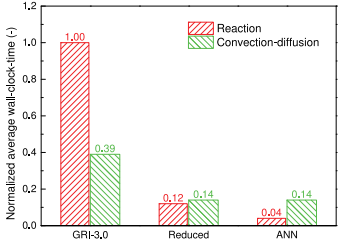
Control

Bottleneck: Curse of dimensionality

Chemistry reduction using machine learning trained from non-premixed micro-mixing modeling: Application to DNS of a syngas turbulent oxy-flame with side-wall effects

Kaidi Wan, Camille Barnaud, Luc Vervisch*, Pascale Domingo

CNRS, CORIA, Normandie Université, INSA de Rouen, Saint-Etienne-du-Rouvray 76801, France



Data-driven framework for input/output lookup tables reduction - with application to hypersonic flows in chemical non-equilibrium

Clément Scherding,[1,*] Georgios Rigas,[2] Denis Sipp,[3] Peter J. Schmid,[4] and Taraneh Sayadi[1,5]

[1] *Institut Jean le Rond d'Alembert, Sorbonne University, France*
[2] *Department of Aeronautics, Imperial College London, UK*
[3] *DAAA, Onera, France*
[4] *Department of Mechanical Engineering, KAUST, SA*
[5] *Institute for Combustion Technology, Aachen University, Germany*

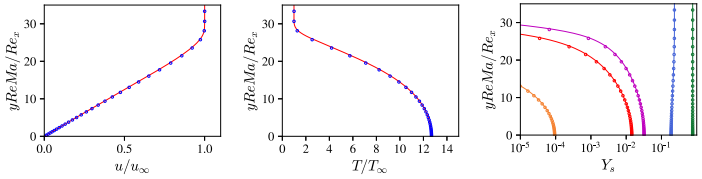


FIG. 15. Comparison of profiles of (a) streamwise velocity, (b) temperature, (c) species mass fractions from left to to right N, NO, O, O_2 and N_2 at $Re_x = 2000$. Solid line and symbols correspond to the solution obtained using Mutation++ and the data-driven model, respectively.

Governing equations

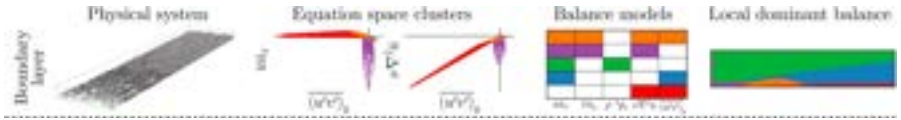
Models

Post-analysis

Control

Learning dominant physical processes with data-driven balance models

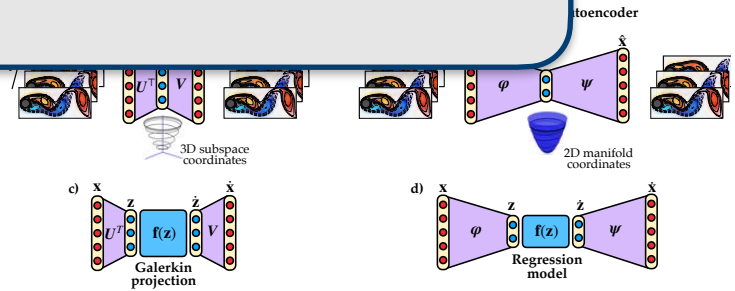
Jared L. Callaham[1✉], James V. Koch[2], Bingni W. Brunton[3], J. Nathan Kutz[4] & Steven L. Brunton[1]



Bottleneck: "i.i.d" hypothesis, postulating unlimited data and invariable environment —> lack of consistency and robustness

Extracting dynamics

Reduced-order Models



Steven L. Brunton · Maziar S. Hemati · Kunihiko Taira

Special issue on machine learning and data-driven methods in fluid dynamics

Governing equations

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \mathbf{u}) = 0$$

Diffusion

Reactions

$$\frac{d\rho_s}{dt} + \nabla \cdot (\rho_s \mathbf{u}) + \nabla \cdot (\rho_s \mathbf{V}_s) = \dot{\omega}_s \quad \forall\, s$$

$$\frac{d\rho \mathbf{u}}{dt} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \tau$$

Incl. diffusive

$$\frac{d\rho e_0}{dt} + \nabla \cdot (\rho h_0 \mathbf{u}) = \nabla \cdot (\tau \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}_{\text{heat}}$$

& state equations and properties

Models

Turbulence

Chemistry

Post-analysis

Extracting dynamics

Reduced-order Models

Control

Machine Learning for Fluid Mechanics

Steven L. Brunton,[1] Bernd R. Noack[2 3] and Petros Koumoutsakos[4]

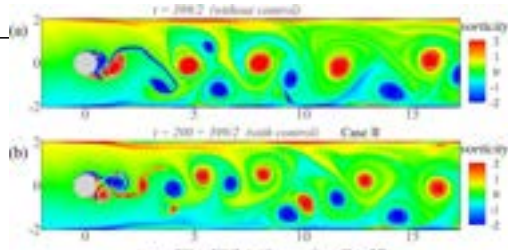
Figure 8

Deep reinforcement learning schematic (left), and application to the study of the collective motion of fish via the Navier-Stokes equations (right; Verma et al. (2018)).Symbols: S_t:state, π_w:policy, W:parameters, $m(S_t), \sigma(S_t)$:mean, standard deviation for action

Applying deep reinforcement learning to active flow control in weakly turbulent conditions

Cite as: Phys. Fluids **33**, 037121 (2021); https://doi.org/10.1063/5.0037371
Submitted: 13 November 2020 • Accepted: 23 February 2021 • Published Online: 19 March 2021

Feng Ren, Jean Rabault and Hui Tang



Type of learning

Supervised Learning

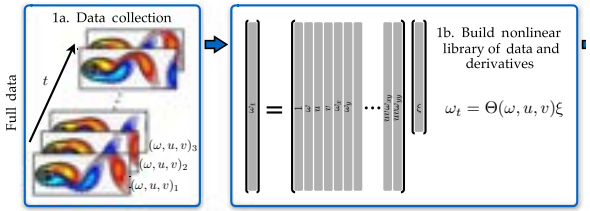
Find a mapping from X —> Y

Regression

- Decision trees
- Random forests
- Neural Networks

Classification

- Linear
- Generalised linear
- Gaussian process



Samuel H. Rudy,[1]* Steven L. Brunton,[2] Joshua L. Proctor,[3] J. Nathan Kutz[1]

Unsupervised Learning

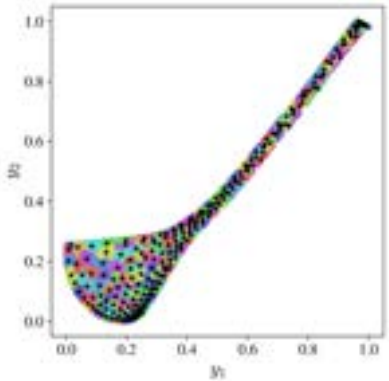
Learning Structure from data : X

Clustering

- K-means
- Spectral clustering

Dimensionality Reduction

- PCA
- Auto-encoders
- Diffusion maps



Semi-supervised Learning

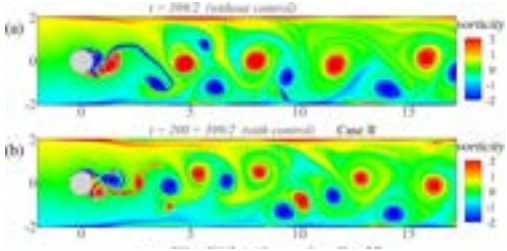
State + action

Reinforcement Learning

- Markov decision process
- Deep RL

Generative Models

- Generative adversarial networks (GANs)

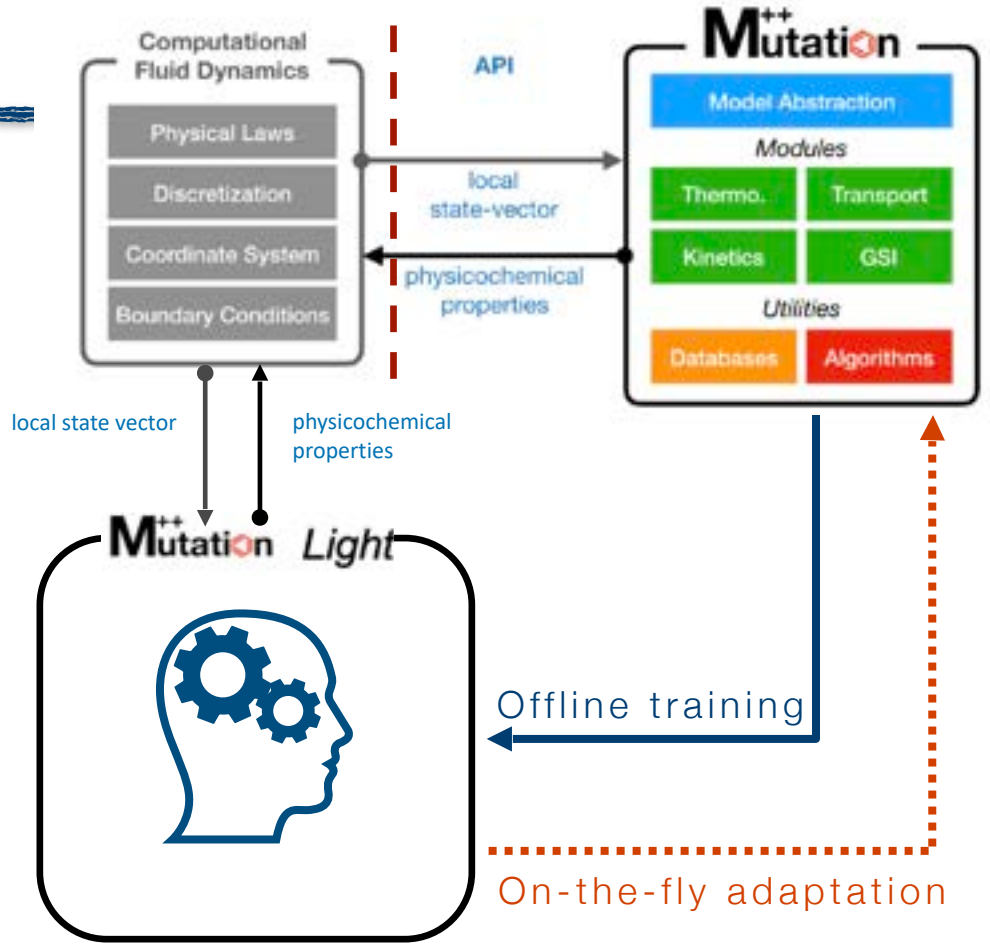


Proposed approach

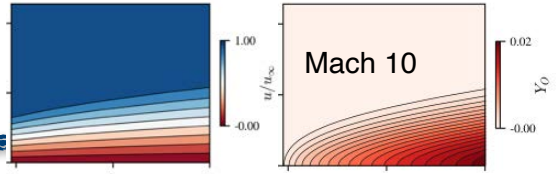
- Flows have history —> most thermodynamic states have been seen previously:
  - Offline training

➢ Learn thermo-chemical model **“on the fly”** —> generalisability

➢ Alternative approach to state-of-the-art learning —> offline training, online testing



Mutation^{++}: Input/Output



- $N = 10^5$ points sampled
- Input: local state vector

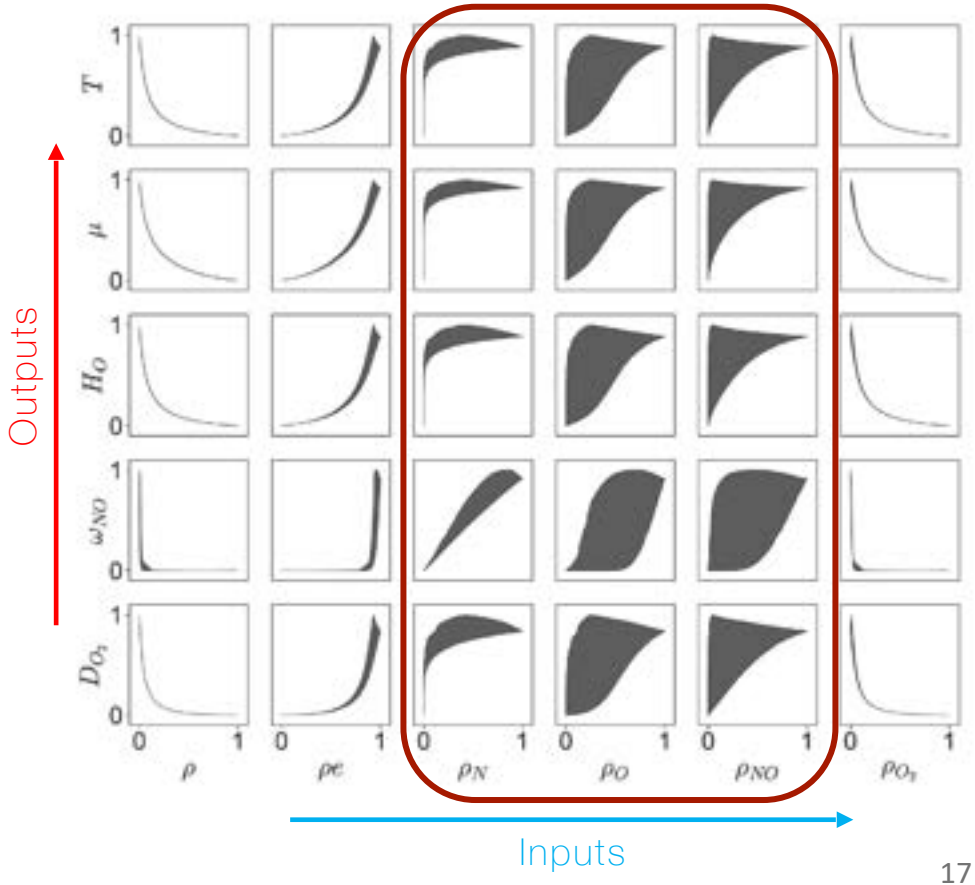
$$\boldsymbol{X} = [\rho,\ \rho e,\ \rho_s] \in \mathbb{R}^{N \times D}$$

- Output: thermochemical properties

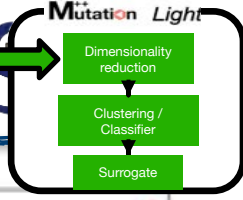
$$\boldsymbol{Z} = [p, T,\ \mu,\ \kappa,\ h_s,\ \omega_s,\ D_s] \in \mathbb{R}^{N \times D_Z}$$

➢ Large spreading of outputs with respect to radicals ρ_N, ρ_O, ρ_{NO}

Active subspaces —> Dimensionality reduction



Dimensionality Reduction $\mathbb{R}^6 \rightarrow \mathbb{R}^2$

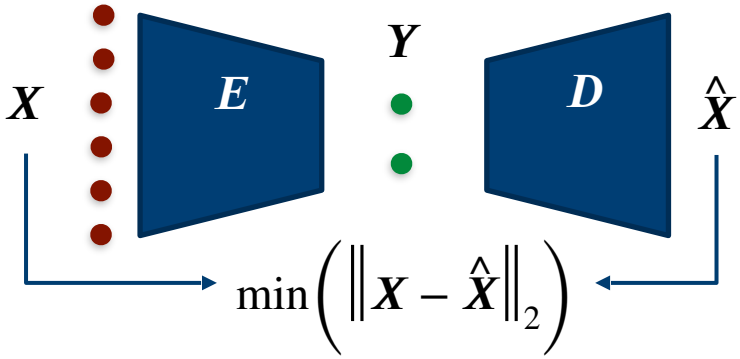


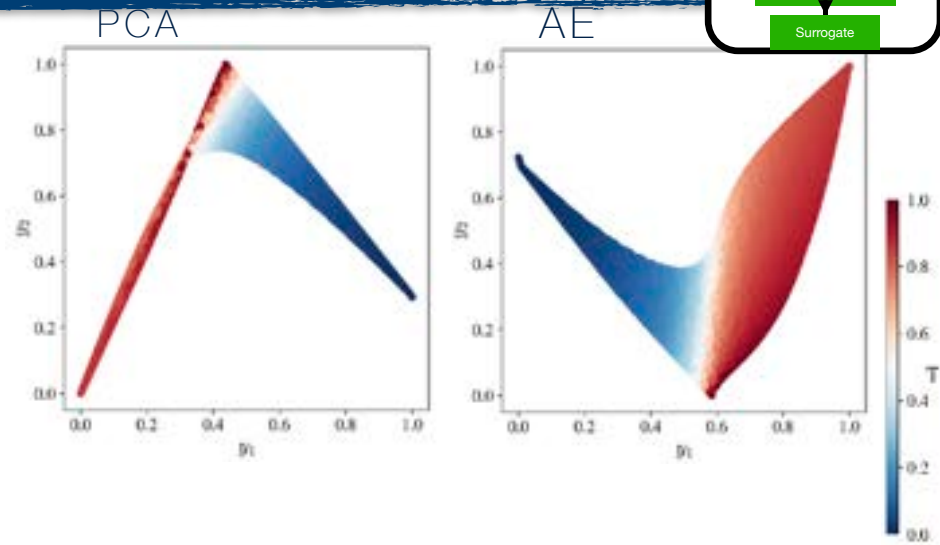
- PCA $\quad \boldsymbol{X^T X = U\Sigma V^T \rightarrow Y = XU_d}$

  $\boldsymbol{Y \in \mathbb{R}^d,\ d < D}$

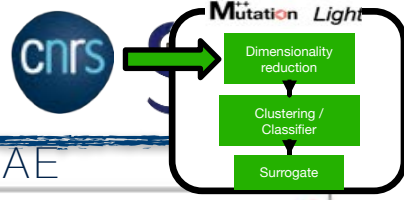
- Nonlinear autoencoder (AE)

$\boldsymbol{Y = E(X);\ \hat{X} = D(Y)}$





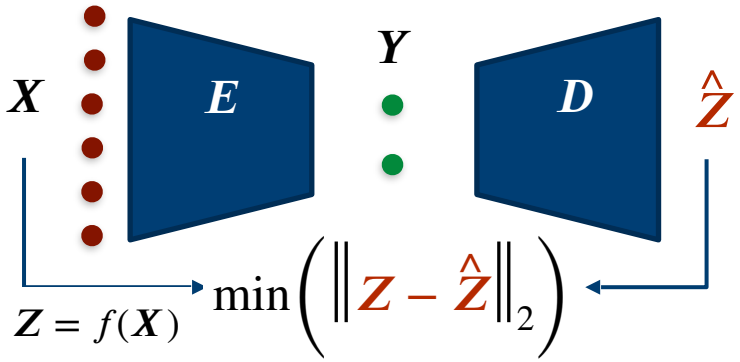
Dimensionality Reduction $\mathbb{R}^6 \rightarrow \mathbb{R}^2$

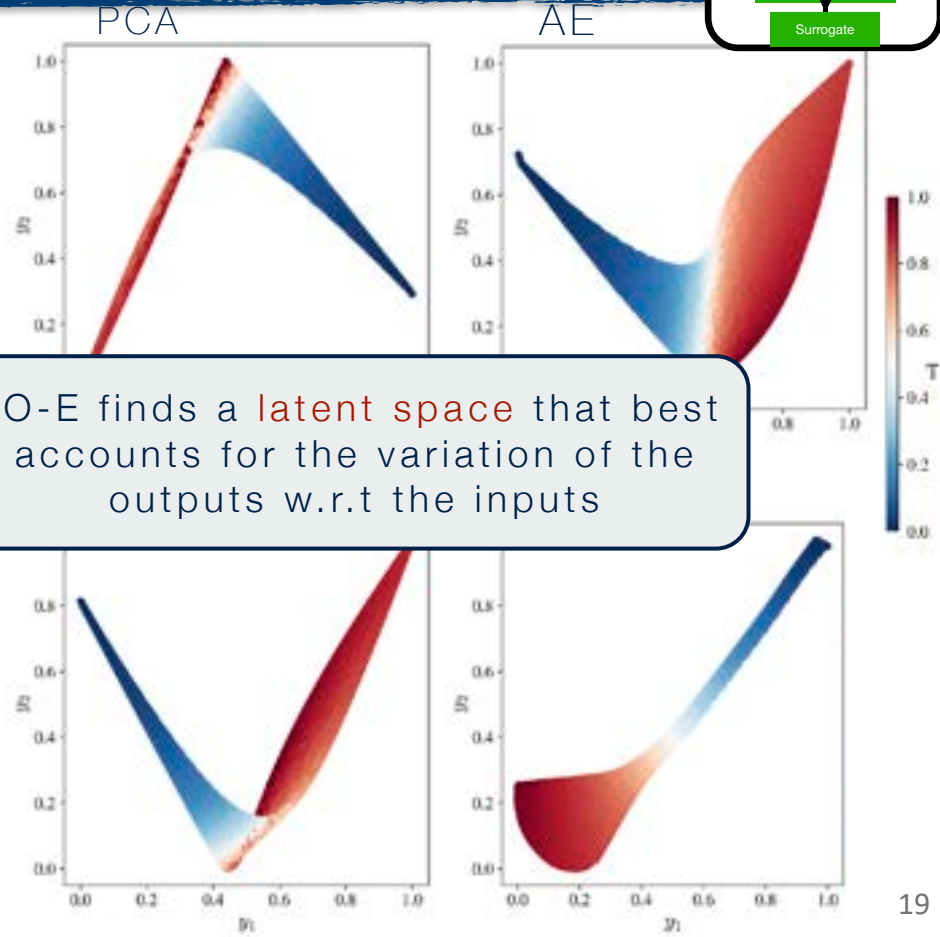


- PLS-SVD $\boldsymbol{X^T Z = U \Sigma V^T \rightarrow Y = X U_d}$

- Input/Output encoder (IO-E)

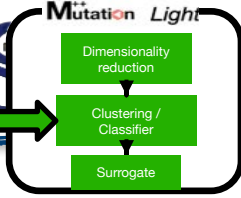
$\boldsymbol{Y = E(X);\ \hat{Z} = D(Y)}$





➢ IO-E finds a latent space that best accounts for the variation of the outputs w.r.t the inputs

Clustering



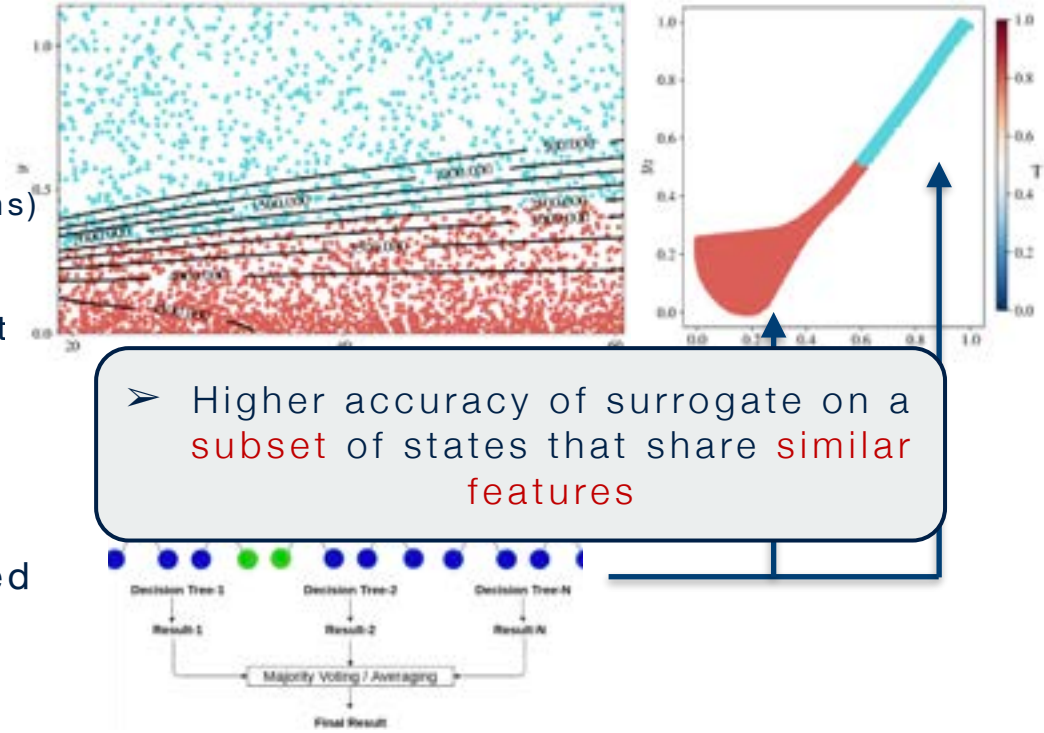
- Outputs have different dynamics depending on their location in the flow

➢ Notion of clusters

- Cluster states in reduced space Y using Newman's algorithm [5]:
  - No a priori # of clusters N_c (vs k-means)

➢ Clusters represent regions at different level of thermochemical equilibrium
  - Freestream : Cold, frozen chemistry
  - Near wall : Hot, finite-rate chemistry

- A random forest classifier is trained in tandem to classify new points



➢ Higher accuracy of surrogate on a subset of states that share similar features

[5] Newman, M. E. (2006). Modularity and community structure in networks. Proceedings of the national academy of sciences, 103(23), 8577-8582.

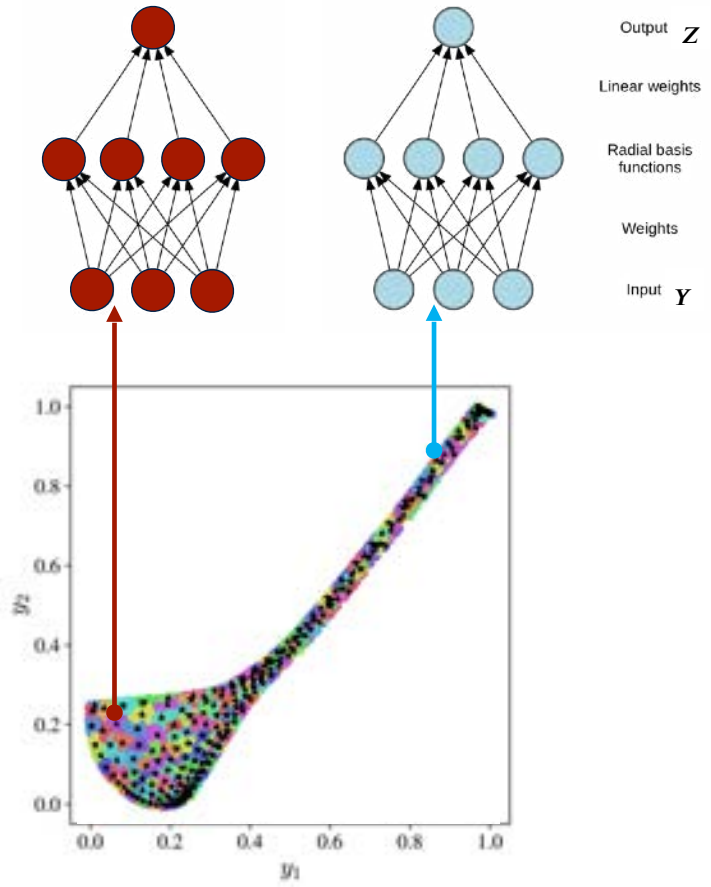
Surrogate

- A surrogate surface (in the reduced space) is build for each cluster C_k using RBFNN

$$\phi(r) = \phi(\| y - c \|), \quad \phi(r) = r^2 \log(r)$$

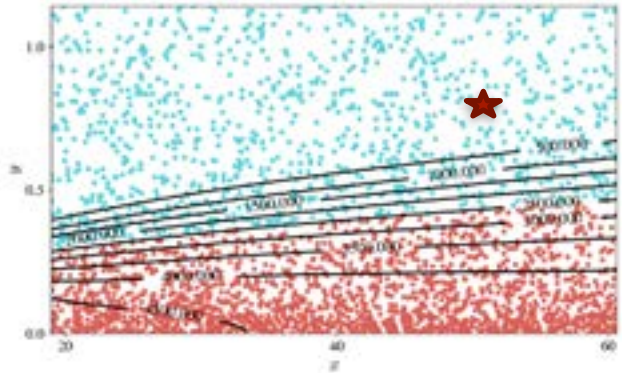
$$z = g_{C_k}(y) = \sum_{i=1}^{N_R} a_i \phi\left(\|y - c_i\|\right)$$

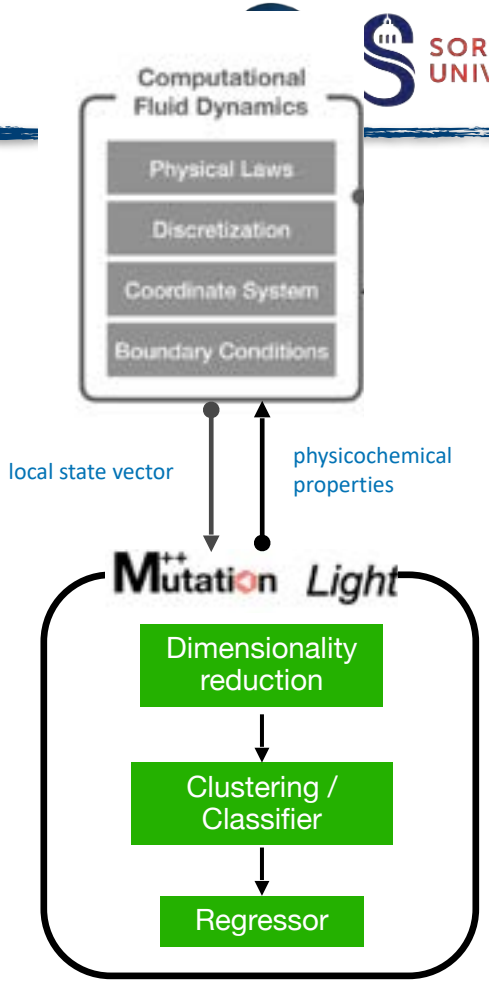
- The N_R centers are determined with k-means of the input/output pairs
  - ➢ avoid overfitting



Coupling with CFD solver

- New local state vector X^t are sent to the model





Coupling with CFD solver

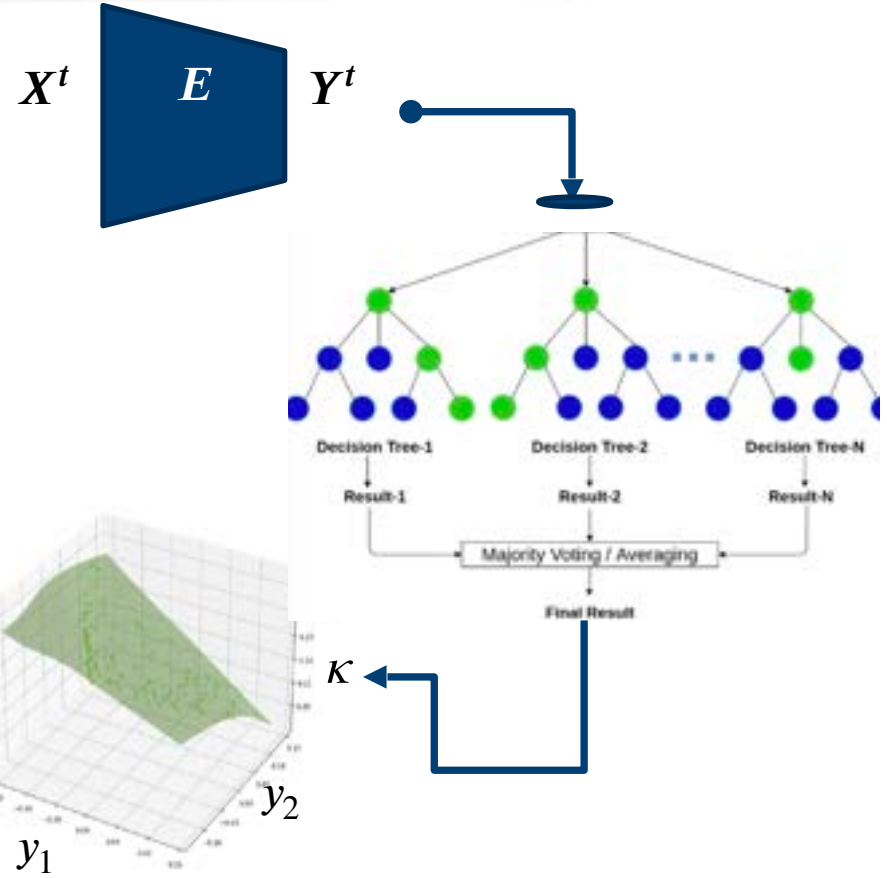
- New local state vector X^t are sent to the model

1. Encoding of new points $Y^t = E(X^t)$

2. Random-forest classifies new points

$C^t = [1,1,2,1 \ldots 2]$

3. Call the corresponding surrogate
4. Send back physicochemical properties to solver

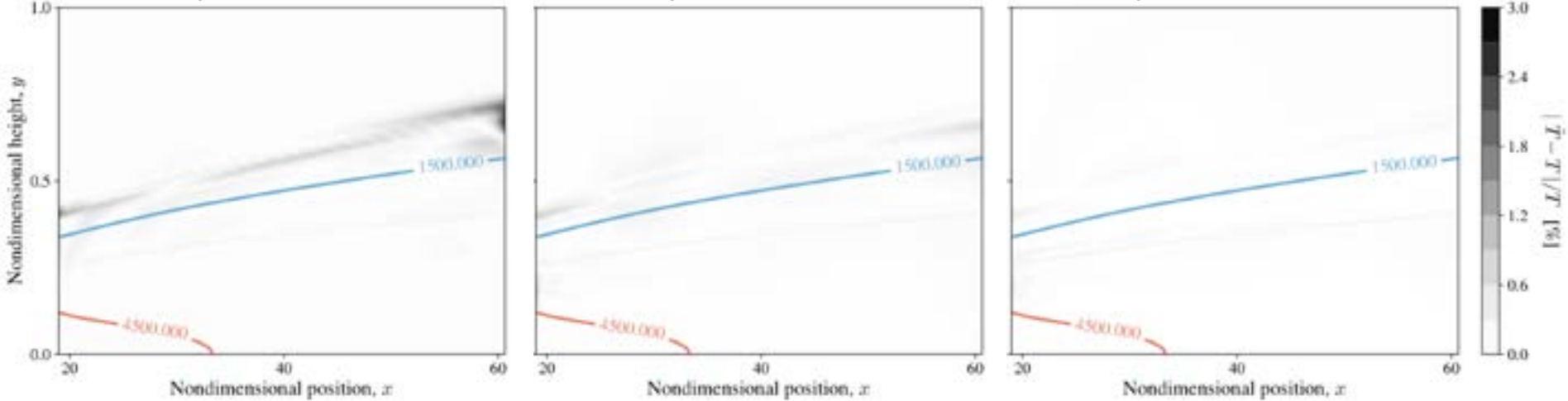


Model accuracy

- Testing of the model in predicting the outputs on the full grid (open-loop prediction)

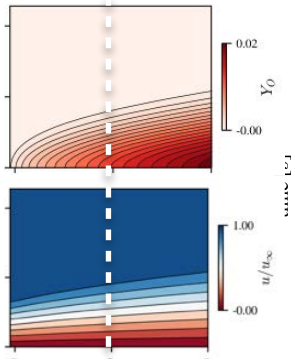
➢ All pre-processing step improve performance while maintaining high accuracy

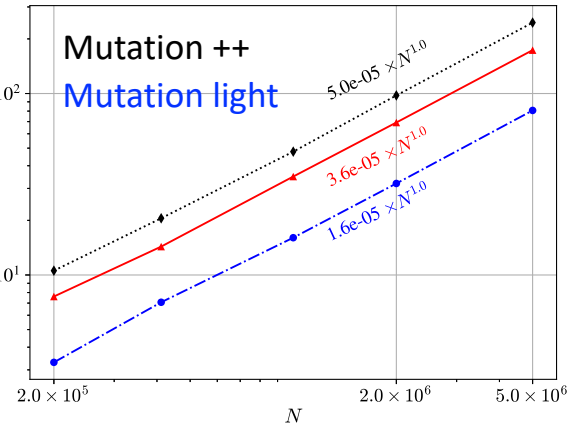
$d = 6,\ N_c = 1,\ N_R = 250$ $d = 2,\ N_c = 1,\ N_R = 250$ $d = 2,\ N_c = 2,\ N_R = 250$

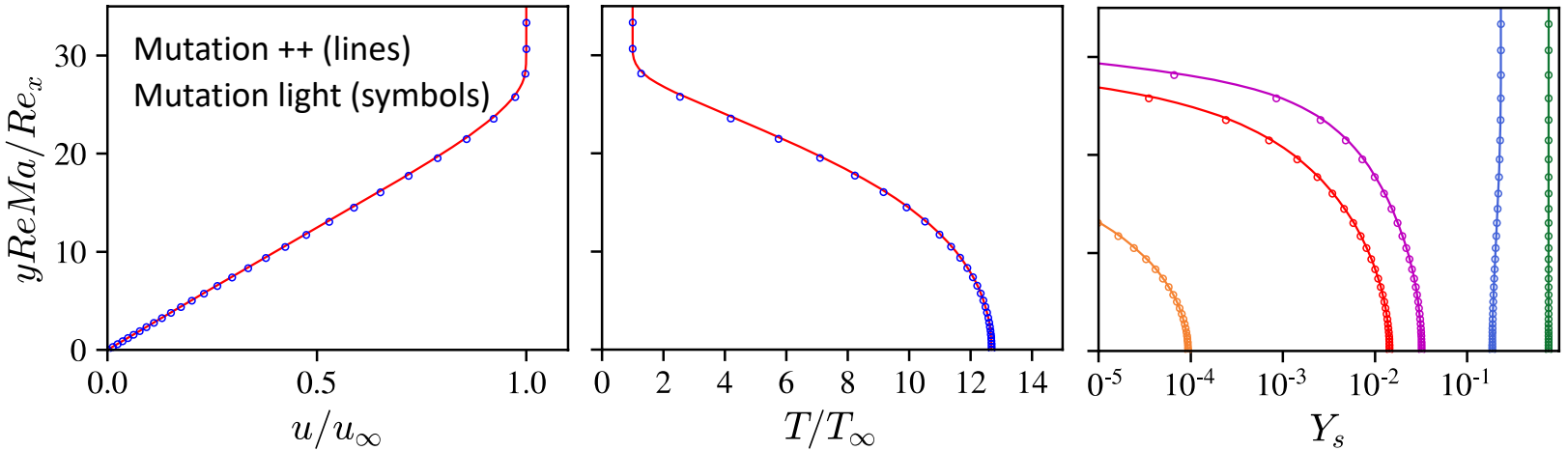


Model stability/performance

- The model replace M++ in the flow solver (closed-loop prediction), starting from the converged solution of BL
  - Solution remains stable after 2 flow-through time
  - Overall accuracy of the solution is maintained
  - Model is 70% faster



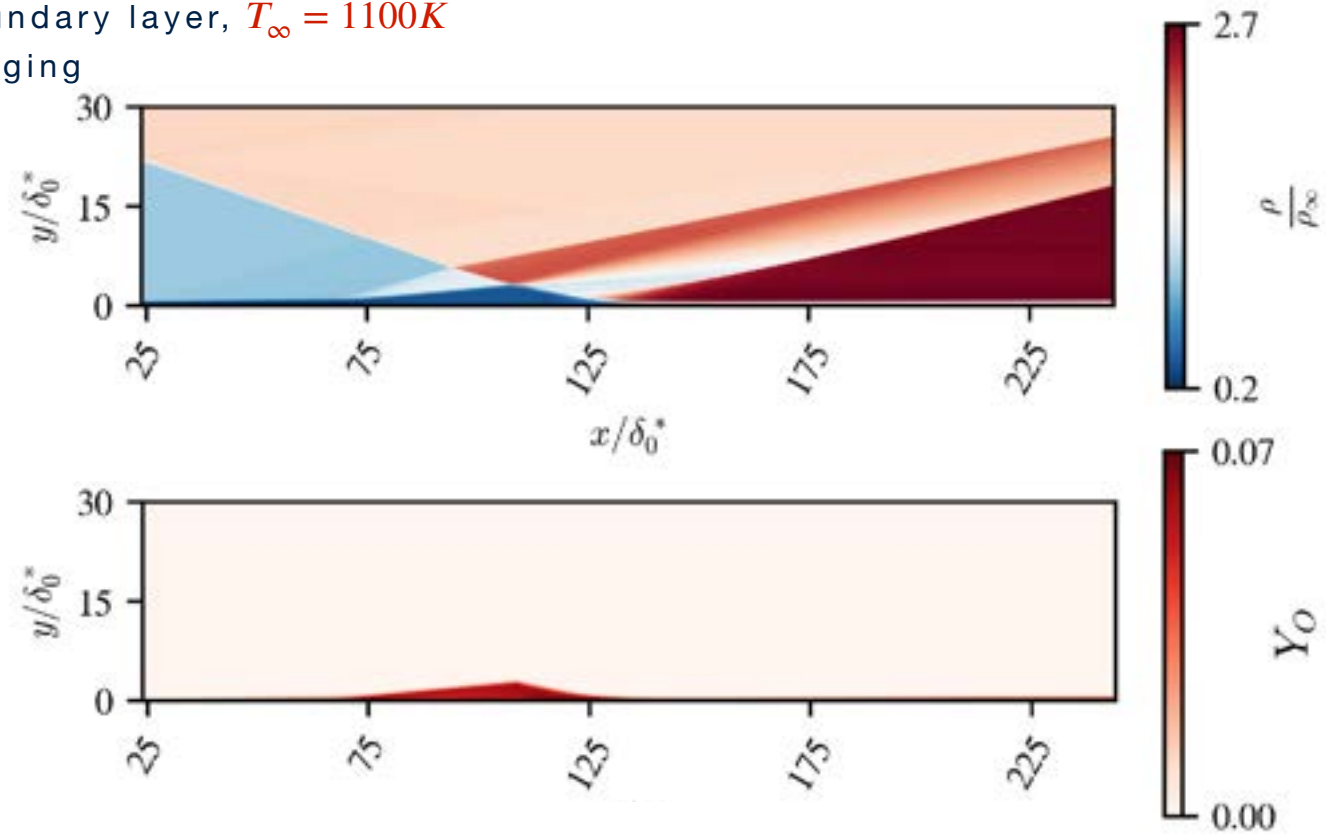




$Ma = 5.92$ **SBLI**

Problem setup

- Mach 5.92 adiabatic boundary layer, $T_\infty = 1100K$
- 13° Oblique shock impinging
- Air-5

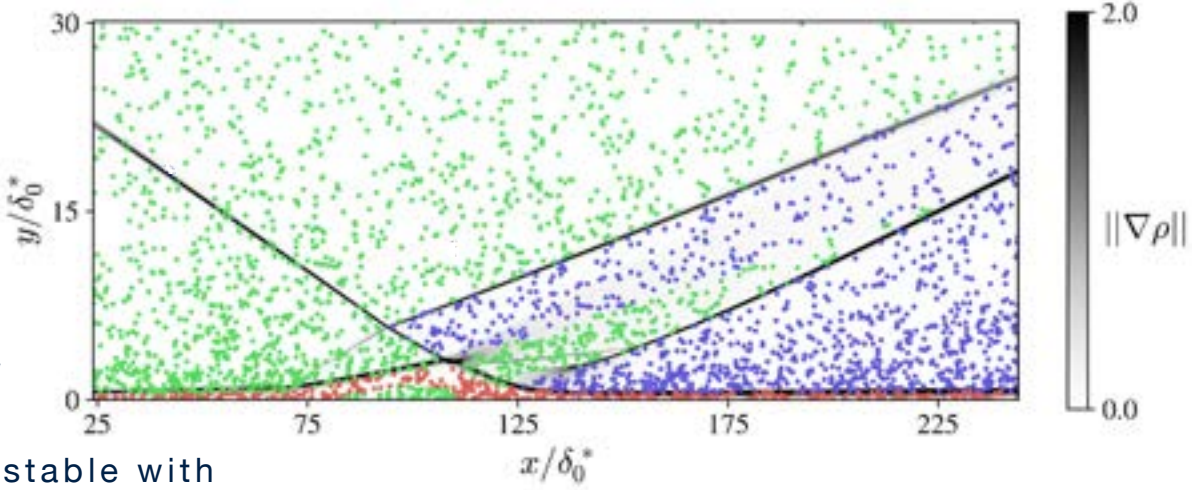


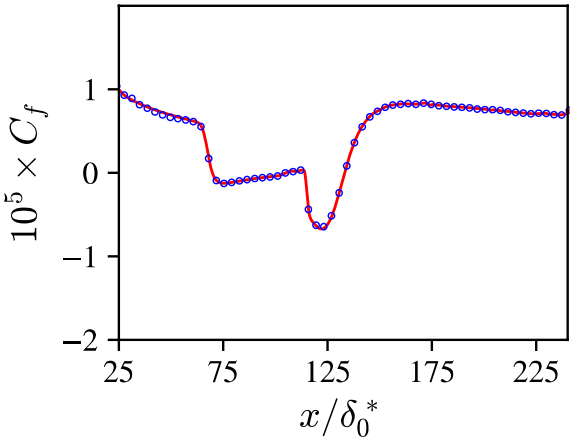
$Ma = 5.92$ **SBLI**

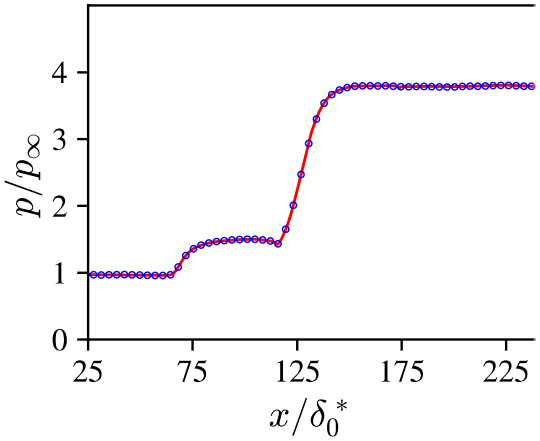
- Application of the algorithm:
  - $d = 3$
  - $N_c = 3$
  - $N_R = 250$

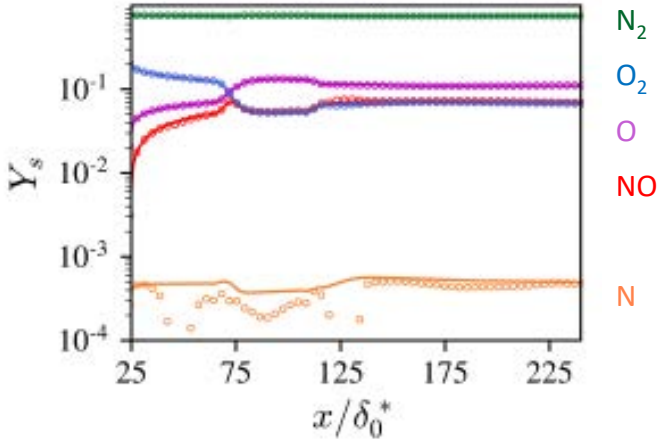
➢ Cluster are aligned with flow features

- Closed-loop simulation remains stable with high accuracy for quantities of interest



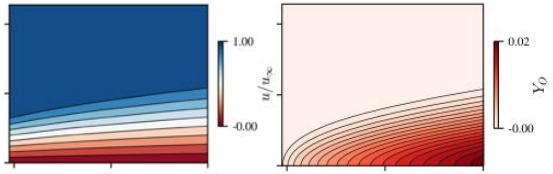


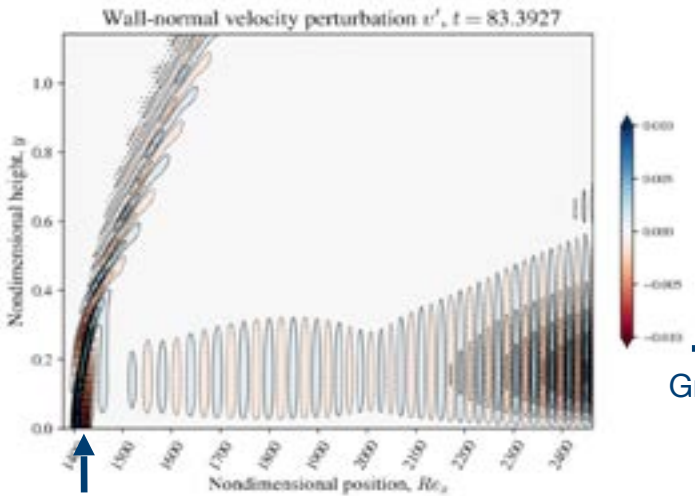




Unsteady flows

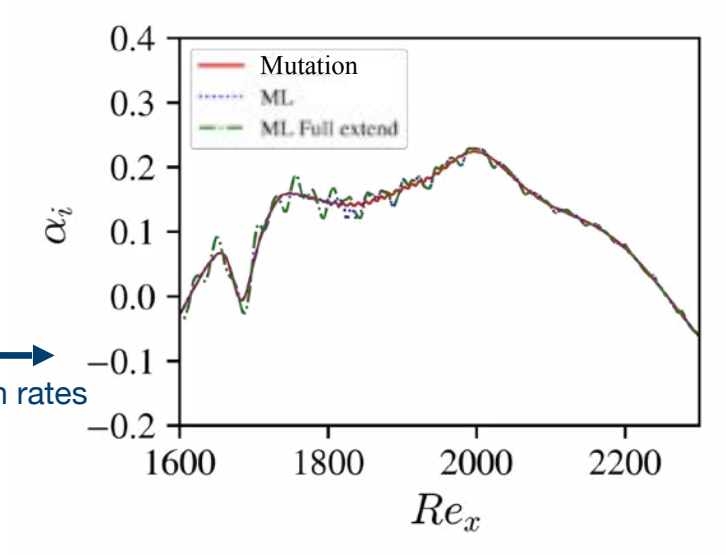
- Mach 10 boundary layer
- Small amplitude perturbations





Blowing & suction strip

Growth rates



Conclusion

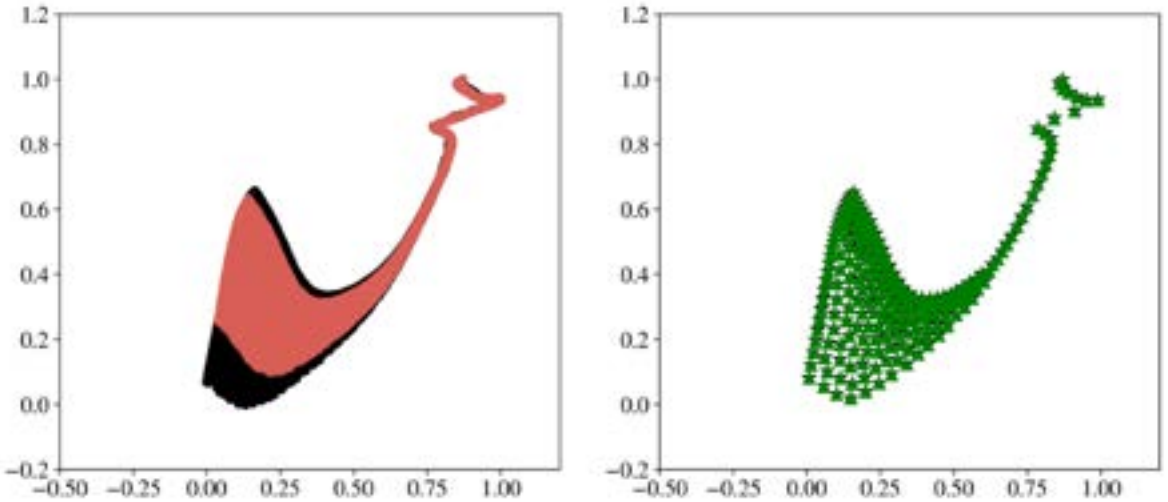
- A novel method for self-learning of reduced look-up table using nonlinear model-reduction, community clustering and surrogate response surfaces

- Testing of the model on $Ma = 10$ adiabatic BL, $Ma = 5.92$ SBLI with finite-chemistry effects (closed-loop simulation)
  - Stability and accuracy where maintained with performance boost

Scherding, C., Rigas, G., Sipp, D., Schmid, P. J., & Sayadi, T. (2022). Data-driven framework for input/output lookup tables reduction--with application to hypersonic flows in chemical non-equilibrium. *Phys. Rev. Fluids*

Way forward

- Optimise implementation for even higher boost in performance
- Implement model **adaptivity** to learn on-the-fly new states never seen before → application to JICF
- Include **thermal non-equilibrium** and **ablation** in the learning process



Thank you for your attention !