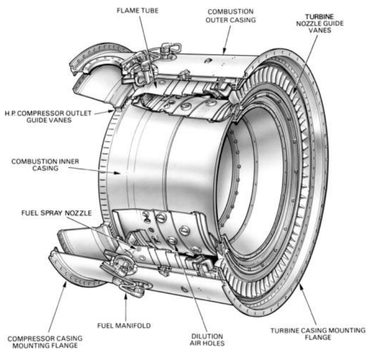
Machine Learning-based Approaches for the Control of Reacting Flows

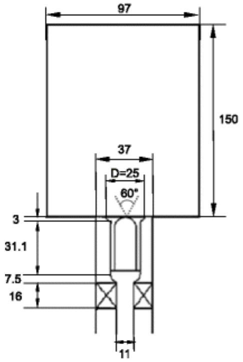
Anh Khoa Doan
Department of Aeronautics
Imperial College London
n.doan@imperial.ac.uk

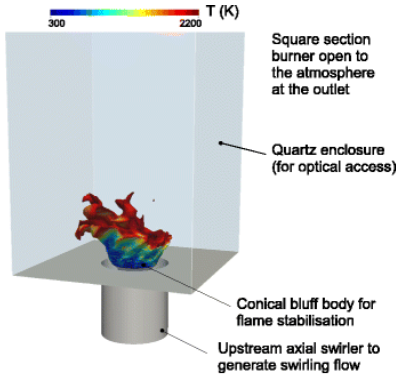
IMPERIAL

Performance and stability of combustor generally guaranteed by *design*

- Geometry and fuel/air conditions: dictates steady flame topology





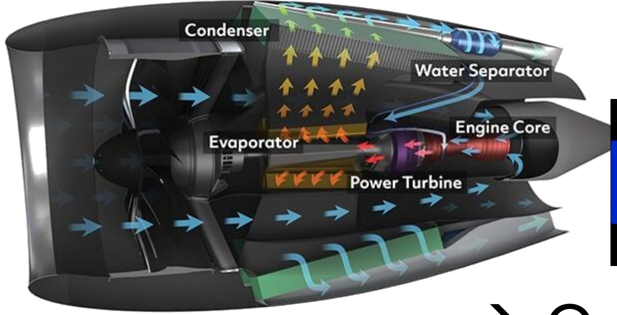


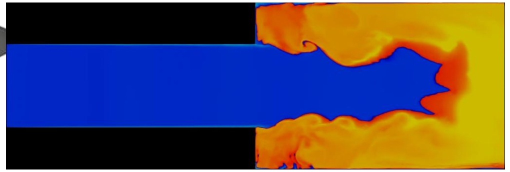
[Soares, Gas Turbines, Butterworth-Heinemann (2008)]
[Giusti et al., Flow Turbul. Combust. 97, 1165-1184 (2016)]

→Limited operations to narrow fuel/condition ranges
→Limited adaptability to out of design operations

- Recent investigations of actuation in combustors

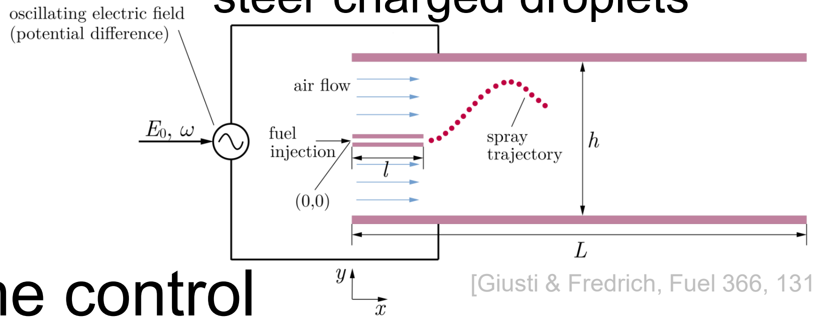
Water/steam injection for hydrogen combustion





[Pratt & Whitney HySIITE concept, RTX (2025)]

Oscillating electric field: able to steer charged droplets



[Giusti & Fredrich, Fuel 366, 131009 (2024)]

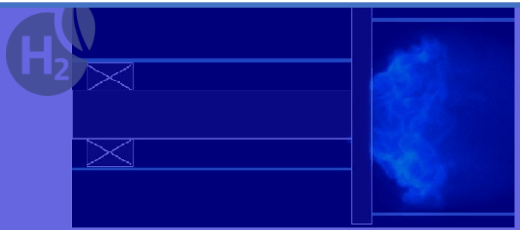
→ Opens avenue for *active* flame control

Turbulent flames are high-dimensional complex multiphysics dynamical systems

- Turbulent flames
  - Complex chaotic dynamics

Leverage developments in machine learning to develop control framework for flame control

- of



→Flashback

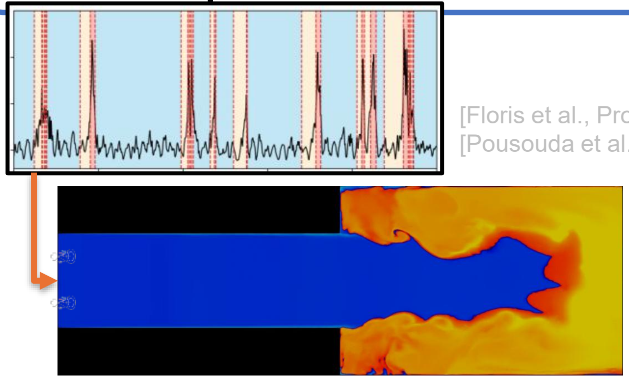
→Blow-off

[Zhang et al., Proc. Comb. Inst., 2021]

→ Limited performance of traditional control

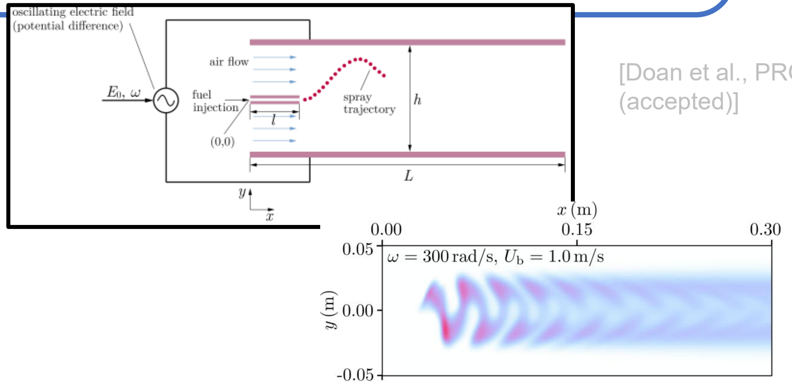
Structure of the seminar

1. Machine Learning to prevent flashback with water injection



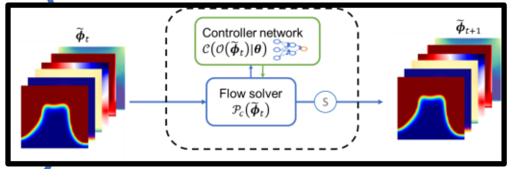
[Floris et al., Proc. Comb. Inst., 2024]
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

2. Machine Learning to control fuel mixing with electric field



[Doan et al., PROCI, 2026 (accepted)]

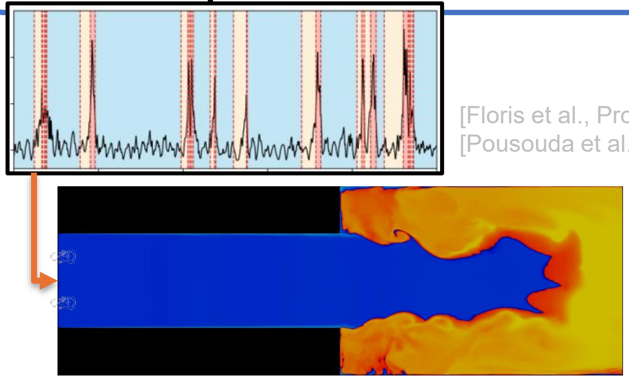
3. Towards unified control development framework with differentiable solver



[Tathawadekar et al., Data-centric Eng., 2023]
[Shehata & Doan, PRFluids, 2026 (under review)]

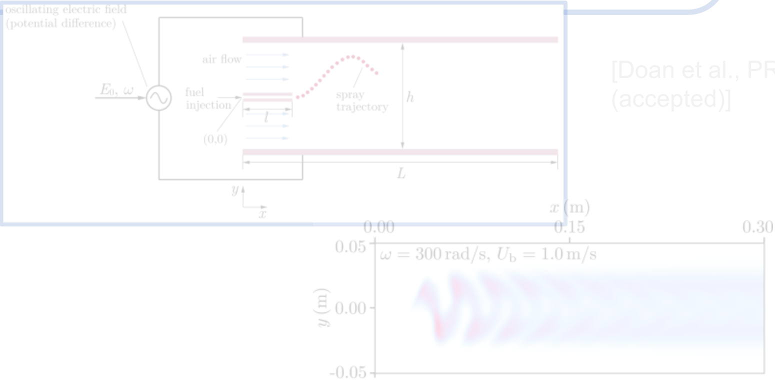
Structure of the seminar

1. Machine Learning to prevent flashback with water injection



[Floris et al., Proc. Comb. Inst., 2024]
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

2. Machine Learning to control fuel mixing with electric field



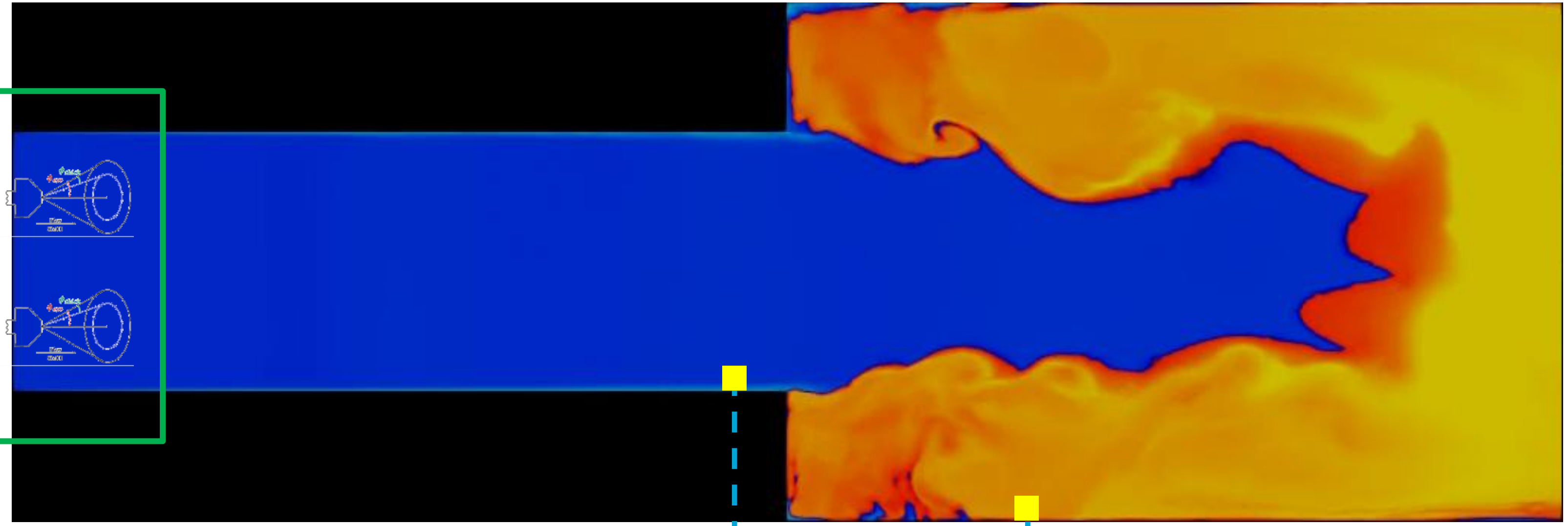
[Doan et al., PROCI, 2026 (accepted)]

3. Towards unified control development framework with differentiable solver

[Tathawadekar et al., Data-centric Eng., 2023]
[Shehata & Doan, PRFluids, 2026 (under review)]

Flashback control framework

Actuator



2. Optimal design?

Gaussian Process-based Optimization

[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

Measurements

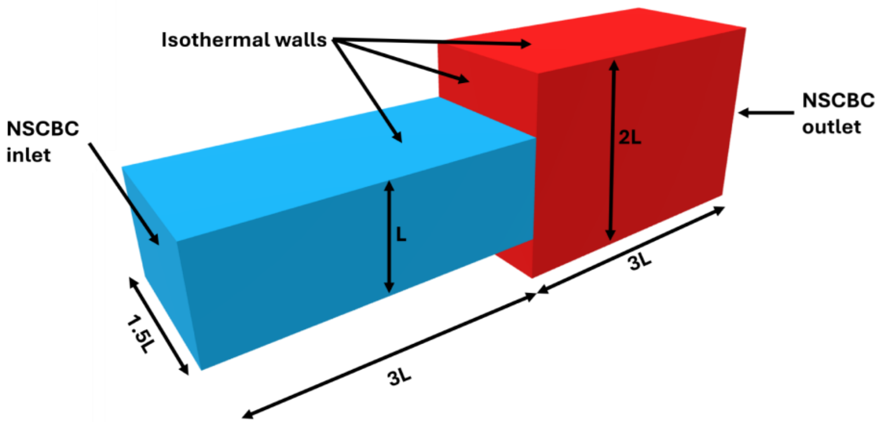
1. What to measure for flashback?

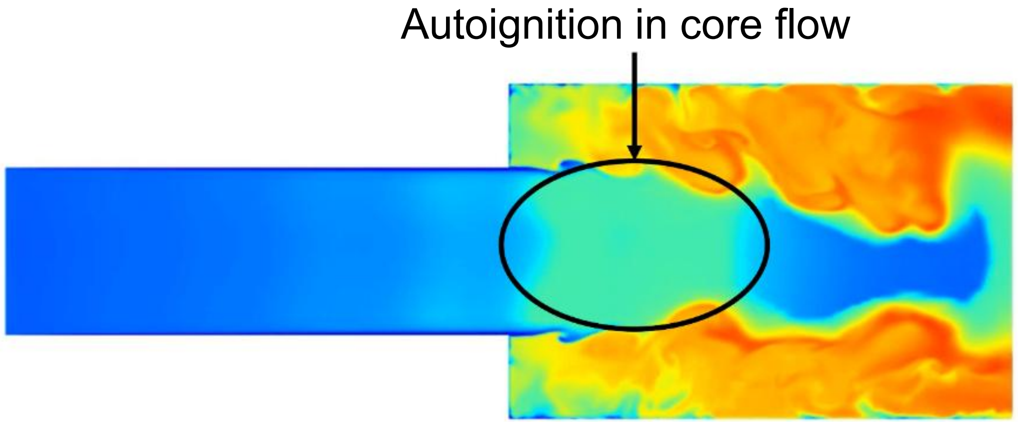
Precursor identification with dimensionality reduction and clustering

[Floris et al., Proc. Comb. Inst., 2024]

Simulation of flashback in hydrogen reheat combustor

- Simplified model of Ansaldo GT36 reheat combustor
  - Lean hydrogen/air burner with $\phi = 0.35$, $p = 20$ atm, $T_{in} = 1180$K
  - $U_{in} = 200$m/s
  - Normally stabilized by autoignition



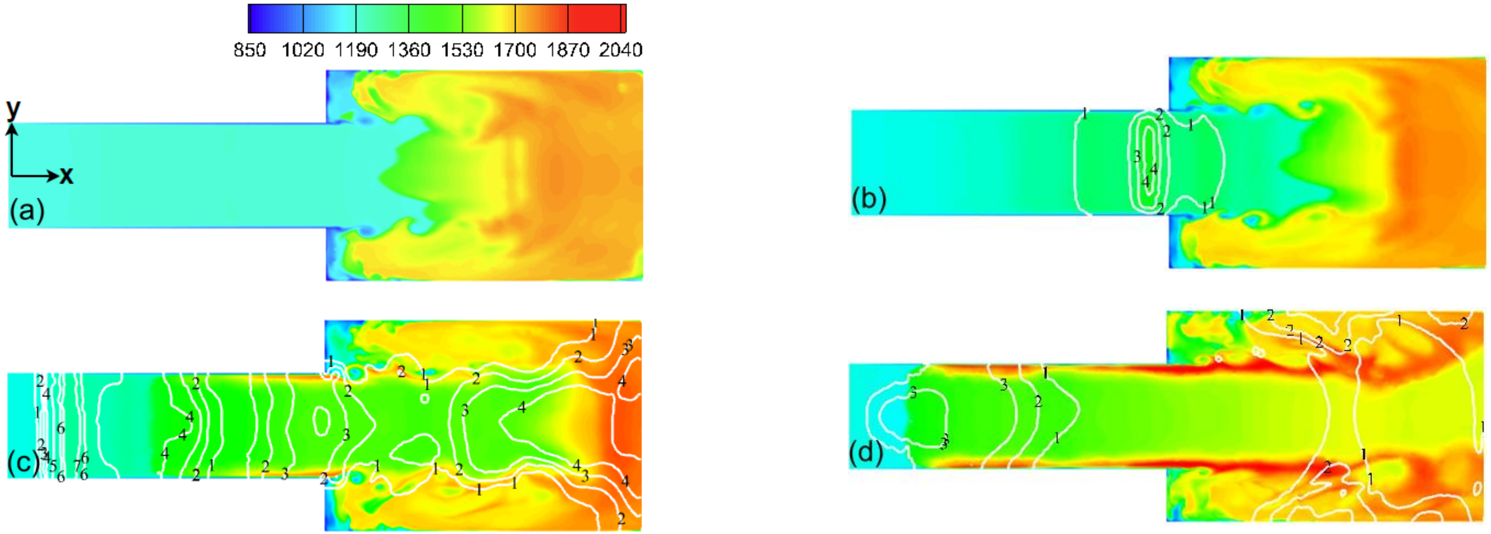


  - LES simulation – Converge CFD (thickened flame model, 11-species mechanism)
  - Total thermochemical/flow state: 17 features

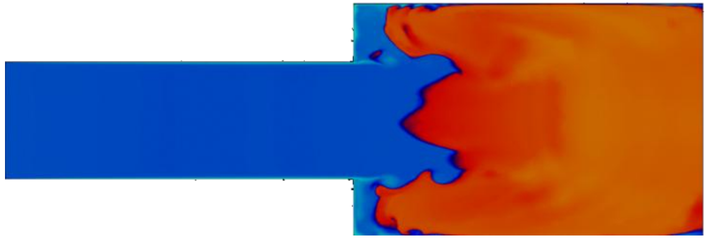
[Floris et al., Proc. Comb. Inst., 2024]

Simulation of flashback in hydrogen reheat combustor

- Shows intermittent flashback due to early autoignition



- Then the burner recovers

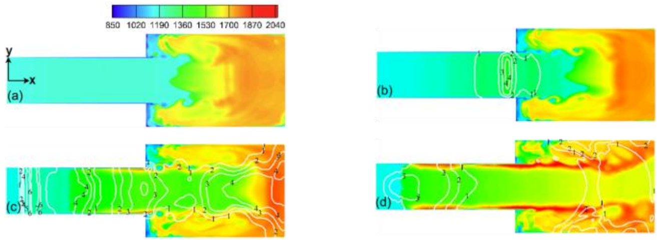


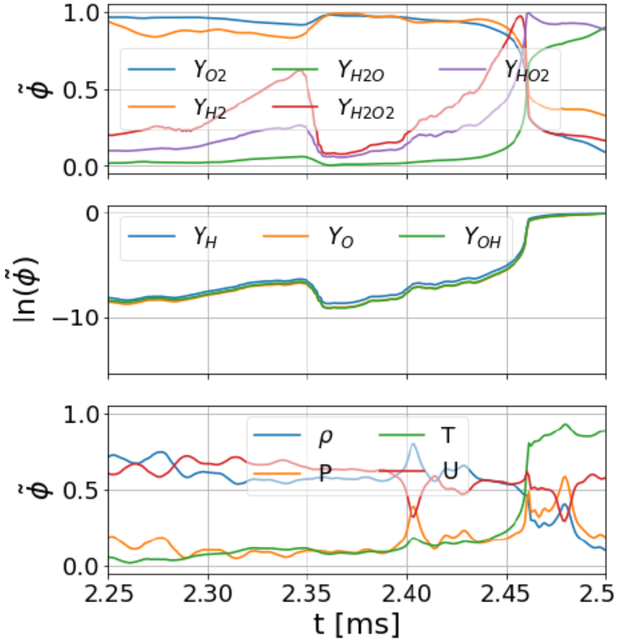
Total time series: 11 flashback events

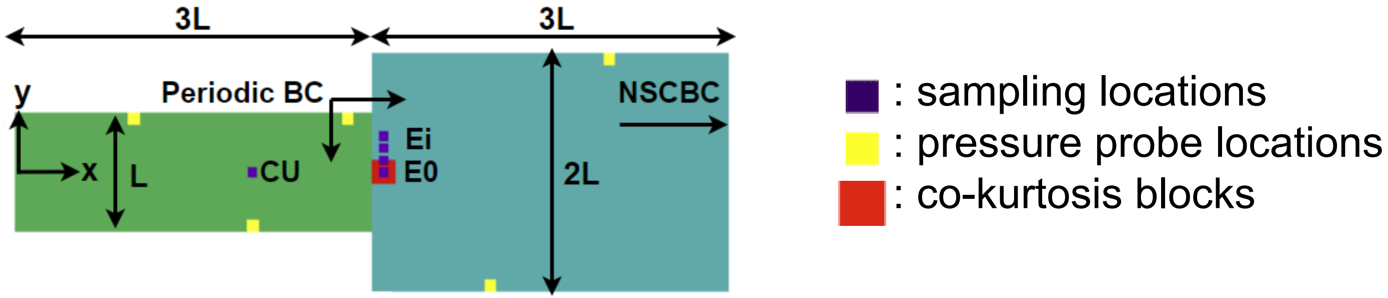
[Floris et al., Proc. Comb. Inst., 2024]

Data-driven analysis of hydrogen flashback mechanism

- Collection of thermochemical/flow state evolution



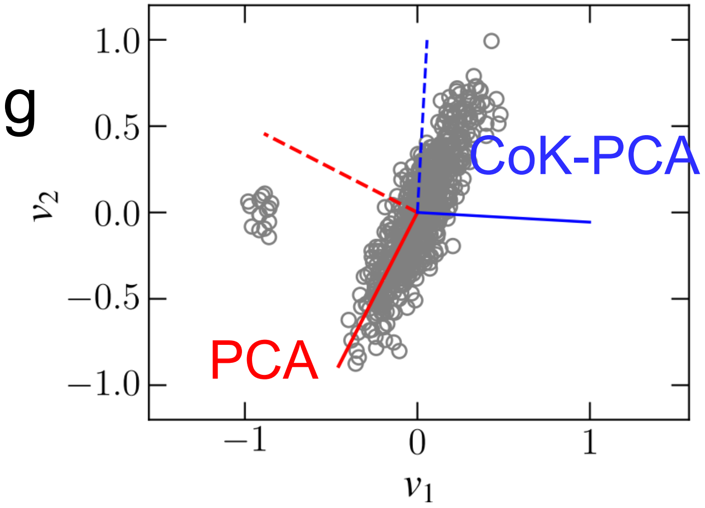




1. Identification of relevant features for flashback with co-kurtosis PCA
   → Provides indication of interesting physical features
2. Precursor identification with modularity clustering
   → Provides precursors

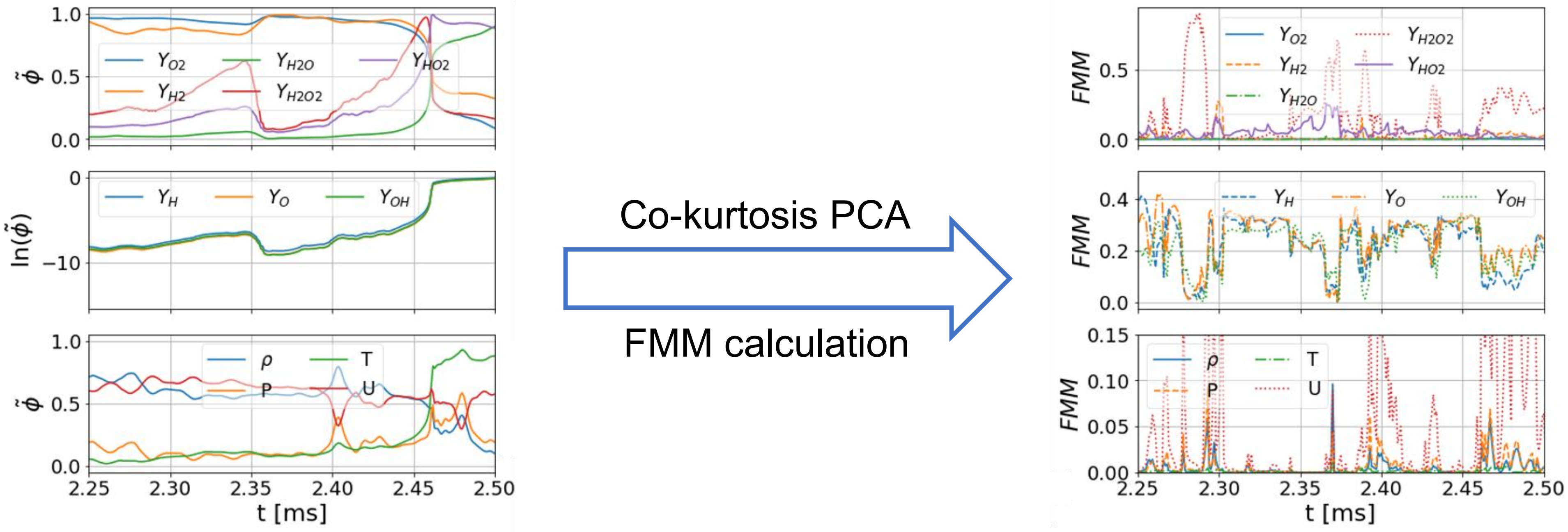
Co-kurtosis Principal Component Analysis consists in applying PCA on the co-kurtosis tensor

- Objective: identify most relevant features in thermochemical and flow state for flashback precursor
- Co-kurtosis PCA
  - Kurtosis: related to “fat tails”
  - Co-kurtosis: related to features undergoing extreme deviations simultaneously
  - PCA applied on the co-kurtosis tensor: sensitive to outlier apparition (precursor)
  - Can compute the relative contribution of features to the principal vector (feature moment matrix - FMM)



[Jonnalagadda et al., CnF 250, (2023)]
[Nayak et al., CnF 259, (2024)]
[Aditya et al., JCP 387, (2019)]

Co-kurtosis PCA on reheat burner allows to identify important features for the onset of flashback

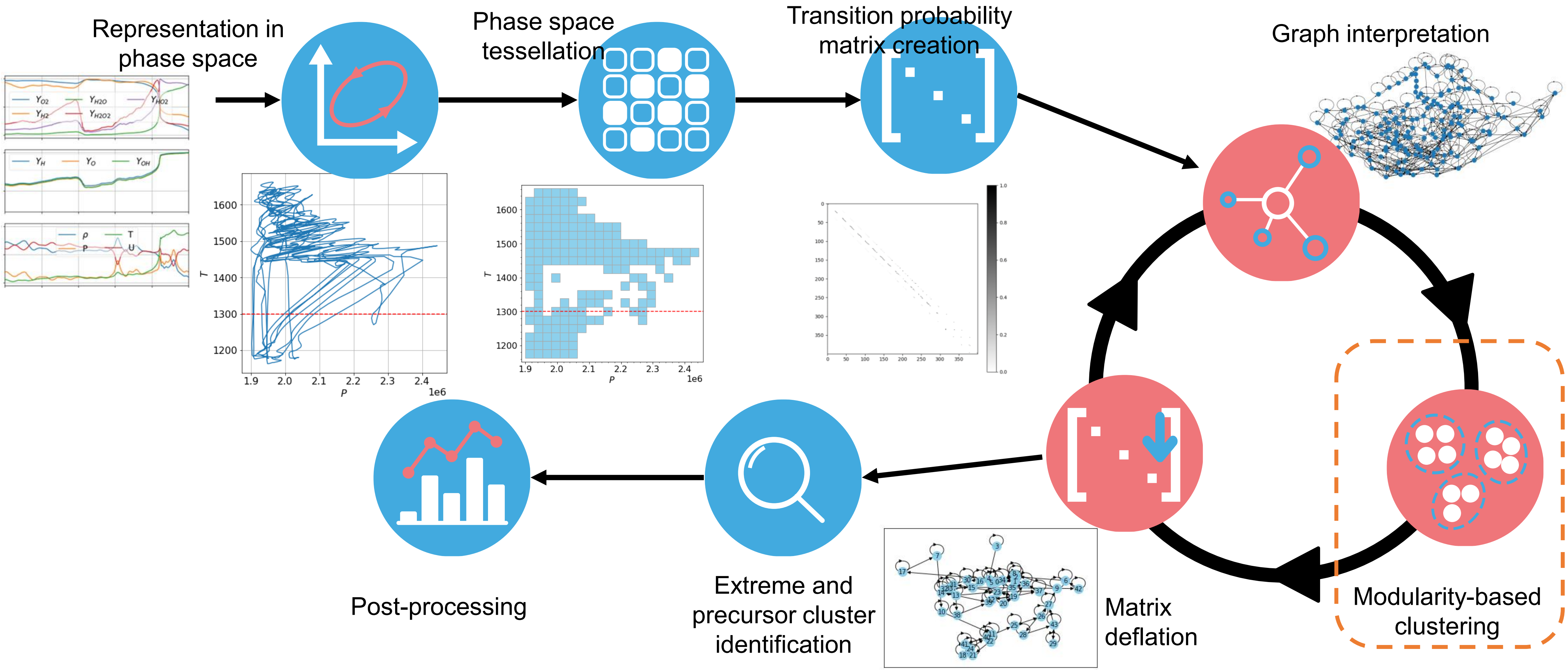


- Identified features:
  - p, ρ, V_x
  - OH, H, O: very similar behaviour → OH kept
  - Strong activity from HO_2, H_2O_2
  - T also kept

→ Features reduced from 17 to 7

[Floris et al., Proc. Comb. Inst., 2024]

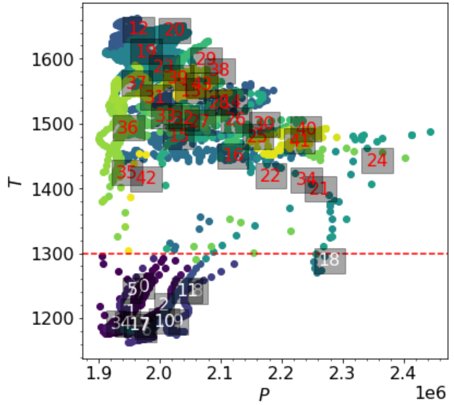
Graph and clustering-based precursor identification method

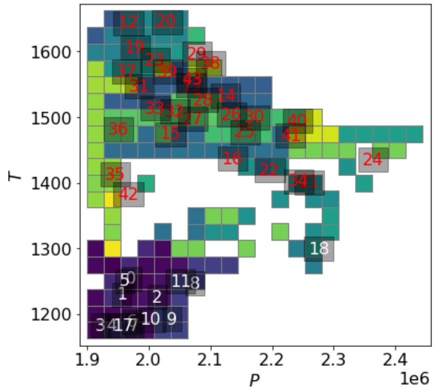


[Floris et al., Proc. Comb. Inst., 2024]

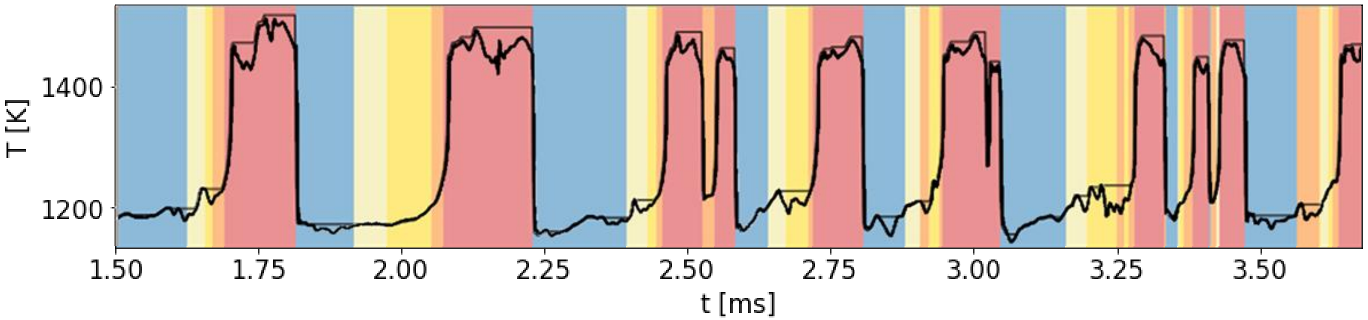
Identified clusters during flashback provides a flashback prediction horizon

- Clusters based on the first 3 flashback events





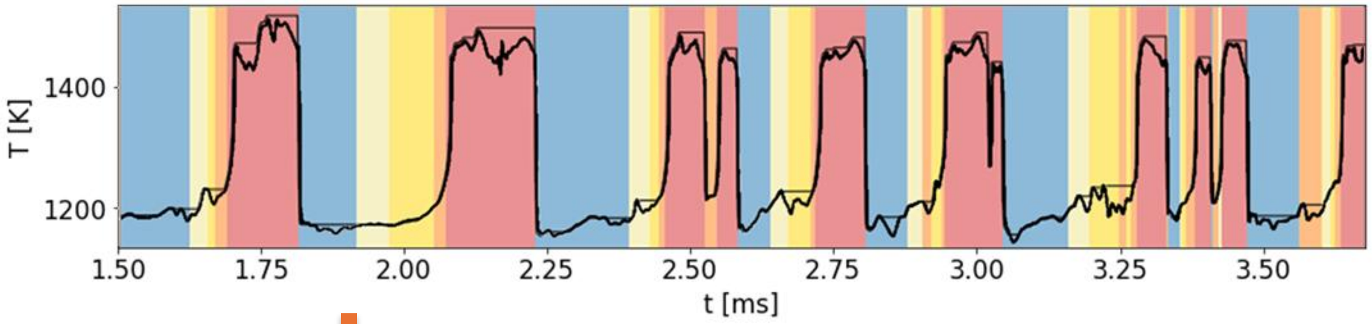
For the remaining flashback



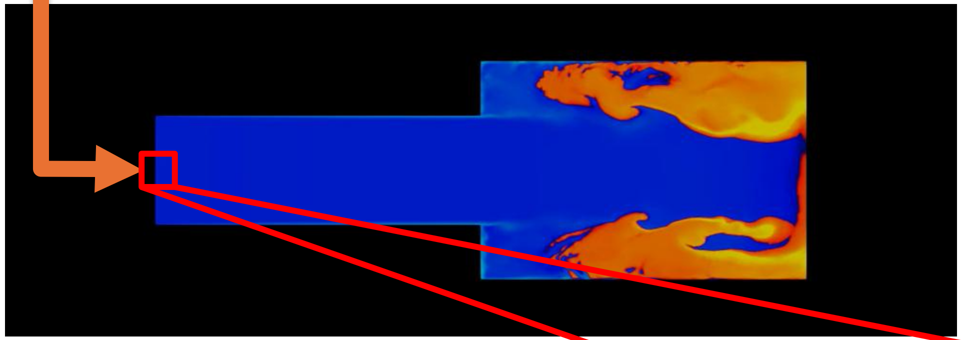
Precursor provide some flashback prediction horizon

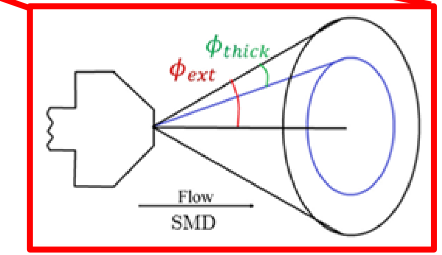
[Floris et al., Proc. Comb. Inst., 2024]

How can we design a flashback mitigation system?



Water injection?



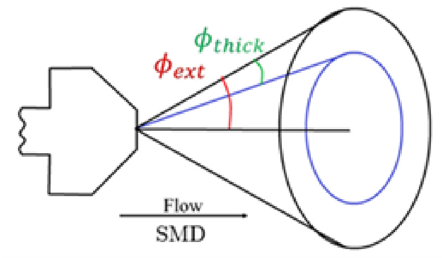


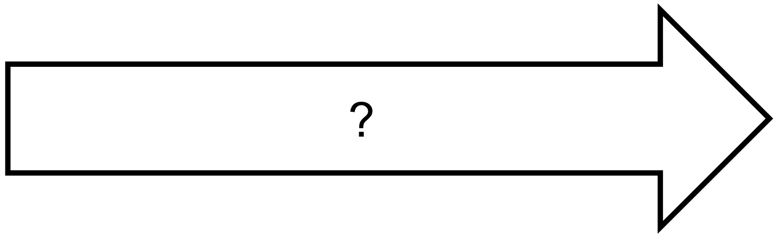
How can we design the water injection optimally?

[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

Development of a surrogate model to design water-injection to mitigate flashback

4 design variables





Performance parameters:

1. Flashback prevented
2. Thermal efficiency η_{th}
3. Evaporation rate η_{vap}
4. Pattern factor PF
5. NOx emission E_{NO_x}

Design of a surrogate model

1. Generate database of 20 simulations
2. Gaussian process regression (one model per performance parameter)
3. Analyse the influence of the design variables based on the surrogate (with Sobol Index)

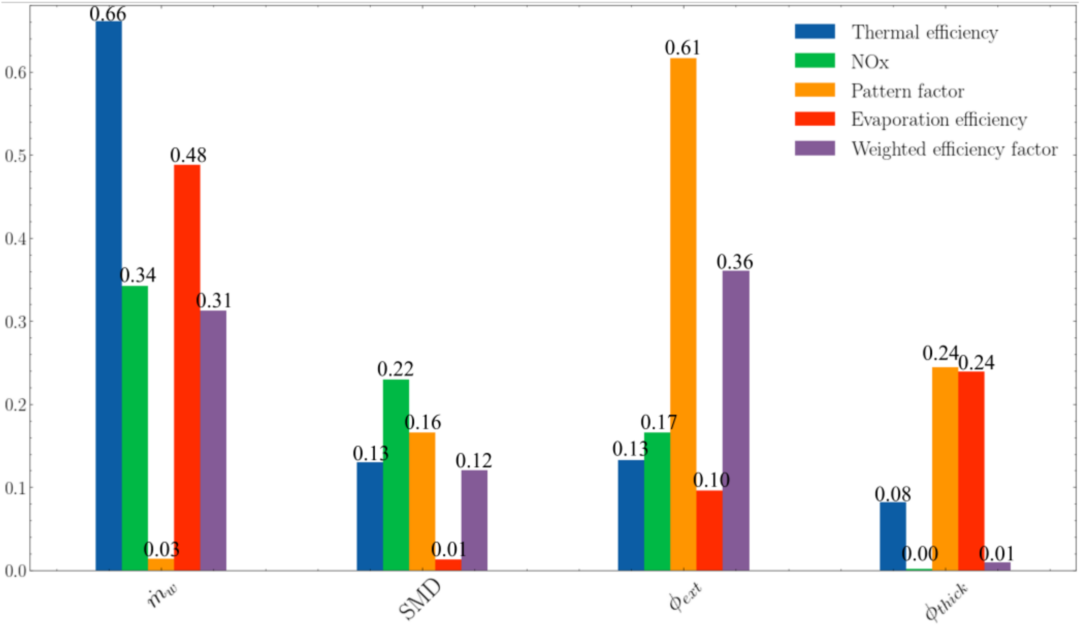
Design parameters	$\dot{m}_w$ (μg/ms)	SMD (μm)	ϕ_{ext} (deg)	ϕ_{thick} (deg)
Min. values	500	2	20	3
Max. values	15,000	20	55	18
Performance parameters	η_{th}	η_{vap}	NO_x	PF

[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

Development of a surrogate model to design water-injection to mitigate flashback

Influence of design parameters deduced from surrogate

First Sobol indices

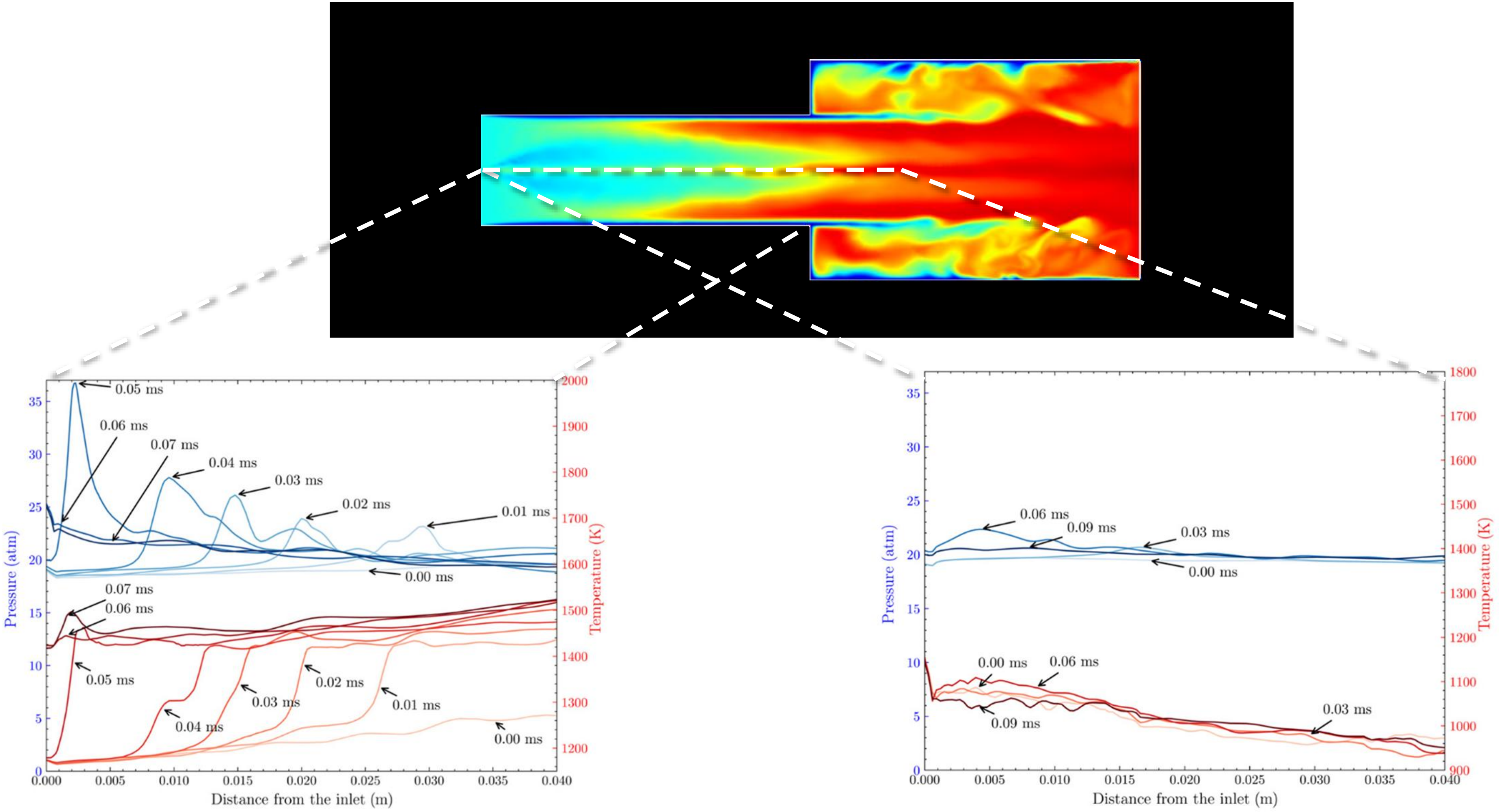


- η_{th}: mostly influenced by $\dot{m}_w$
- E_{NO_x}: joint influence of $\dot{m}_w$, SMD and ϕ_{ext}
- PF: mostly influenced by droplet distribution through ϕ_{ext} and ϕ_{thick}
- η_{vap}: mostly influenced by $\dot{m}_w$ and ϕ_{thick}

⇨ Surrogate used for design optimization of performance $\mathcal{L}(\eta_{th}, \eta_{vap}, PF, E_{NO_x})$

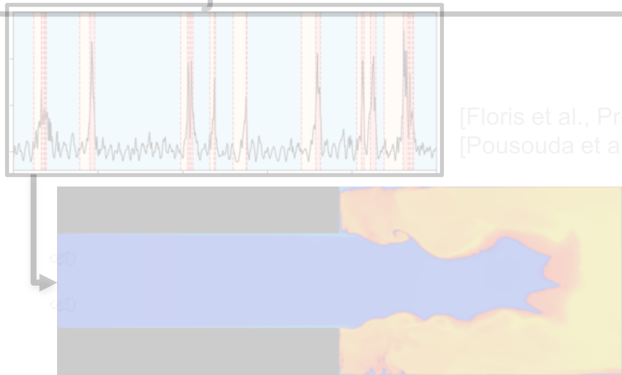
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

Designed water injection system prevents flashback



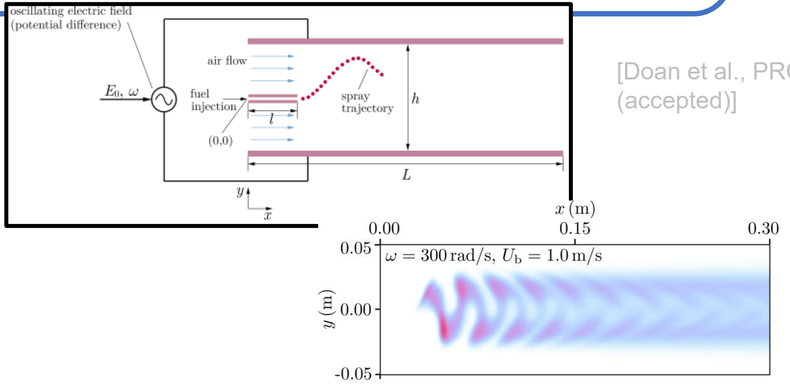
Structure of the seminar

1. Machine Learning to prevent flashback with water injection



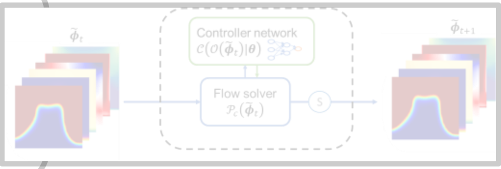
[Floris et al., Proc. Comb. Inst., 2024]
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

2. Machine Learning to control fuel mixing with electric field



[Doan et al., PROCI, 2026 (accepted)]

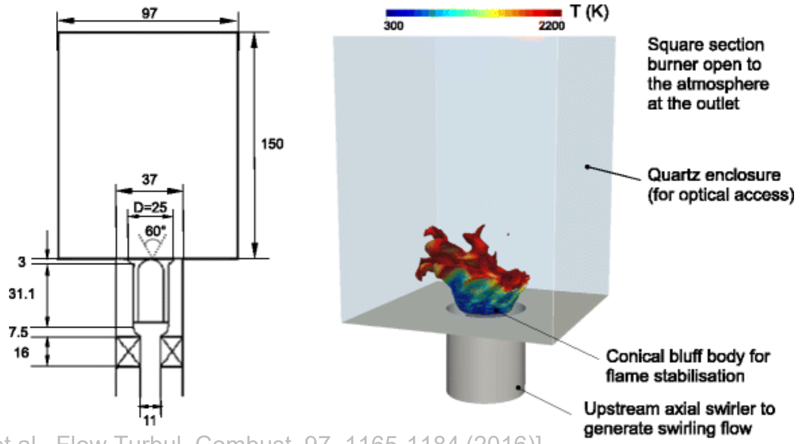
3. Towards unified control development framework with differentiable solver



[Tathawadekar et al., Data-centric Eng., 2023]
[Shehata & Doan, PRFluids, 2026 (under review)]

Fuel stratification control through charged droplet trajectory control

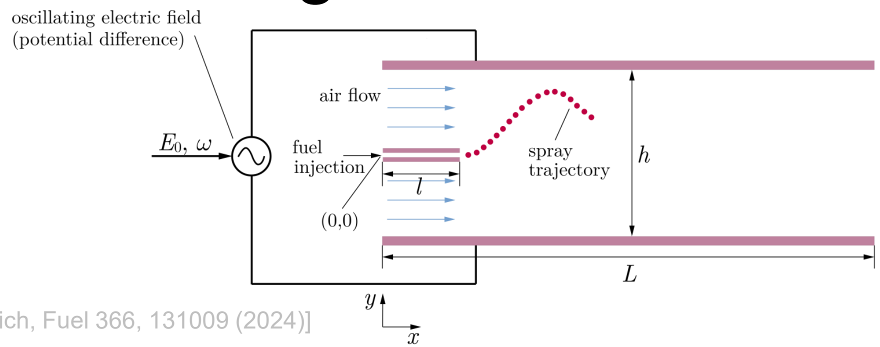
- Fuel-air mixing: constrained by combustor, injector and chamber geometry



[Giusti et al., Flow Turbul. Combust. 97, 1165-1184 (2016)]

→ Designed for specific conditions
→ Limited operations to narrow fuel/condition ranges

- Oscillating electric field: able to steer charged droplets



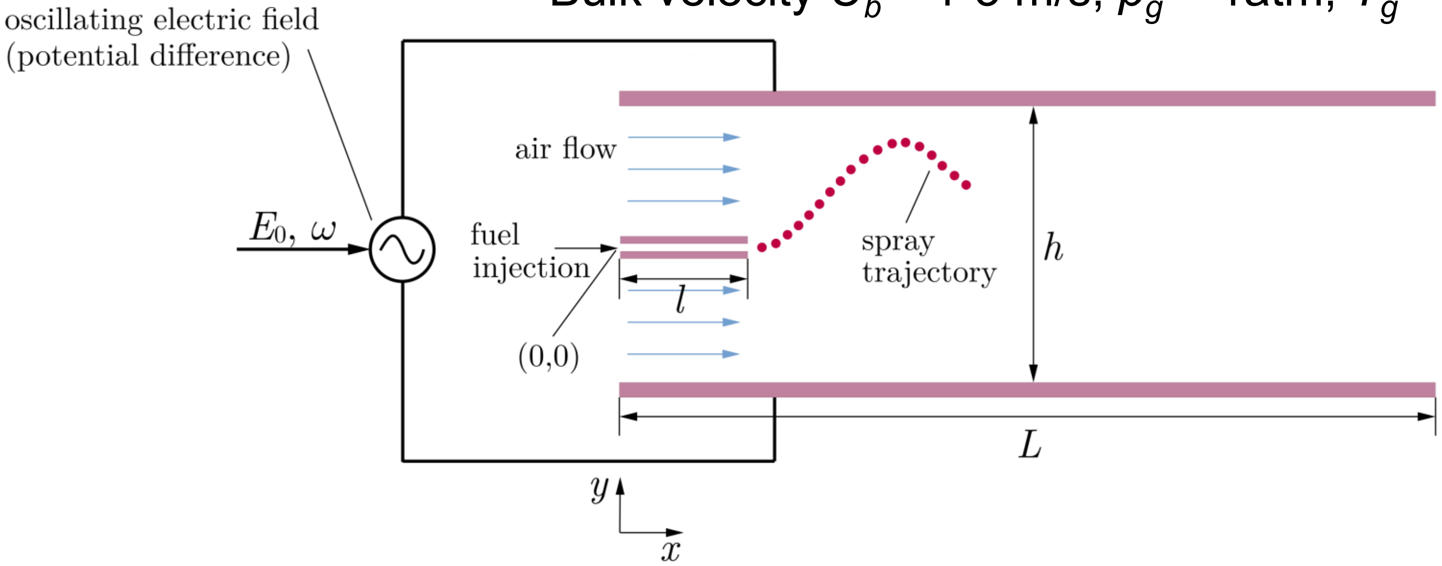
→ Potential for fuel stratification control

[Giusti & Fredrich, Fuel 366, 131009 (2024)]

Simulation Framework

Large Eddy Simulation

- Eulerian-Lagrangian framework for dilute prays
- Channel Flow L = 0.3m h = 0.1m, Grid: 300 × 50
- Bulk velocity U_b = 1-3 m/s, p_g = 1atm, T_g = 600K



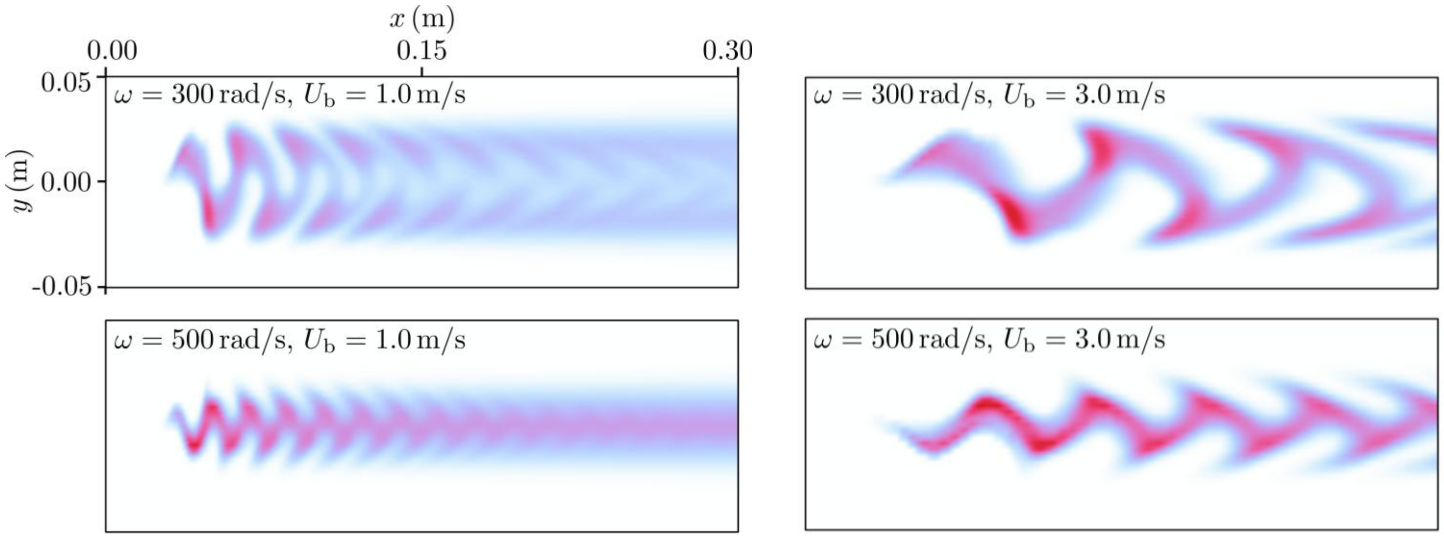
- Injection distance l = 0.025m
- Fuel mass flow rate: JetA@0.0068 g/s
- Droplet: droplet model from [1], Velocity 1.5U_b, d_0 = 50μm, $\rho_{q,d,0}$ = -1 C/m^3

[1] Lawson & Giusti, Int. J. Multiph. Flow 366, 105289 (2025)

Electric Field Effects on Fuel Vapour Profile

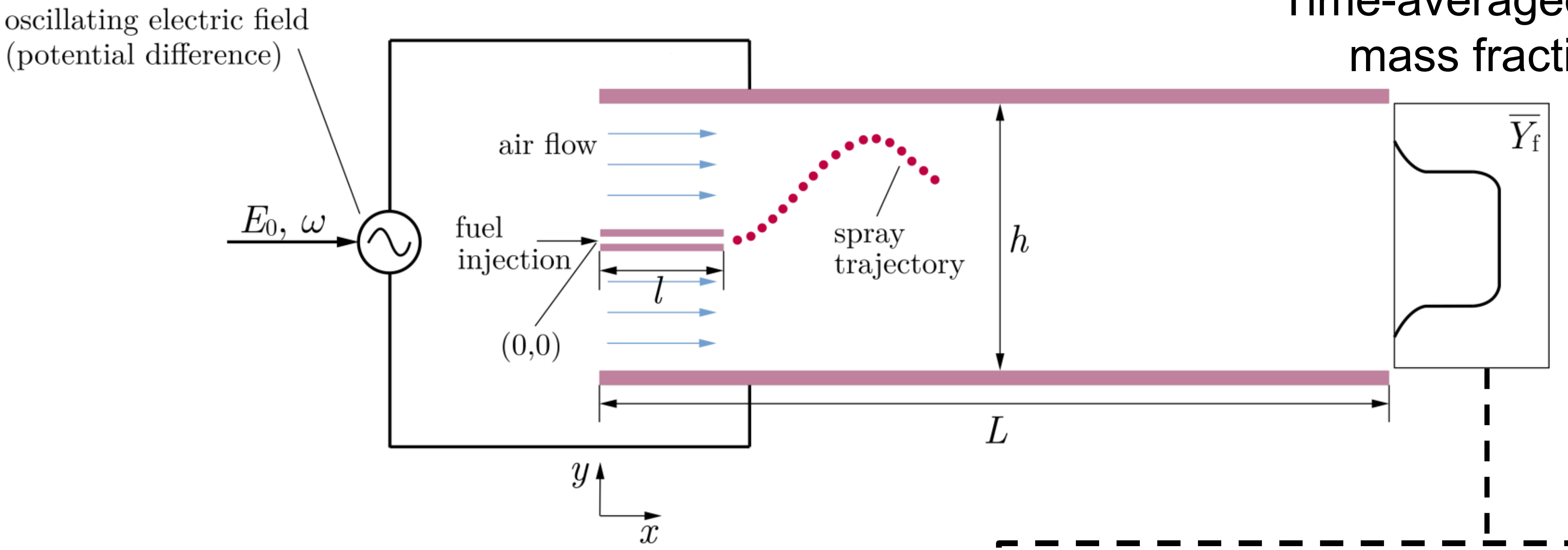
Instantaneous fuel mass fraction

E_0=1MV/m



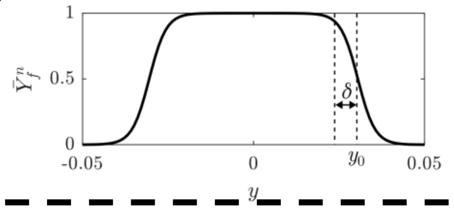
- U_b↑: longer oscillation wavelength
- ω↑ : smaller oscillation wavelength and amplitude

Control Framework



Time-averaged fuel vapour mass fraction profile

$\bar{Y}_f$, Exit fuel vapour target profile



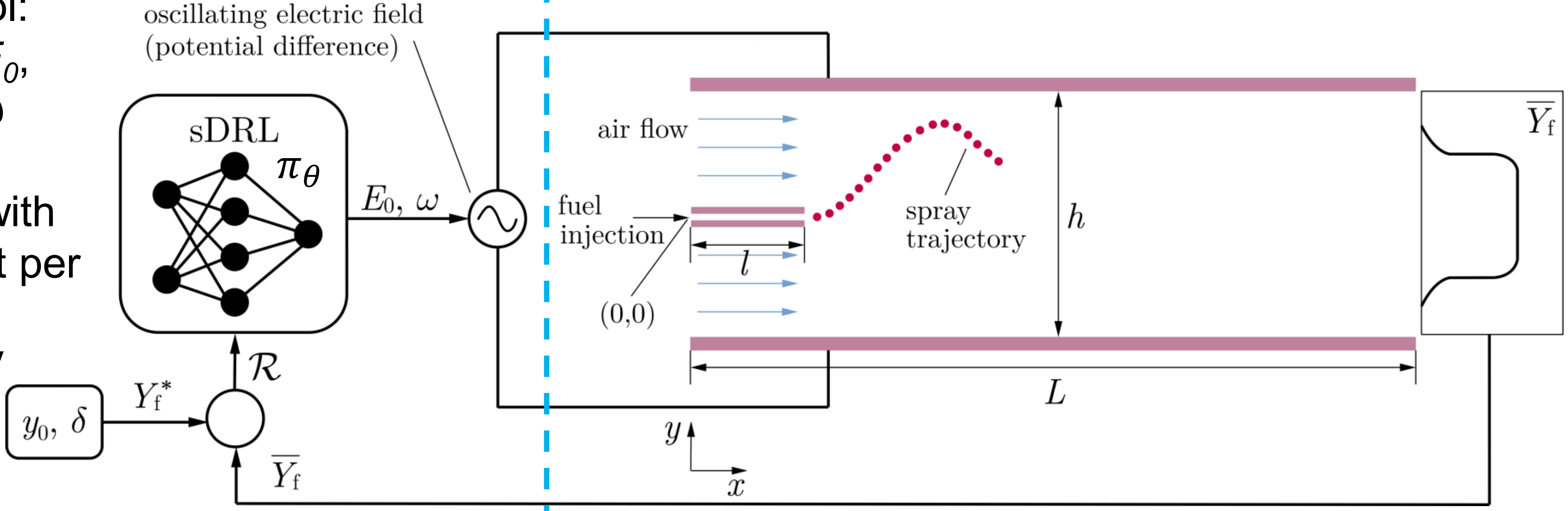
2 parameters: y_0 and δ

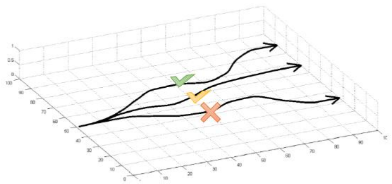
Control Framework

Single-step Deep Reinforcement Learning (sDRL)

- sDRL control: Amplitude E_0, frequency ω
- One agent interaction with environment per episode
- Agent policy π_θ trained through policy optimization

$$\nabla_\theta J(\theta) \approx \frac{1}{N}\sum_{n}^{N}\left[\sum_{t=t_0}^{T}\nabla_\theta \log\left(\pi_\theta\left(a_{n,t}|s_{n,t}\right)\right)R_n(\tau)\right]$$

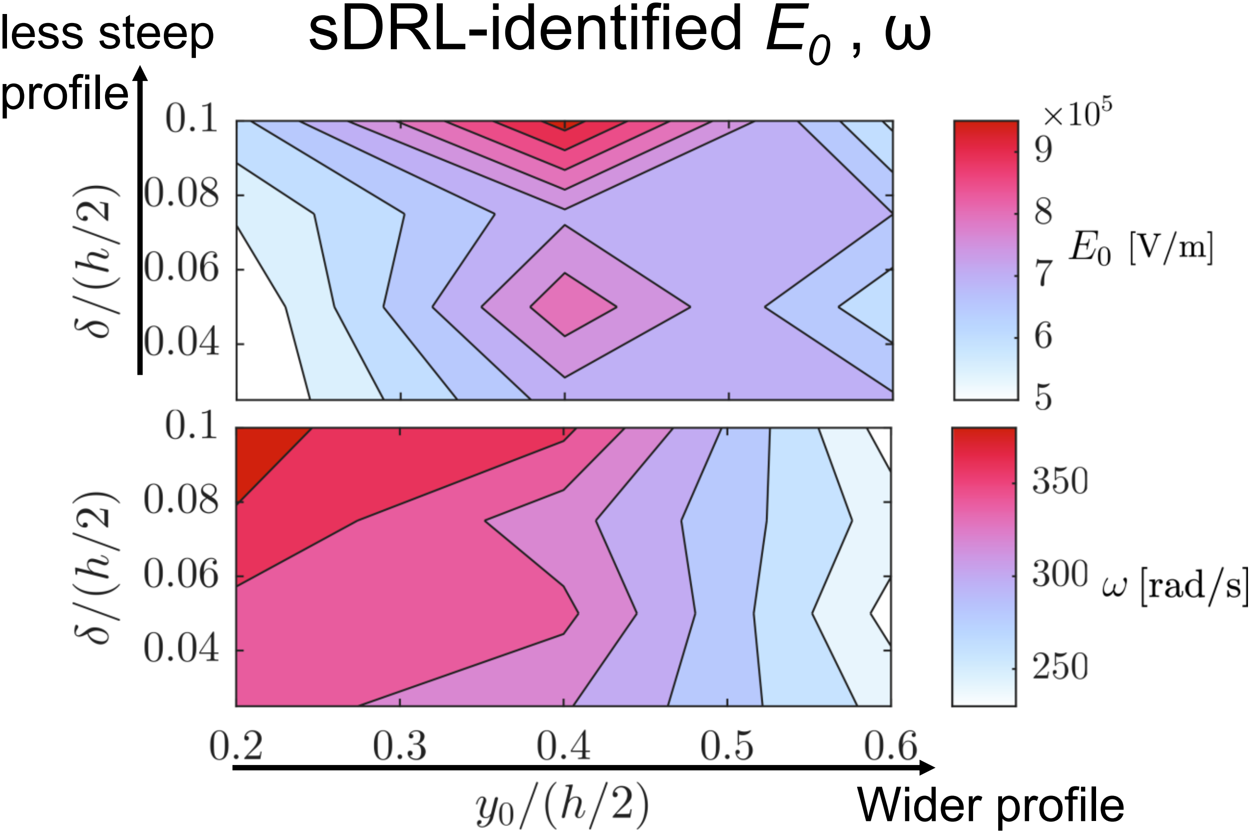


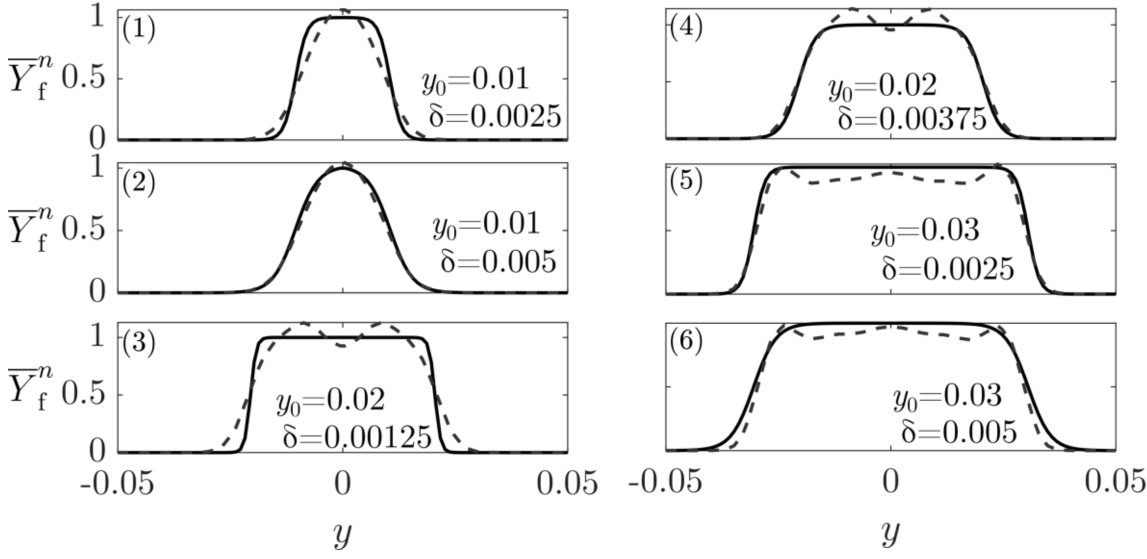


sDRL used to identify optimal E_0,ω for given y_0, δ

sDRL-identified optimal electric field parameters

sDRL-identified E_0 , ω





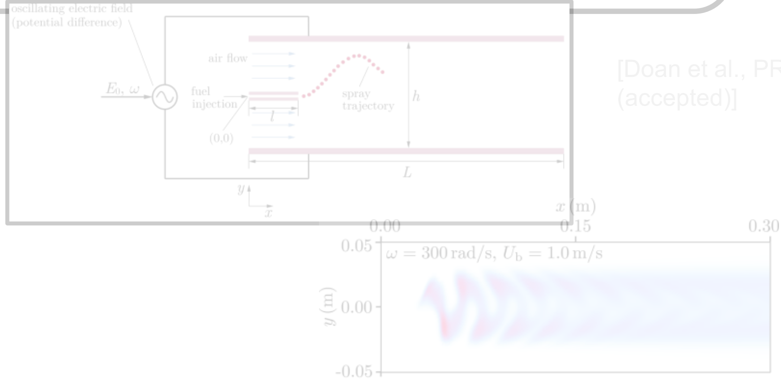
Also extended to 3D configuration

Structure of the seminar

1. Machine Learning to prevent flashback with water injection

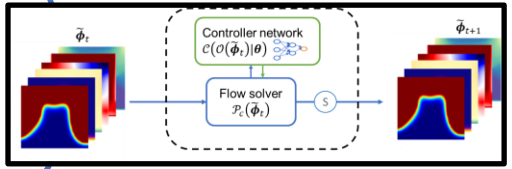
[Floris et al., Proc. Comb. Inst., 2024]
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

2. Machine Learning to control fuel mixing with electric field



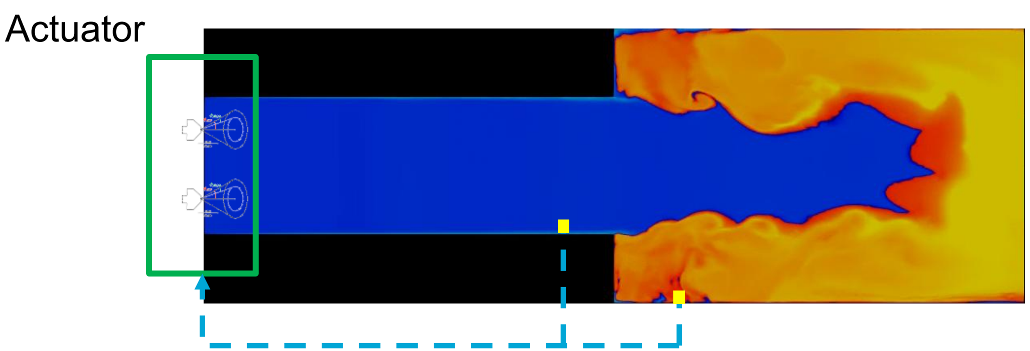
[Doan et al., PROCI, 2026 (accepted)]

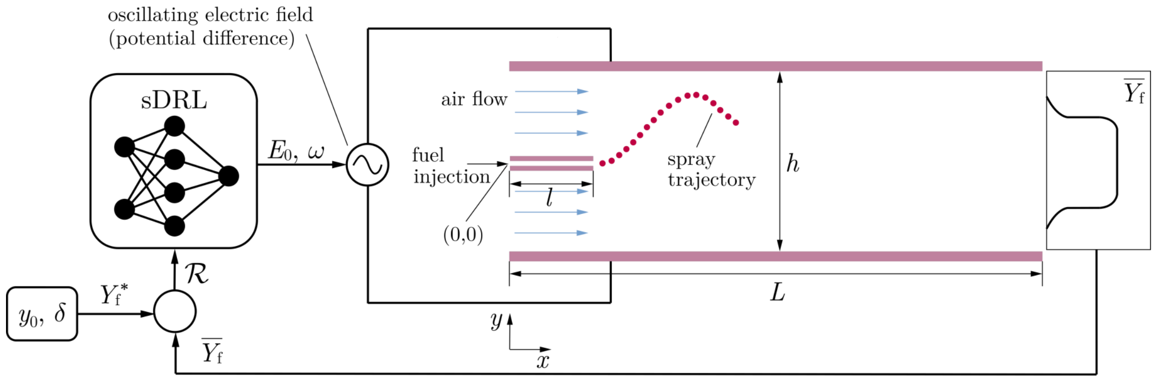
3. Towards unified control development framework with differentiable solver



[Tathawadekar et al., Data-centric Eng., 2023]
[Shehata & Doan, PRFluids, 2026 (under review)]

Flame control poses large challenges for DRL

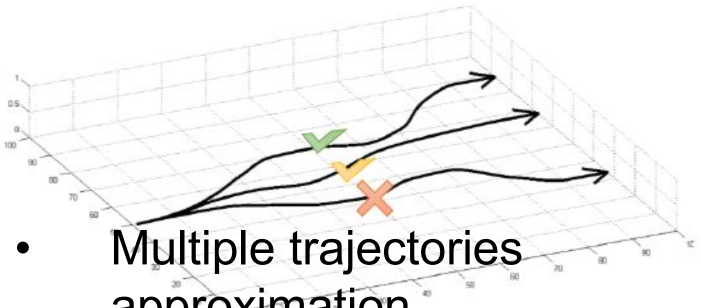




(Long) time-delay between actuator input and effect on flow
→ Challenging for many control algorithms, including reinforcement learning

Approximated policy gradient for DRL:

$$\nabla_\theta J(\theta) \approx \frac{1}{N} \sum_{n}^{N} \left[\sum_{t=t_0}^{T} \nabla_\theta \log\left(\pi_\theta\left(a_{n,t} \middle| s_{n,t}\right)\right) R_n(\tau) \right]$$

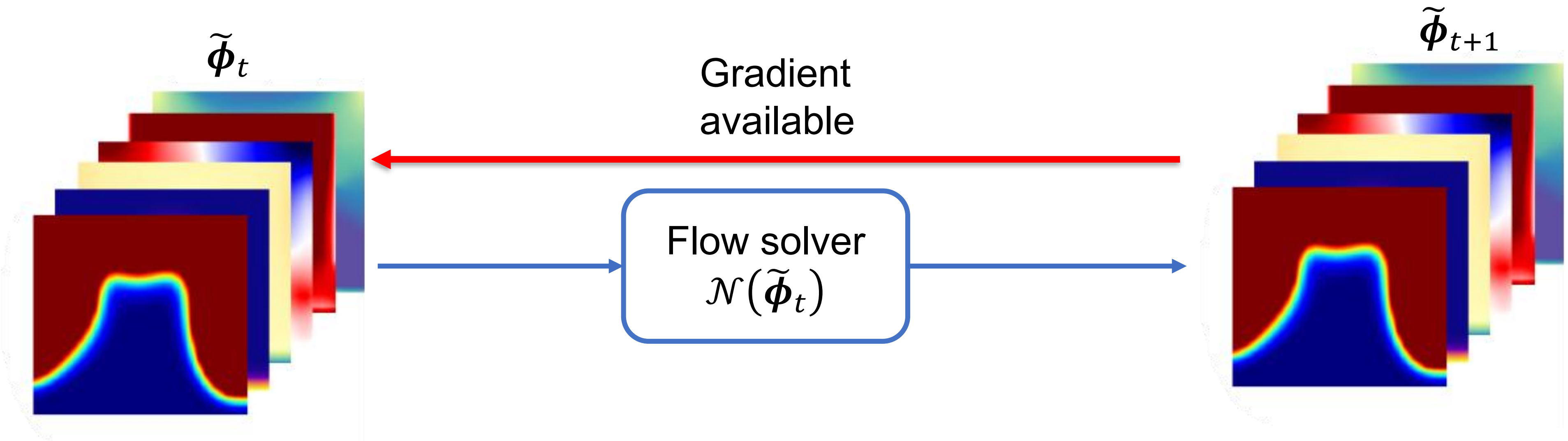


- Multiple trajectories approximation
- Mini-batch approximation

Extremely data-intensive

Differentiable solver propagates gradient through its operations

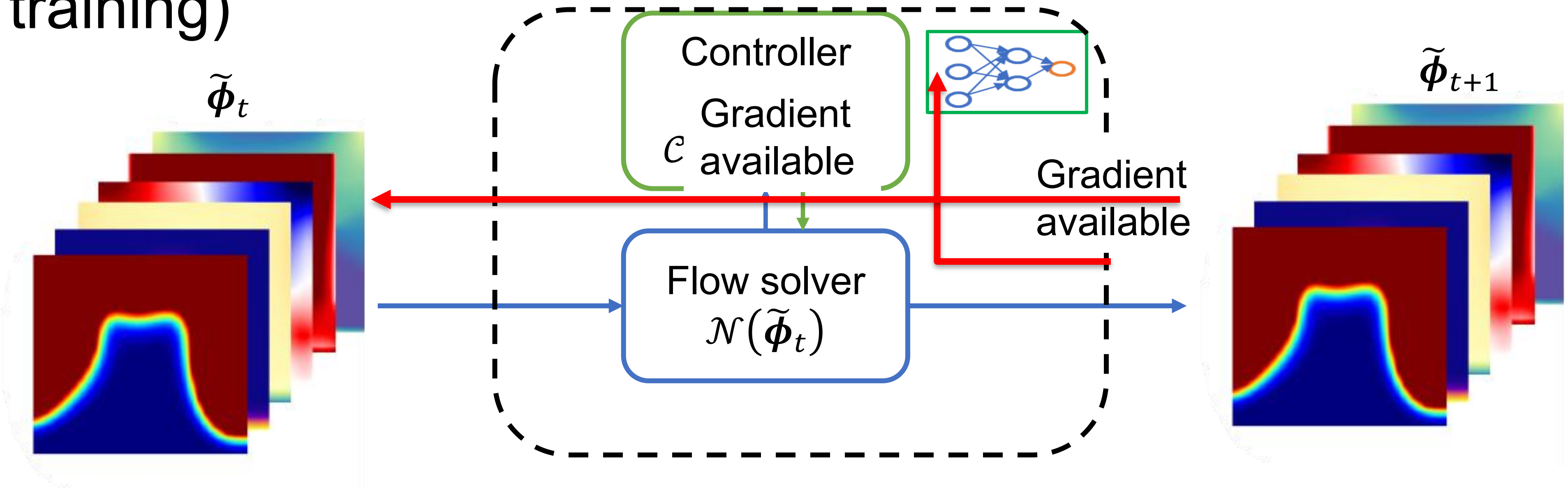
- Recently, differentiable flow solver appeared
  - Jaxcfd, jaxfluids, phiflow, PICT, …
  - Maintain automatic differentiation capabilities through solver operation
- Effectively, similar to algorithmic adjoint



[Tathawadekar et al., DCE, (2023)]

Differentiable solver provides seamless gradients for neural network training

- Recently, differentiable flow solver appeared
  - Jaxcfd, jaxfluids, phiflow, …
  - Maintain automatic differentiation capabilities through solver operation
- Effectively, similar to algorithmic adjoint
- Allows for seamless embedding of neural network (and their training)



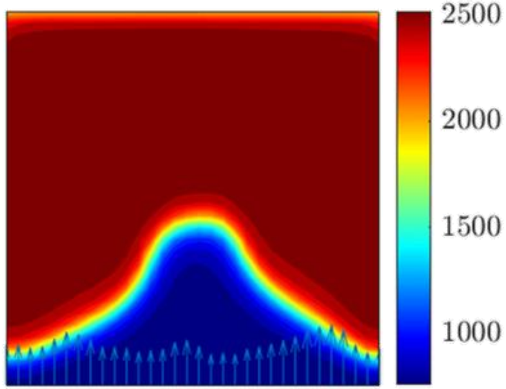
Differentiable solver leveraged for two flow control problems

Test case: flame shape control

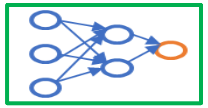
[Tathawadekar et al., DCE, (2023)]

Standard Bunsen flame

Arbitrary initial T field



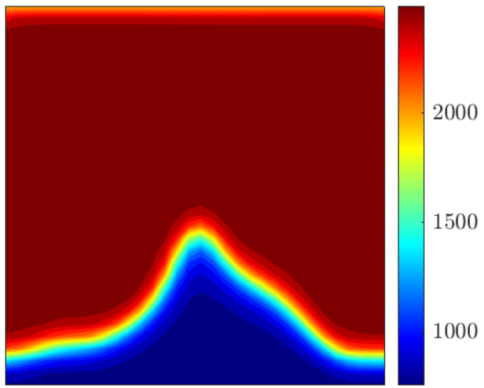
Inlet velocity profile control $\boldsymbol{u}^c(0,t)$



?

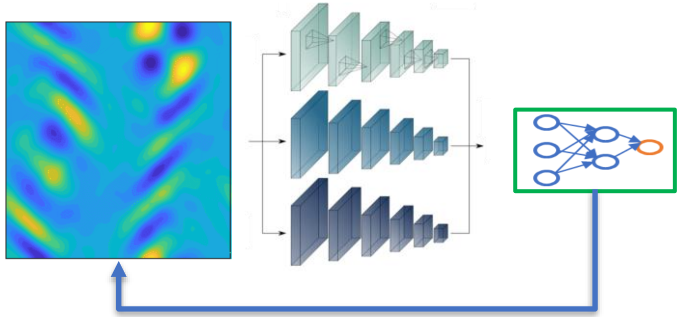
Based on temperature observation $\boldsymbol{T}(x,t)$

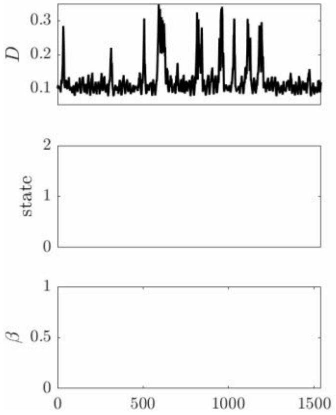
Target final T state

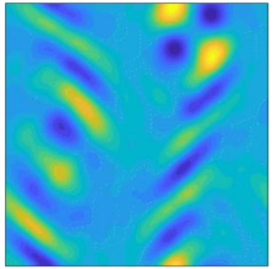


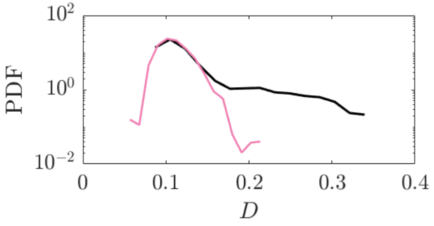
Test case: Extreme events control in Kolmogorov flow

[Shehata & Doan., PRFluids, (under review)]



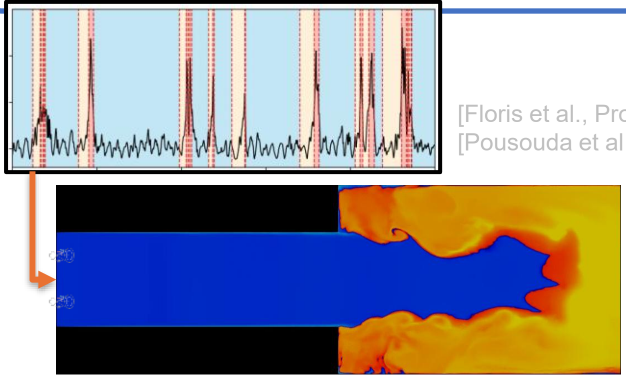






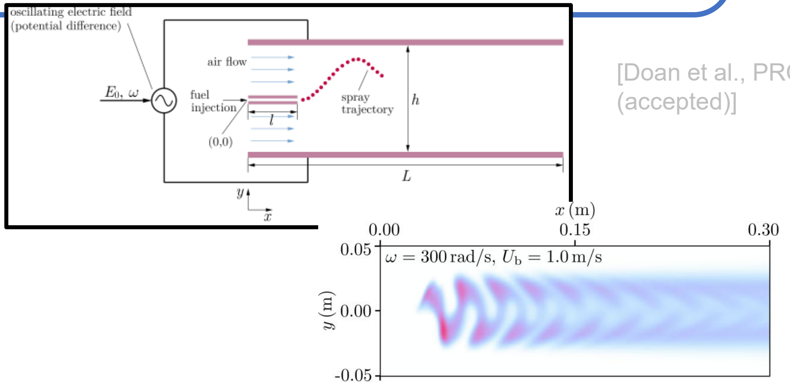
Structure of the seminar

1. Machine Learning to prevent flashback with water injection



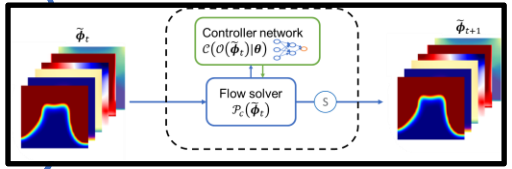
[Floris et al., Proc. Comb. Inst., 2024]
[Pousouda et al., J. Eng. Gas Turbines Power, 2025]

2. Machine Learning to control fuel mixing with electric field



[Doan et al., PROCI, 2026 (accepted)]

3. Towards unified control development framework with differentiable solver



[Tathawadekar et al., Data-centric Eng., 2023]
[Shehata & Doan, PRFluids, 2026 (under review)]

Summary & Perspectives

- Machine learning: promising new approaches to exploit "actuators" for flame control
- Flashback prevention
  - Informed by precursors obtained with dimensionality reduction: CoK-PCA and modularity-based clustering
  - GP-based design of optimal water injection
- Fuel stratification control
  - Reinforcement Learning-control of electric field
- First step towards unified control framework development with differentiable solver

Summary & Perspectives

- Still many challenges
  - Integration of precursor/control techniques into unified framework
  - Applicability to realistic configurations
  - Robustness of identified control approach?

Thank you for your attention!

Questions?

n.doan@imperial.ac.uk

Interested in this research?
Postdoc position available soon

Acknowledgement to
Y. Shehata, A. Giusti, N. S. Lavrati (Imperial College London)
A. Konduri (IISc Bangalore)
B. Mohammadikalakoo, M. Floris, P. Pousouda, I. Langella (TU Delft)
N. Tathawadekar (TU Munich, GE Aviation)
N. Thuerey (TU Munich)

ERC Starting Grant CONTEXT
Grant n. 1011612942

Funded by the European Union

European Research Council
Established by the European Commission