CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

High performance learning for computational physics

Quels bénéfices de l'apprentissage en grande dimension pour les méta-modèles physiques?

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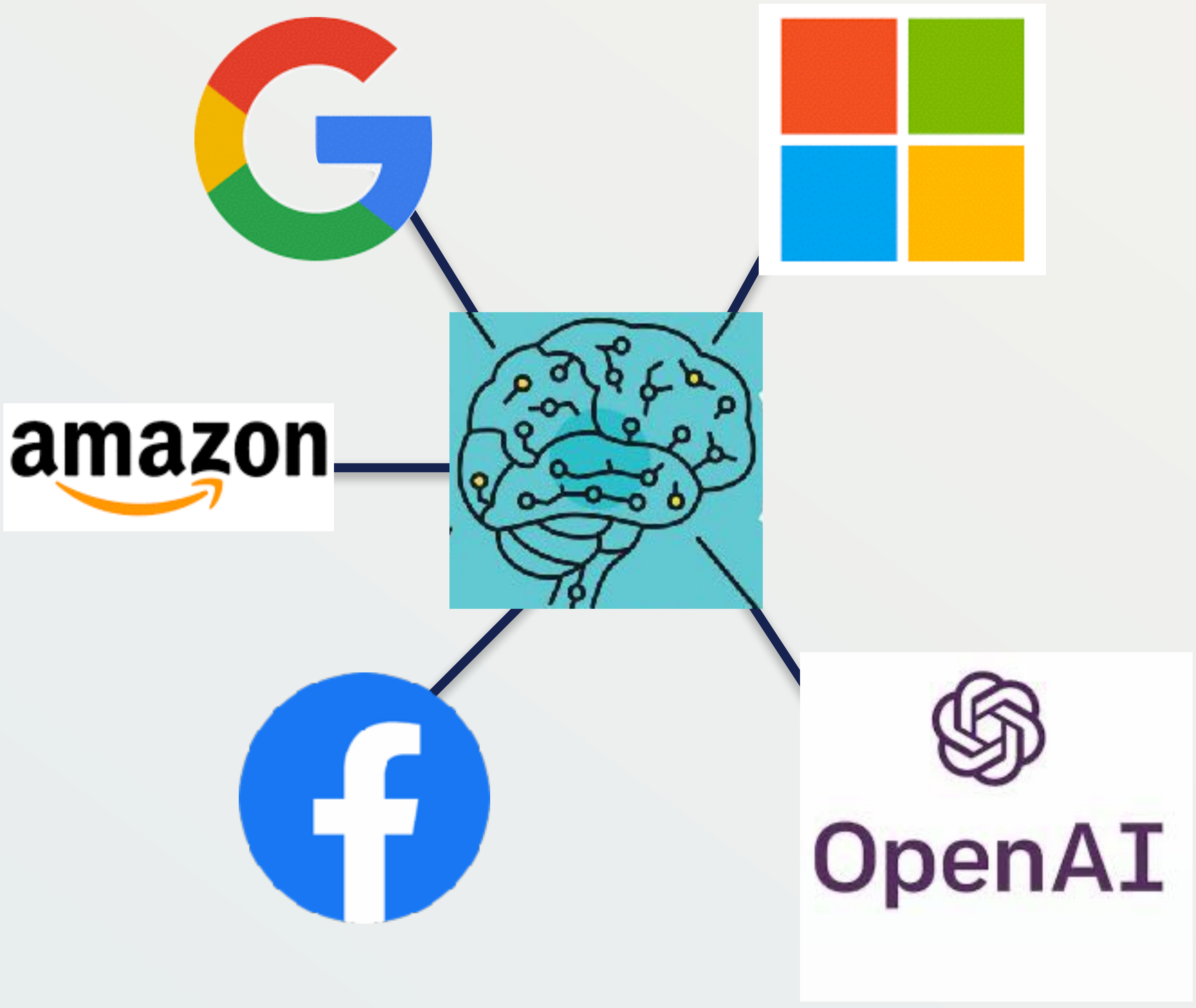
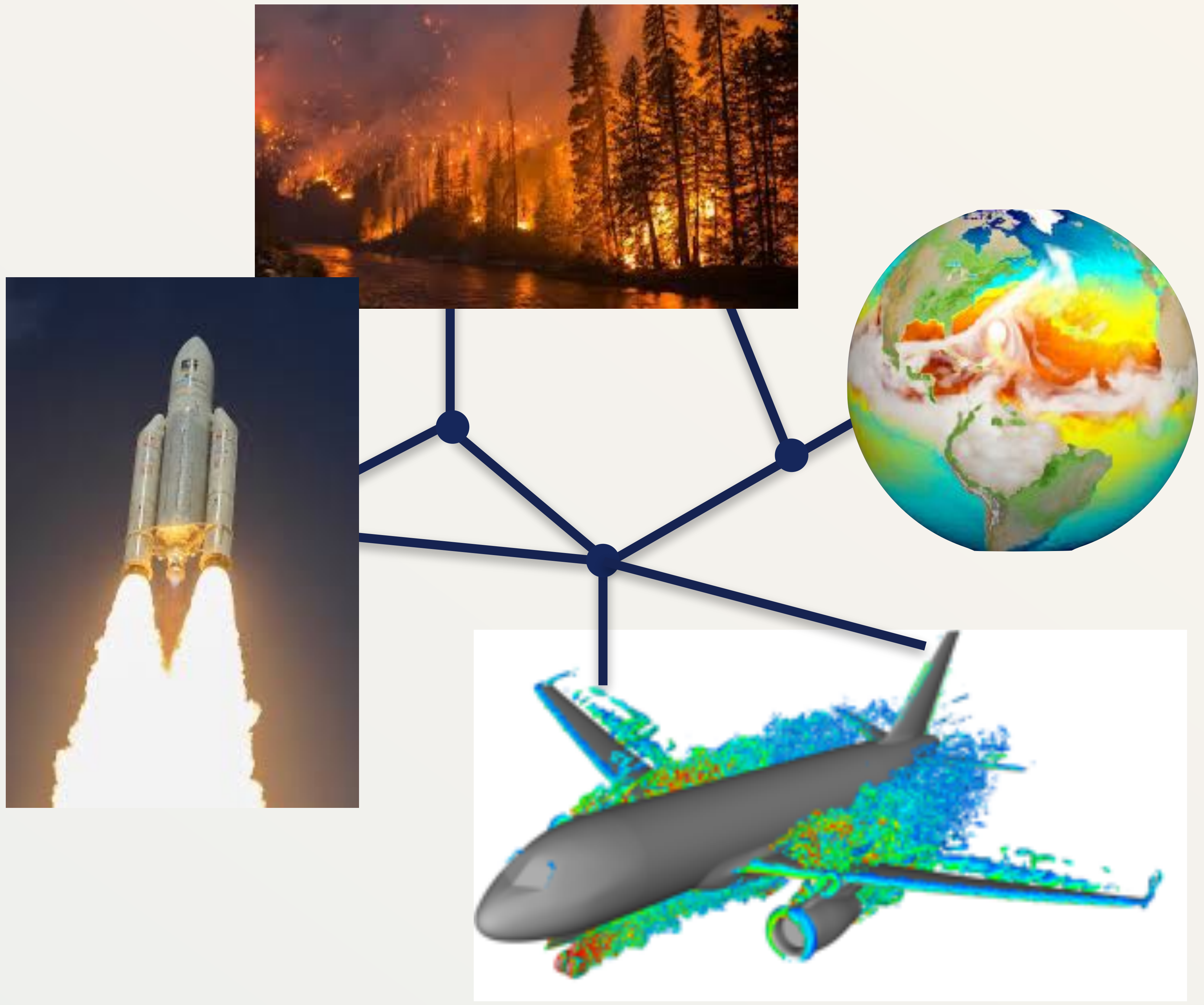
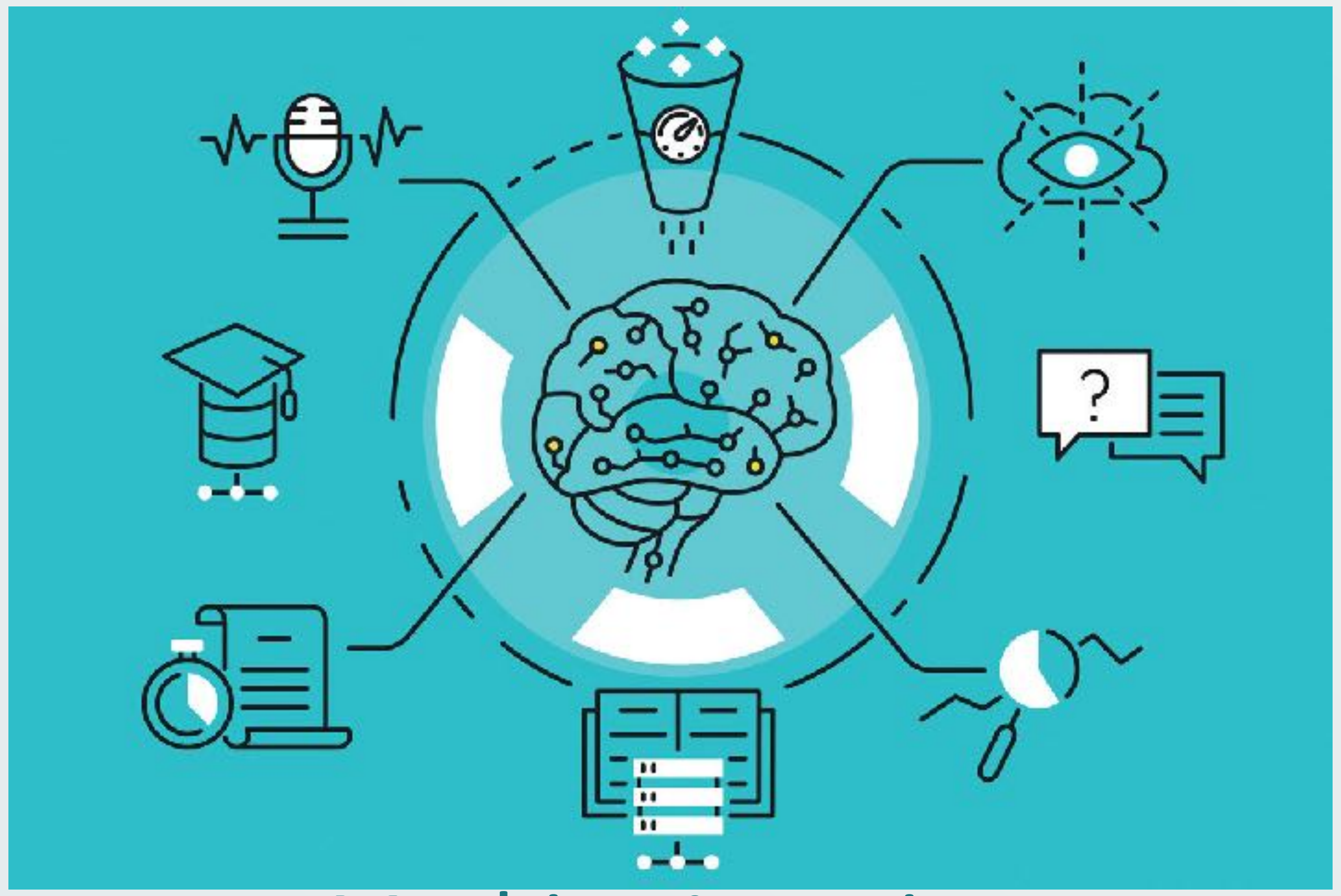
Réunion "Méta-modèles en grande dimension"

Acknowledgments: N. Cazard, V. Xing, L. Drozda, A. Cellier, E. Gullaud, D. Dupuy, Q. Douasbin, A. Misdariis, N. Odier, P. Mohanamuraly, R. Paugam, M. Rochoux, T. Poinsot, M. Bauerheim (ISAE)



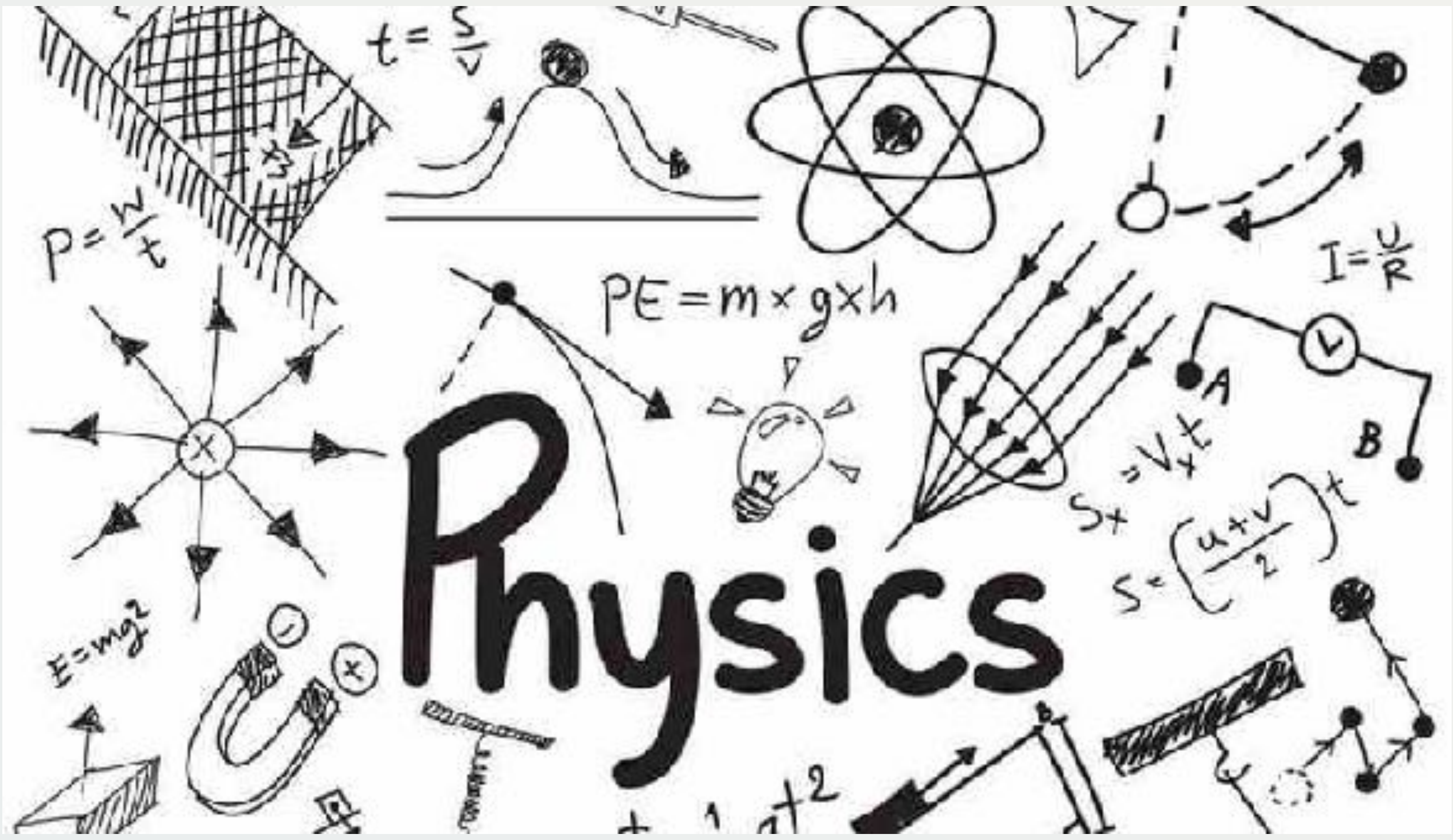
?



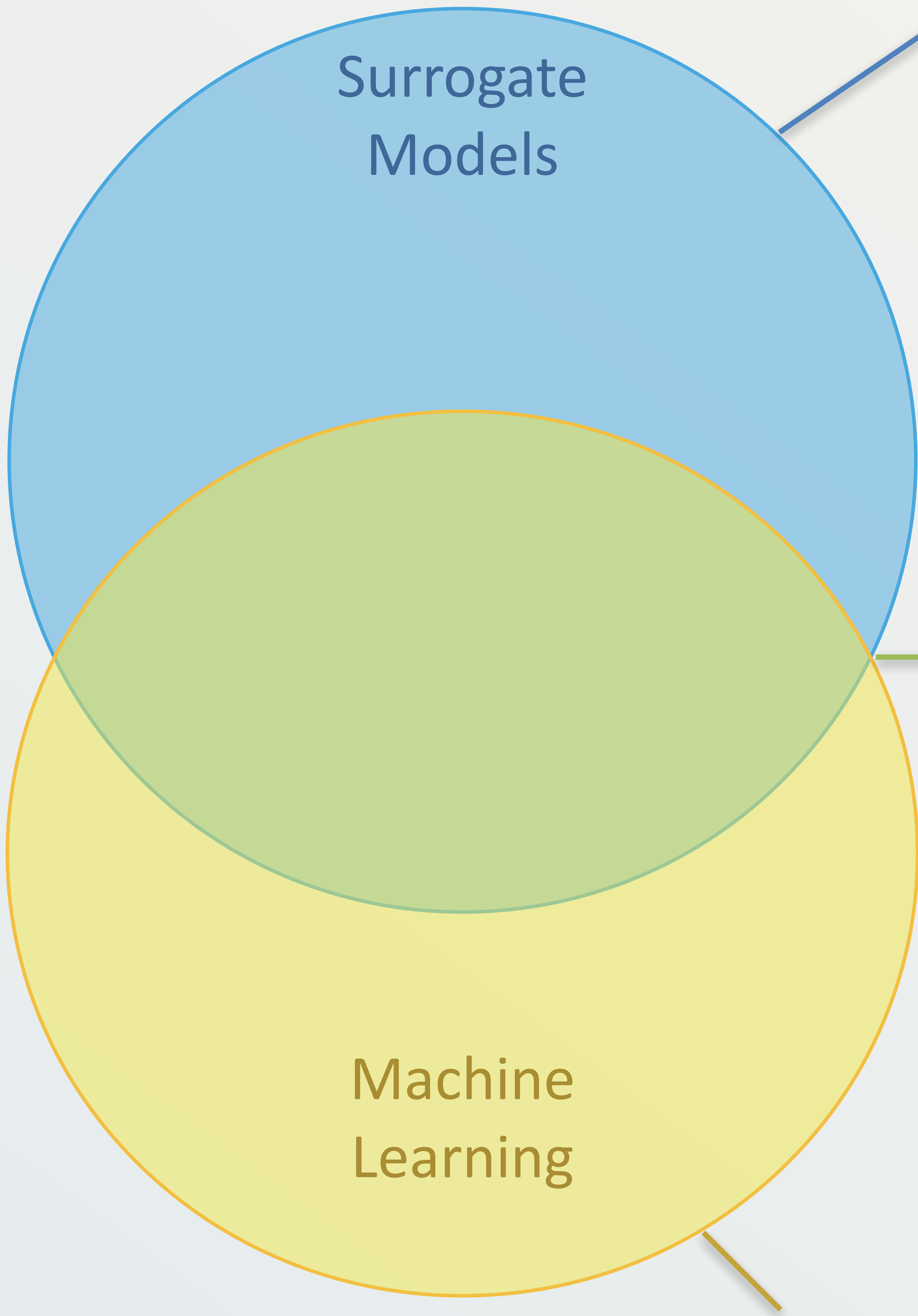


Machine Learning

?

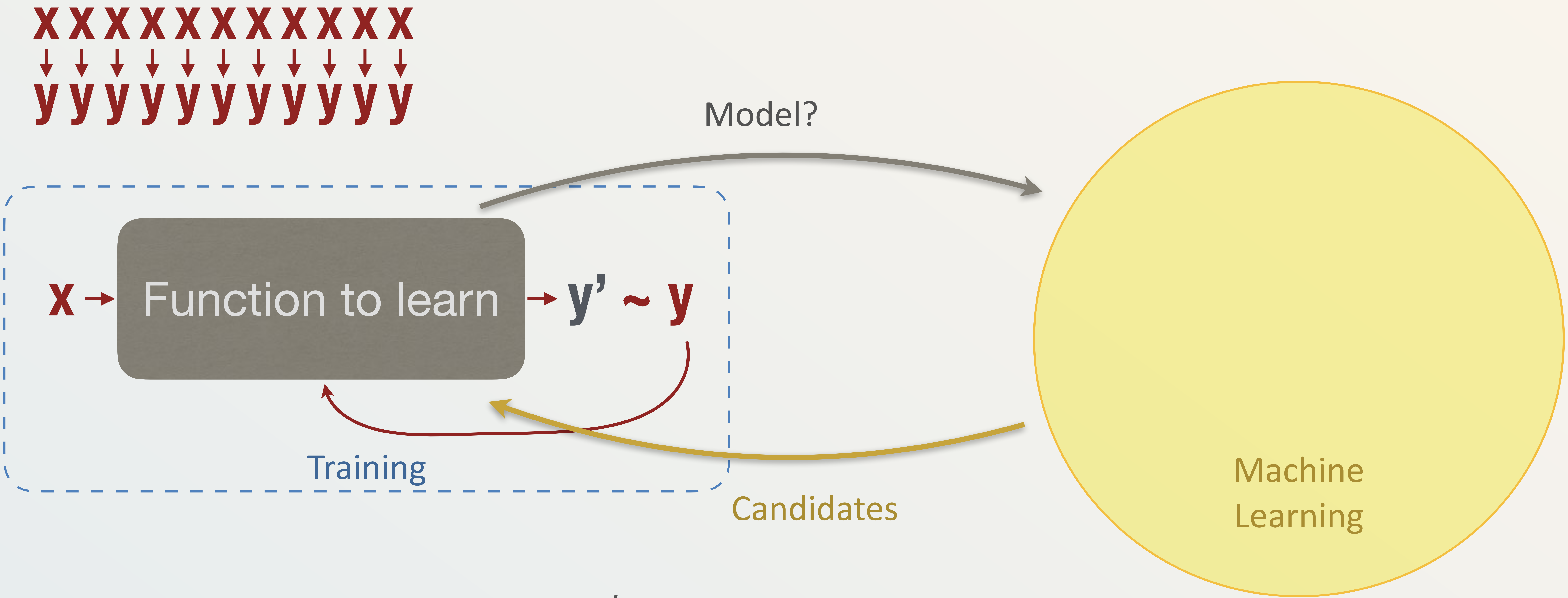


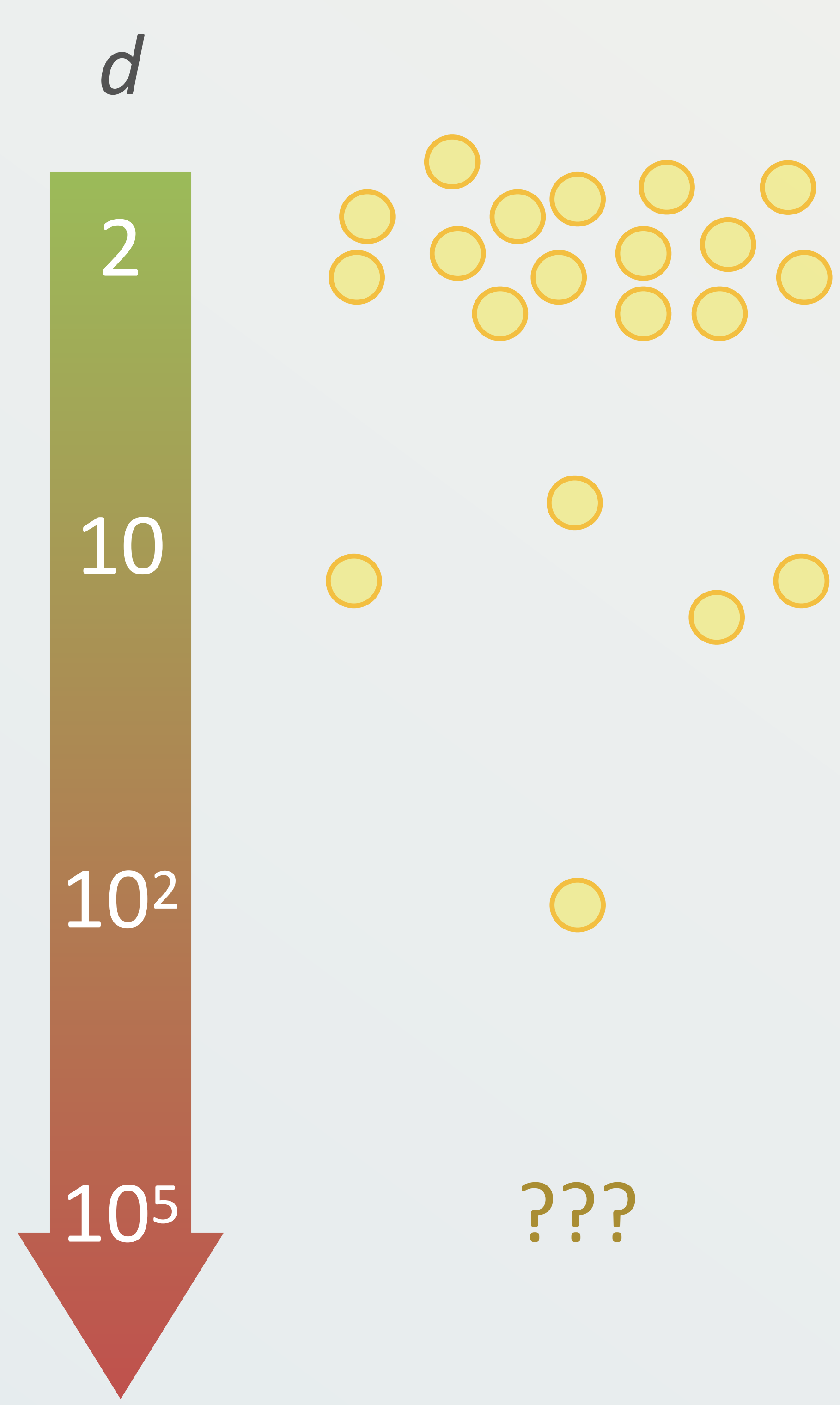
Focus on uncertainty
Design of experiments
…



- Least-squares approximation
- Polynomial fits
- Kriging == Gaussian Process Regression
- …

Historically a strong interest in categorical problems
…





<u>Model?</u>
N number of samples
d dimension of *X*
…

Can I interest you in a dimensionality reduction technique?

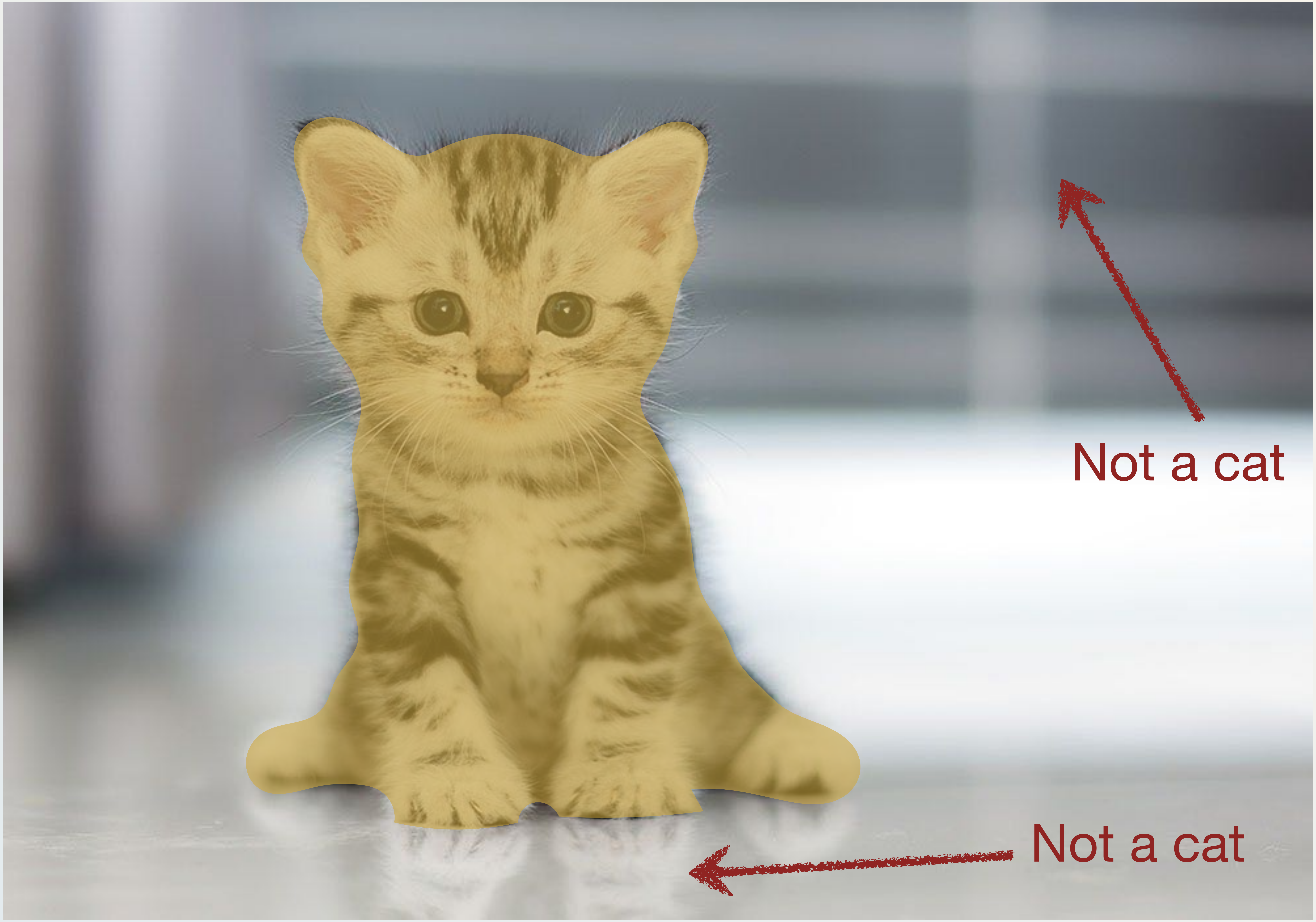
Clustering

PCA

SOM

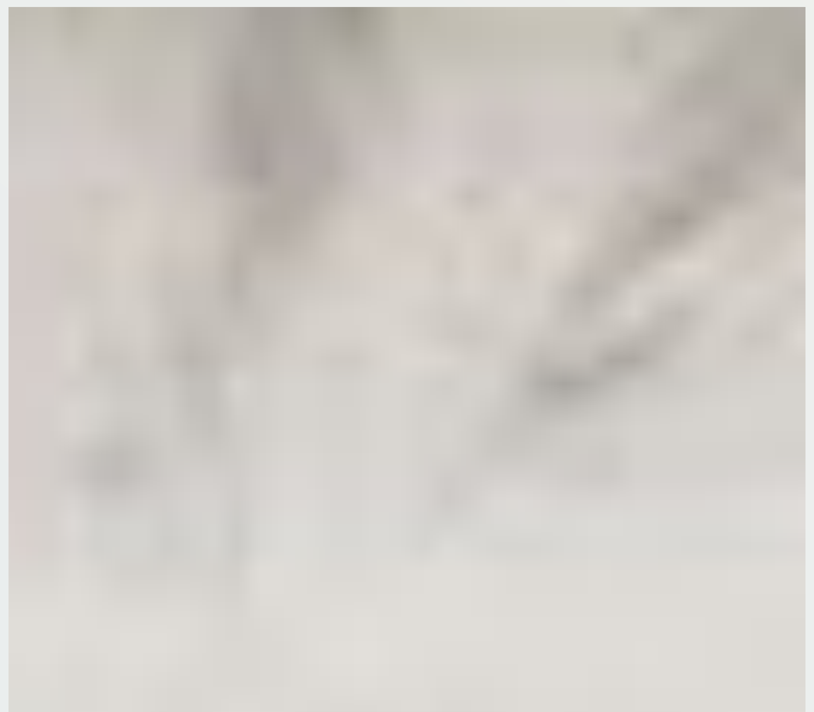
POD

…



What pixels belong to the cat?

50 x 50 pixels x 3 colors = 7500 dimensions…



Cat? No

Jeez, that's hard!

How come you knew before?

Cat? Yes

Context !

Machine Learning

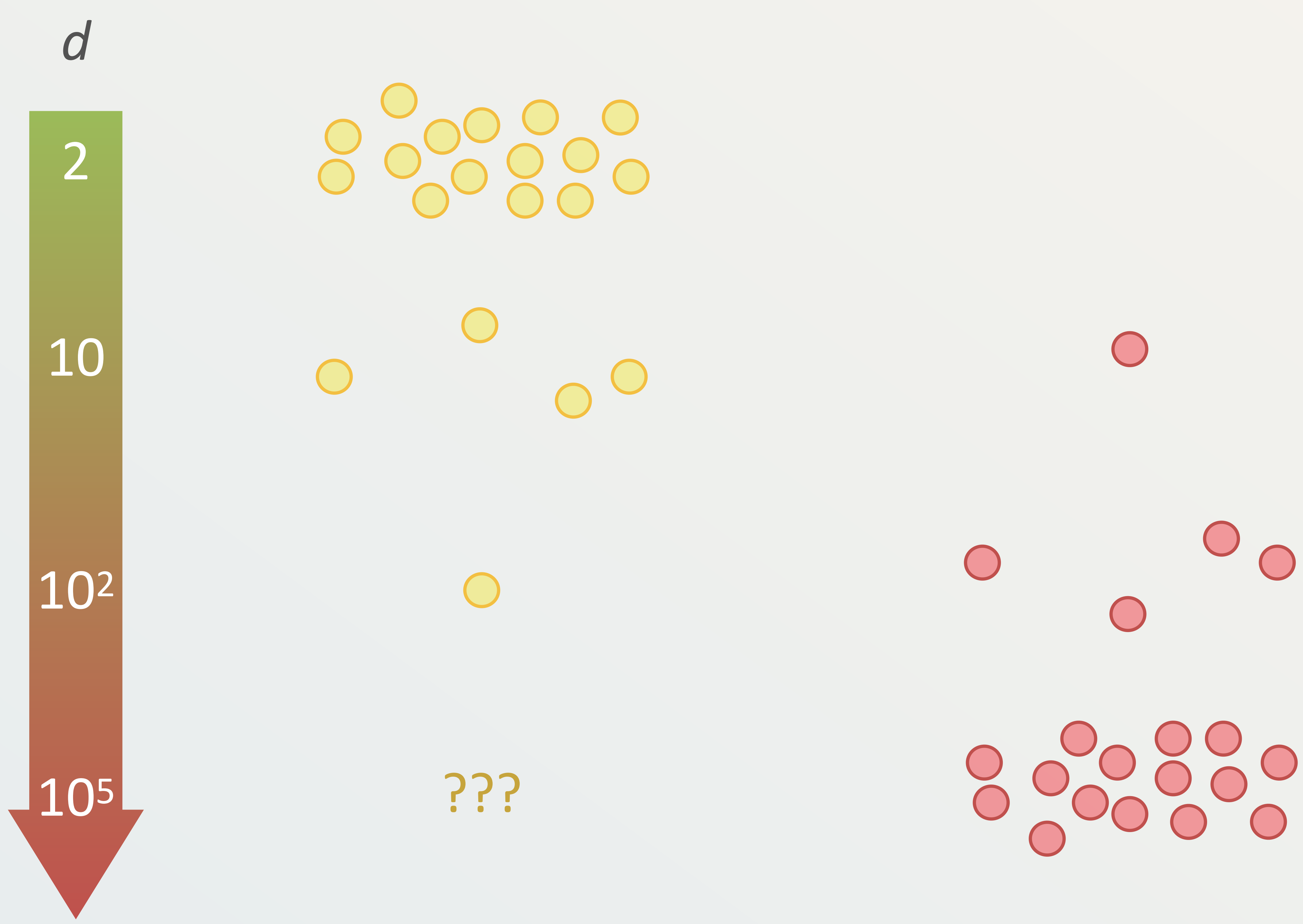
Feature / Representation / Deep Learning

Model?

N number of samples

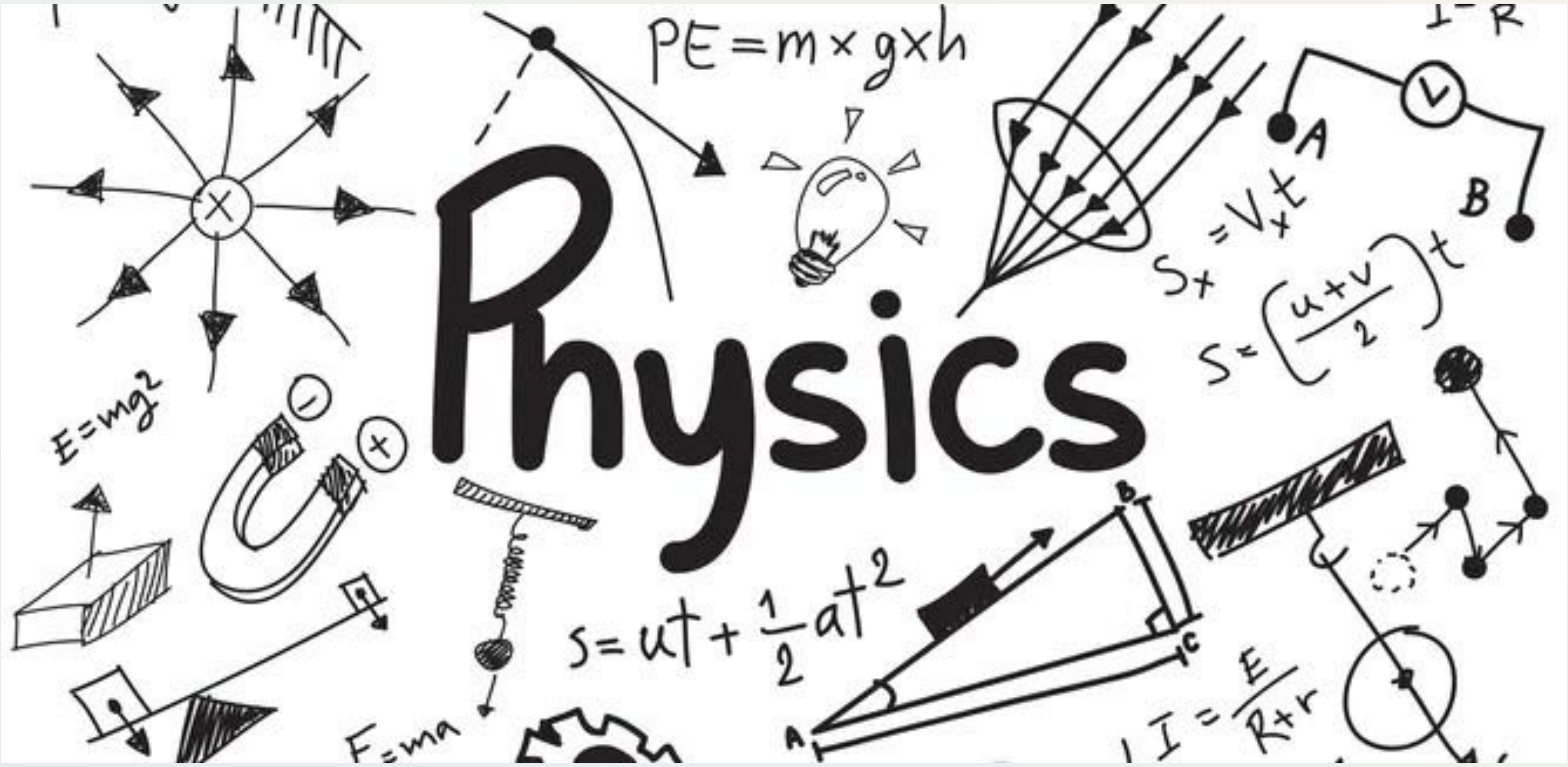
d dimension of *X*

…



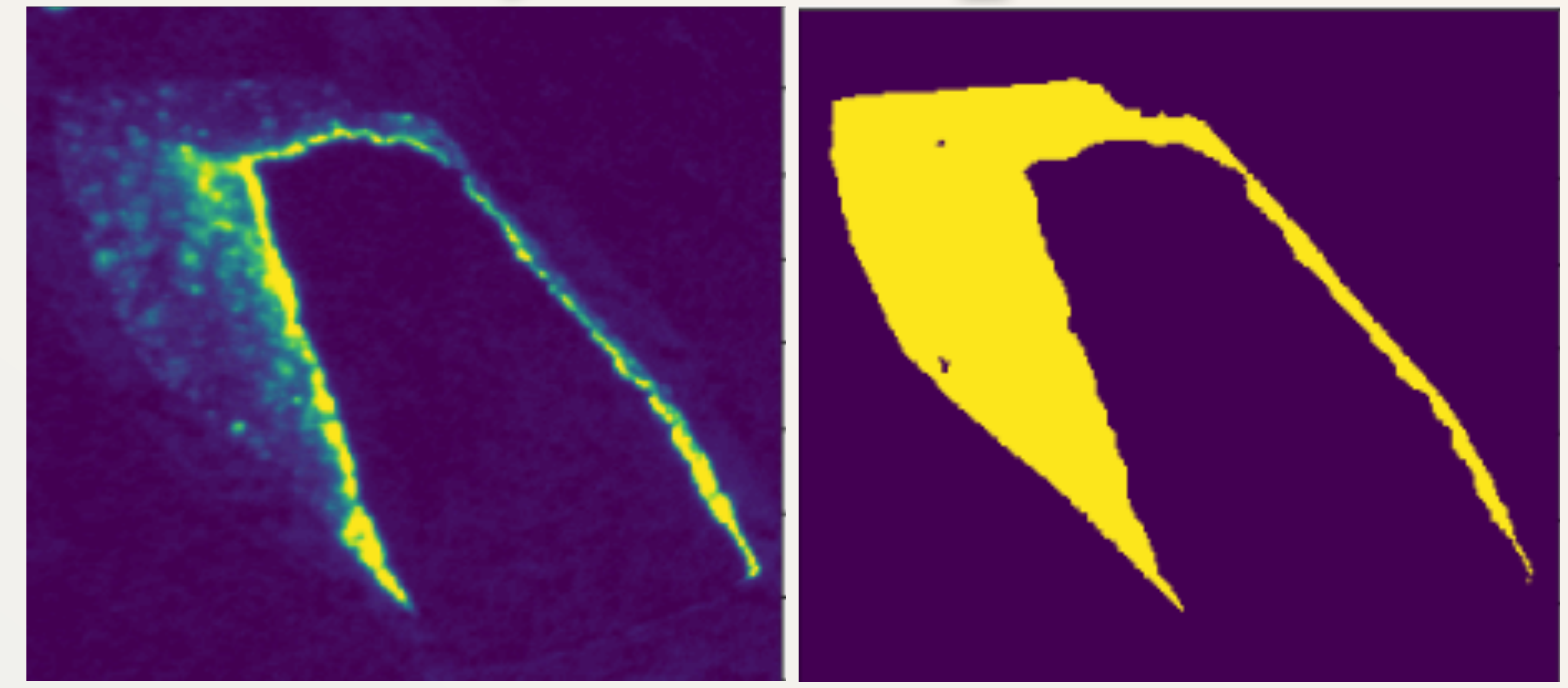
Automatic discovery of representations needed from raw data

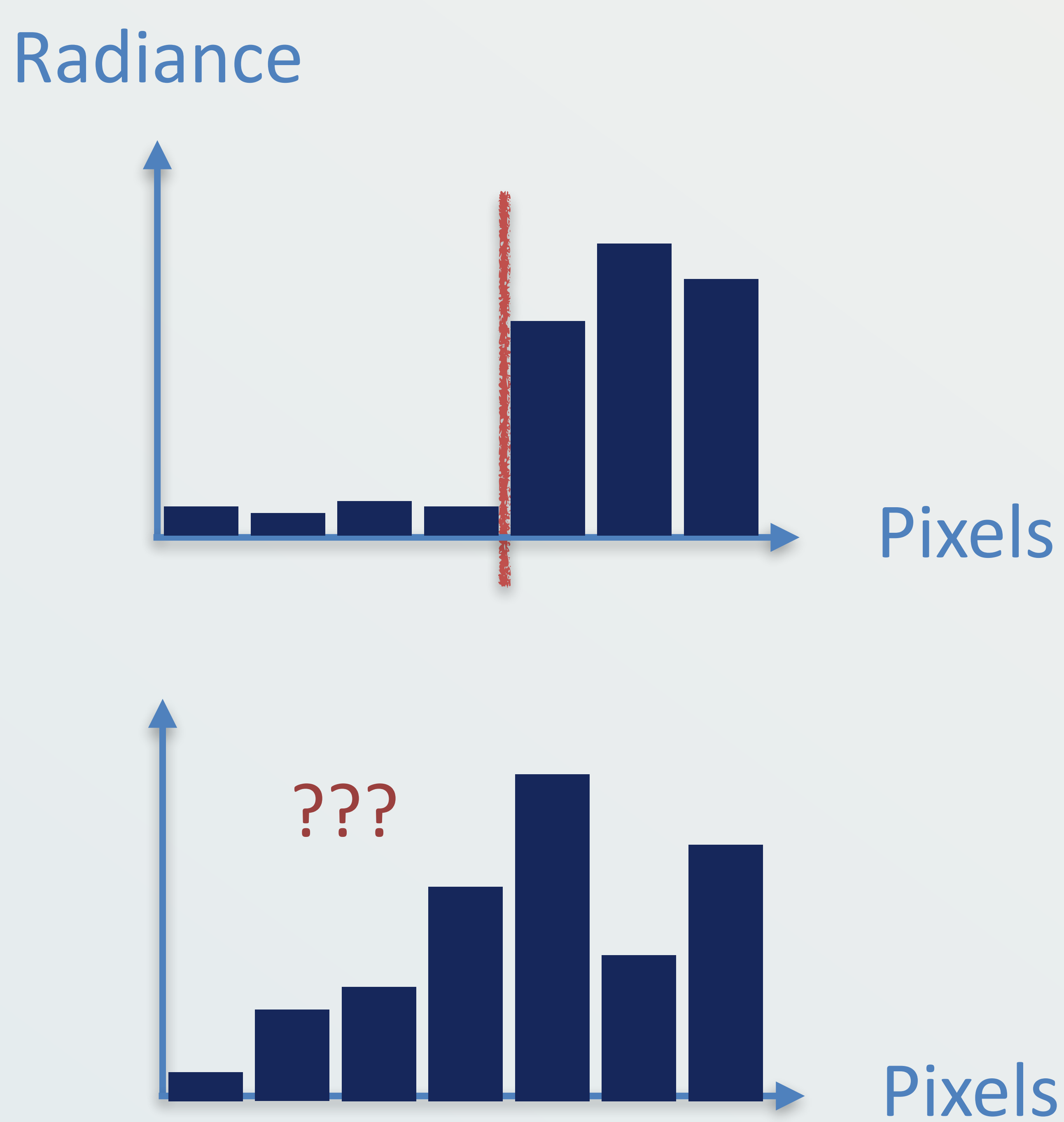
Back to

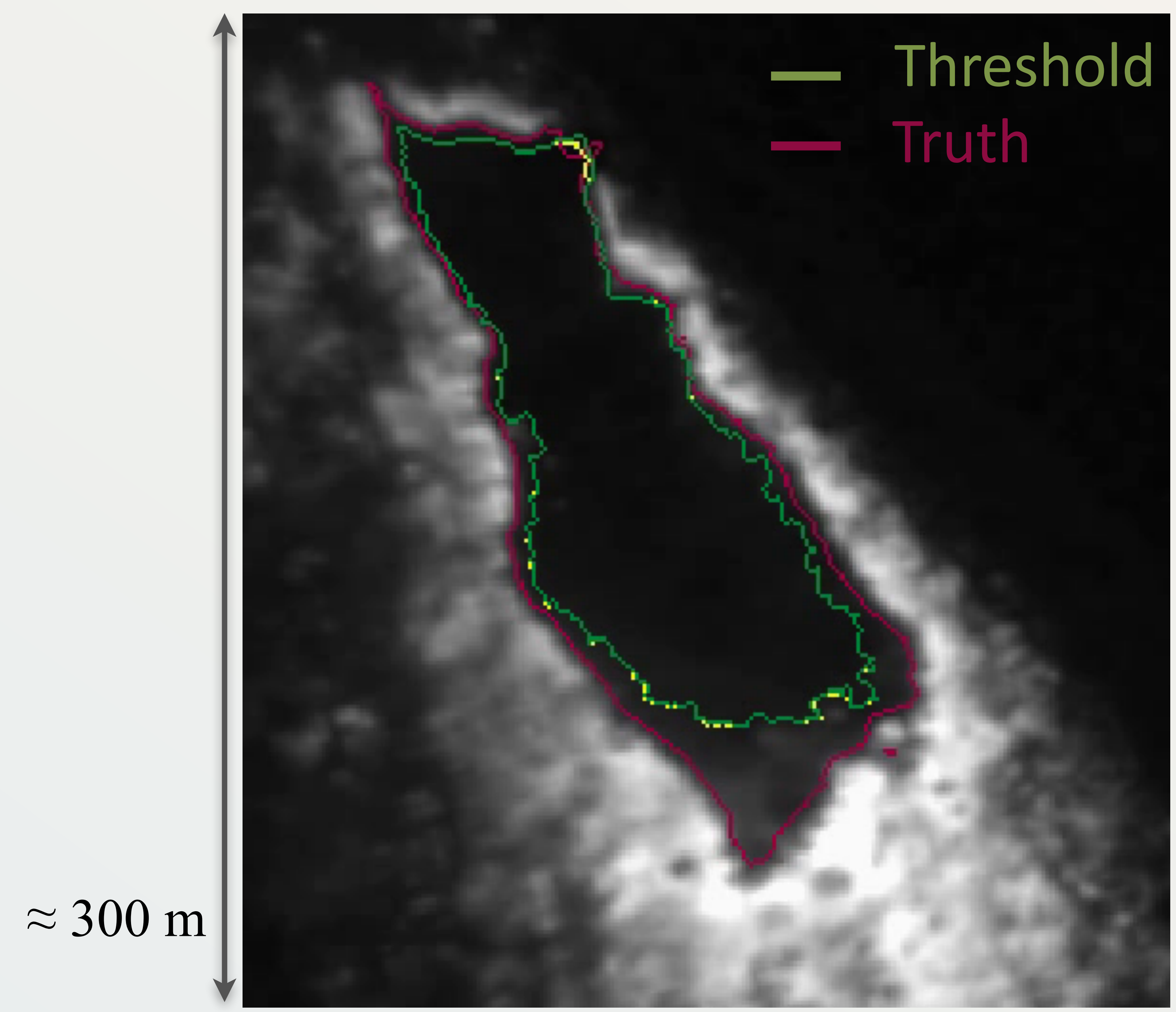


Radiance

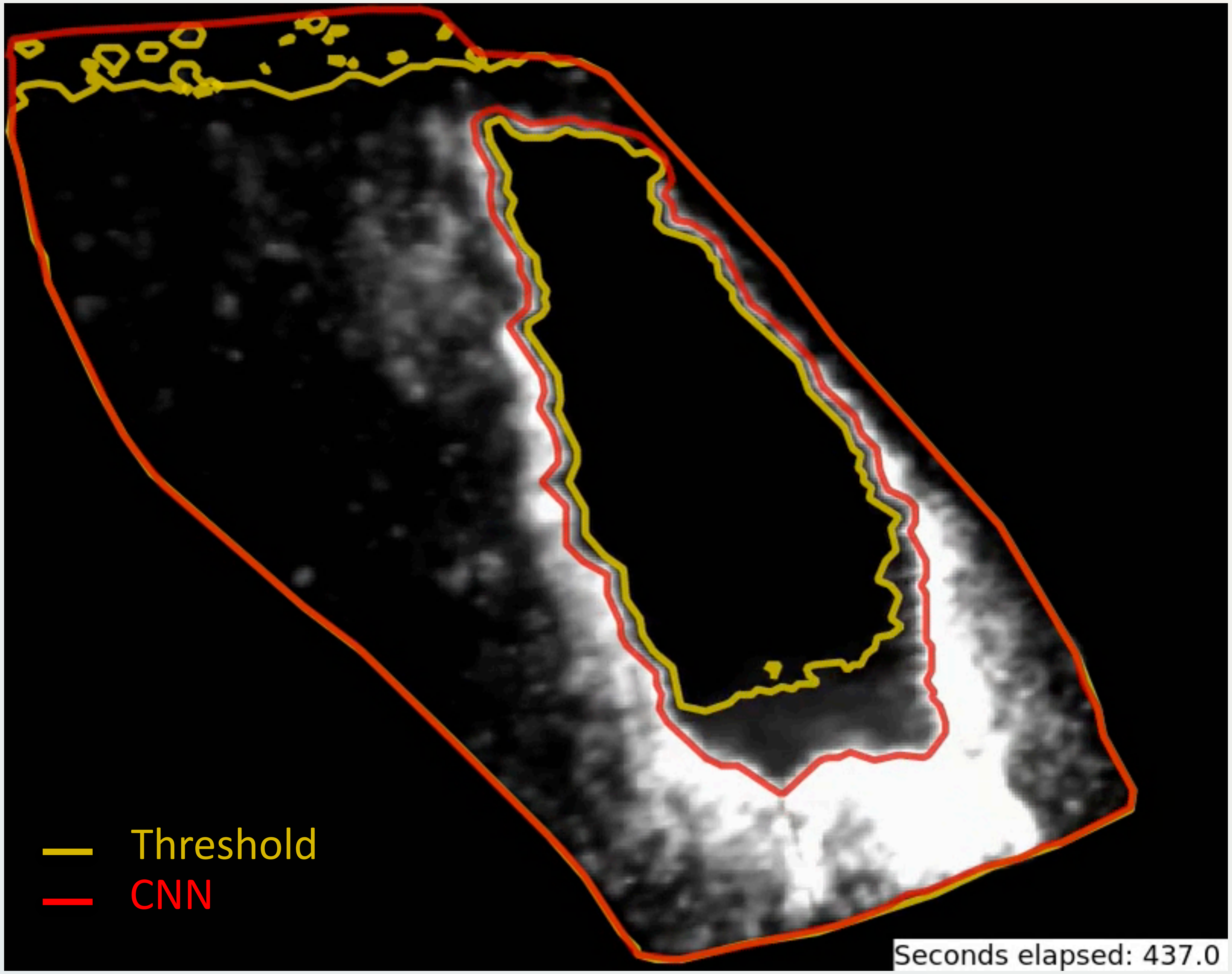
Mask







Fieldwork campaign organized by Prof. Martin Wooster (Dept of Geog. University College London) in Kruger National Park, 2014 South Africa.
Ongoing work performed at Cerfacs by R. Paugam, N. Cazard, M. Rochoux



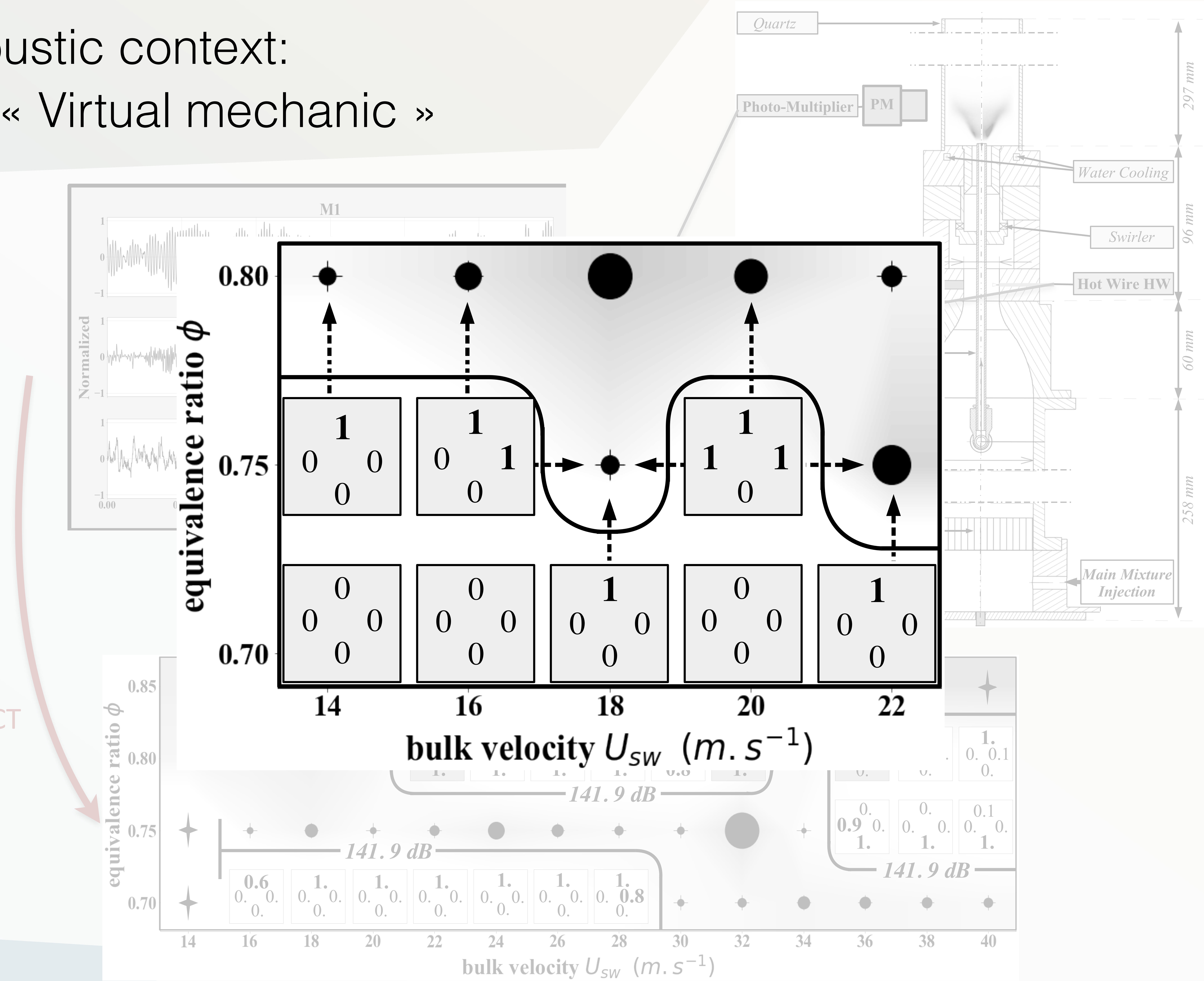
Context awareness is crucial here

Deep Learning enables automatic extraction of features from context

Fieldwork campaign organized by Prof. Martin Wooster (Dept of Geog. University College London) in Kruger National Park, 2014 South Africa.
Work performed at Cerfacs by R. Paugam, N. Cazard, M. Rochoux

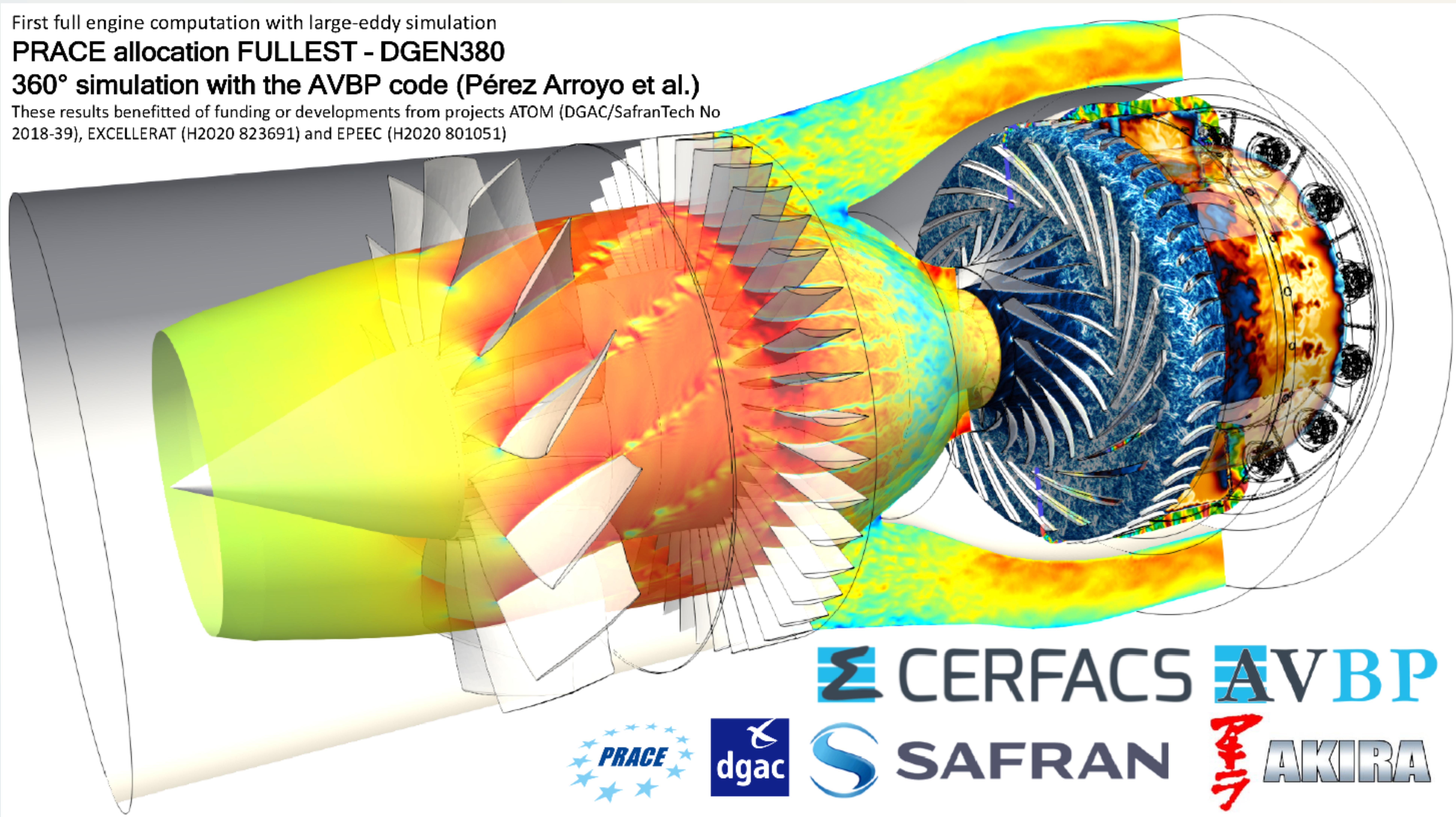
Acoustic context: the « Virtual mechanic »

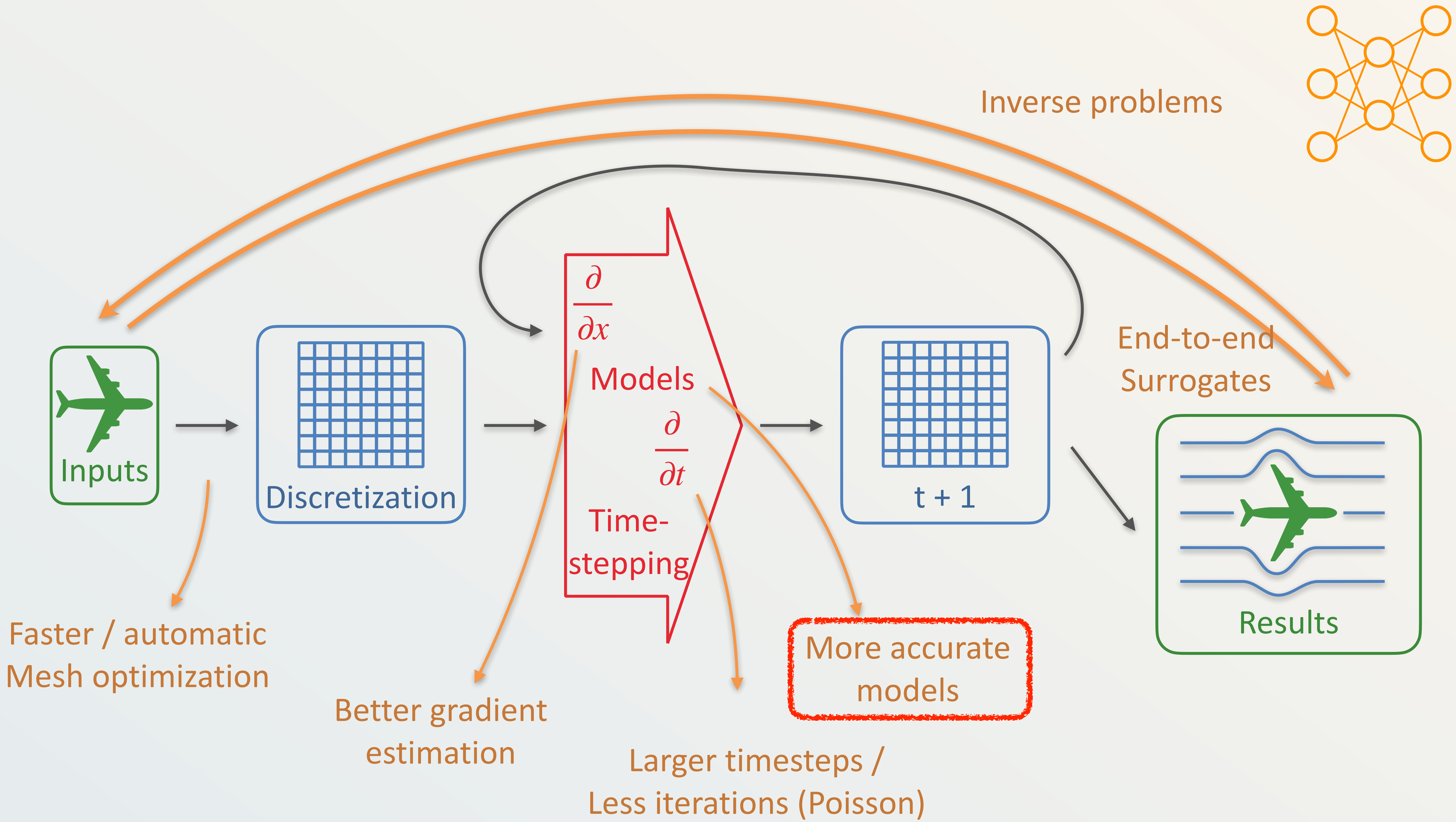
PREDICT



Cellier, A. et al. "Detection of Precursors of Combustion Instability using Convolutional Recurrent Neural Networks" Combustion and Flame (accepted for publication) (2021).

What about CFD?

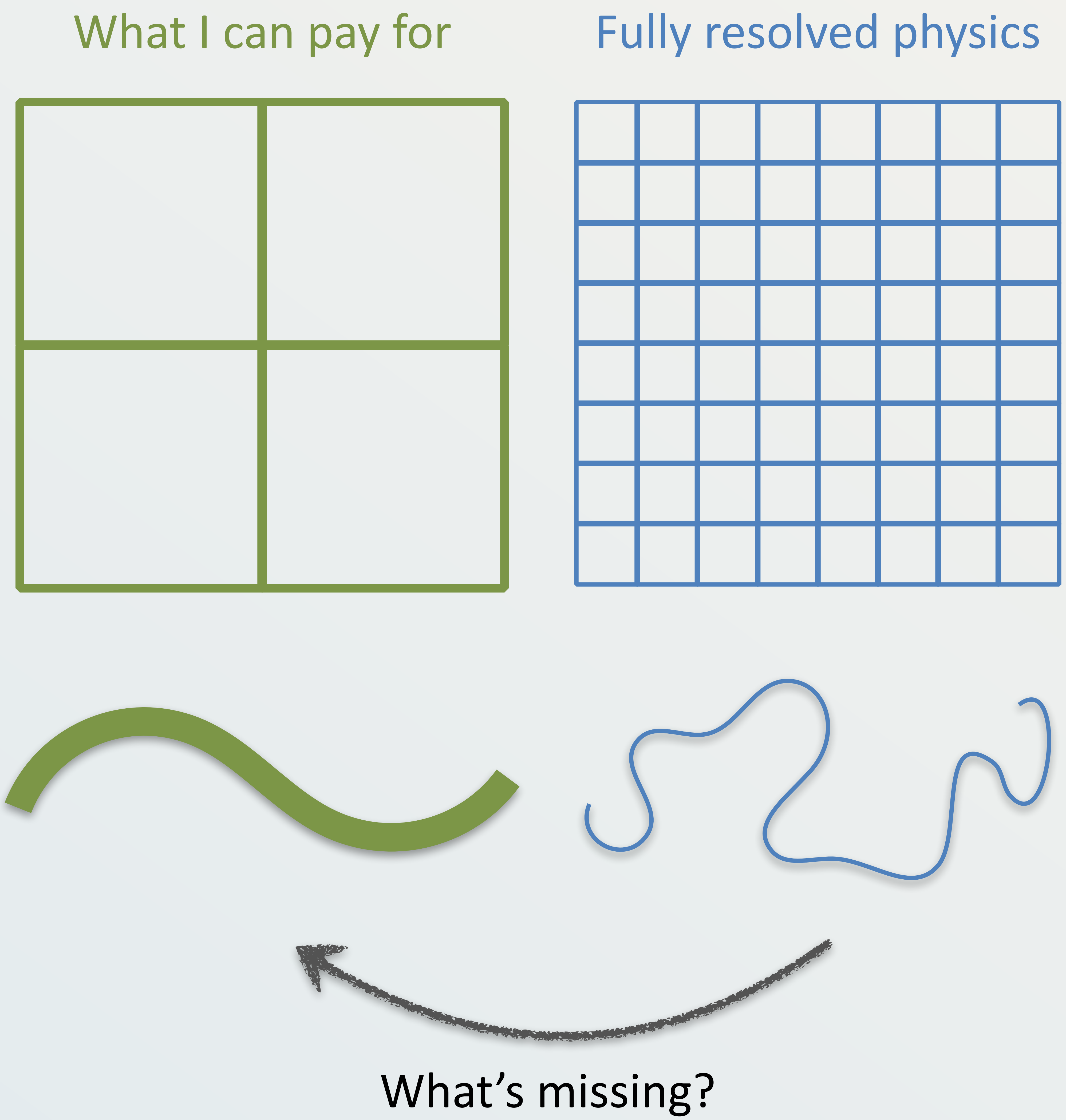


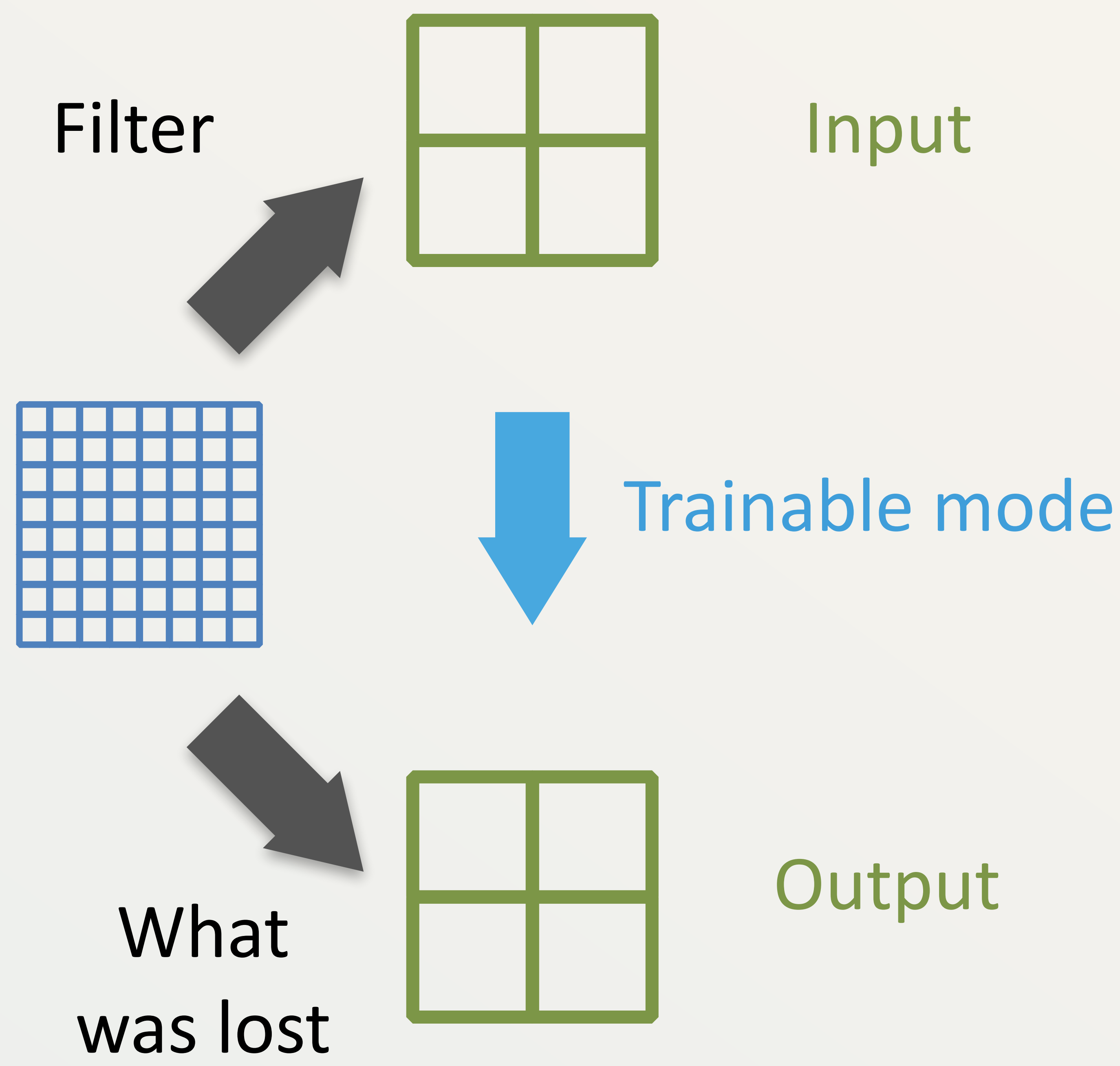


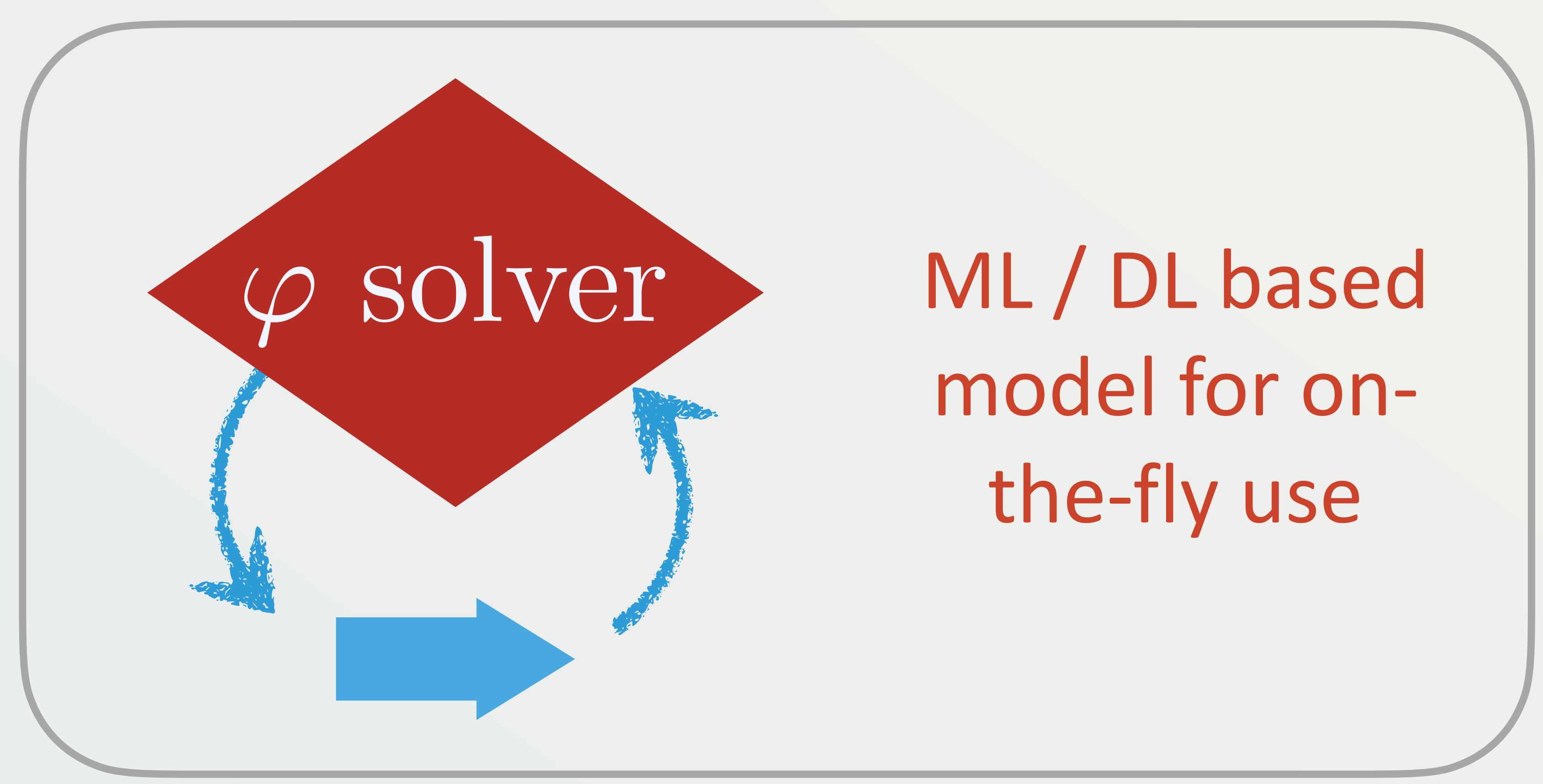
Where should we look?
Unclear: literature still hesitant

Much research on hybrid techniques

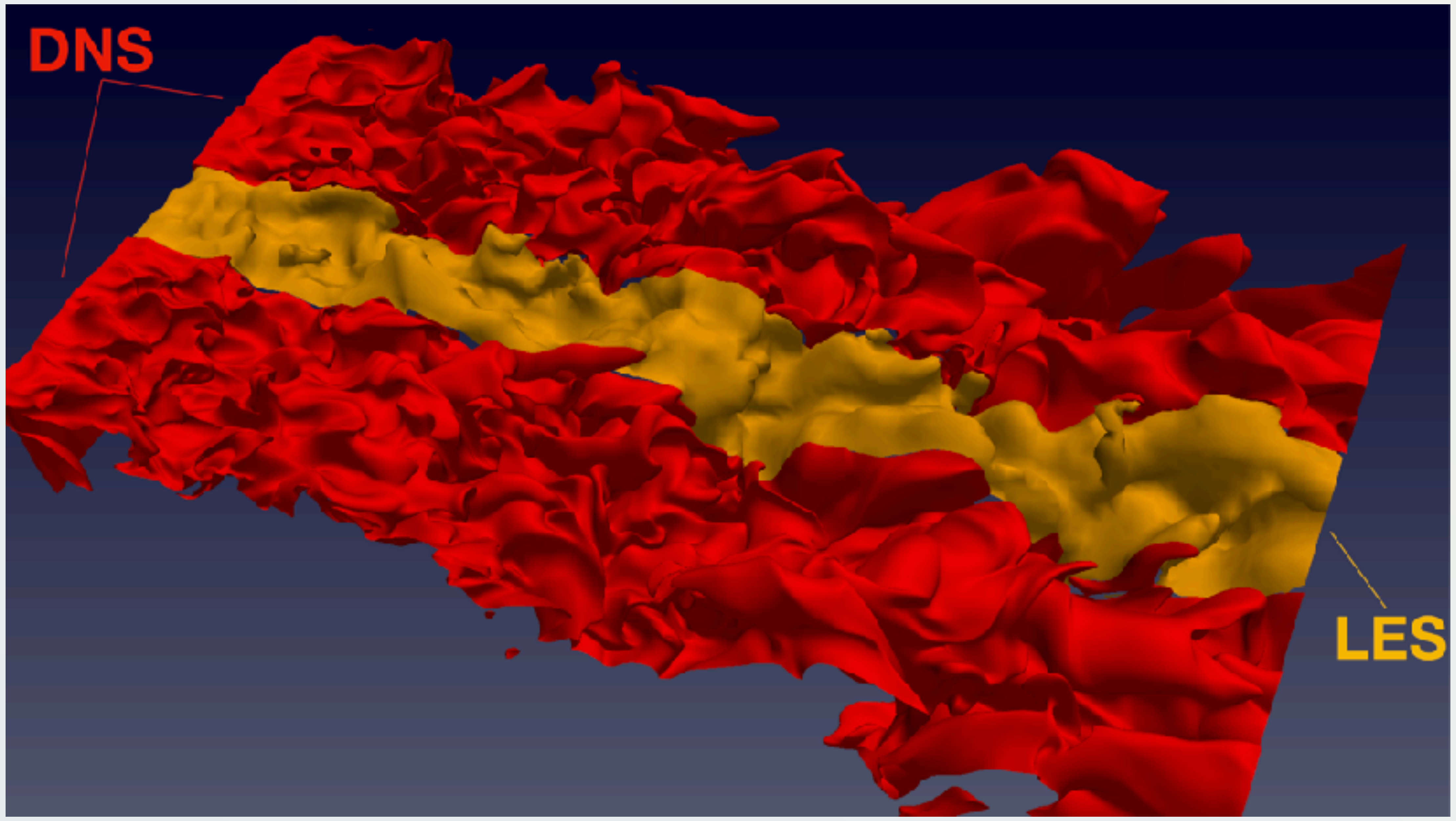
Subgrid-scale models

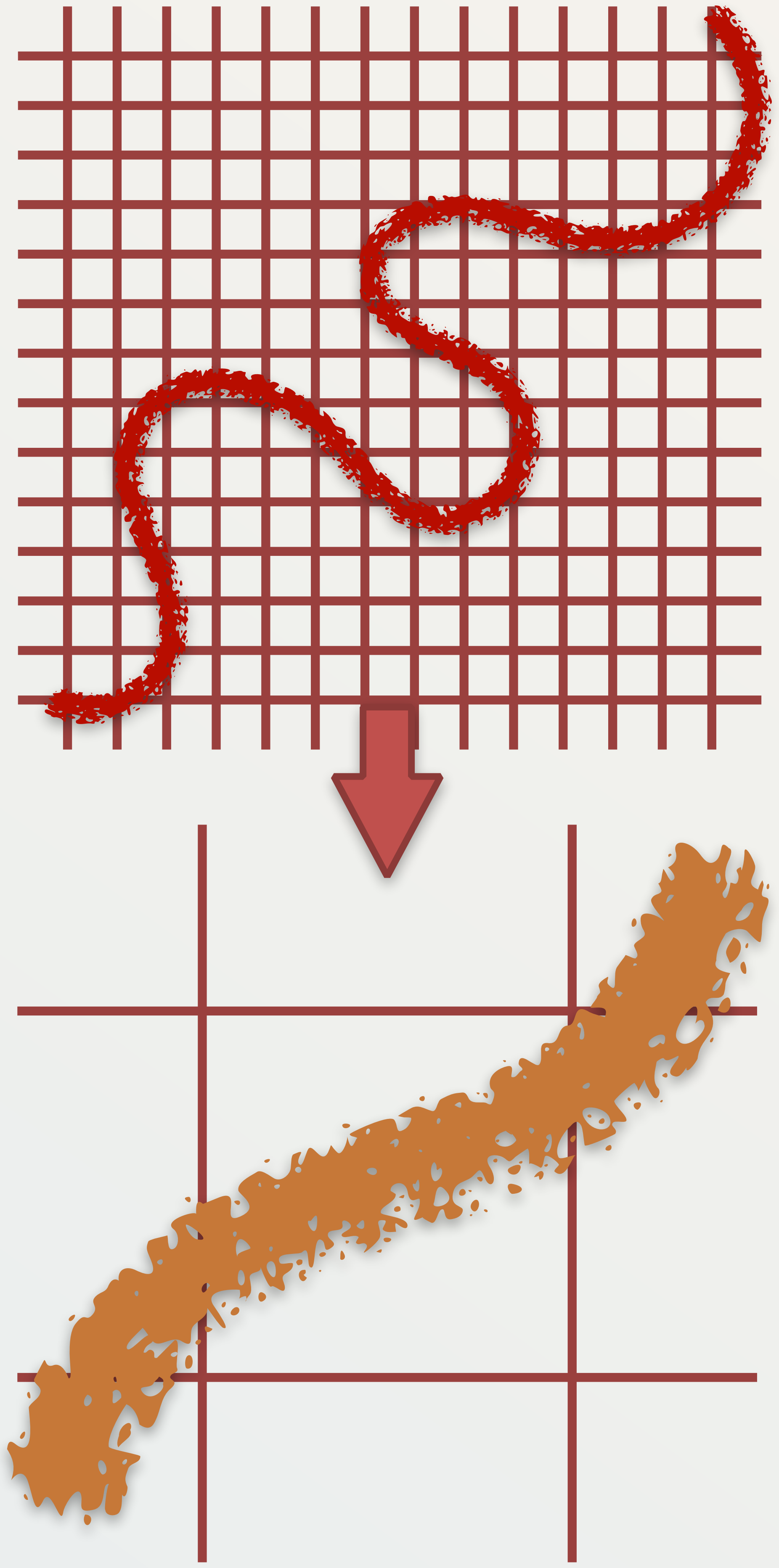






Combustion SGS





DNS: Resolved flame

LES: *e.g.* Artificially thickened flame [1]

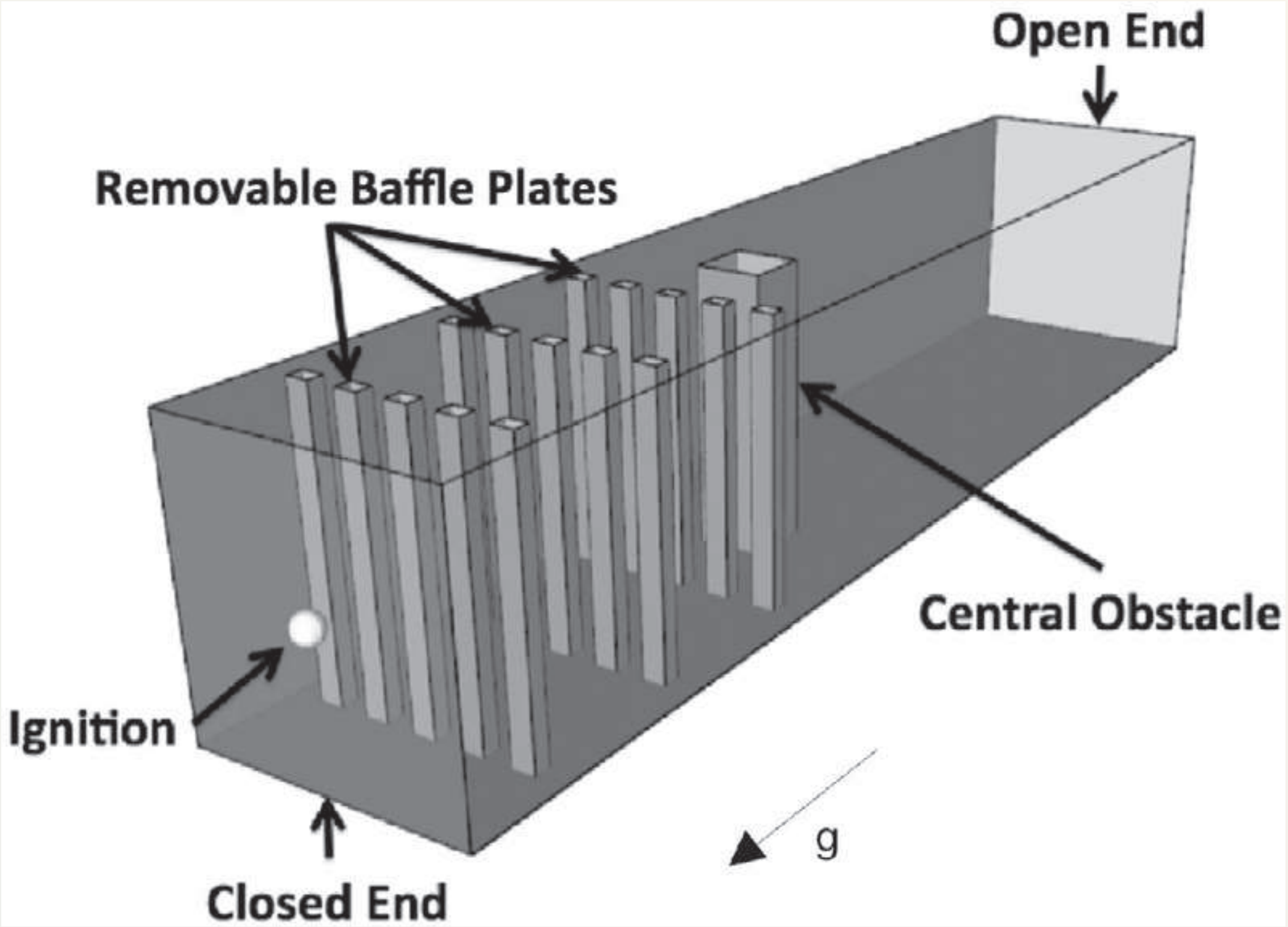
[1] Butler, T. D. & O'Rourke, P. J. (1977). Symp. (Int.) Combust. 16, 1503 – 1515.

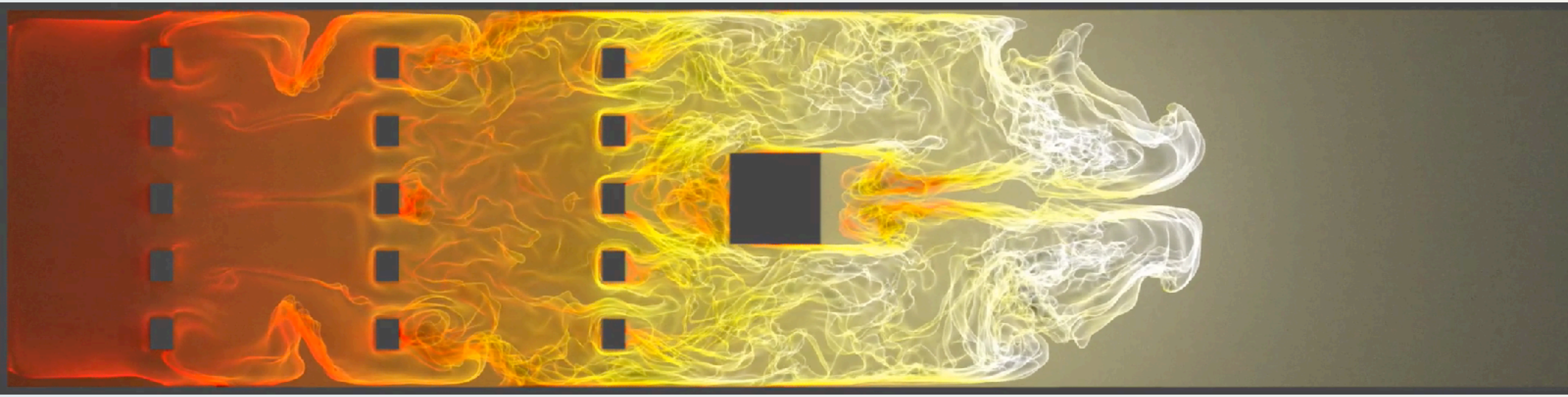
Ongoing PhD of Victor Xing, Cerfacs

Very large scale combustion

- Context: safety of industrial complexes in combustible gas leaks

- Reactive LES of very large domains (LEFEX: EDF, AirLiquide, Total)





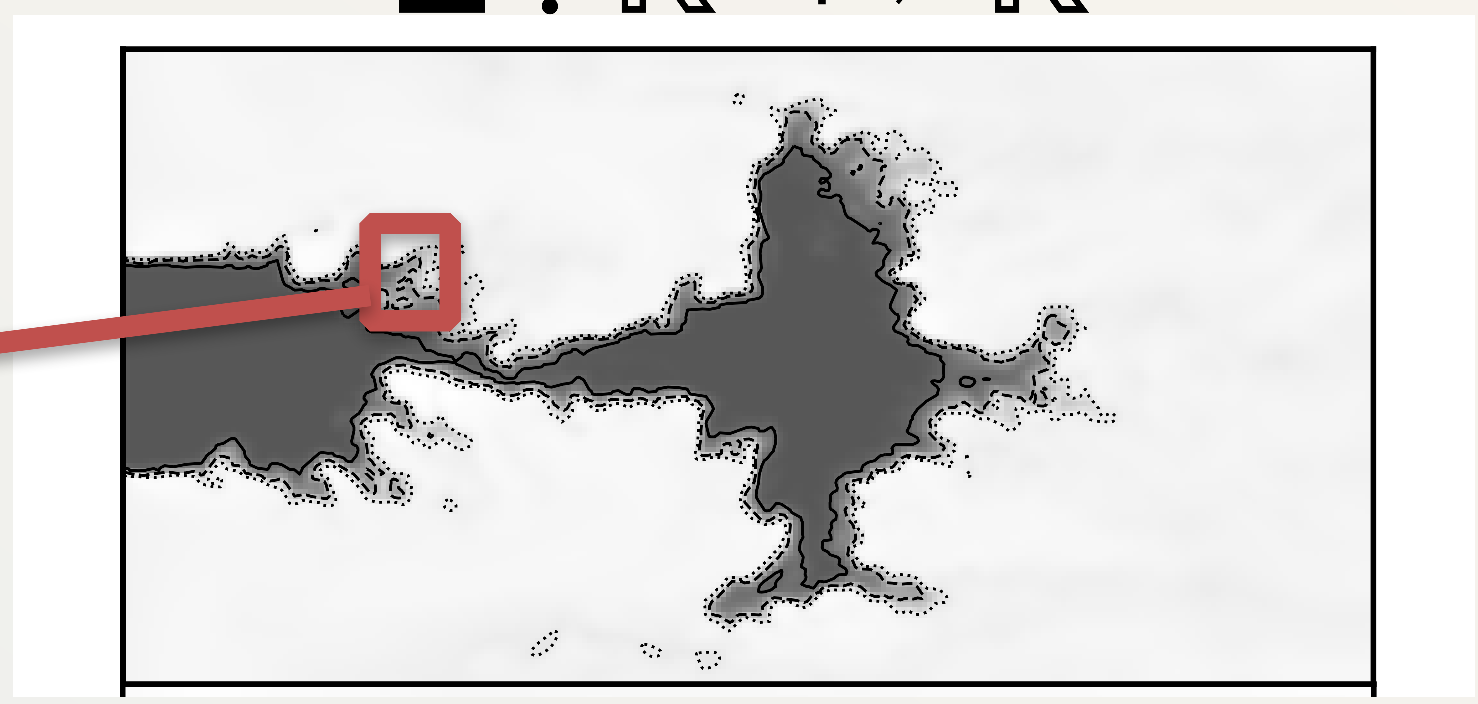
E. Gullaud & Q. Douasbin, Post-Docs

Efficiency functions f - local to global

LOCAL FORMULATIONS:

- 1989 - Gouldin (fractal)
- 2000 - Colin *et al.*
- 2002 - Charlette *et al.*

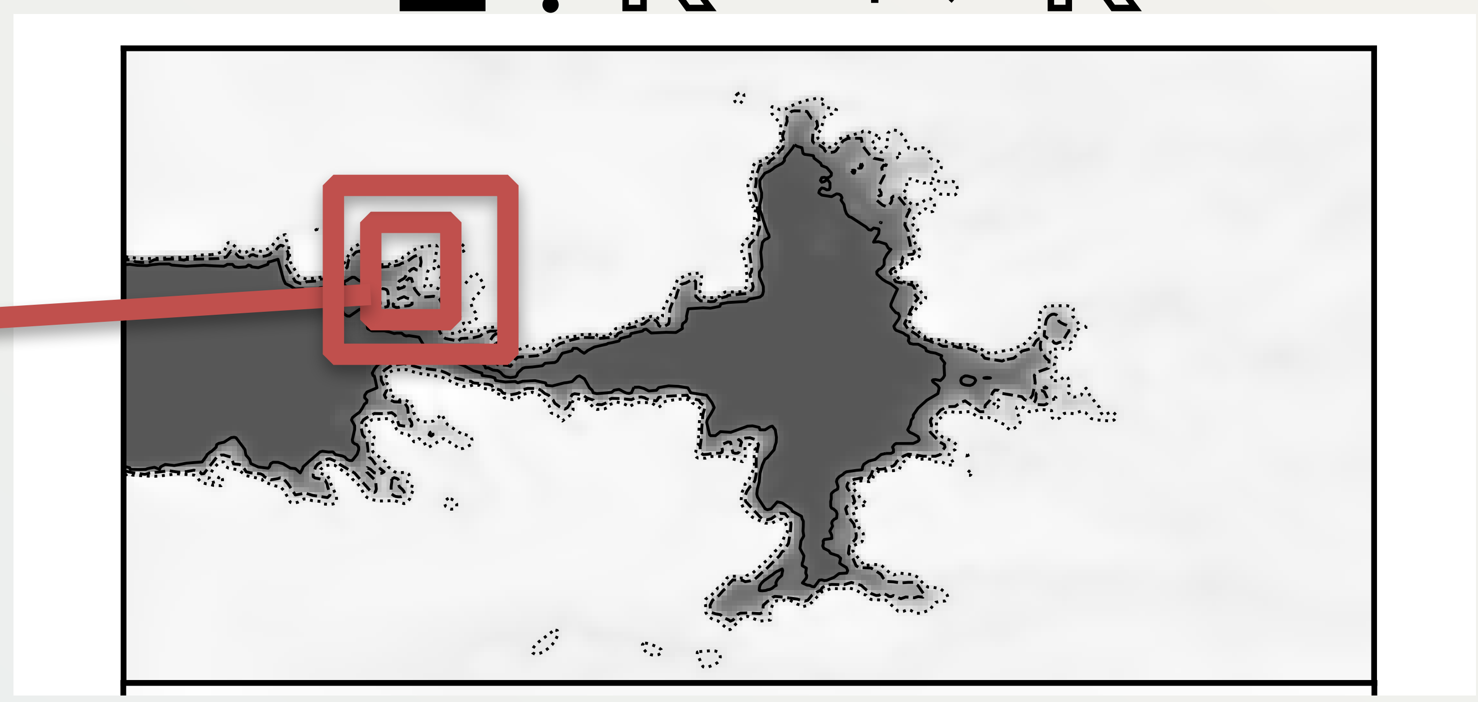
$$\Xi : \mathbb{R}^k \mapsto \mathbb{R}$$



DYNAMIC FORMULATIONS:

- 2011 - Wang *et al.*
- 2015 - Veynante & Moureau

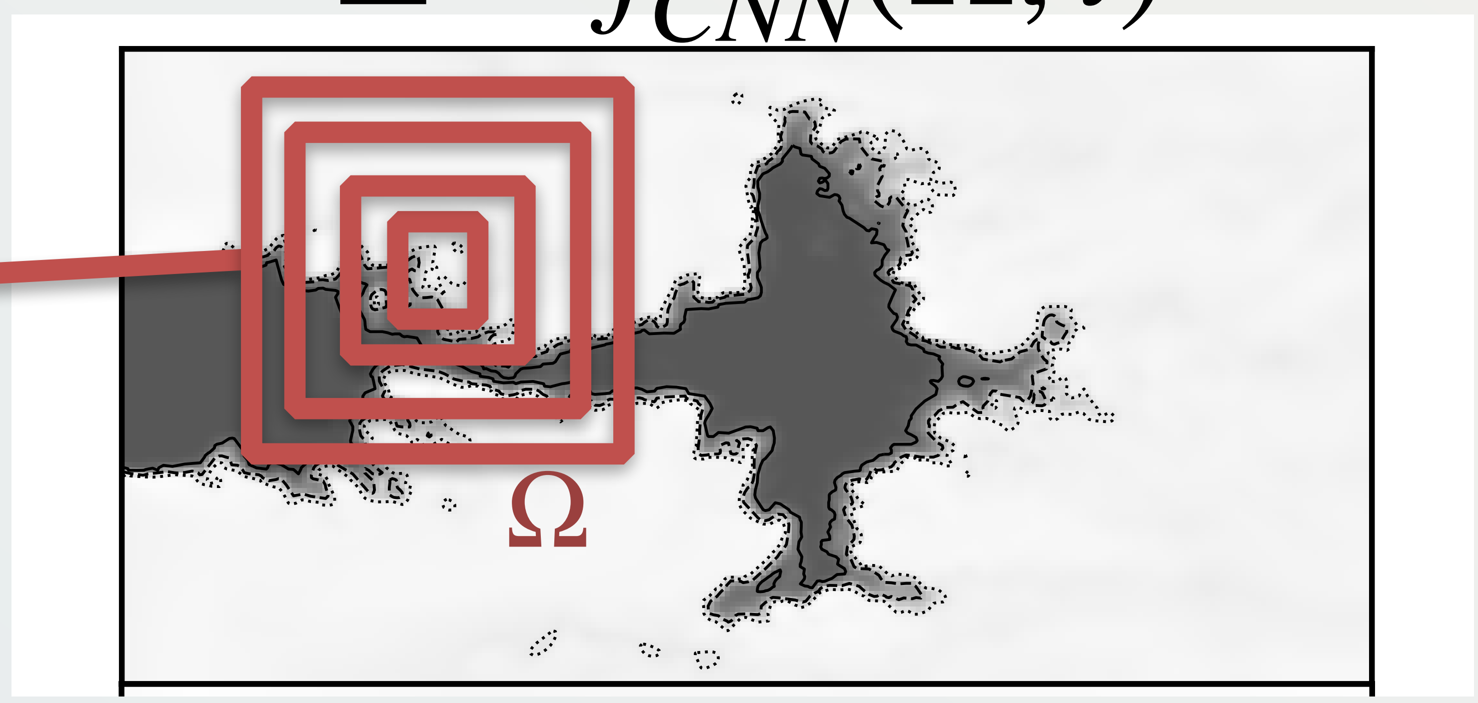
$$\Xi : \mathbb{R}^{2k} \mapsto \mathbb{R}$$



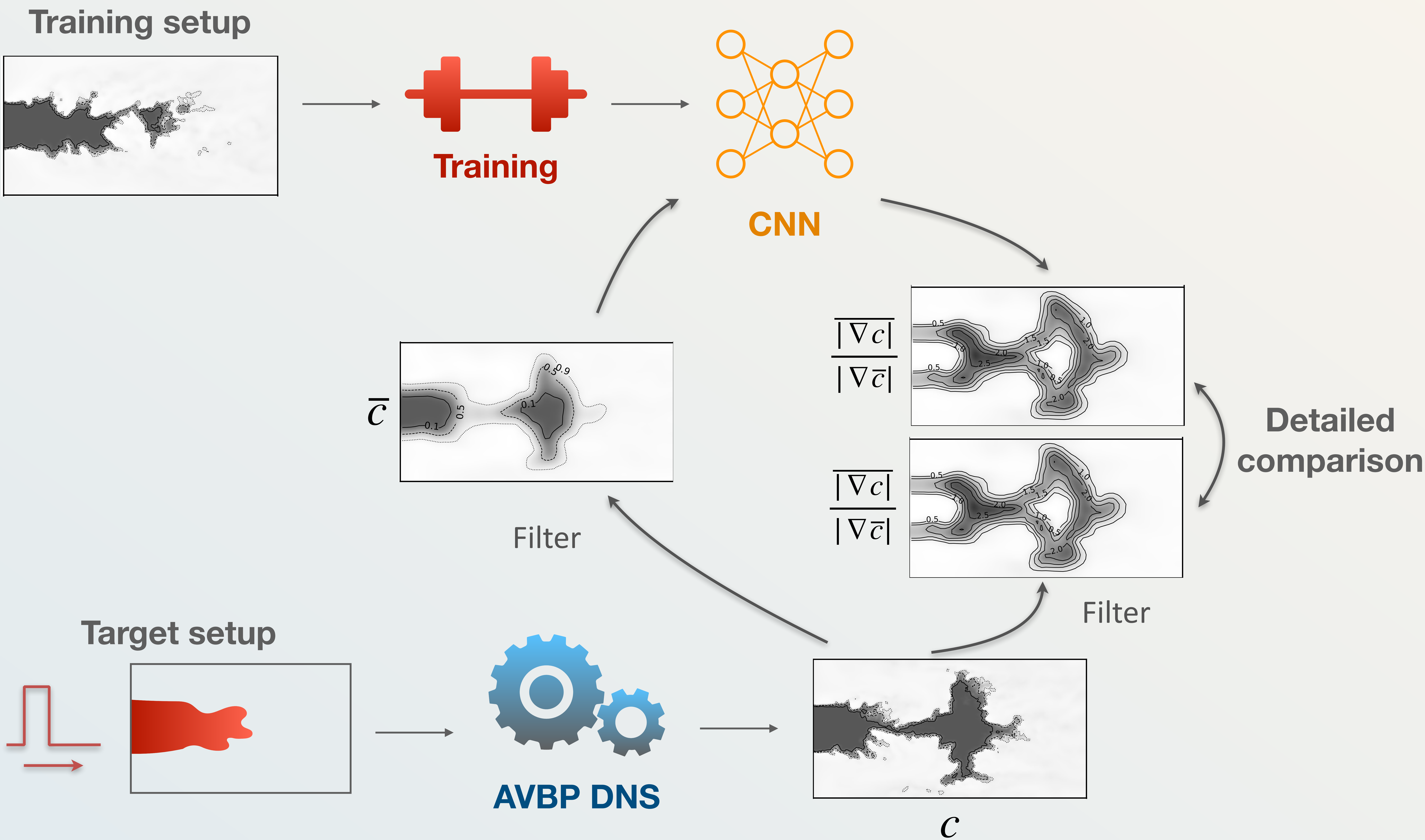
CNN FORMULATION:

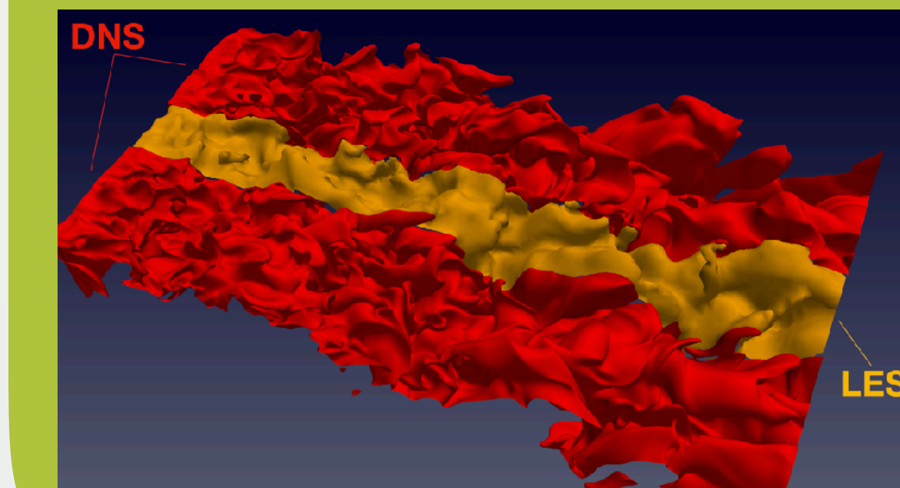
- 2019 - Lapeyre et al.

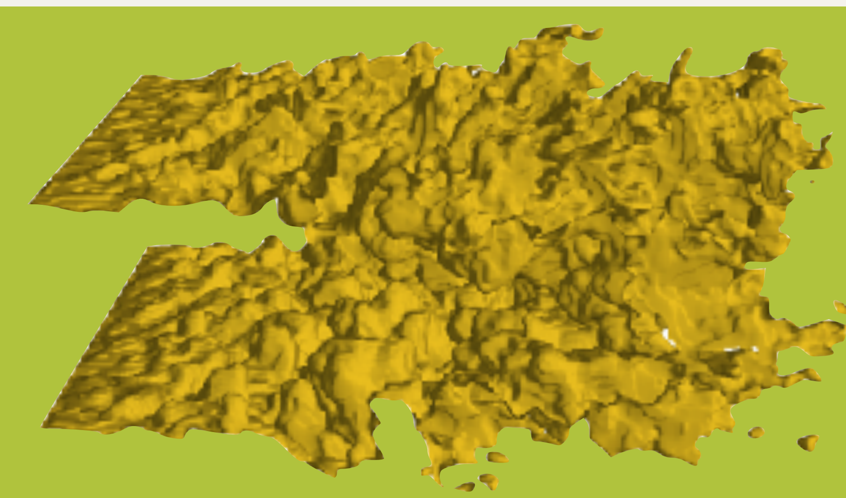
$$\Xi = f_{CNN}(\Omega, t)$$

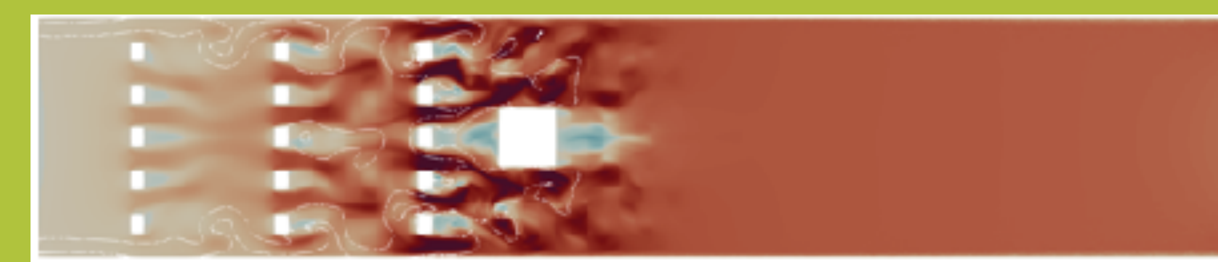


A priori strategy

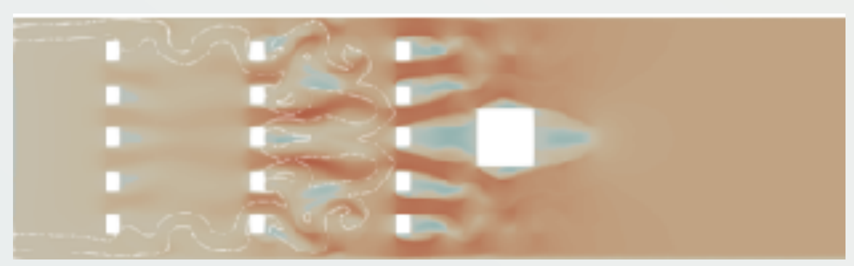
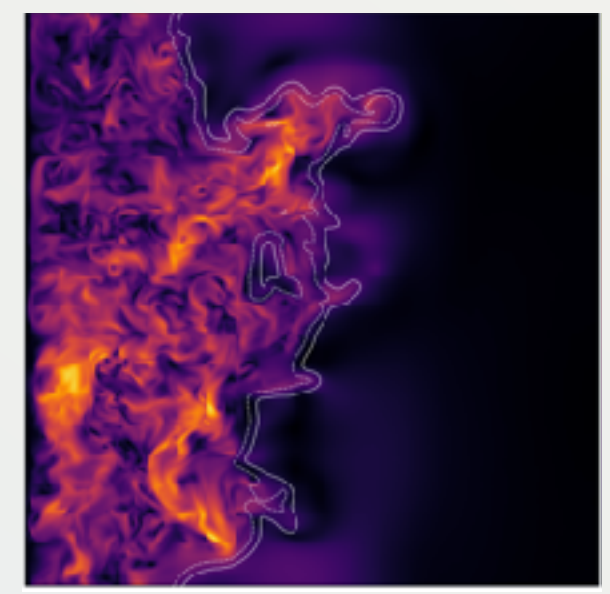




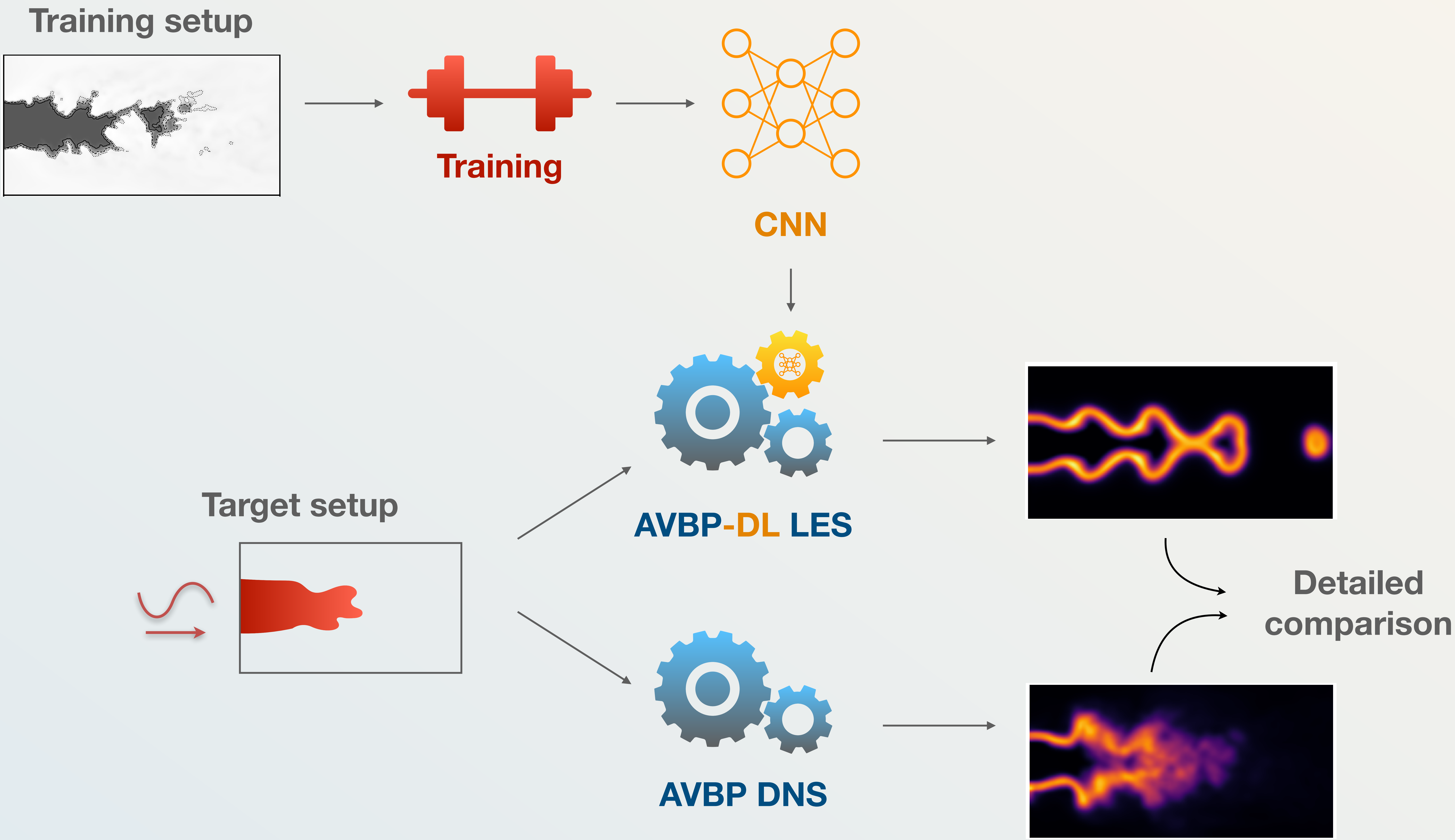




Training Database

Testing Database	 Similar config	 Different config
Differences	Turbulent realisation Flow dynamics Geometry variations …	Flow regimes Chemistry Geometry Scale …
	Close generalisation	Further generalisation

A posteriori strategy



AVBP-DL LES

CPU : Navier-Stokes solver
(AVBP)

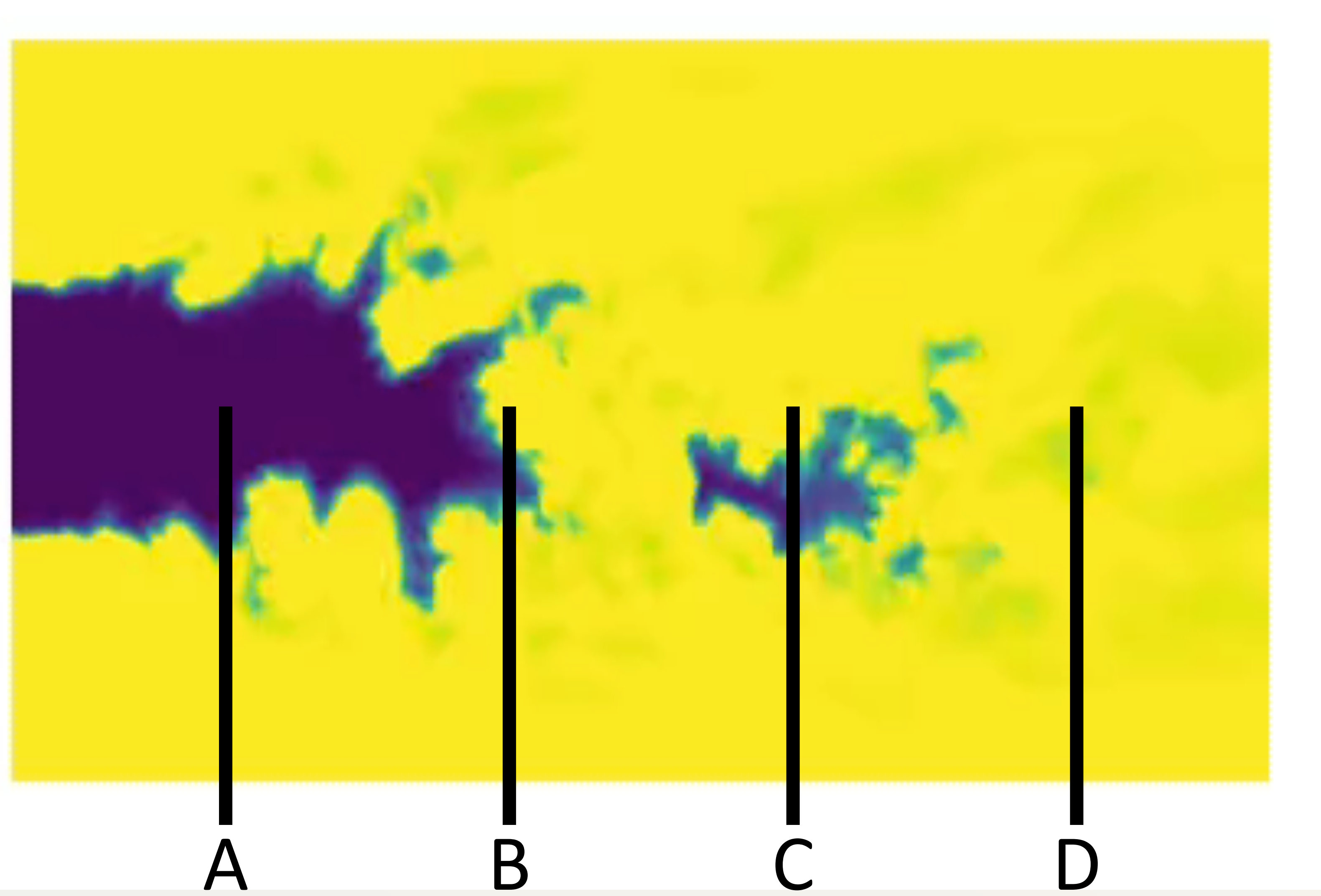
$\overline{c}$

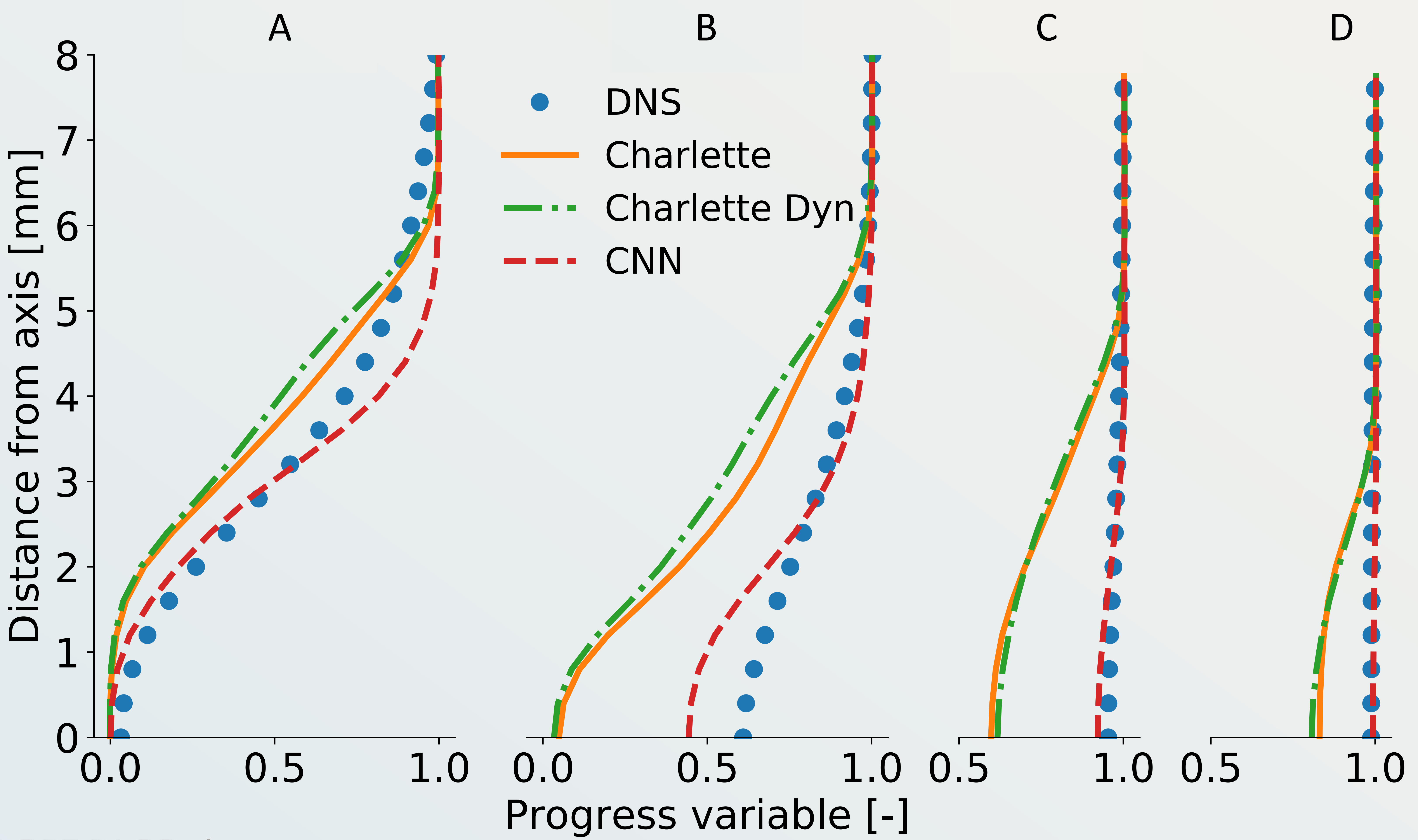
$f_{CNN}(\overline{c})$

GPU : CNN
(TensorFlow)

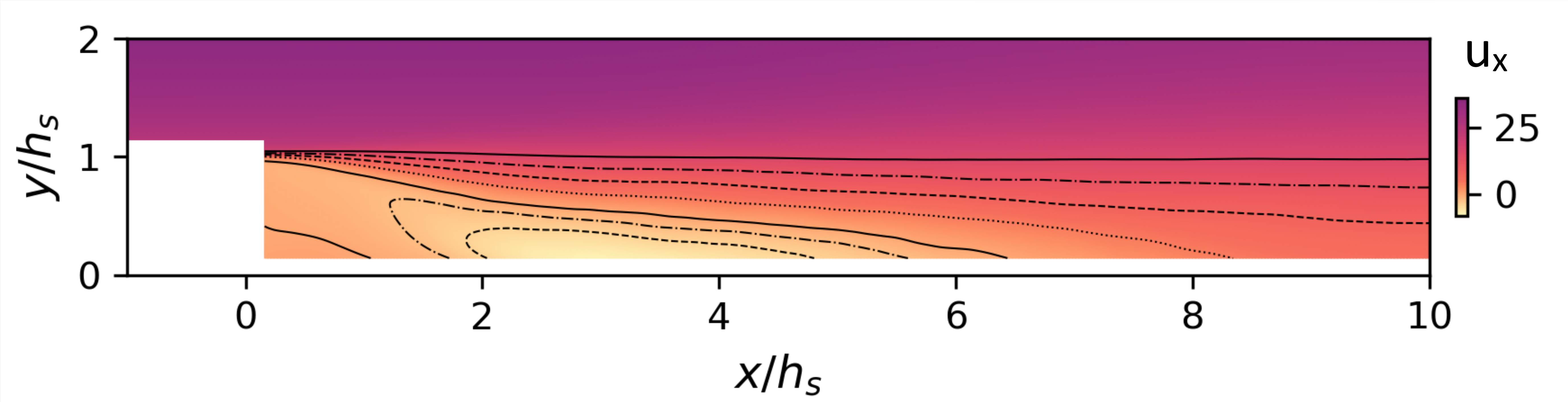
A posteriori results

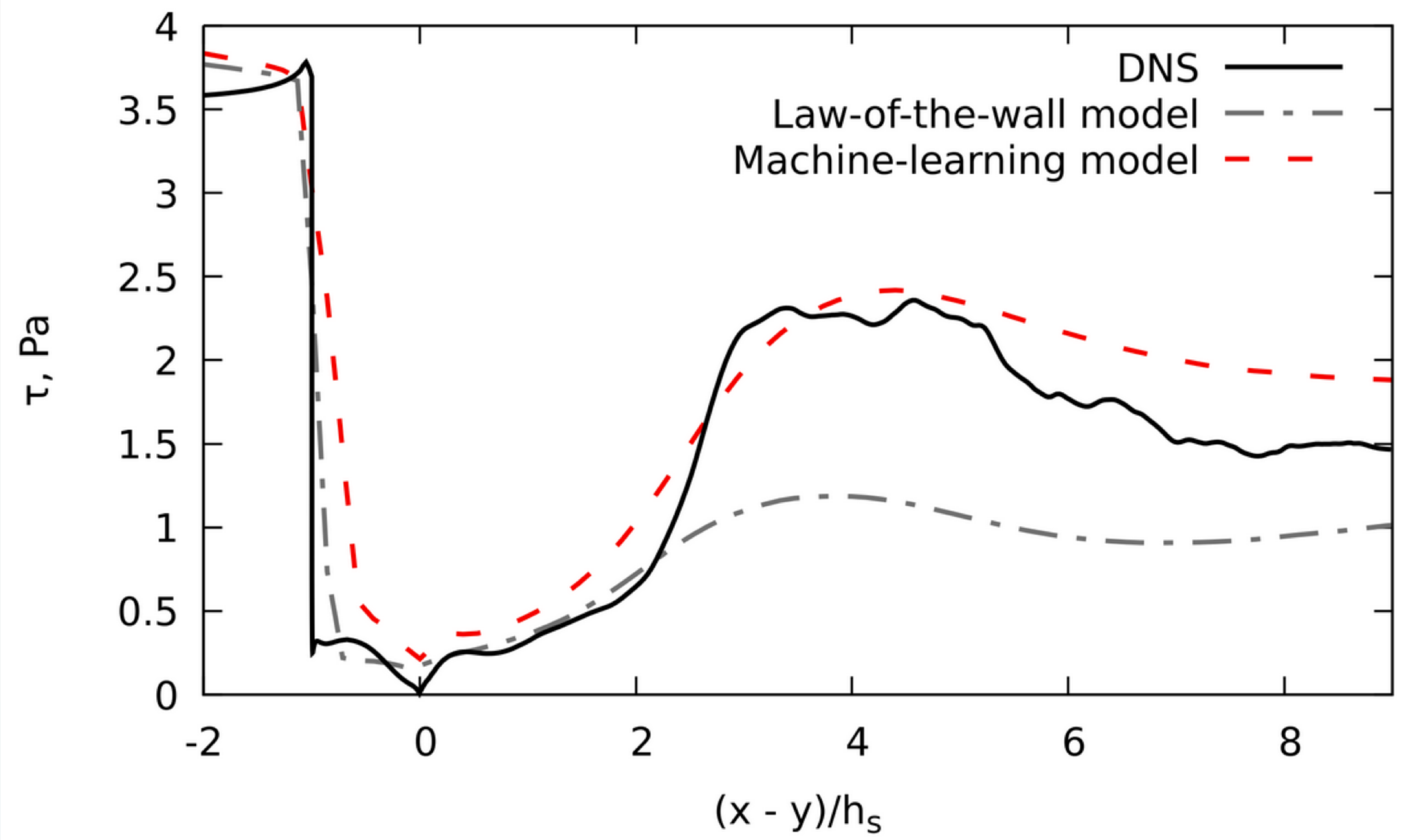
- CNN performs better than than state-of-the-art models on this setup



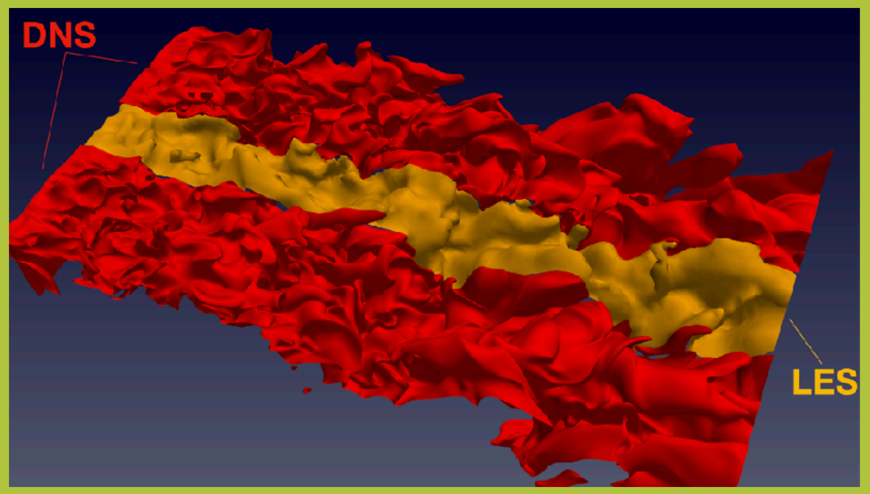


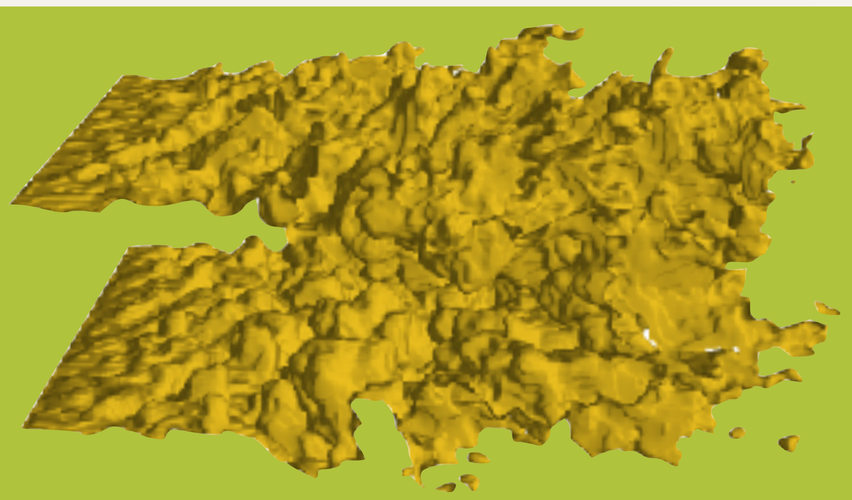
A posteriori

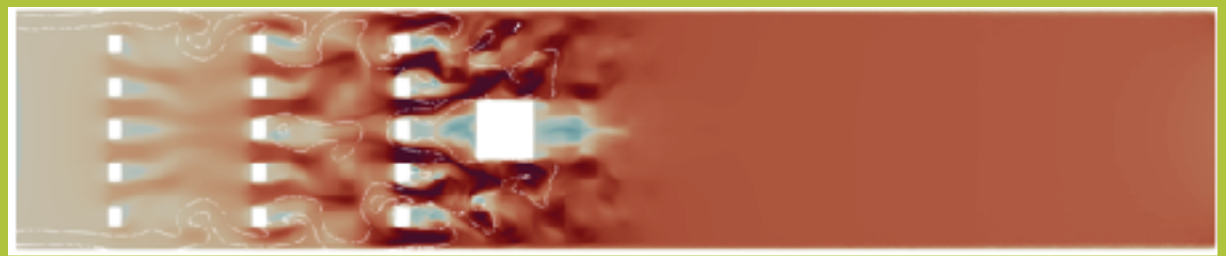


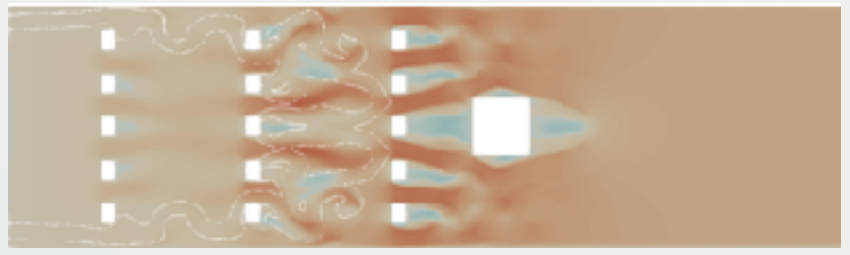
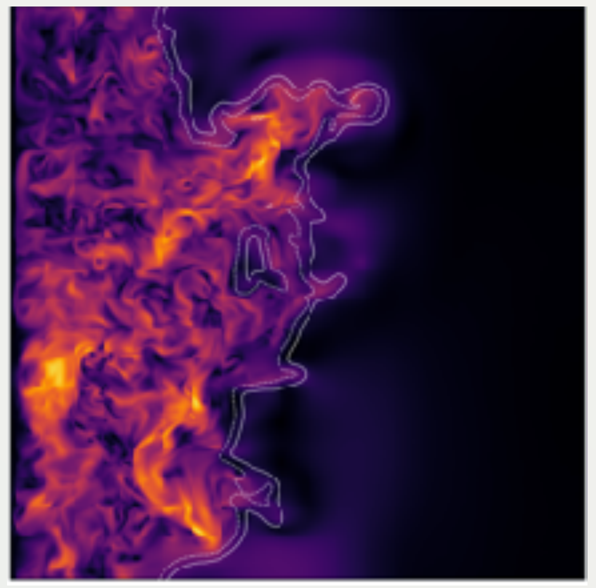
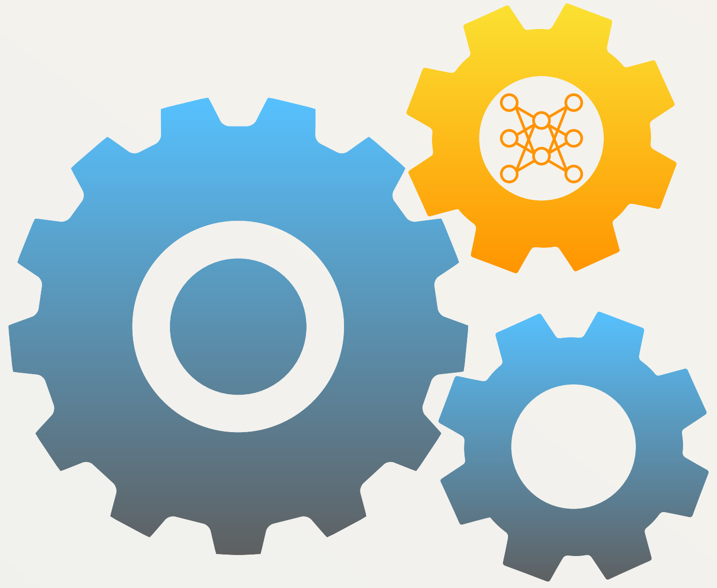


Training Database



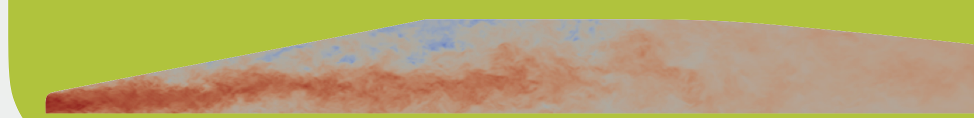




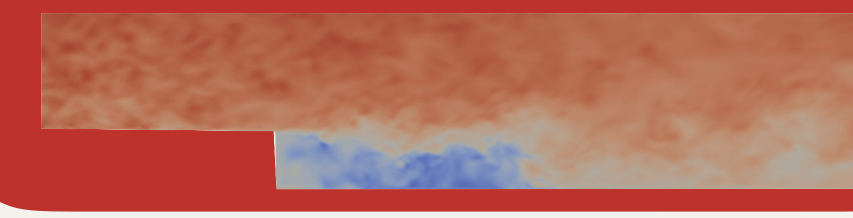
	Similar config	Different config	In-solver
Testing Database			
Differences	Flow dynamics Geometry variations …	Flow regimes Chemistry Geometry Scale …	
	Close generalisation	Further generalisation	Does the learning still hold in a feedback loop? Solver <-> Model
	A priori		A posteriori

Post-mortem

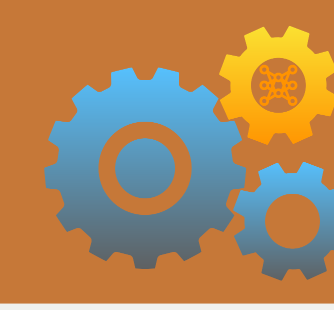
Training Database



A priori Testing



A posteriori Testing



In the loop

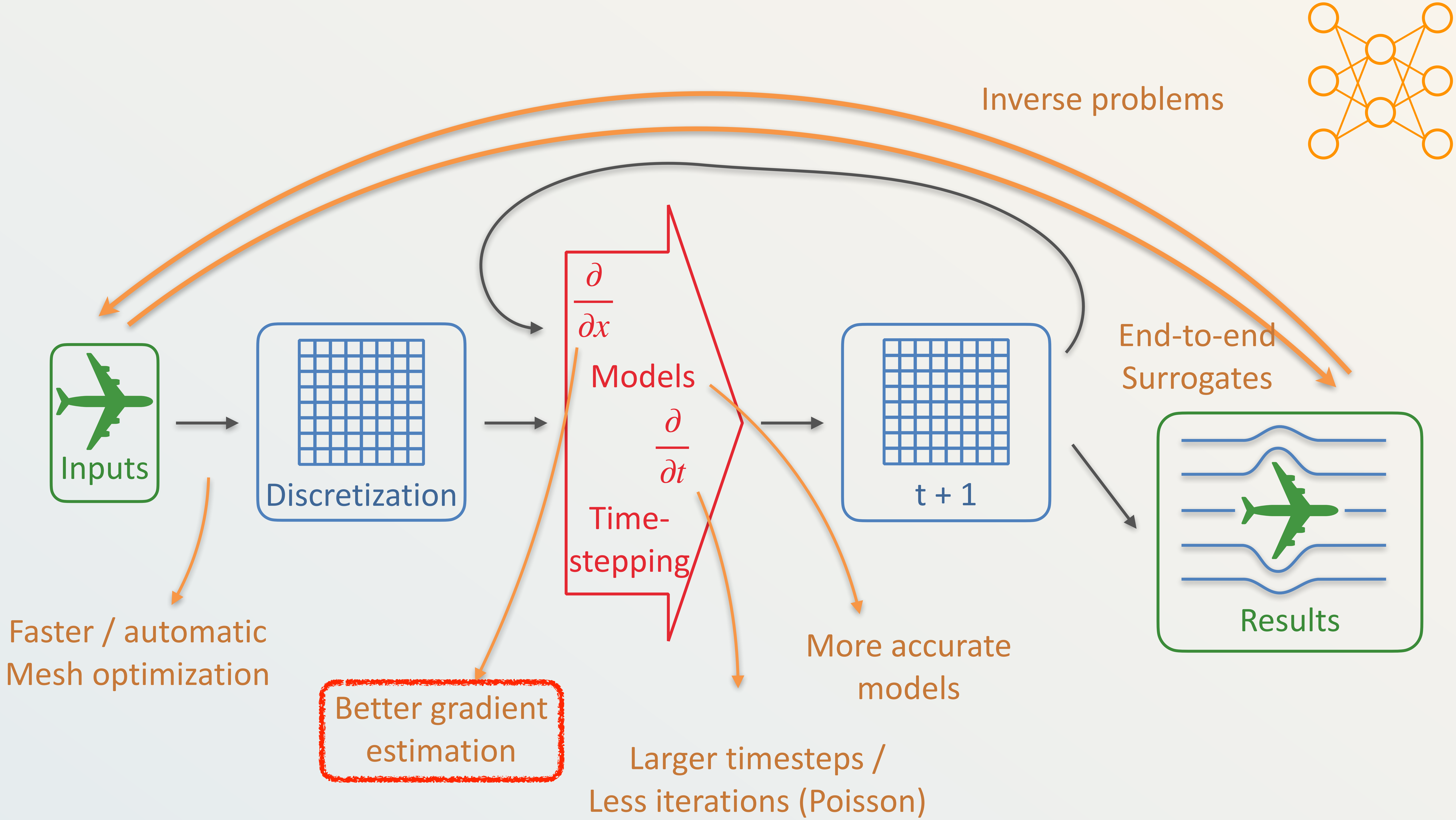
Reinforcement Learning

(*e.g.* work from [1])

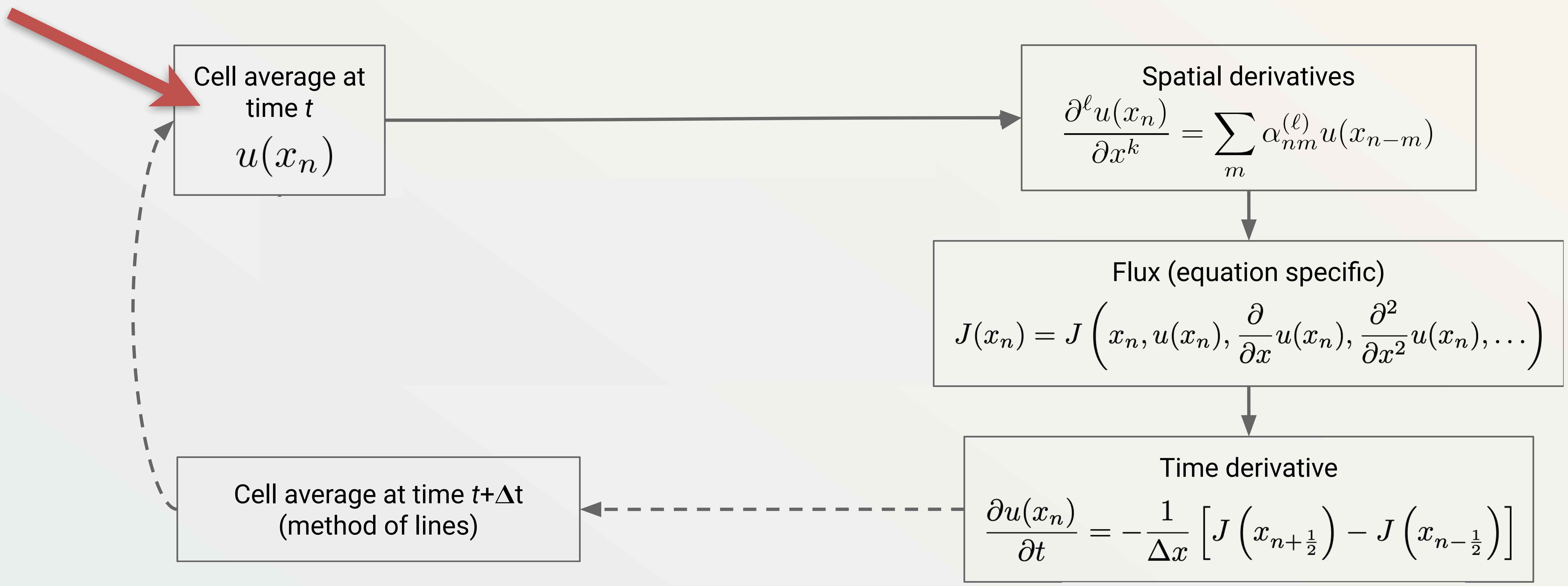
=> Search for behaviour that maximises your true objective
(here: in code performance)

Train for your objective directly *through* the solver

[1] Novati, G., de Laroussilhe, H. L., & Koumoutsakos, P. (2021). Automating turbulence modelling by multi-agent reinforcement learning. *Nature Machine Intelligence*, *3*(1), 87-96.

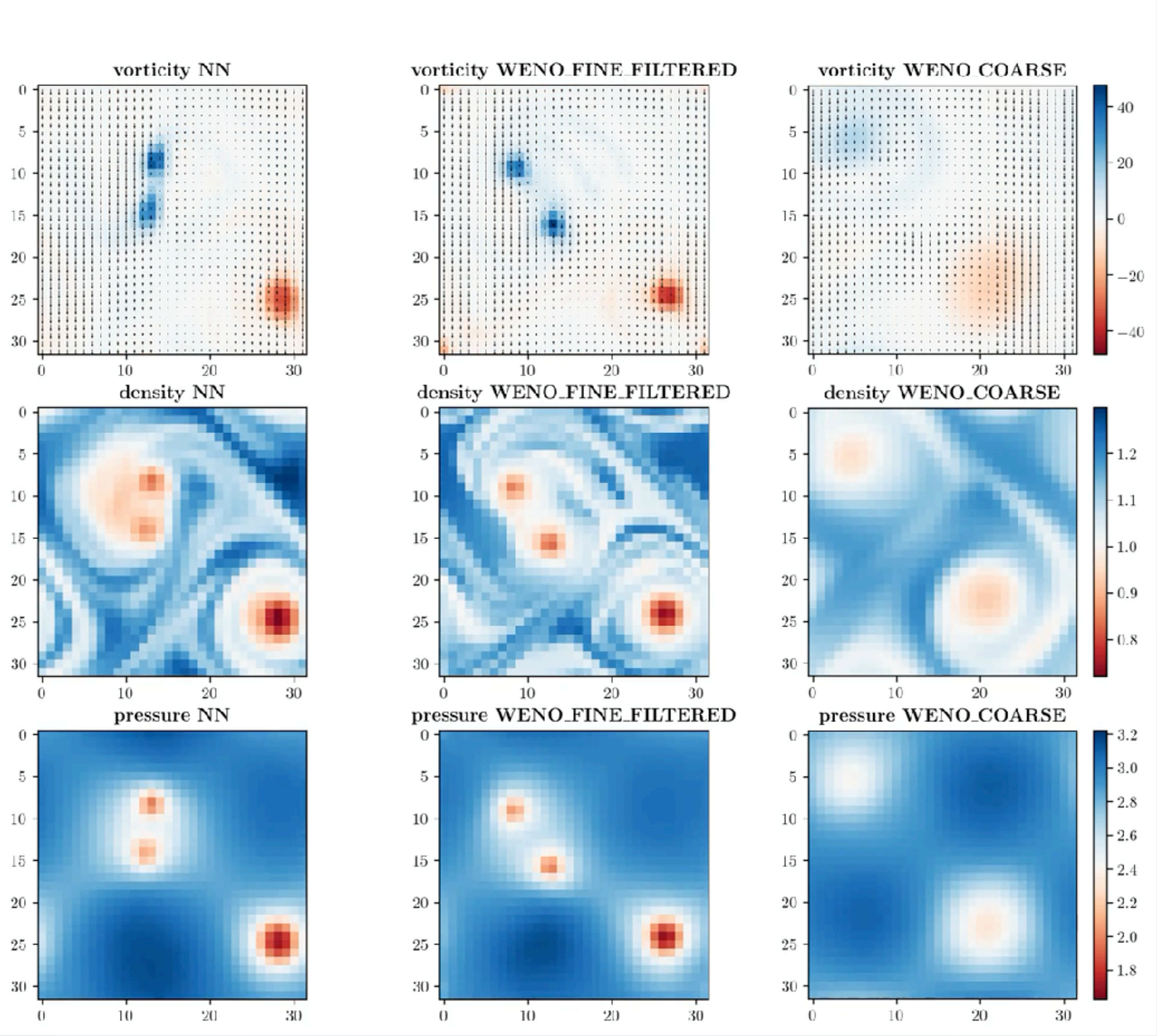


An example of training through the solver

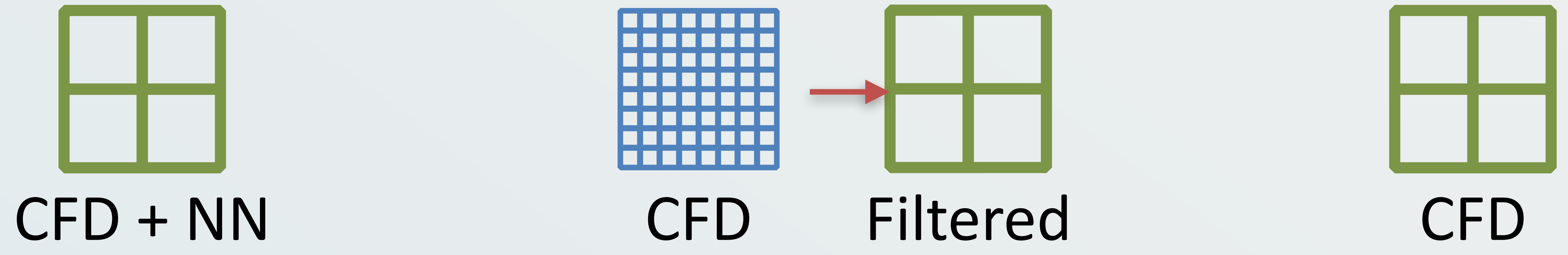


To train *through* the solver,
it must be *differentiable.*

Bar-Sinai, Y., Hoyer, S., Hickey, J., & Brenner, M. P. (2019). Learning data-driven discretizations for partial differential equations. *Proceedings of the National Academy of Sciences*, *116*(31), 15344-15349.

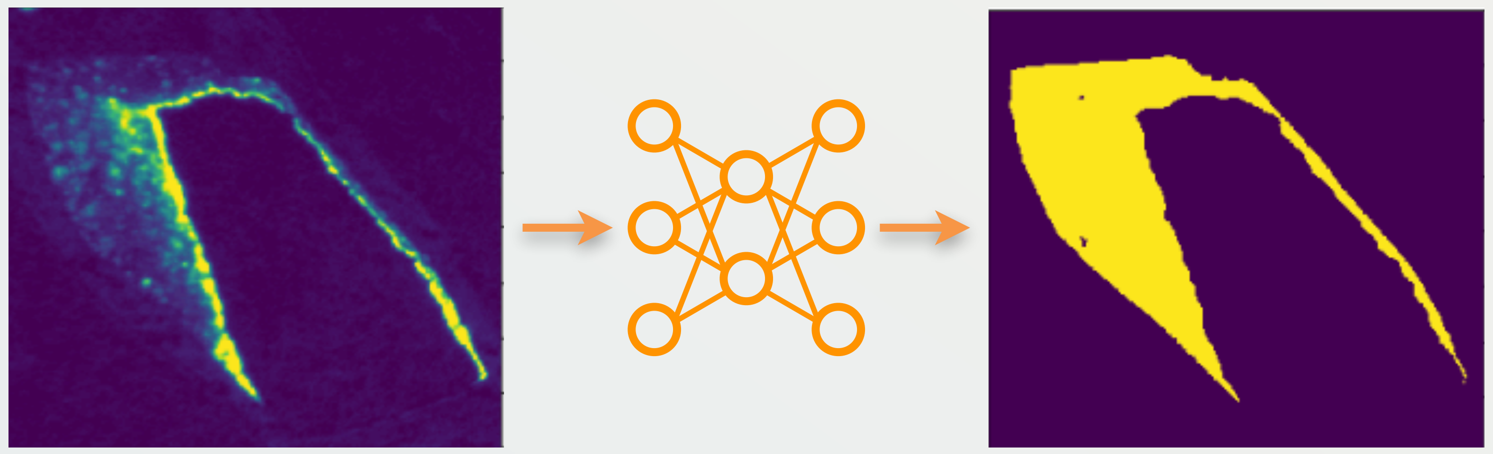


CFD solver rewritten in Julia



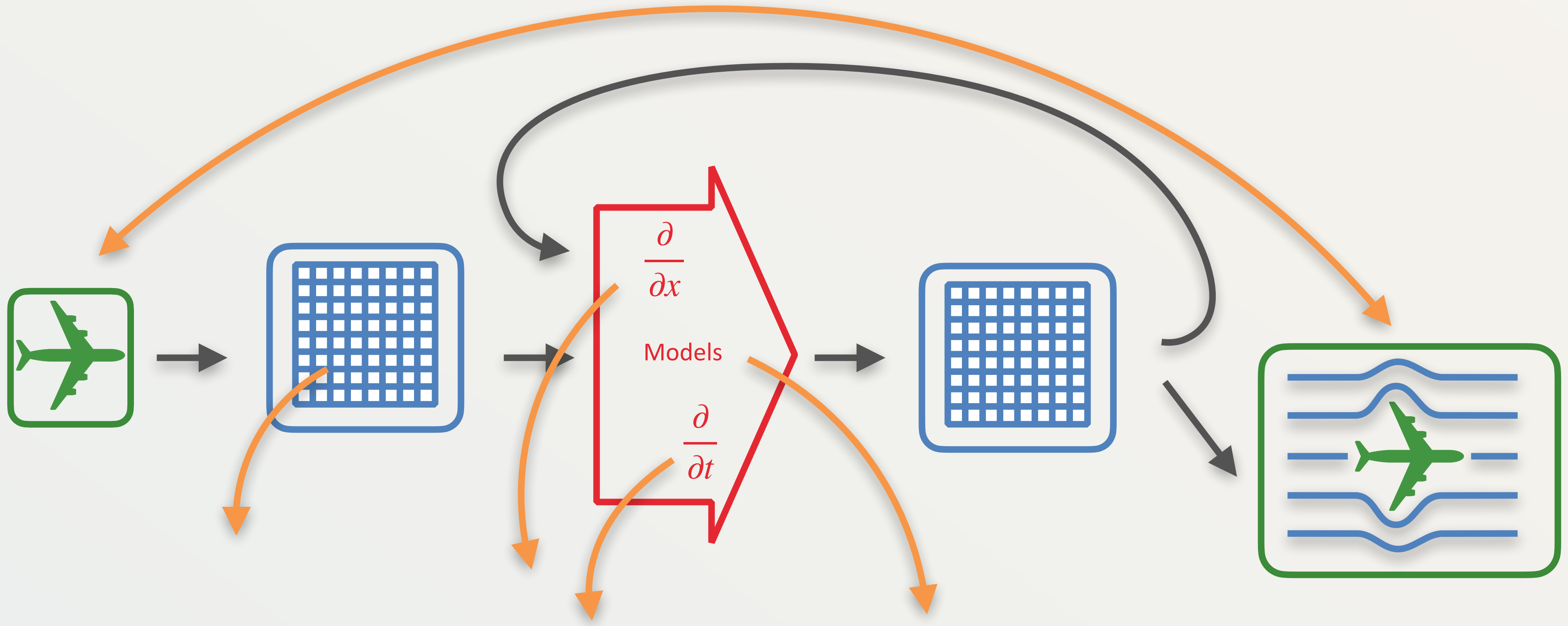
Ongoing PhD of Luciano Drozda, Cerfacs

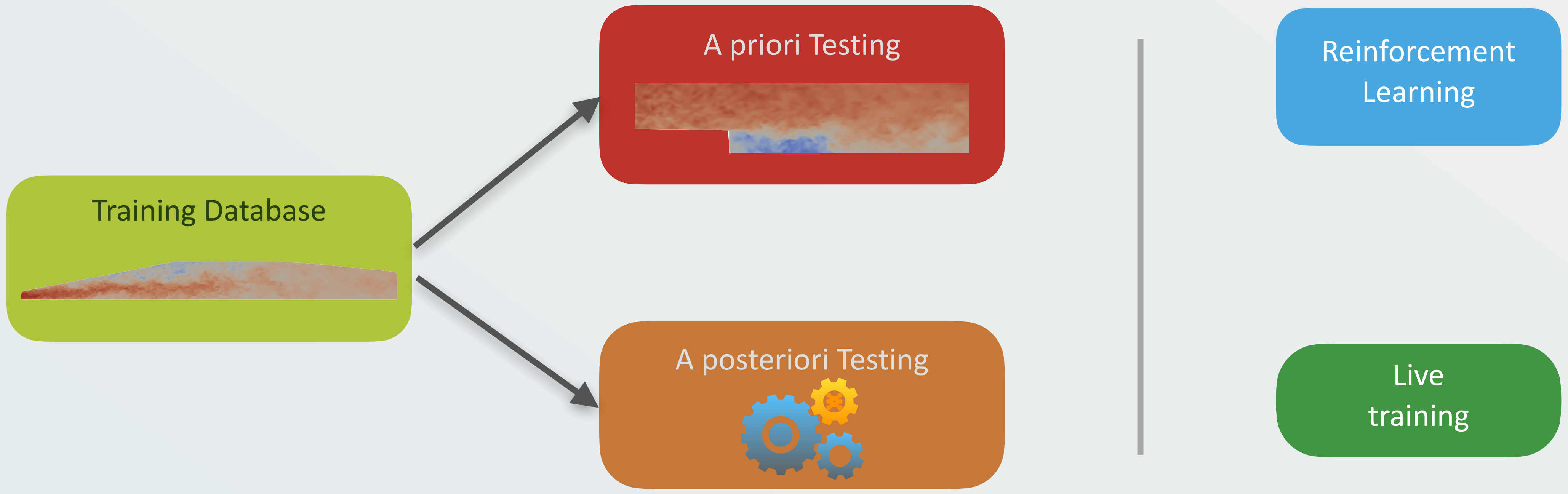
Key take-aways



Neural networks are versatile
But they excel at *extracting context*

There are many ways this can help CFD
It's an active and exciting field of research!





We're not even sure what method to train with for best efficiency / generalisation

This domain won't advance as fast as the hype.
Hang in there if you're interested in the science!

Thank you

- Recent Papers:
  - Besombes, C. *et al.* (2021). Producing realistic climate data with GANs. Nonlinear Processes in Geophysics, 28, 347–370.
  - Xing V. *et al.* (2021). Generalization Capability of Convolutional Neural Networks for Progress Variable Variance and Reaction Rate Subgrid-Scale Modeling. Energies 14(16):5096.
  - Cellier, A. e*t al.* (2021). Detection of precursors of combustion instability using convolutional recurrent neural networks. Combustion and Flame, Volume 233, 111558.
  - Lapeyre, C.J. e*t al.* (2019). Training convolutional neural networks to estimate turbulent sub-grid scale reaction rates. Combustion and Flame, 203, 255-264.
- Conferences:
  - Yewgat, A., Busby, D., Chevalier, M., Lapeyre, C. & Teste, O. (2020) Deep-CRM: A New Deep Learning Approach for Capacitance Resistive Models. 17th European Conference on the Mathematics of Oil Recovery, September 14-17 2020.
  - Lapeyre, C. J., Cazard, N., Roy, P. T., Ricci, S., & Zaoui, F. (2019). Reconstruction of Hydraulic Data by Machine Learning. SimHydro 2019, Nice, France, June 12-14, arXiv:1903.01123.
  - Lapeyre, C.J., Misdariis, A., Cazard, N., Xing, V., Veynante, D. & Poinsot, T. (2019). A convolutional neural network-based efficiency function for sub-grid flame-turbulence interaction in LES. 16th International Conference on Numerical Combustion, May 6-8 2015, Avignon France.
  - Ronan Paugam, Melanie Rochoux, Nicolas Cazard, Corentin Lapeyre, William Mell, Joshua Johnston, and Martin Wooster: Computing High Resolution Fire Behavior Metrics from Prescribed Burn using Handheld Airborne Thermal Camera Observations. The 6th International Fire Behaviour and Fuels Conference, Marseilles, May 2019.
  - Ronan Paugam, Melanie Rochoux, Nicolas Cazard, Corentin Lapeyre, William Mell, Joshua Johnston, and Martin Wooster. Journée de télédétection et incendie Organisée par IRSTEA, Aix, Decembre 2018.
  - Lapeyre, C.J., Misdariis, A., Cazard, N, Poinsot, T. Replacing a sub-grid closure model with a trained deep convolutional neural network. HiFiLeD Symposium, November 14-16th 2018, Brussels Belgium.
- Other:
  - Lapeyre, C.J., Misdariis, A., Cazard, N. & Poinsot, T (2018). A-posteriori evaluation of a deep convolutional neural network approach to subgrid-scale flame surface estimation. Proc. CTR Summer Program, 349-358.