Data-driven modelling of reactive flows

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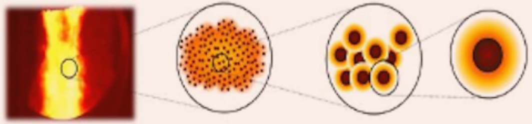
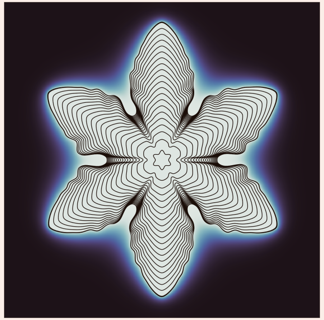
Complex flows

Sustainable & renewable research —> motivates the study of complex flows

Space reentry



Solid fuel combustion



Interfacial flows

- Moving interfaces
- Transfer across interfaces
- Phase-change
- Reactions (chemistry)

Flower.jl: our in-house julia package

In-house code developed in julia[1] —> high-level dynamic programming language.

- **Sharp interface limit** → level set function to track the interface
- **Cut Cell method** → heat equation, incompressible Navier-Stokes equations, convection diffusion equation, free-surface flows
- **Phase change** → Stefan condition, normal motion of the interface controlled by the temperature field
- **Adjoint capabilities** → optimization procedure using continuous adjoint derivation for two phase Stefan problems
- **Derivative free optimisation techniques**

[1] J. Bezanson, A. Edelman, S. Karpinski, V. B. Shah. SIAM Review, 2017.

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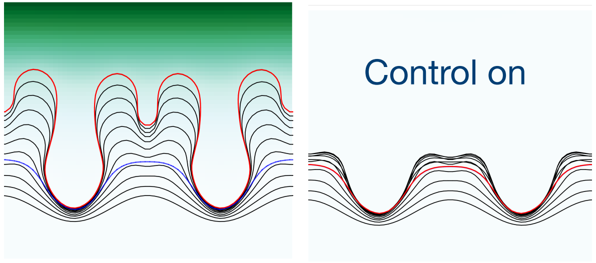
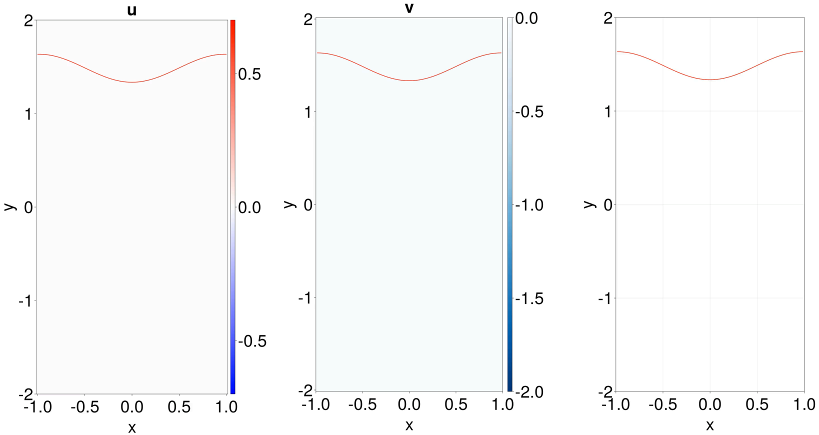
Some of the recent results

- Phase-change: Mullins-Sekerka instability & RB instability



- Free surface flows: drop formation



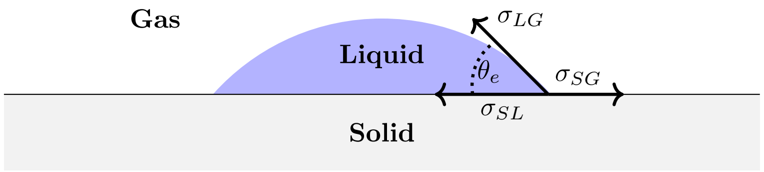
Work in progress

SOLVER:

- Multi-level **DD methods** & **hierarchical solvers** —> fast linear algebra solves —> efficient solve for 3D complex configurations
- Making use of GPU/CPU architectures —> targeting ARM-based CPUs

Physics:

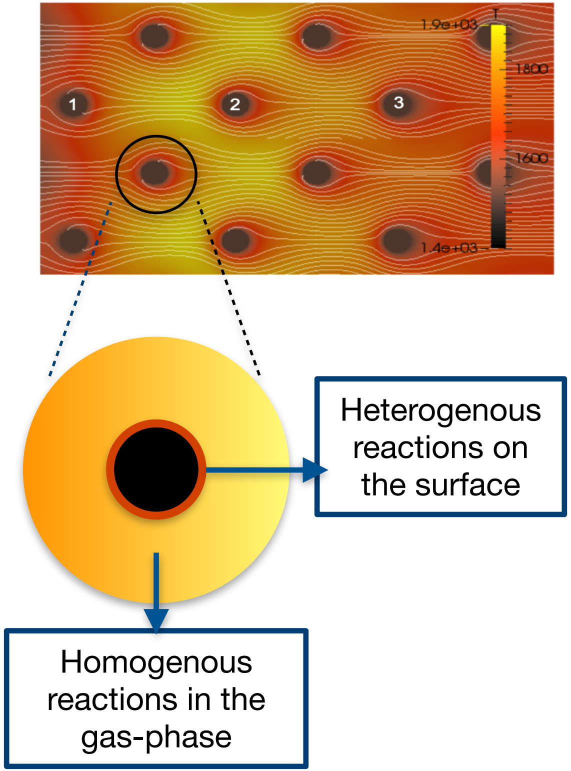
- Implementing **contact lines** —> three-phase problems



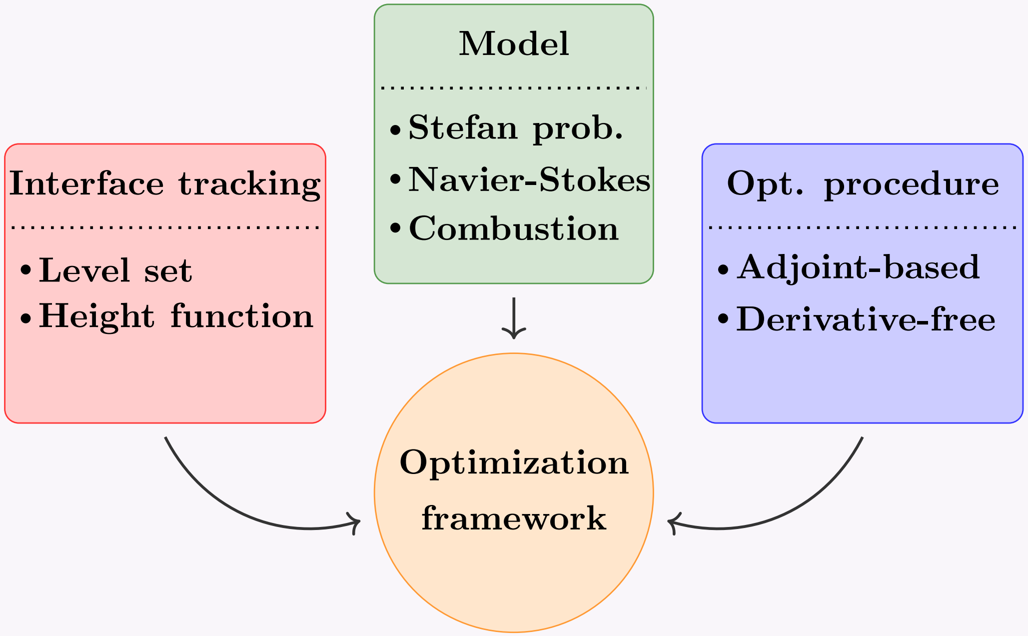
Chemical reactions : Apophis.jl - package

- Large mechanisms to represent all the chemical reactions
- **Sensitivity analysis** & **UQ** of any QoI with respect to the chemical models in 0D & 1D
- This capability is being added to Flower.jl to perform the analyse in a multi-dimensional setting

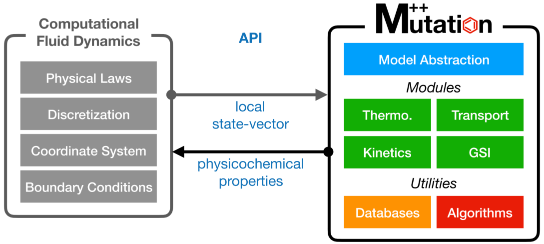
Joint project with RWTH - Aachen University



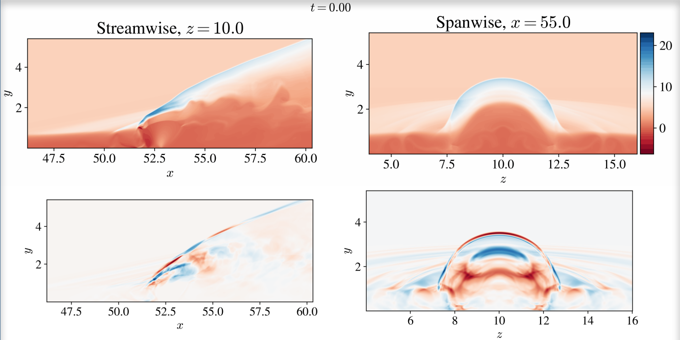
Flower.jl


Model
• Stefan prob.
• Navier-Stokes
• Combustion
Interface tracking
• Level set
• Height function
Opt. procedure
• Adjoint-based
• Derivative-free
Optimization framework

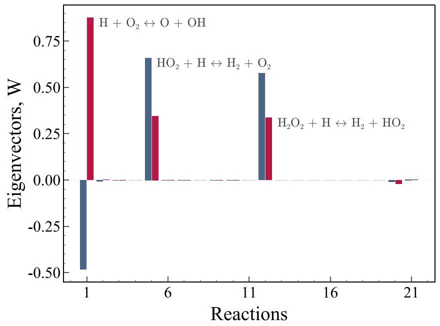
Dedicated methods



Model design



ROM



UQ

- Model design
- Model order reduction
- Multi-query application :
  - Optimisation
  - Data assimilation
  - Uncertainty quantification

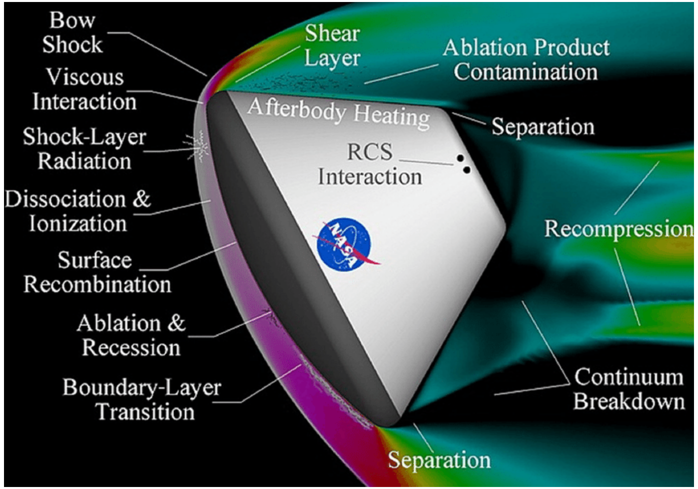
Reentry

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

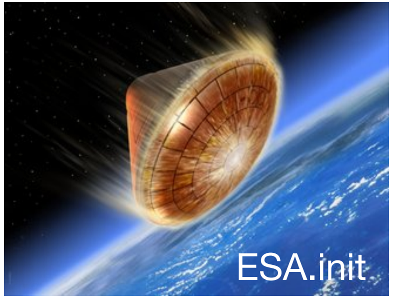
→ **Flow**

Due to high-speeds reactions are in non-equilibrium

What is the impact of chemistry on the flow dynamics?



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



Physicochemical modeling of reactive flow

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

Compressible Navier-Stokes

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

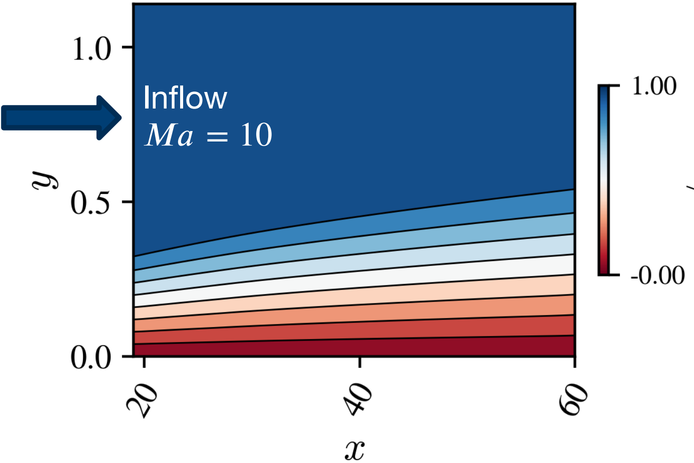
Reactions

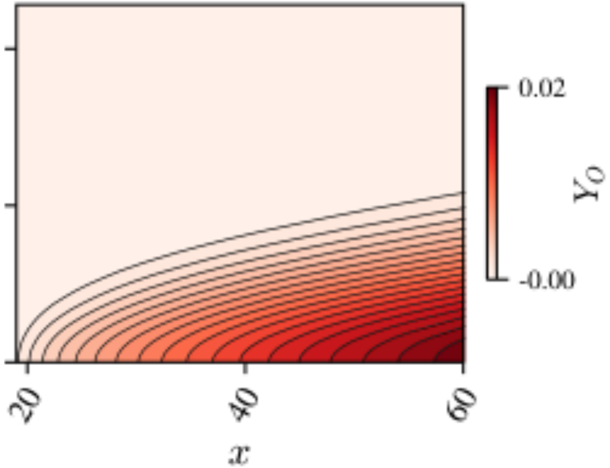
Species diffusion

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

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

+diffusive

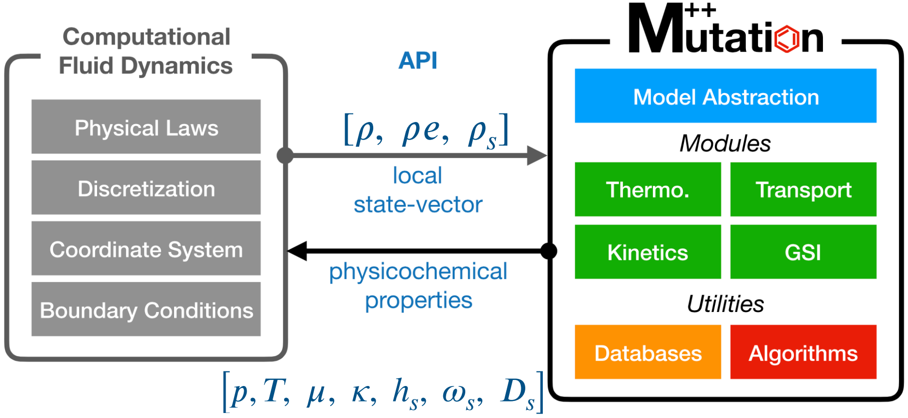


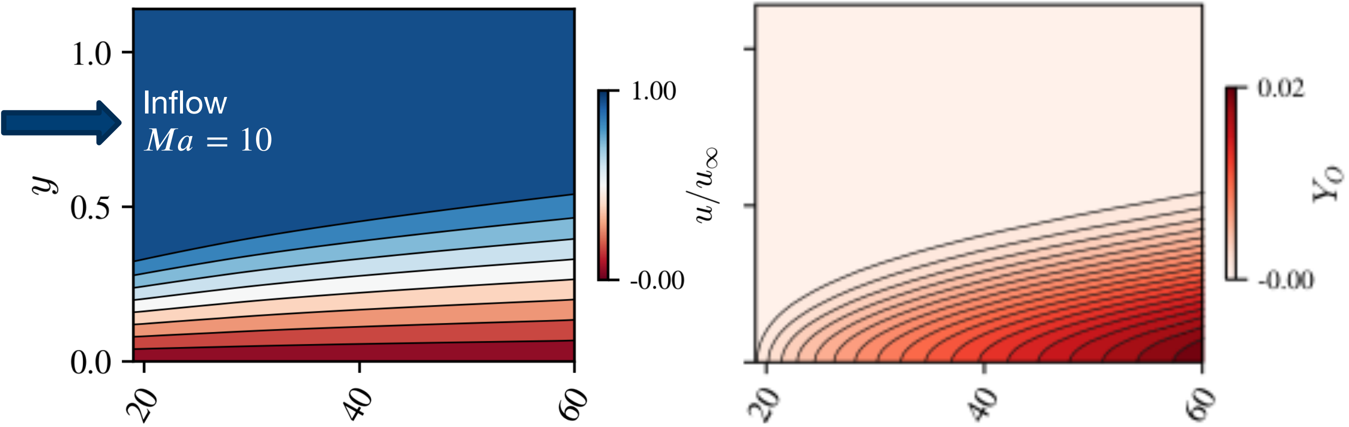


How to evaluate local thermodynamic quantities?

Thermodynamic – transport – kinetics need to be modelled accurately

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

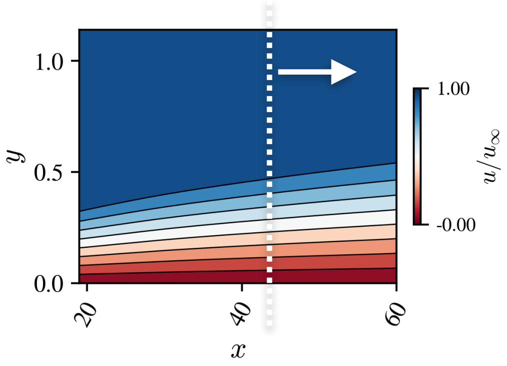


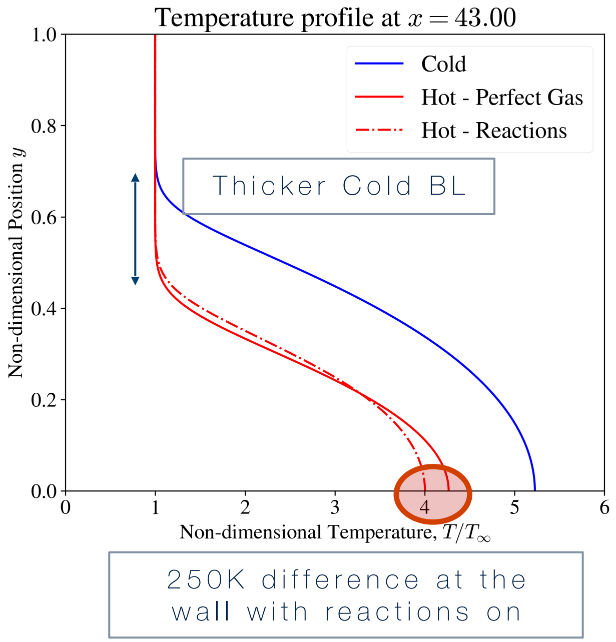


[4] - Scoggins, J. B., Leroy, V., Bellas-Chatzigeorgis, G., Dias, B., & Magin, T. E. (2020). Mutation++: Multicomponent thermodynamic and transport properties for ionized gases in C++. SoftwareX, 12, 100575.

Influence of finite-rate chemistry

- 2D preliminary setup
  - Hot : $T_\infty = 947K$
  - Cold : $T_\infty = 62.5K$





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

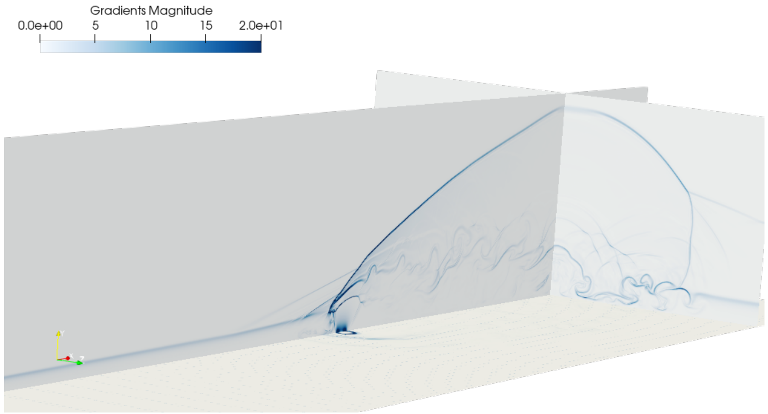
[1] - Candler, G. V. (2019). *Annual Review of Fluid Mechanics*, *51*, 379-402.
[2] – Di Renzo, M., & Urzay, J. (2021). *JFM*, *912*.
[3] – Marxen, O., Iaccarino, G., & Magin, T. E. (2014). *JFM*, *755*, 35-49.

Application of interest: JICF

- Conditions from Erdem [4] experimental test campaign

	Cold case
Mach number	5
Reynolds number	26,200
Free-stream temperature	62.5 K
Free stream pressure	1210 Pa
Wall temperature	5.22 - quasi adiabatic
Jet Mach number	1
Jet Temperature ratio	4
Jet Pressure ratio	29
Jet Momentum ratio	1.16

- Domain and grid

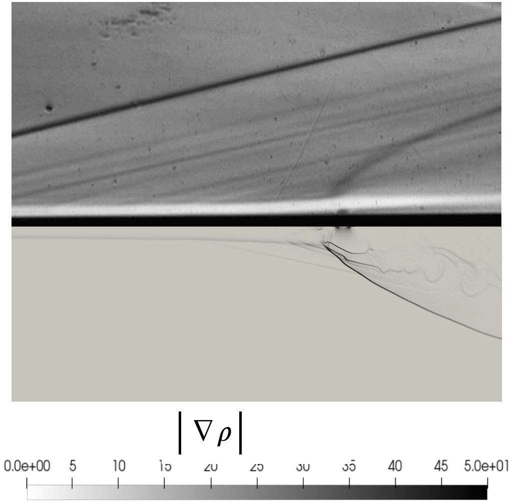


	+ units	N
X	14	2132
Y	1	697
Z	14	1024
Total	-	1.5×10^9

[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.

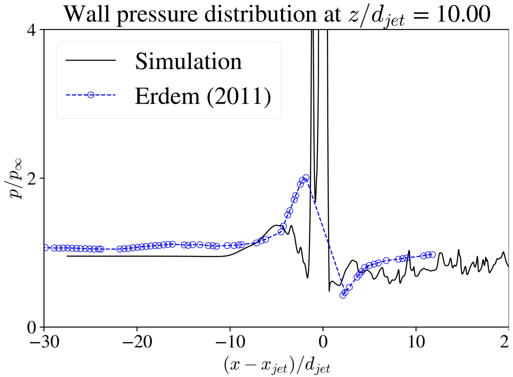
Validation – Comparison with experiment

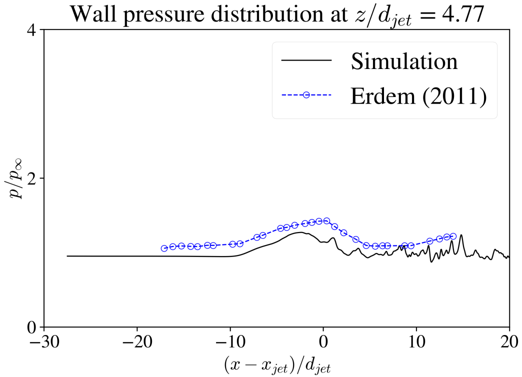
- Qualitative
  - ➢ Very good agreement in shock location and separation length
- Pressure distribution on the wall
  - ➢ Trend and values match closely experimental data



Experimental Schlieren

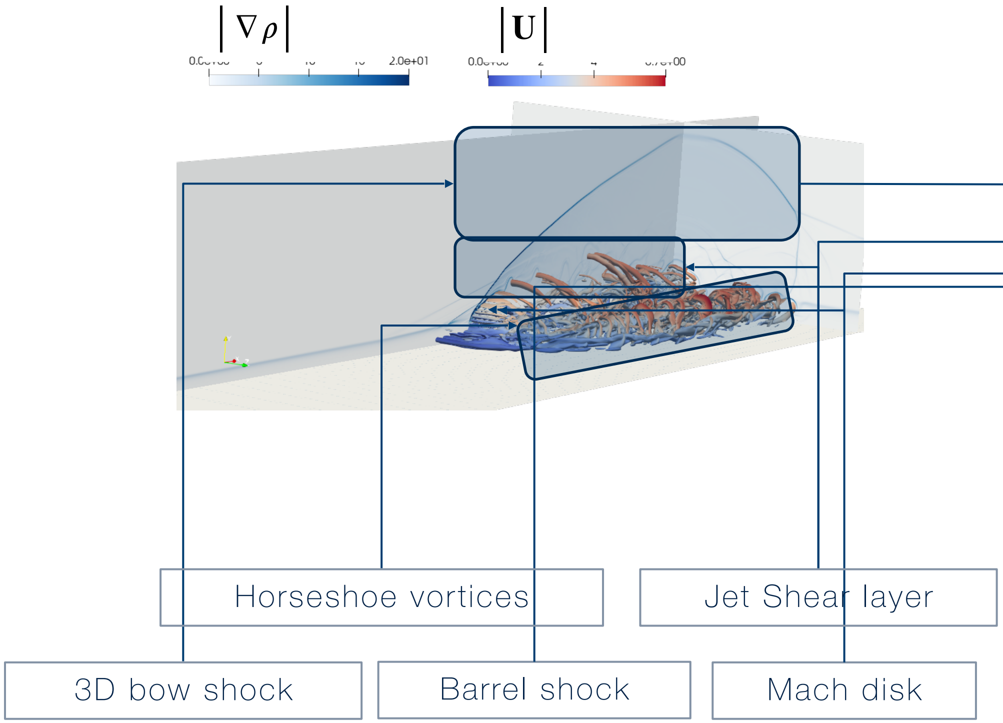
Numerical Schlieren



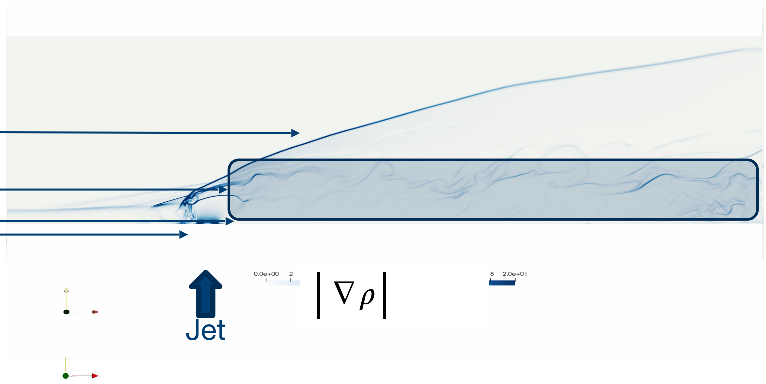


Flow features

- 3D flowfield



- Dynamics $St = \frac{fd_j}{u_\infty}$

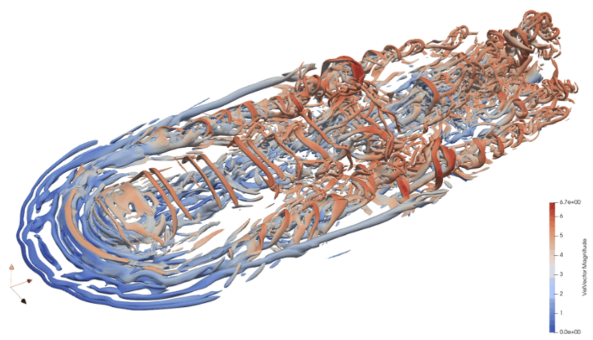


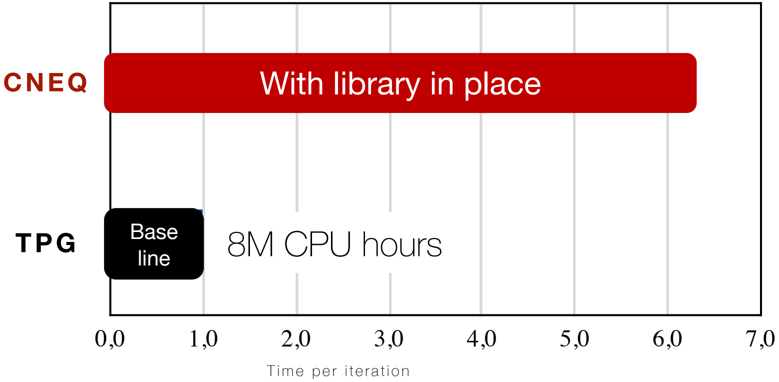
  - Unsteadiness of shock structure coupled with shear layer at $St \approx 0.6$
  - Horseshoe vortices at $St \approx 1.3$

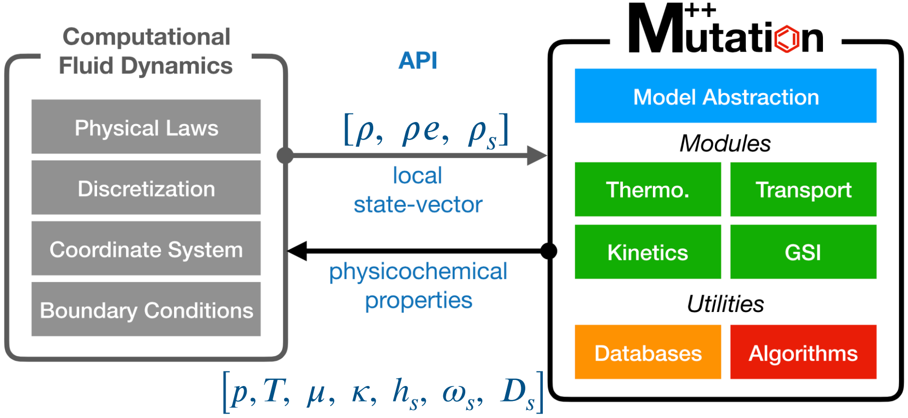
➢ Good agreement with available literature [5,6,7]

[5] – Kawai, S., & Lele, S. K. (2010). Large-eddy simulation of jet mixing in supersonic crossflows. *AIAA journal*, *48*(9), 2063-2083.
[6] – Miller, W. A., Medwell, P. R., Doolan, C. J., & Kim, M. (2018). Transient interaction between a reaction control jet and a hypersonic crossflow. *Physics of Fluids*, *30*(4), 046102
[7] – Chai, X., Iyer, P. S., & Mahesh, K. (2015). Numerical study of high speed jets in crossflow. *Journal of Fluid Mechanics*, *785*, 152-188.

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

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

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

Incl. diffusive

& state equations and properties

Models

Turbulence

Chemistry

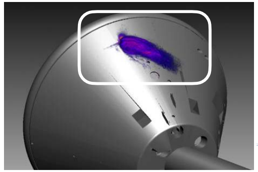
Post-analysis

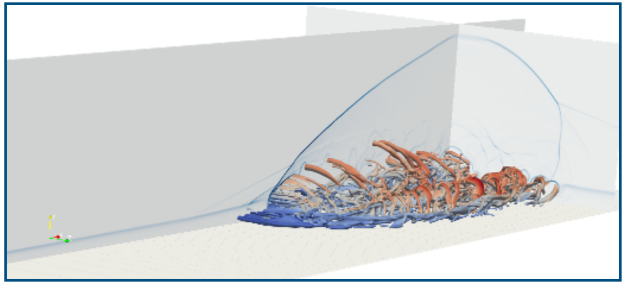
Extracting dynamics

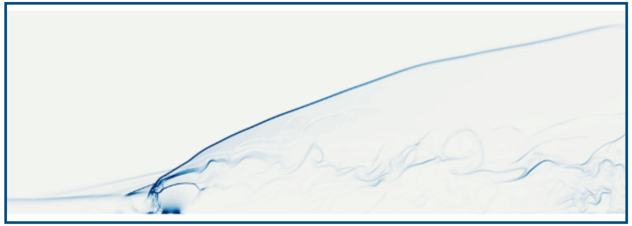
Reduced-order Models

Control

Ivey et al. 2011







Governing equations

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Diffusion

Reactions

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& state equations and properties

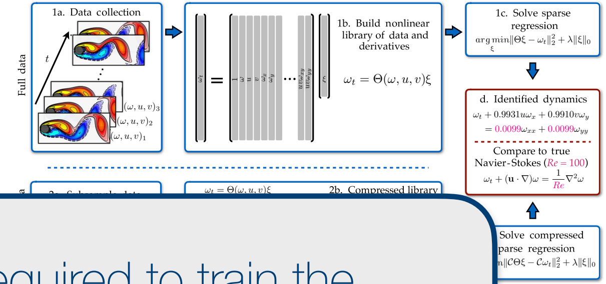
Models

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]



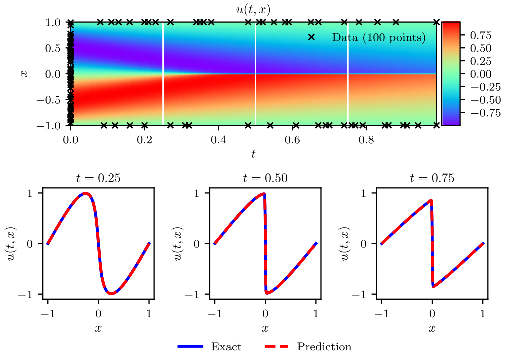
Bottleneck: large amount of data required to train the models for *multi-scale multi-physics* problems!

...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

Post-analysis

Control

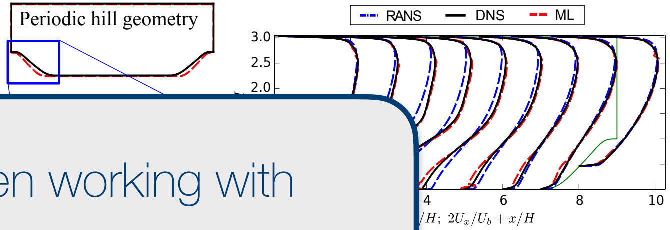
Extracting dynamics

Reduced-order Models

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

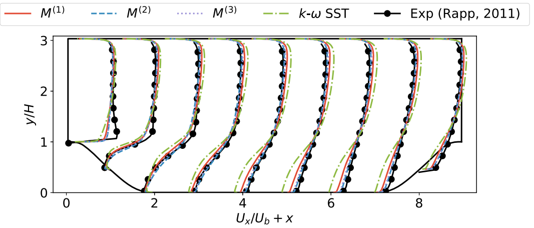
Turbulence Modeling in the Age of Data

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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Diffusion — Reactions — Incl. diffusive

& state equations and properties

Models

Improve Speed, while keeping accuracy

Turbulence

Chemistry

Post-analysis

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Reduced-order Models

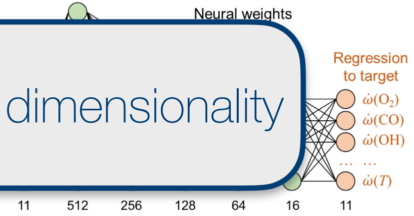
Control

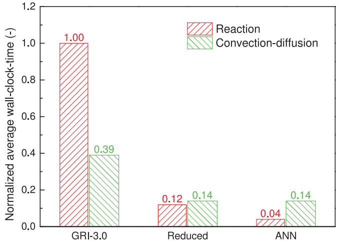
Bottleneck: Curse of dimensionality

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*

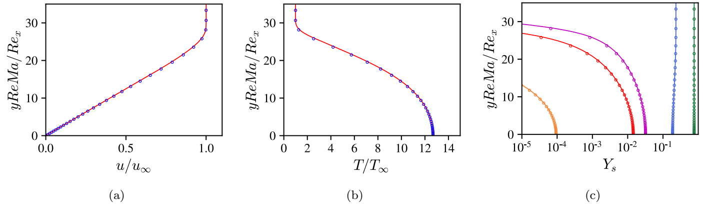


FIG. 15. Comparison of profiles of (a) streamwise velocity, (b) temperature, (c) species mass fractions from left to to right N, NO, O, O_2 and N_2 at $Re_x = 2000$. Solid line and symbols correspond to the solution obtained using Mutation++ and the data-driven model, respectively.

Governing equations

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& state equations and properties

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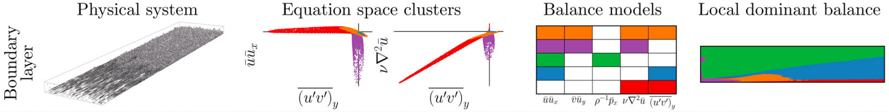
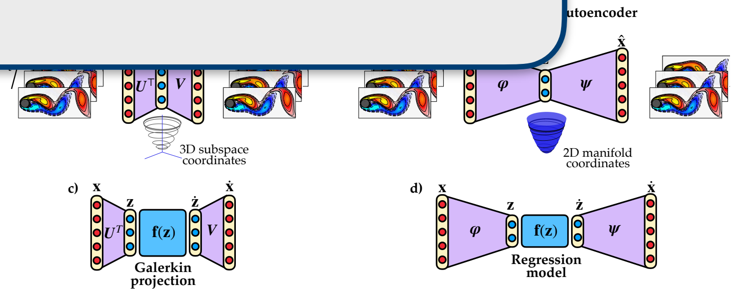
Learning dominant physical processes with data-driven balance models

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*



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

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

Governing equations

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

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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]

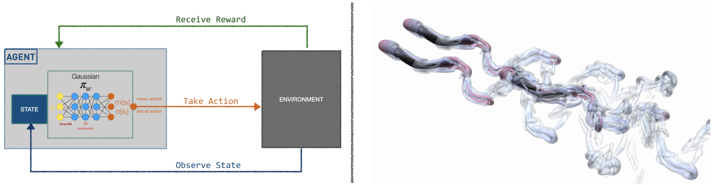


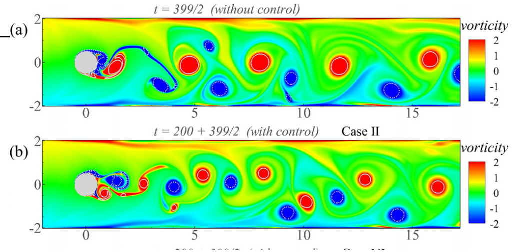
Figure 8

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

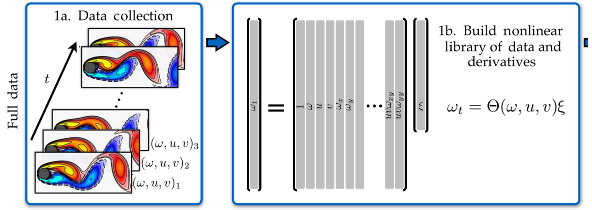


Supervised Learning

Find a mapping from X —> Y

Regression
- Decision trees
- Random forests
- Neural Networks

Classification
- Linear
- Generalised linear
- Gaussian process



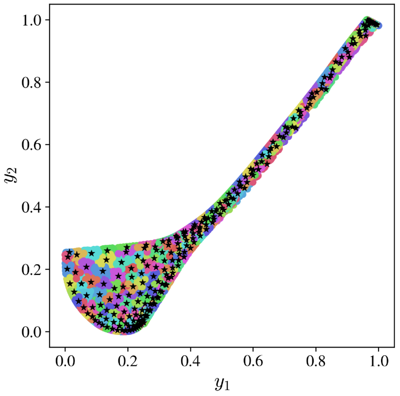
Samuel H. Rudy,[1]* Steven L. Brunton,[2] Joshua L. Proctor,[3] J. Nathan Kutz[1]

Unsupervised Learning

Learning Structure from data : X

Clustering
- K-means
- Spectral clustering

Dimensionality Reduction
- PCA
- Auto-encoders
- Diffusion maps

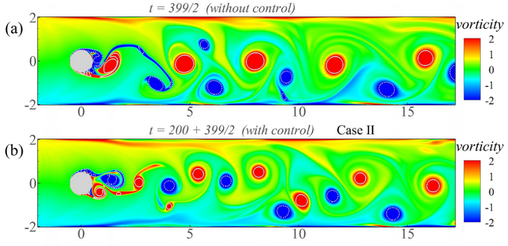


Semi-supervised Learning

State + action

Reinforcement Learning
- Markov decision process
- Deep RL

Generative Models
- Generative adversarial networks (GANs)

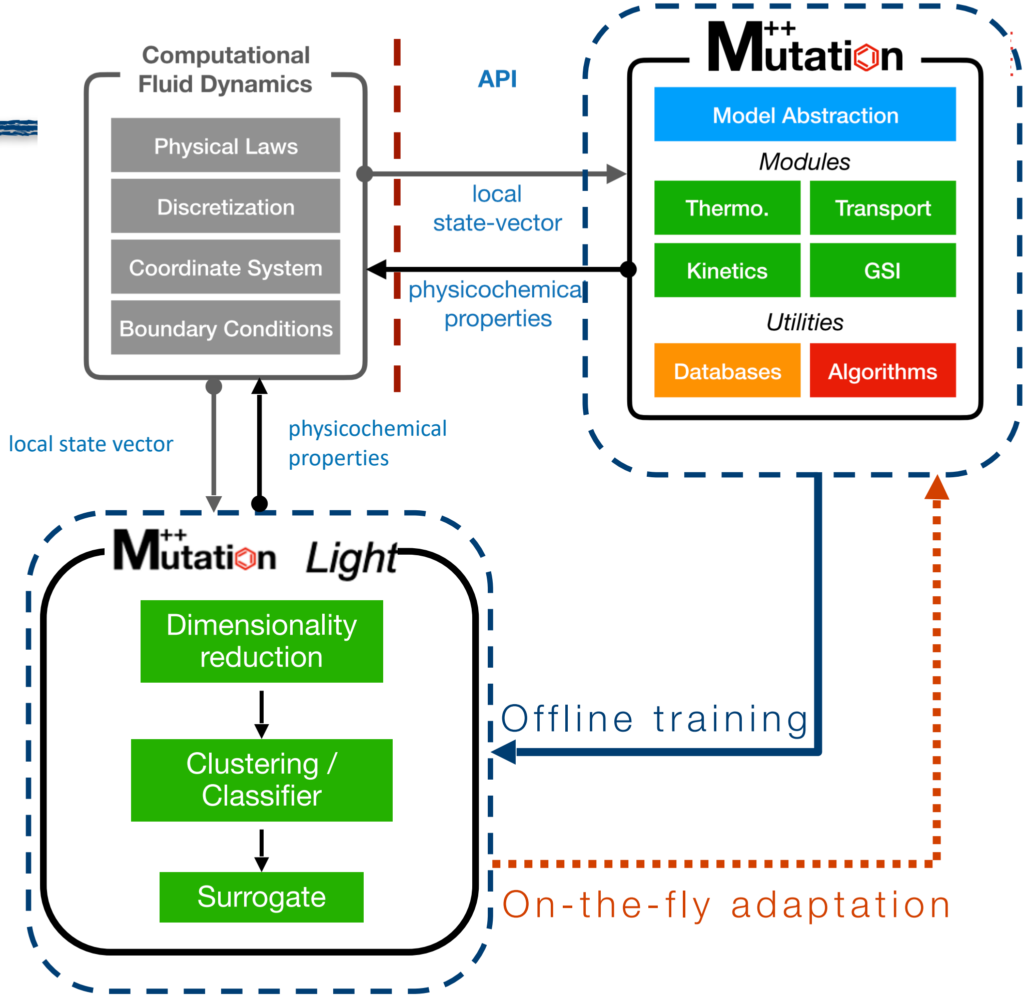


Proposed approach

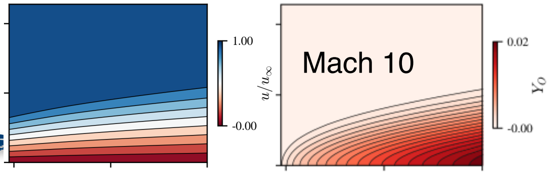
- Flows have history: most thermodynamic states have been seen previously
- Thermodynamic states are constrained to a low-dimensional manifold due to hydrodynamic

➢ Learn thermo-chemical model "**on the fly**"

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



Mutation++: Input/Output



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

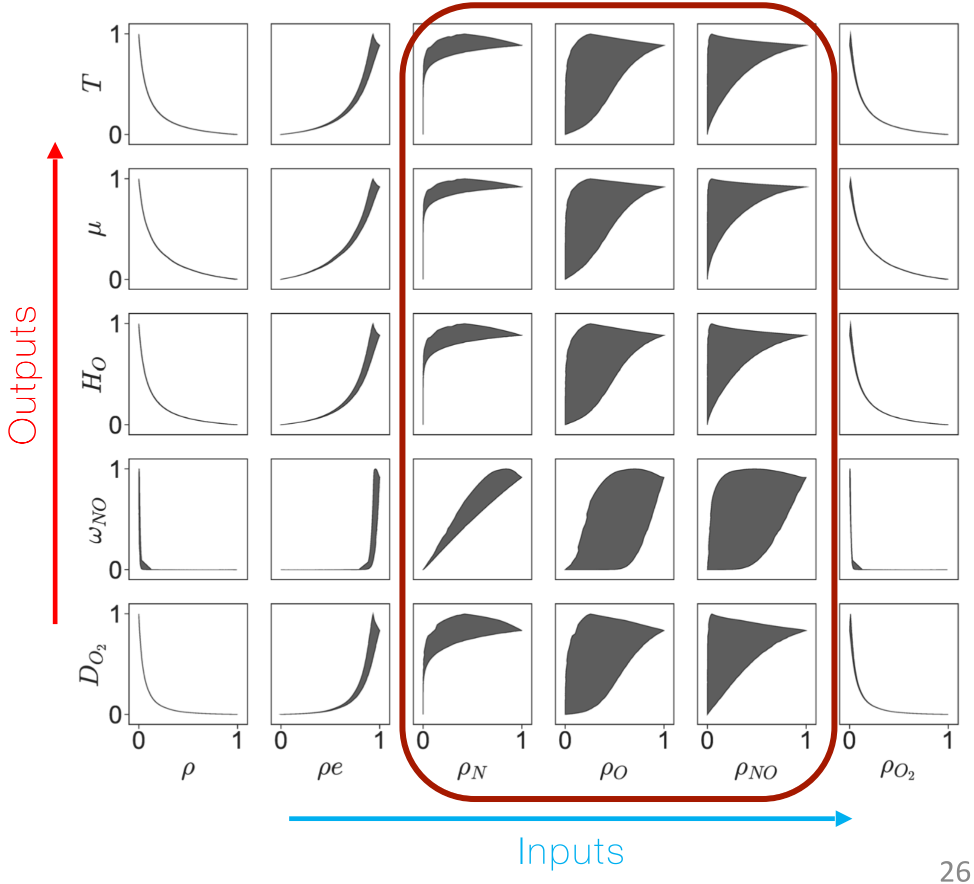
$$\boldsymbol{X} = [\rho,\ \rho e,\ \rho_s] \in \mathbb{R}^{N \times D}$$

- Output: thermochemical properties

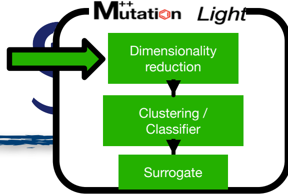
$$\mathbf{Z} = [p, T,\ \mu,\ \kappa,\ h_s,\ \omega_s,\ D_s] \in \mathbb{R}^{N \times D_Z}$$

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

Active subspaces —> Dimensionality reduction

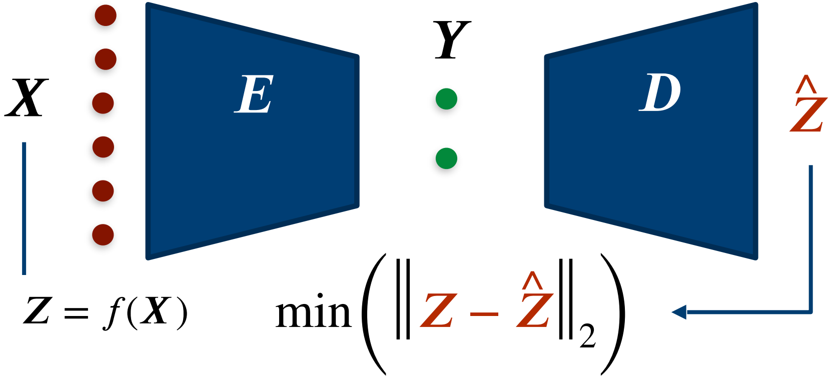


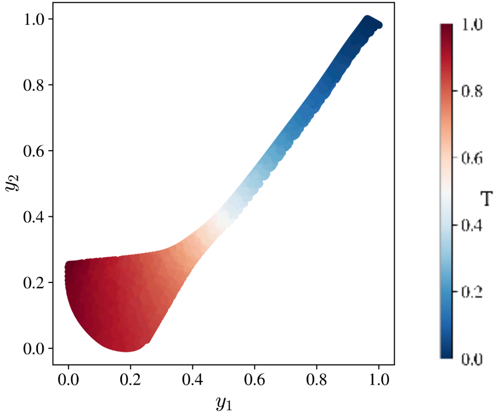
Dimensionality Reduction $\mathbb{R}^6 \rightarrow \mathbb{R}^2$



Nonlinear dimensionality reduction:

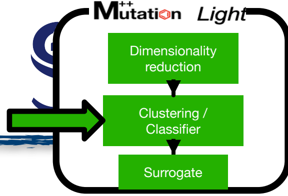
- IO - autoencoder





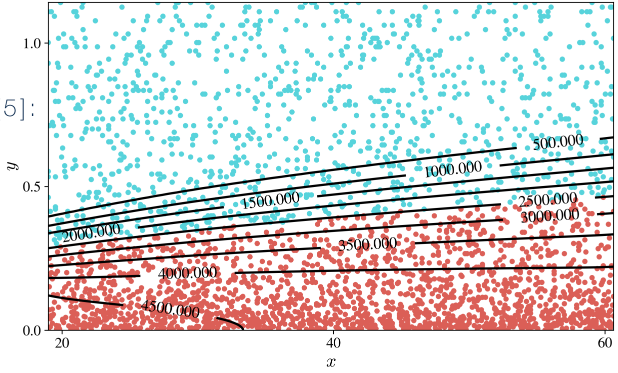
➢ IO-E finds a latent space that best accounts for the variation of the outputs w.r.t the inputs

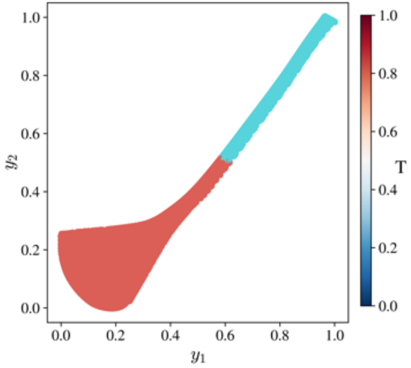
Clustering



- Outputs have different dynamics depending on their location in the flow
- ➢ Notion of clusters

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





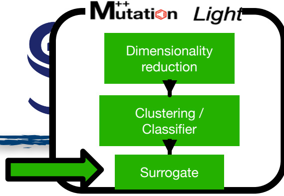
- ➢ Clusters represent regions at different level of thermochemical equilibrium
  - – Freestream : Cold, frozen chemistry
  - – Near wall : Hot, finite-rate chemistry

- 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

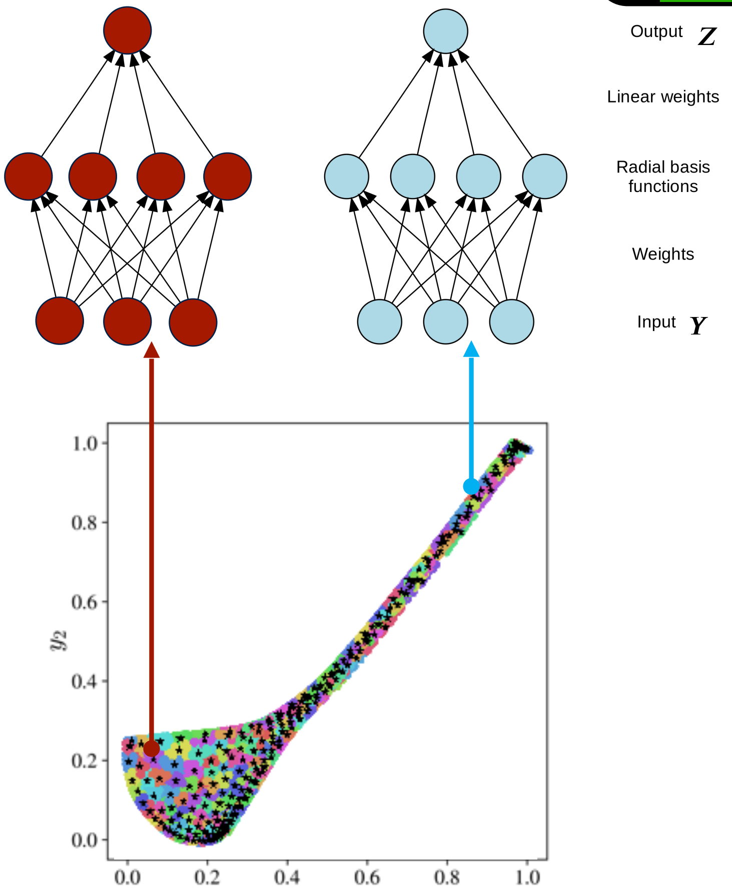


- A surrogate surface (in the reduced space) is build for each cluster C_k using RBFNN

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

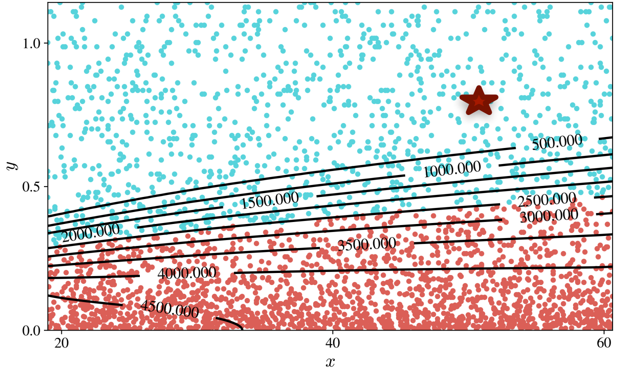
$$z = g_{C_k}(y) = \sum_{i=1}^{N_R} a_i \phi\left(\|y - c_i\|\right)$$

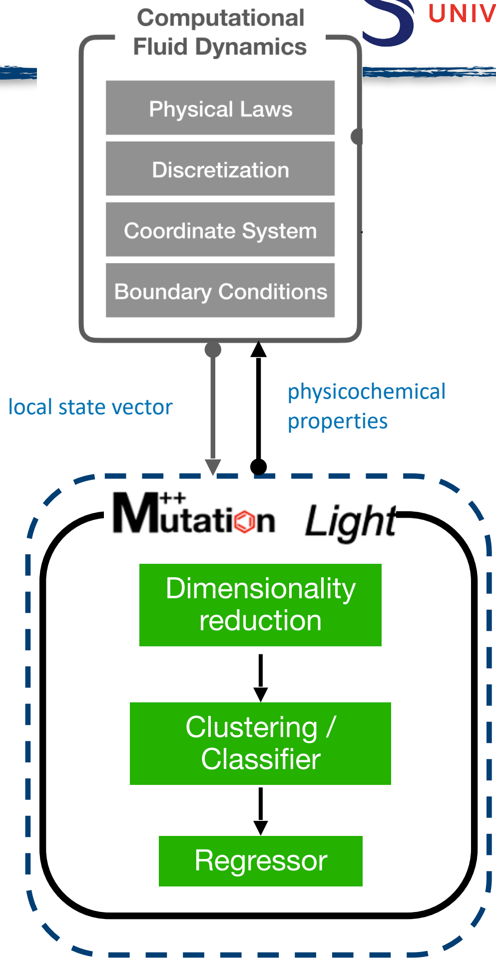
- The N_R centers are determined with k-means of the input/output pairs
  - ➢ avoid overfitting



Coupling with CFD solver

- New local state vector $\boldsymbol{X}^t$ are sent to the model





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Coupling with CFD solver

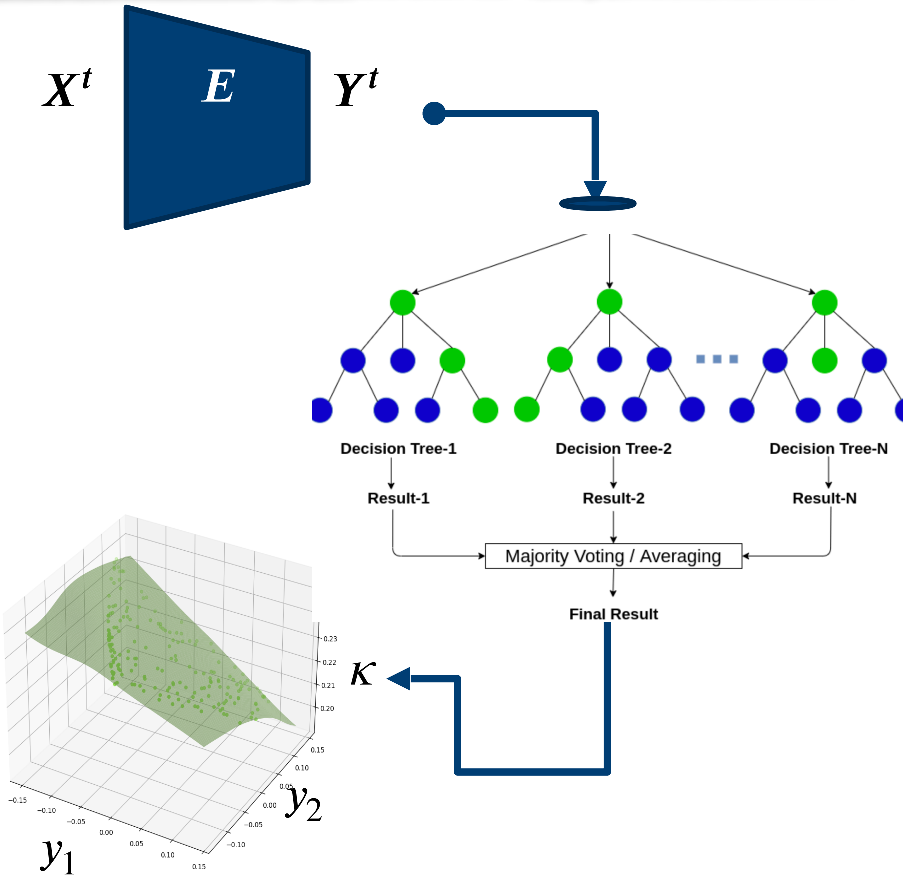
- New local state vector $\boldsymbol{X}^t$ are sent to the model

1. Encoding of new points $\boldsymbol{Y}^t = \boldsymbol{E}(\boldsymbol{X}^t)$

2. Random-forest classifies new points

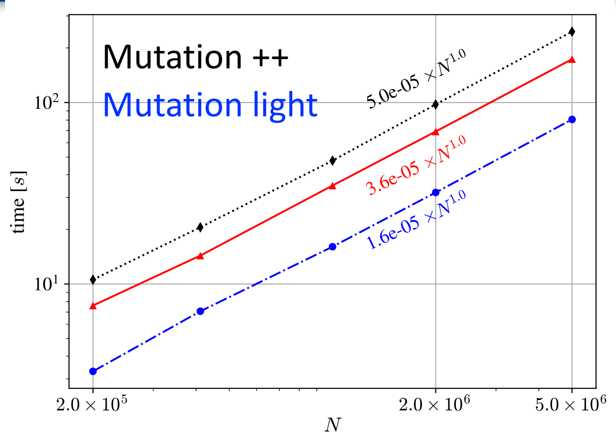
$$C^t = [1,1,2,1\ldots2]$$

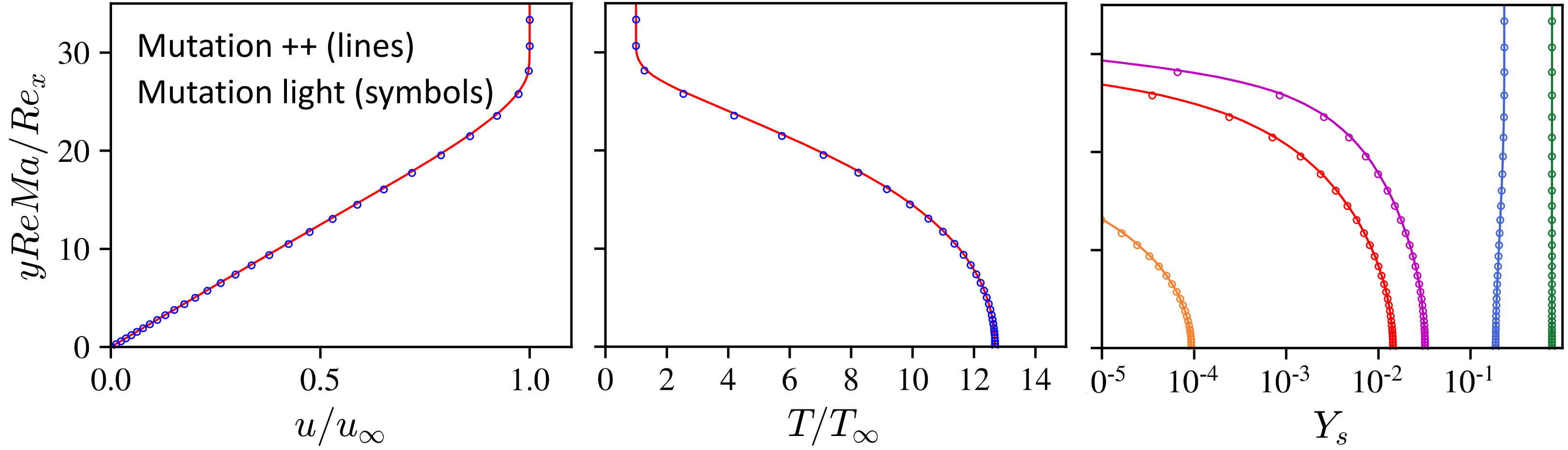
3. Call the corresponding surrogate
4. Send back physicochemical properties to solver



Model stability/performance

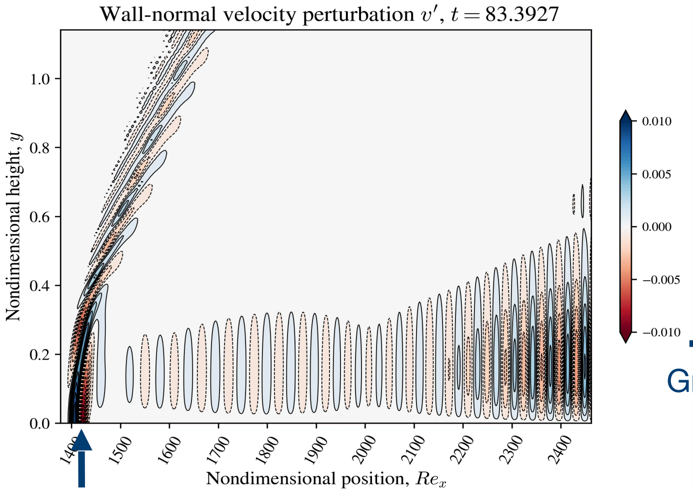
- The model replace M++ in the flow solver (closed-loop prediction), starting from the converged solution of case A
  - ➢ Solution remains stable after 2 flow-through time
  - ➢ Overall accuracy of the solution is maintained
  - ➢ Model is 70% faster





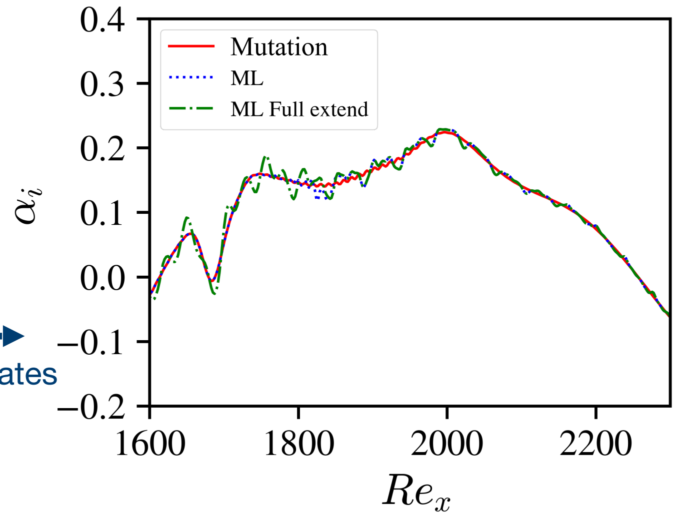
Unsteady flows

- Mach 10 boundary layer
- Small amplitude perturbations



Blowing & suction strip

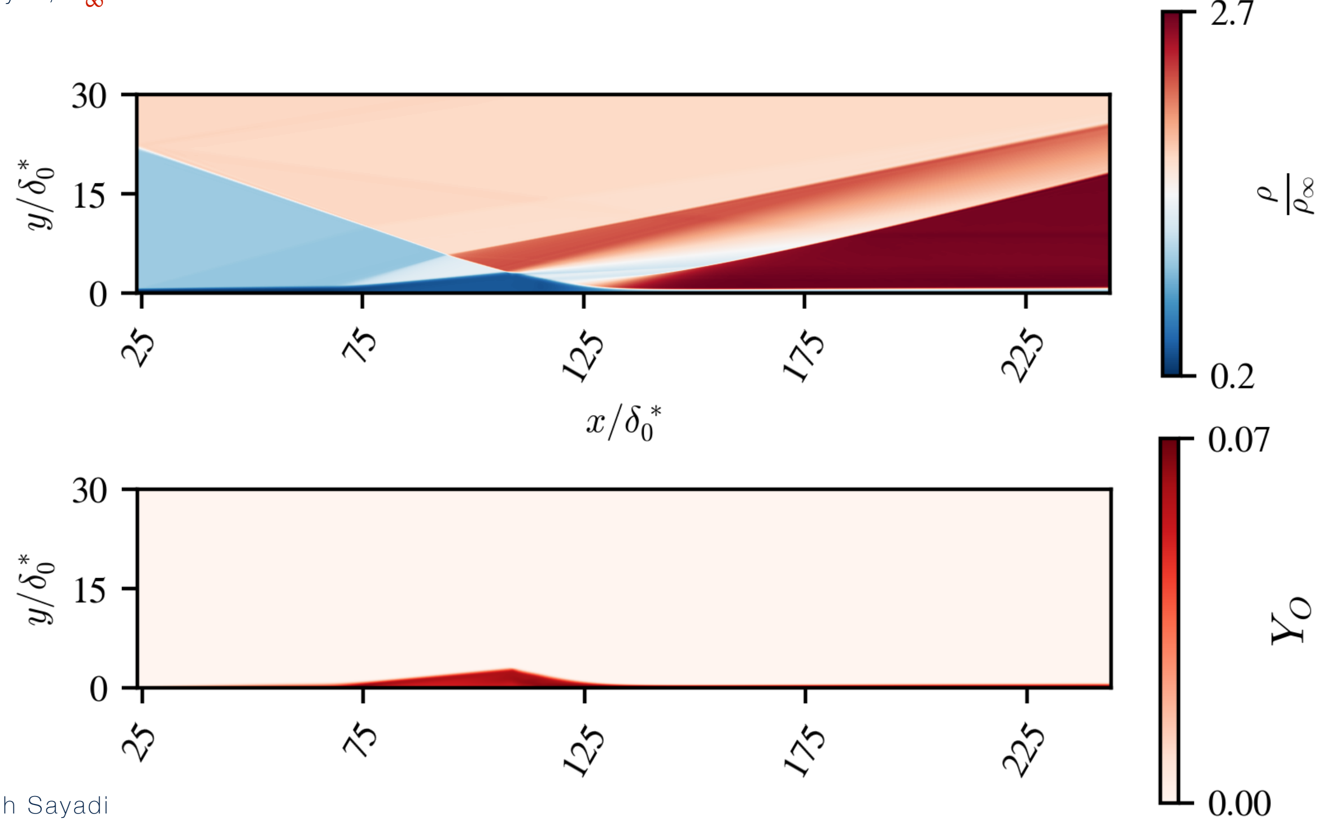
Growth rates



$Ma = 5.92$ SBLI

Problem setup

- Mach 5.92 adiabatic boundary layer, $T_\infty = 1100K$
- 13° Oblique shock impinging
- Air-5 $S = \{O_2, N_2, NO, N, O\}$

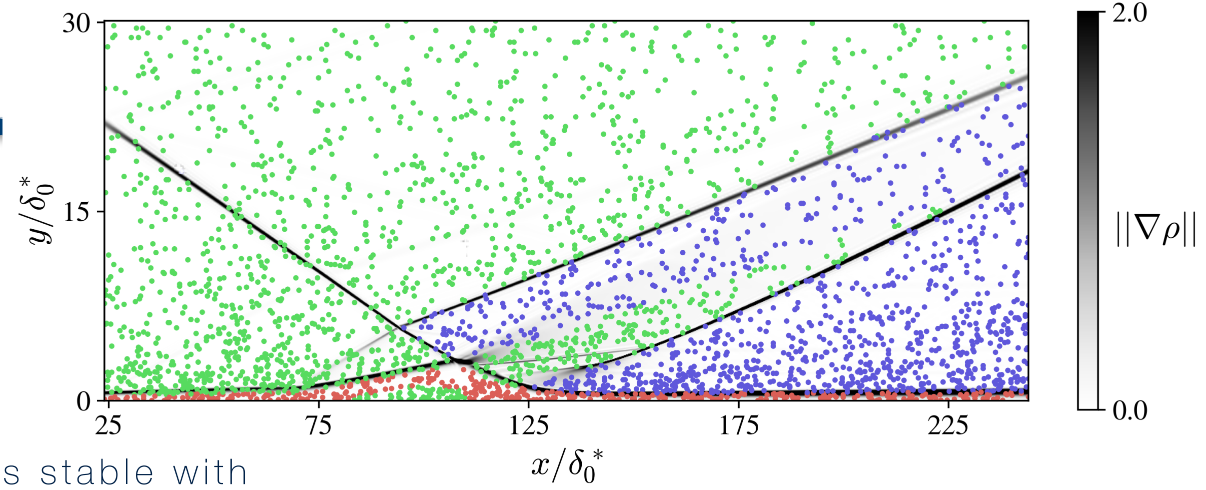


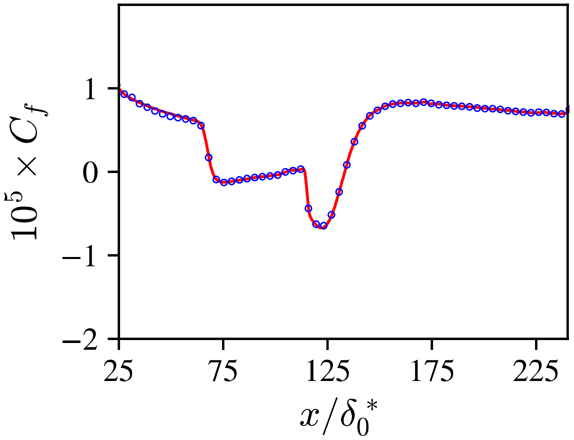
$Ma = 5.92$ SBLI

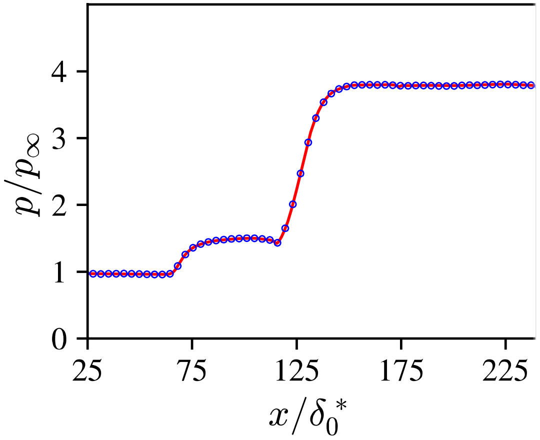
- Application of the algorithm:
  - $d = 3$
  - $N_c = 3$
  - $N_R = 250$

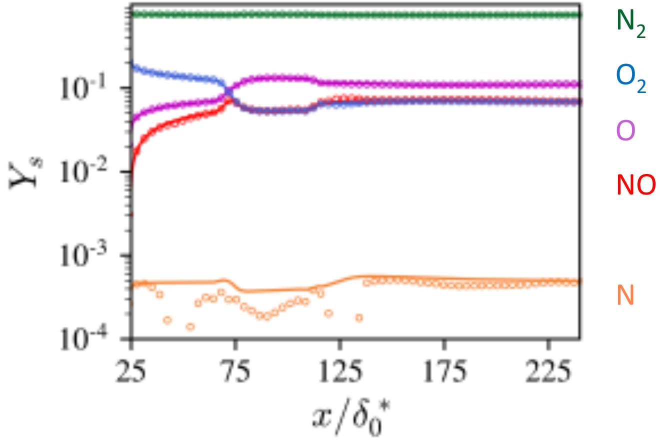
➢ Cluster are aligned with flow features

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









Conclusion

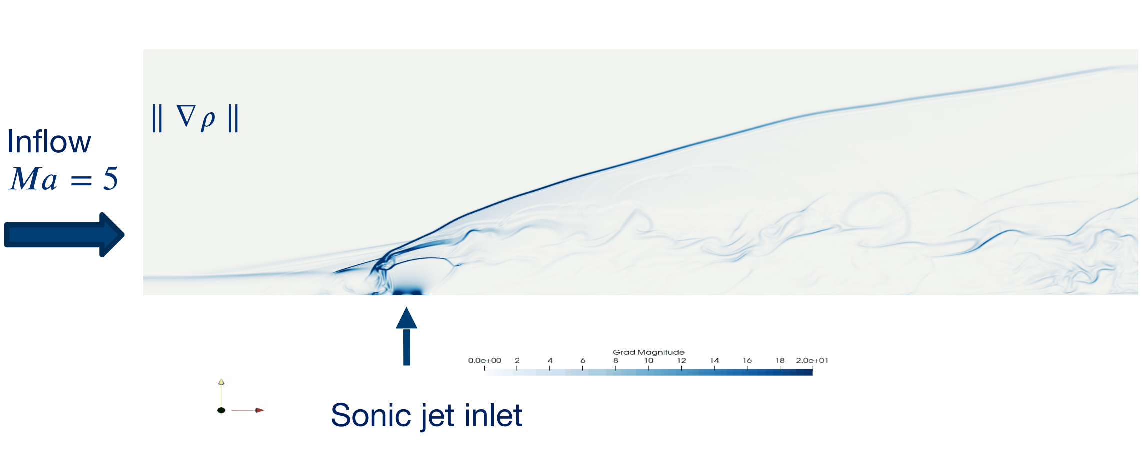
- A novel method for self-learning of reduced look-up table using nonlinear model-reduction, community clustering and surrogate response surfaces

- 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

- Optimize 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

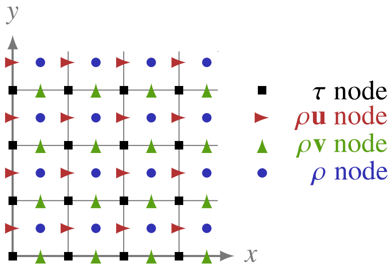


Thank you for your attention !

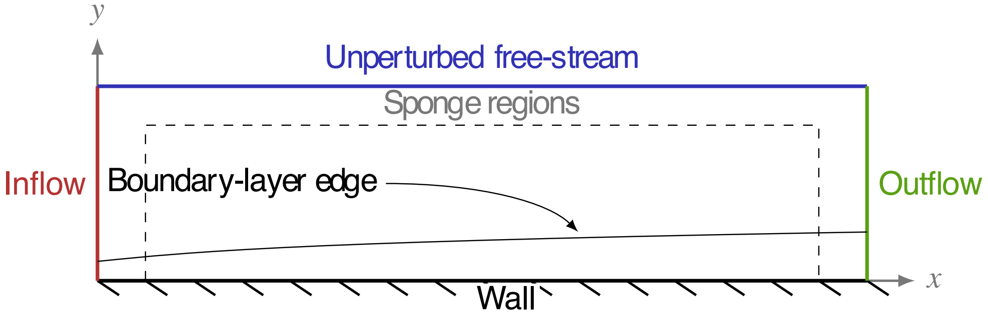
Computational tools

A high-order finite-difference DNS code for boundary layers (and more)

- Fortran-90 compressible Navier-Stokes DNS/LES solver[1]
  - Compact 4th/6th order finite-difference scheme
  - Explicit 3rd/4th order Runge-Kutta time integration
  - Staggered grid
  - Curvilinear coordinates
  - Boundary-layer setup: no-slip non-catalytic wall (also forcing, jet)



- Mutation++ library[2]
  - Thermodynamics
  - Kinetics
  - Transport

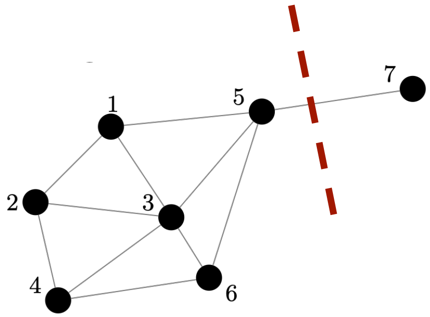


- Artificial-diffusion shock-capturing model[3]

[1] Nagarajan et al., JCP 191 (2003)
[2] Scoggins et al., SoftwareX 12 (2020)
[3] Kawai et al., JCP 229 (2010)

Newman algorithm

- Network: comprised of nodes, edges and weights



- Adjacency matrix

$$\mathbf{A}_{ij} = \begin{cases} 1, & \textbf{if there is an edge } \textit{from i to j} \\ 0, & \textbf{otherwise} \end{cases}$$

A

0	1	1	0	1	0	0
1	0	1	1	0	0	0
1	1	0	1	1	1	0
0	1	1	0	0	1	0
1	0	1	0	0	1	1
0	0	1	1	1	0	0
0	0	0	0	1	0	0

- Modularity: fraction of edges between communities – expected fraction of such edges

$$Q = \frac{1}{m} \sum_{ij} \left[A_{ij} - \frac{k_i k_j}{m} \right] s_i s_j$$

- Define $\mathbf{s} \rightarrow s_i = +1, -1$

$$Q = \frac{1}{4m} \mathbf{s}^T \mathbf{B} \mathbf{s}$$

- Spectral optimization of Q
  - Find **s** that maximises *Q* for a given **B**

$$Q = \sum_i a_i \mathbf{v}_i^T \mathbf{B} \sum_j a_j \mathbf{v}_j = \sum_i \beta_i (\mathbf{v}_i^T \cdot \mathbf{s})^2$$

β eigenvalues, $\mathbf{v}$ eigenvector } $\mathbf{B}$

Q is maximised when $\mathbf{s} \parallel \mathbf{v}_1 : \; \mathbf{s} \cdot \mathbf{v}_1 = 1$

- Fine-tuning: moving vertices between communities to increase the modularity
- If more than 2 communities: **Repeated bisection**