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

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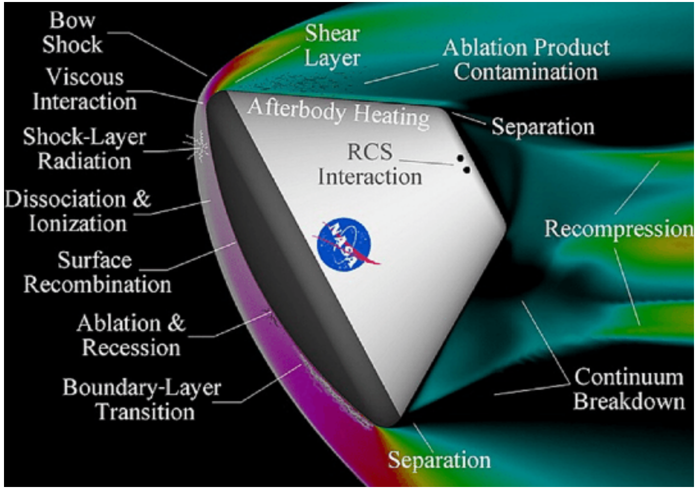
# Motivation

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

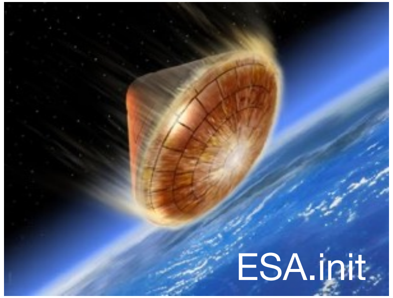
- Multiple complex phenomena interacting
  - Shock waves
  - Separation
  - Transition
  - **Chemistry**

  (Shock waves, Separation, Transition → **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

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

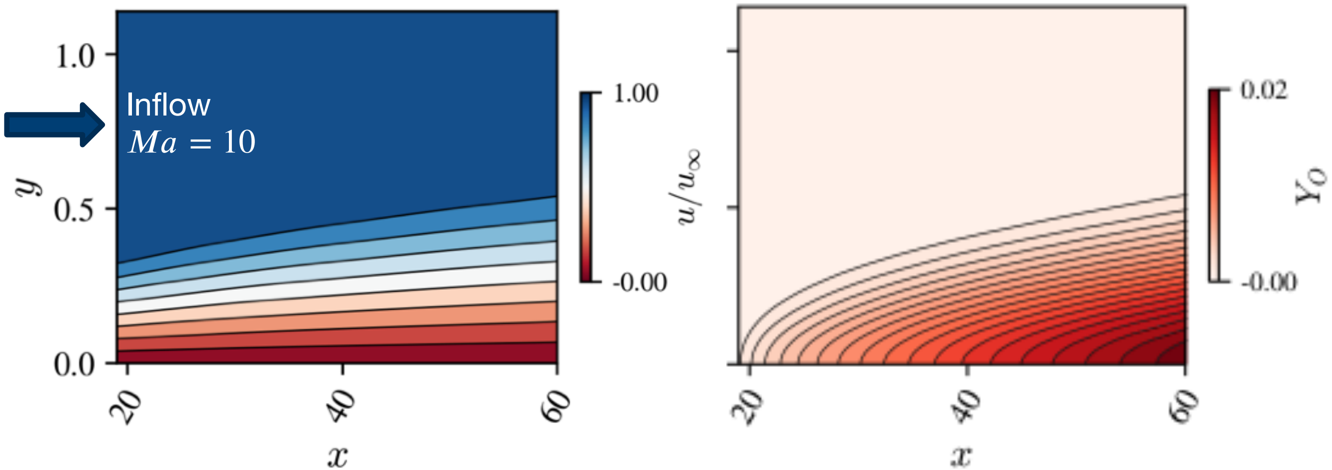
Reactions

Species diffusion

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

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

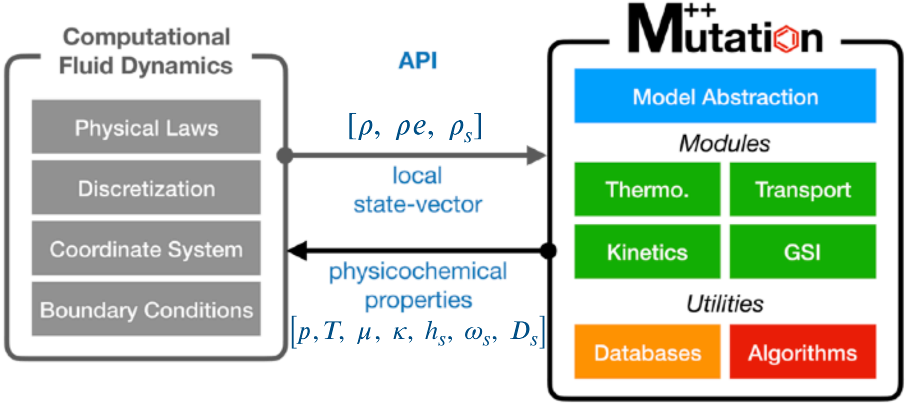
+diffusive

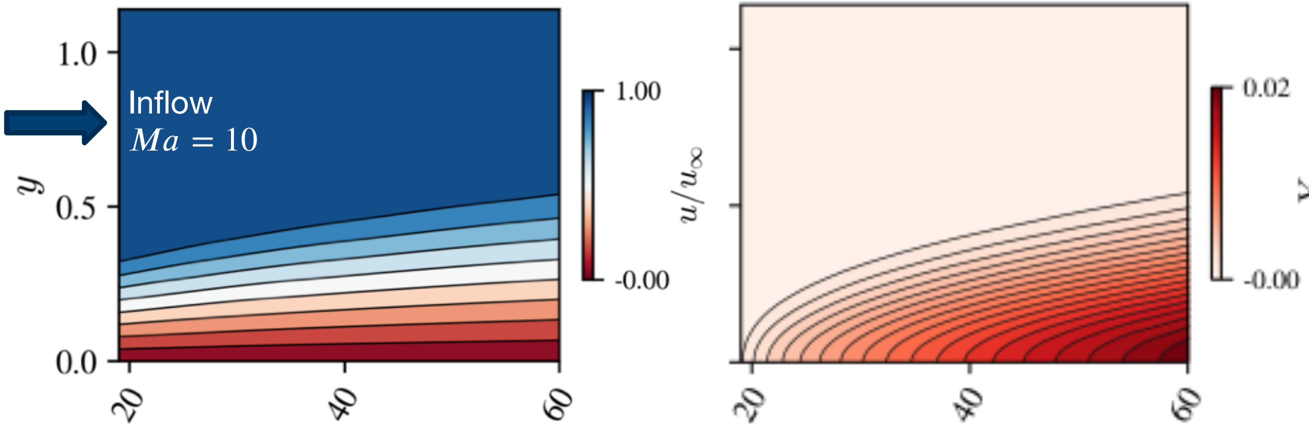


# Physicochemical modeling of hypersonic flow

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

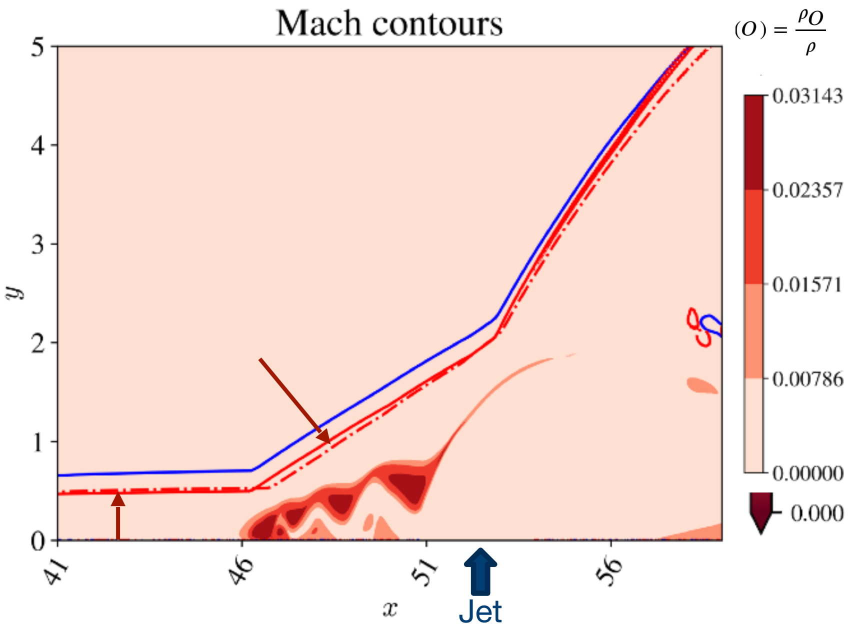
[4] - Scoggins, J. B., Leroy, V., Bellas-Chatzigeorgis, G., Dias, B., & Magin, T. E. (2020). Mutation++: Multicomponent thermodynamic and transport properties for ionized gases in C++. SoftwareX, 12, 100575.

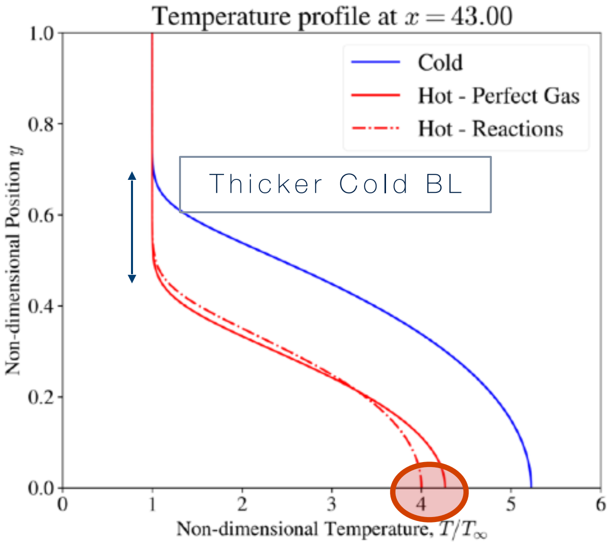
# Influence of finite-rate chemistry

- 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

250K difference at the wall with reactions on

Endothermic dissociation → weaker interaction

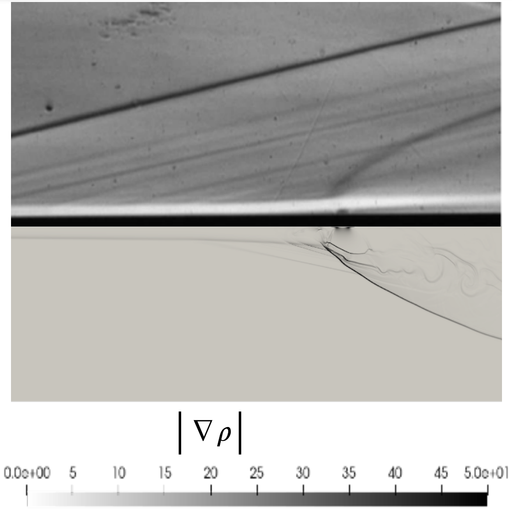
- Chemical non-equilibrium in hypersonic flows
  – Order-one influence on quantities of interests (stability, heating, transition) [1,2,3]
  – Limited experimental/numerical data


[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

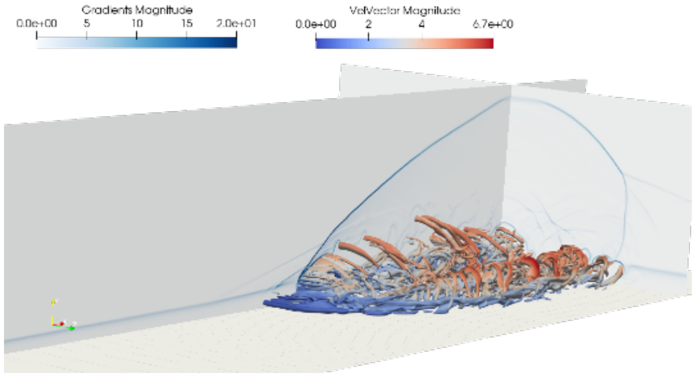
- Grid

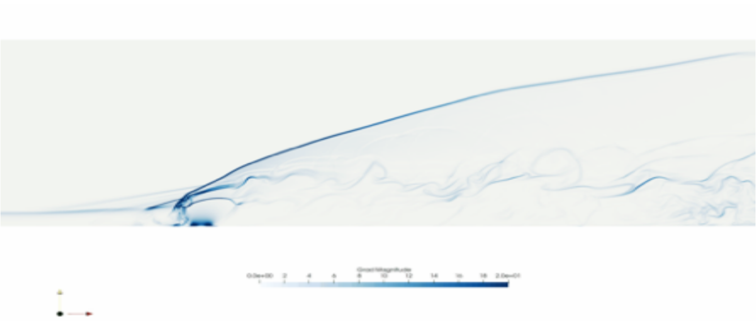
| | + units | N |
|---|---|---|
| X | 14 | 2132 |
| Y | 1 | 697 |
| Z | 14 | 1024 |
| Total | - | $1.5 \times 10^9$ |




Experimental Schlieren [4]

Numerical Schlieren

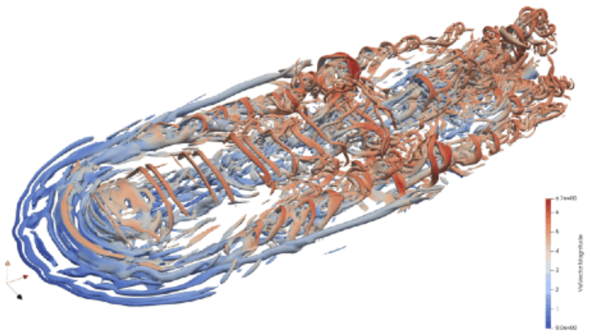


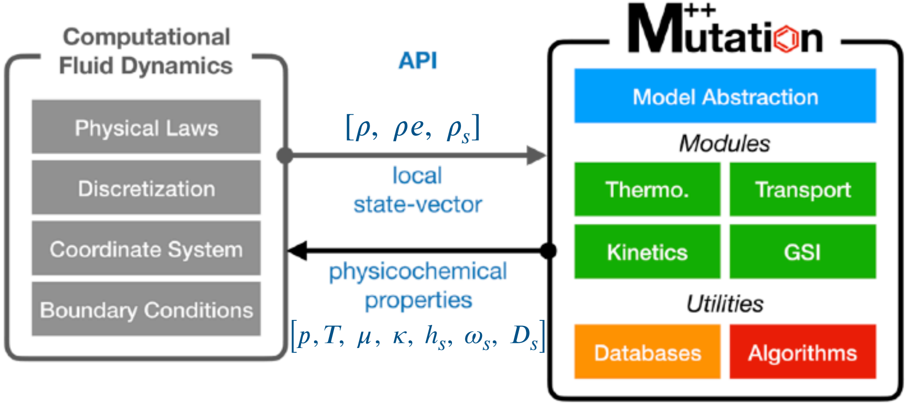



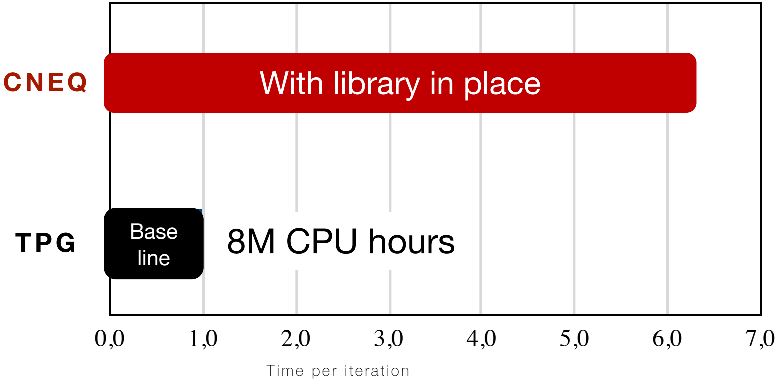


[4] – Erdem, Erinc. (2011). ACTIVE FLOW CONTROL STUDIES AT MACH 5: MEASUREMENT AND COMPUTATION. Manchester EScholar - The University of Manchester. The University of Manchester, 2011.

# 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**

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

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

Diffusion — Reactions

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

Incl. diffusive

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

& state equations and properties

**Models**

Turbulence

Chemistry

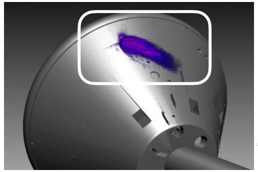
**Post-analysis**

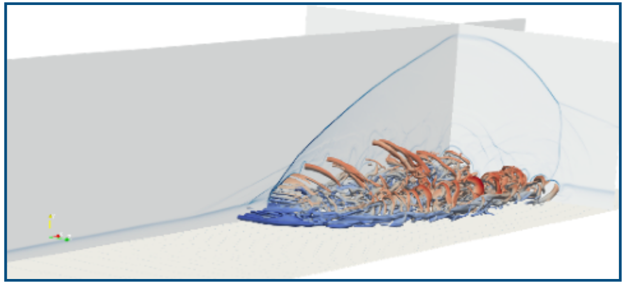
Extracting dynamics

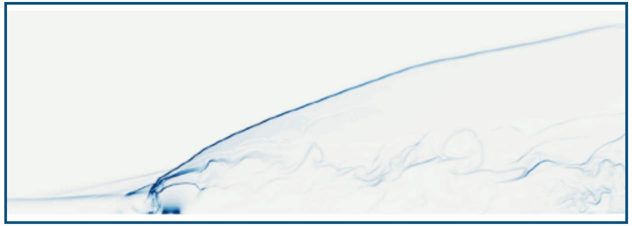
Reduced-order Models

**Control**

Ivey et al. 2011





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& state equations and properties

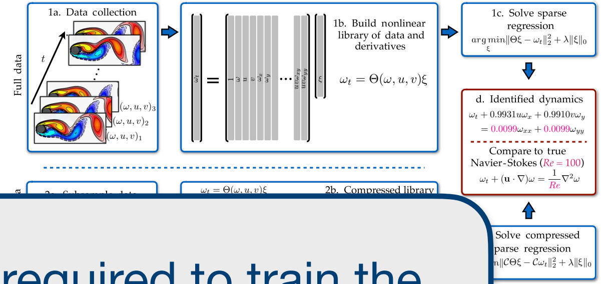
Models

Post-analysis

Control

Data-driven discovery of partial differential equations

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



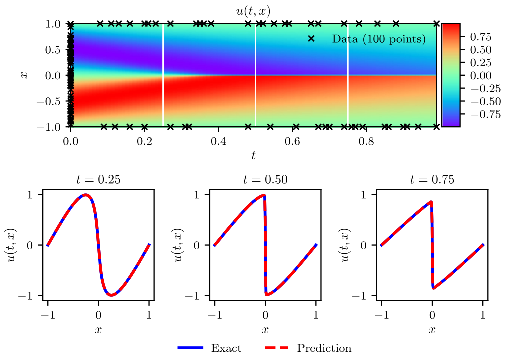

**Bottleneck:** large amount of data required to train the models for multi-scale multi-physics problems!

...nvolving

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

Extracting dynamics

Reduced-order Models



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Diffusion

Reactions

Incl. diffusive

& state equations and properties

**Models**

*Improve predictability*

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

Post-analysis

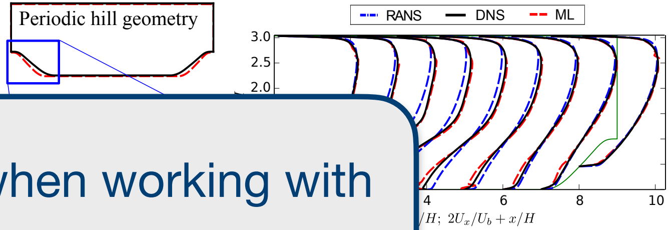
Extracting dynamics

Reduced-order Models

Control

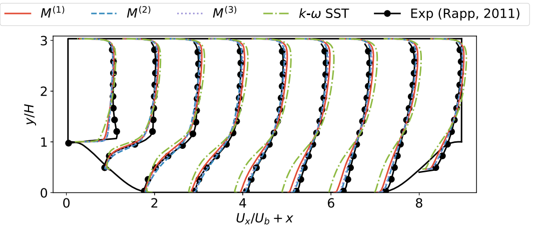
# Turbulence Modeling in the Age of Data

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




…sing
Sparse Symbolic Regression

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



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& state equations and properties

**Models**

Turbulence

Chemistry

*Improve Speed, while keeping accuracy*

Post-analysis

Extracting dynamics

Reduced-order Models

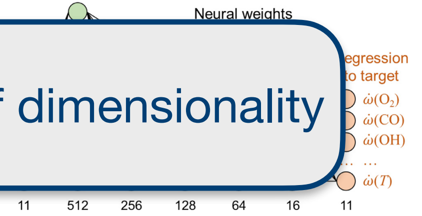
Control

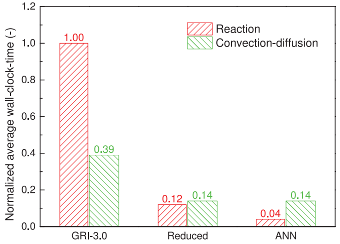
## <u>**Bottleneck:**</u> Curse of dimensionality

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*

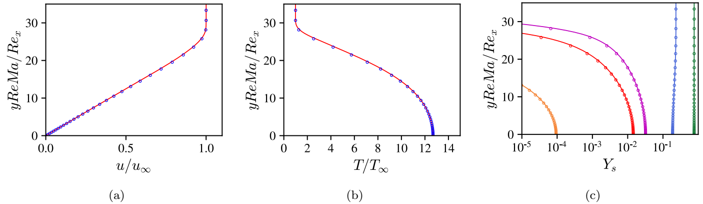



FIG. 15. Comparison of profiles of (a) streamwise velocity, (b) temperature, (c) species mass fractions from left to to right $N$, $NO$, $O$, $O_2$ and $N_2$ at $Re_x = 2000$. Solid line and symbols correspond to the solution obtained using Mutation++ and the data-driven model, respectively.

Governing equations

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Diffusion

Reactions

Incl. diffusive

& state equations and properties

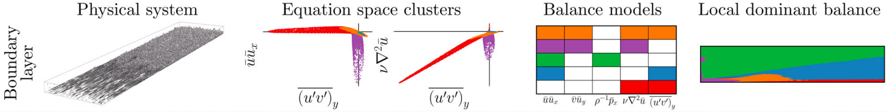
Models

**Post-analysis**

Control

# Learning dominant physical processes with data-driven balance models

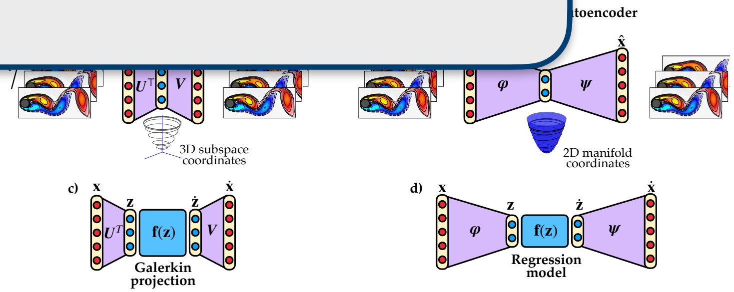
Jared L. Callaham [1✉], James V. Koch[2], Bingni W. Brunton [3], J. Nathan Kutz[4] & Steven L. Brunton[1]




**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

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

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& 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]

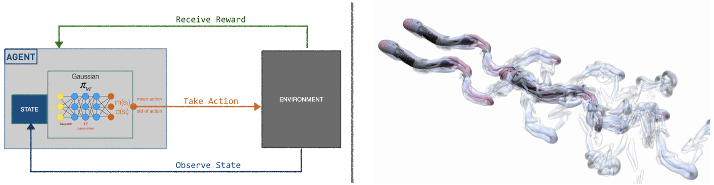


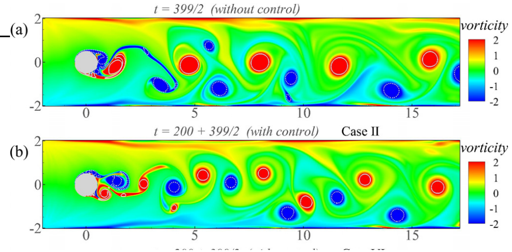

**Figure 8**

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, $\pi_w$: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



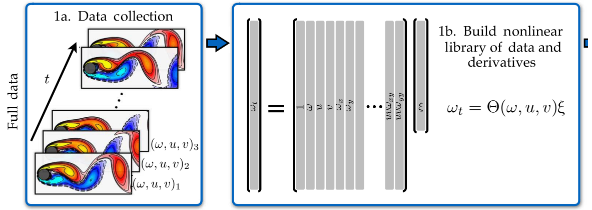
# Type of learning

## Supervised Learning

**Find a mapping from X —> Y**

**Regression**
- Decision trees
- Random forests
- Neural Networks

**Classification**
- Linear
- Generalised linear
- Gaussian process



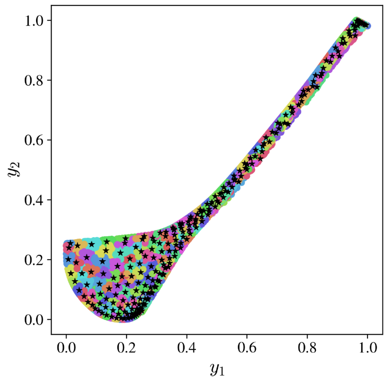

Samuel H. Rudy,[1]* Steven L. Brunton,[2] Joshua L. Proctor,[3] J. Nathan Kutz[1]

## Unsupervised Learning

**Learning Structure from data : X**

**Clustering**
- K-means
- Spectral clustering

**Dimensionality Reduction**
- PCA
- Auto-encoders
- Diffusion maps

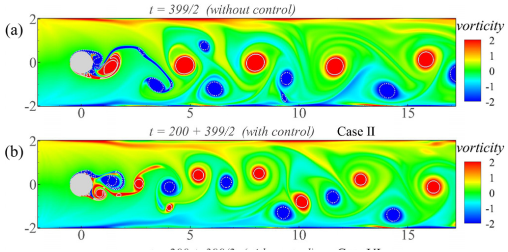



## Semi-supervised Learning

**State + action**

**Reinforcement Learning**
- Markov decision process
- Deep RL

**Generative Models**
- Generative adversarial networks (GANs)

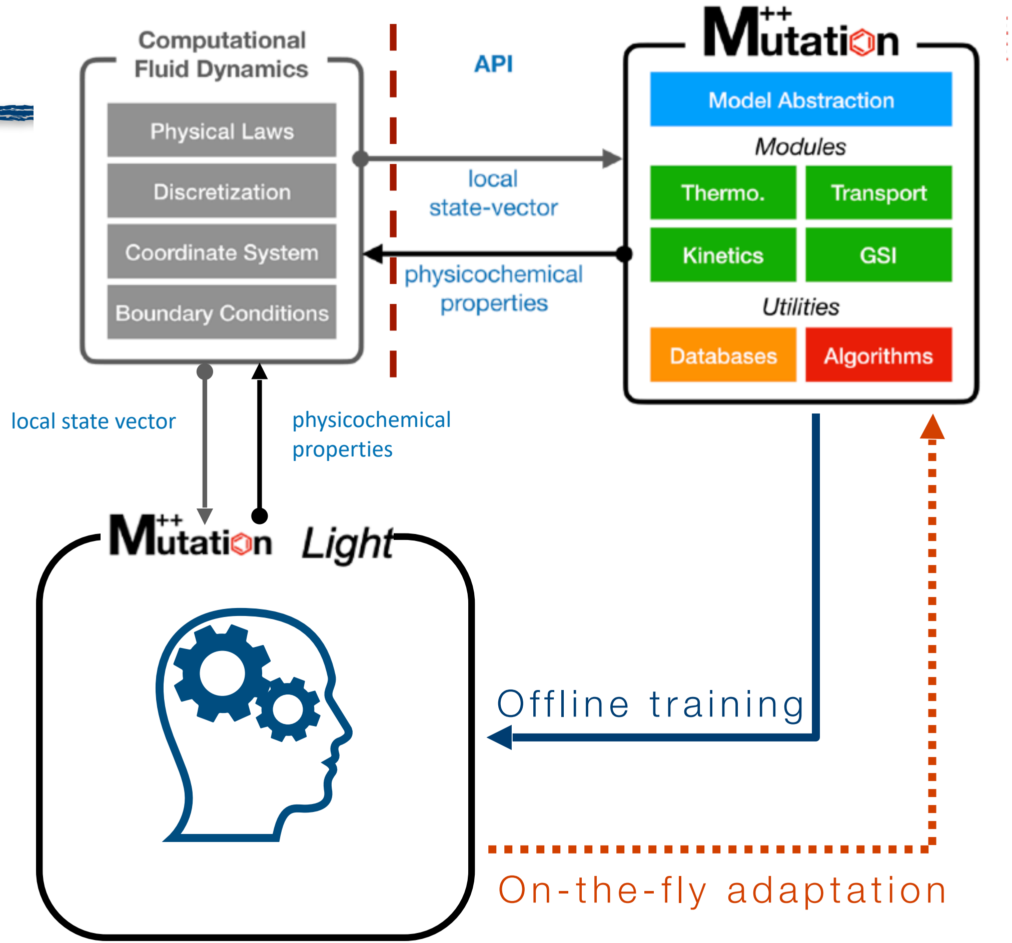


# Proposed approach

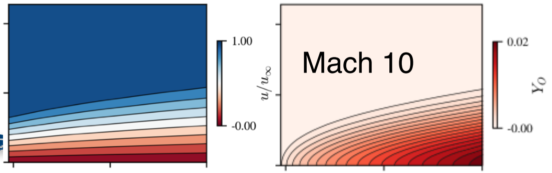
- Flows have history —> most thermodynamic states have been seen previously:
  - Offline training

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

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



# Mutation++: Input/Output



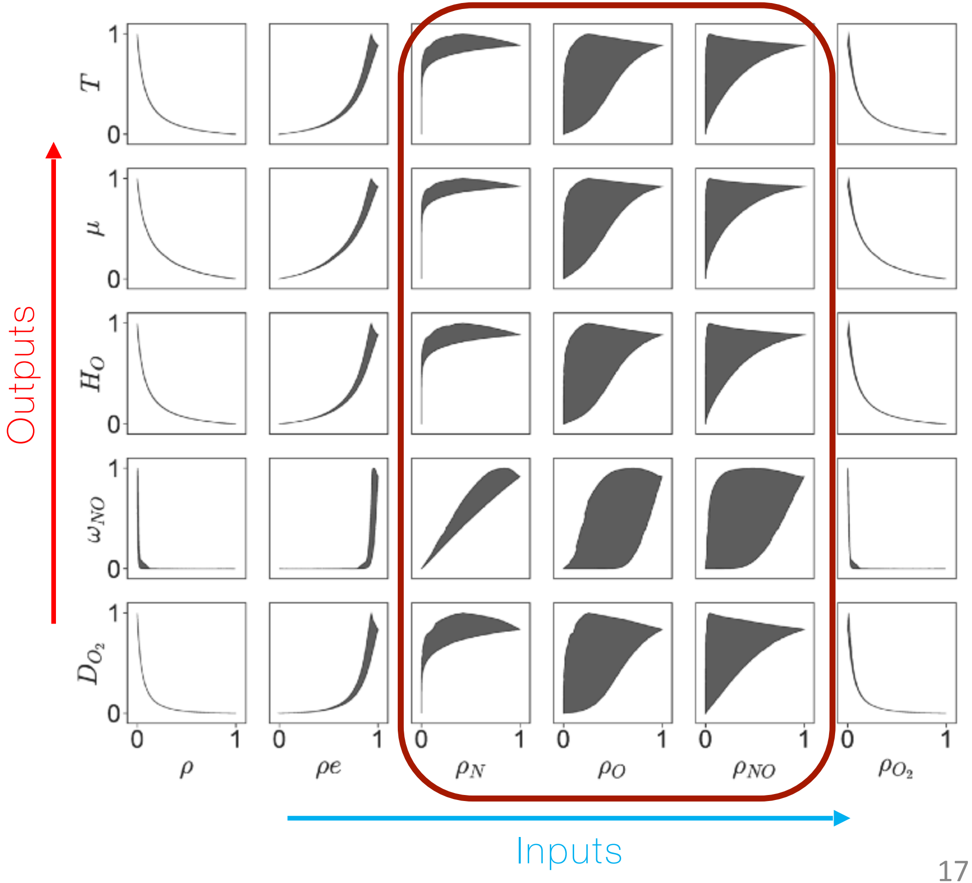

- $N = 10^5$ points sampled
- Input: local state vector

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

- Output: thermochemical properties

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

➢ Large spreading of outputs with respect to radicals $\rho_N,\ \rho_O,\ \rho_{NO}$




**Active subspaces** —> Dimensionality reduction

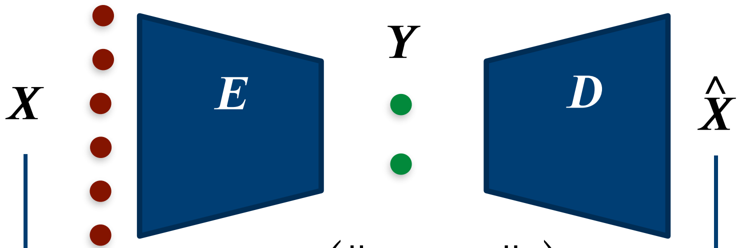
# Dimensionality Reduction $\mathbb{R}^6 \rightarrow \mathbb{R}^2$

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

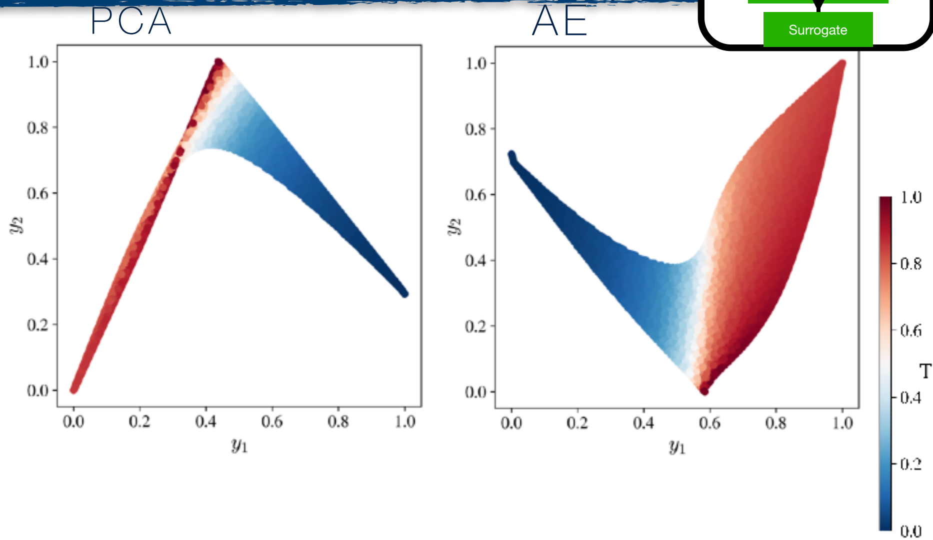
  $Y \in \mathbb{R}^d,\ d < D$

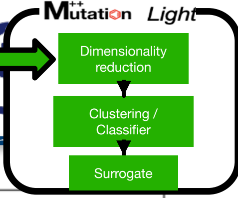
- Nonlinear autoencoder (AE)

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




$$\min\left(\left\|X - \hat{X}\right\|_2\right)$$



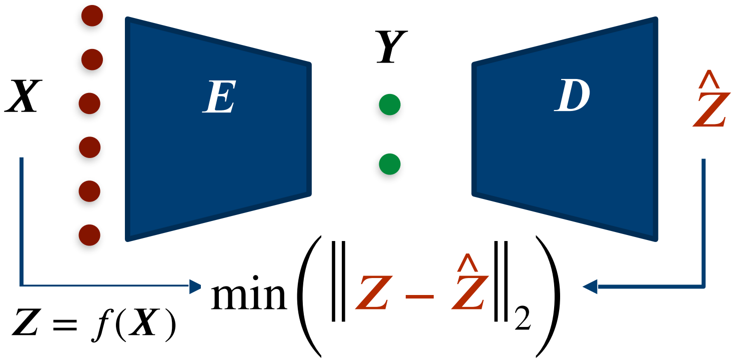



# Dimensionality Reduction $\mathbb{R}^6 \rightarrow \mathbb{R}^2$

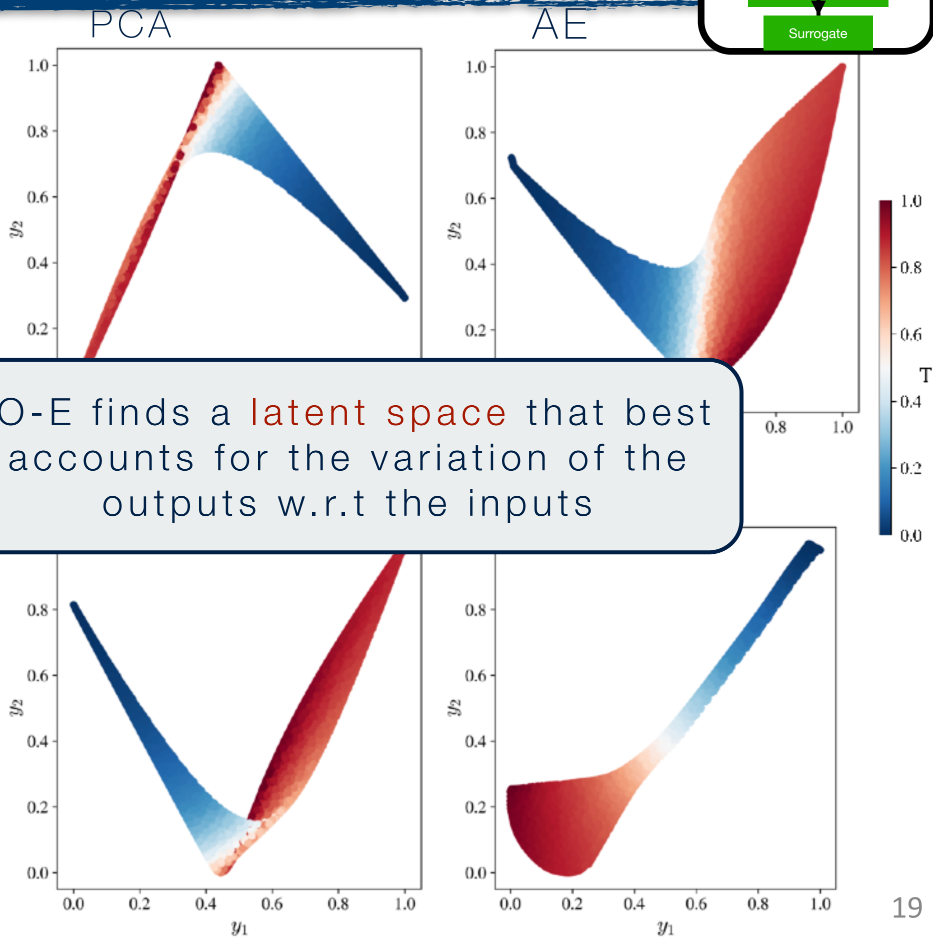
- PLS-SVD $X^T Z = U\Sigma V^T \rightarrow Y = XU_d$

- Input/Output encoder (IO-E)

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

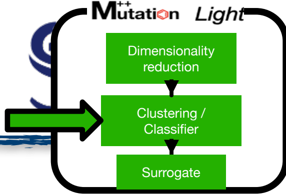



$$\min\left(\left\|Z - \hat{Z}\right\|_2\right)$$




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

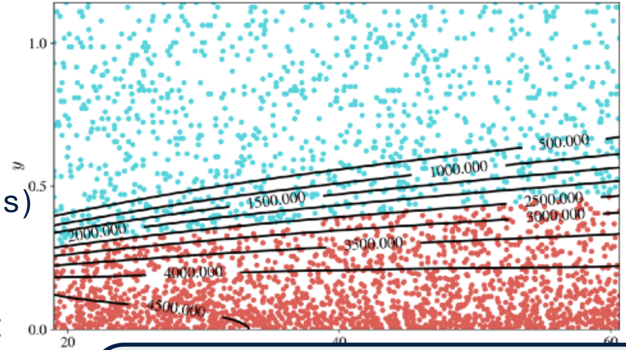
# Clustering

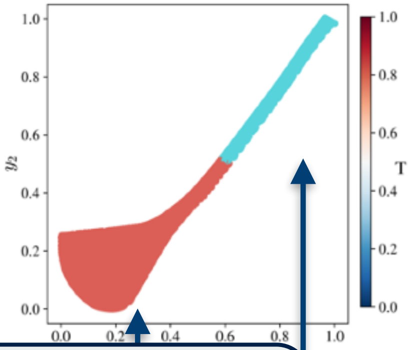



- Outputs have different dynamics depending on their location in the flow

➢ Notion of clusters

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

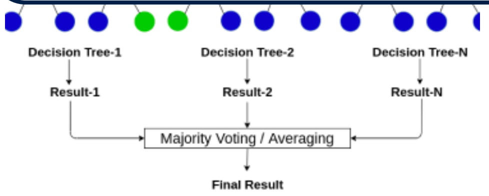


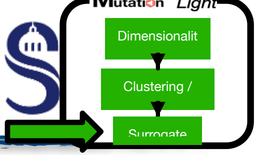

➢ Clusters represent regions at different level of thermochemical equilibrium
  - Freestream : Cold, frozen chemistry
  - Near wall : Hot, finite-rate chemistry

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

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




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



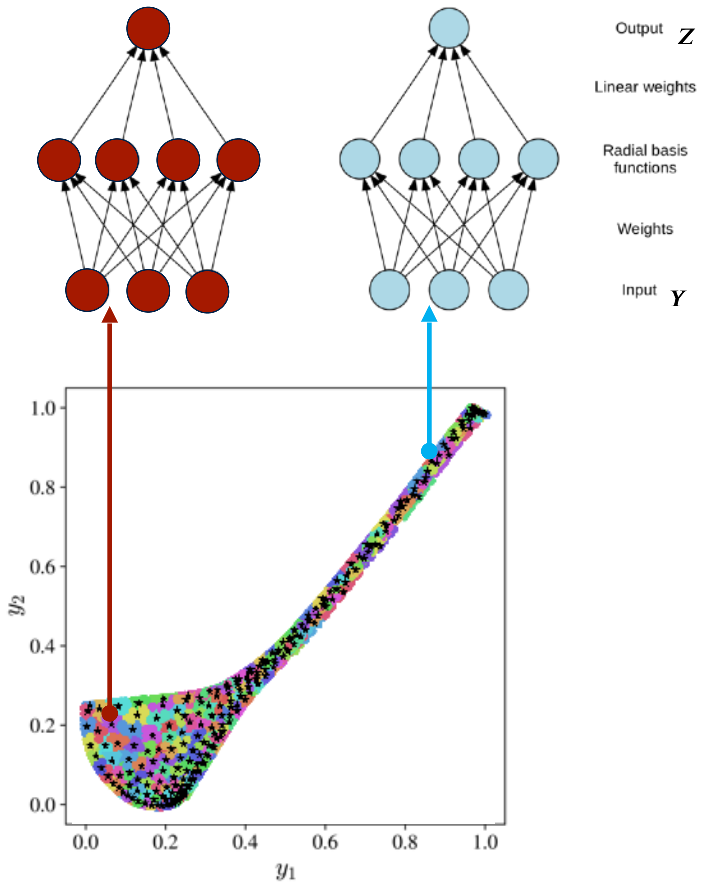

# Surrogate

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

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

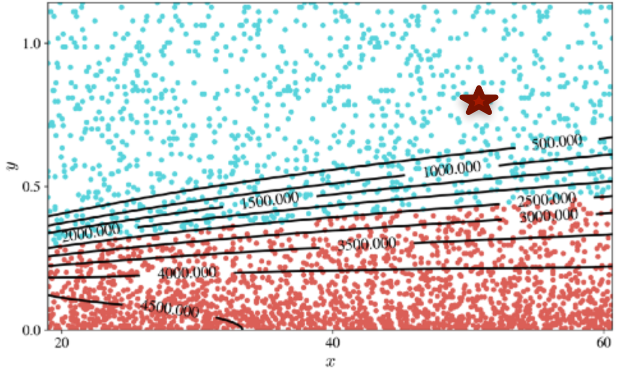
$$z = g_{C_k}(y) = \sum_{i=1}^{N_R} a_i \phi\left(\|y - c_i\|\right)$$

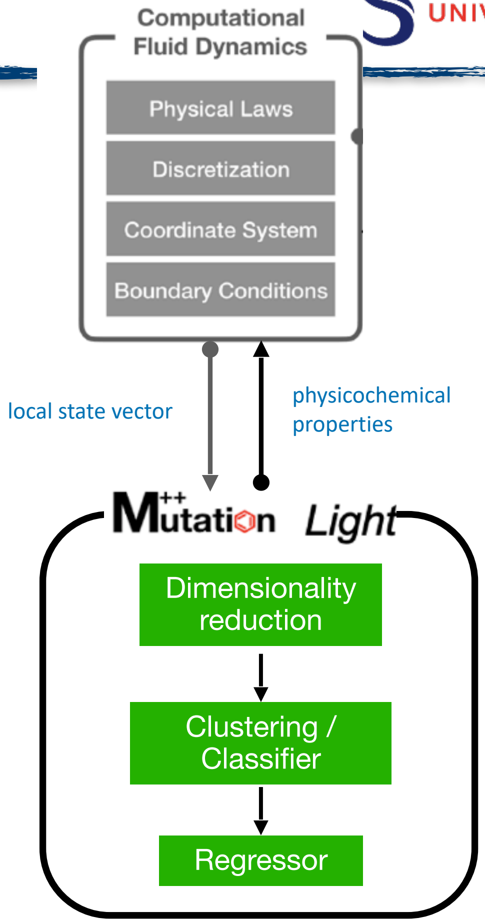
- The $N_R$ centers are determined with k-means of the input/output pairs
  - ➢ avoid overfitting



# Coupling with CFD solver

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



# Coupling with CFD solver

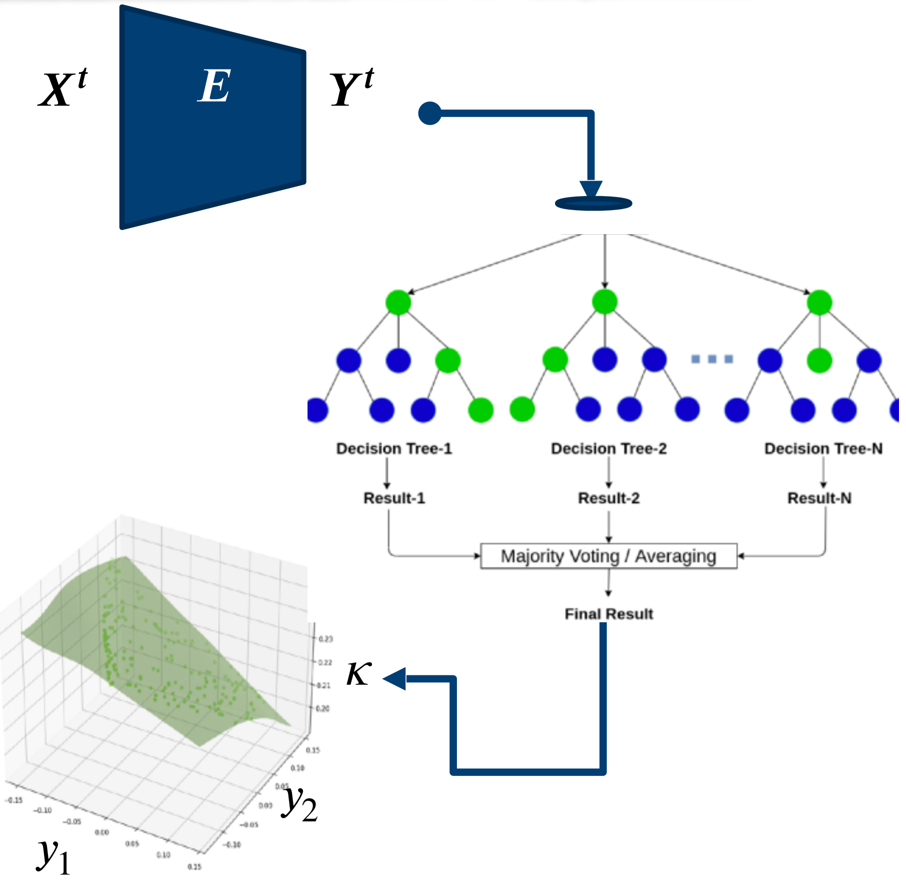
- New local state vector $X^t$ are sent to the model

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

2. Random-forest classifies new points

$C^t = [1,1,2,1\ldots2]$

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

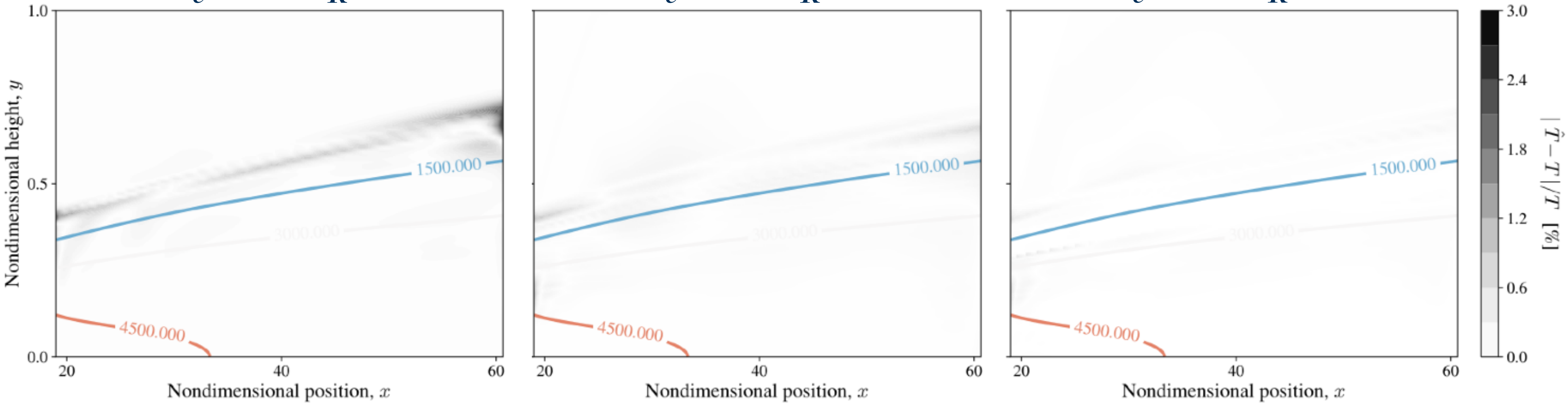


# Model accuracy

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

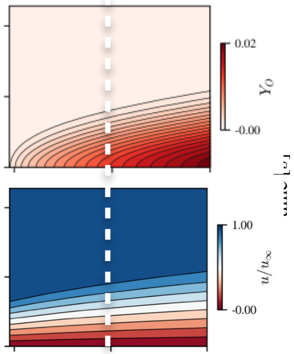
➢ All pre-processing step improve performance while maintaining high accuracy

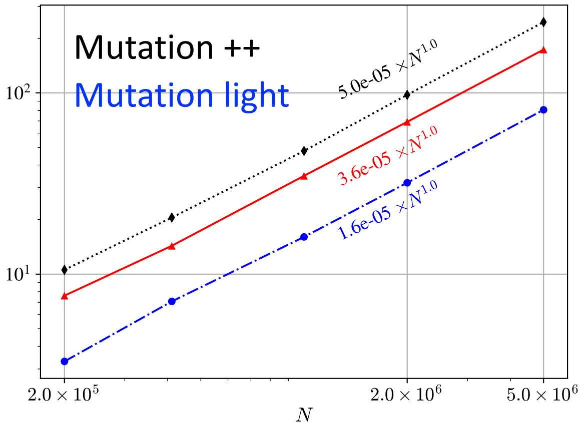
$d = 6,\ N_c = 1,\ N_R = 250$ $d = 2,\ N_c = 1,\ N_R = 250$ $d = 2,\ N_c = 2,\ N_R = 250$

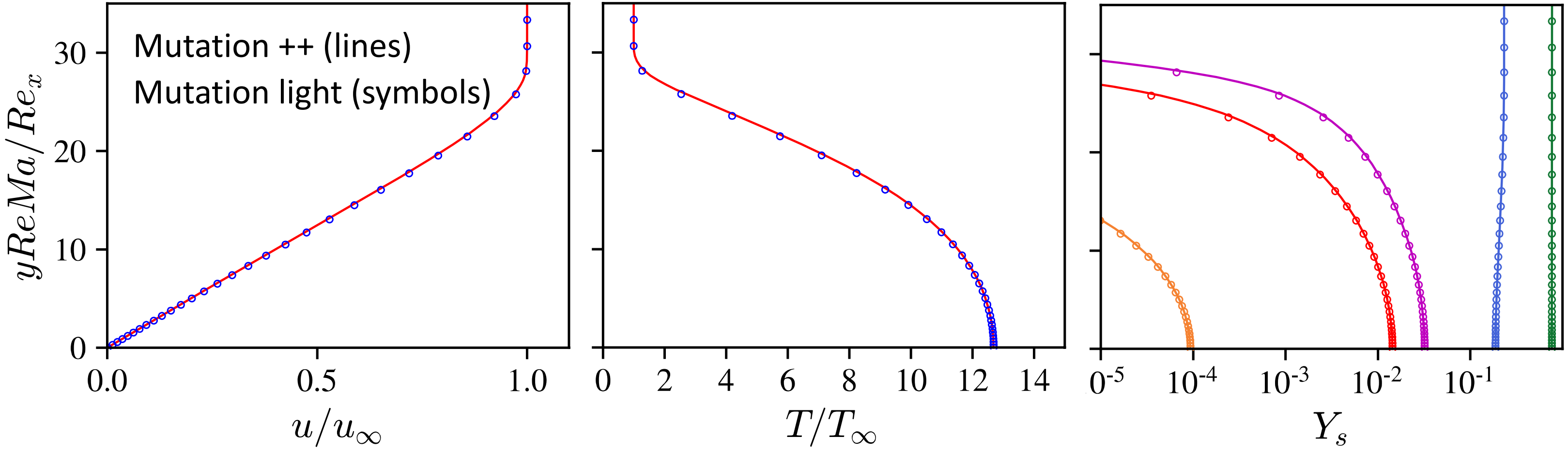


# Model stability/performance

- 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



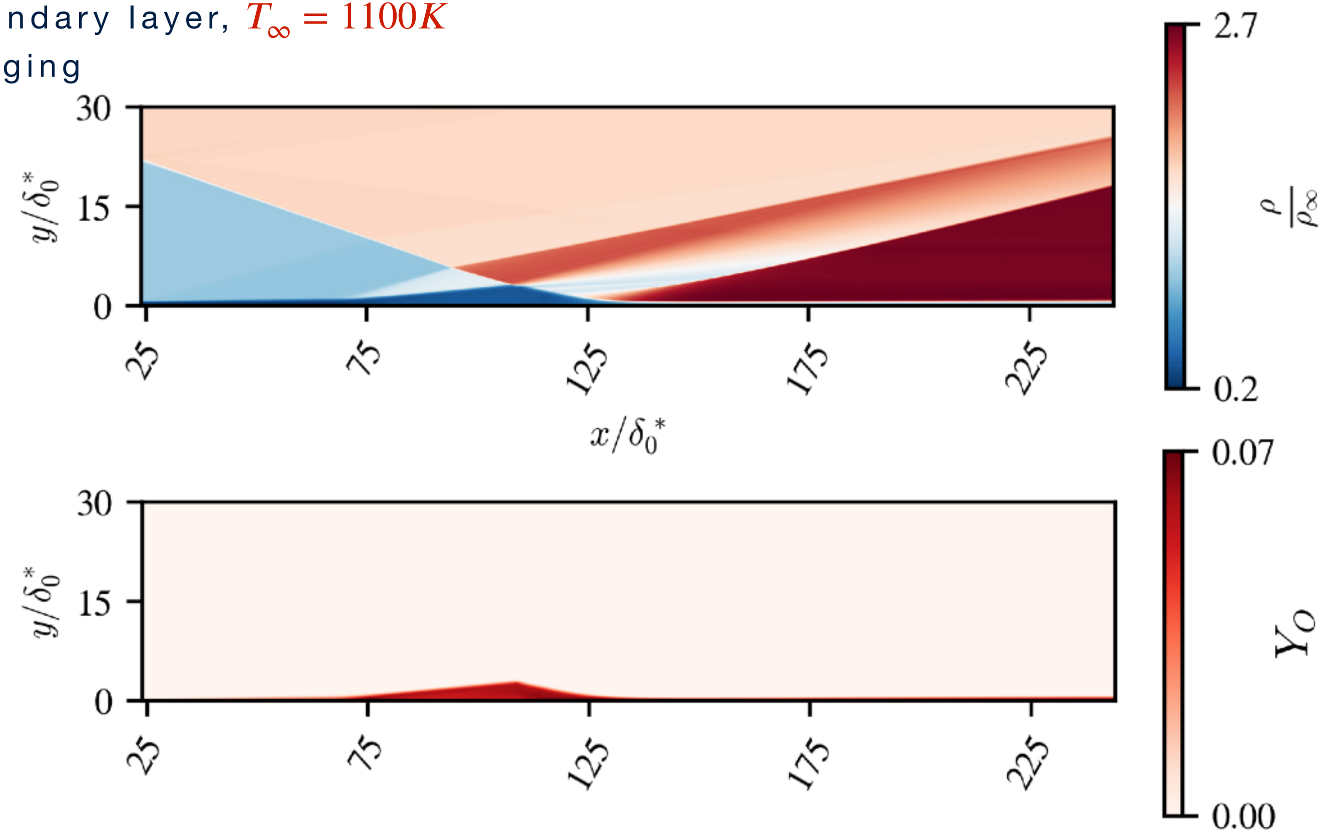



# $Ma = 5.92$ SBLI

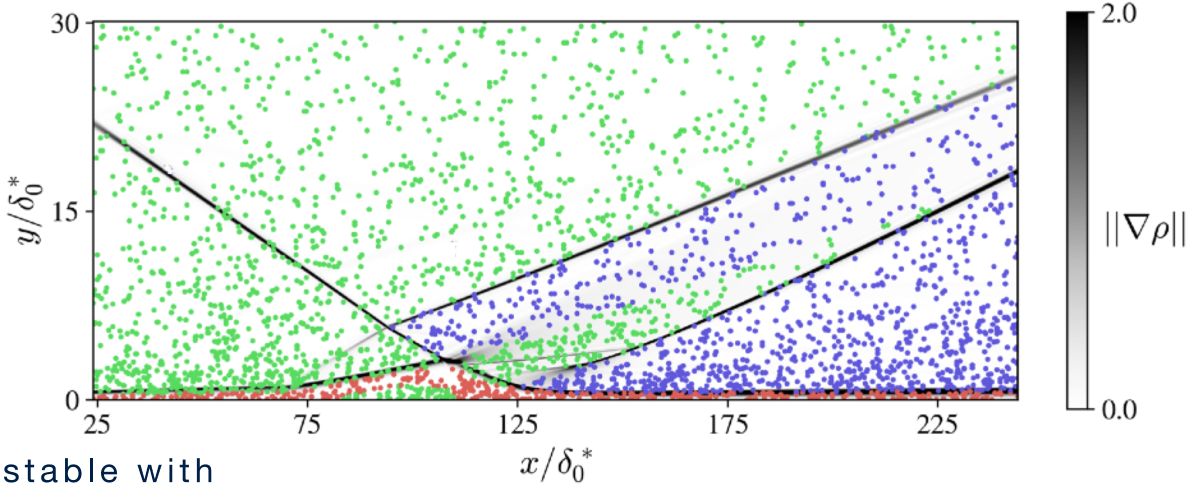
## Problem setup

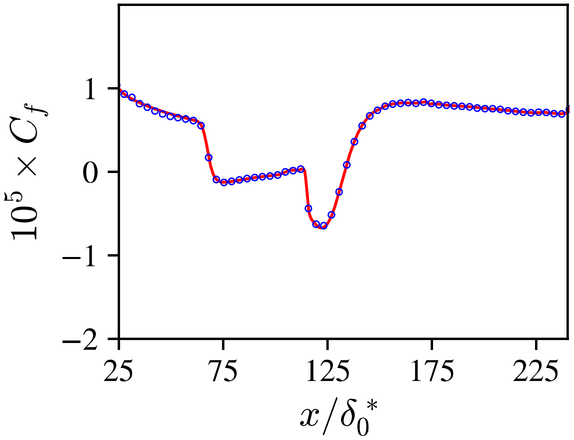
- Mach 5.92 adiabatic boundary layer, $T_\infty = 1100K$
- 13° Oblique shock impinging
- Air-5

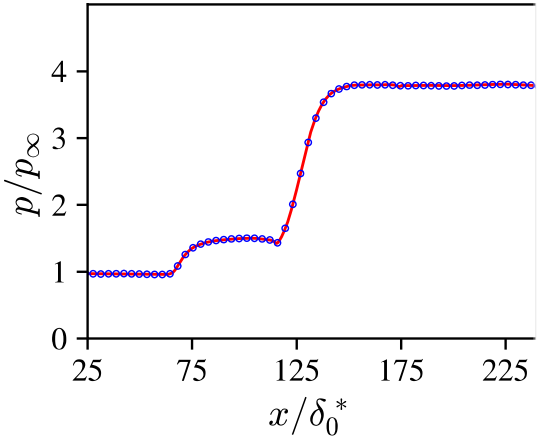


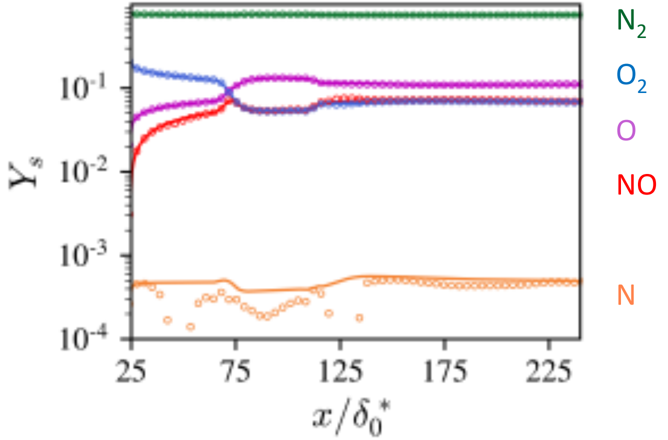
# $Ma = 5.92$ SBLI

- 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



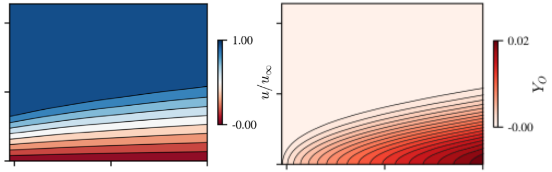



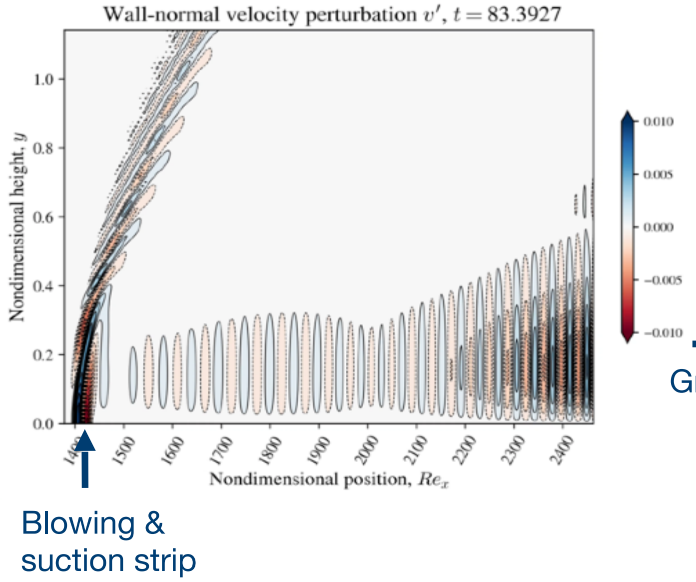



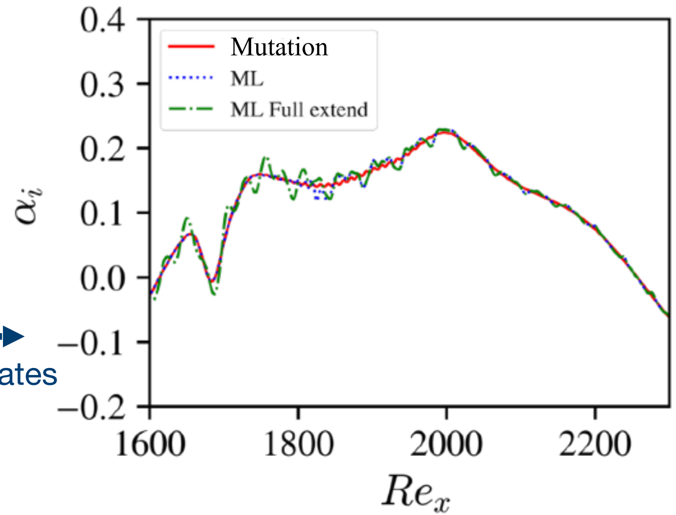
# Unsteady flows

- Mach 10 boundary layer
- Small amplitude perturbations




Growth rates



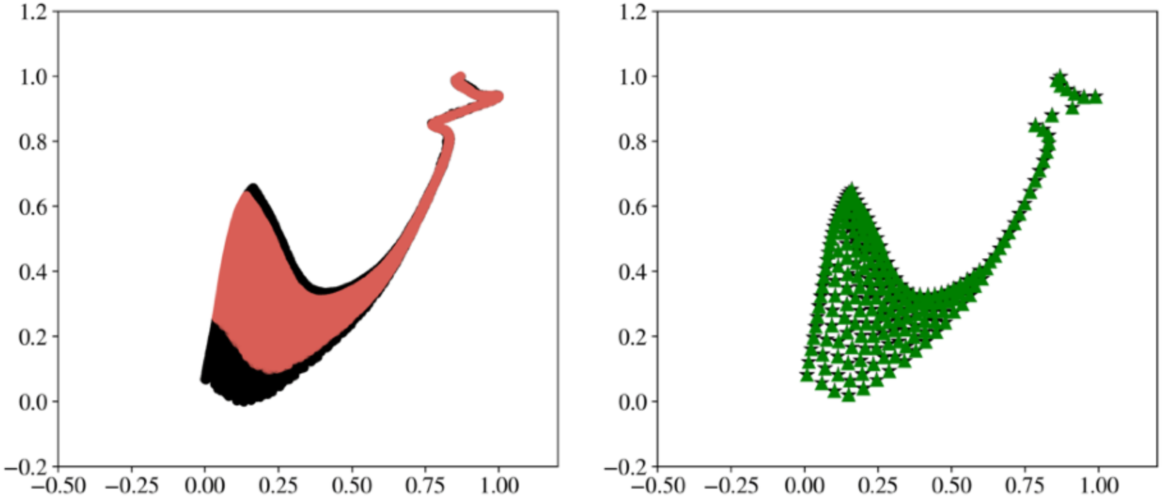
# Conclusion

- 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 !