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HELIOS

High performance learning for computational physics

Exploring strategies to exploit machine learning in HPC-CFD

Corentin Lapeyre

MAGISTER • 2020.09.15

Acknowledgments: A. Misdariis, N. Cazard, C. Besombes, V. Xing, E. Gullaud, L. Drozda, T. Poinsot, M. Bauerheim (ISAE), R. Selmi (TOTAL) and many more contributors…

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Comment l'Intelligence Artificielle va changer nos vies
Libération
inter
N°1
VOYAGE AU CŒUR DE L'IA
HORS-SÉRIE
Comment l'Intelligence Artificielle change nos vies
Libération
inter
N°2
L'IA AU CŒUR DE L'HUMAIN
Avec Alain Damasio, Yuval Noah Harari, Cathy O'Neil...


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Intelligence artificielle
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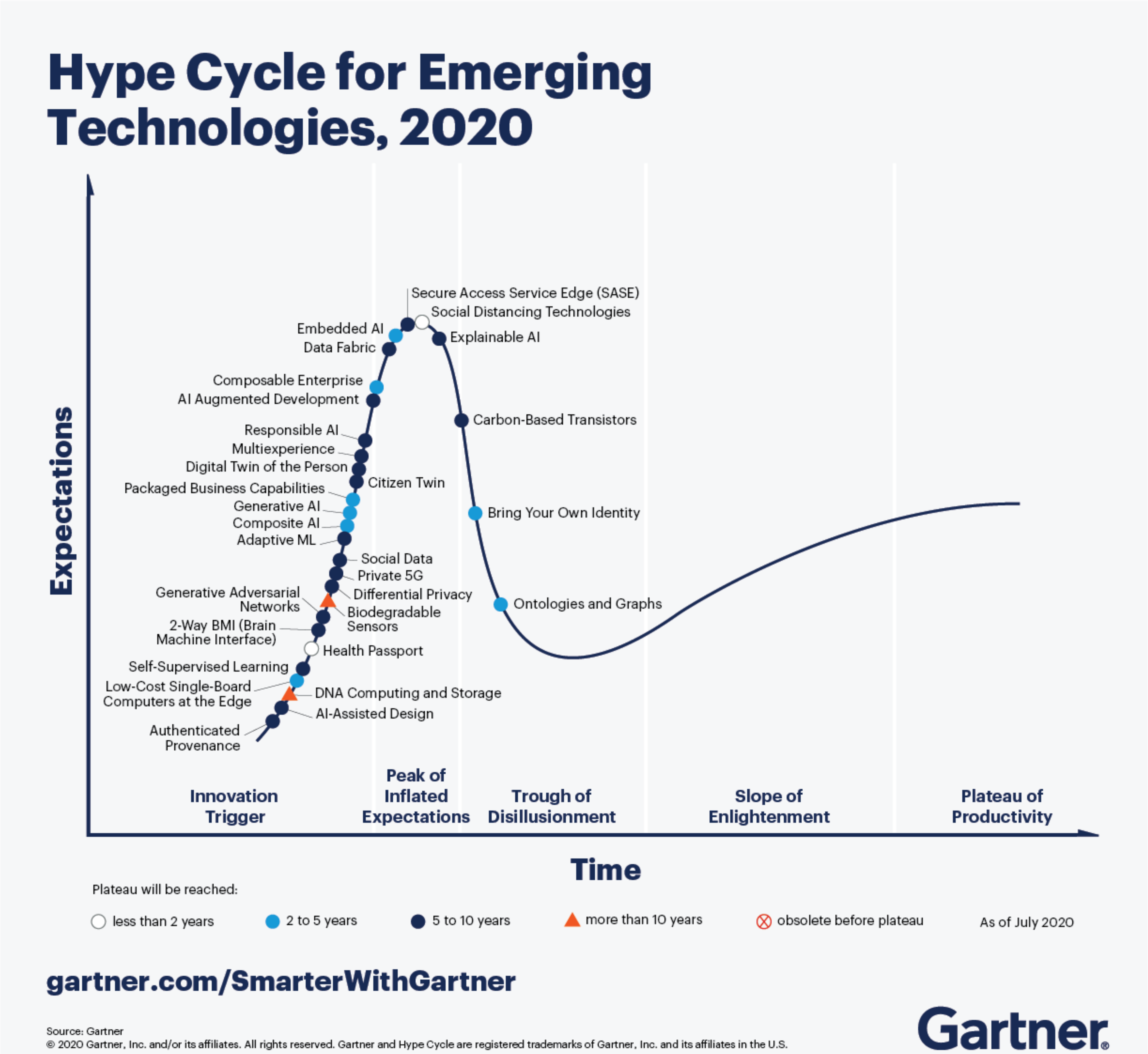
La révolution qui devrait être au cœur de la présidentielle
Avec Thomas L. Friedman, Charles-Edouard Bouée et Yann Le Cun


COMMENT S'INFORMENT LES ADOS
SPÉCIAL MODE
L'OBS
LE PARI DE L'INTELLIGENCE ARTIFICIELLE
PAR
CÉDRIC VILLANI


Courrier international
INTELLIGENCE ARTIFICIELLE
LA MACHINE À FANTASMES
EN SUPPLÉMENT 2017, L'ANNÉE EN CARTOONS
INFLUENCE — LE BEL AUTOMNE FRANÇAIS
ÉCONOMIE — BITCOIN, UN FLÉAU ÉCOLOGIQUE
Les robots vont-ils détruire nos emplois et nos vies ? Pour en finir avec les idées reçues, le décryptage de la MIT Technology Review
Voyage
Acapulco, mon paradis perdu

...

The hype


Hype Cycle for Emerging Technologies, 2020
Expectations
Secure Access Service Edge (SASE)
Social Distancing Technologies
Embedded AI
Data Fabric
Explainable AI
Composable Enterprise
AI Augmented Development
Carbon-Based Transistors
Responsible AI
Multiexperience
Digital Twin of the Person
Citizen Twin
Packaged Business Capabilities
Generative AI
Composite AI
Adaptive ML
Bring Your Own Identity
Social Data
Private 5G
Differential Privacy
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Biodegradable Sensors
Ontologies and Graphs
2-Way BMI (Brain Machine Interface)
Health Passport
Self-Supervised Learning
Low-Cost Single-Board Computers at the Edge
DNA Computing and Storage
AI-Assisted Design
Authenticated Provenance
Innovation Trigger
Peak of Inflated Expectations
Trough of Disillusionment
Slope of Enlightenment
Plateau of Productivity
Time
Plateau will be reached:
less than 2 years
2 to 5 years
5 to 10 years
more than 10 years
obsolete before plateau
As of July 2020
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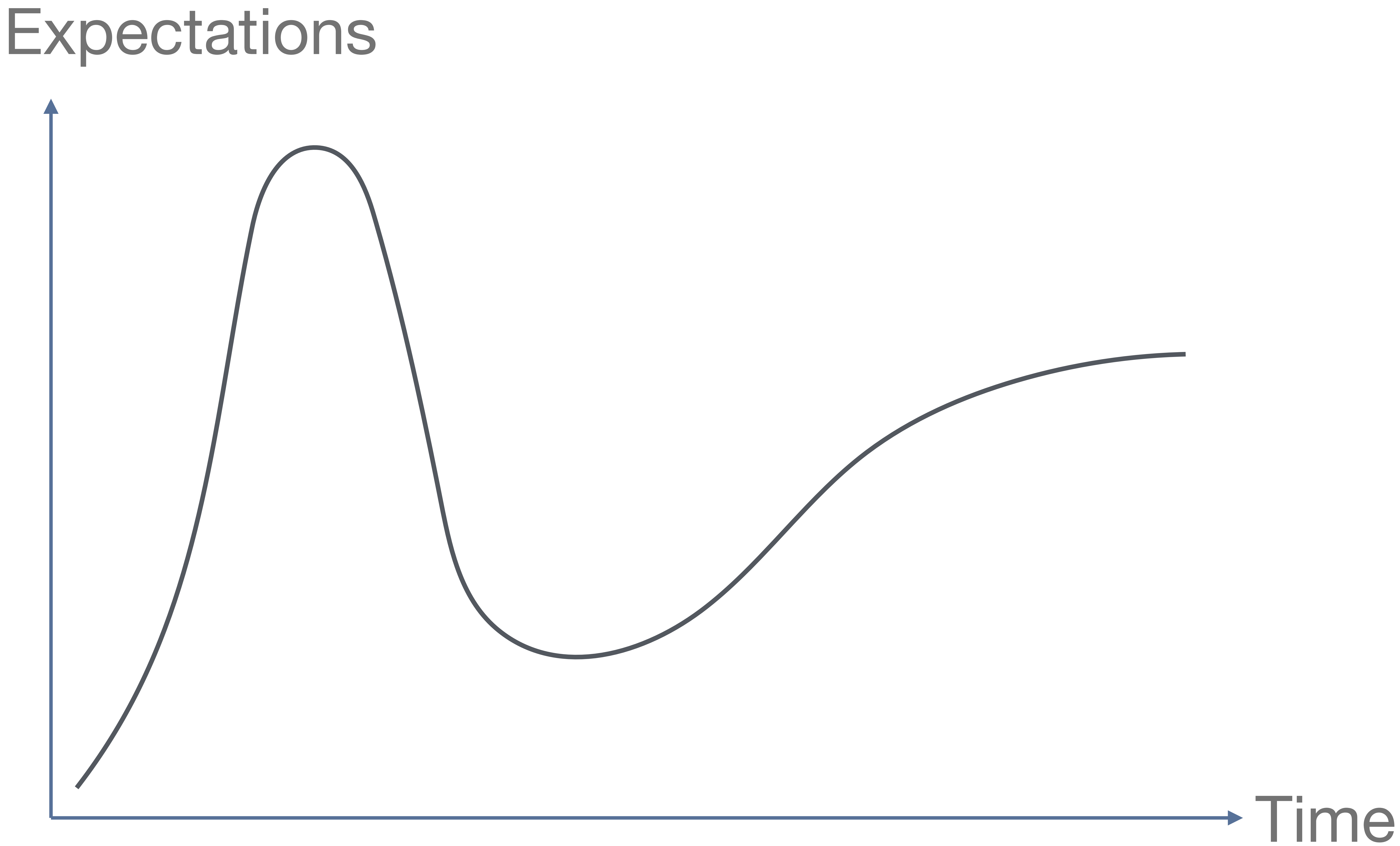

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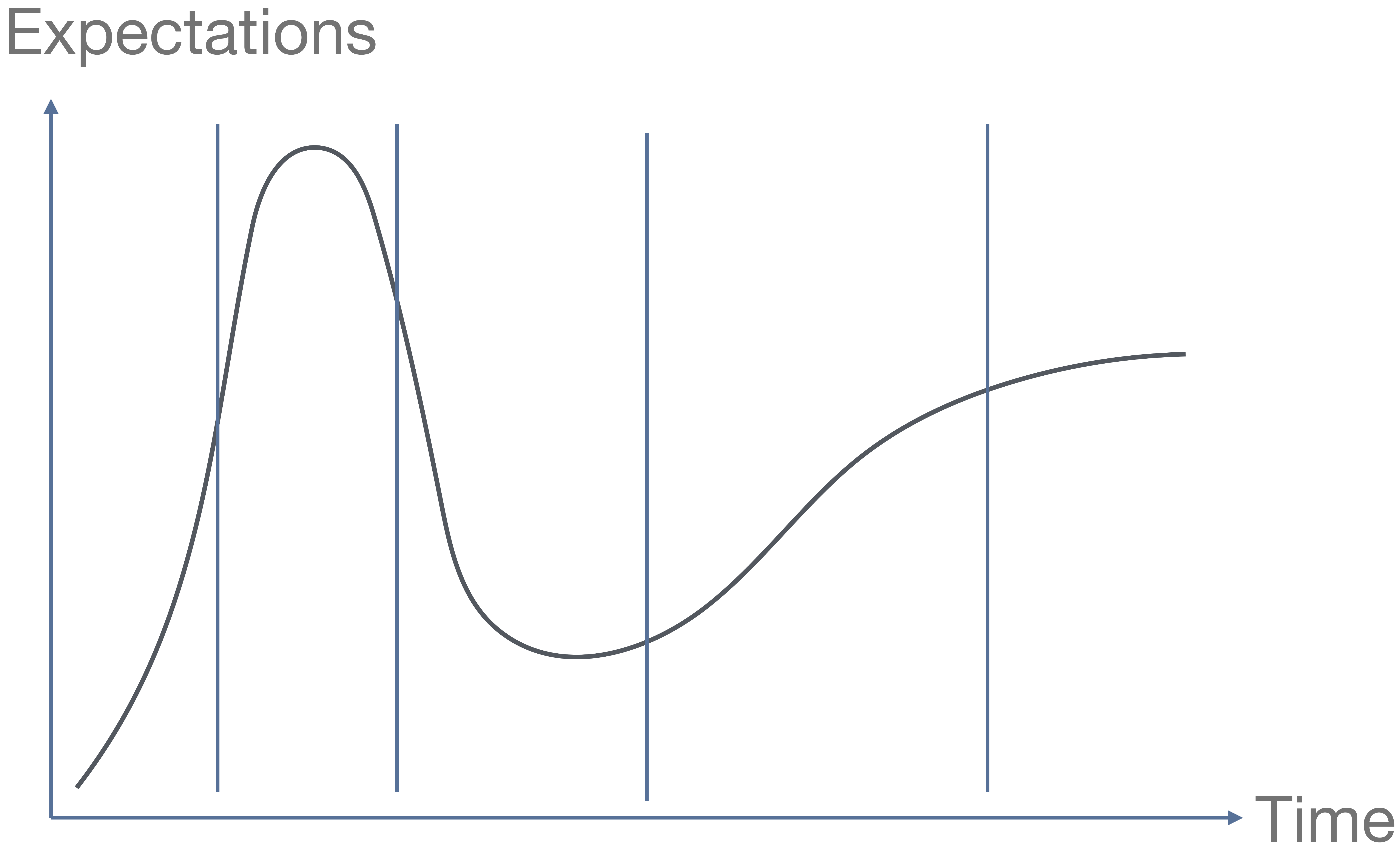

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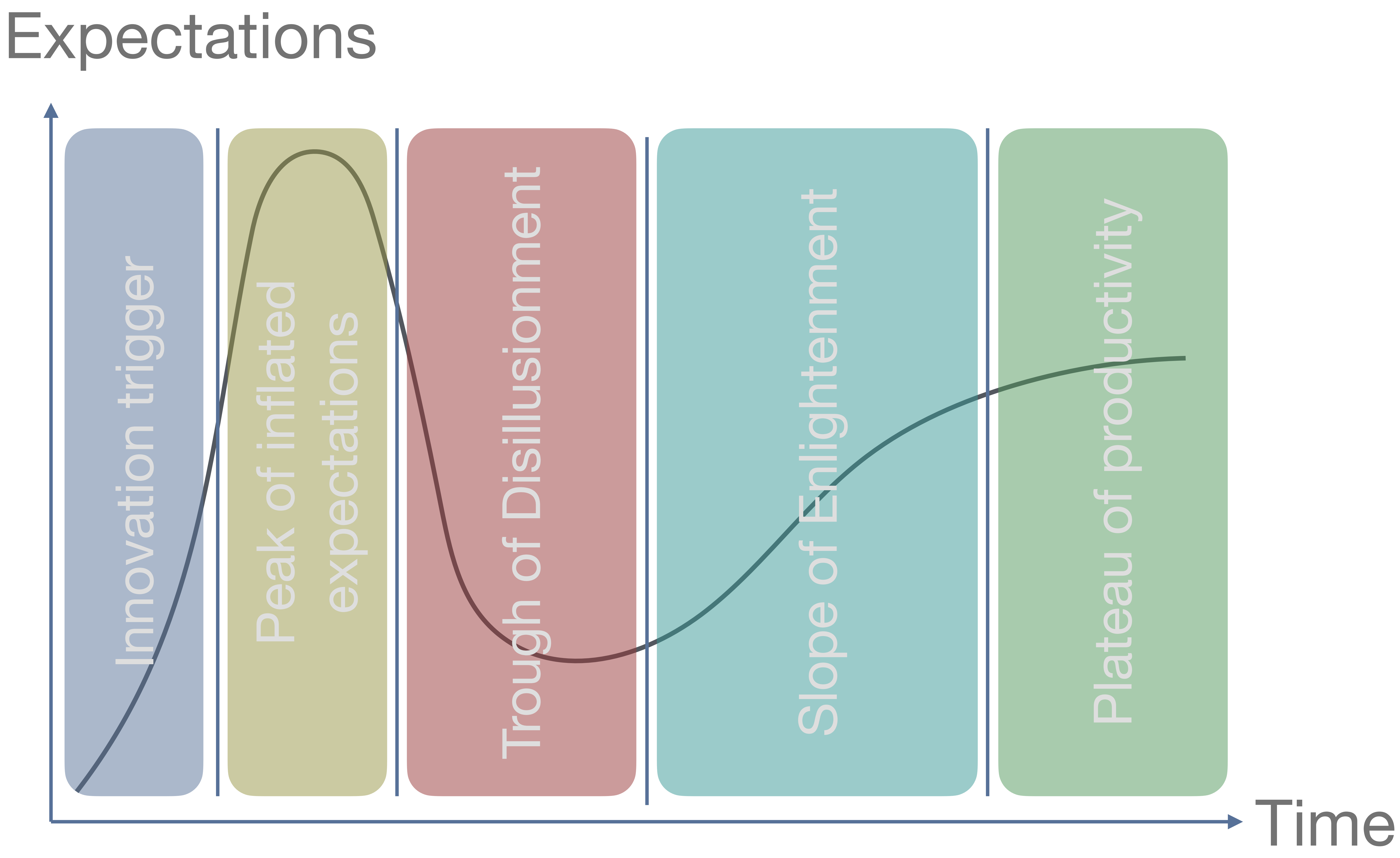
Expectations
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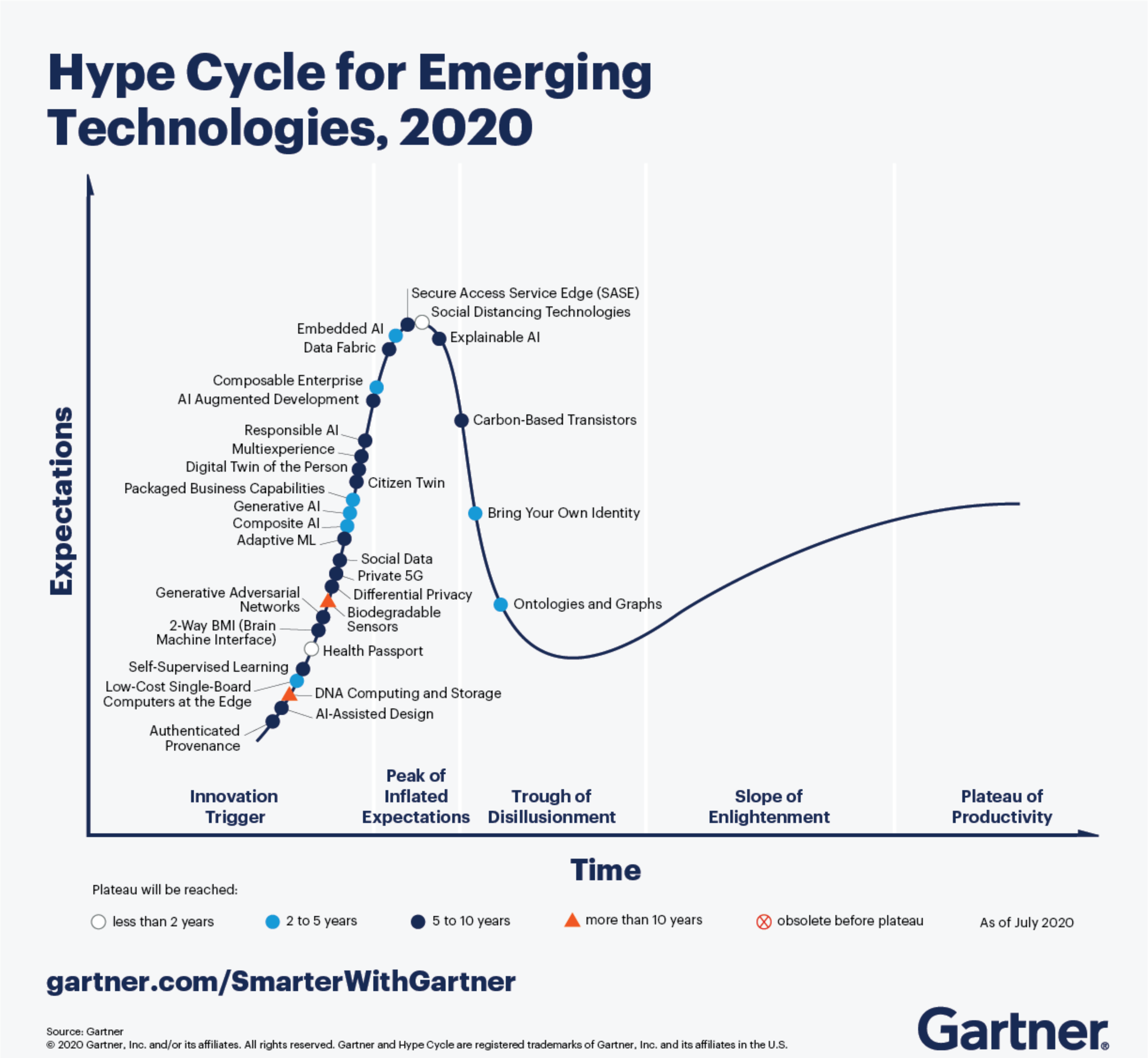
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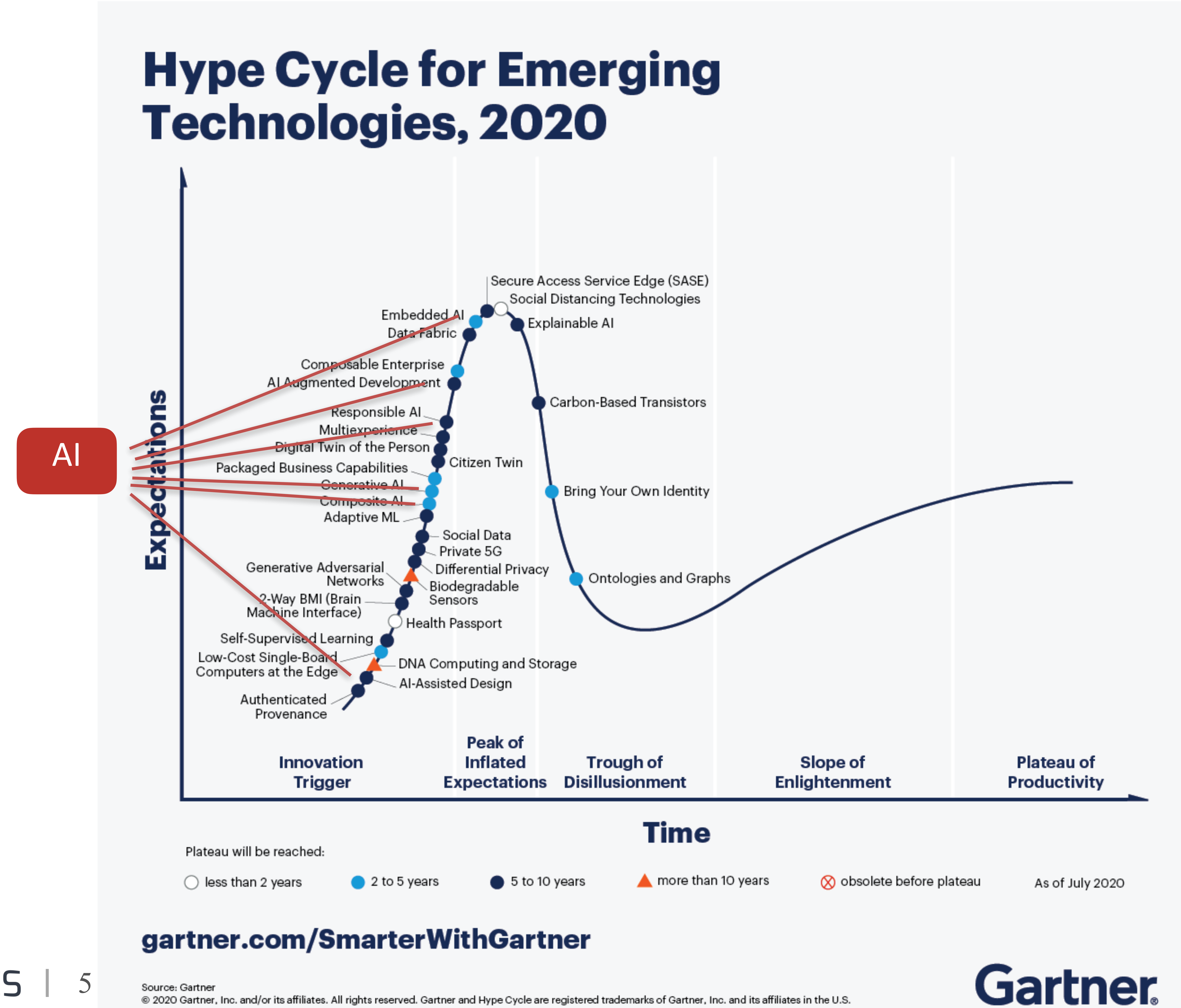
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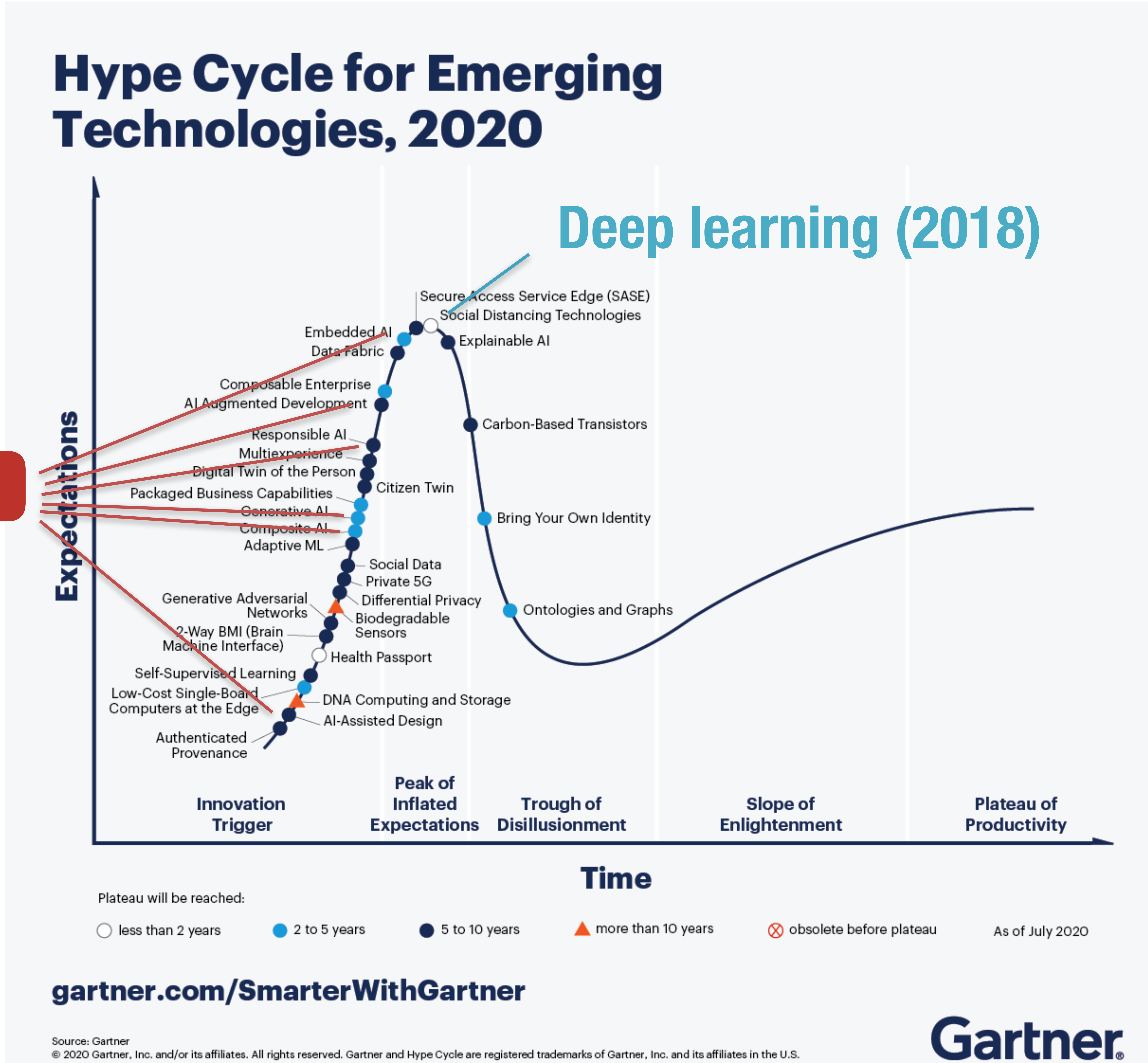
AI

The hype

AI



Hype Cycle for Emerging Technologies, 2020
Deep learning (2018)
Expectations
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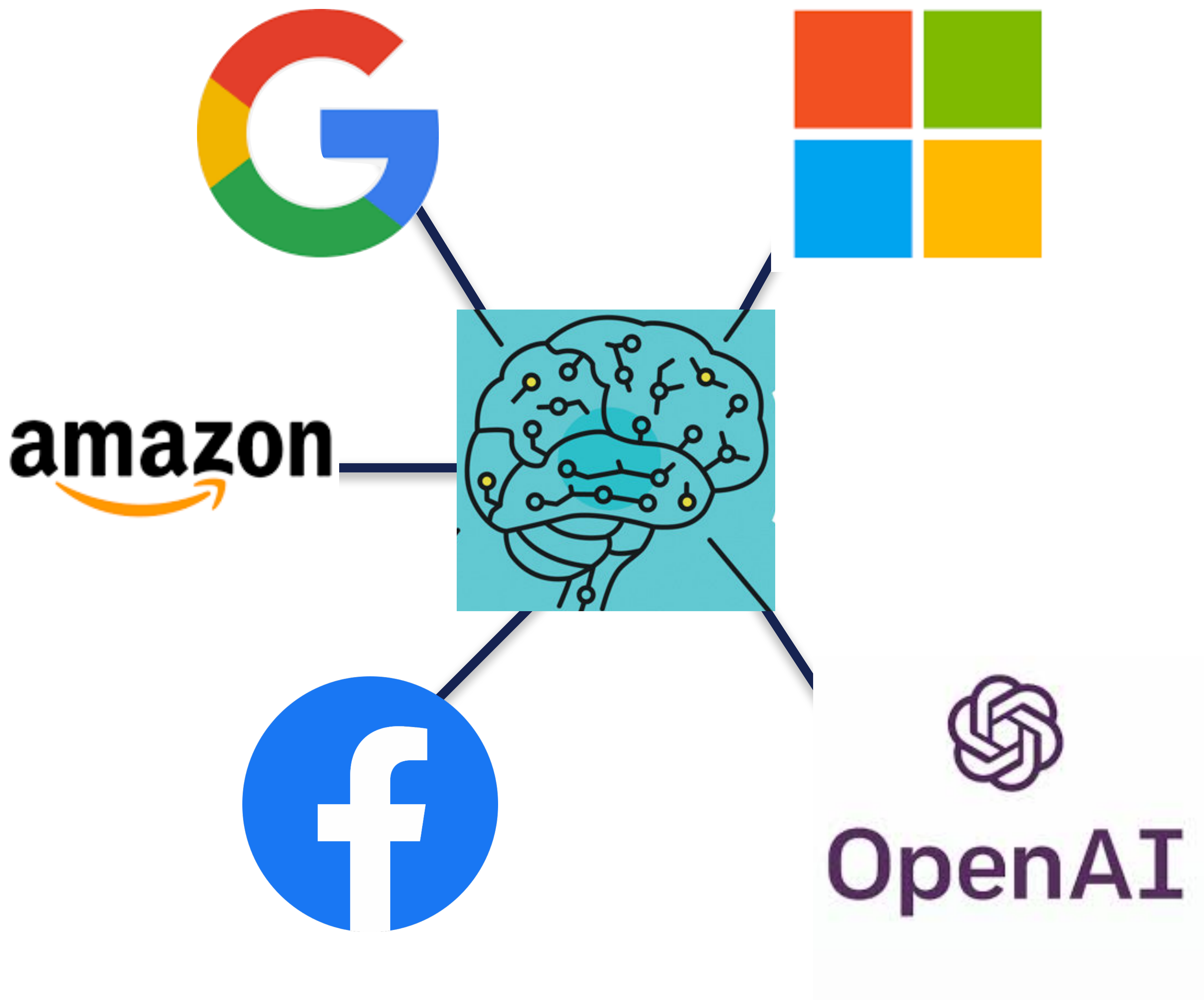
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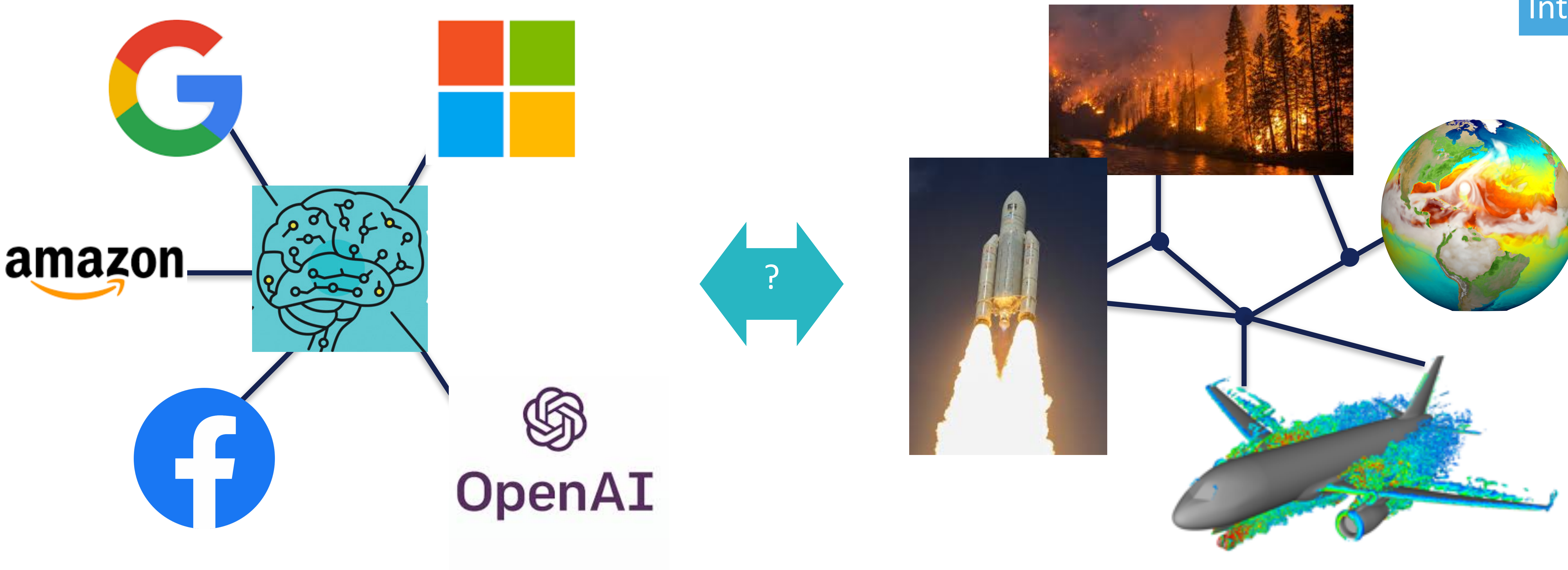
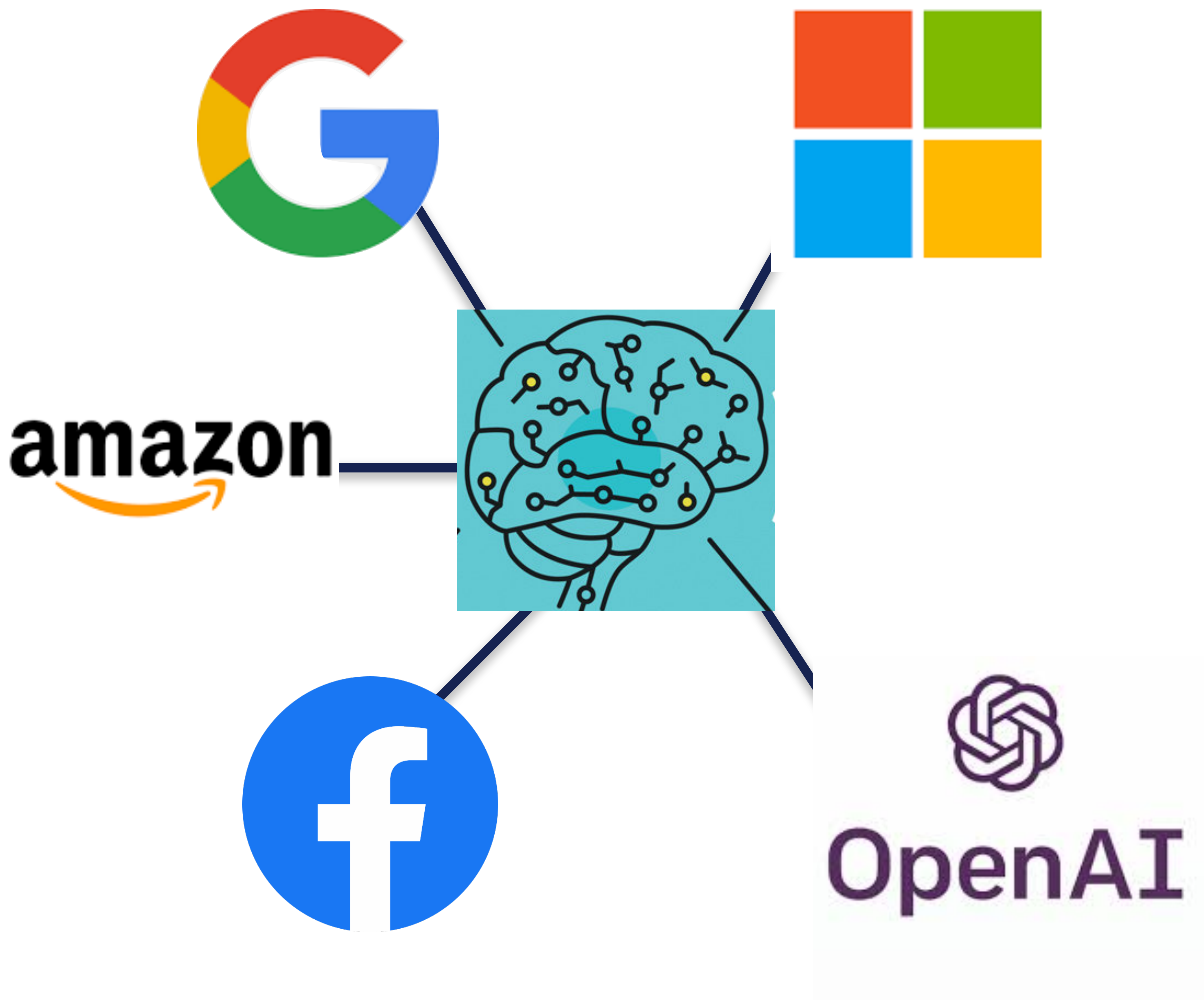


How is Data Science (DS) relevant to the Physical sciences?
A.k.a. how do we separate the hype from what's truly useful?



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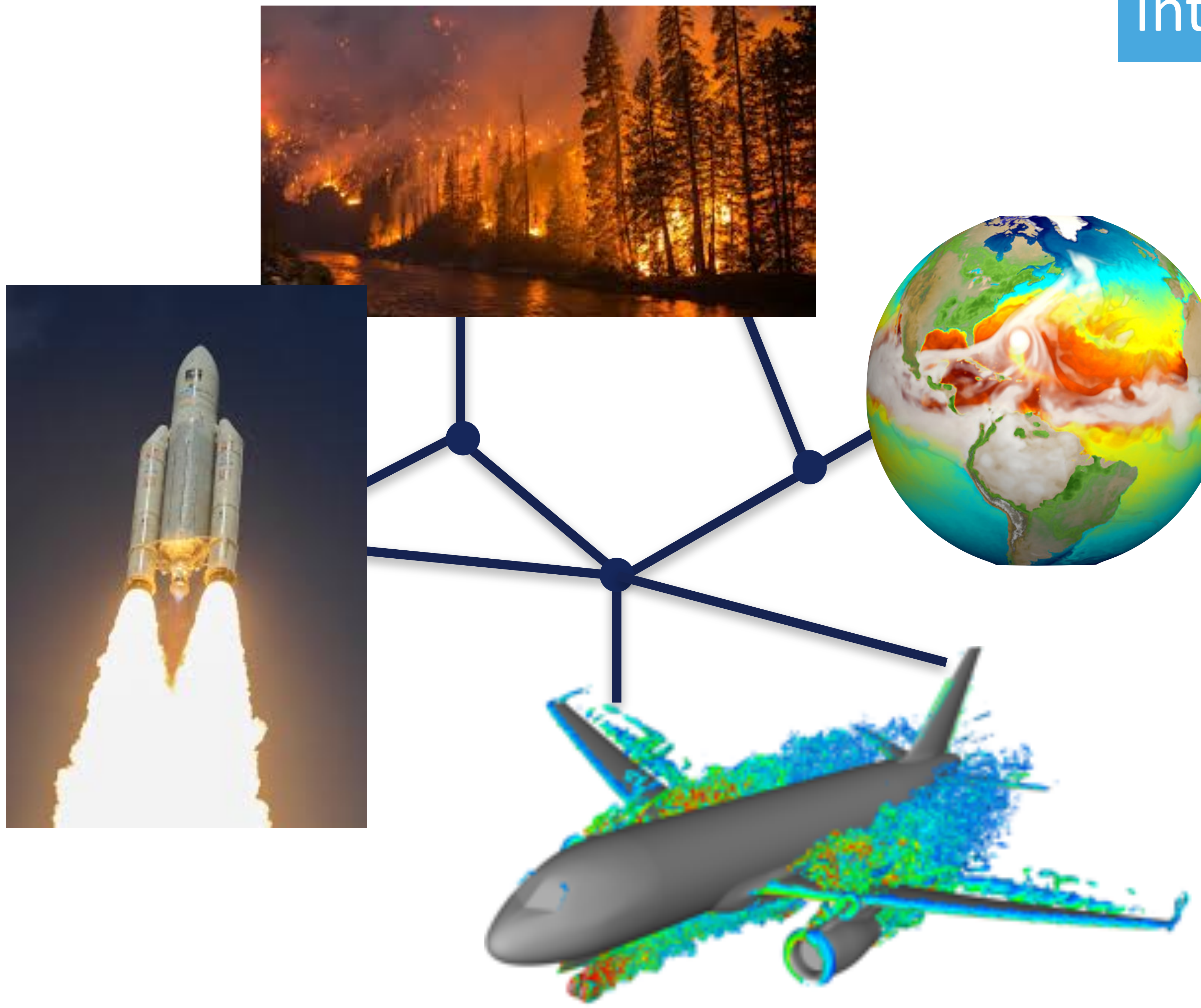

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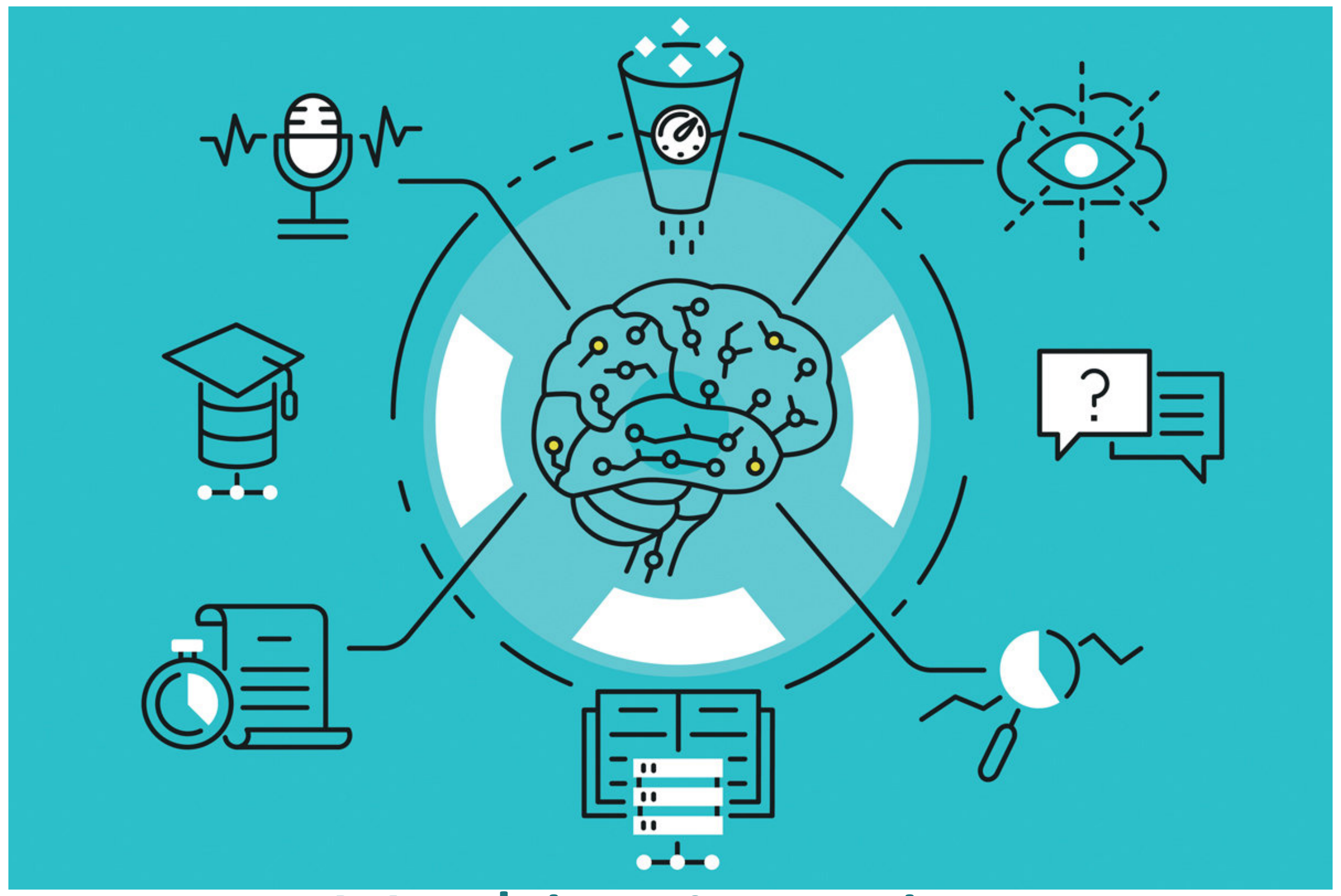
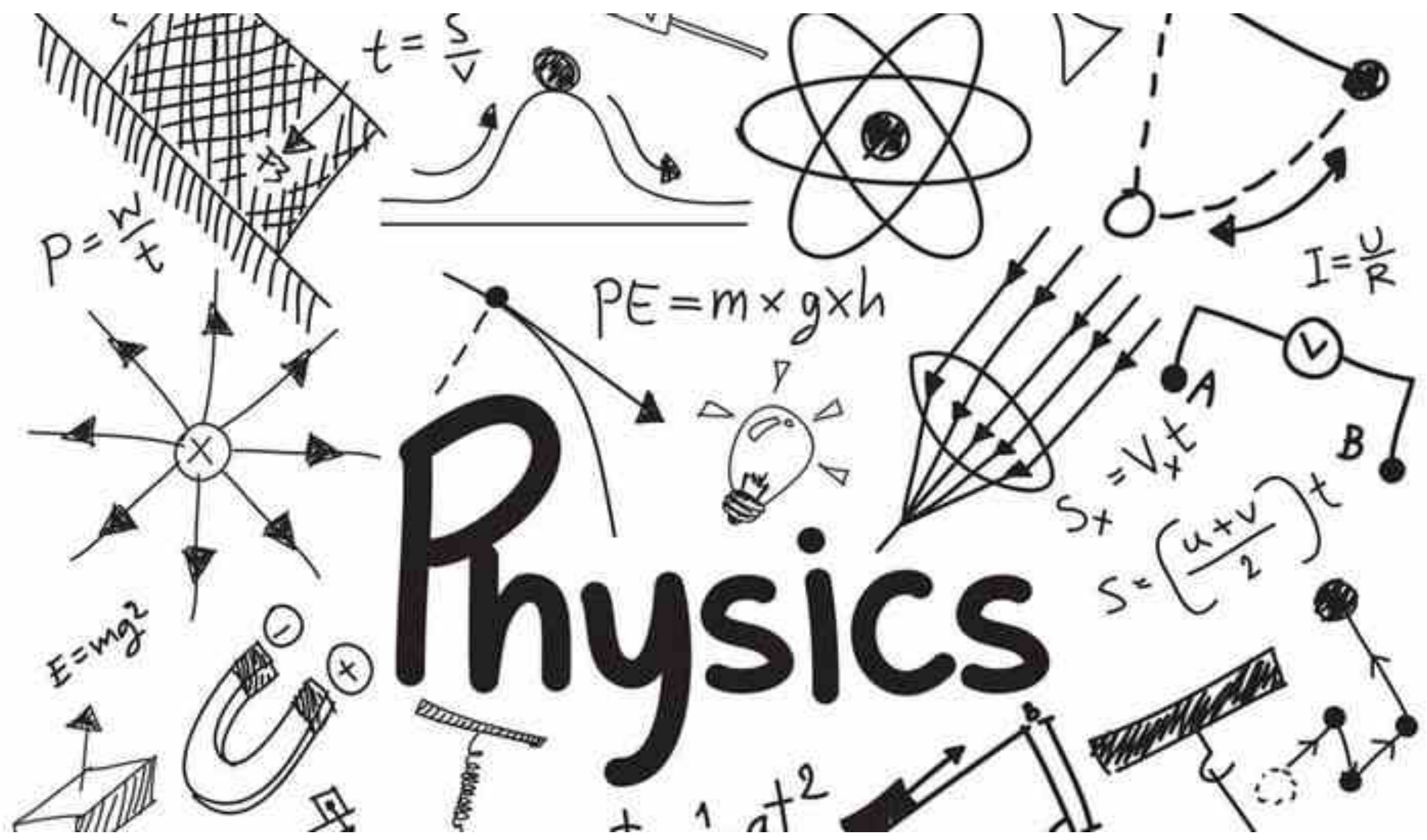


Machine Learning

?



Machines that learn ?

The Data Science landscape

Statistics: The science of collecting, displaying, and analysing data

oxfordreference.com

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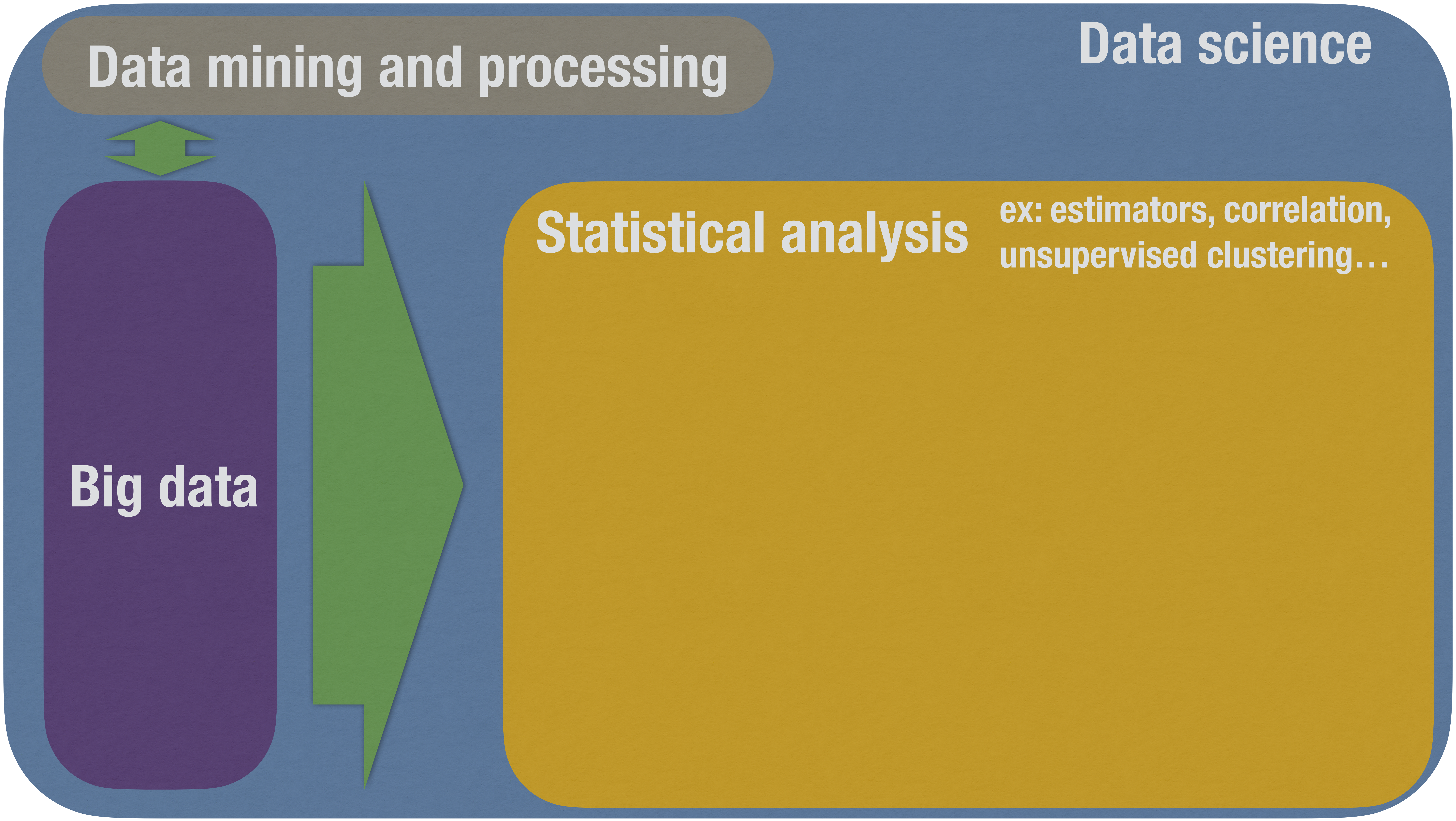

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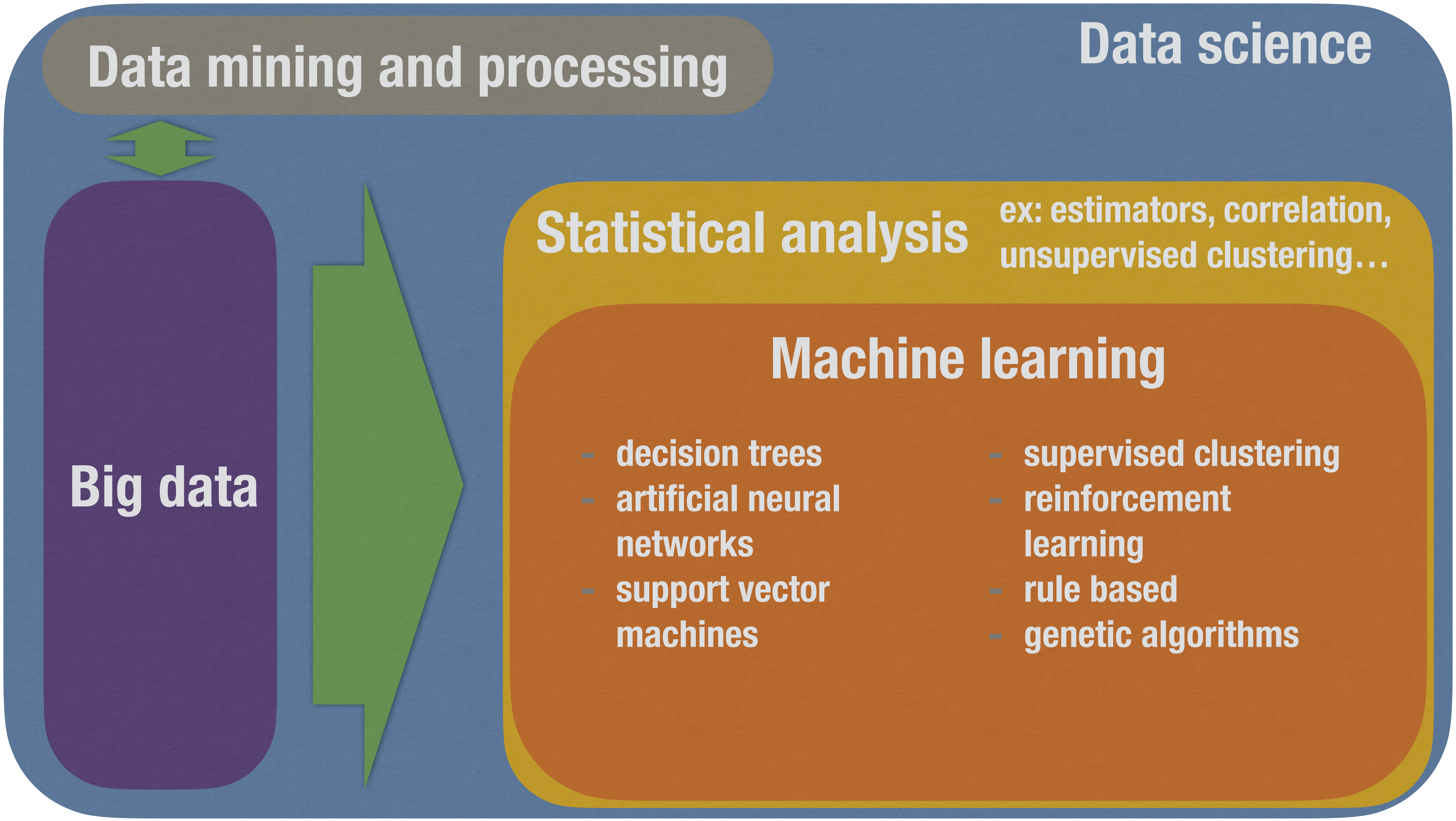

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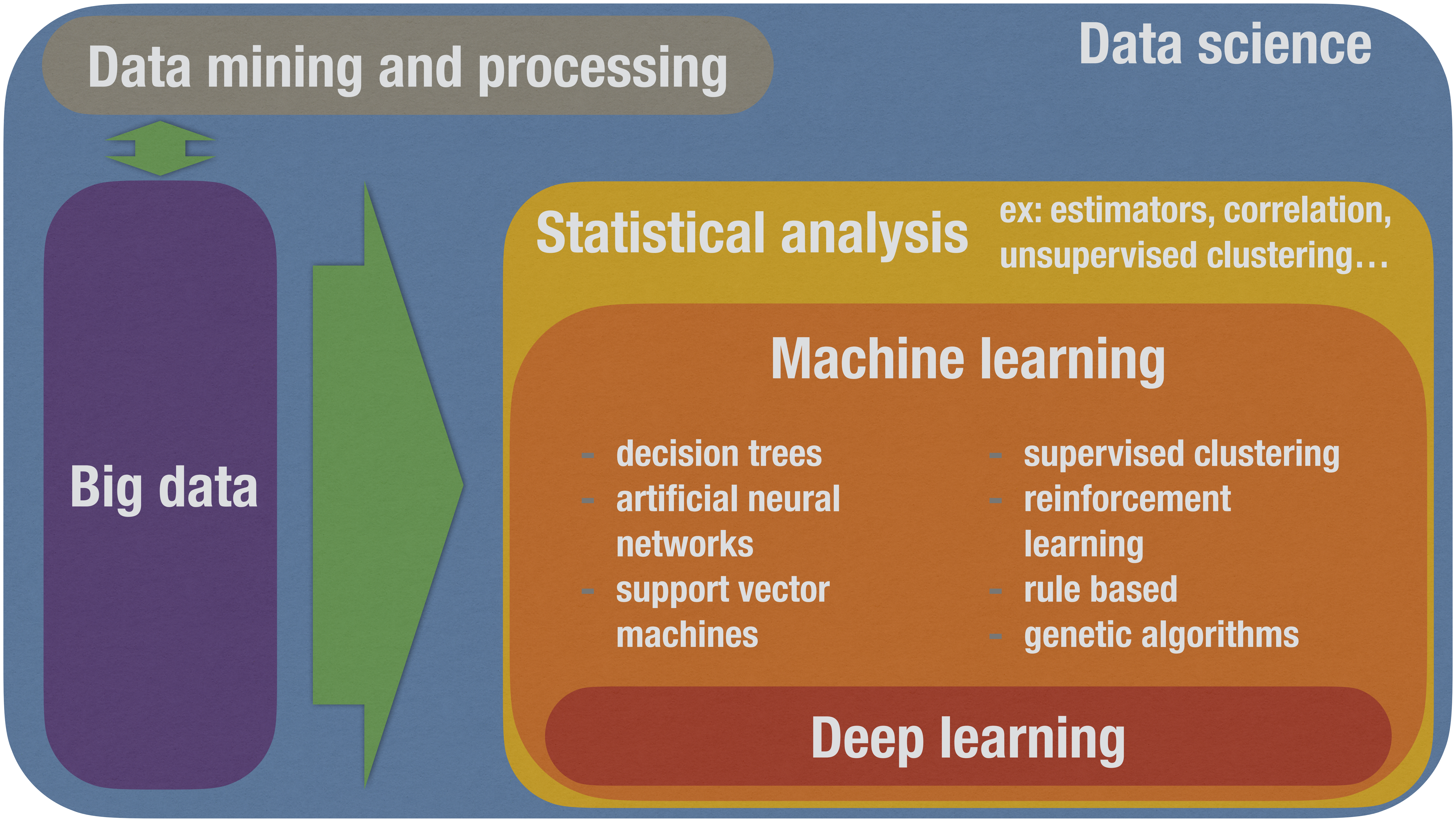

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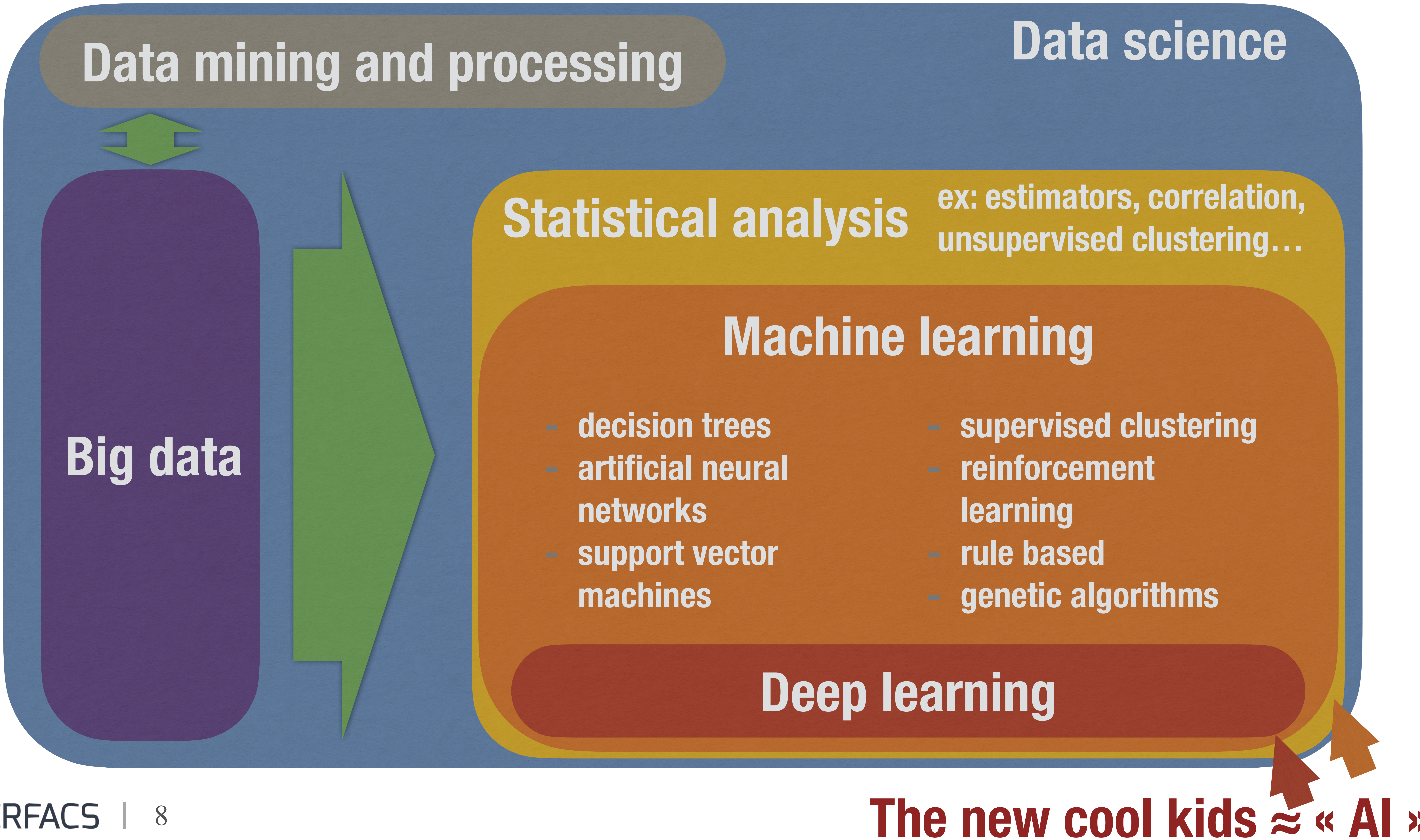


What is *learning*?


Multiplication Square

X	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	6	7	8	9	10
2	2	4	6	8	10	12	14	16	18	20
3	3	6	9	12	15	18	21	24	27	30
4	4	8	12	16	20	24	28	32	36	40
5	5	10	15	20	25	30	35	40	45	50
6	6	12	18	24	30	36	42	48	54	60
7	7	14	21	28	35	42	49	56	63	70
8	8	16	24	32	40	48	56	64	72	80
9	9	18	27	36	45	54	63	72	81	90
10	10	20	30	40	50	60	70	80	90	100

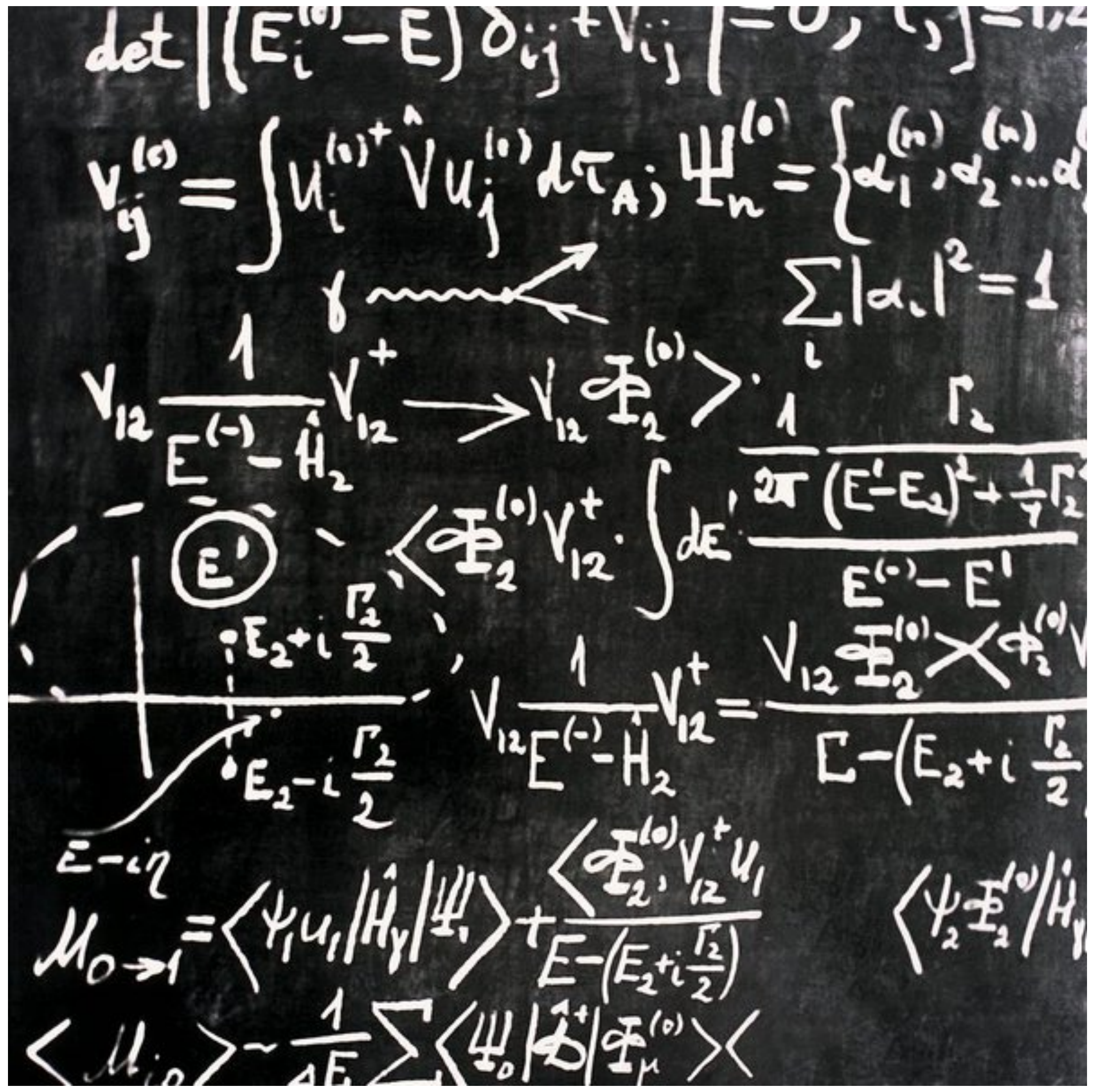
Learn by heart

What is *learning*?

Learn by heart

What is *learning*?

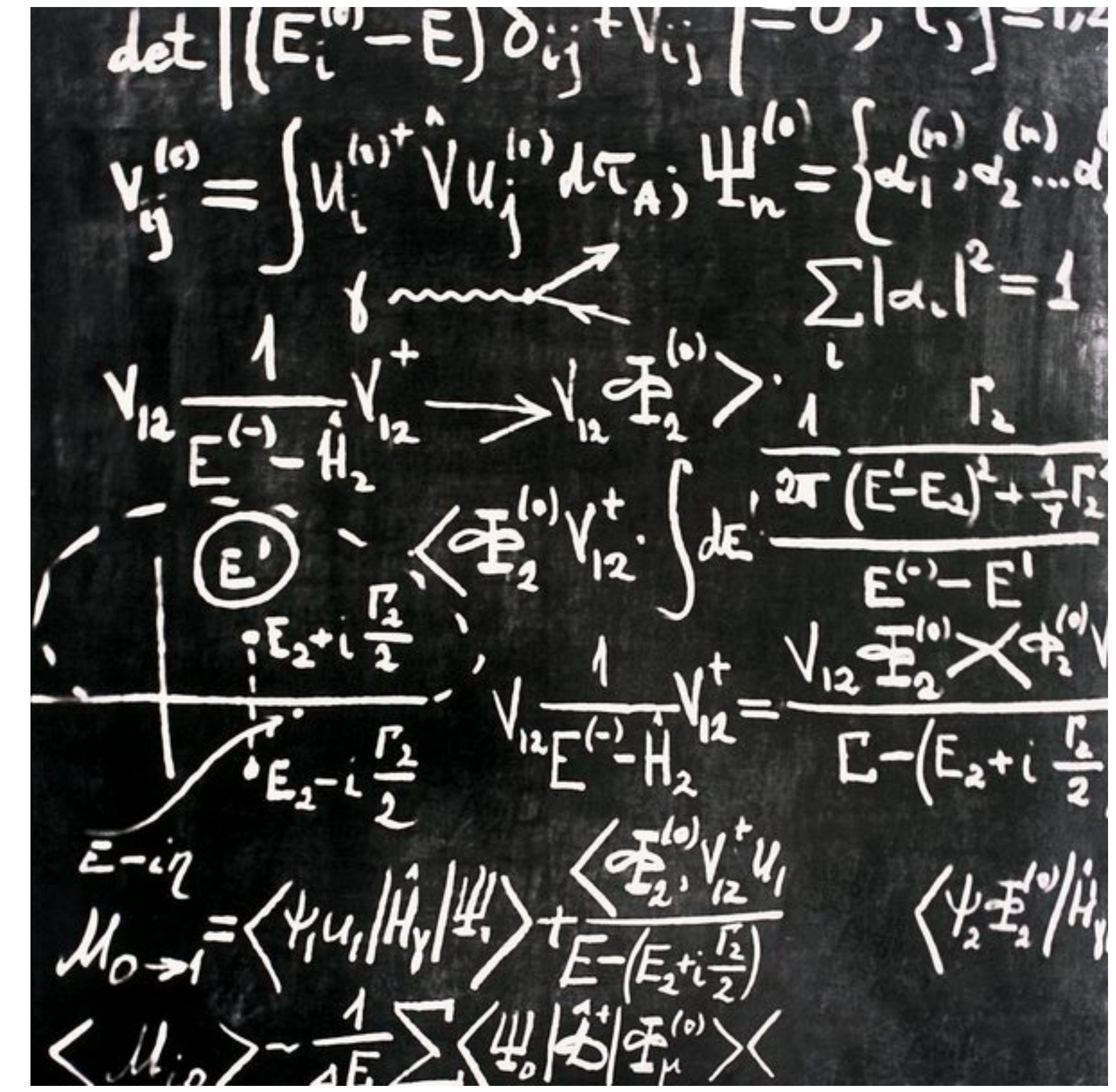
Learn by heart



Learn abstract concepts

What is *learning*?

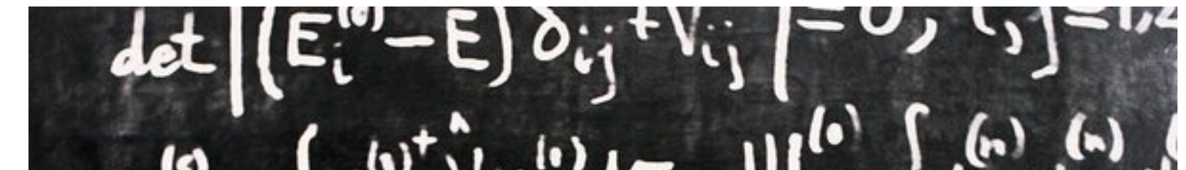
Learn by heart

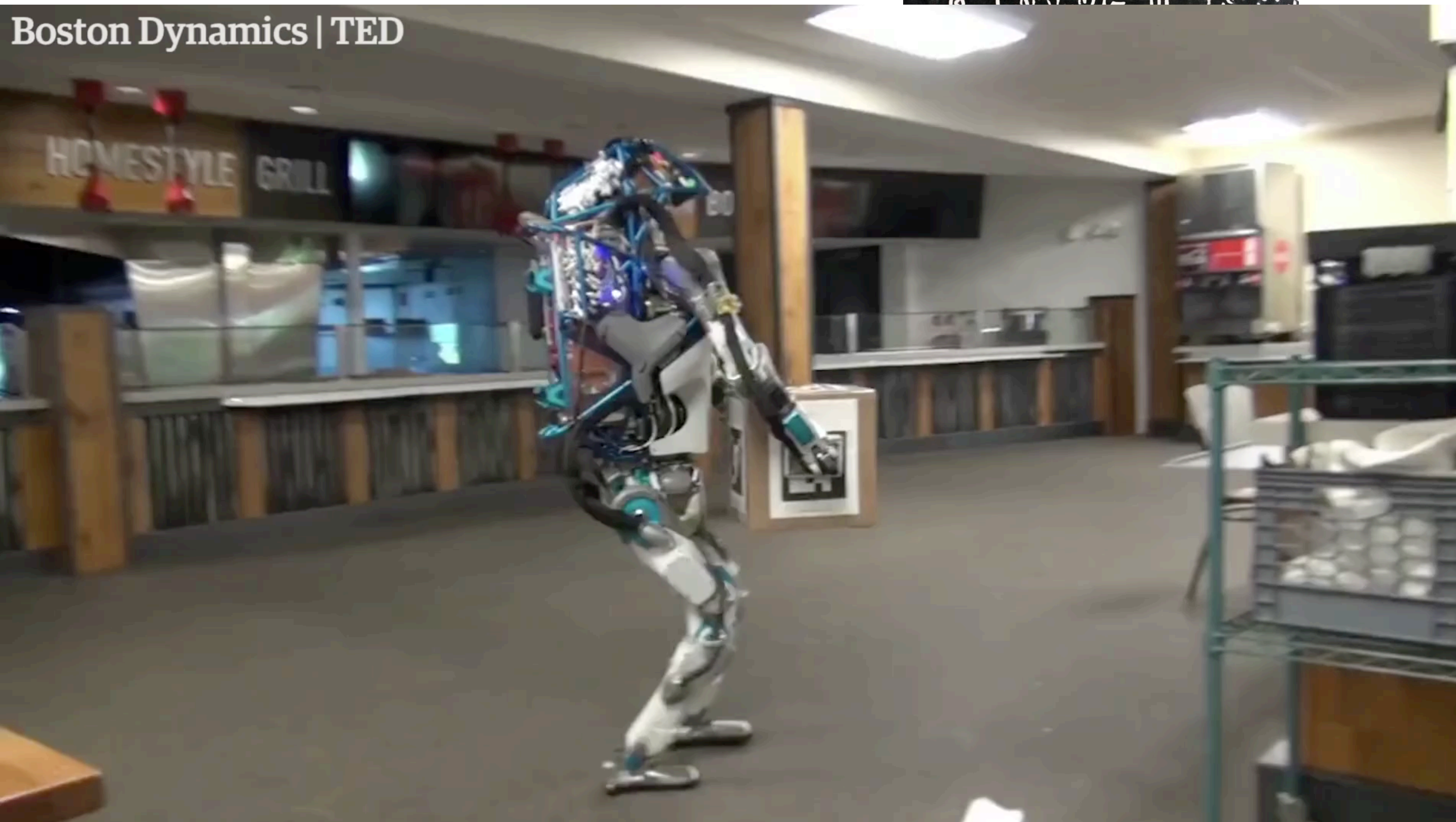


Learn abstract concepts

Learn motor skills

What is *learning*?





Learn motor skills

How about *machine* learning?

At it's heart: *Bayesian Inference:*

(just like humans! [1])

Hypothesis H

Evidence E

$$P(H|E) \propto P(E|H) \cdot P(H)$$

[1] Dehaene, S. (2020). How We Learn: Why Brains Learn Better Than Any Machine... for Now. Penguin.

How about *machine* learning?

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Prior

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Hypothesis H

Evidence E

$$\underbrace{P(H|E)}_{\text{Posterior}} \propto \underbrace{P(E|H)}_{\text{Likelihood}} \cdot \underbrace{P(H)}_{\text{Prior}}$$

- Procedure:
  - Choose Prior (*e.g.* « linear relation »)
    - Compute Likelihood
    - Evaluate Posterior
  - Repeat (with new Prior)

- *Priori beliefs* (H) are updated according to *evidence* (E), using Bayes' rule

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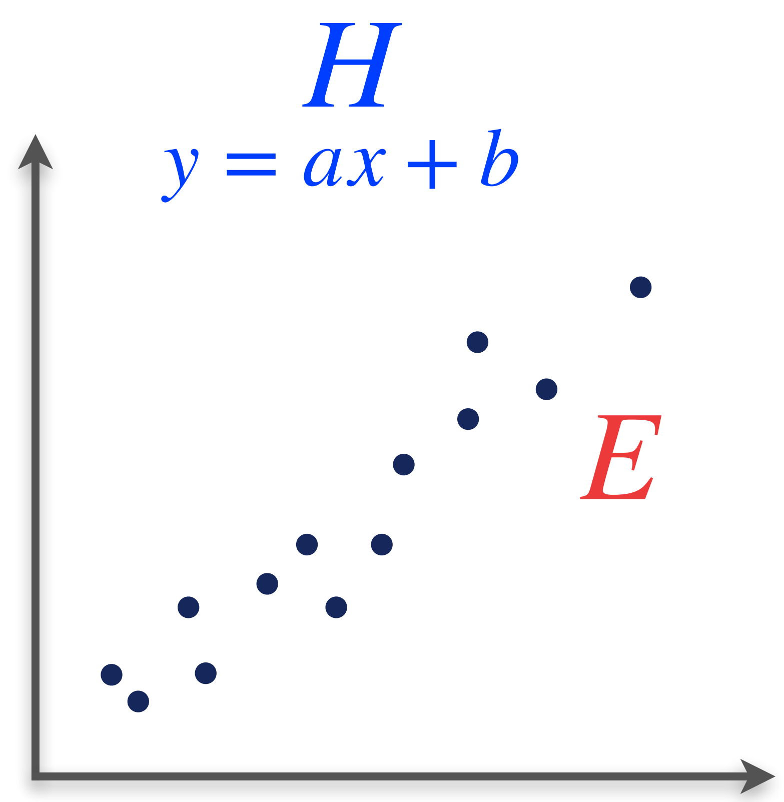
How about *machine* learning?

Often called « glorified curve-fitting »

Objective: find the prior beliefs (H) that lead to the best posterior $P(H \mid E)$



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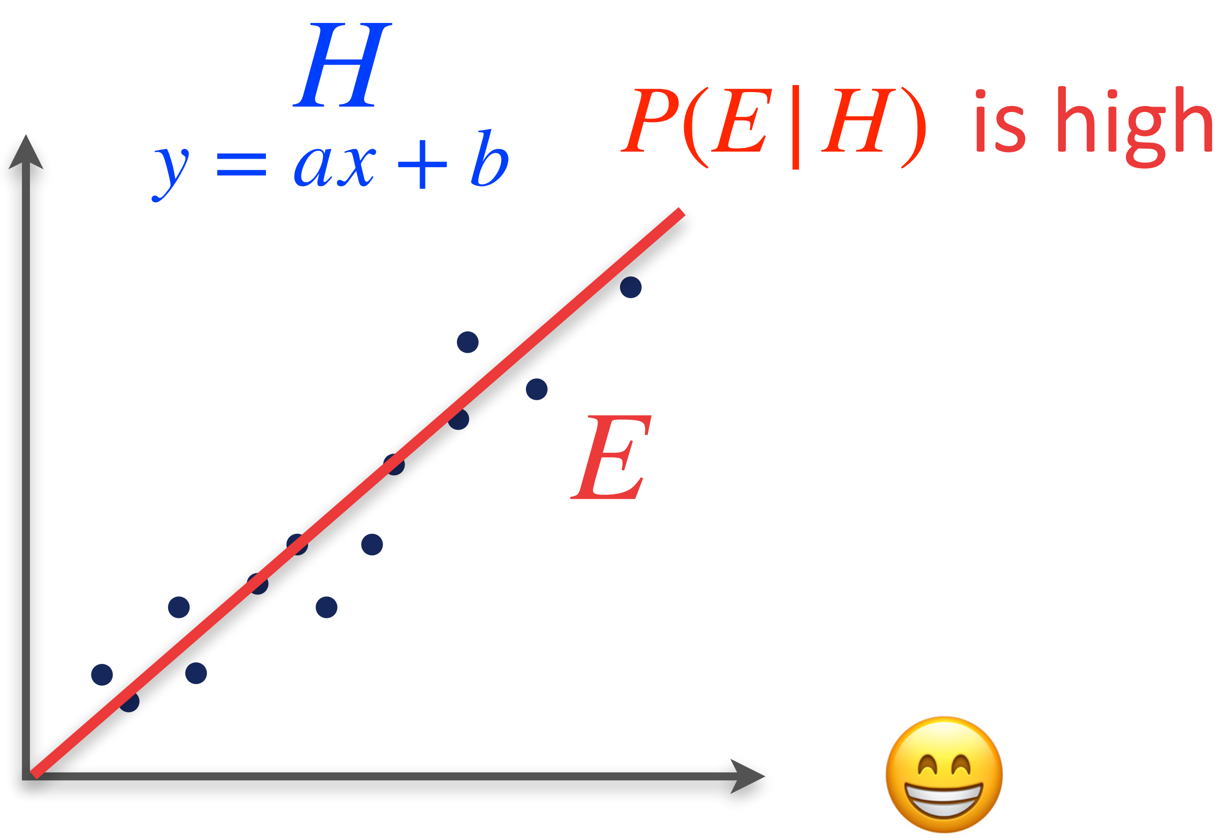

Conclusion: my hypothesis is supported by the data, so I'm now more confident in it

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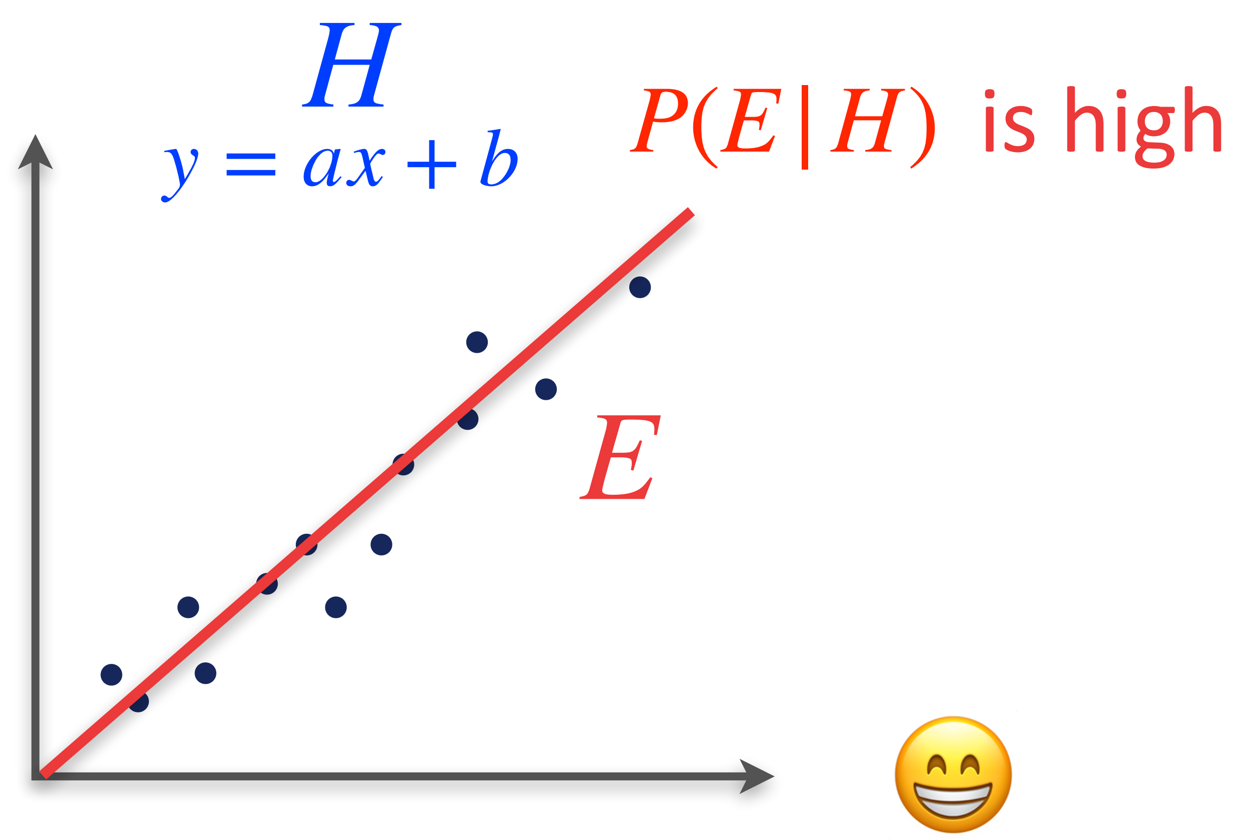

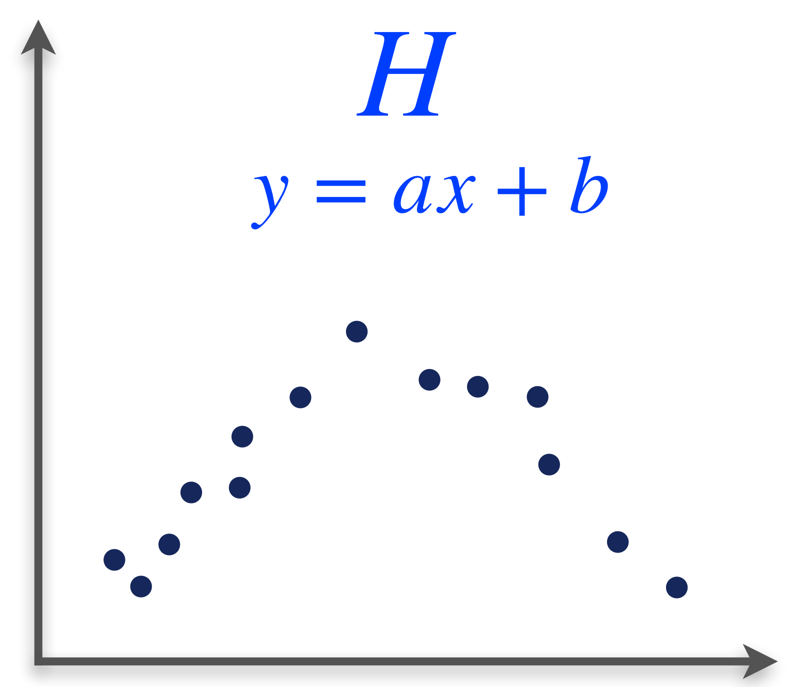

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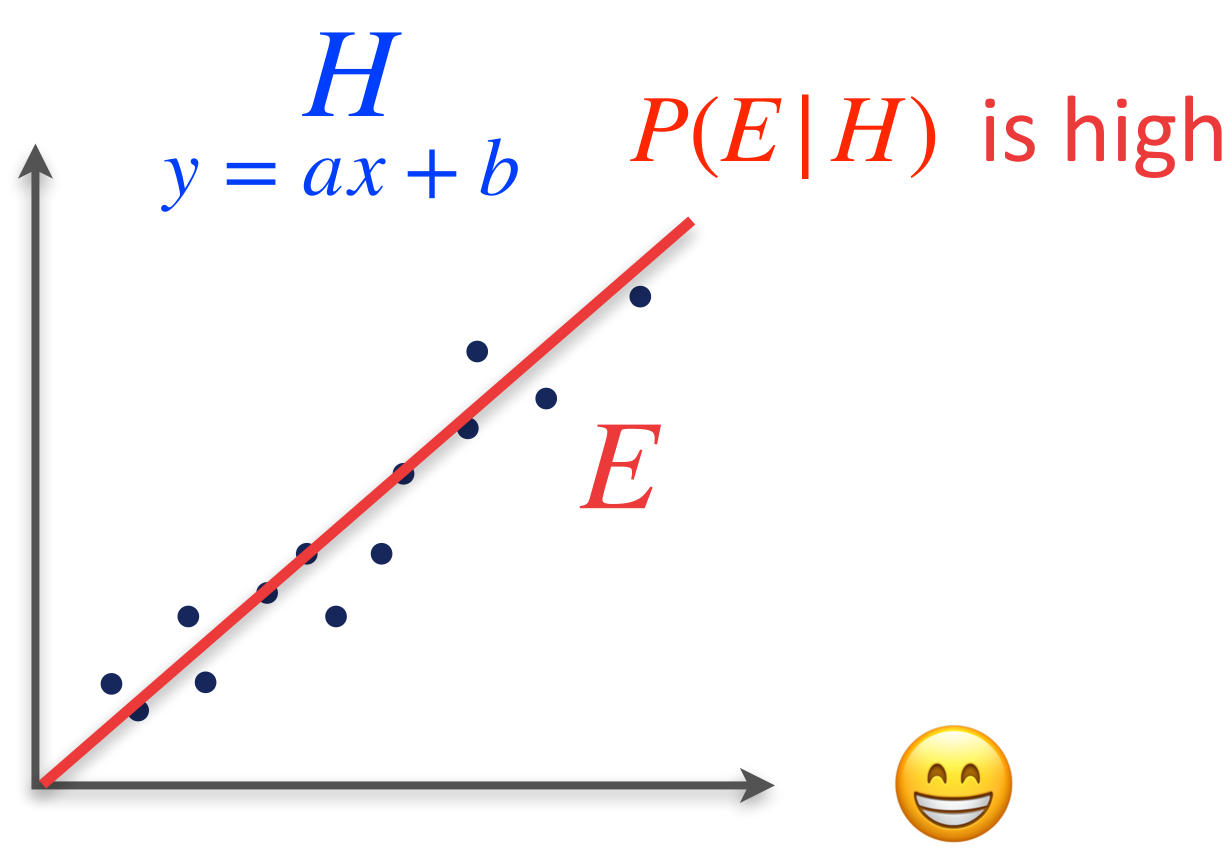

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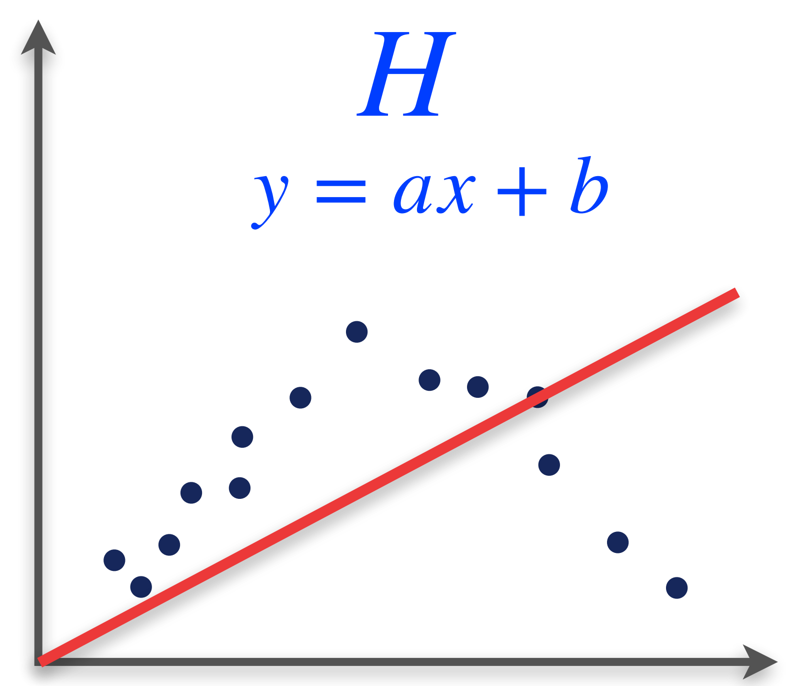

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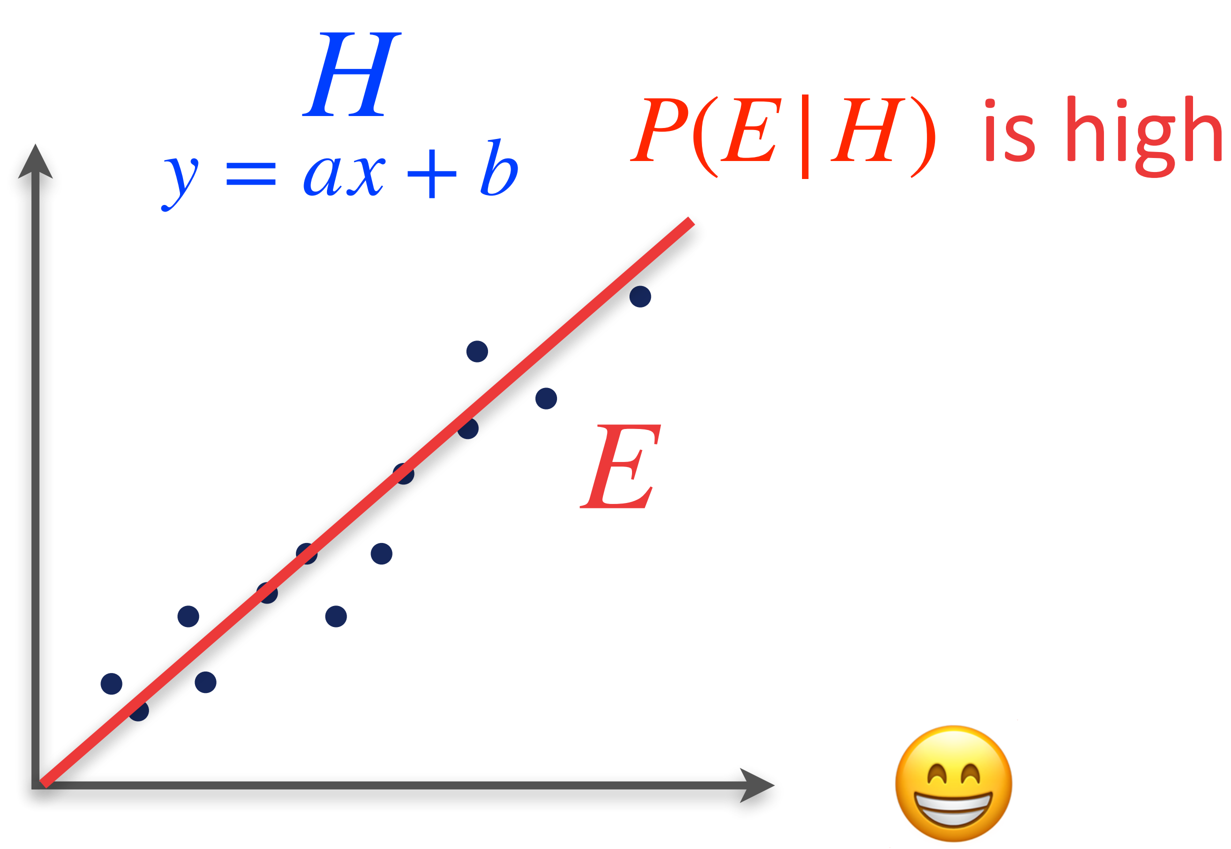

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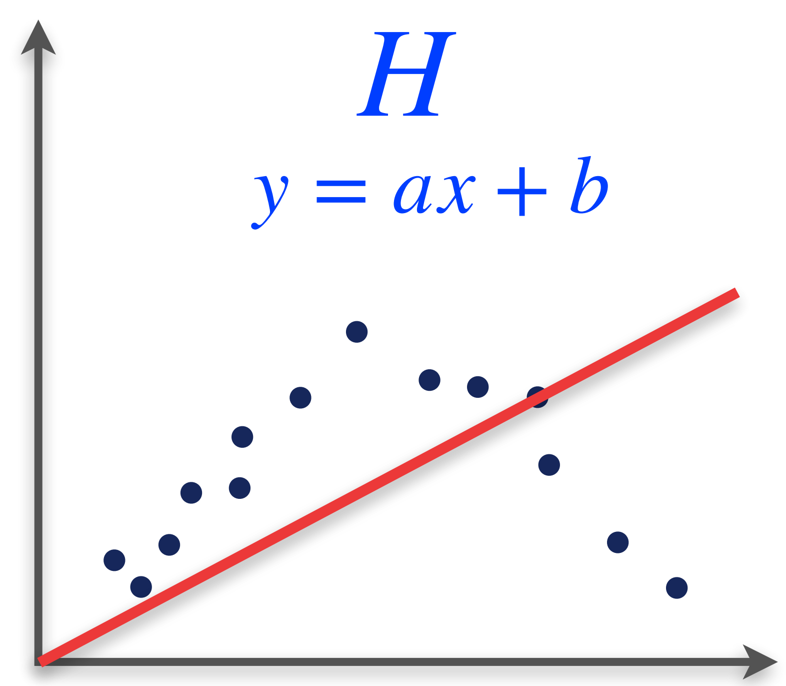

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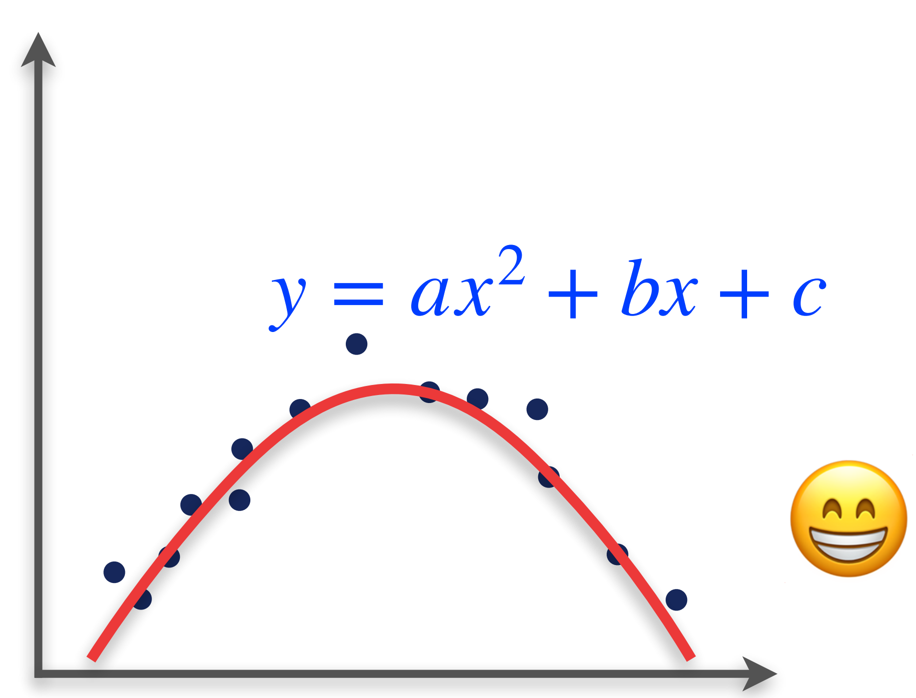
The no-free lunch theorem [1]
« there are no a priori distinctions between learning algorithms »



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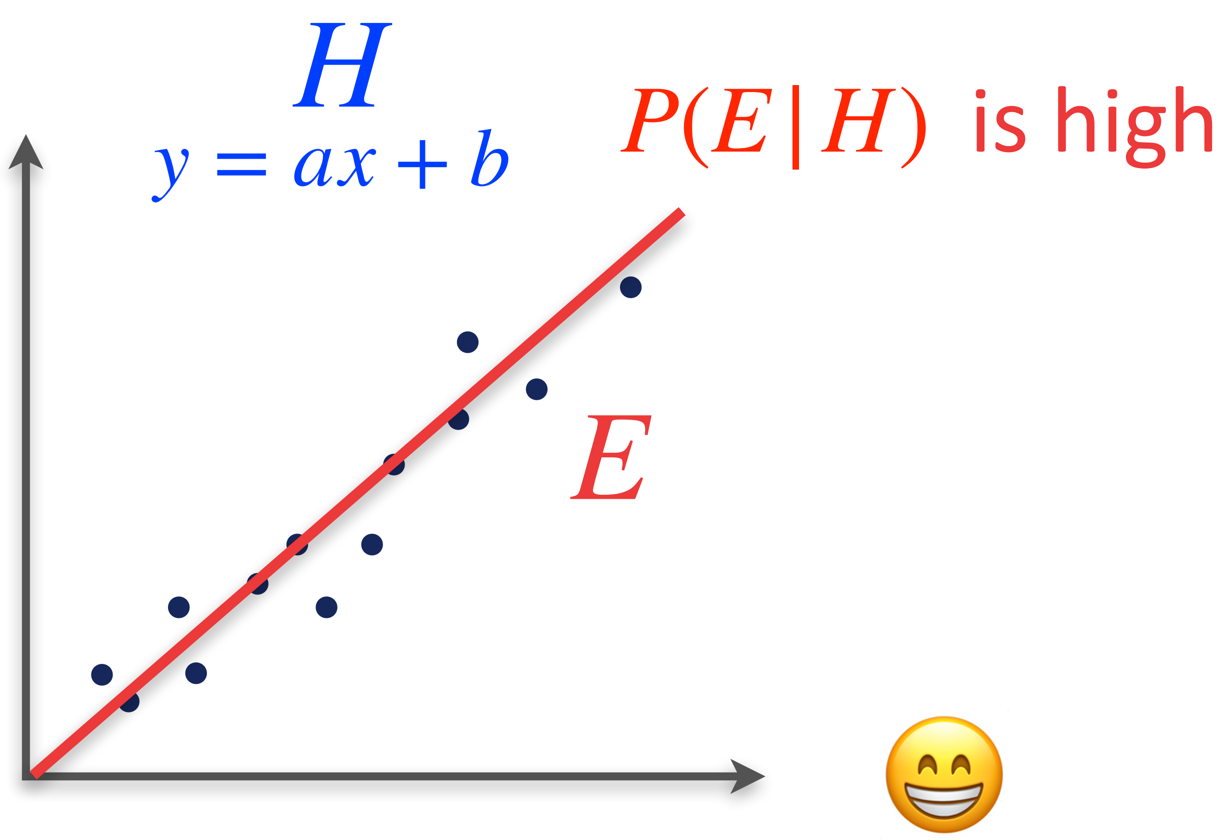

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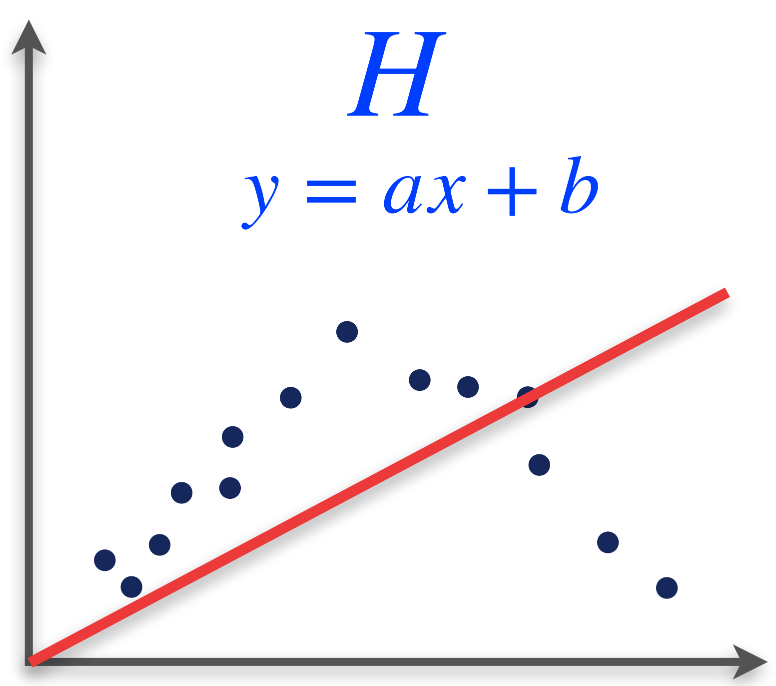

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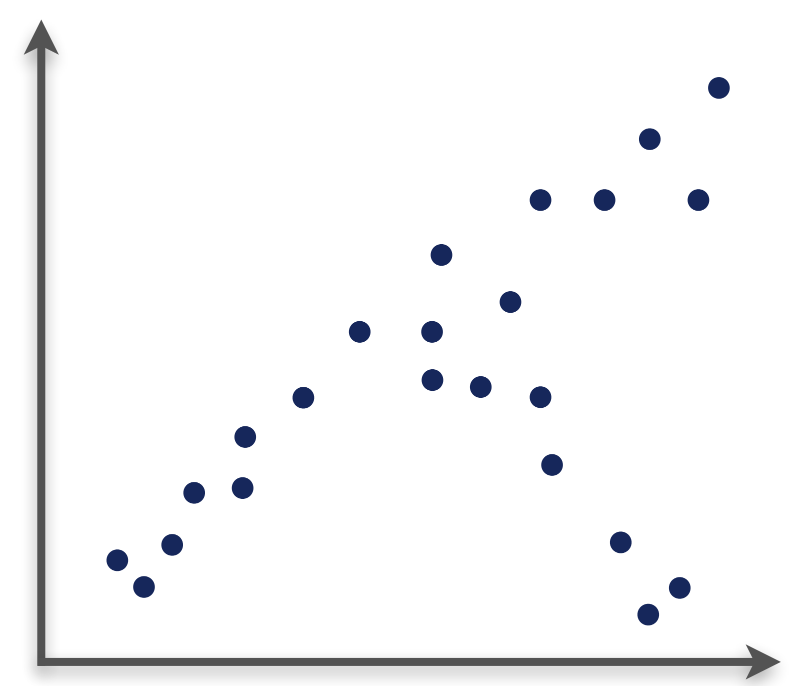

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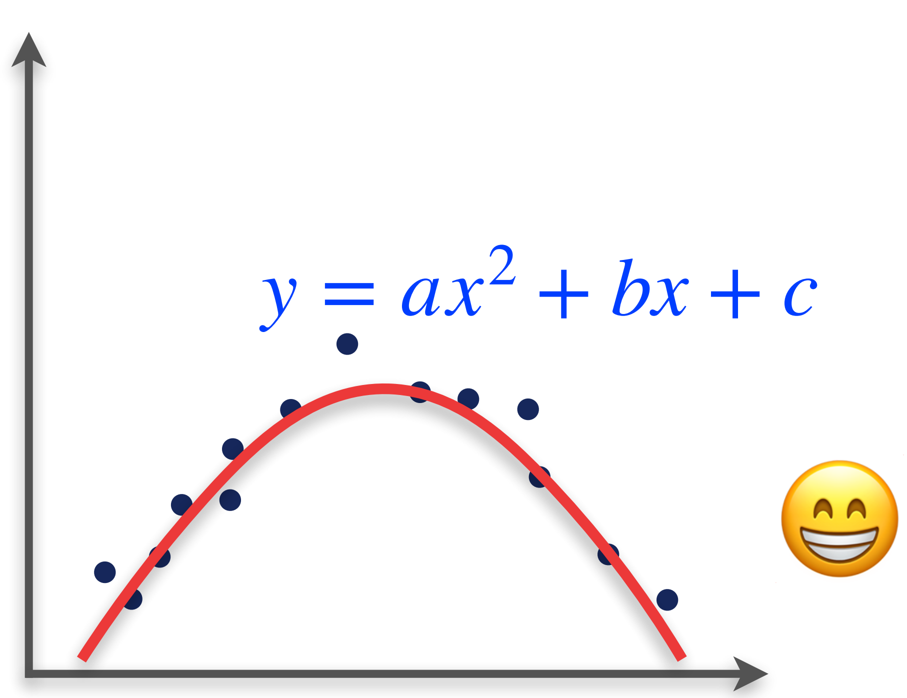

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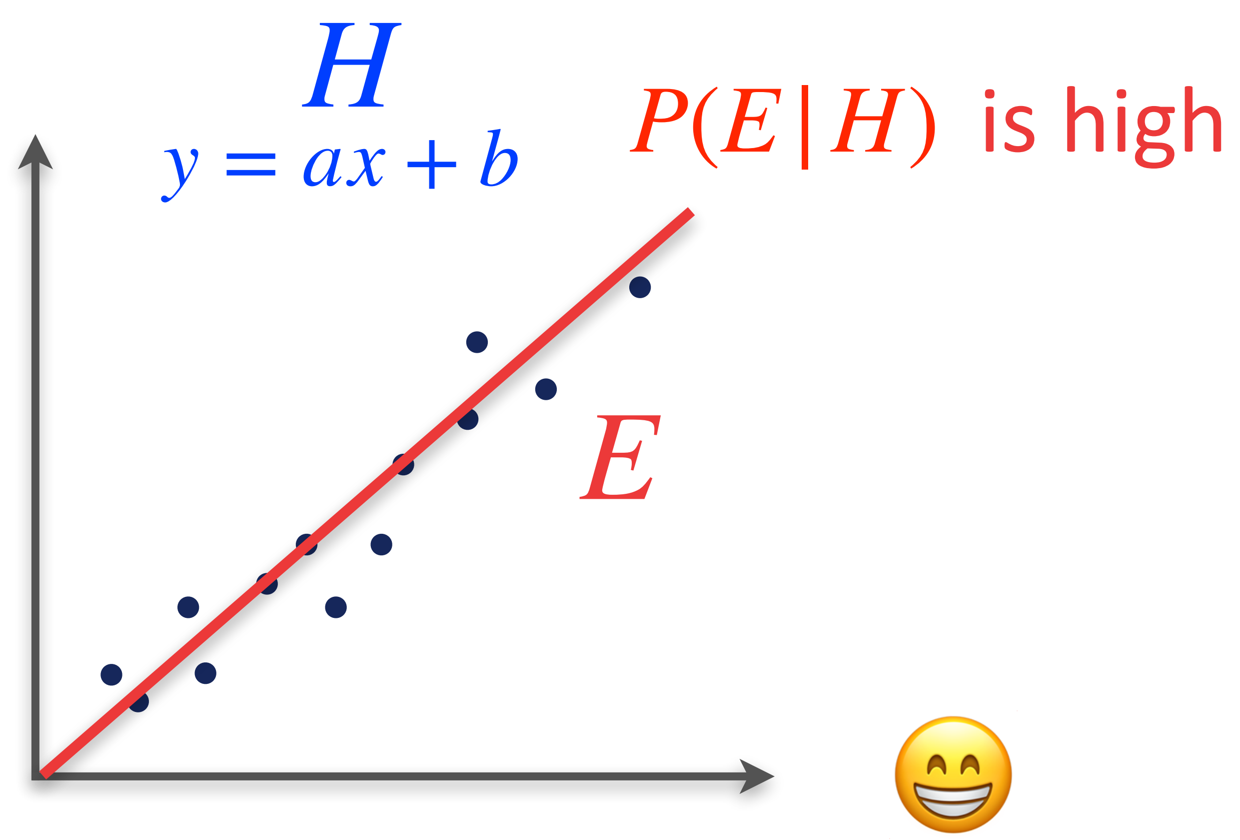

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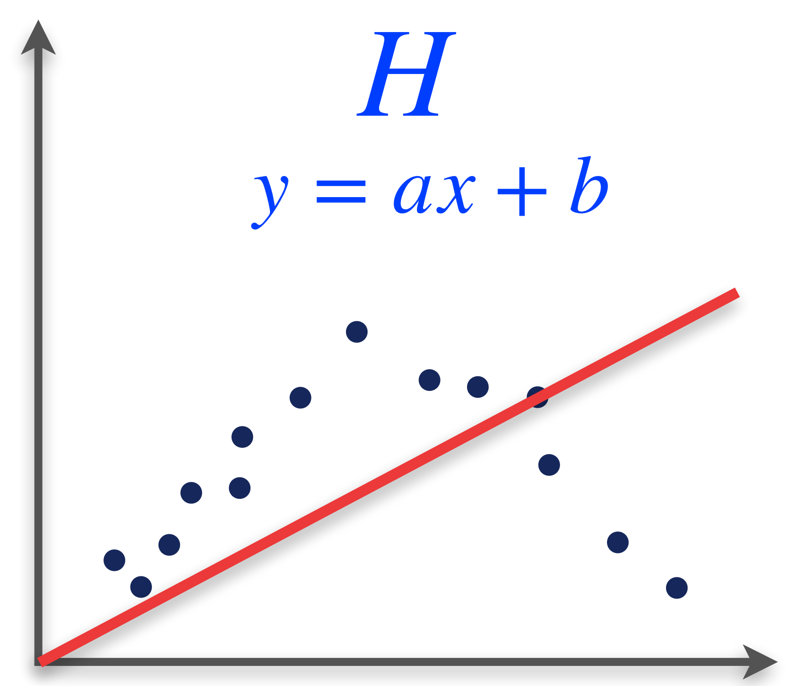

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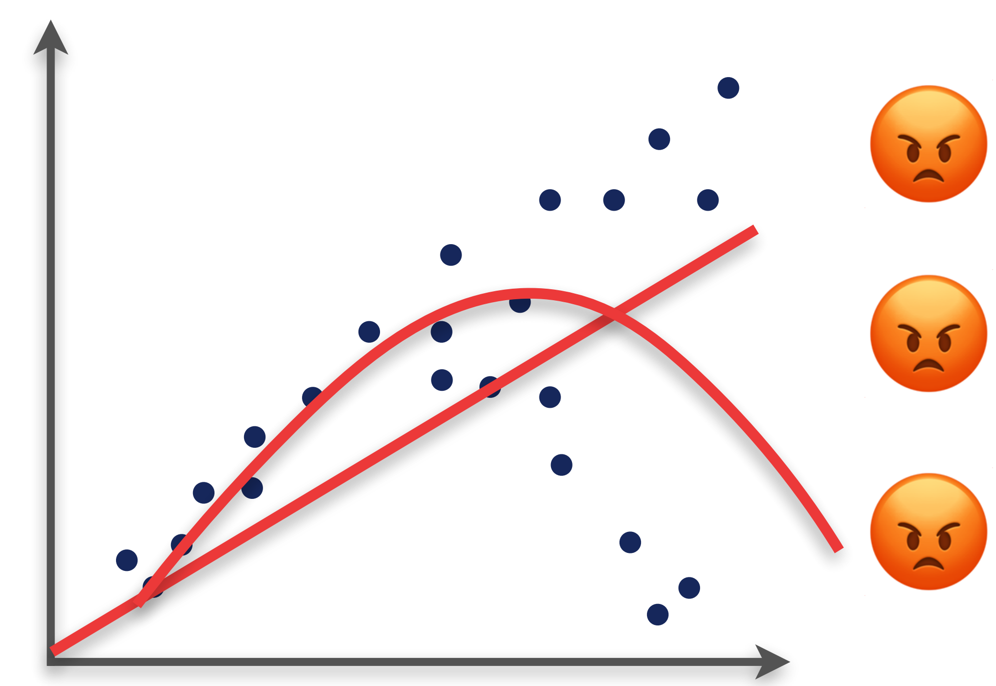
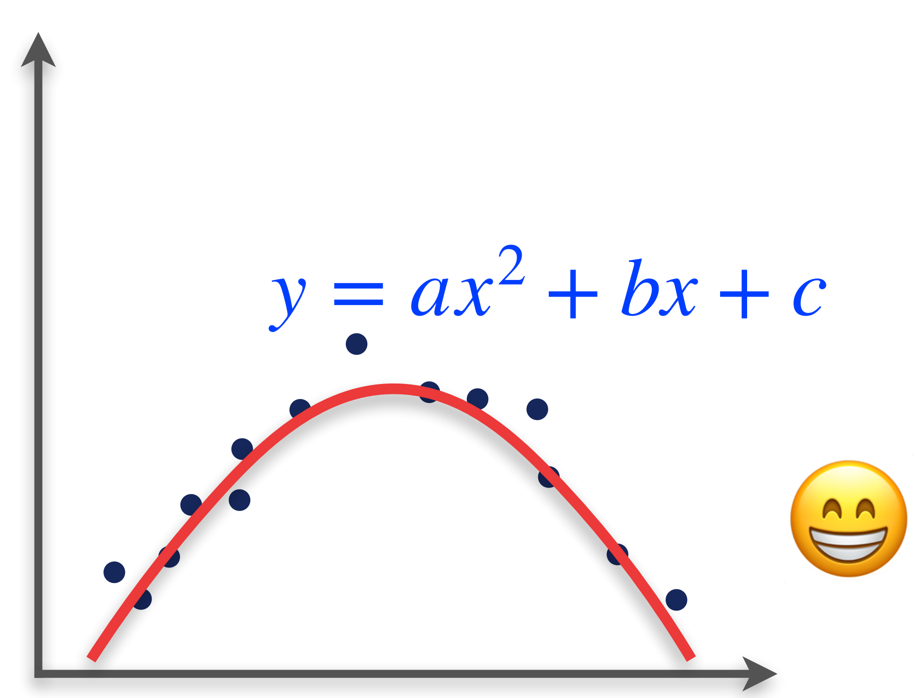


Conclusion:
Nothing works!

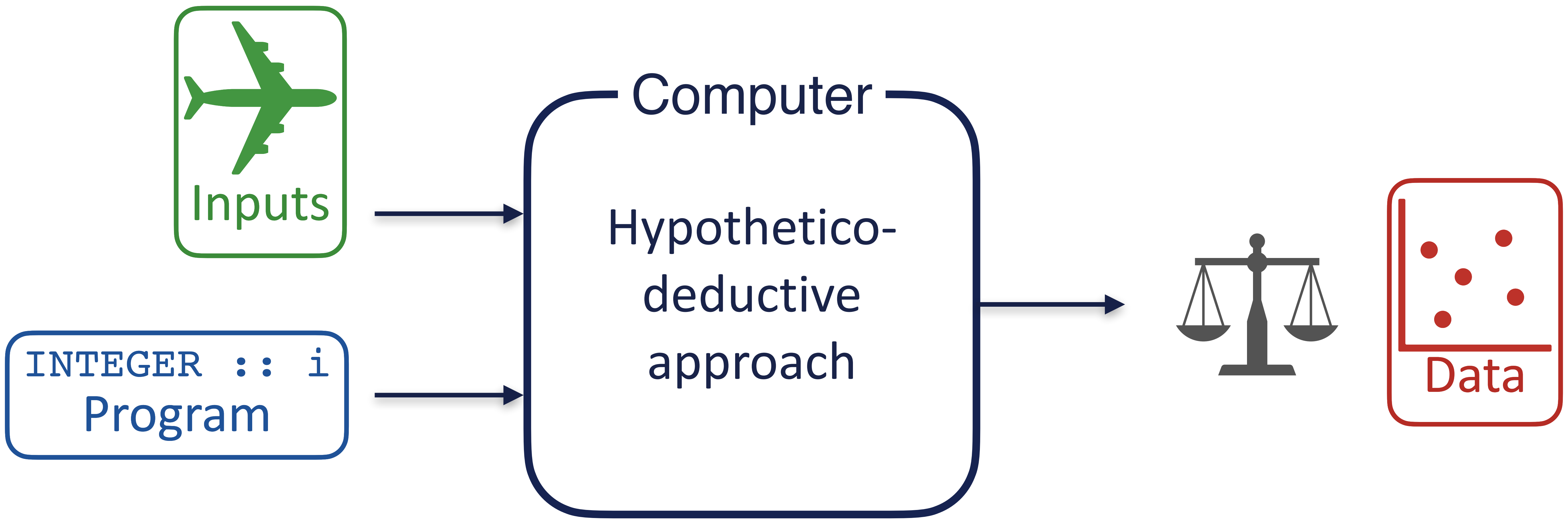
The no-free lunch theorem [1]
« there are no a priori distinctions between learning algorithms »



Some problems are ill-posed:
There is a fundamental ambiguity that cannot be resolved

[1] Wolpert, David H. "The lack of a priori distinctions between learning algorithms." Neural computation 8.7 (1996): 1341-1390.

Learning: a paradigm shift



Breiman, L. (2001). Statistical modeling: The two cultures. *Statistical science*, *16*(3), 199-231.

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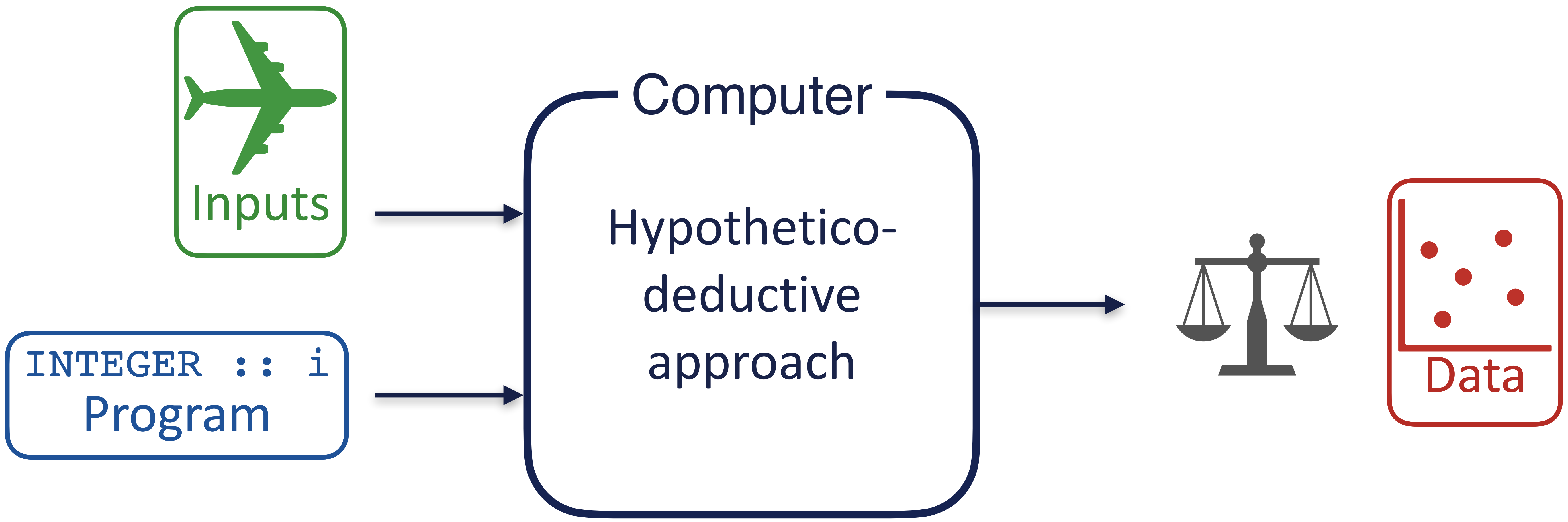

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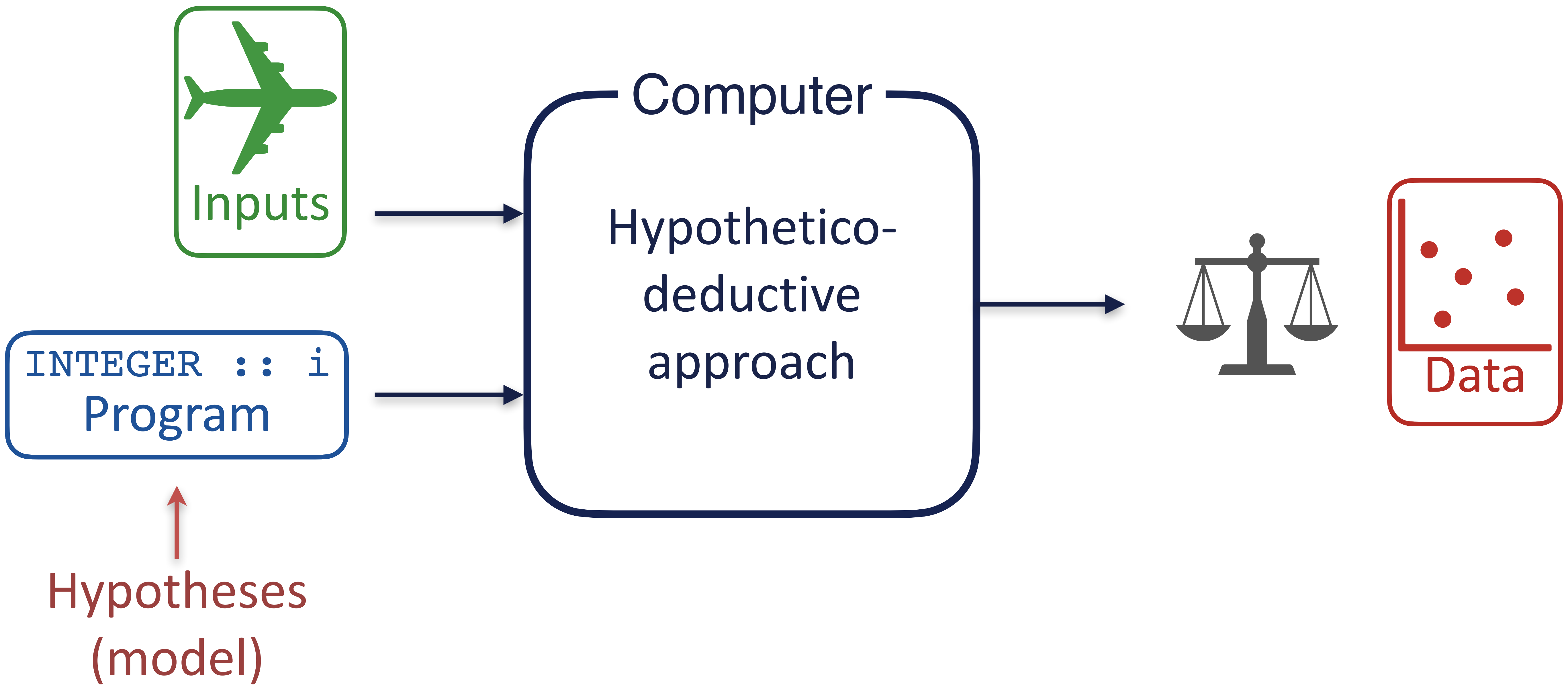

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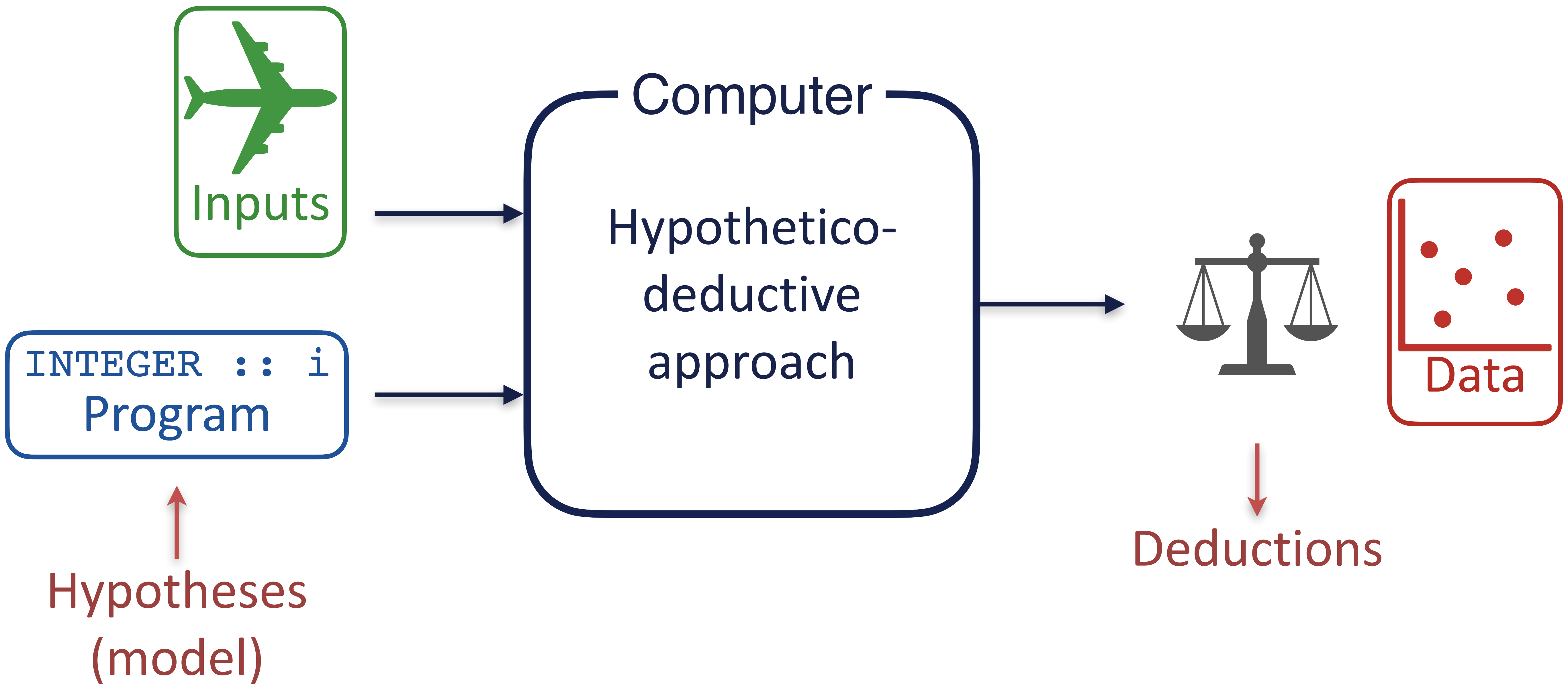

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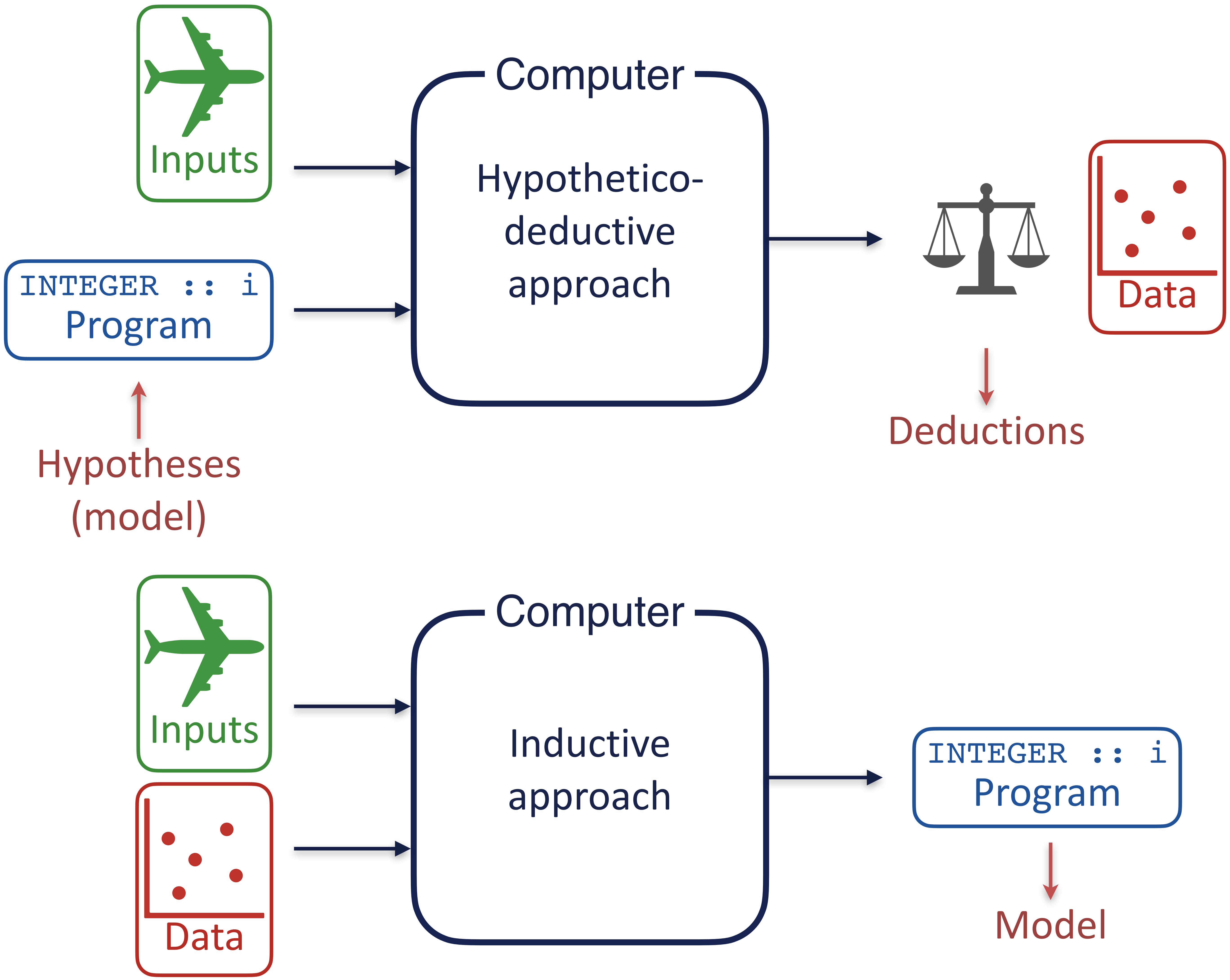

The scientific method is historically a deductive approach. **The data validates the model.**

Data-driven approaches are *inductive*. **The model is the output.**

Breiman, L. (2001). Statistical modeling: The two cultures. *Statistical science*, *16*(3), 199-231.

Machine Learning

AlphaZero …

Uses of AI

OpenAI

DeepMind

Uses of AI

Machine Learning

AlphaZero …

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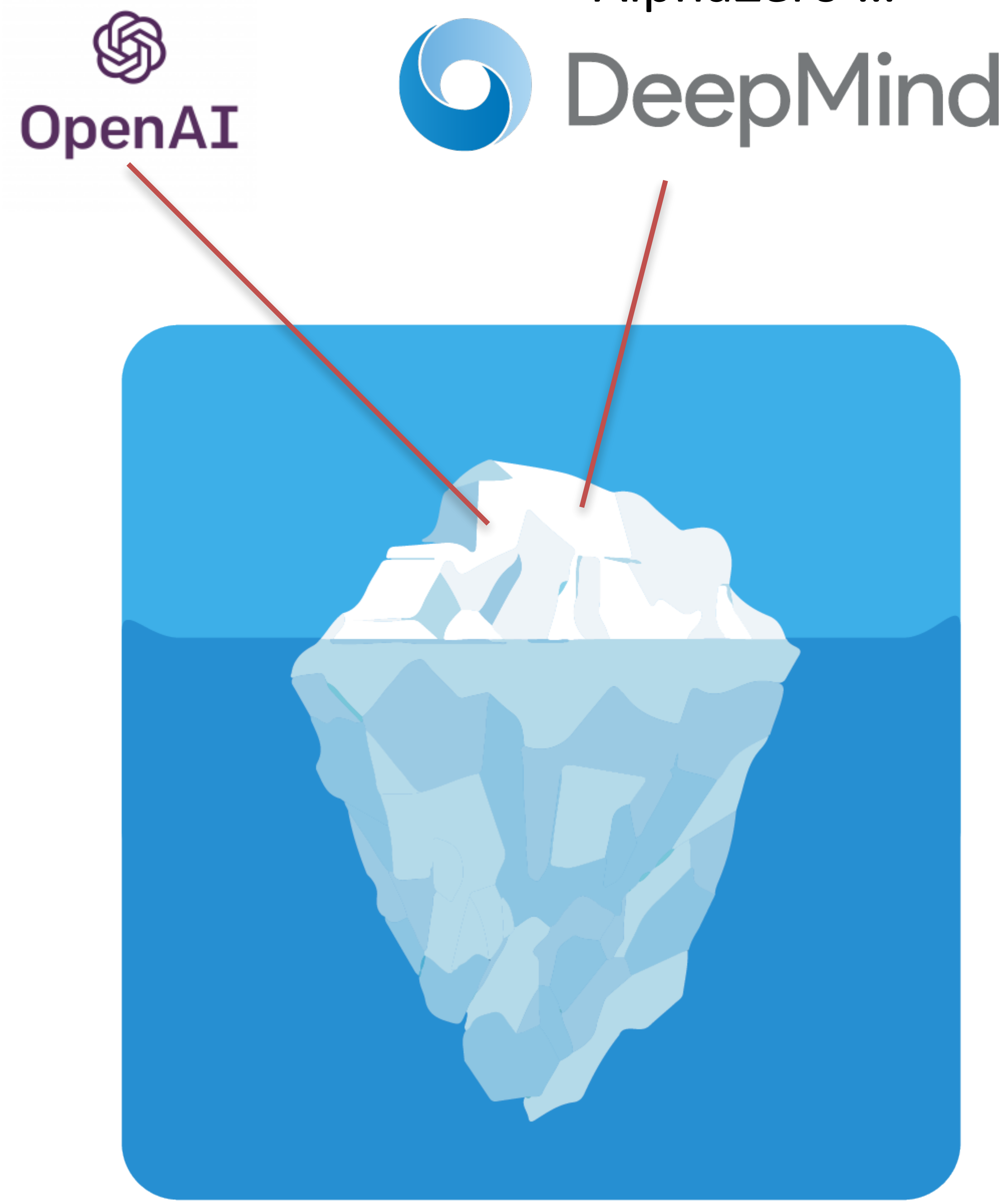
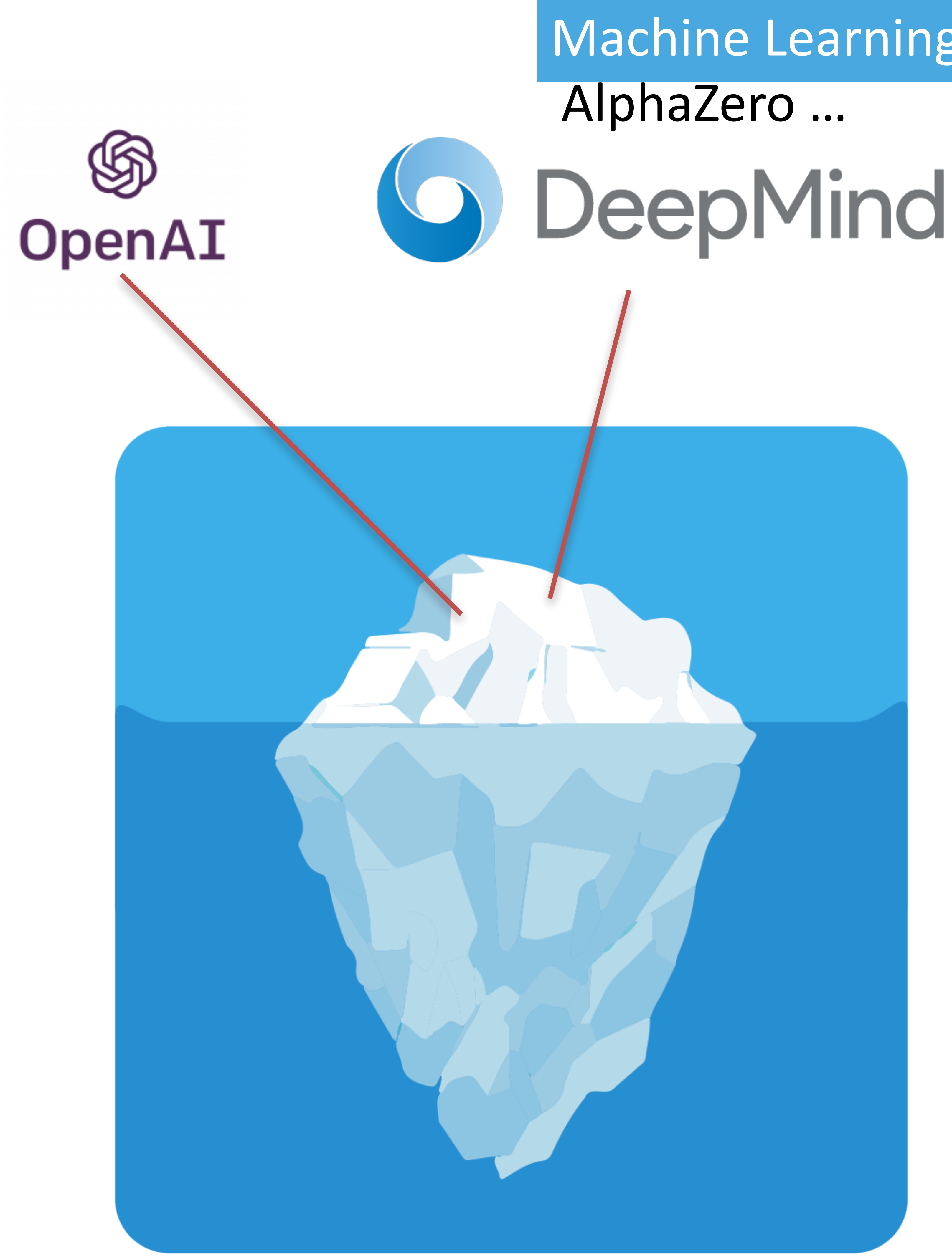


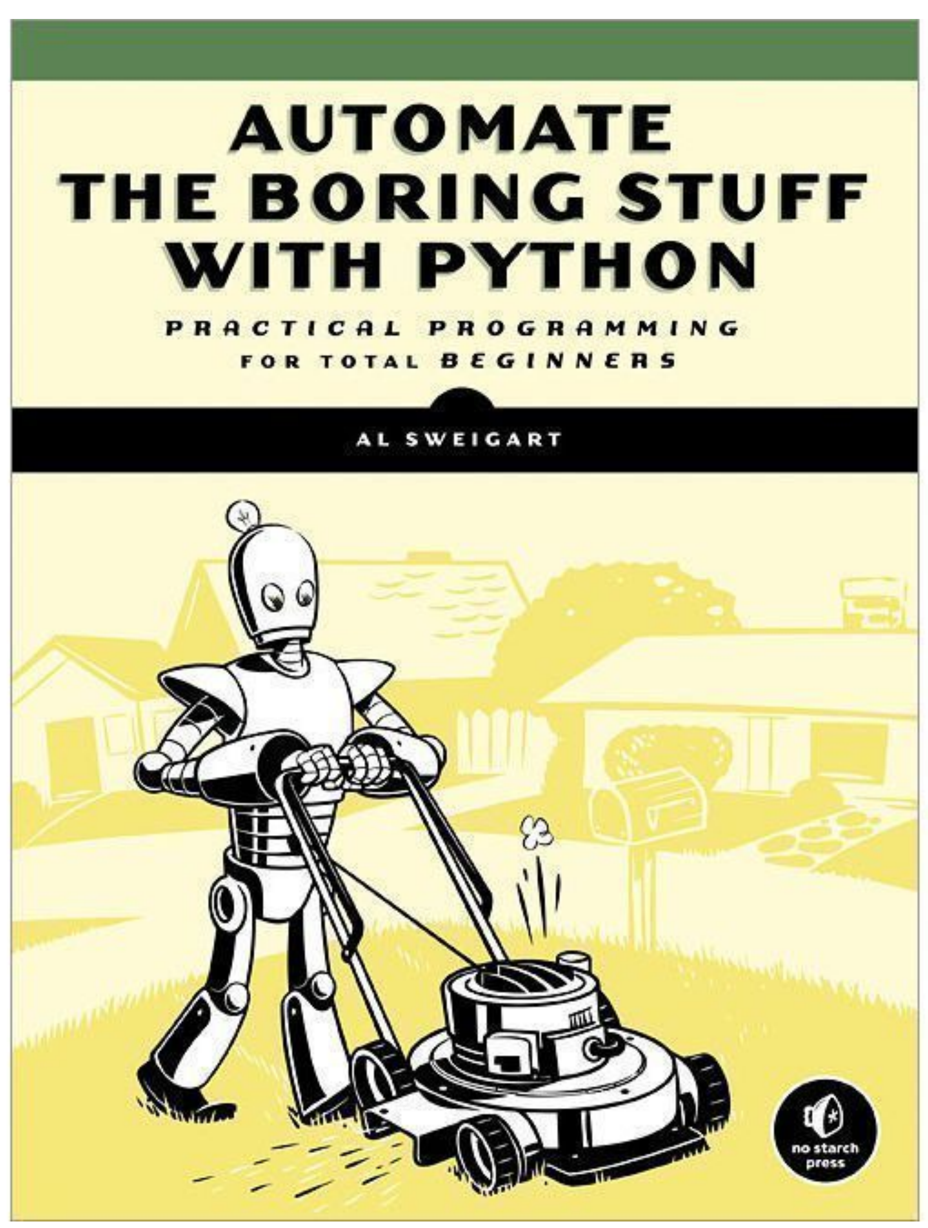
Uses of AI

- Shiny « superhuman » algorithms make headlines

- But most applications « automate the boring stuff ».



Just like regular programming does!



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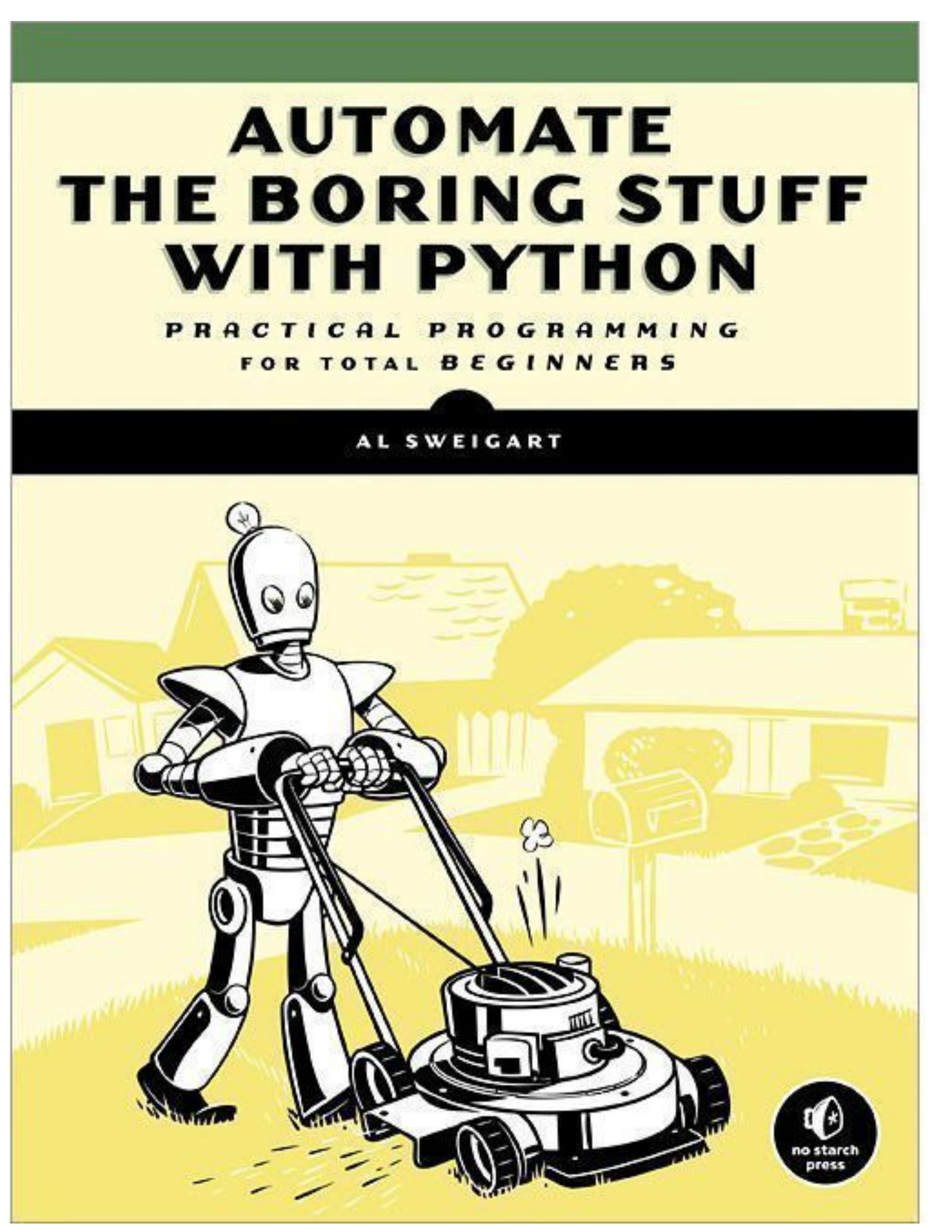

amazon

300 Million Images / Day + ...

100 Billion Words / Day + ...

+ ...

Intelligence vs Experience

- One definition of intelligence: $$\text{Intelligence} = \frac{\text{Skill}}{\text{Experience}}$$
  (from F. Chollet)

[1]: Silver, D., Hubert, T., Schrittwieser, J., Antonoglou, I., Lai, M., Guez, A., ... & Lillicrap, T. (2017). Mastering chess and shogi by self-play with a general reinforcement learning algorithm.

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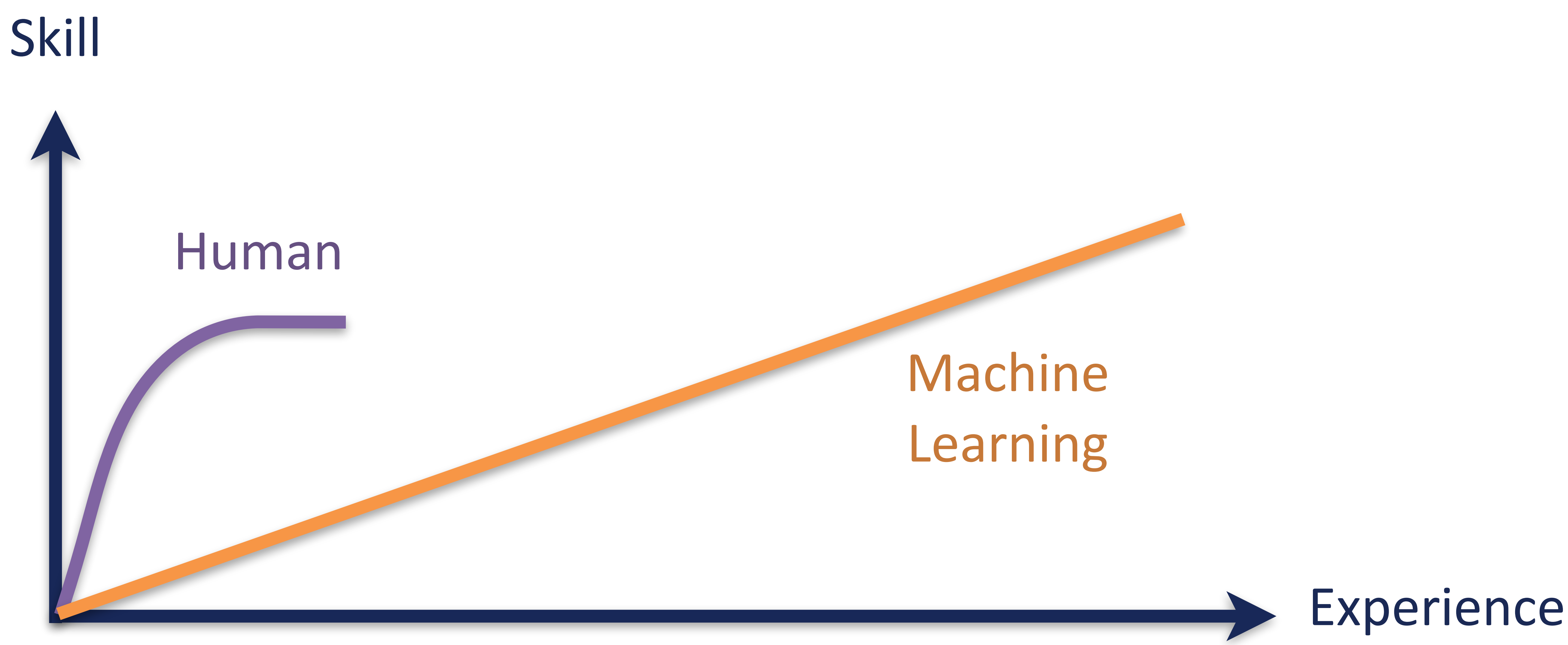

Alpha Zero[1] needs 21 Million games of Go during training

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training takes ≈24h

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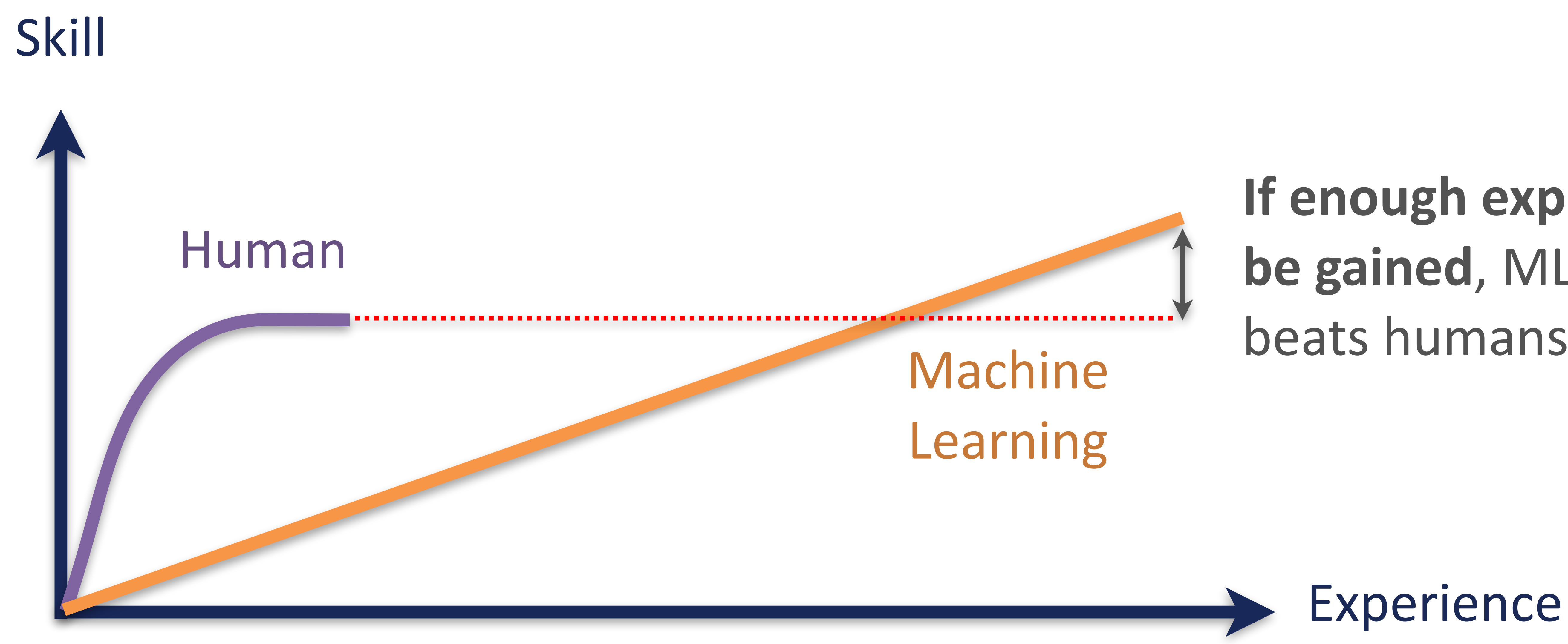

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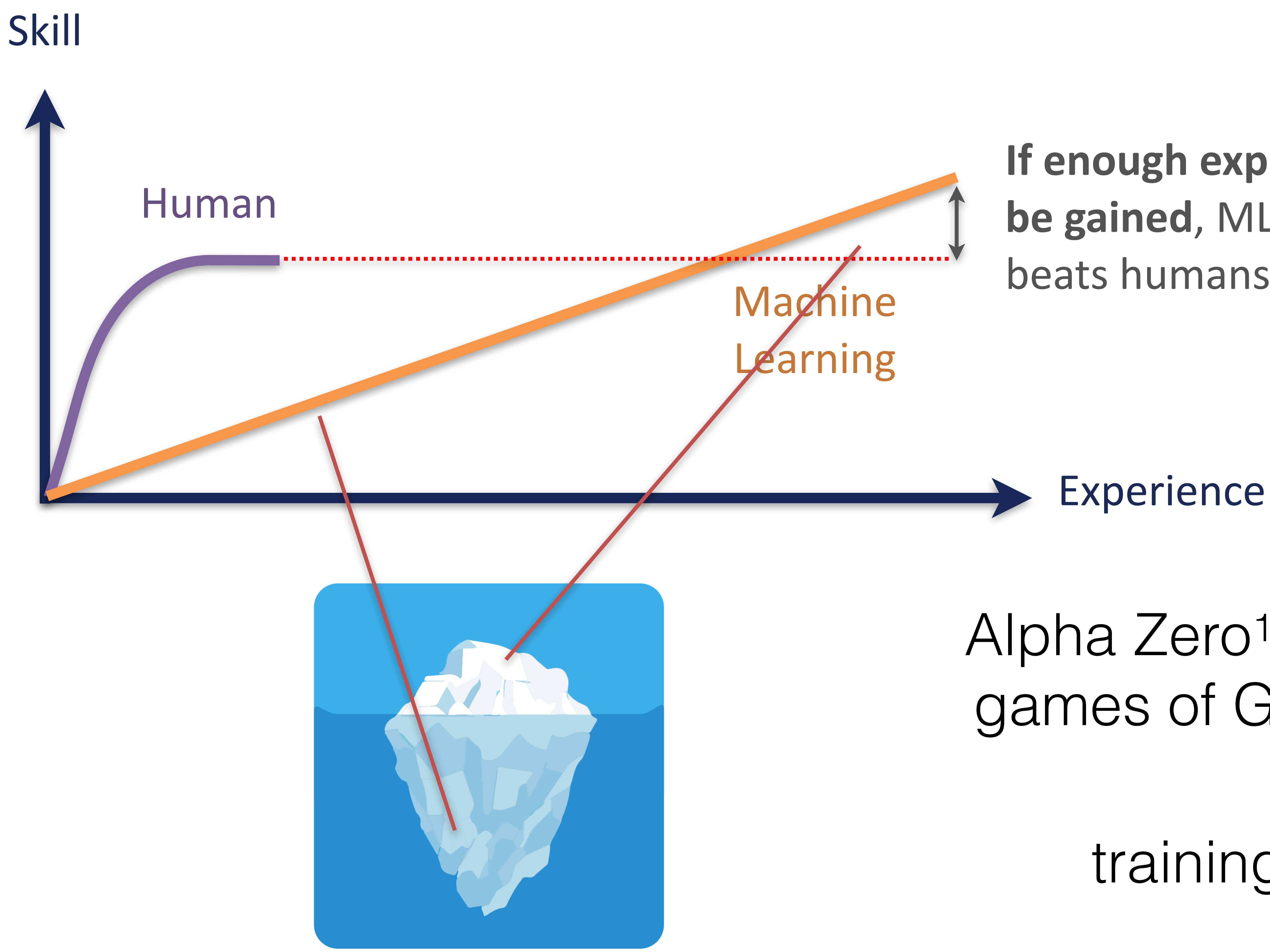

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Finding a good ML problem

Focus on problems that would be difficult to solve with traditional programming

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Neural networks ≈ « intuition machines ». If you can do it but you don't know how, you can't code it. Example:

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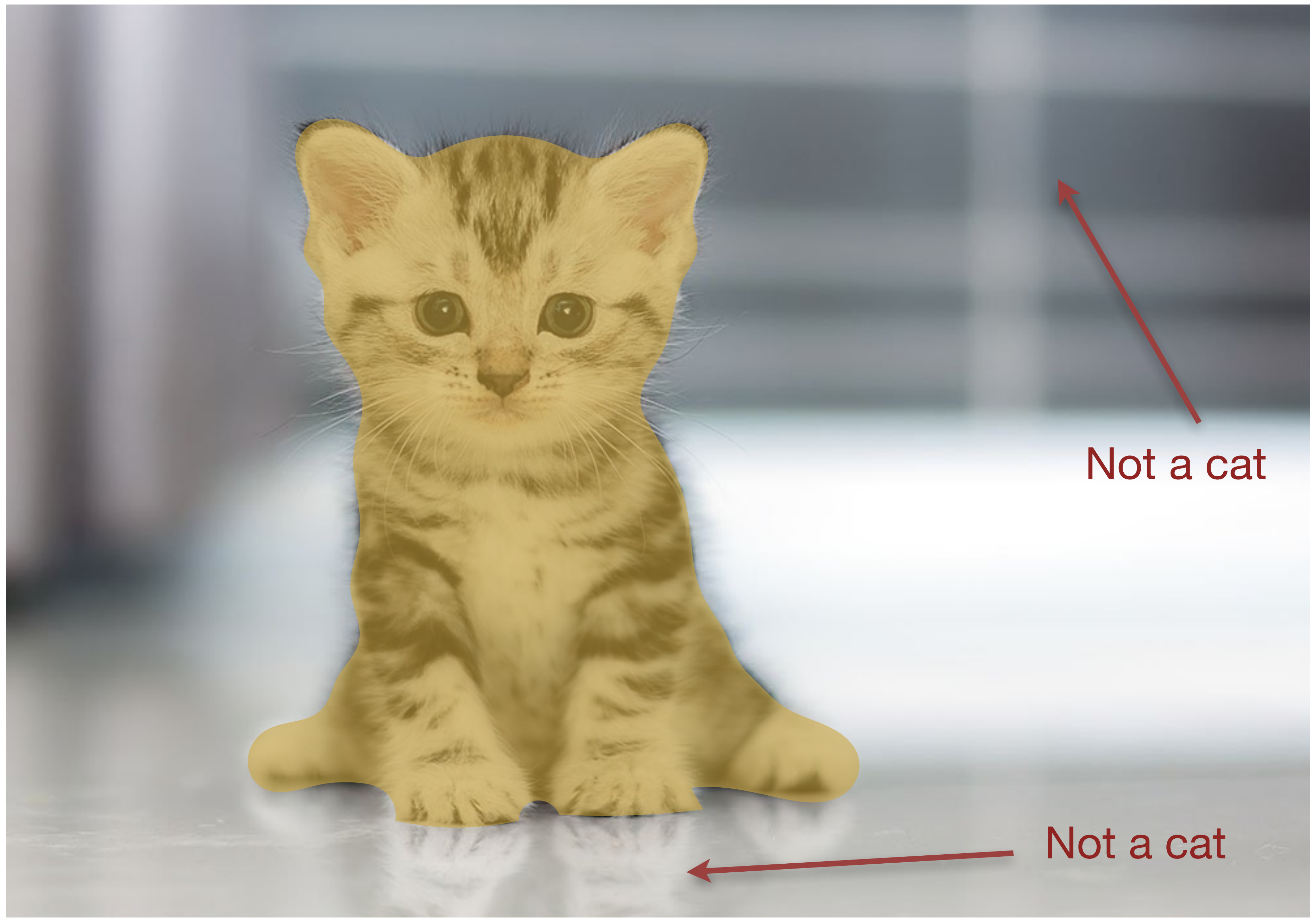

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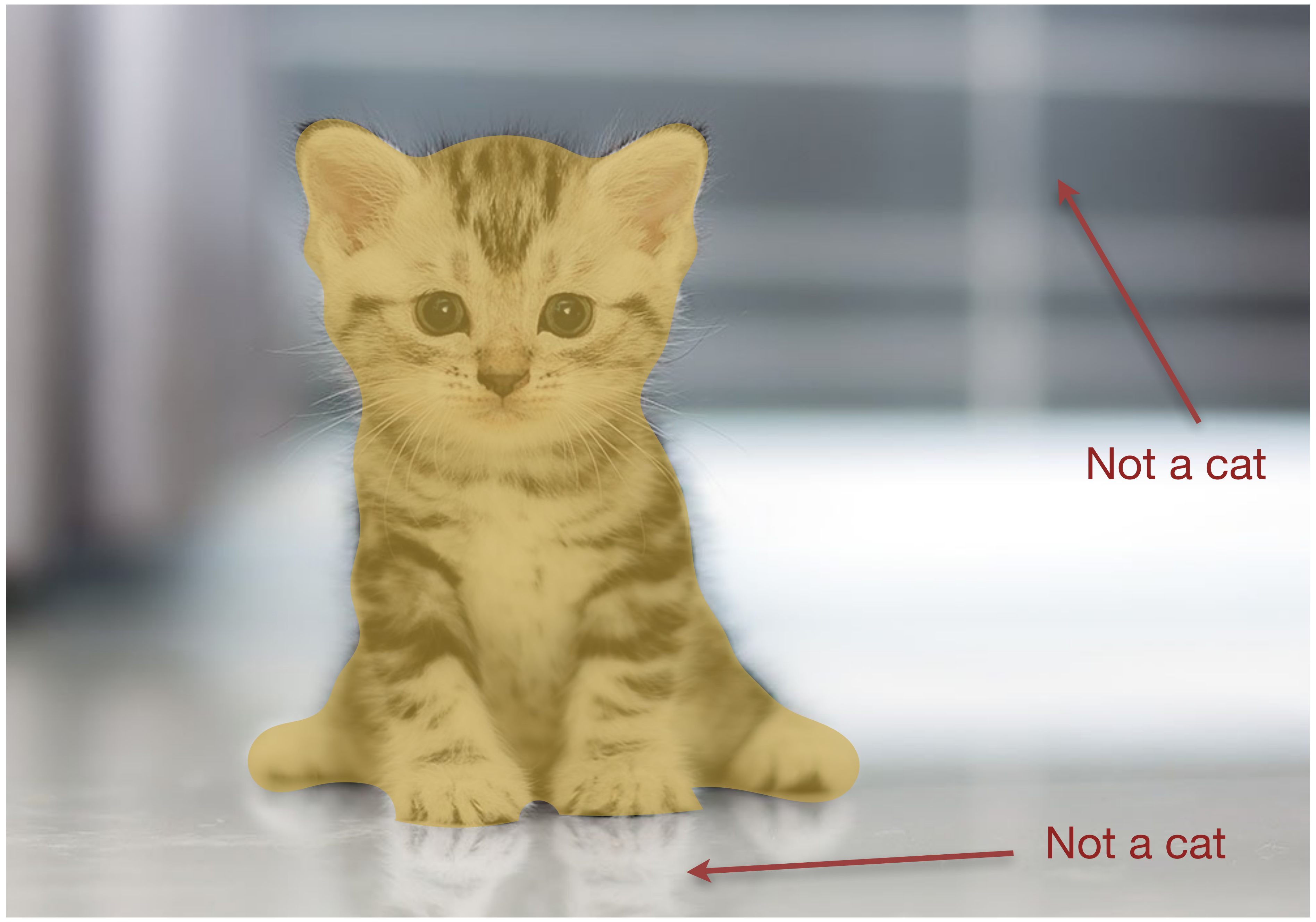

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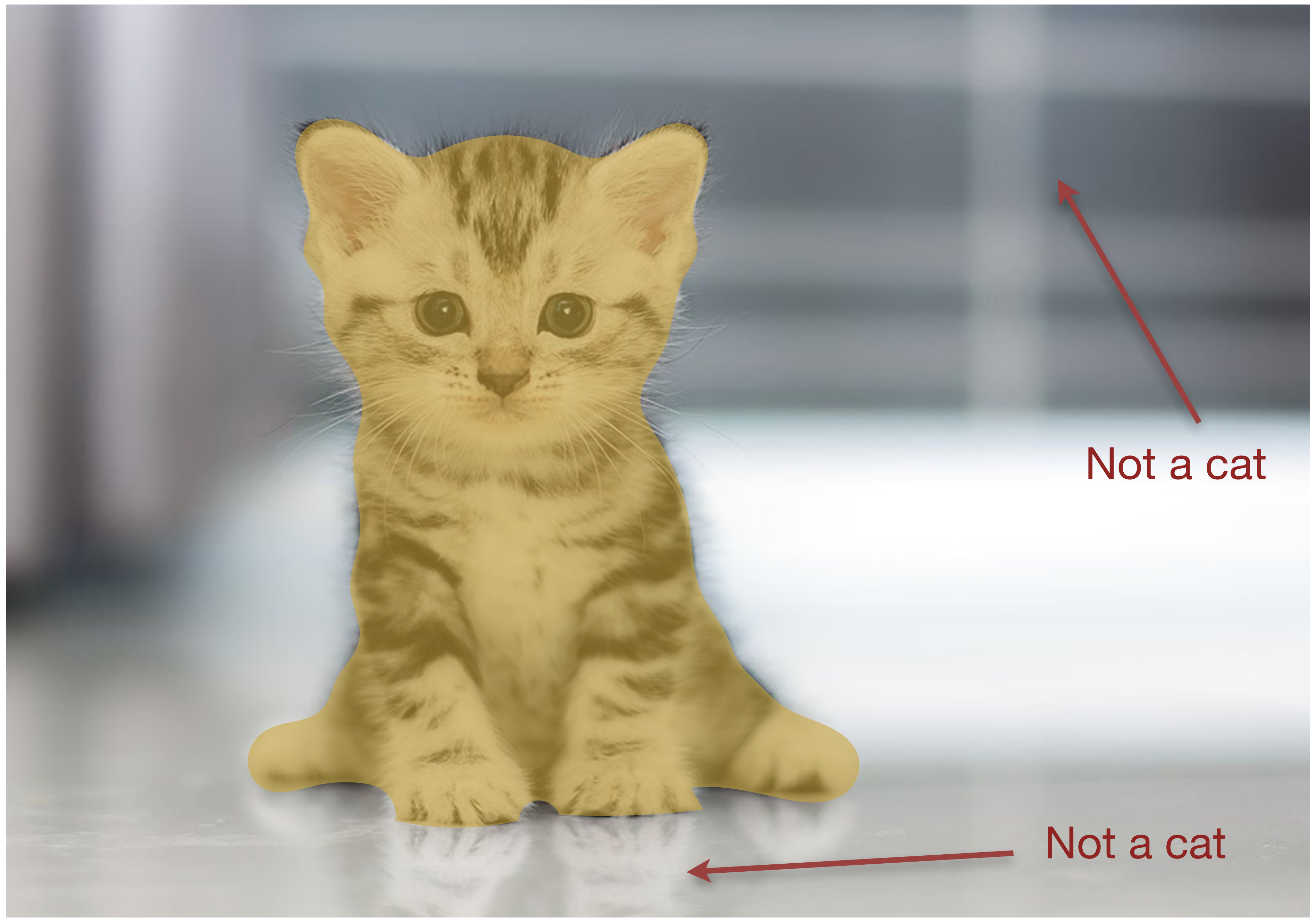

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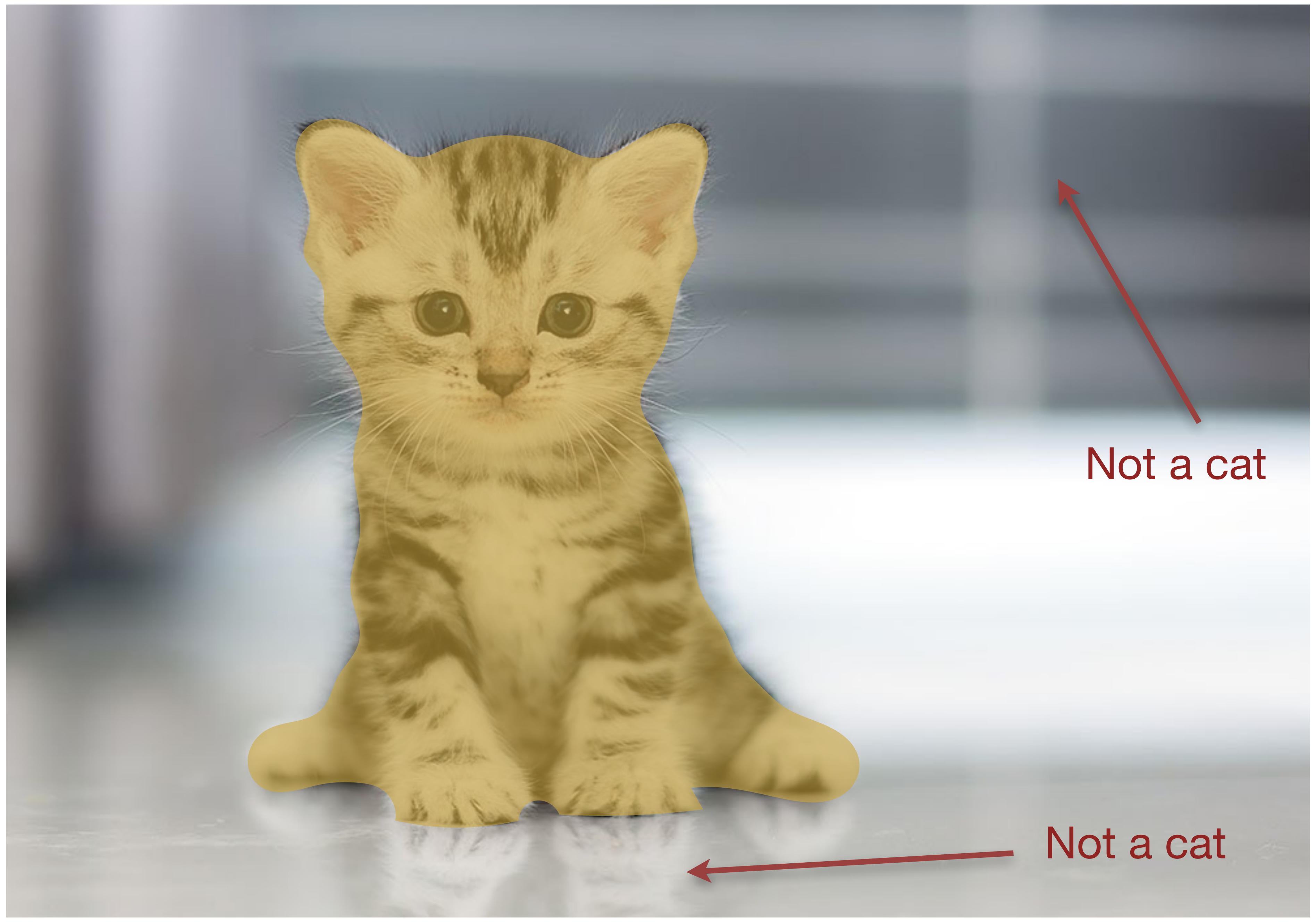

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Ok, but what is a lot?

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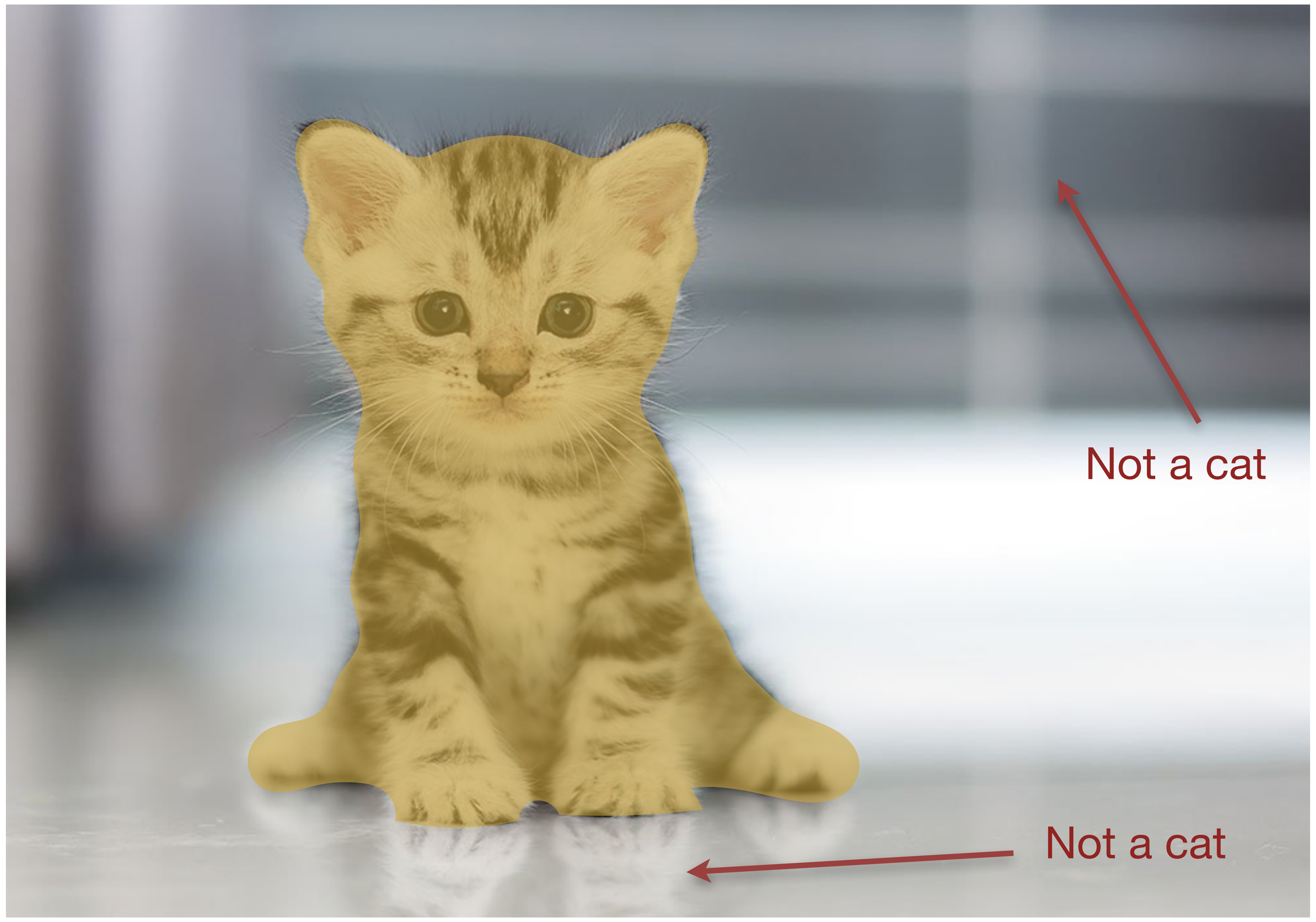


Where's the cat?

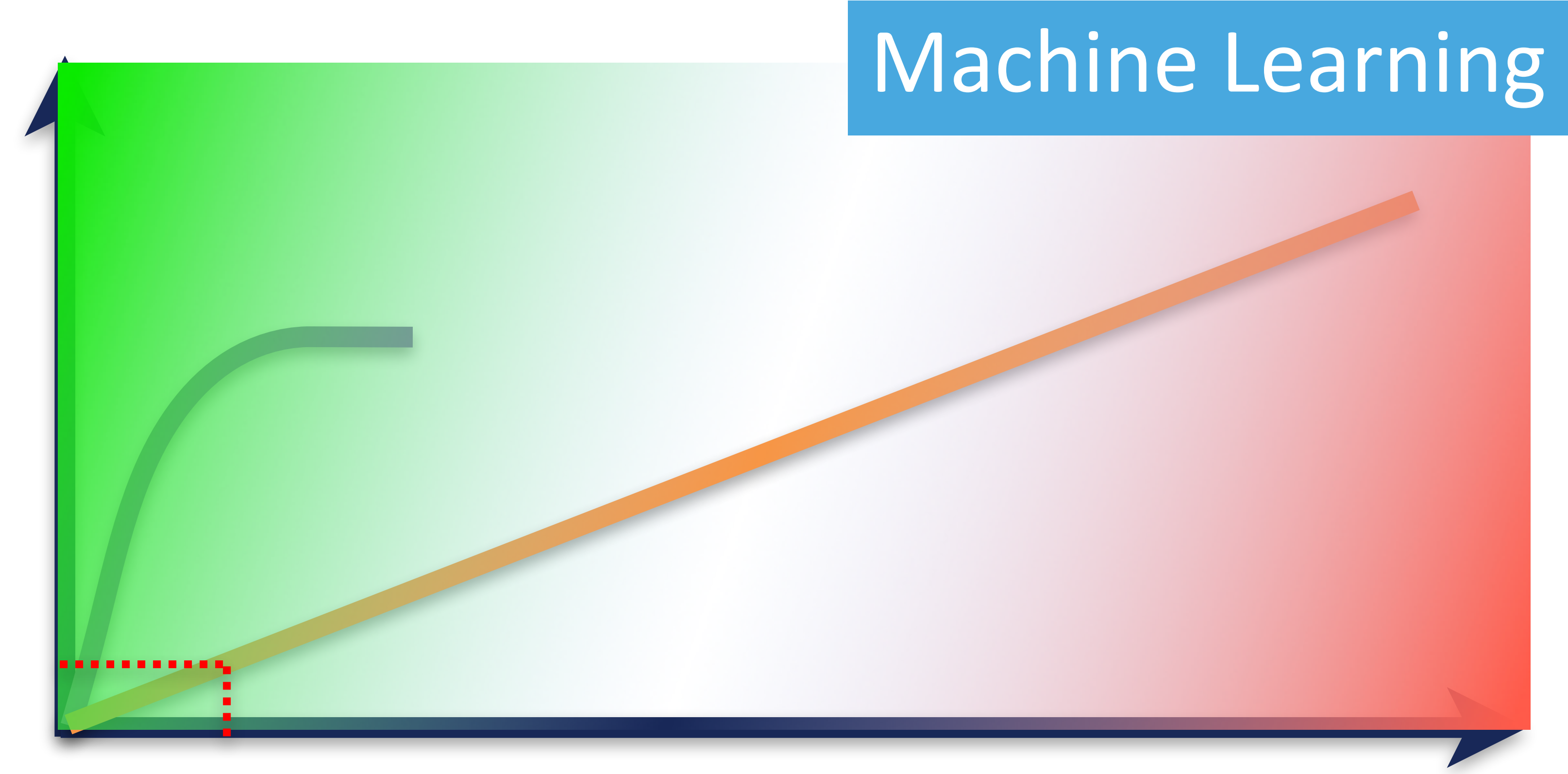
Know the problem before focusing on the data

Get lots of data

Don't let ML do the hard work of choosing features

Ok, but what is a lot?

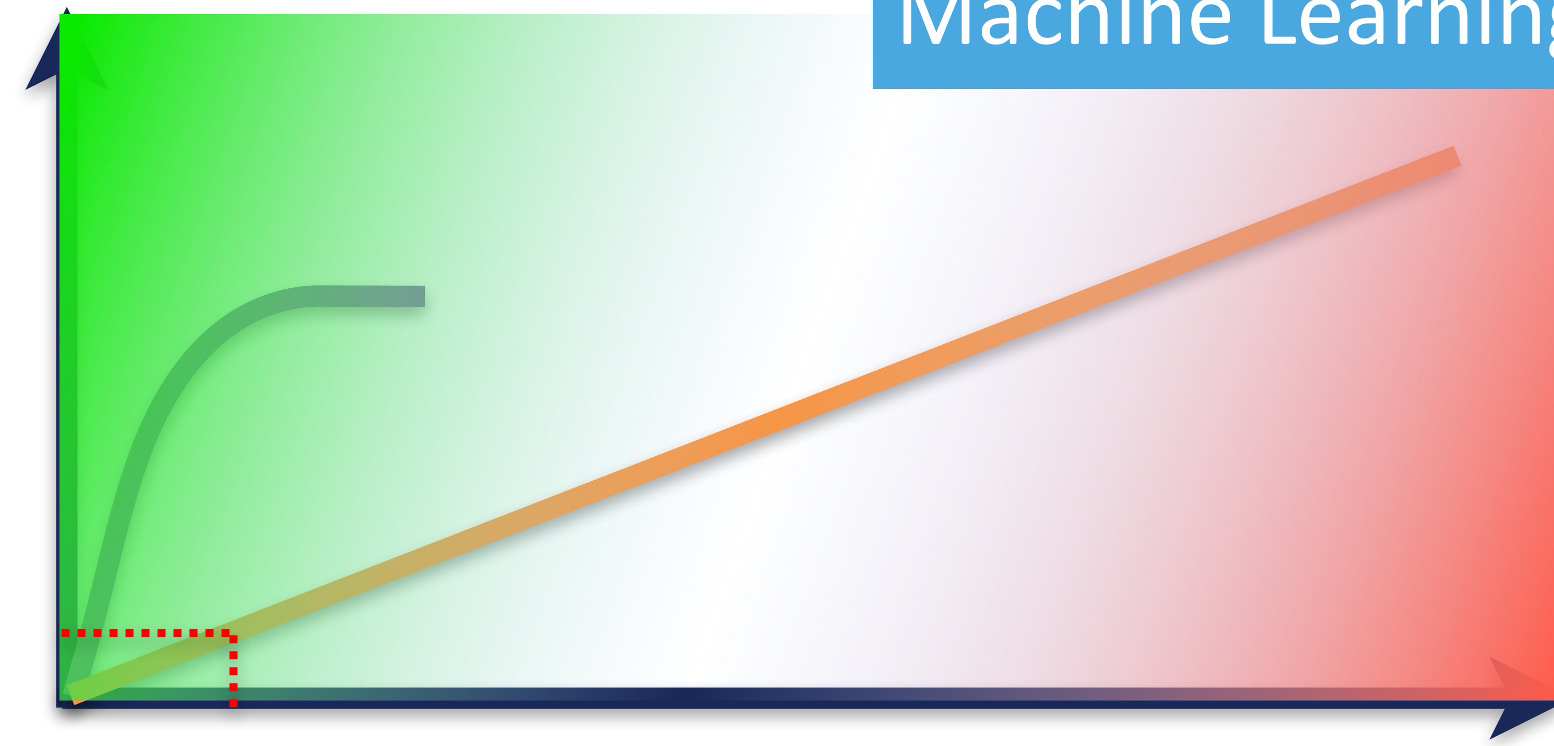
How much data?



Low intelligence + low experience
= low skill

How much data?

https://scikit-learn.org/



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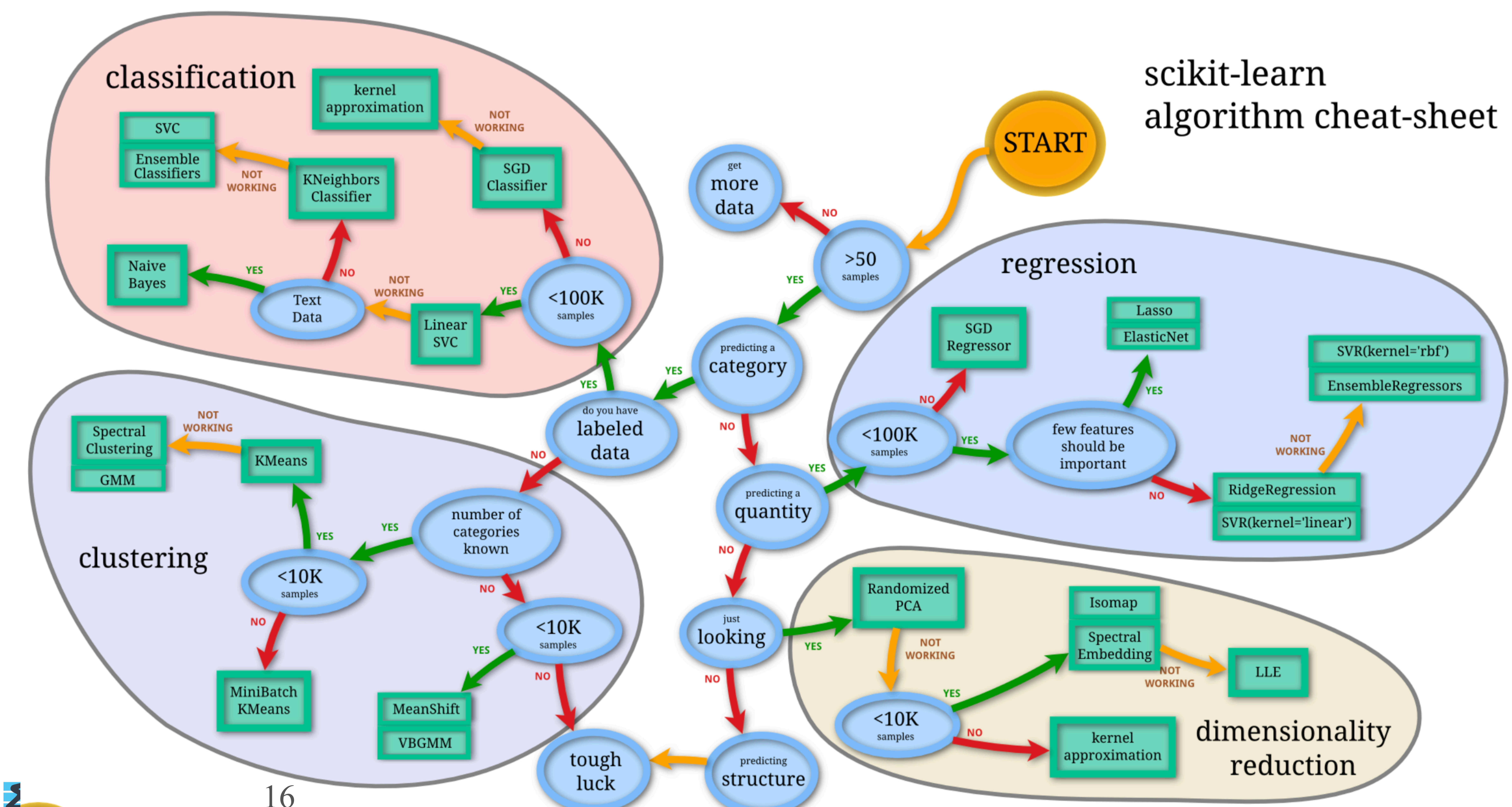

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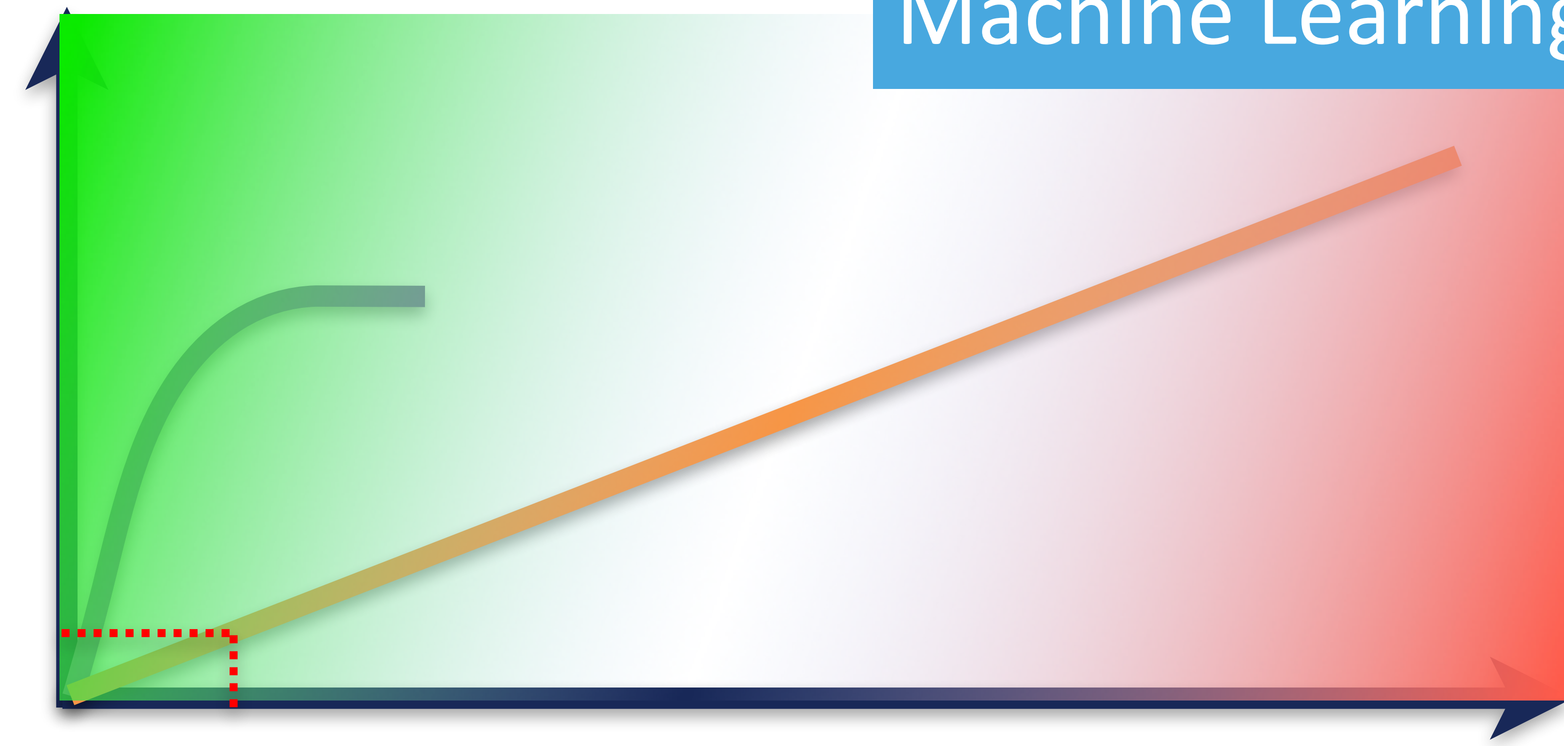
Machine Learning



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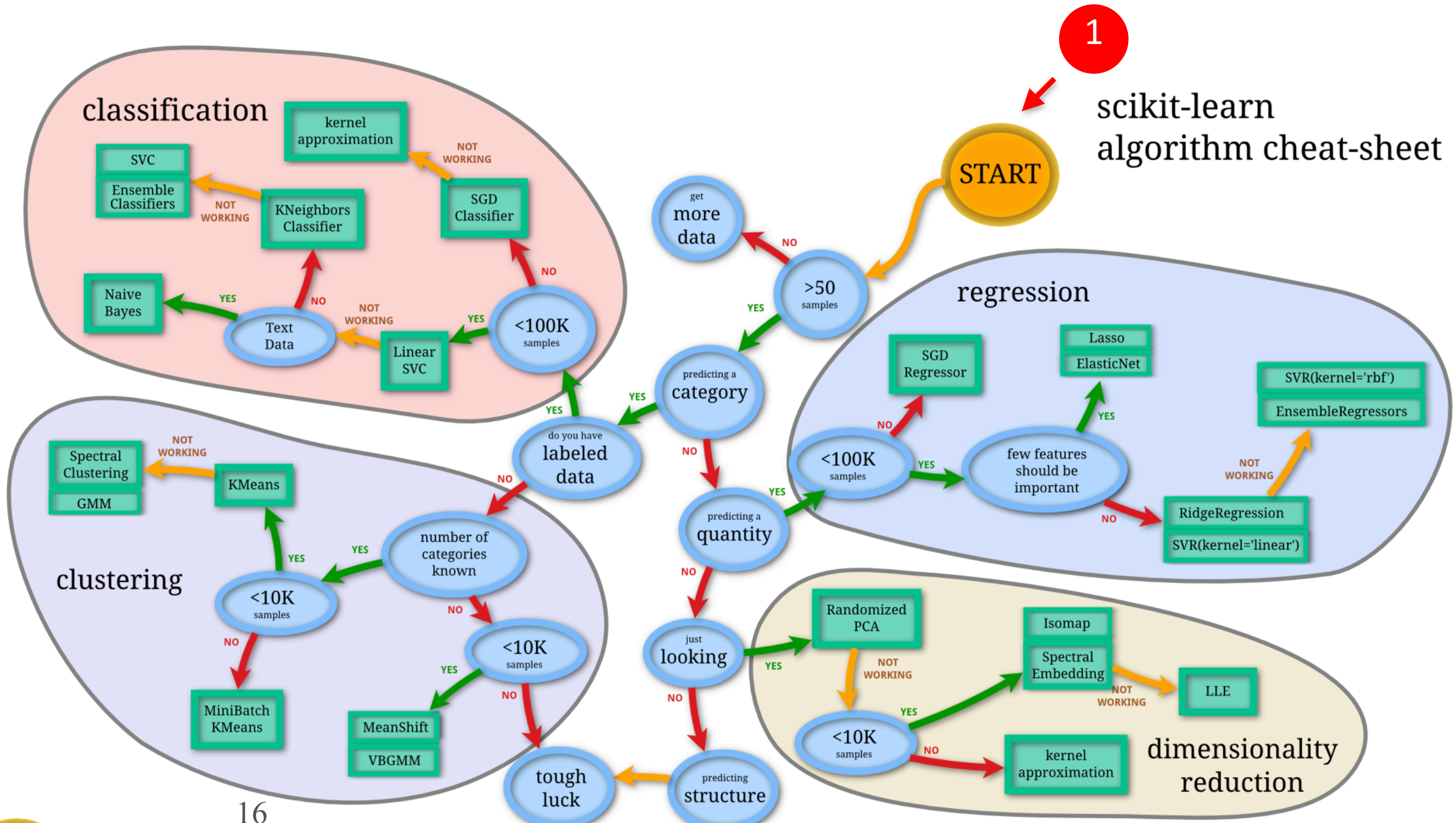

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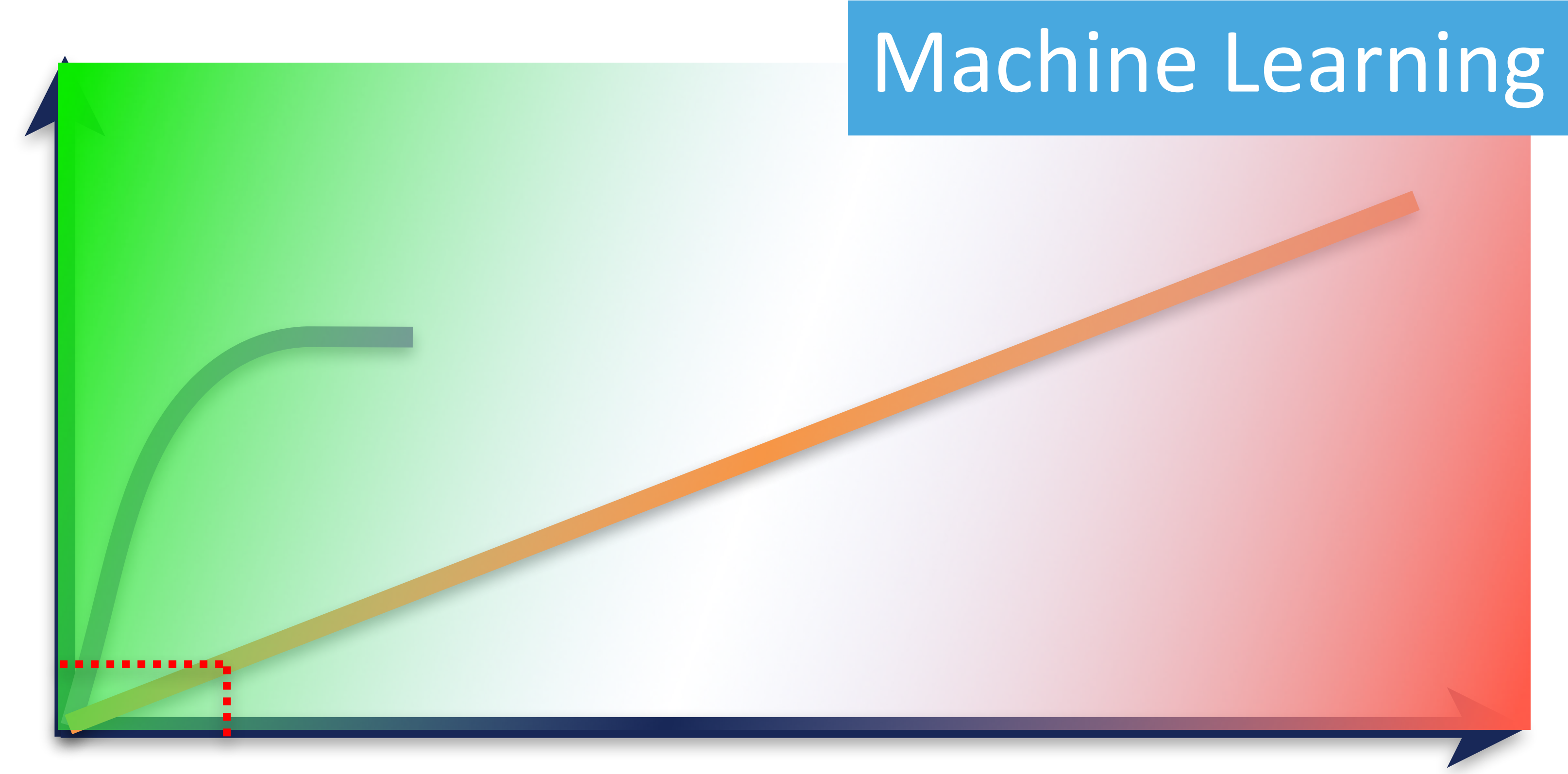

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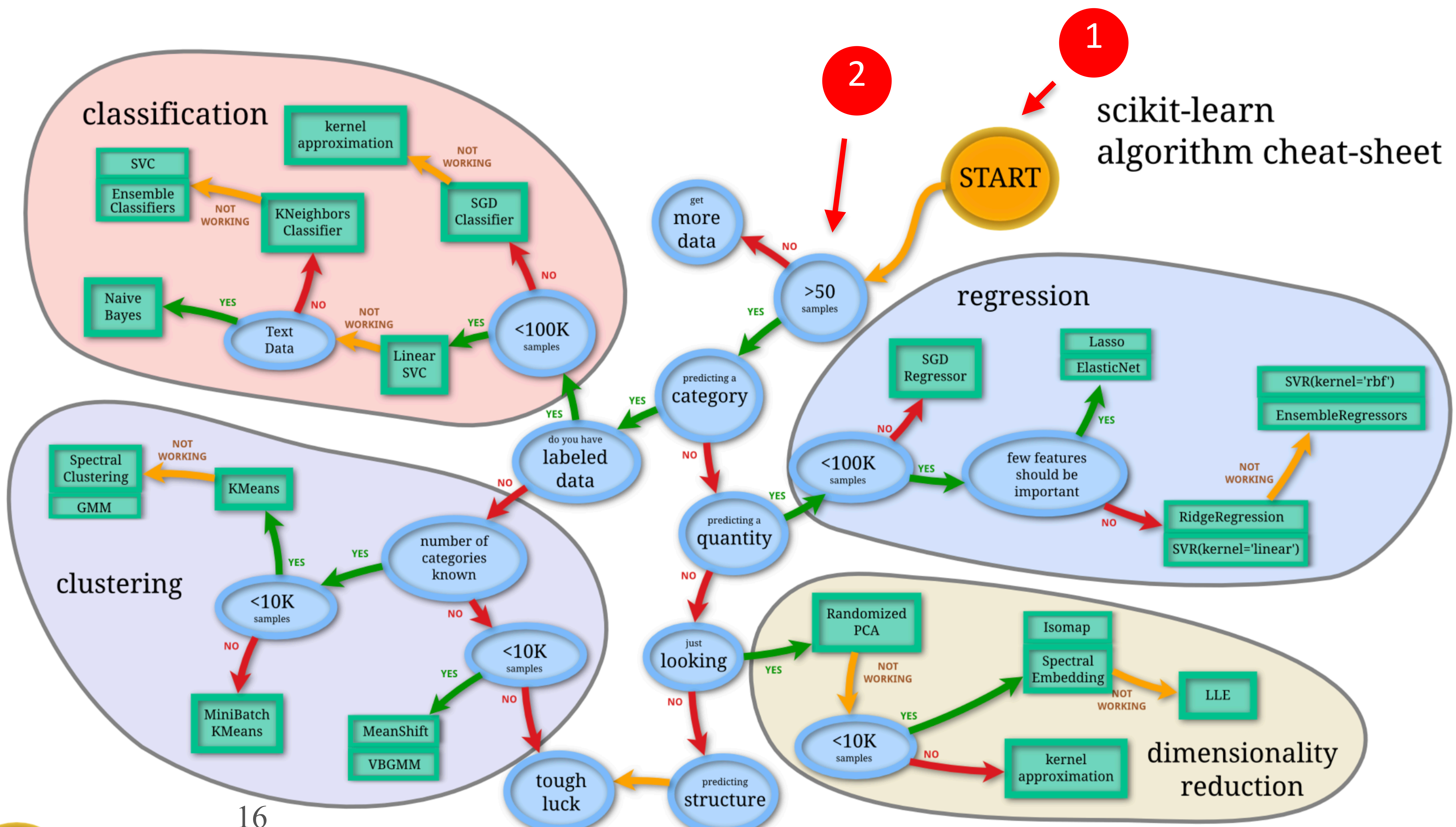

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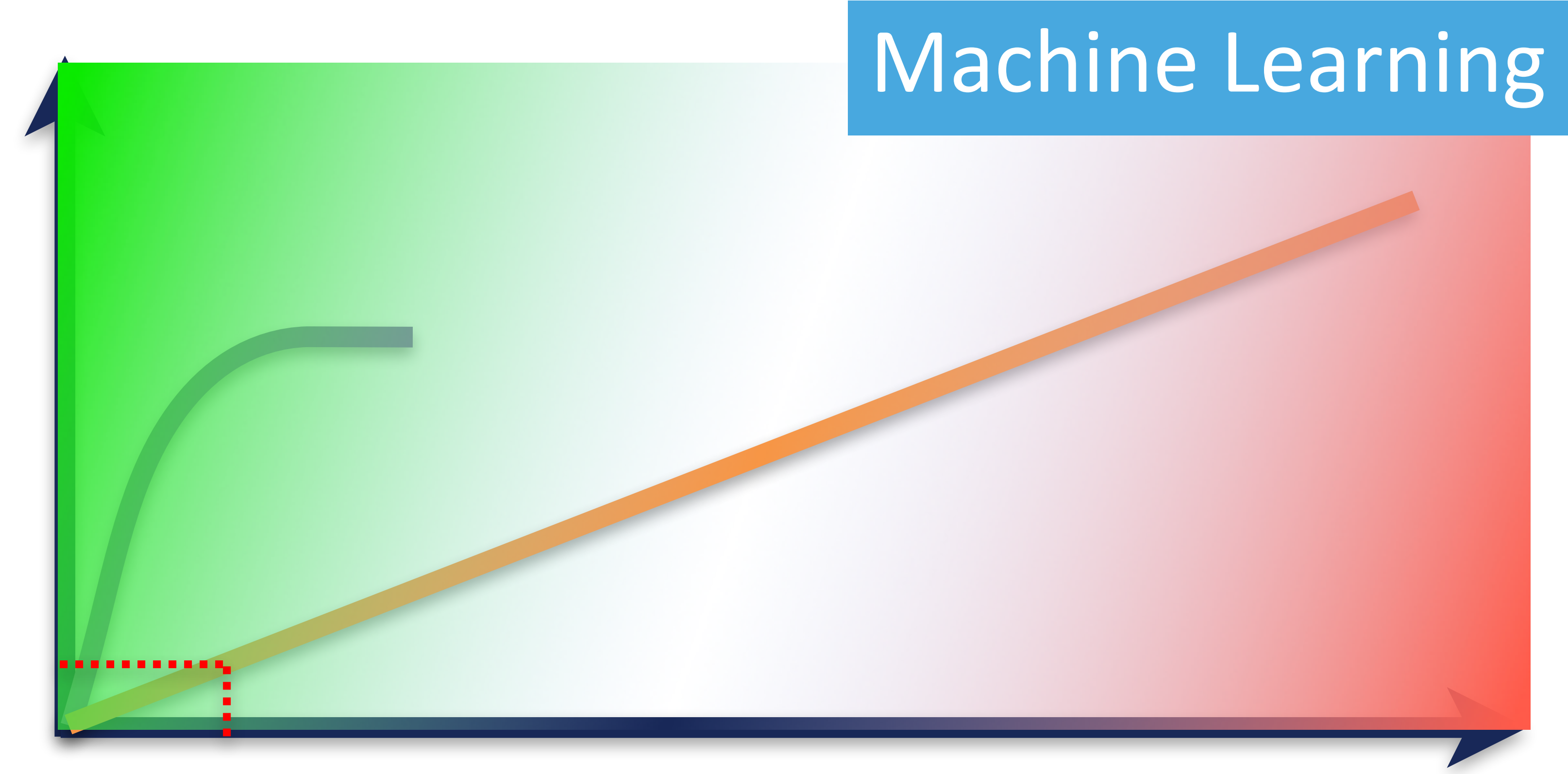

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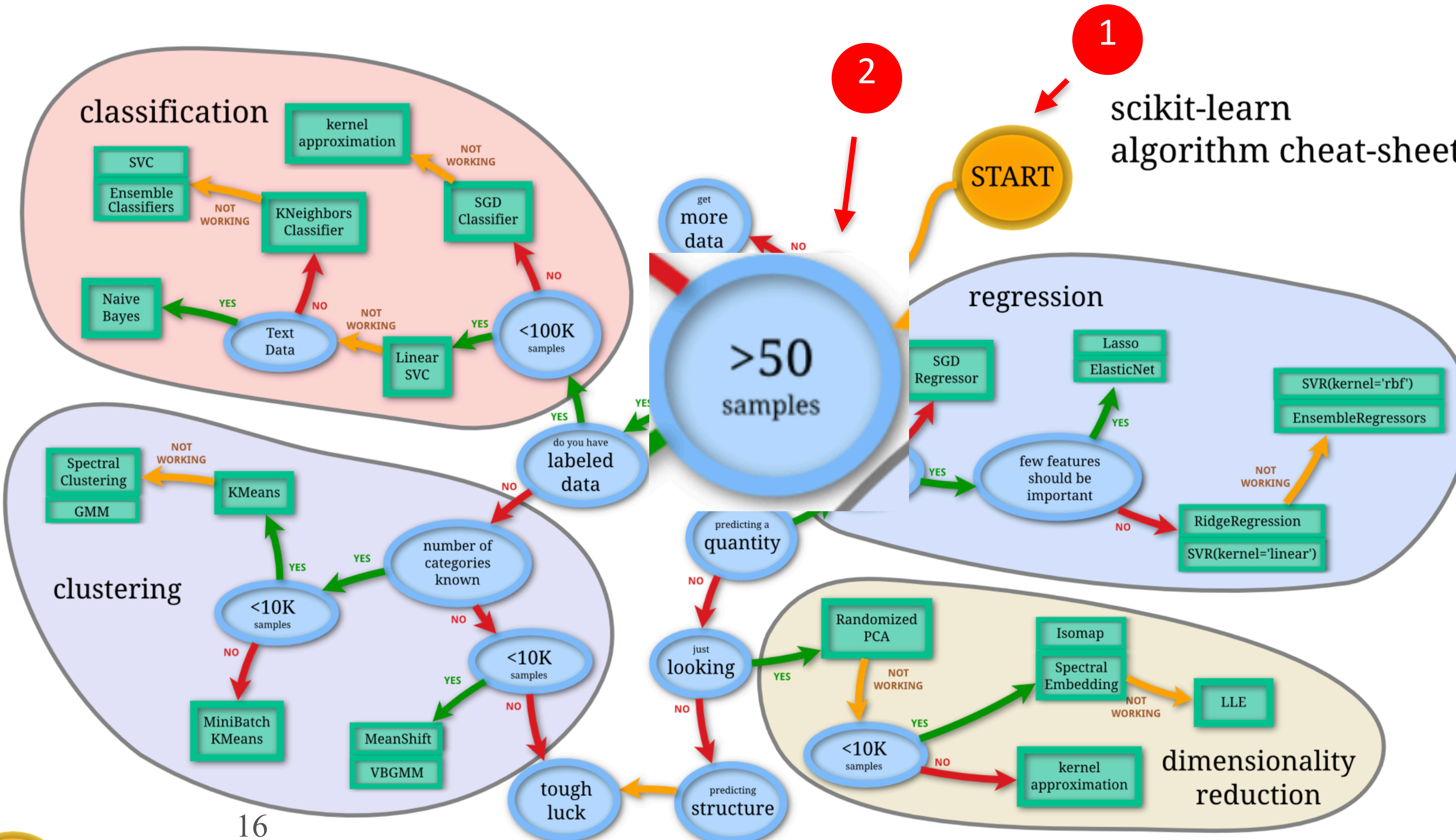

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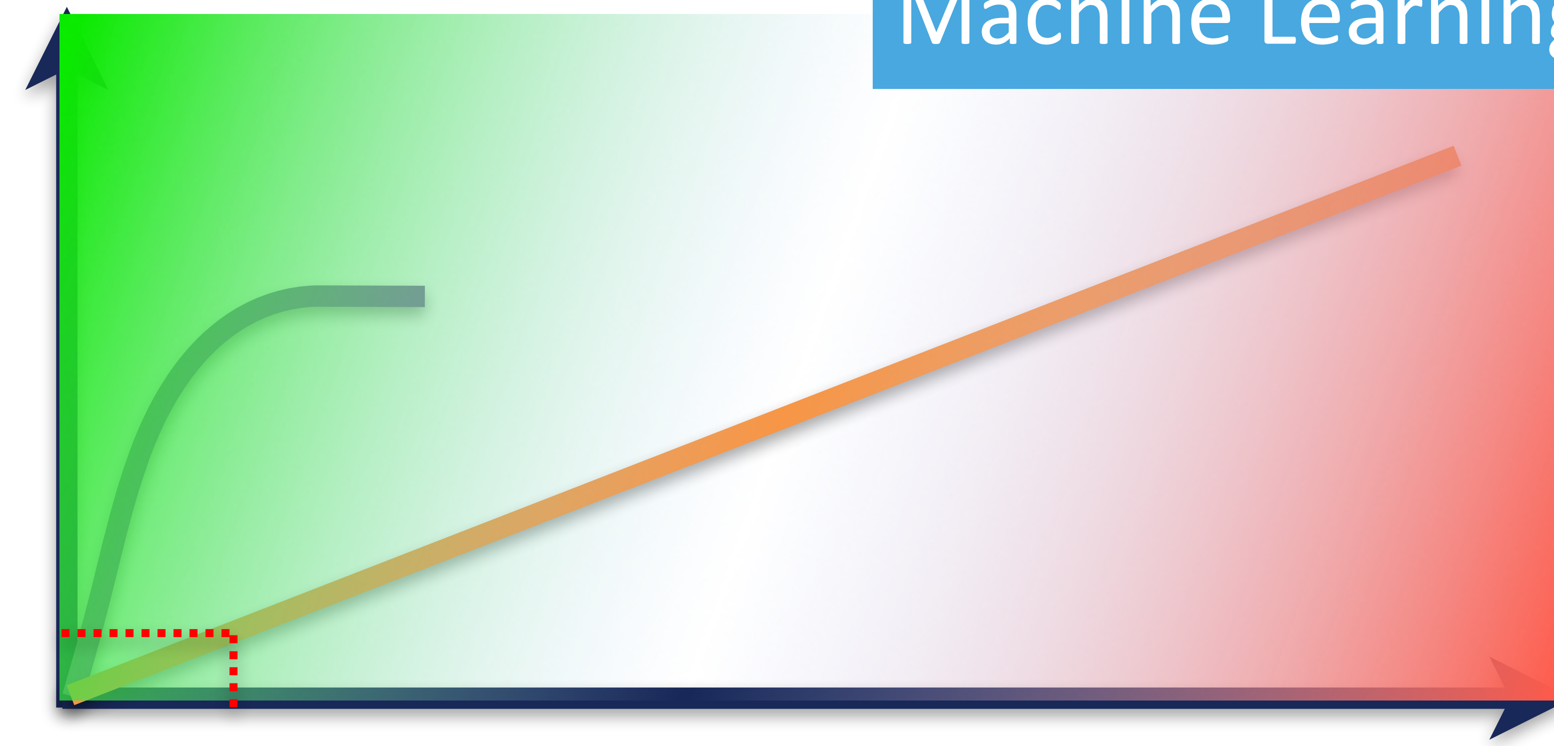

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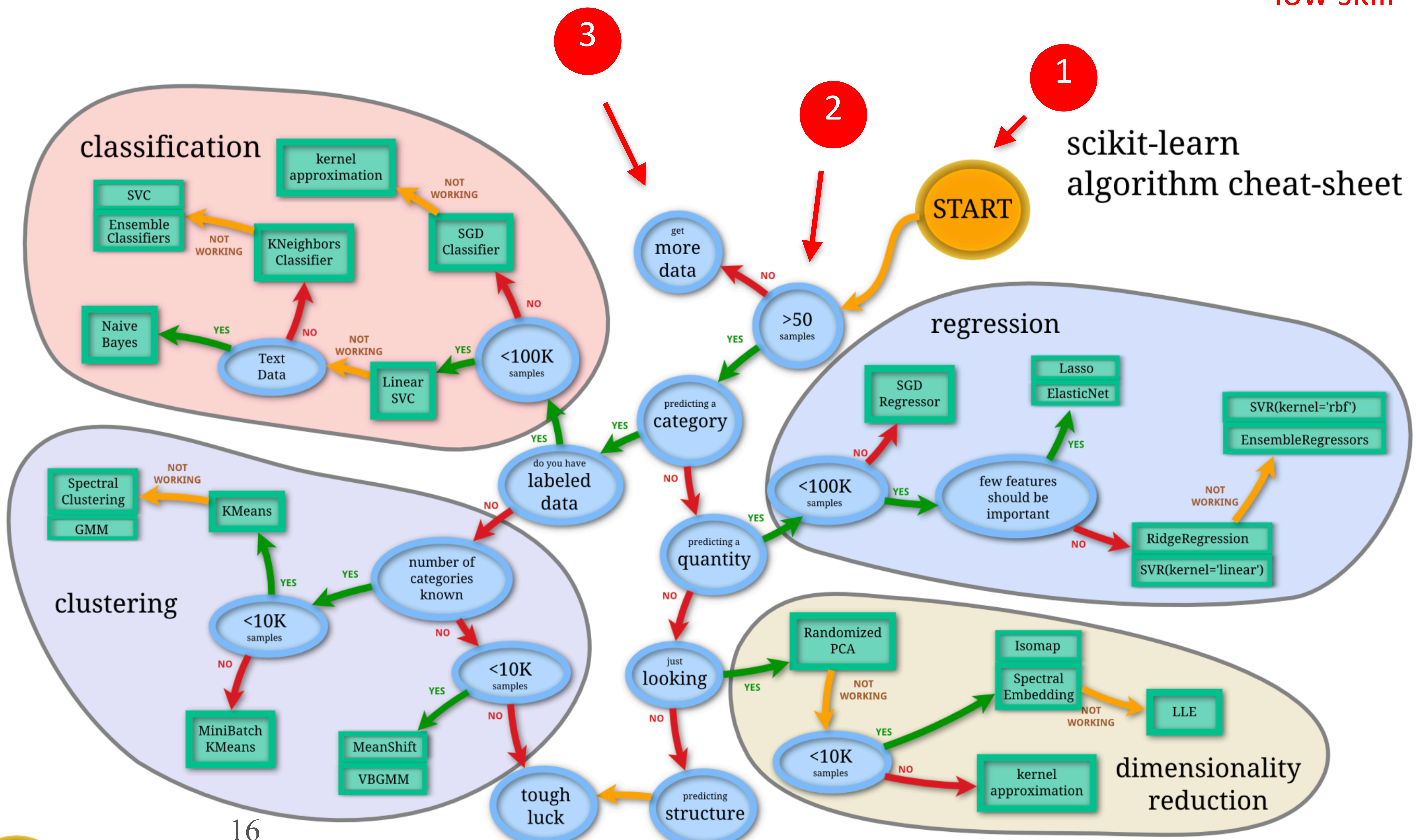
ML can't help you



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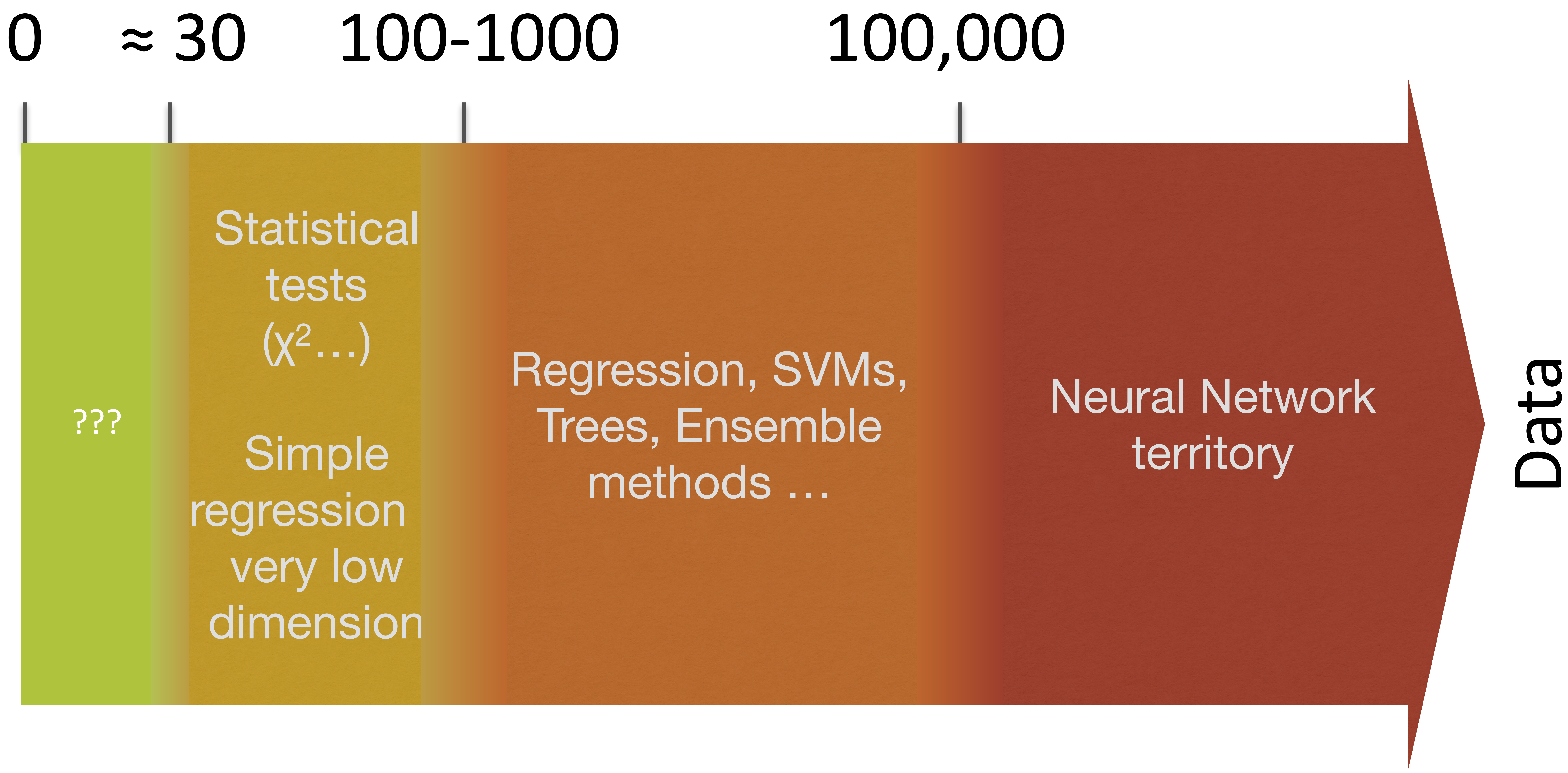
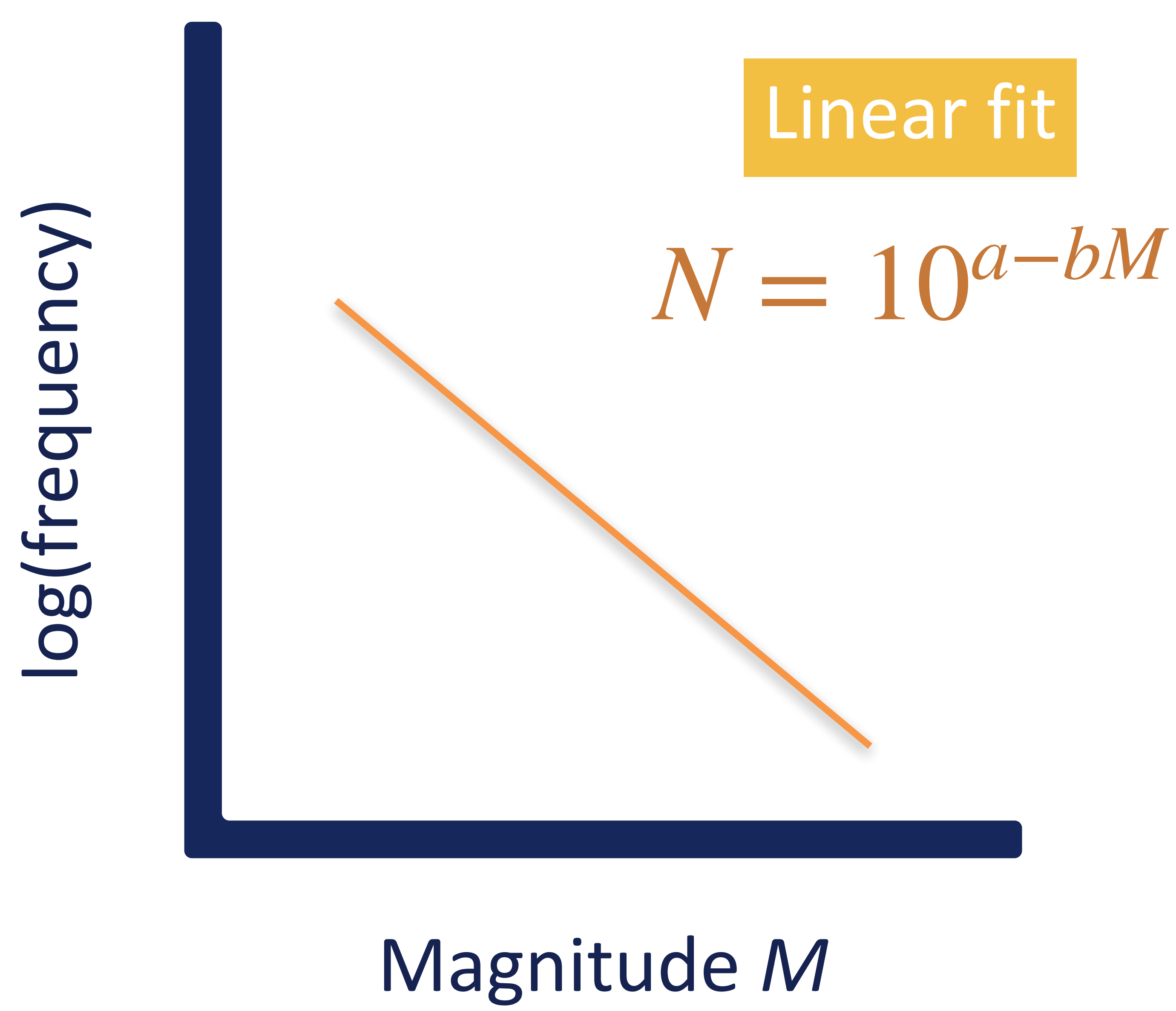


Not enough data … ?

Earthquake frequency:
The Gutenberg-Richter Law



N. Silver, The Signal and the Noise, 2012

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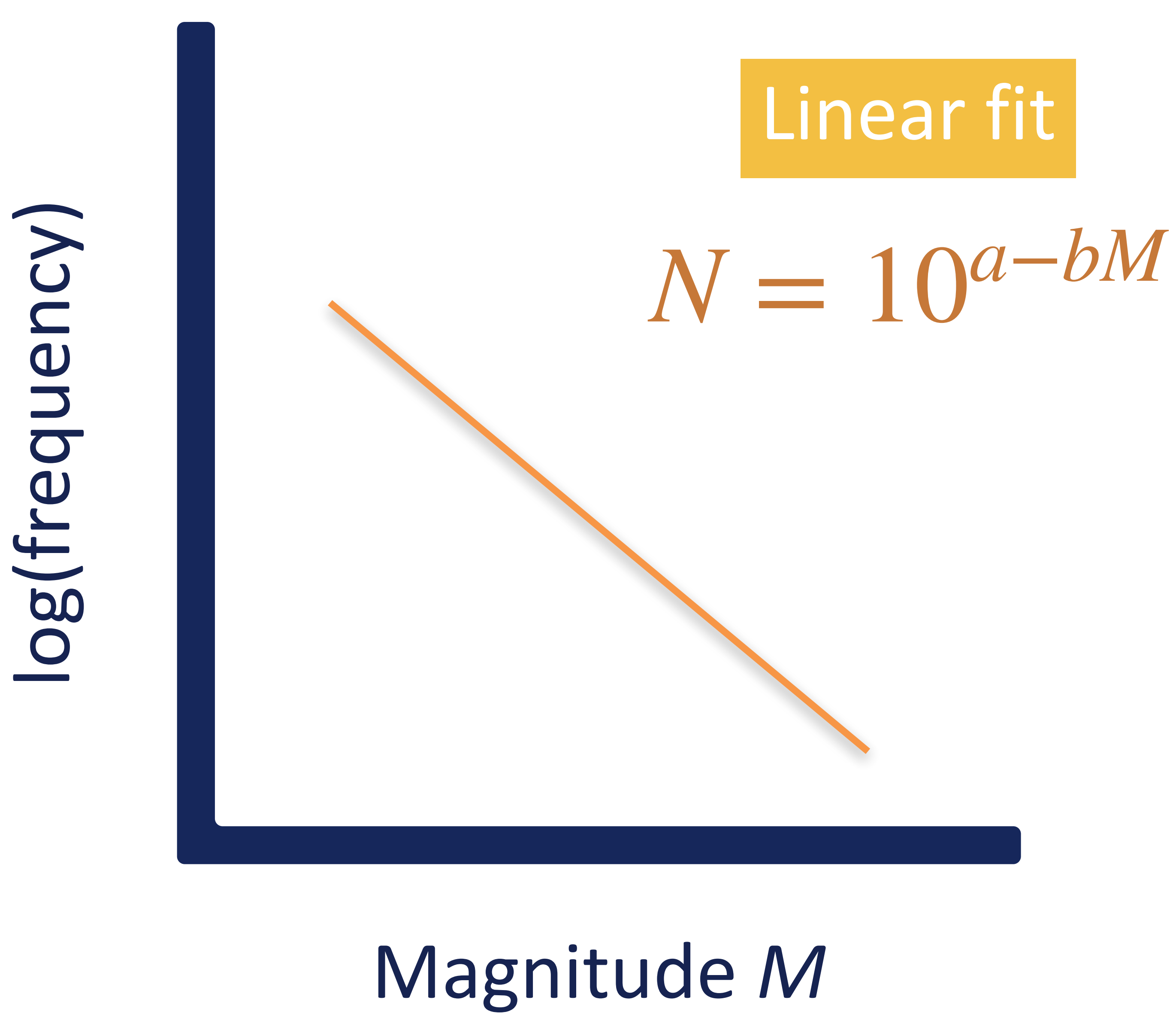
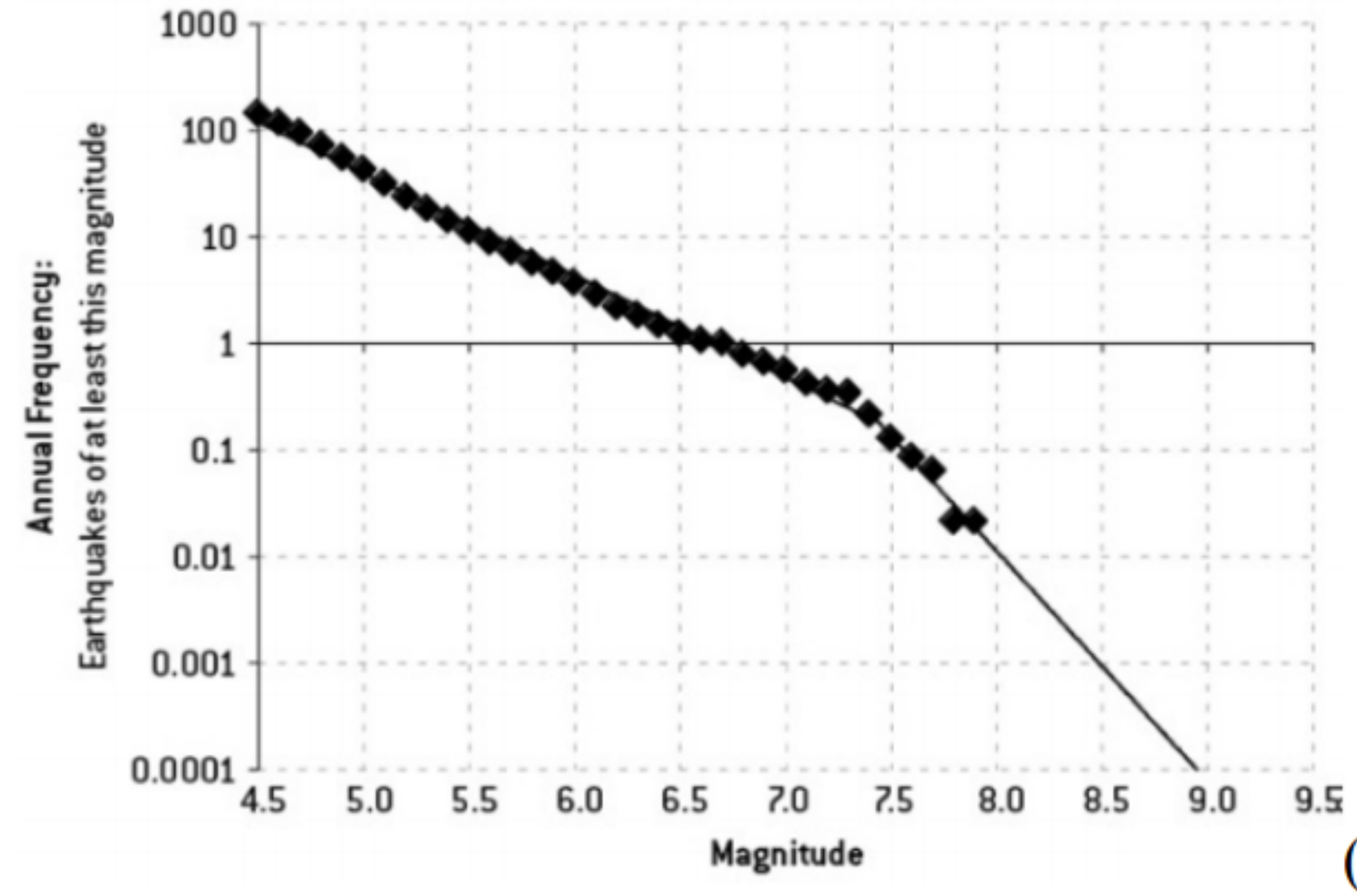


Tōhoku area
(near Fukushima)



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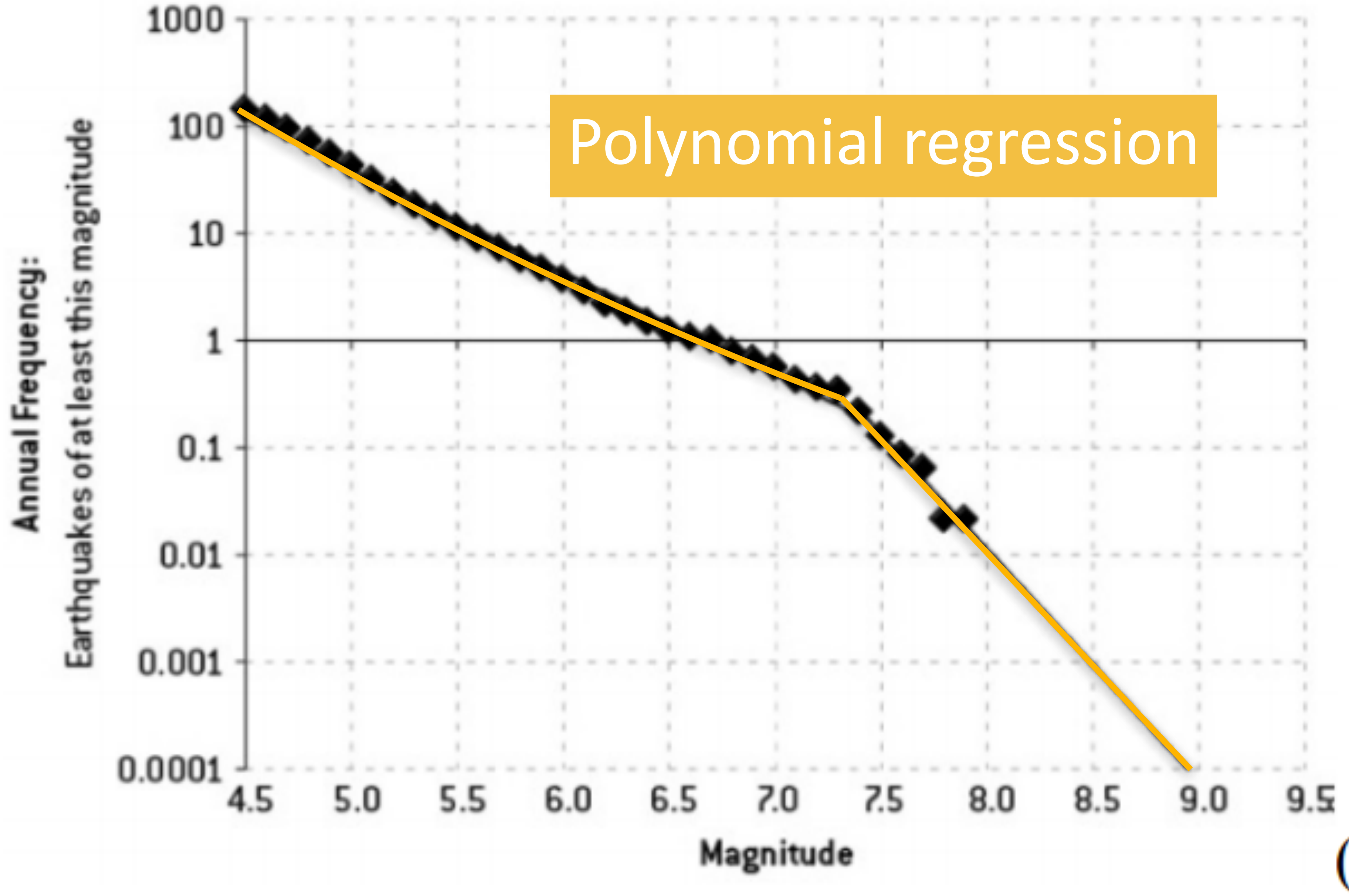

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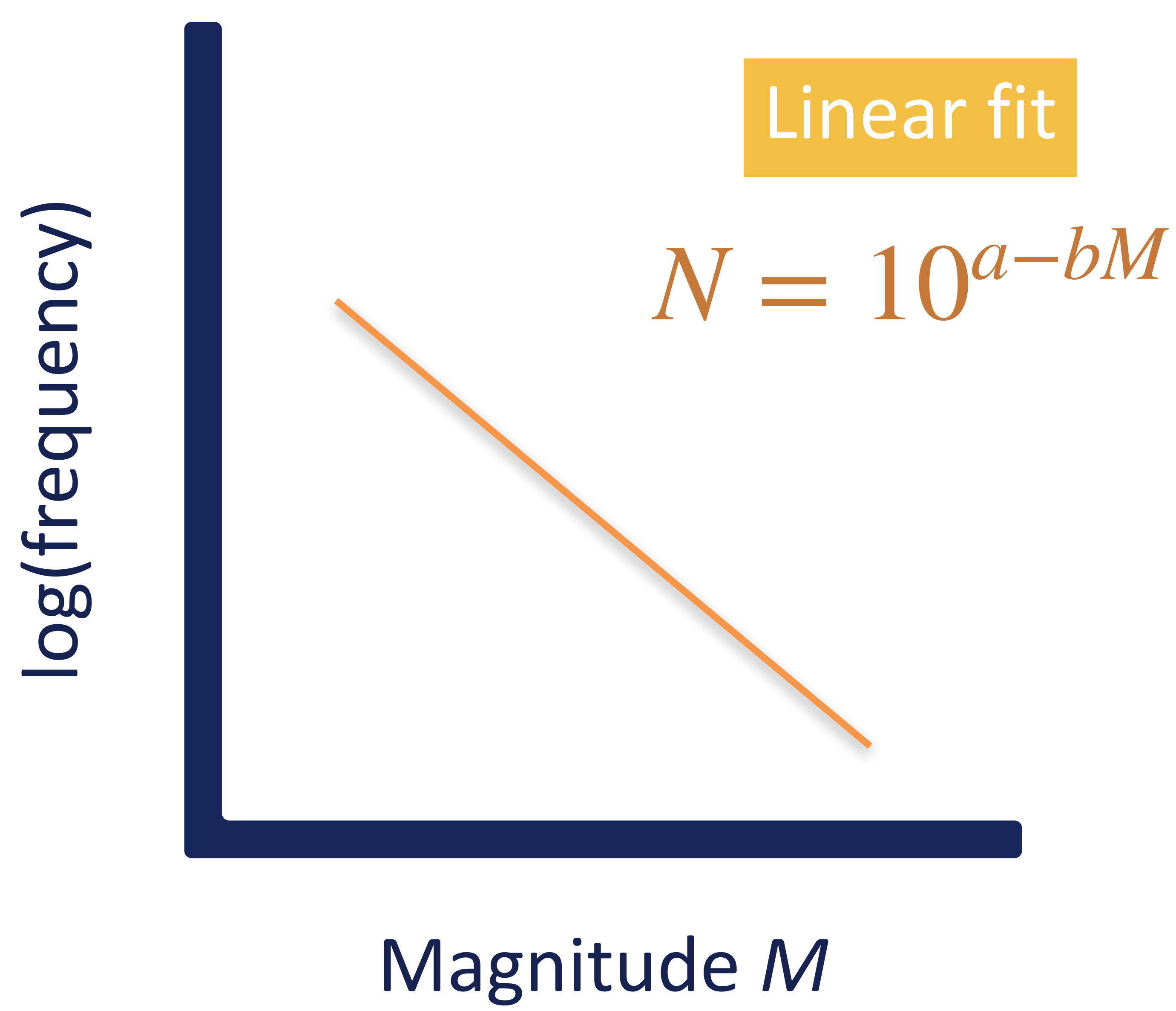

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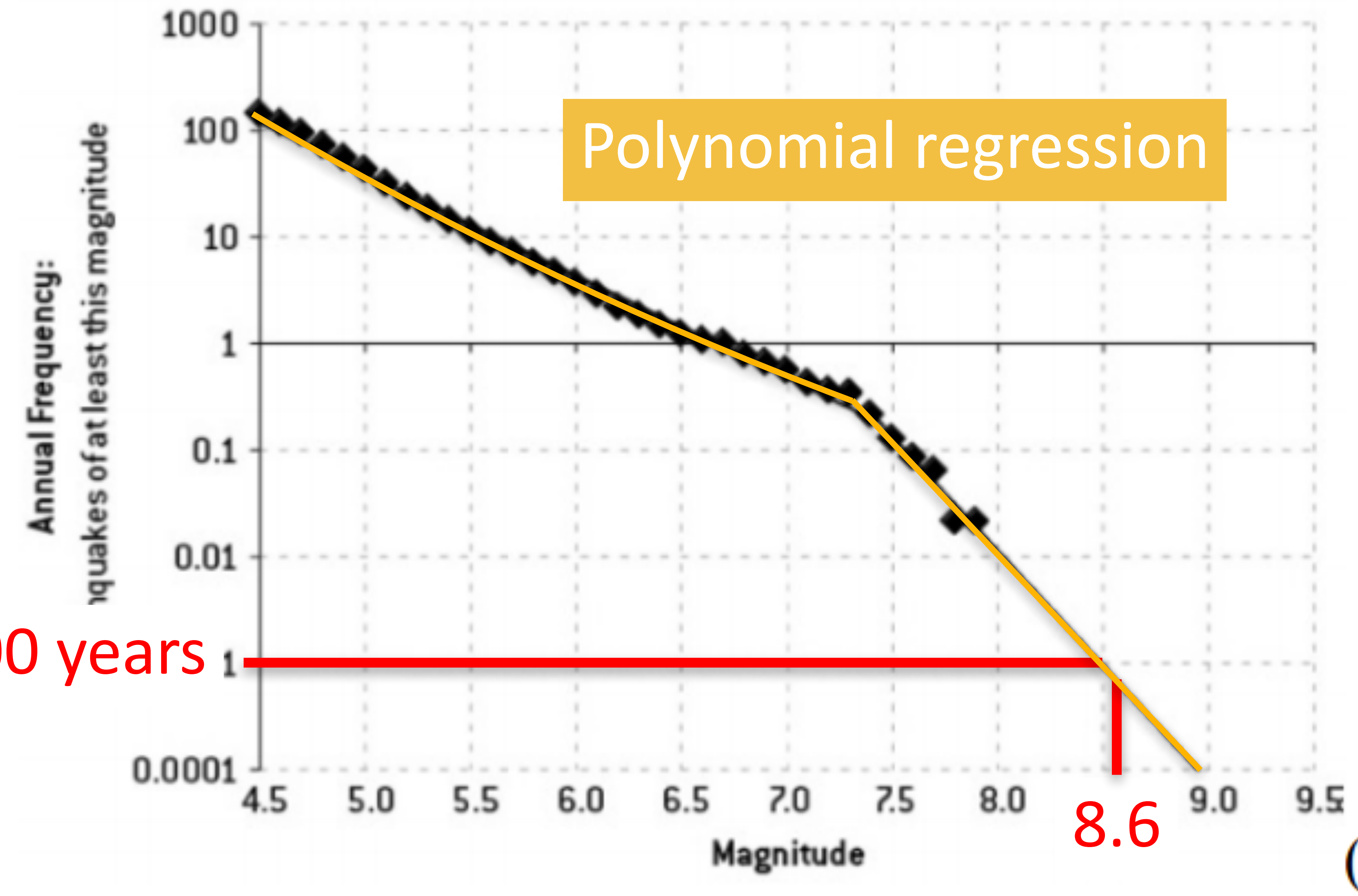
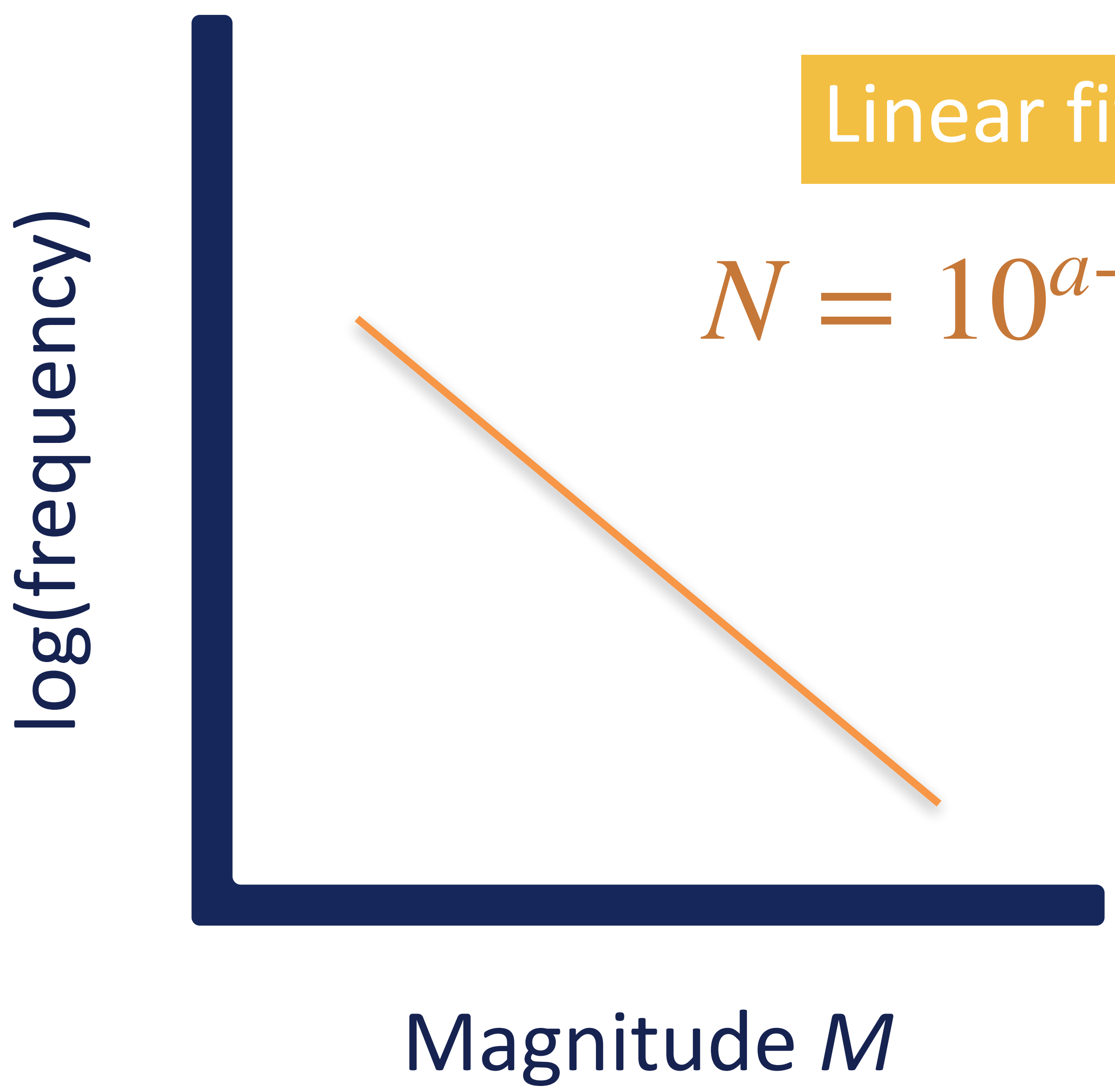


Earthquake frequency:
The Gutenberg-Richter Law

Linear fit

$$N = 10^{a-bM}$$



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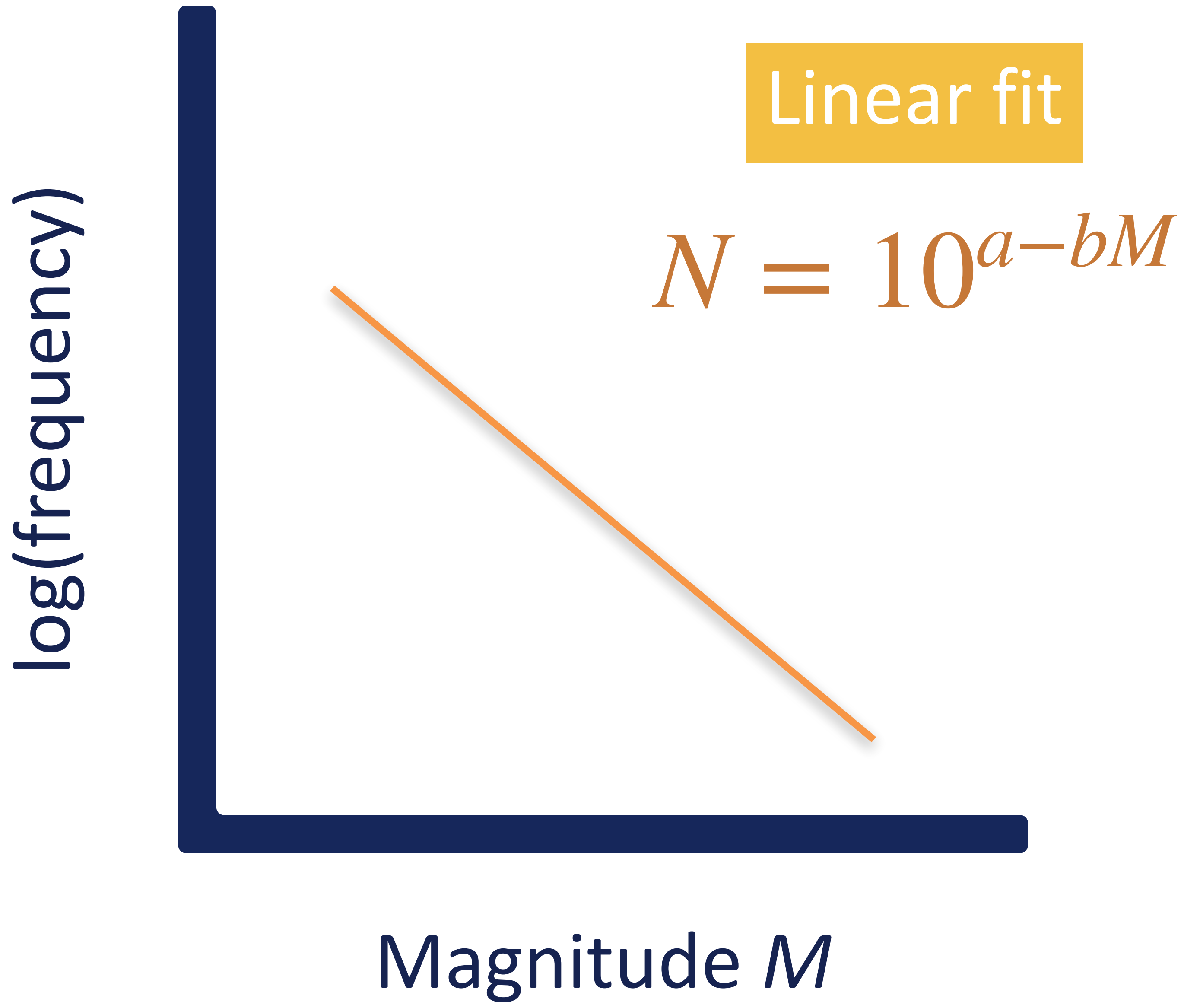

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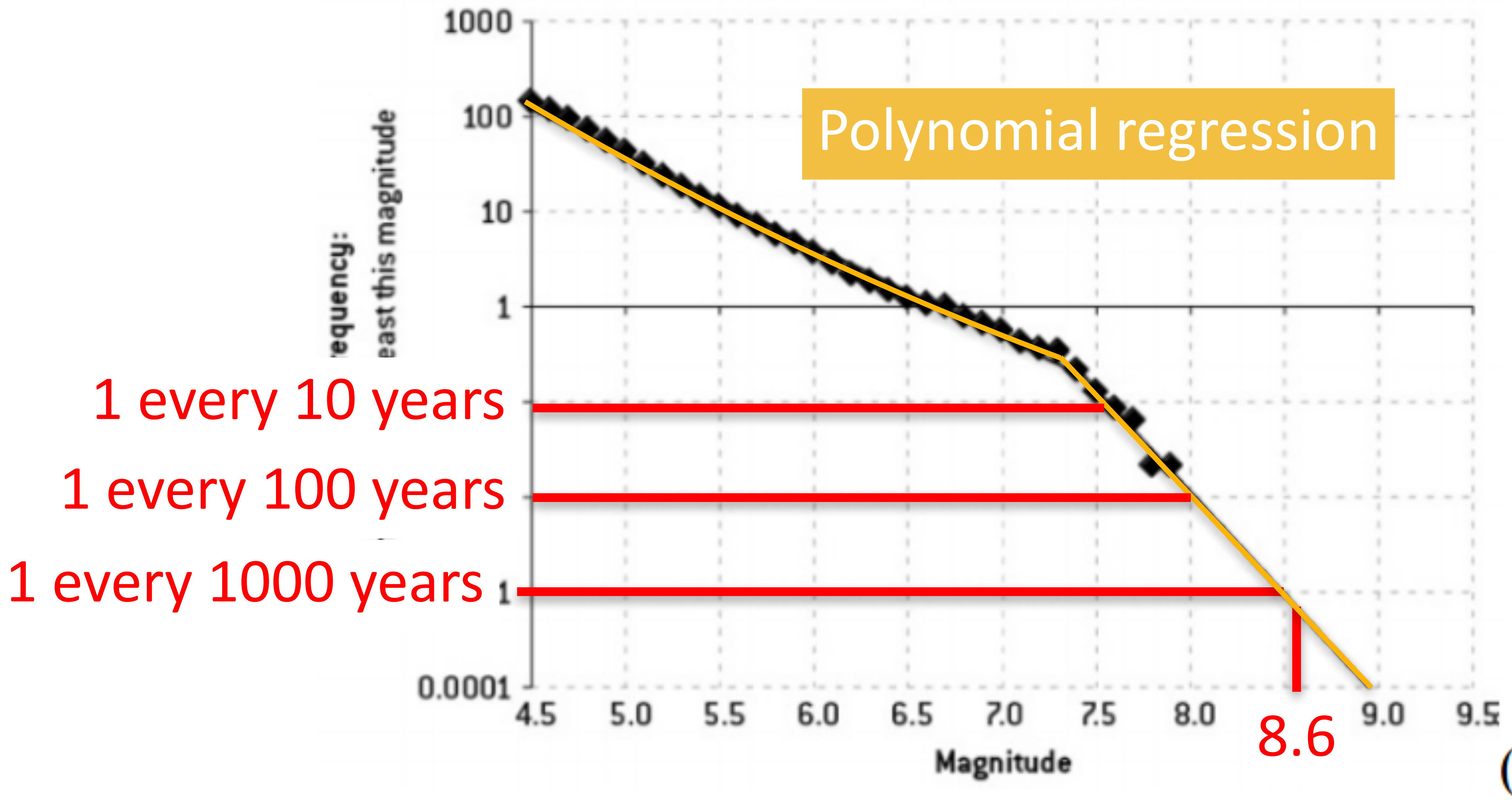

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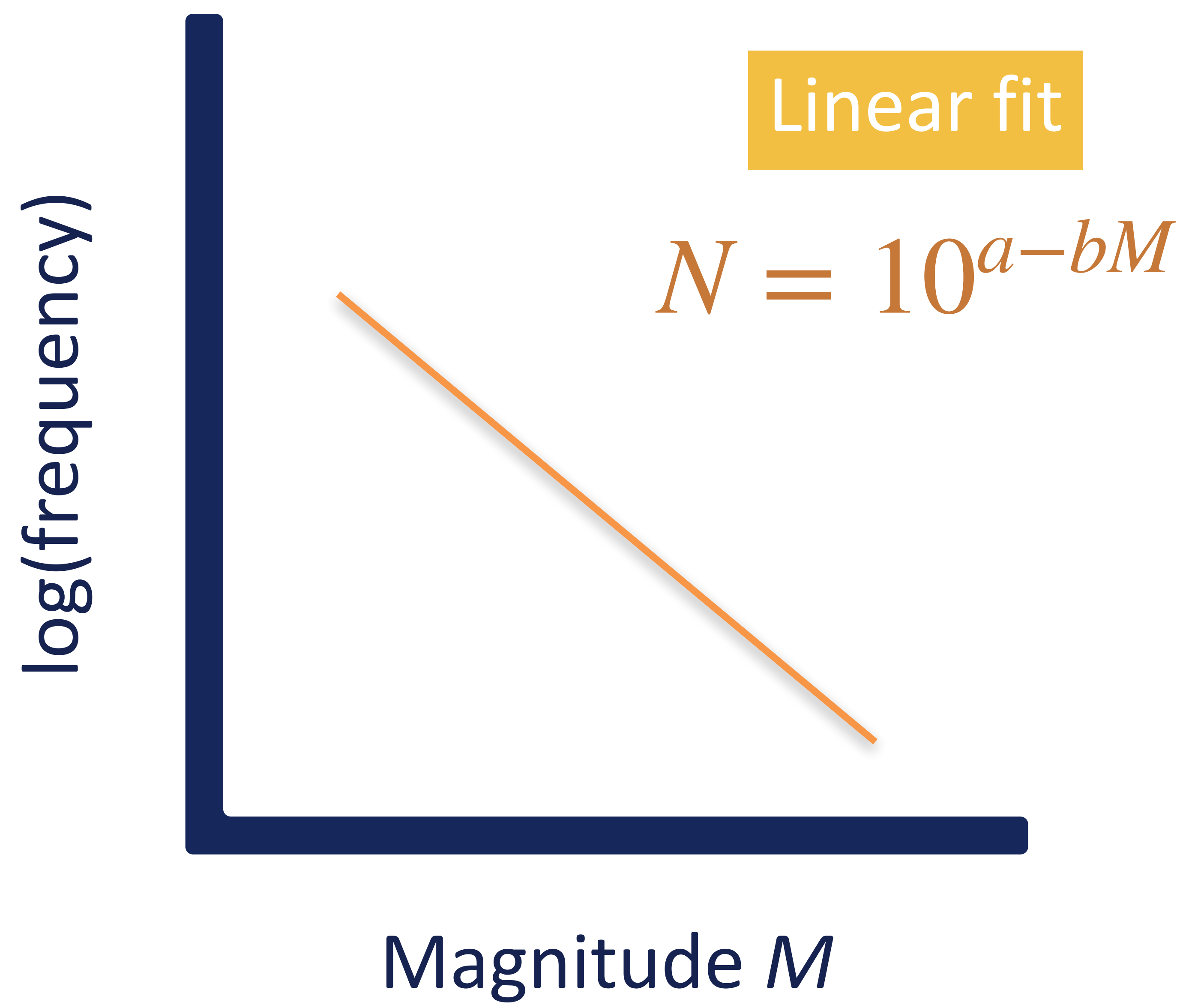

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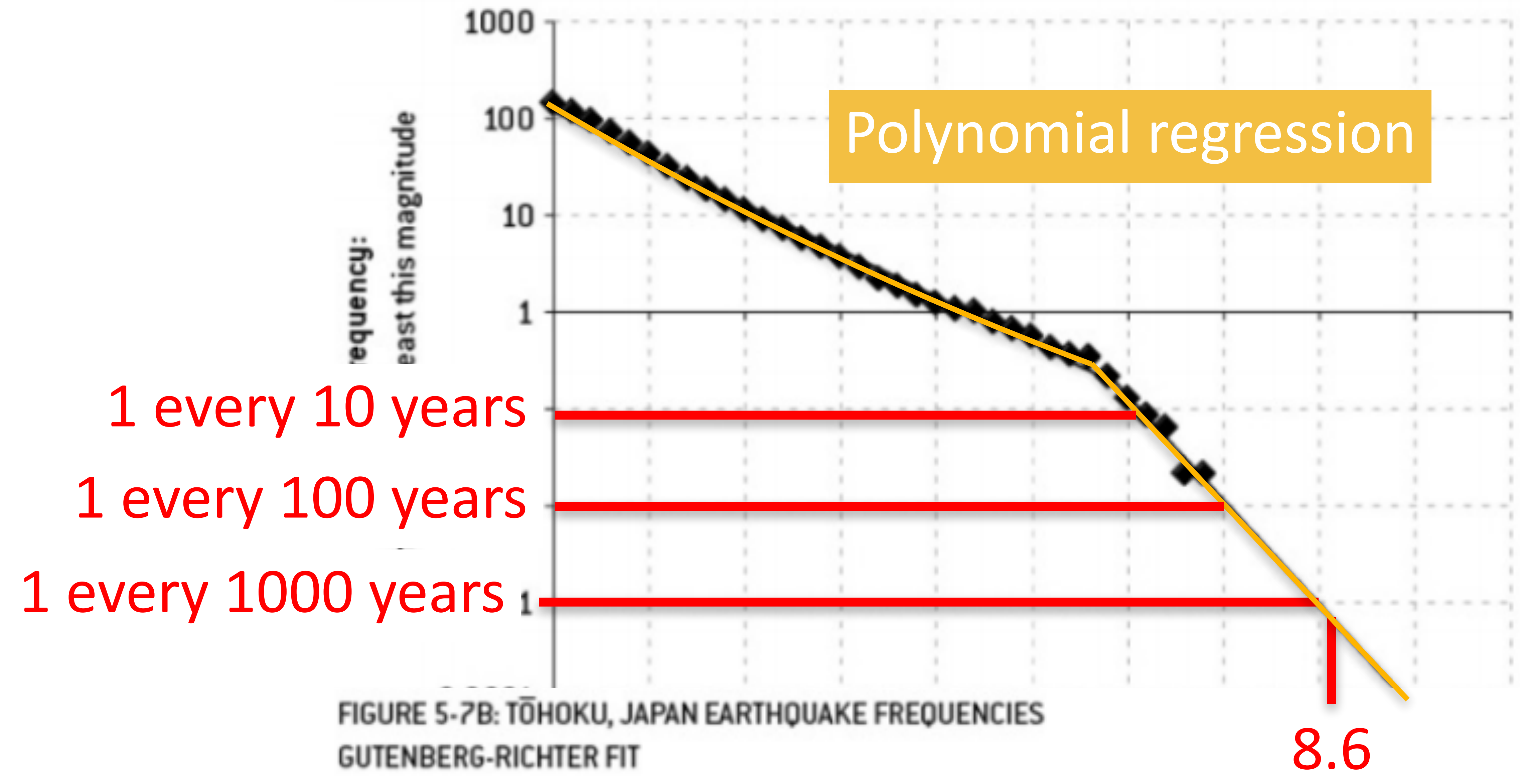
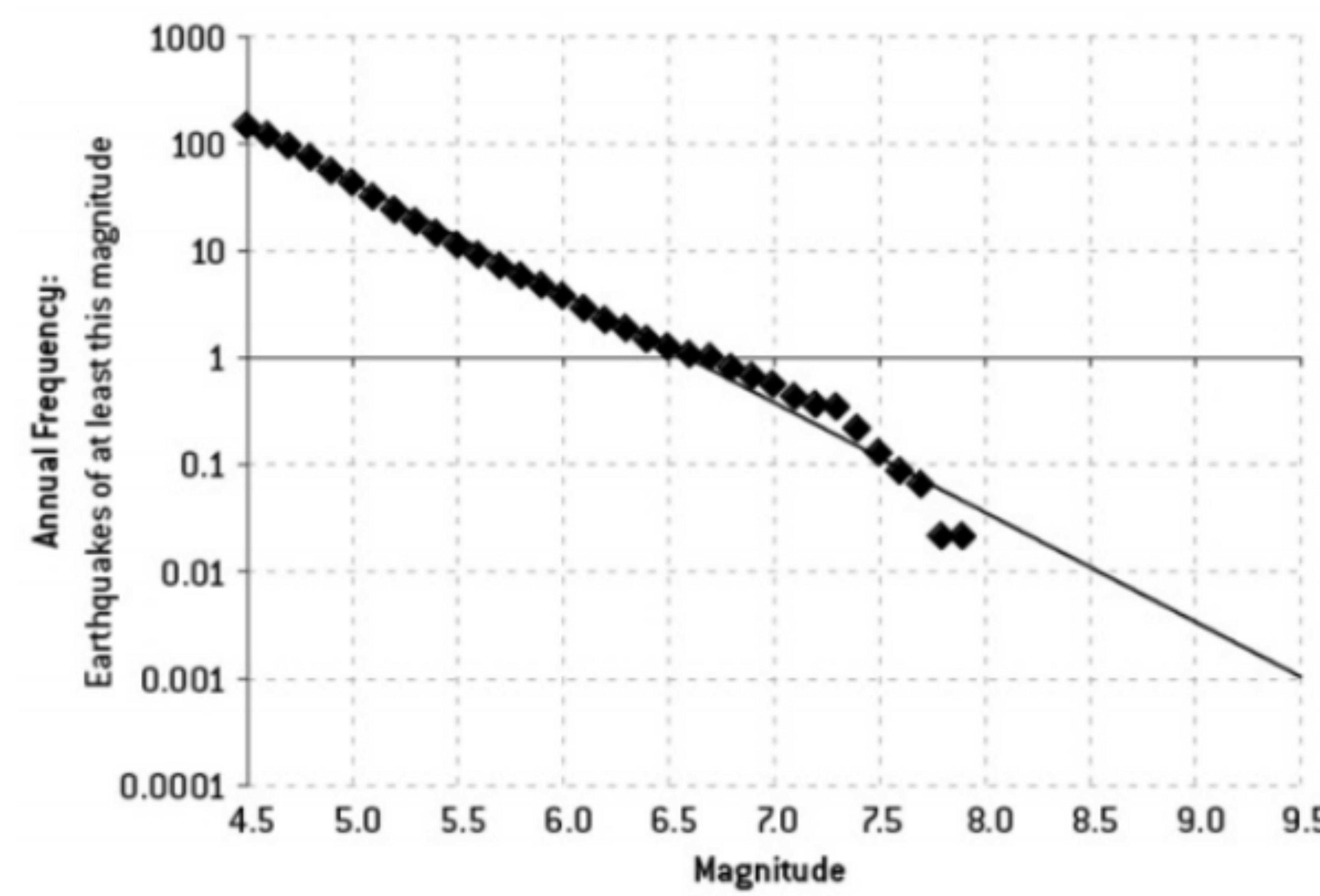


FIGURE 5-7B: TŌHOKU, JAPAN EARTHQUAKE FREQUENCIES
GUTENBERG-RICHTER FIT



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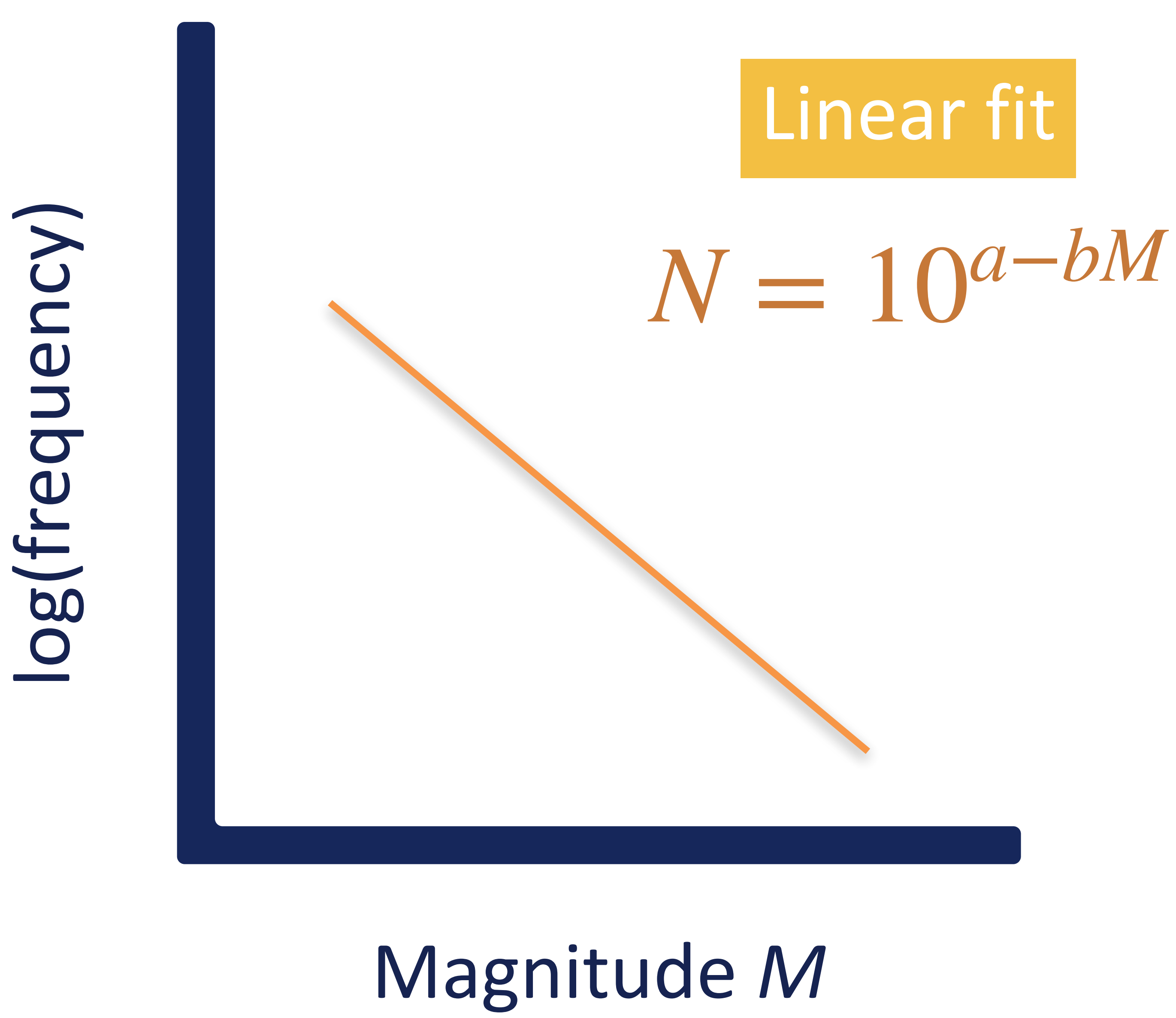

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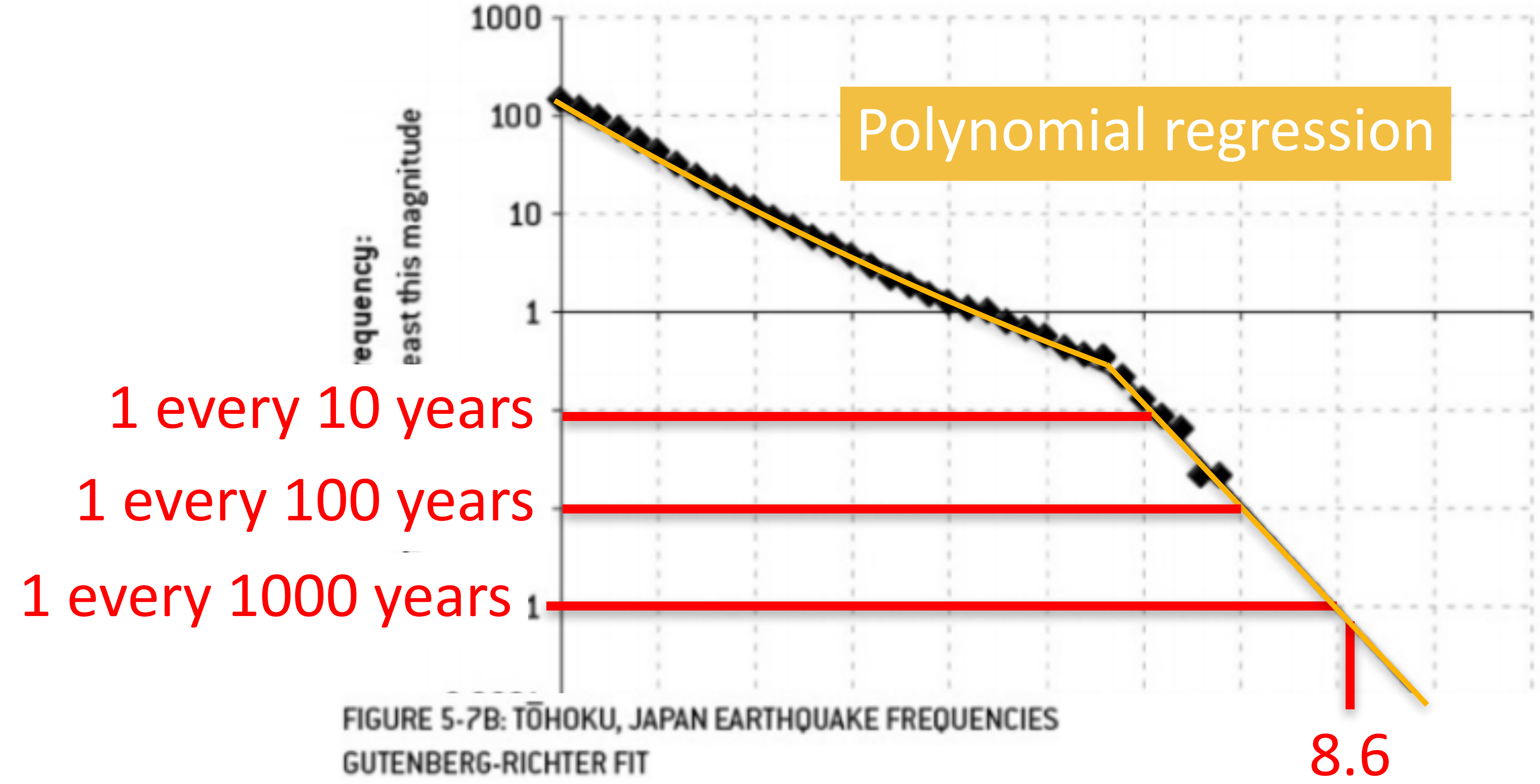

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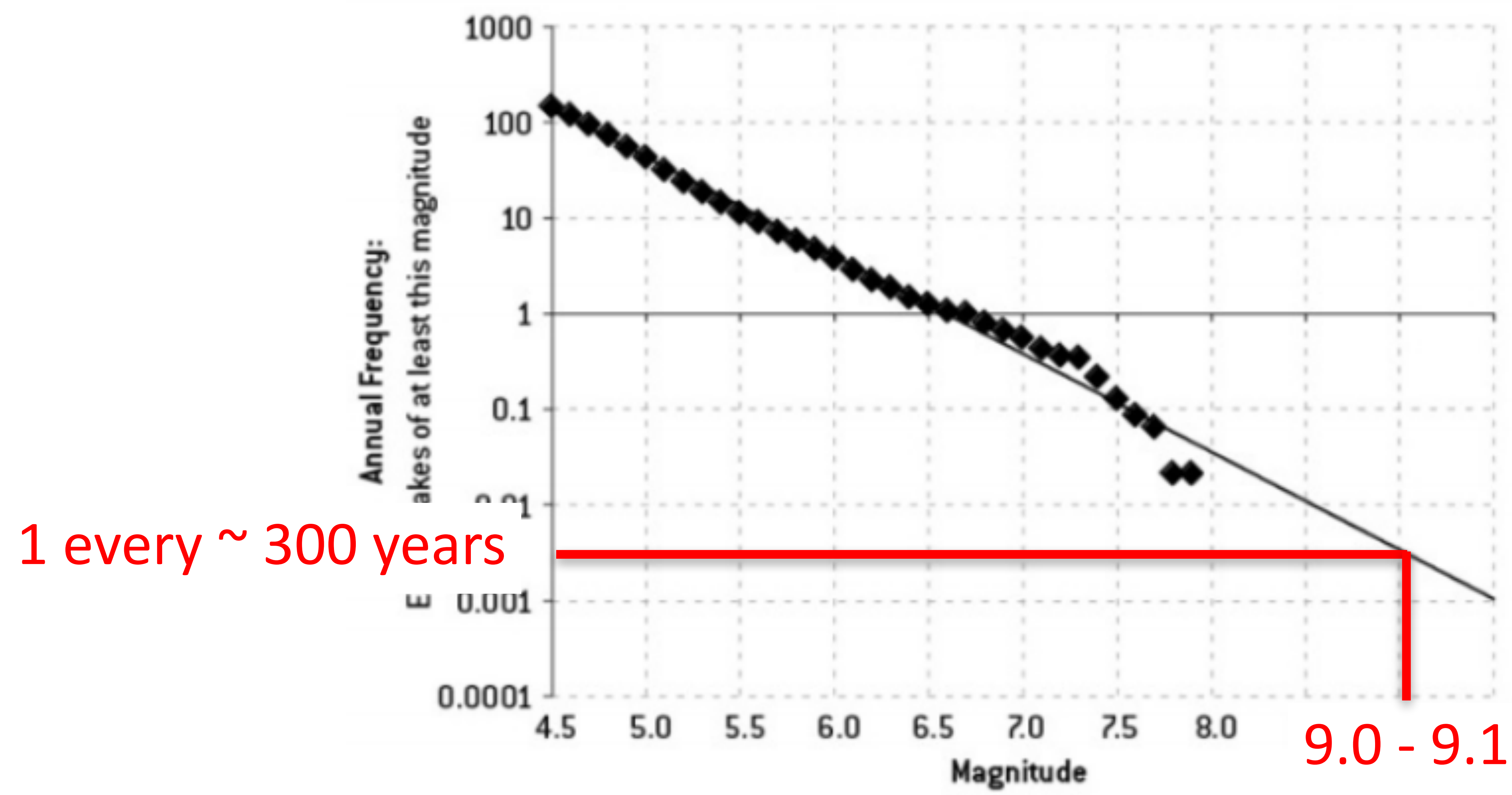

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Case Studies of AI in CFD

AI for « better » CFD…?

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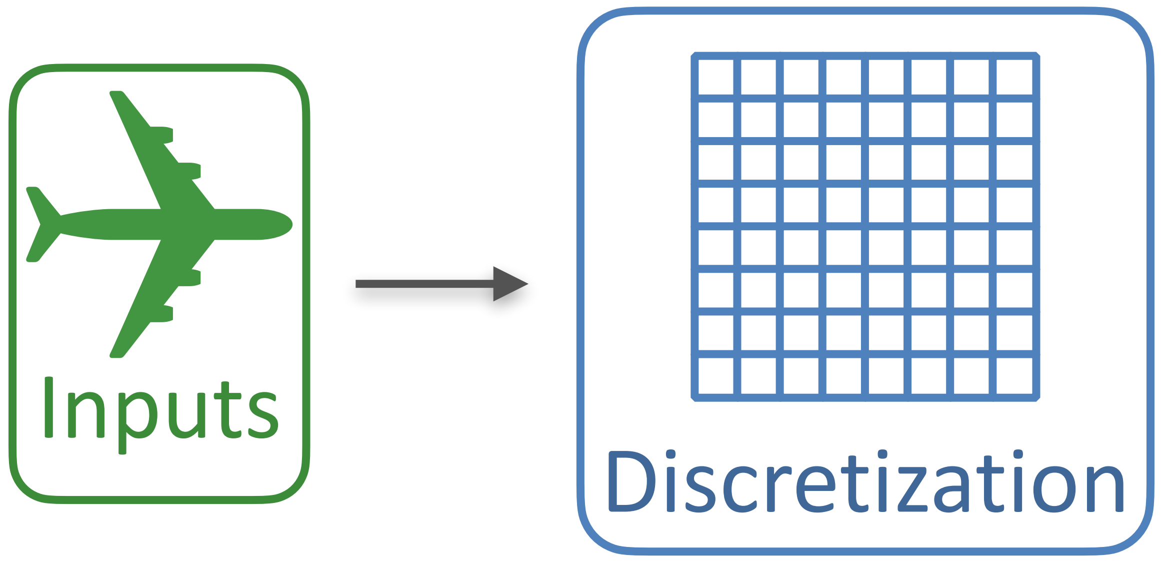

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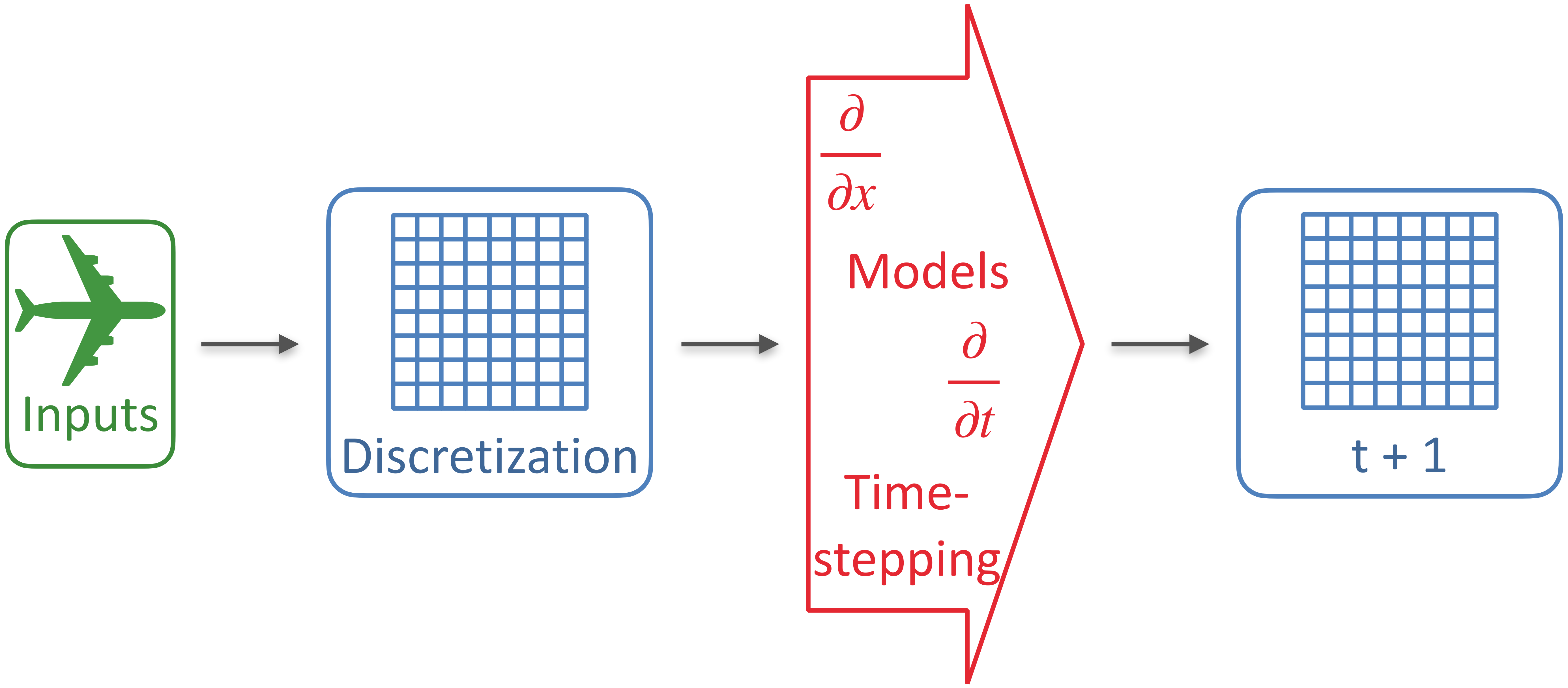

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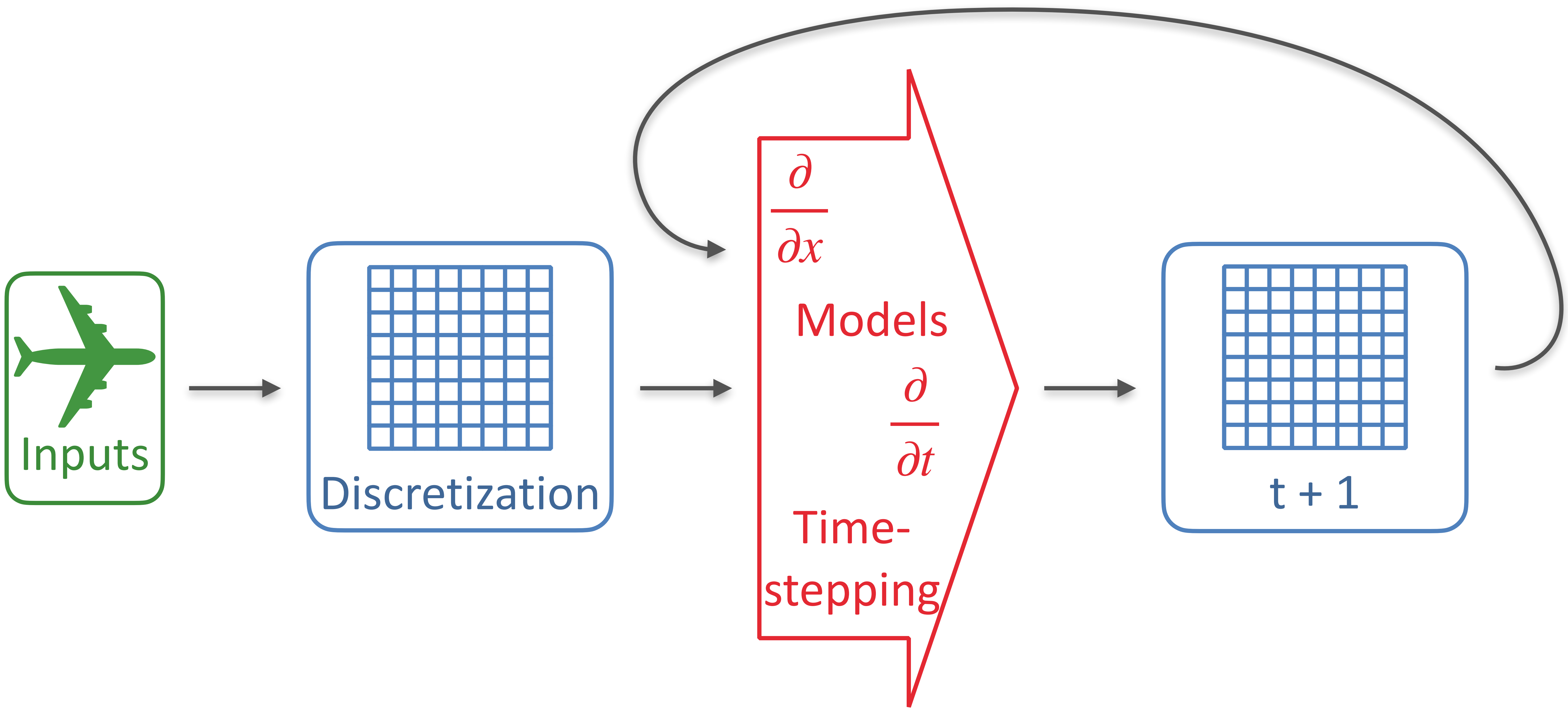

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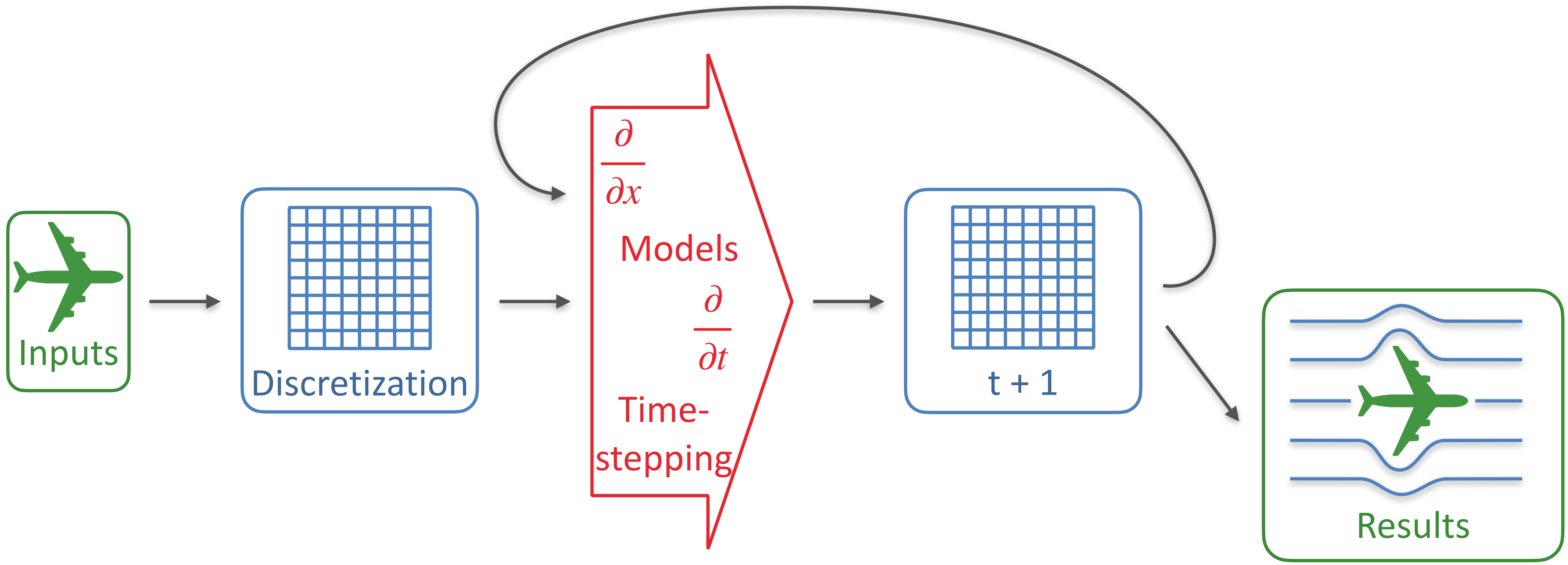

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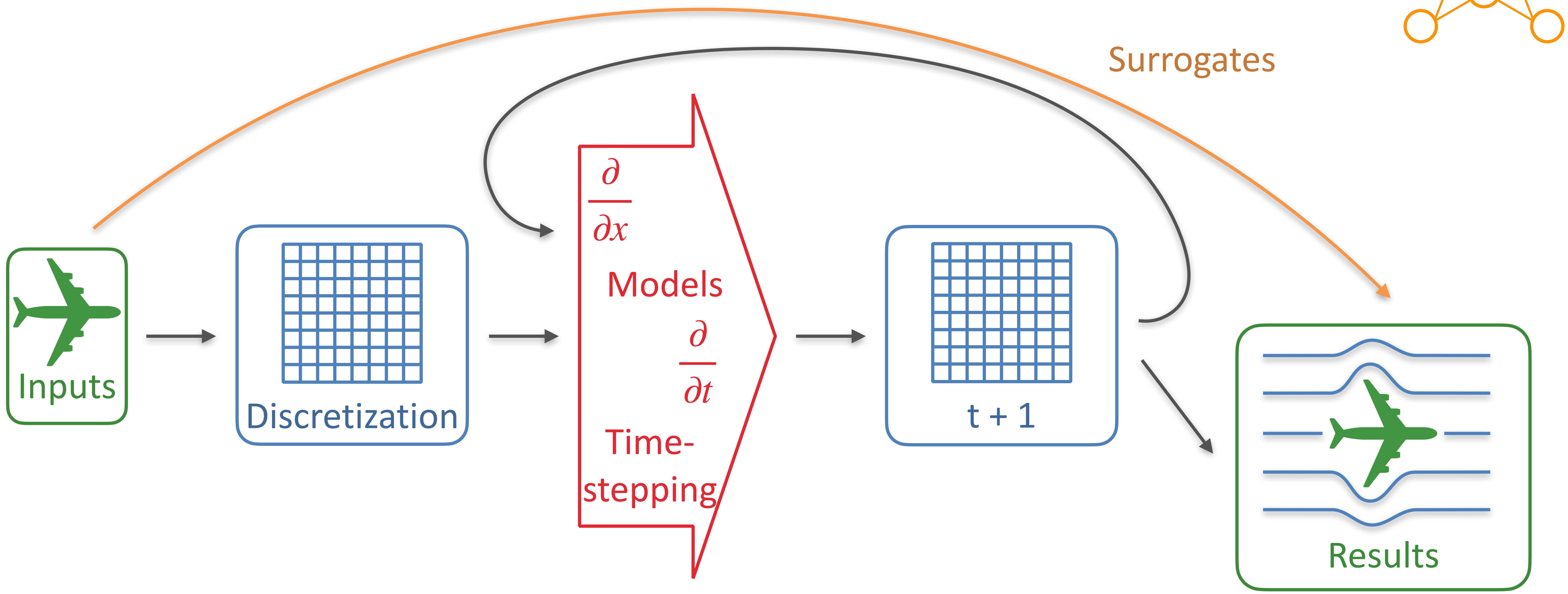

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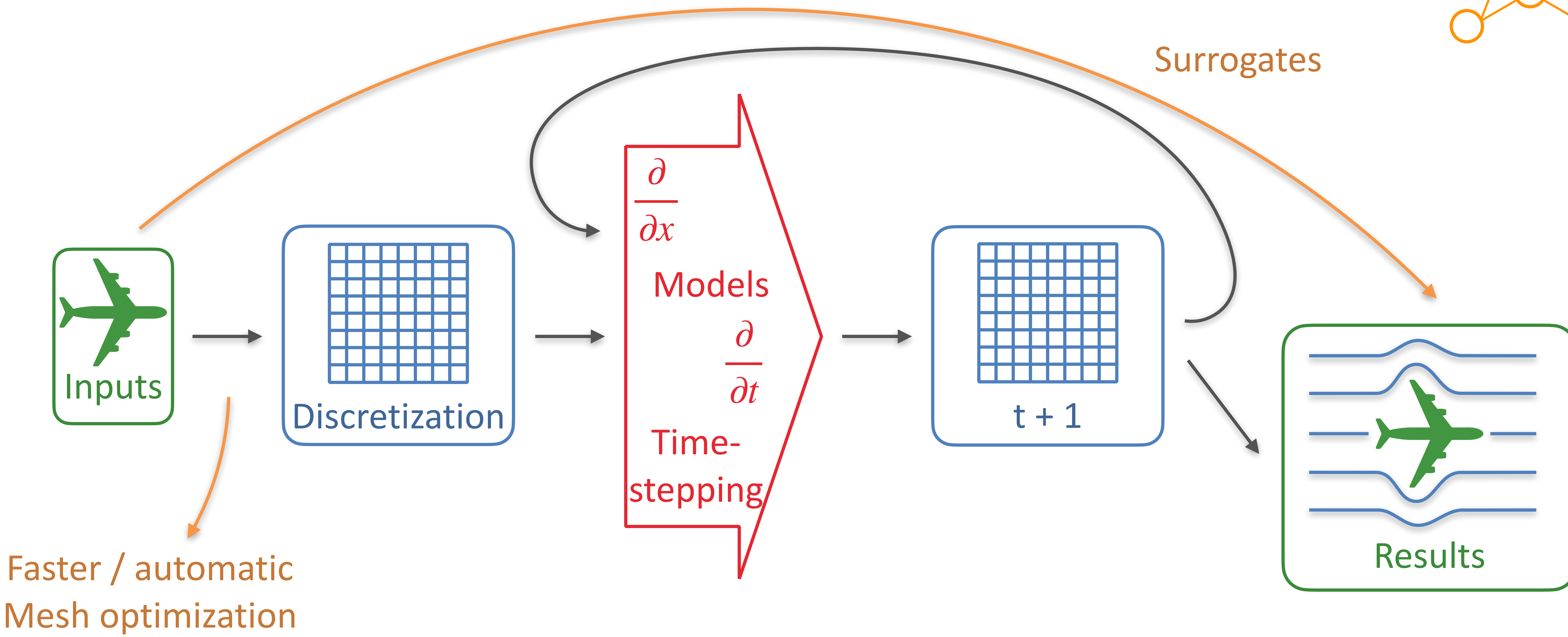

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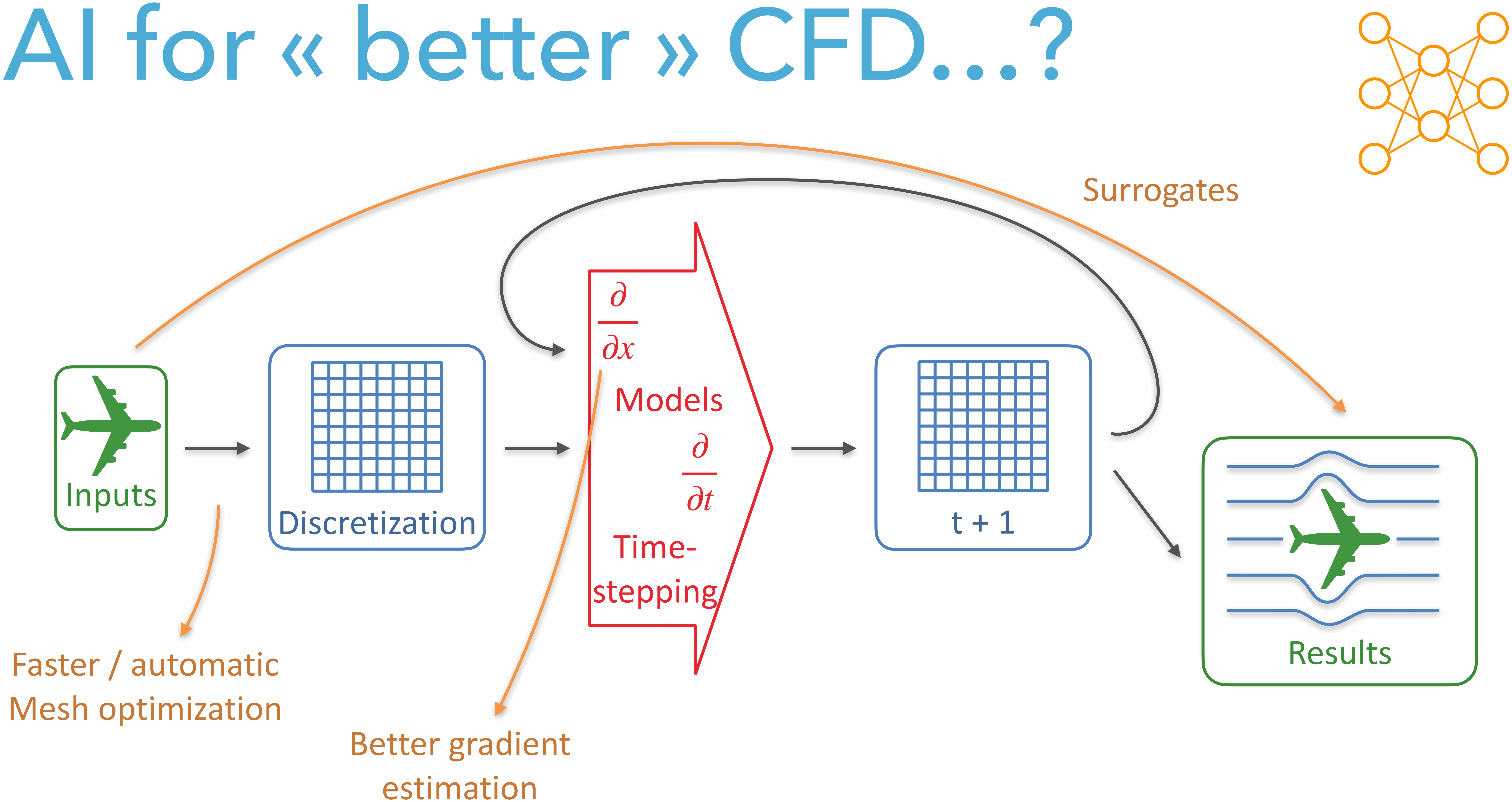

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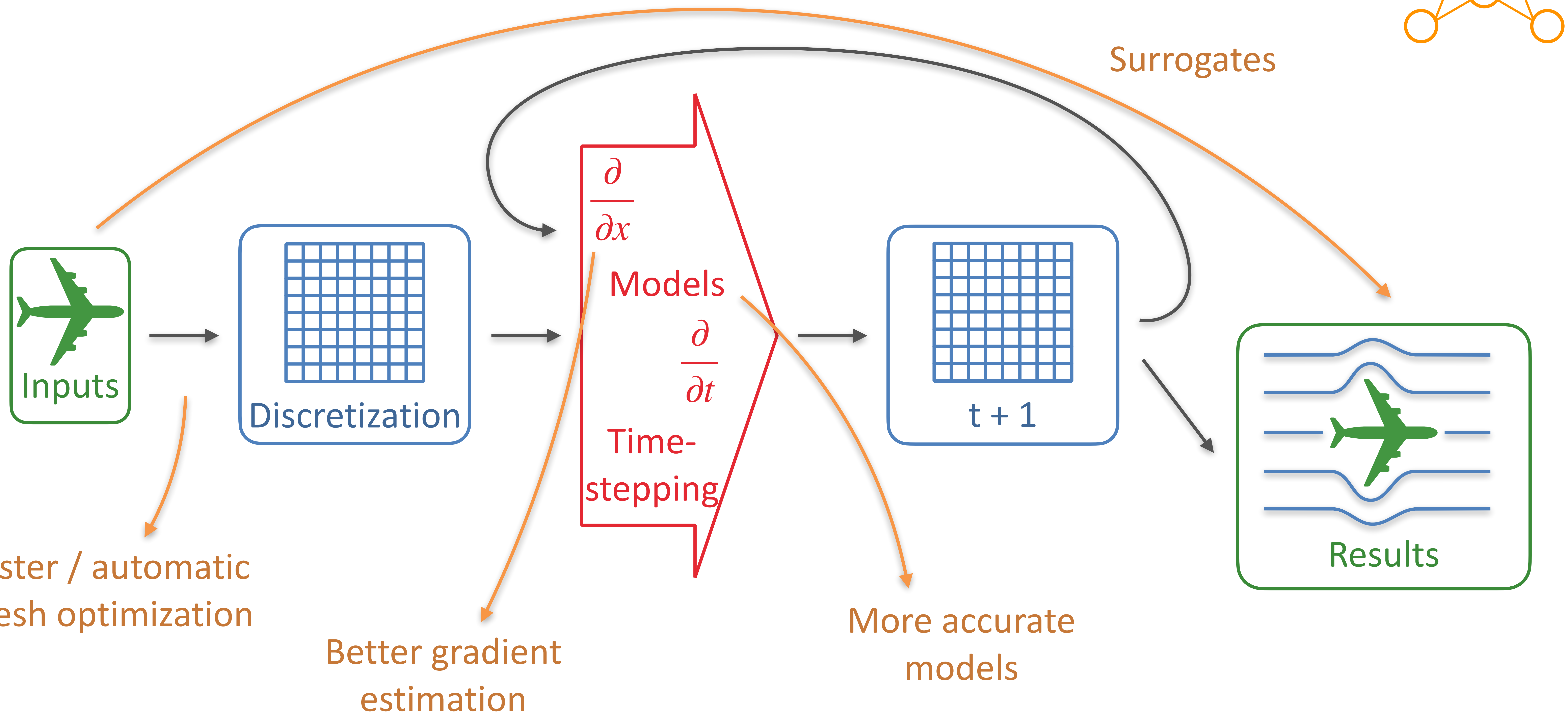
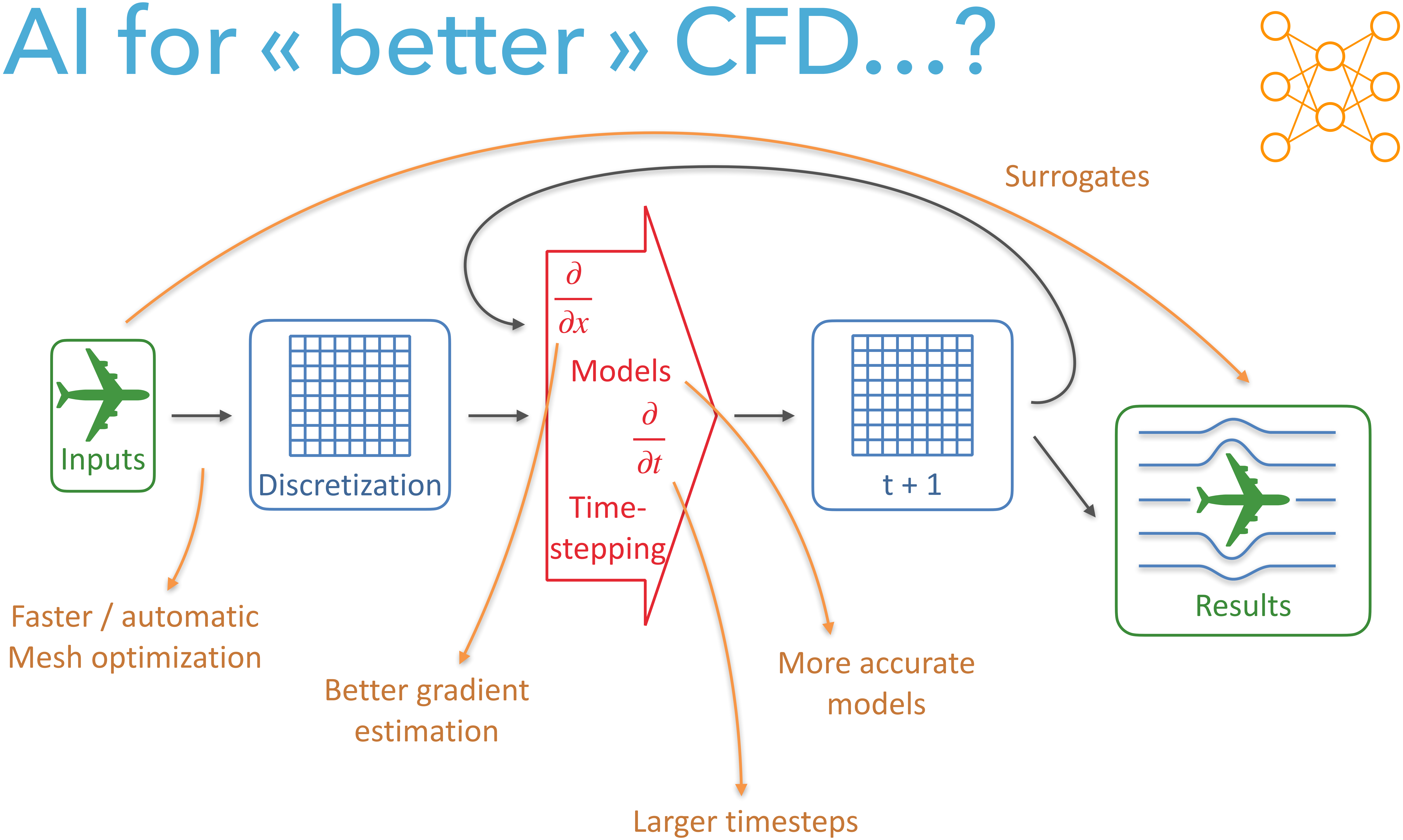
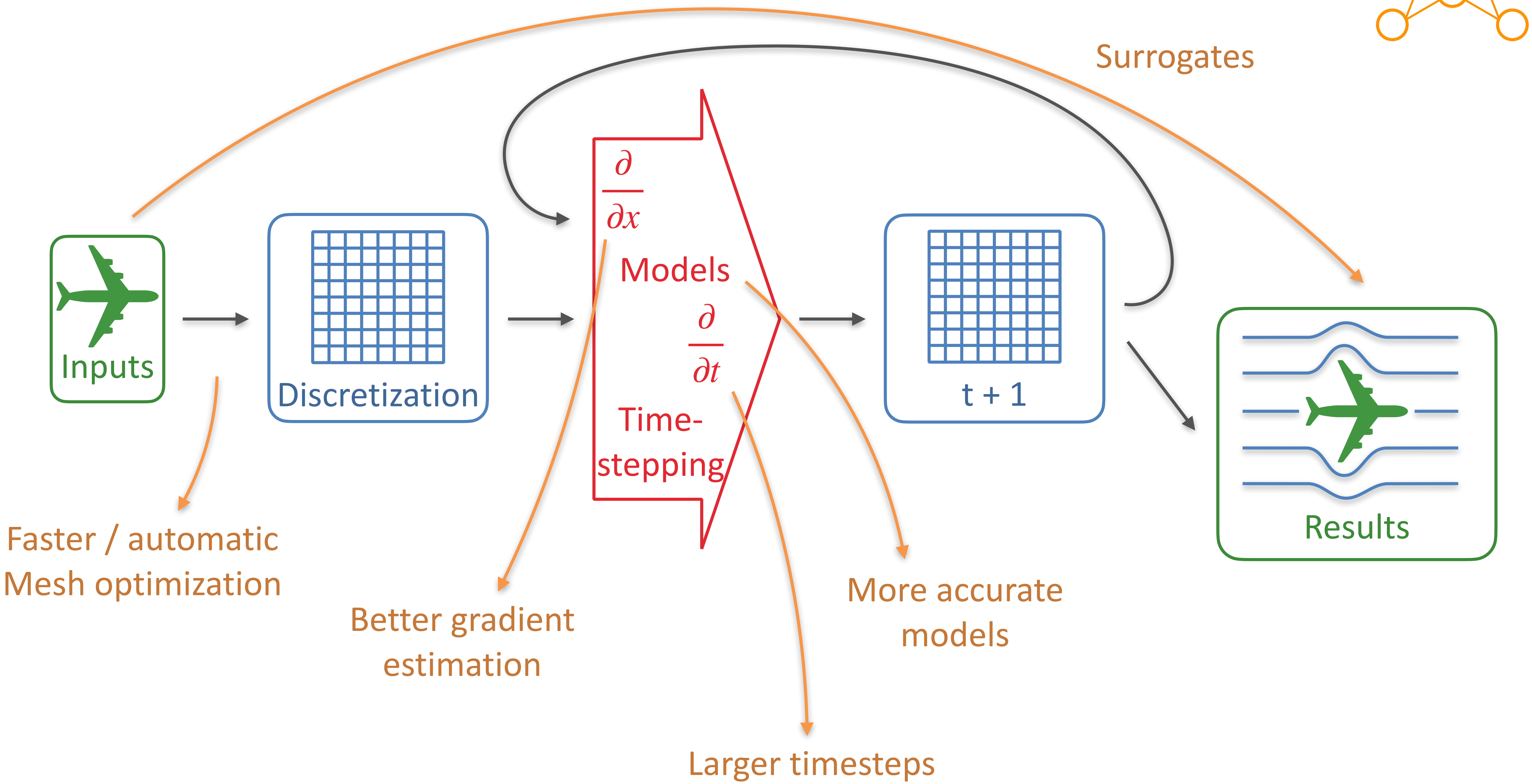


AI for « better » CFD...?

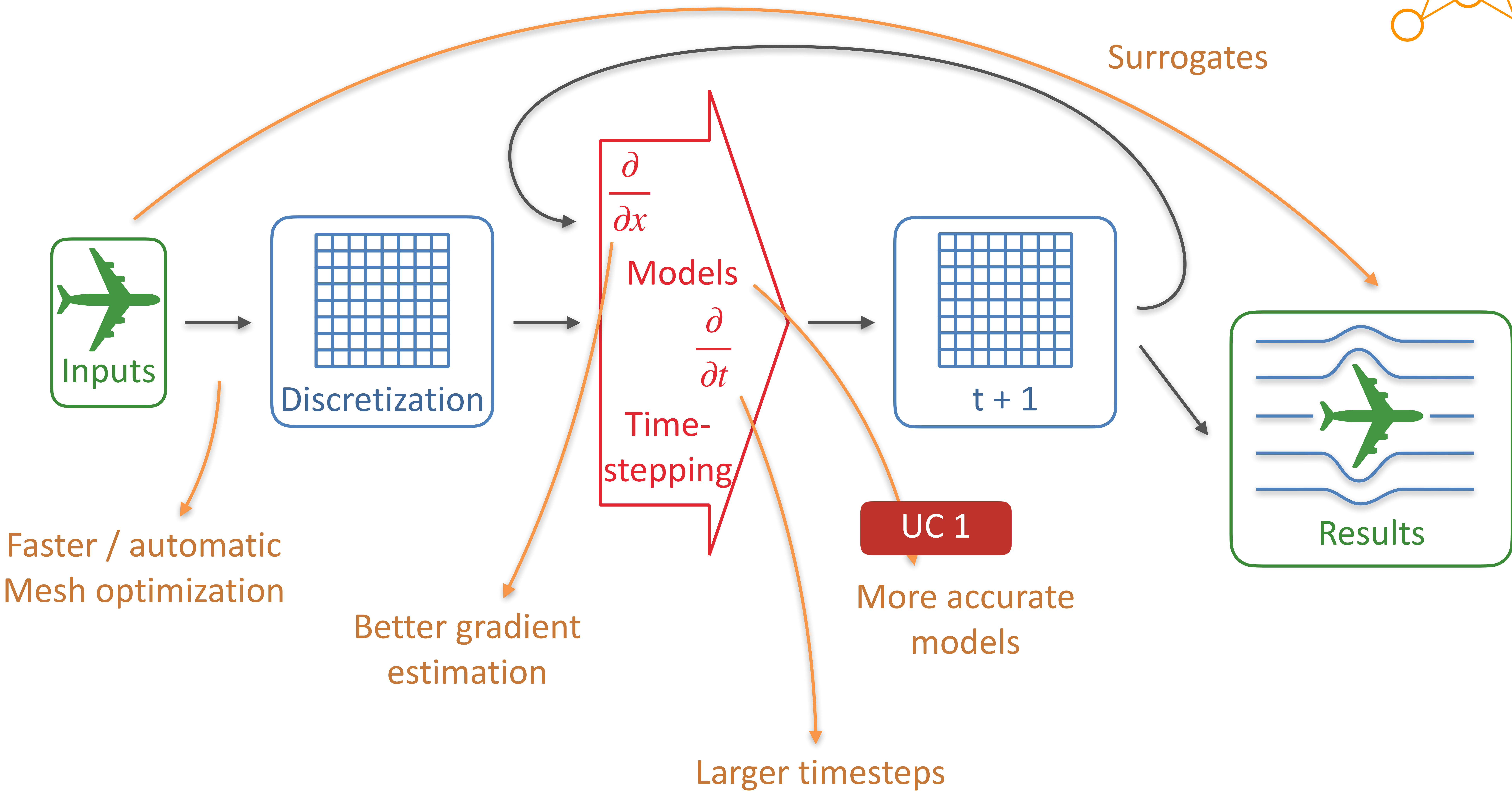


AI for « better » CFD...?



- Many degrees of AI « intrusion » in CFD are possible
- It is not yet clear which is the best way to go!

AI for « better » CFD...?



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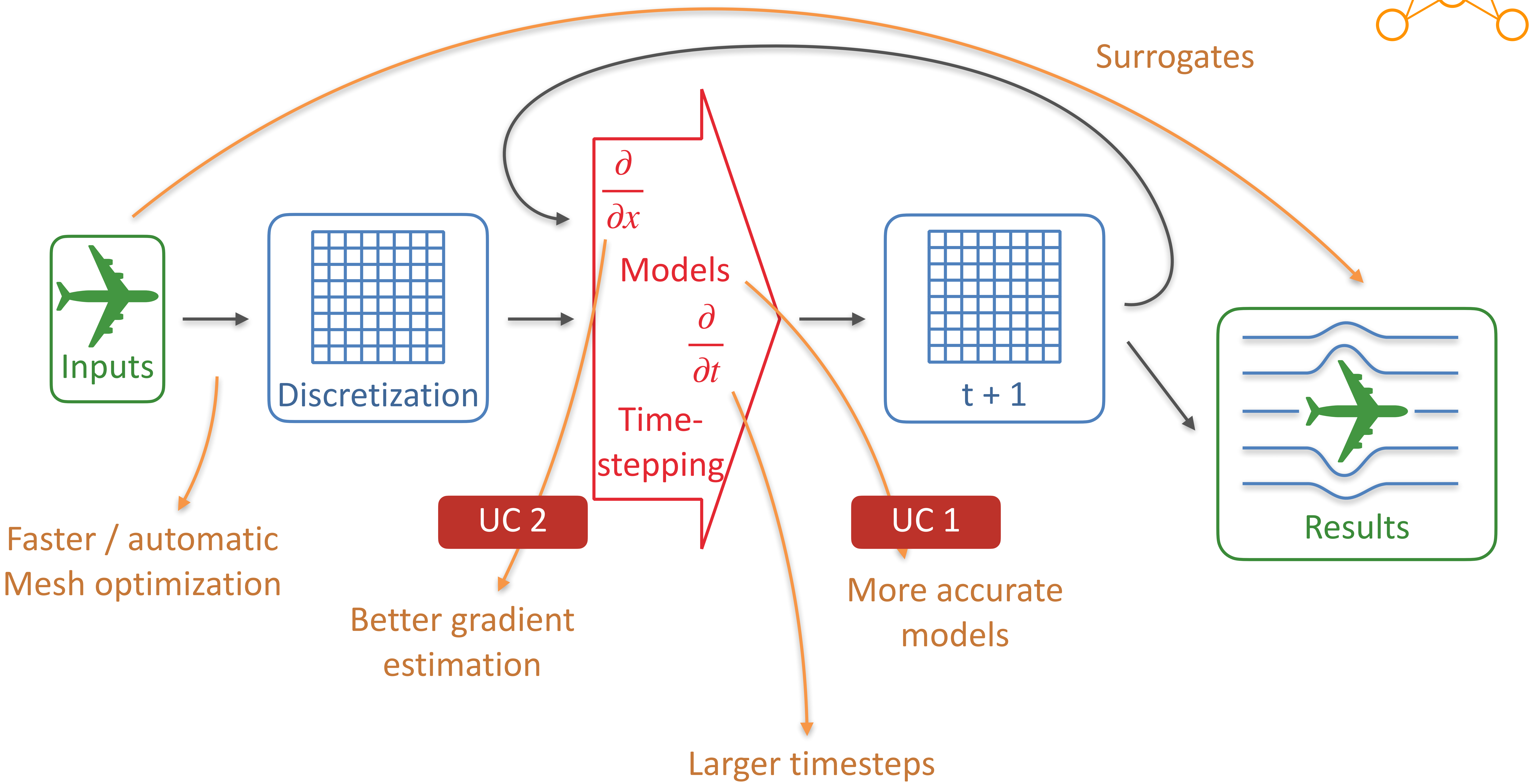
AI for « better » CFD…?



- Many degrees of AI « intrusion » in CFD are possible
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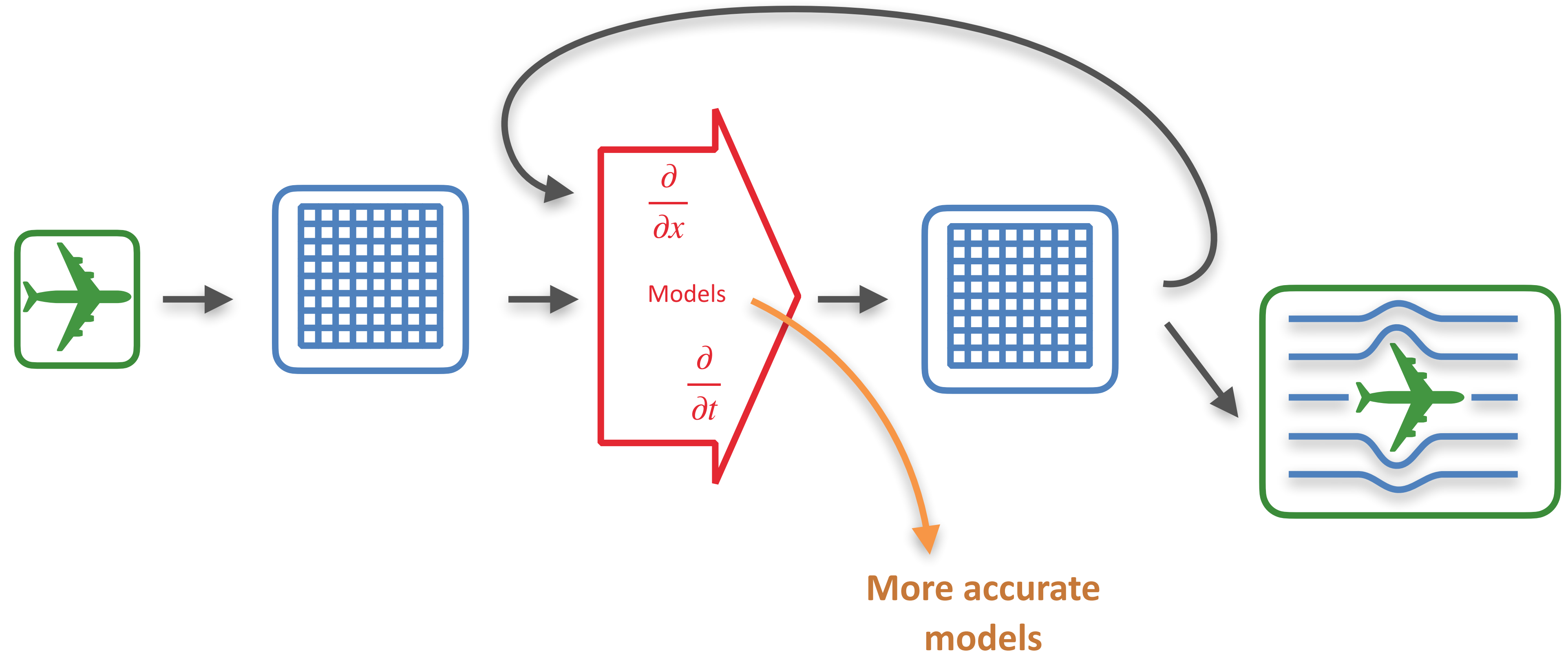


1. Subgrid-scale modeling with CNNs

Ongoing PhD of Victor Xing, Cerfacs

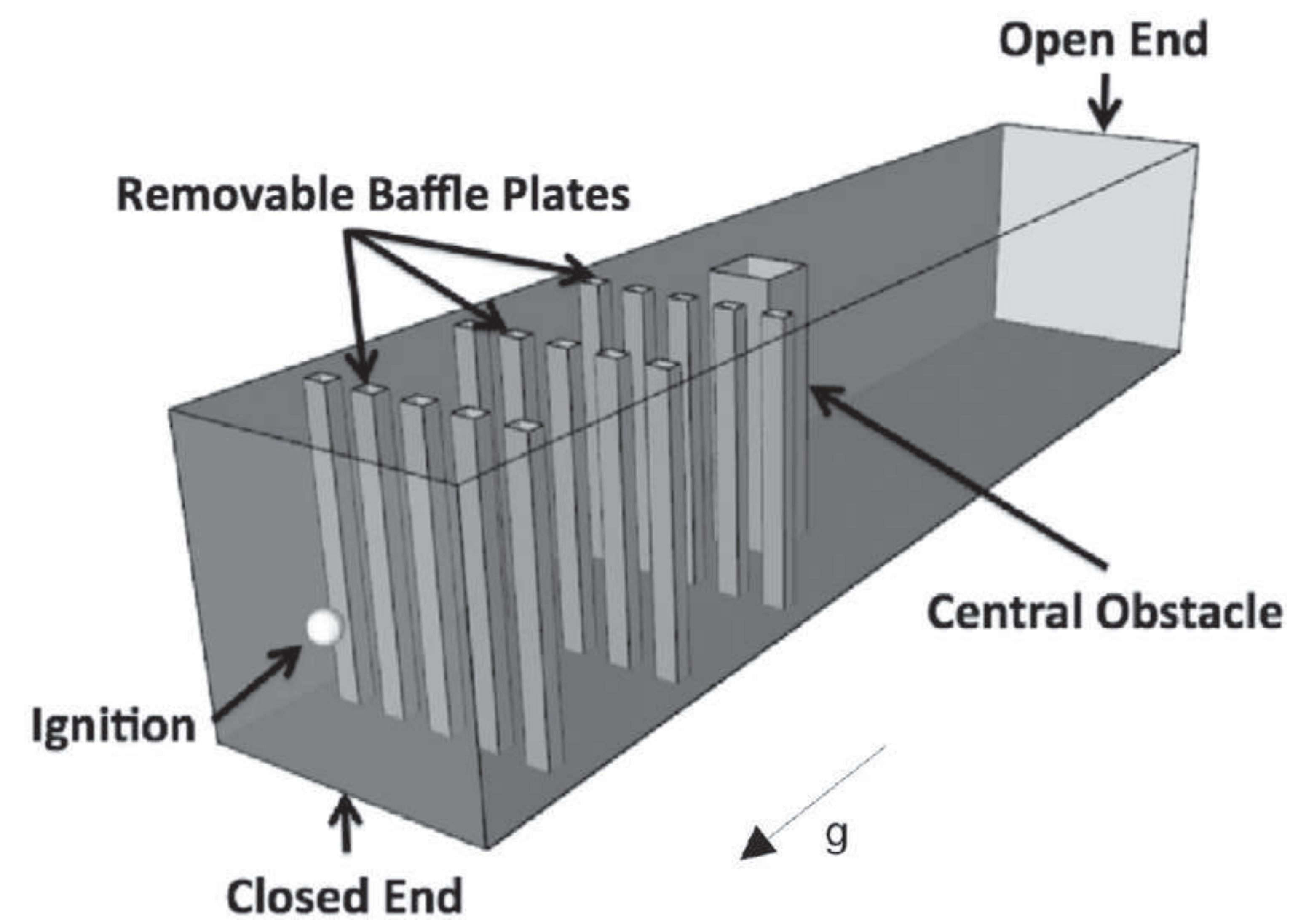
Lapeyre, C.J., Misdariis, A., Cazard, N. & Poinsot, T (2018). A-posteriori evaluation of a deep convolutional neural network approach to subgrid-scale flame surface estimation. Proc. CTR Summer Program, 349-358.

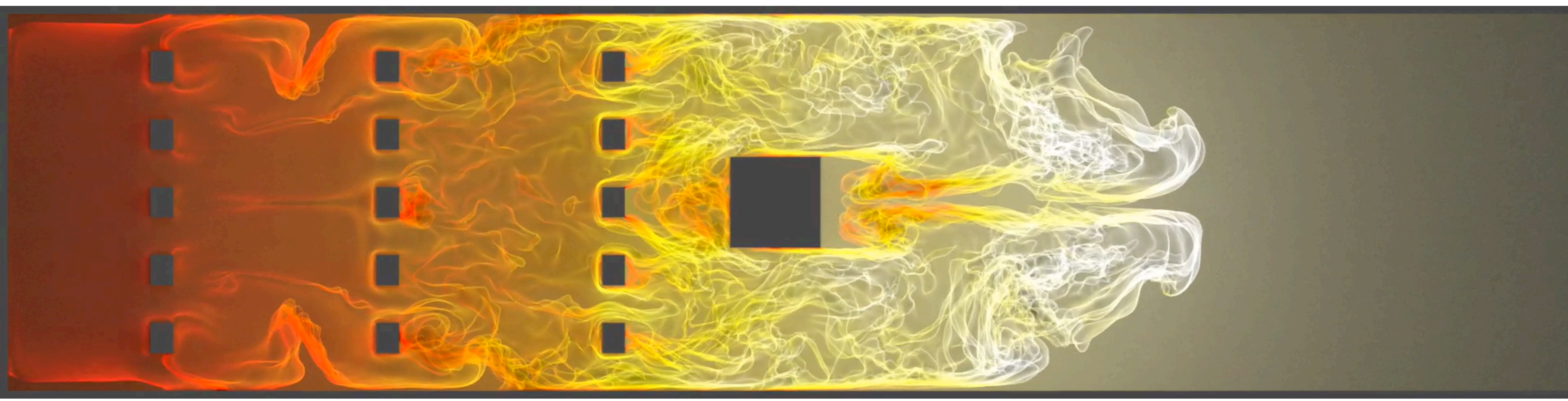
Lapeyre, C.J., Misdariis, A., Cazard, N., Veynante, D. & Poinsot, T. (2019). Training convolutional neural networks to estimate turbulent sub-grid scale reaction rates. *Combustion and Flame*, 203, 255-264

Very large scale combustion

- Context: safety of industrial complexes in combustible gas leaks

- Reactive LES of very large domains





Elsa Gullaud, Post-Doc 2019

Very large scale combustion

- Context: safety of industrial complexes in combustible gas leaks
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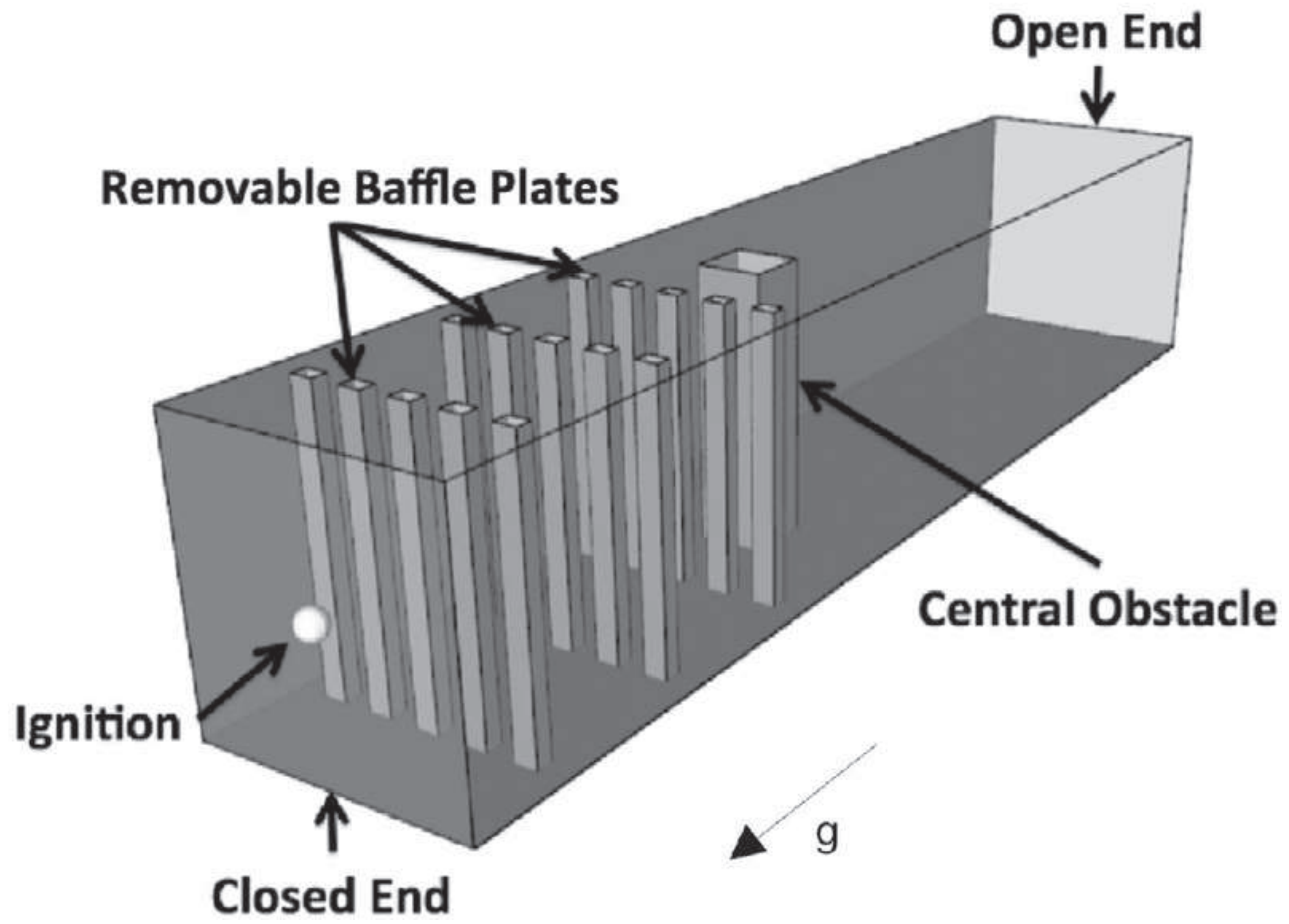
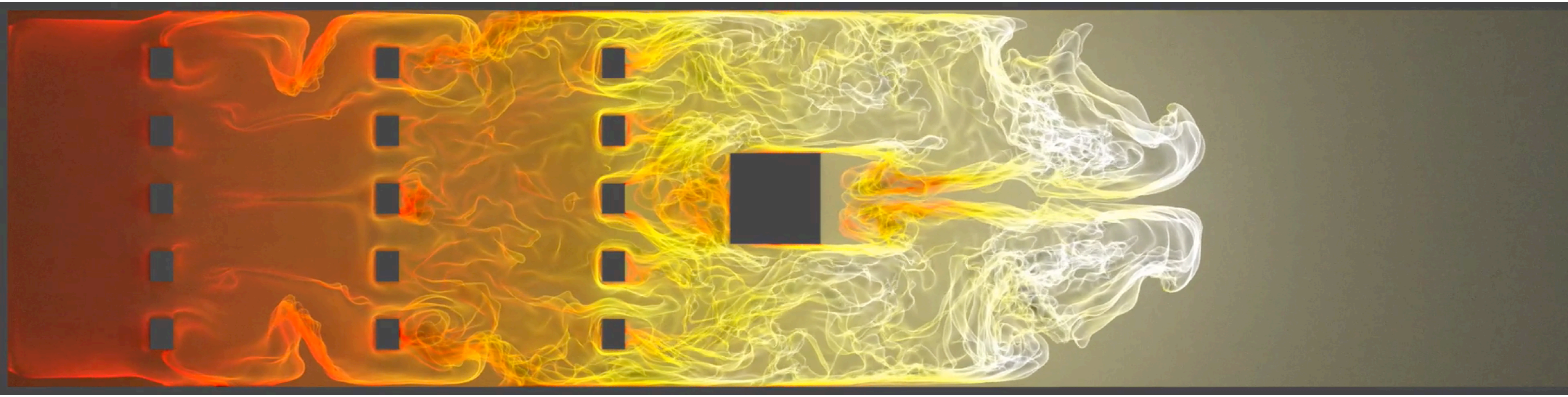
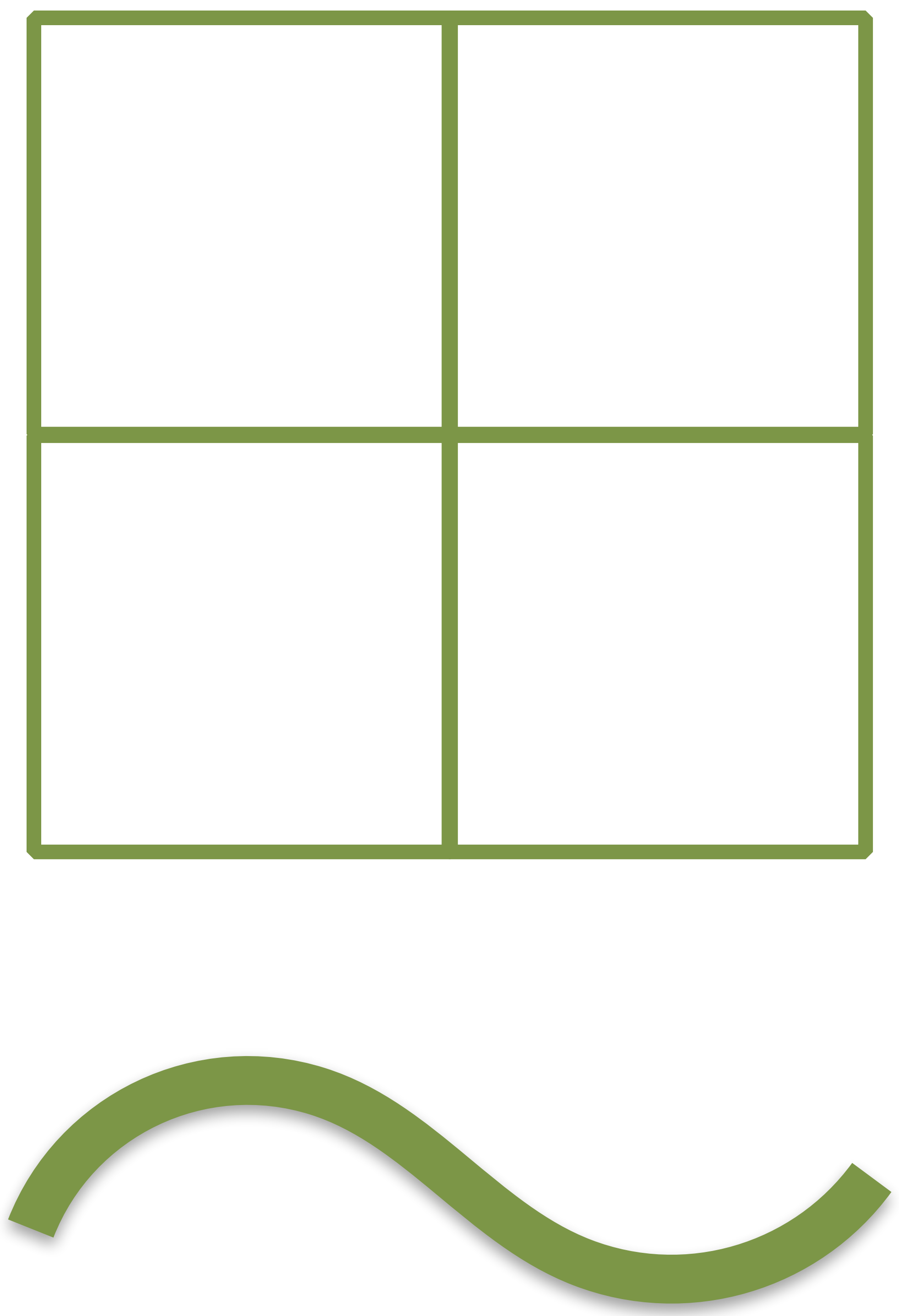




Elsa Gullaud, Post-Doc 2019

Subgrid-scale models

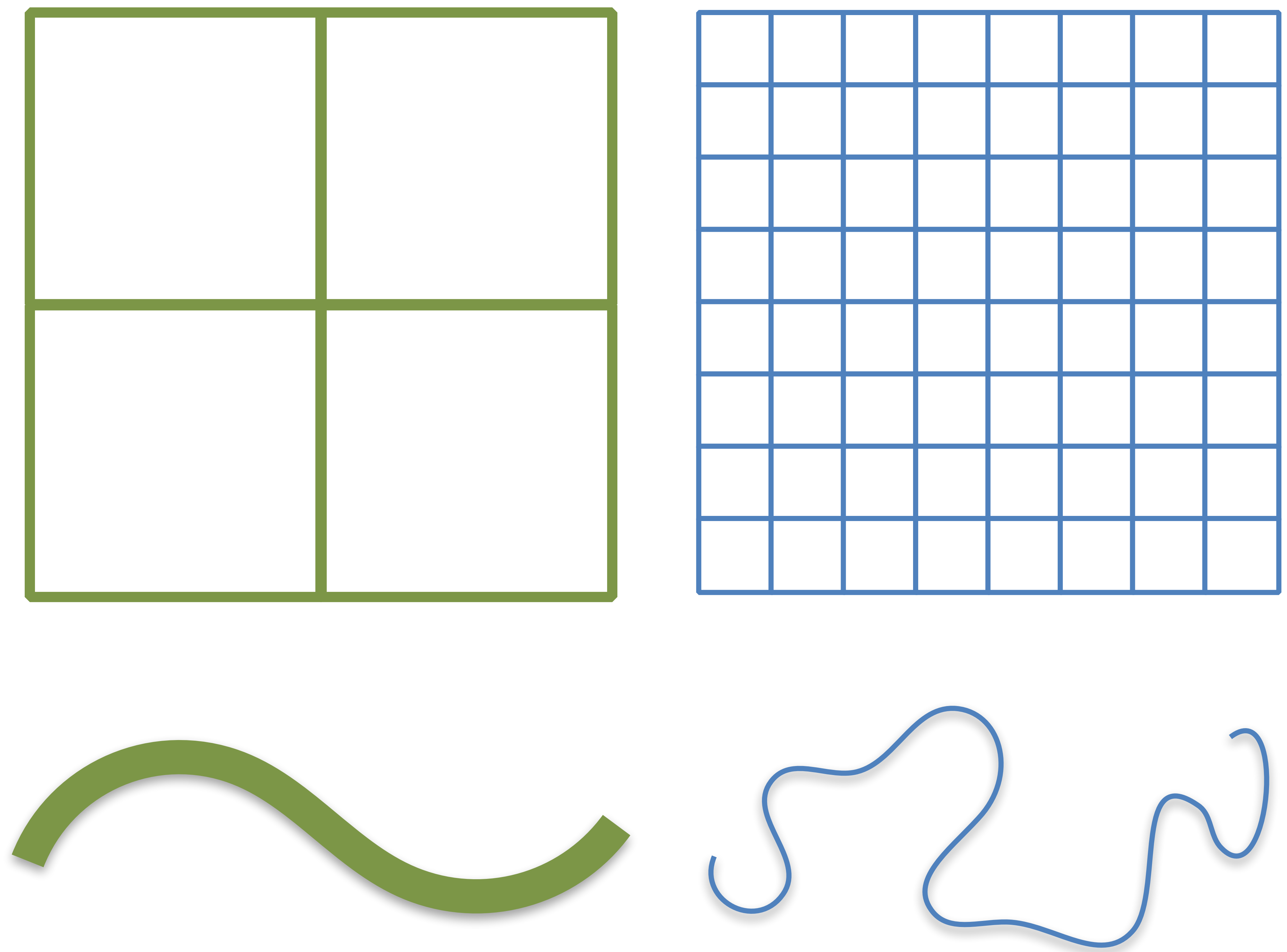
What I can pay for



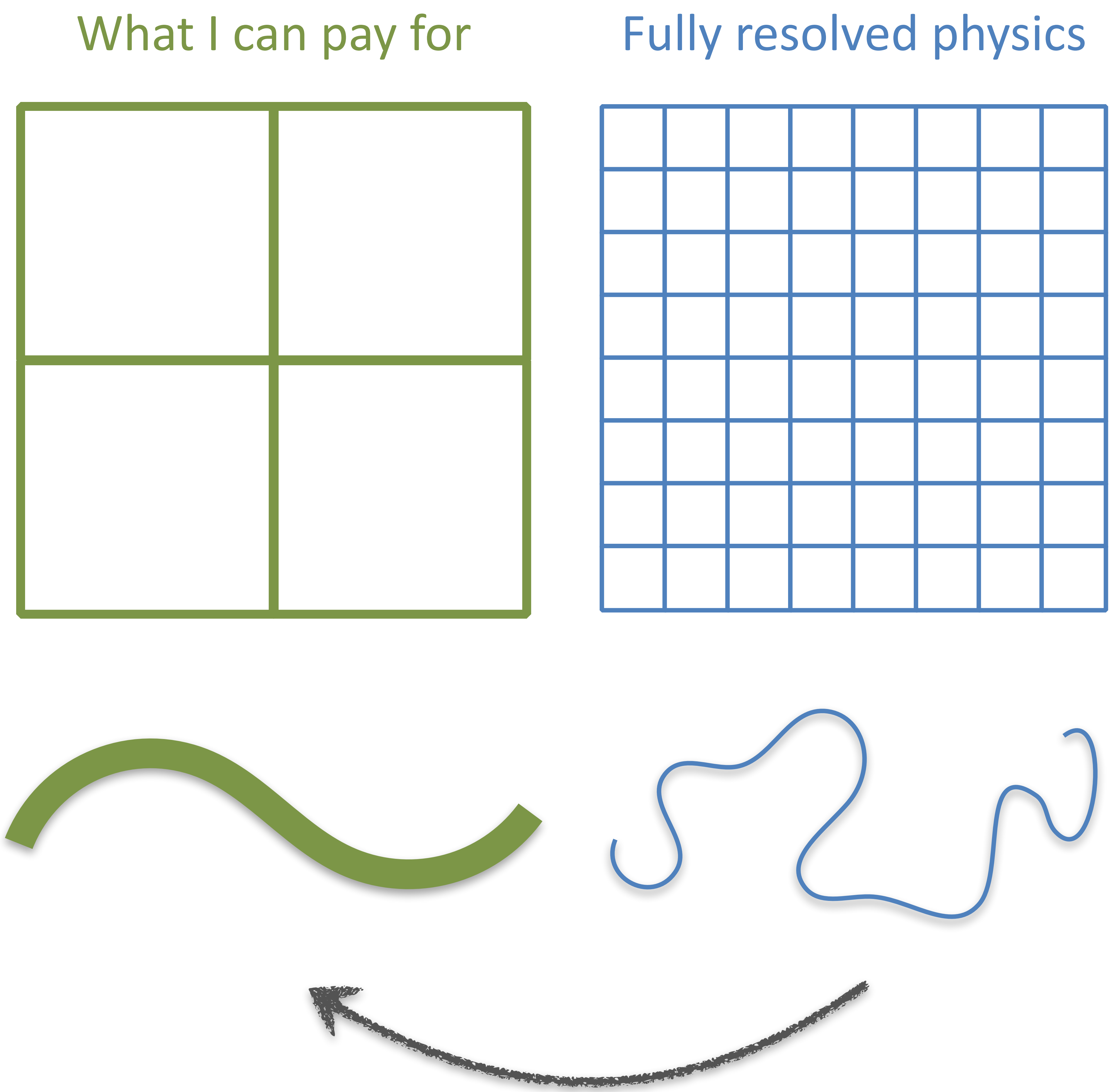
Subgrid-scale models

What I can pay for

Fully resolved physics

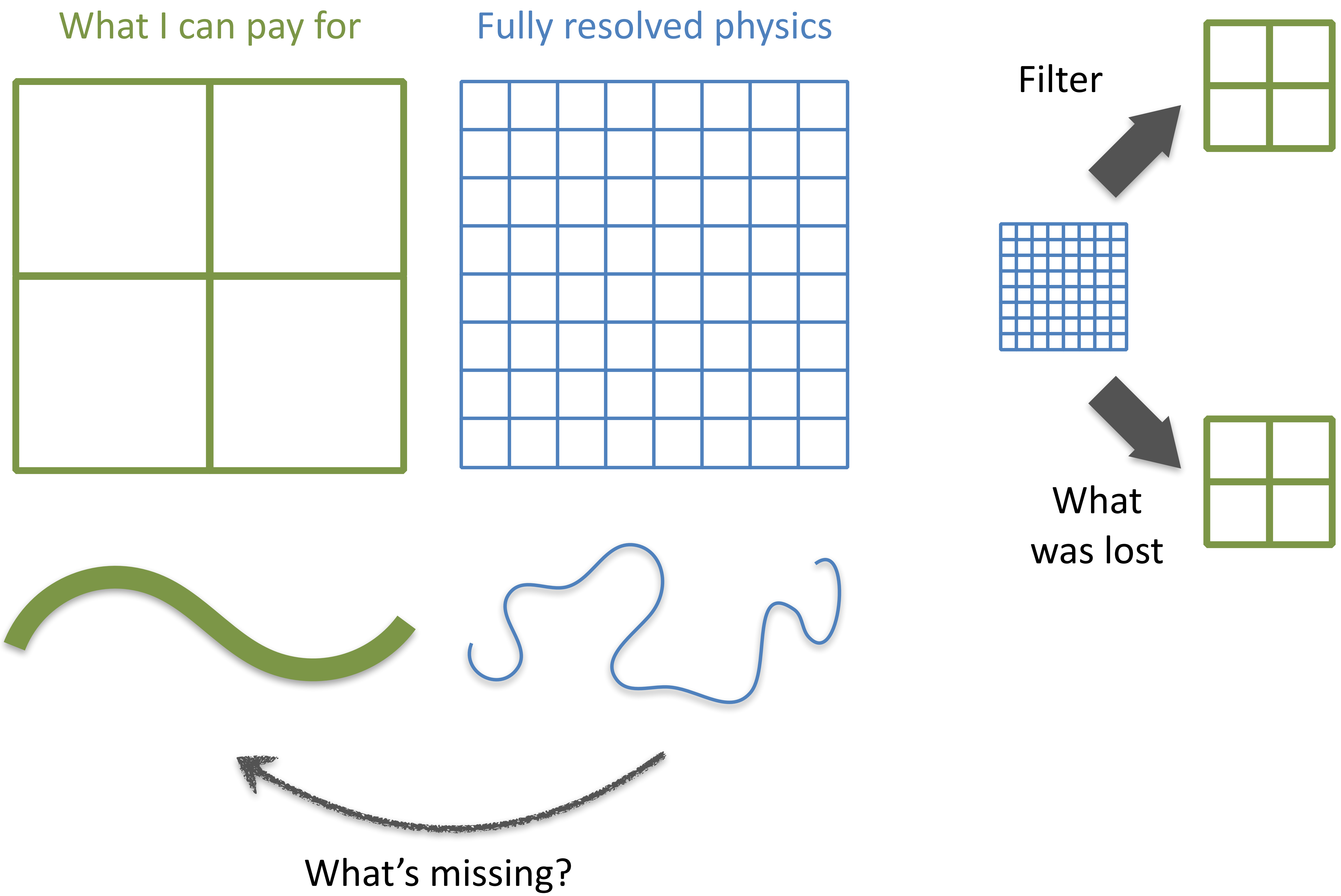


Subgrid-scale models

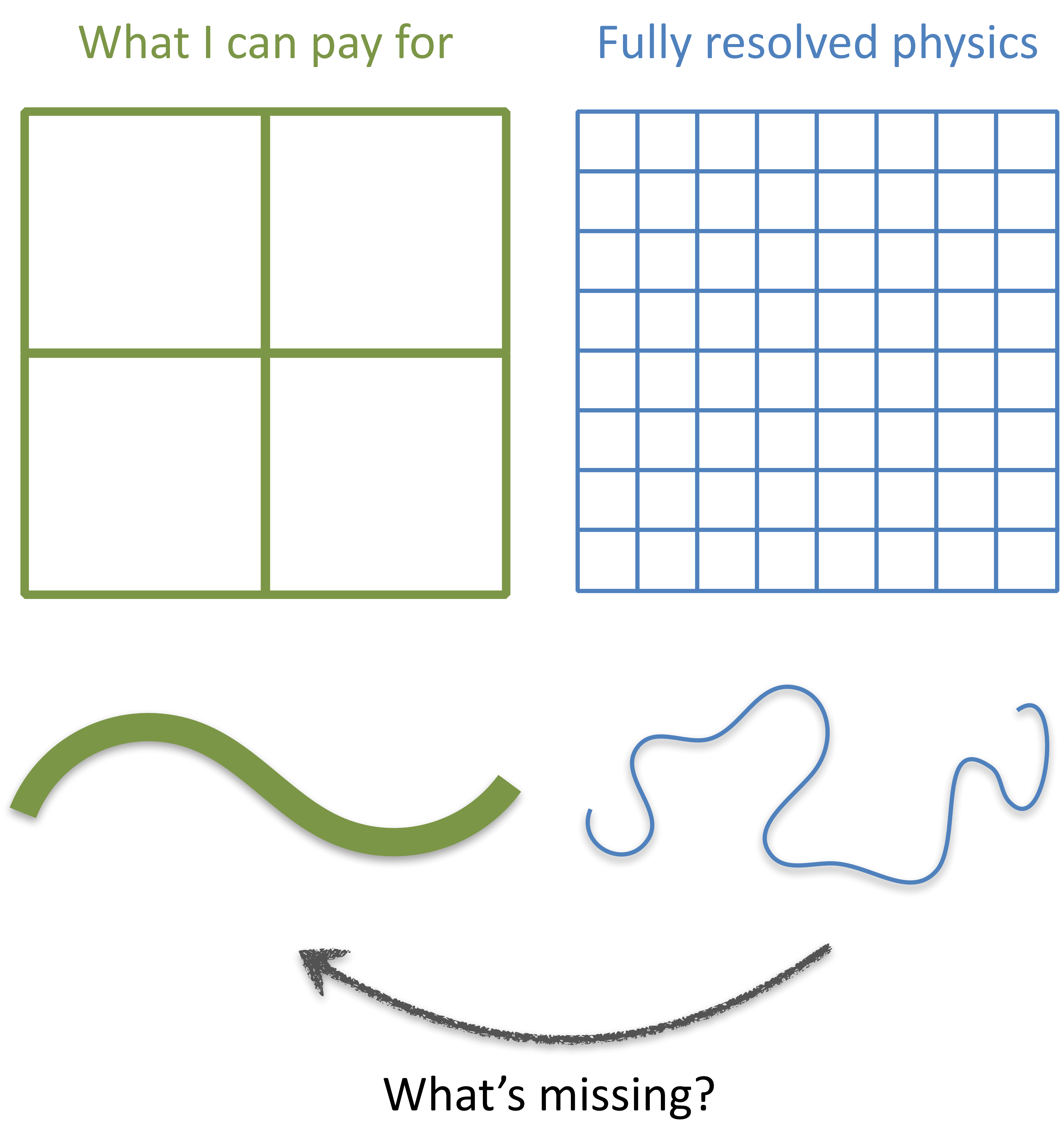


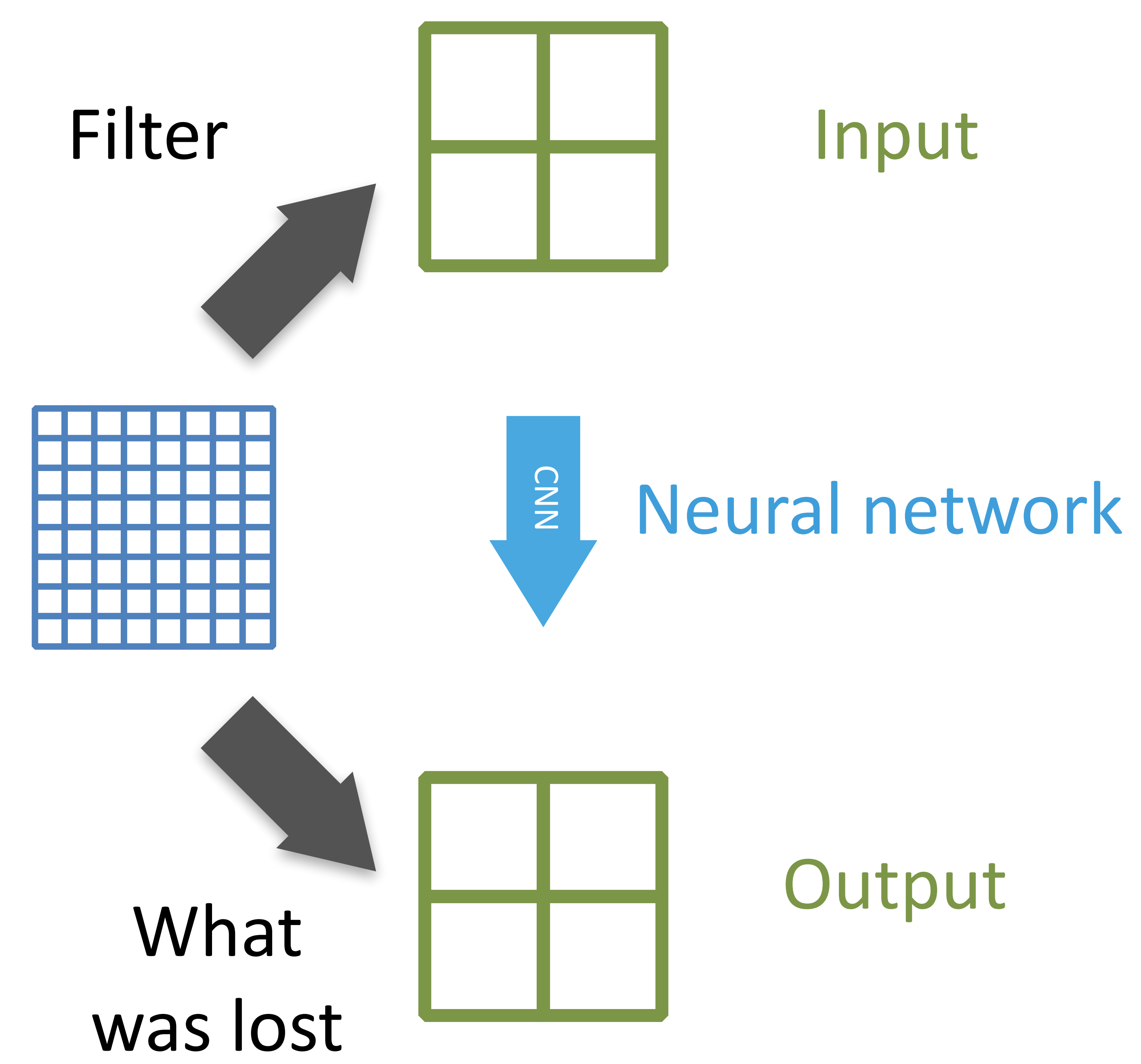
What's missing?

Subgrid-scale models

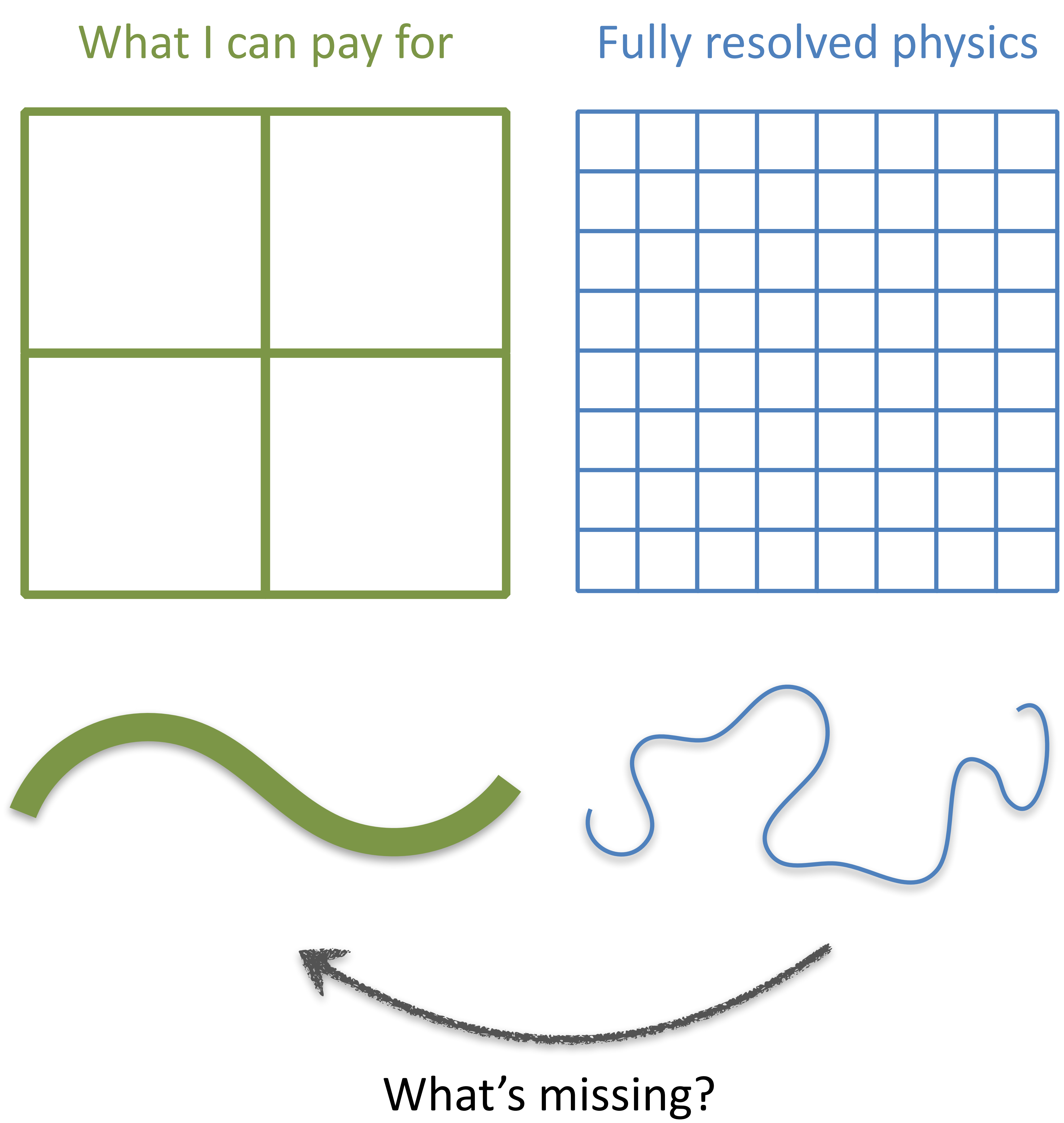


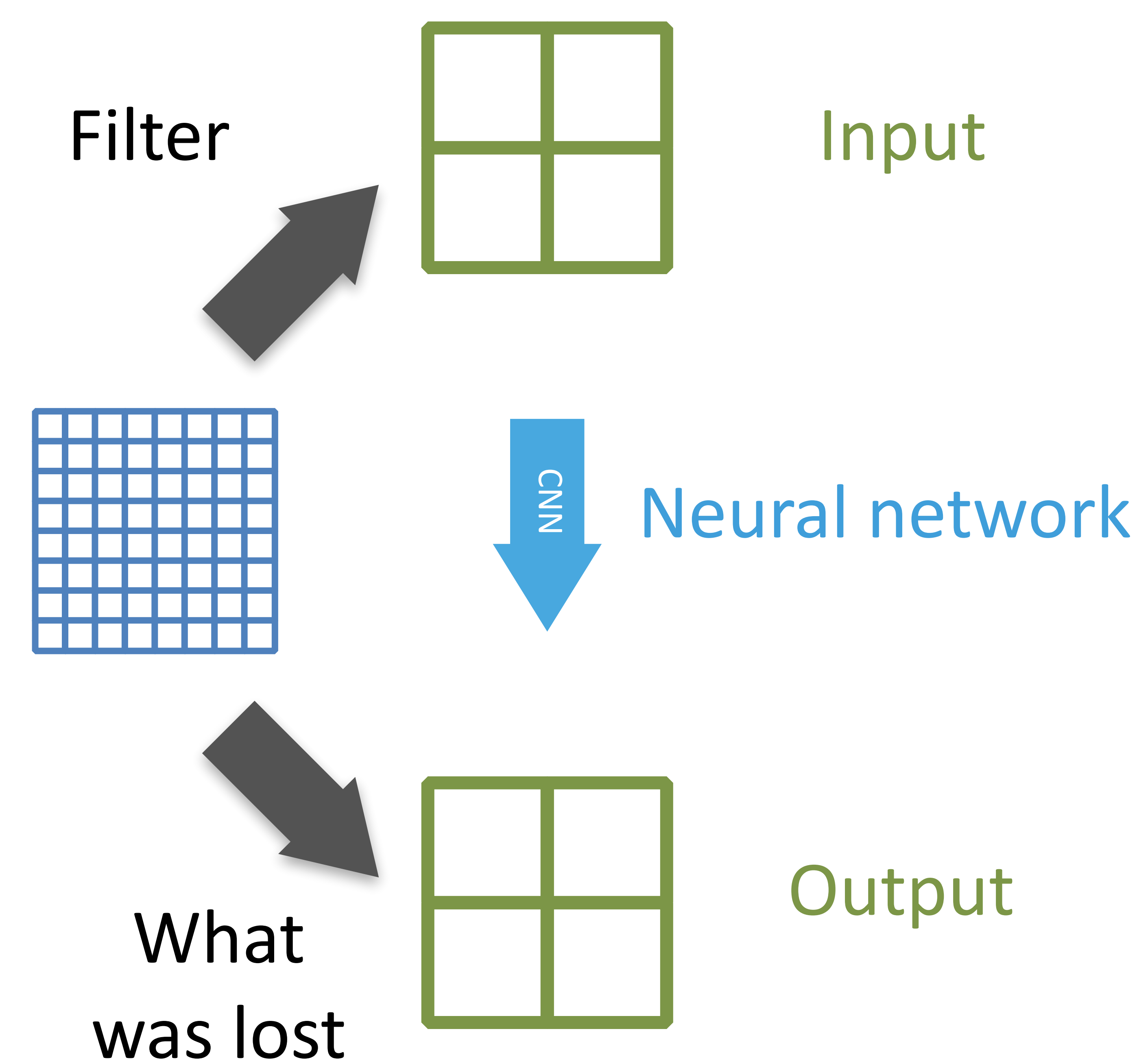
Subgrid-scale models

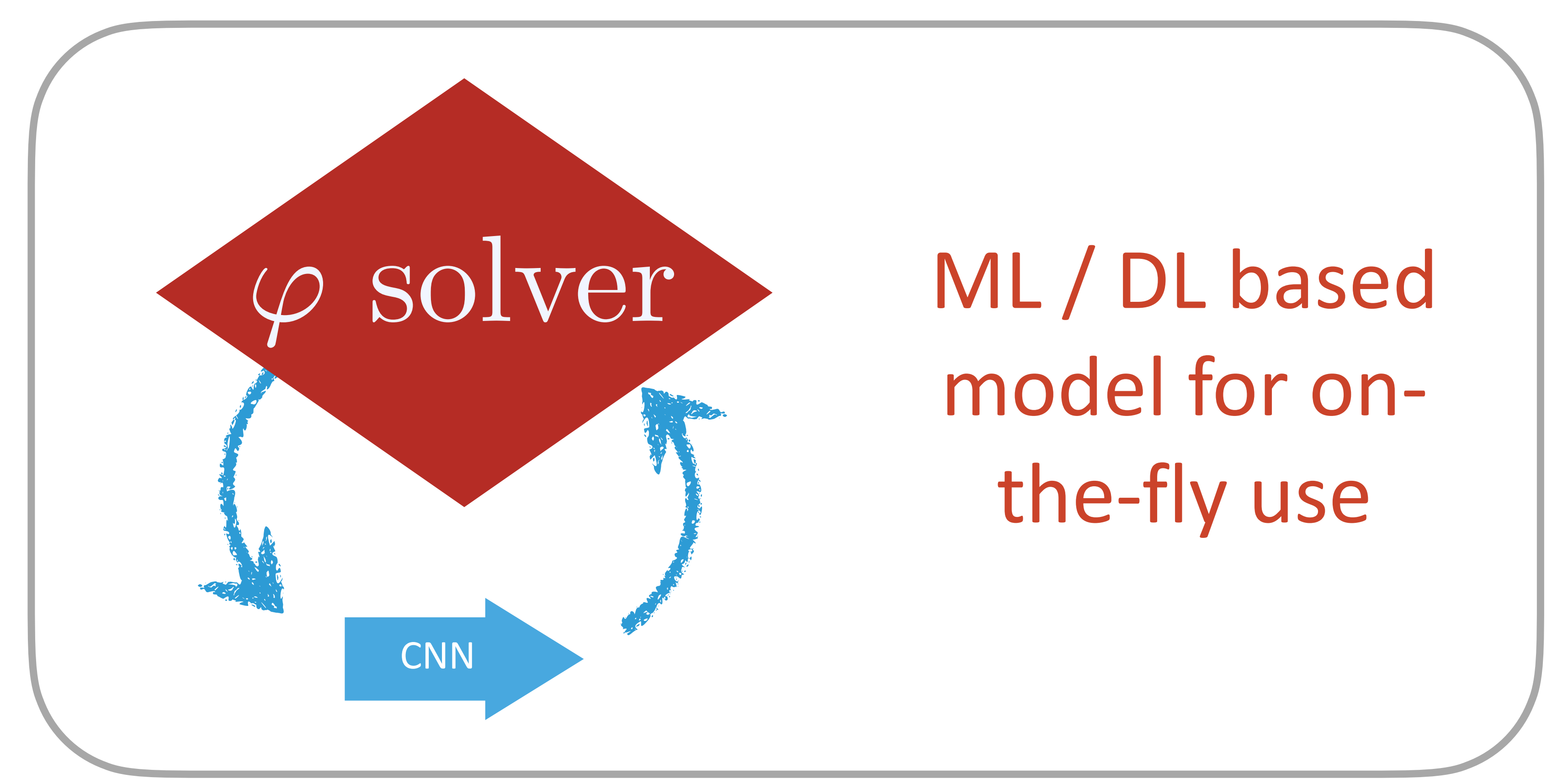




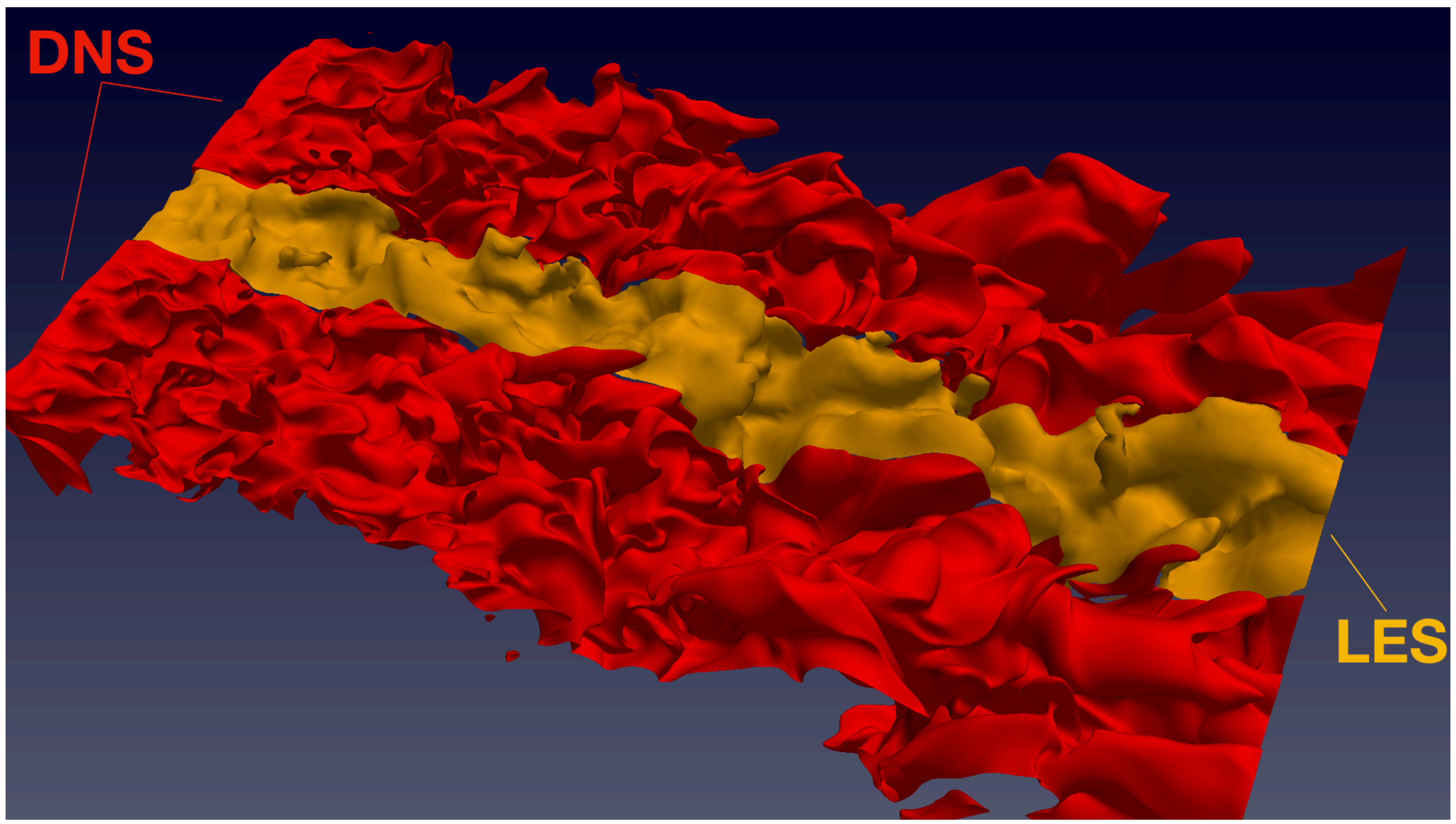
Subgrid-scale models

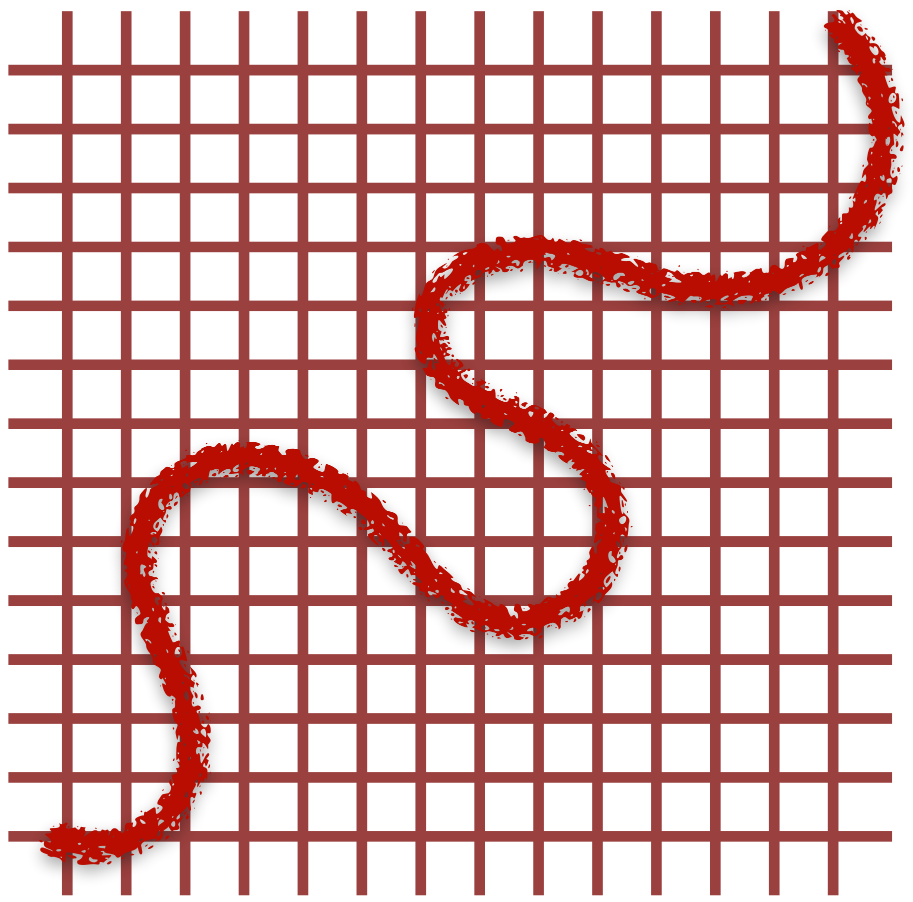






Combustion SGS

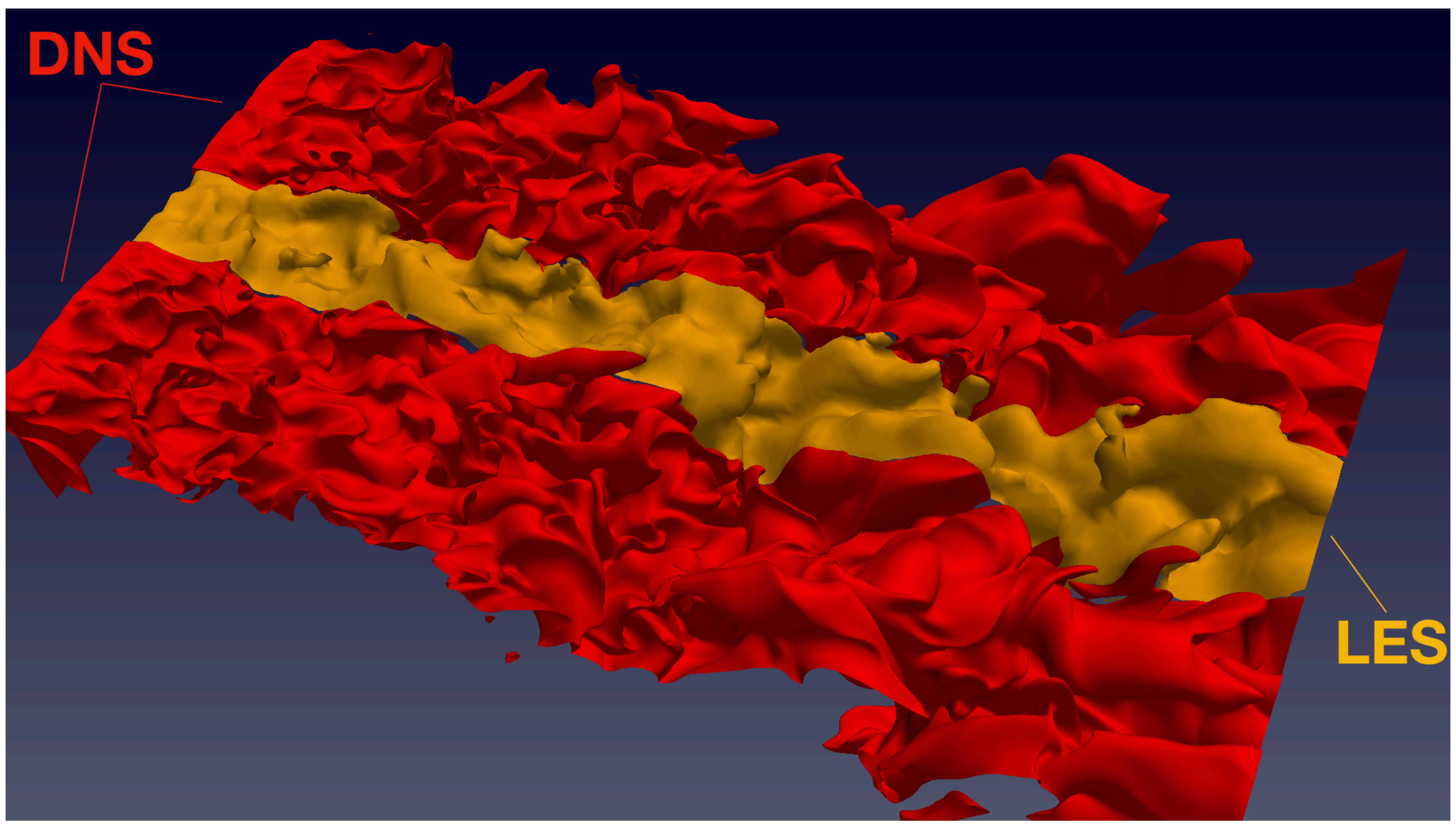


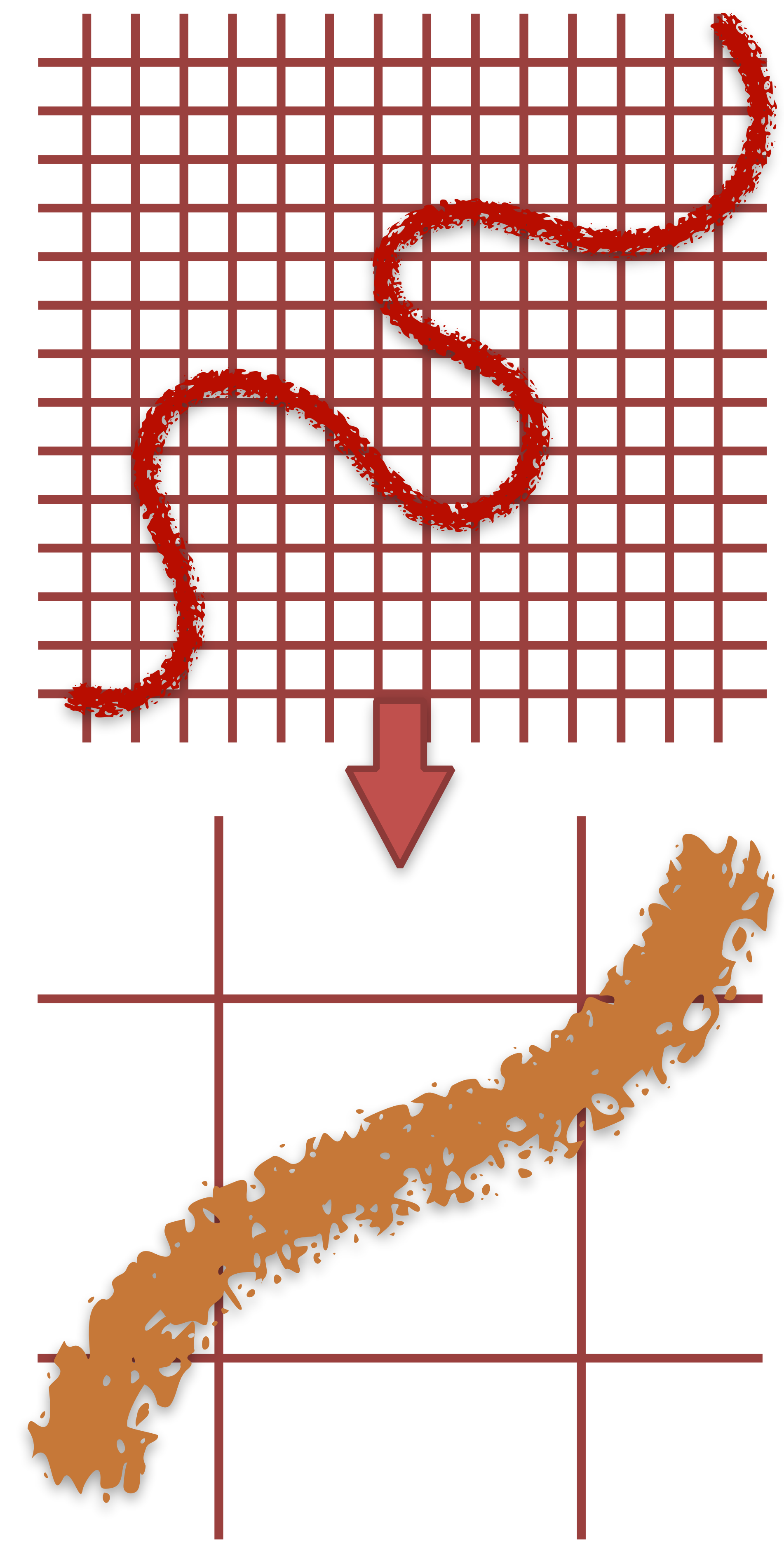


DNS:
Resolved
flame

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

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.

Efficiency functions f - local to global

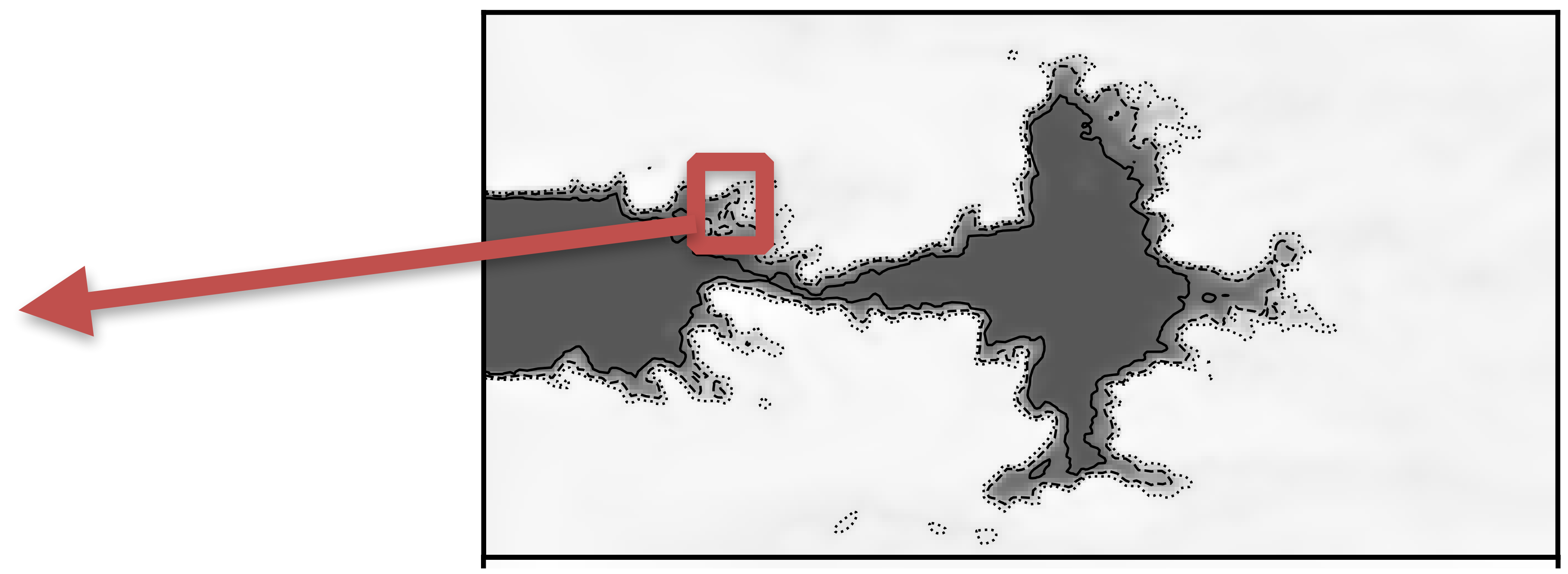
LOCAL FORMULATIONS:

1989 - Gouldin (fractal)

2000 - Colin *et al.*

2002 - Charlette *et al.*

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



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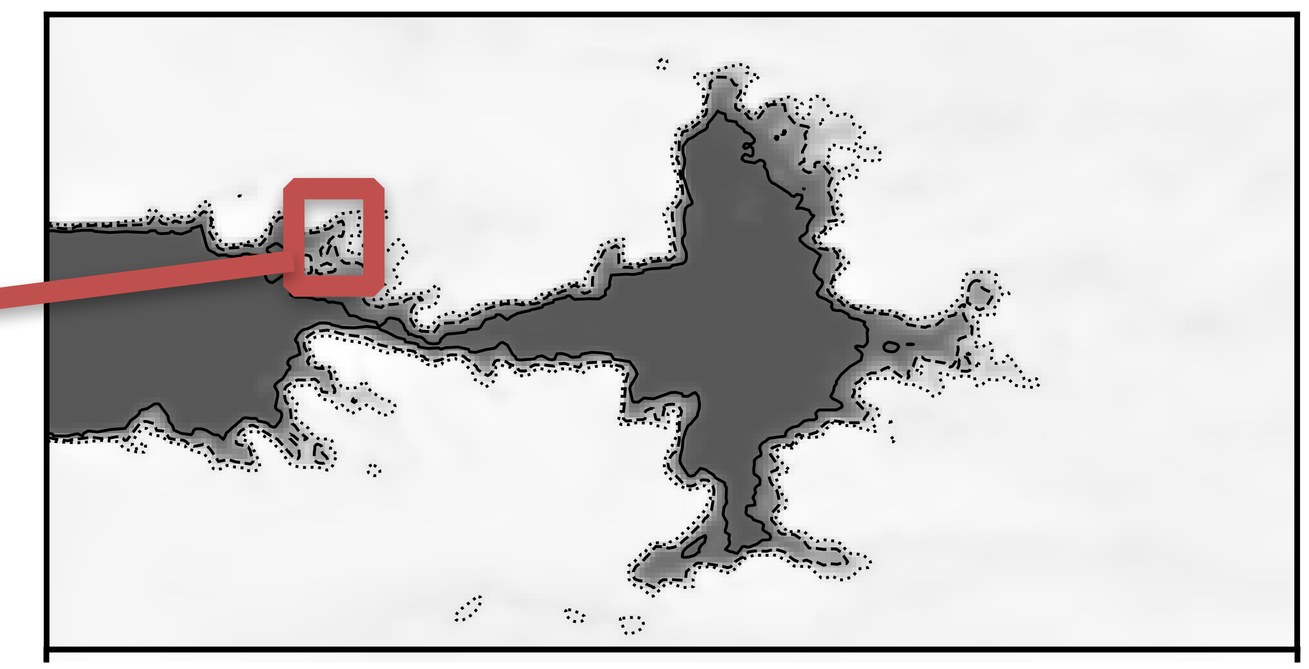

DYNAMIC FORMULATIONS:

2011 - Wang *et al.*

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

Efficiency functions f - local to global

LOCAL FORMULATIONS:

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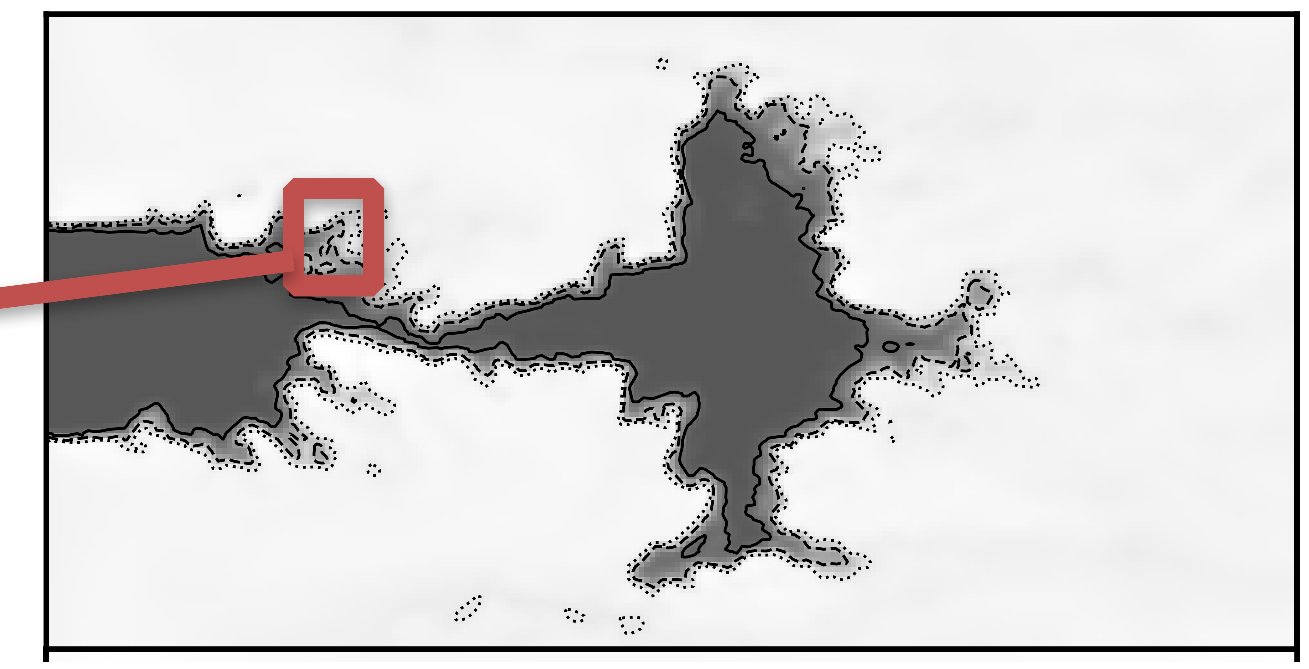


DYNAMIC FORMULATIONS:

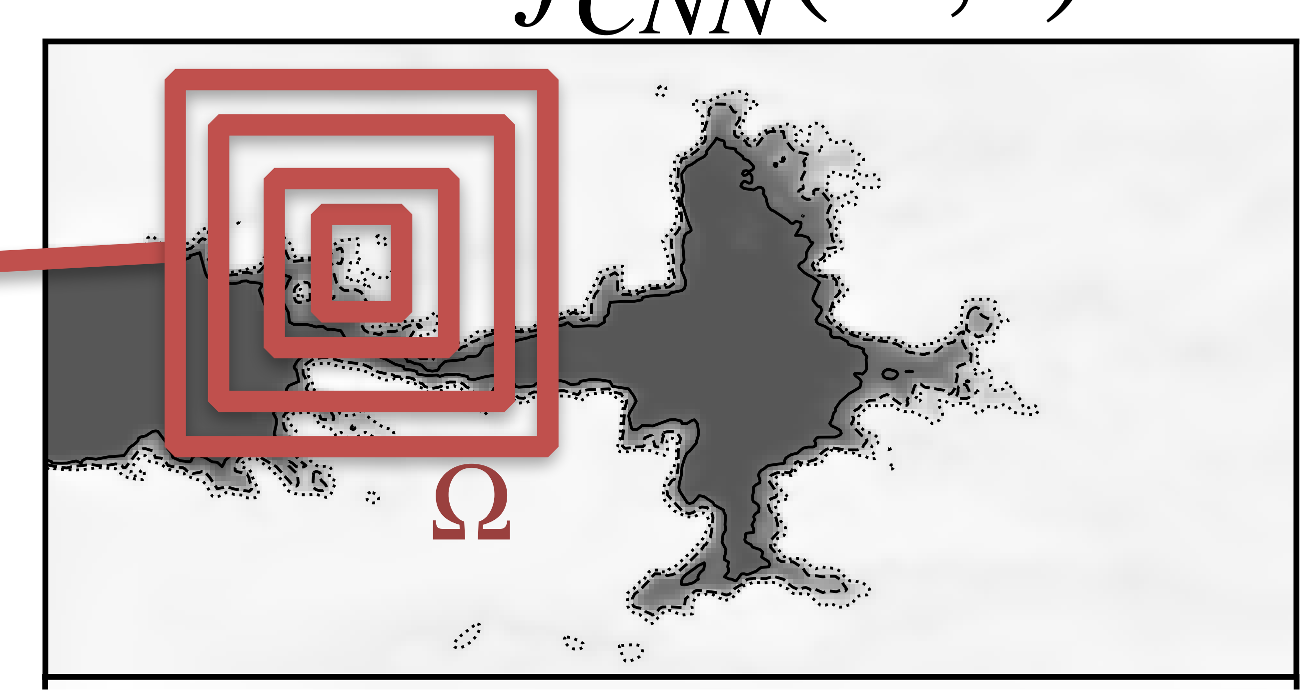
2011 - Wang *et al.*

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

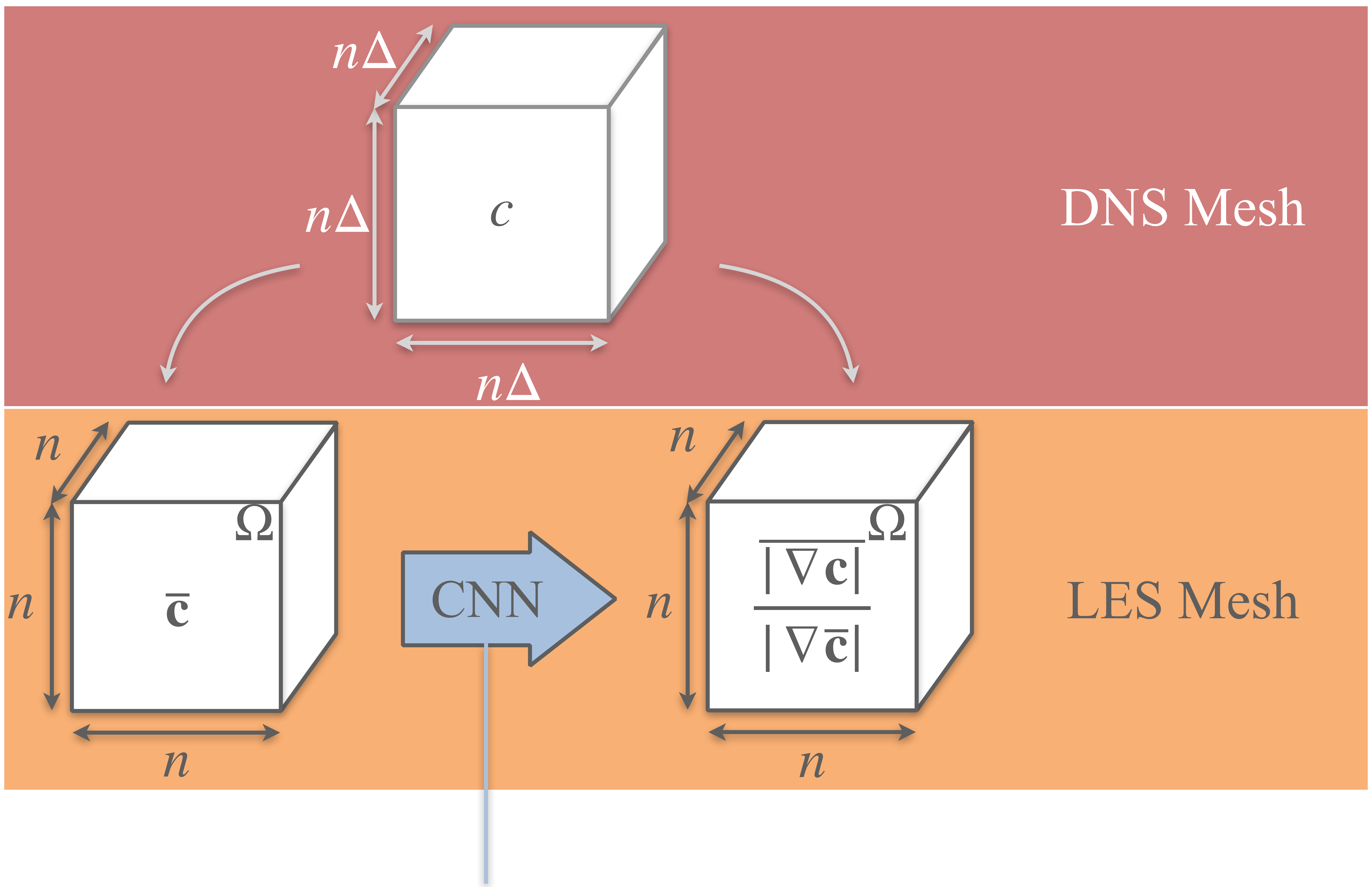
CNN FORMULATION:

2019 - Lapeyre *et al.*

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



Building the dataset



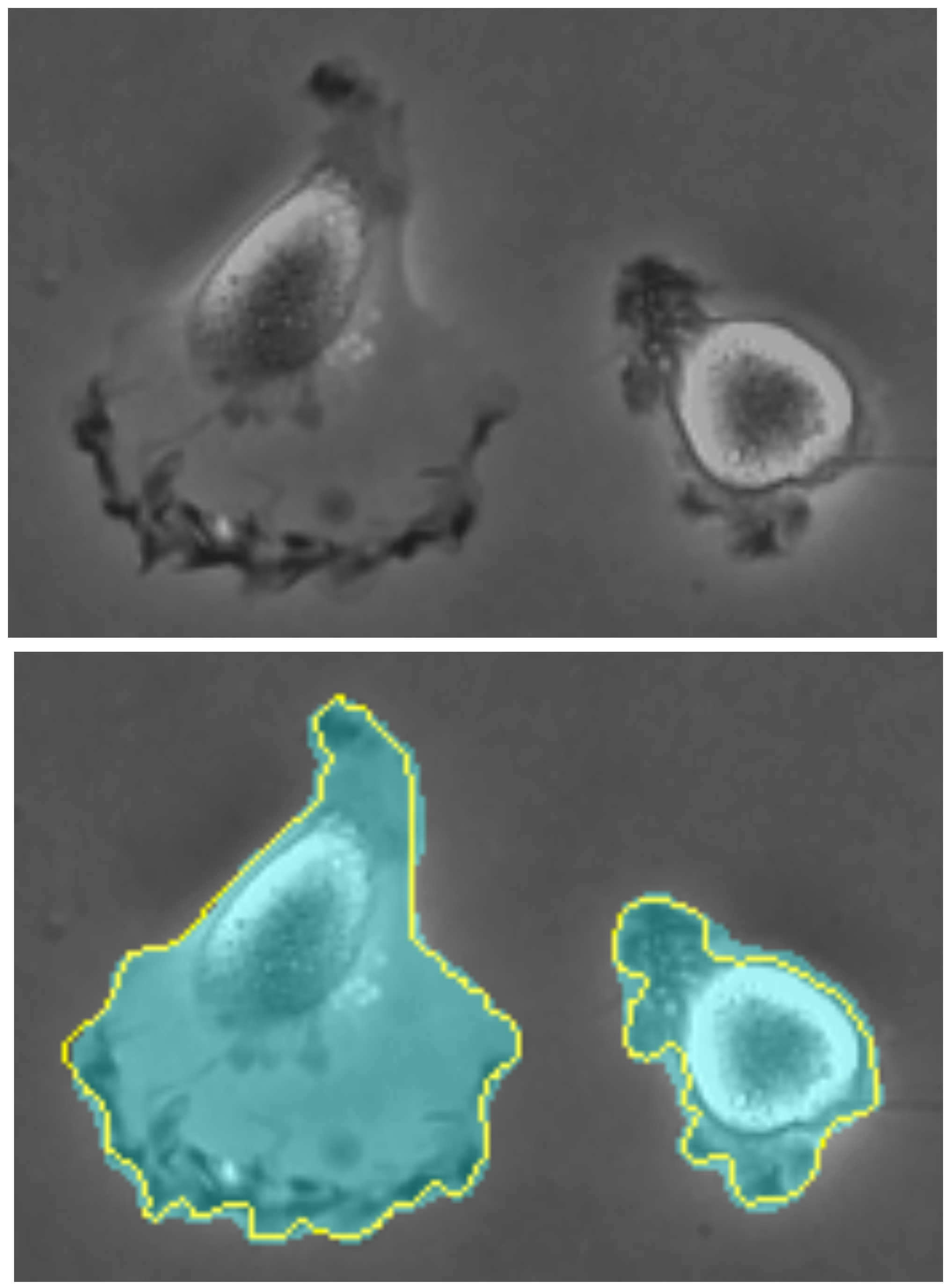
Convolutional neural network

Gaussian filtering equivalent to flame thickening Δ

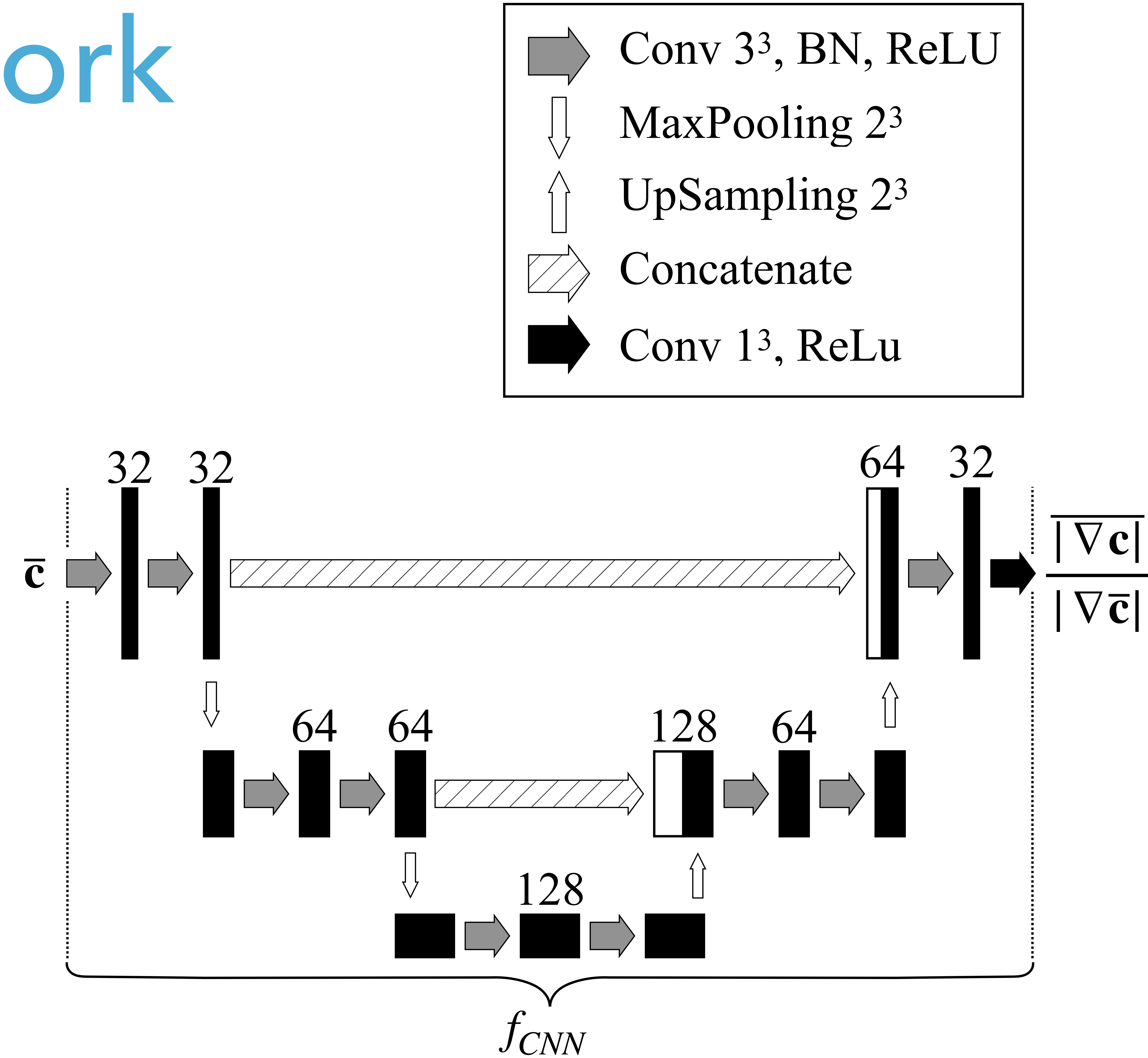
$$F_\Delta(n) = \begin{cases} e^{-\frac{1}{2}\left(\frac{n}{\sigma}\right)^2} & \text{if } n \in [1,N] \\ 0 & \text{otherwise} \end{cases}$$

Neural network

Input



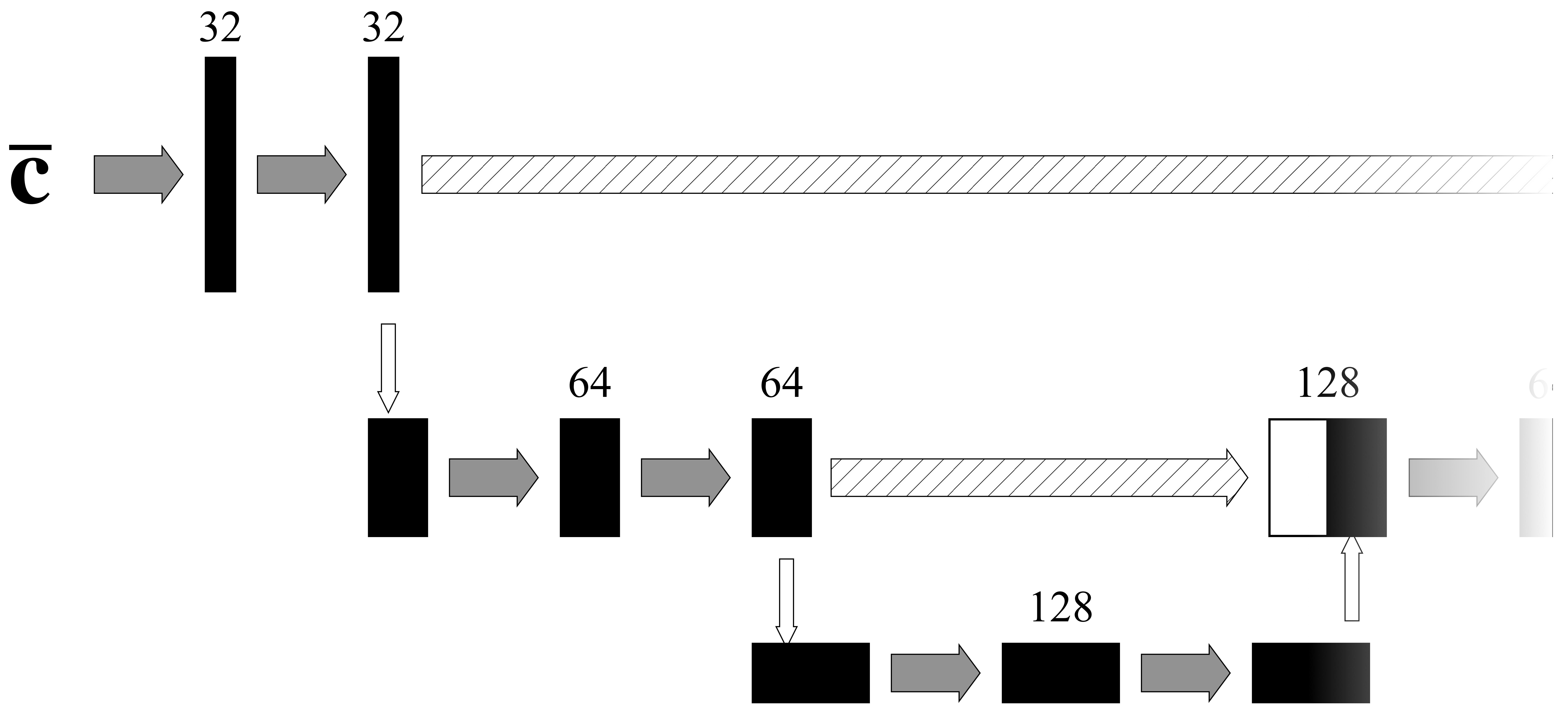
Segmented image



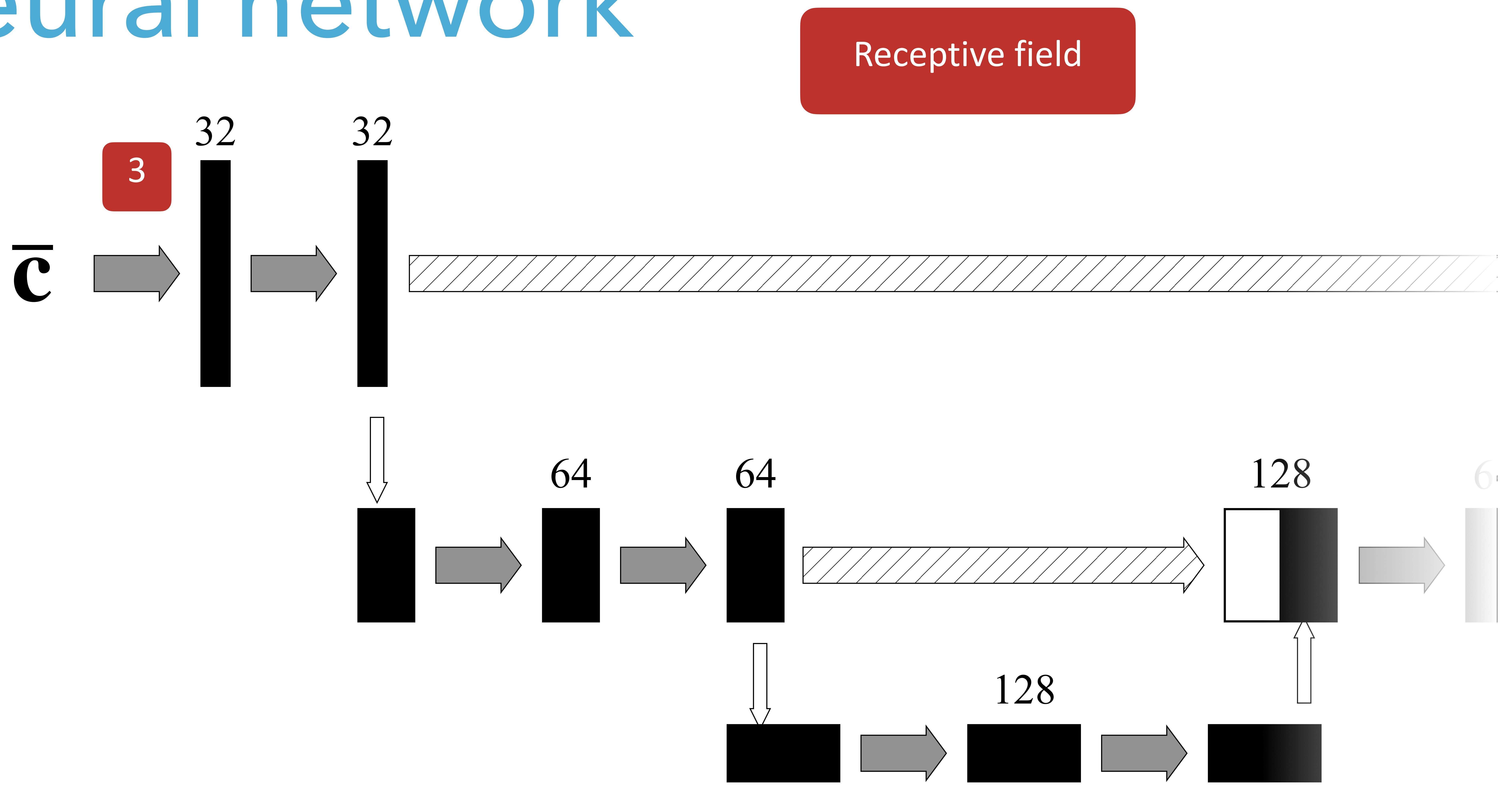
Architecture is adapted from a medical image segmentation network [9]

Ronneberger, O., Fischer, P., & Brox, T. (2015, October). U-net: Convolutional networks for biomedical image segmentation. In *International Conference on Medical image computing and computer-assisted intervention* (pp. 234-241). Springer, Cham.

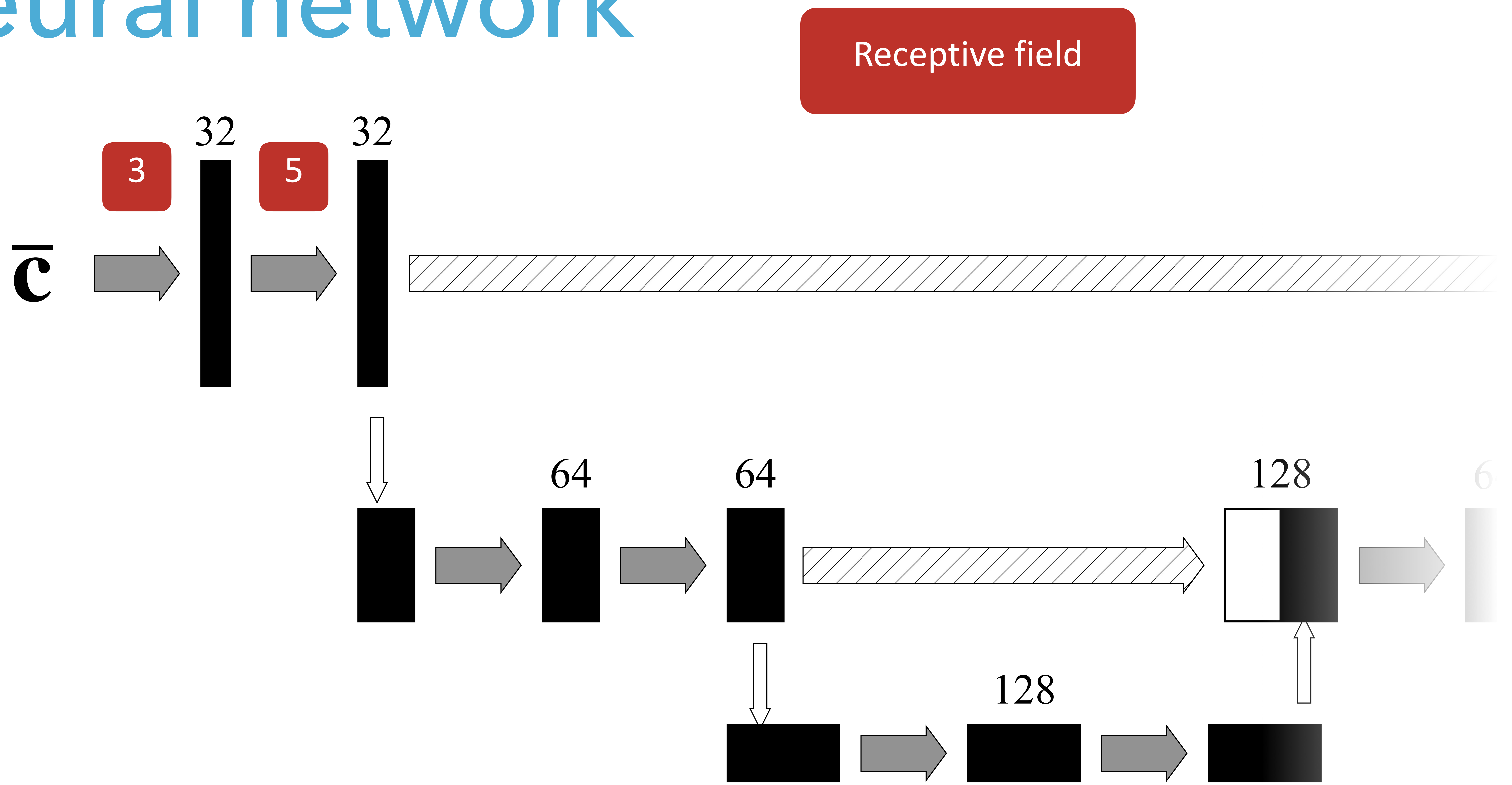
Neural network



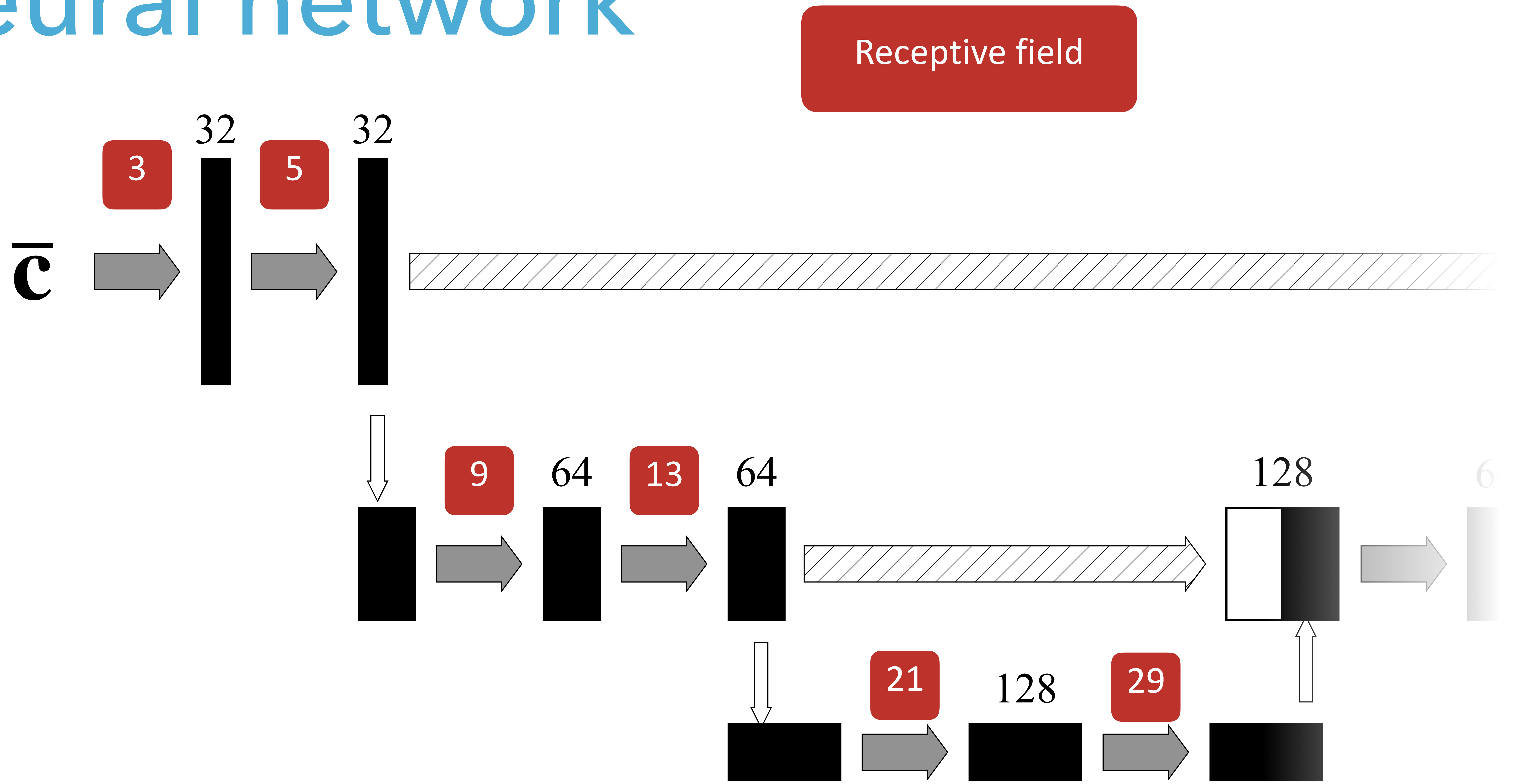
Neural network



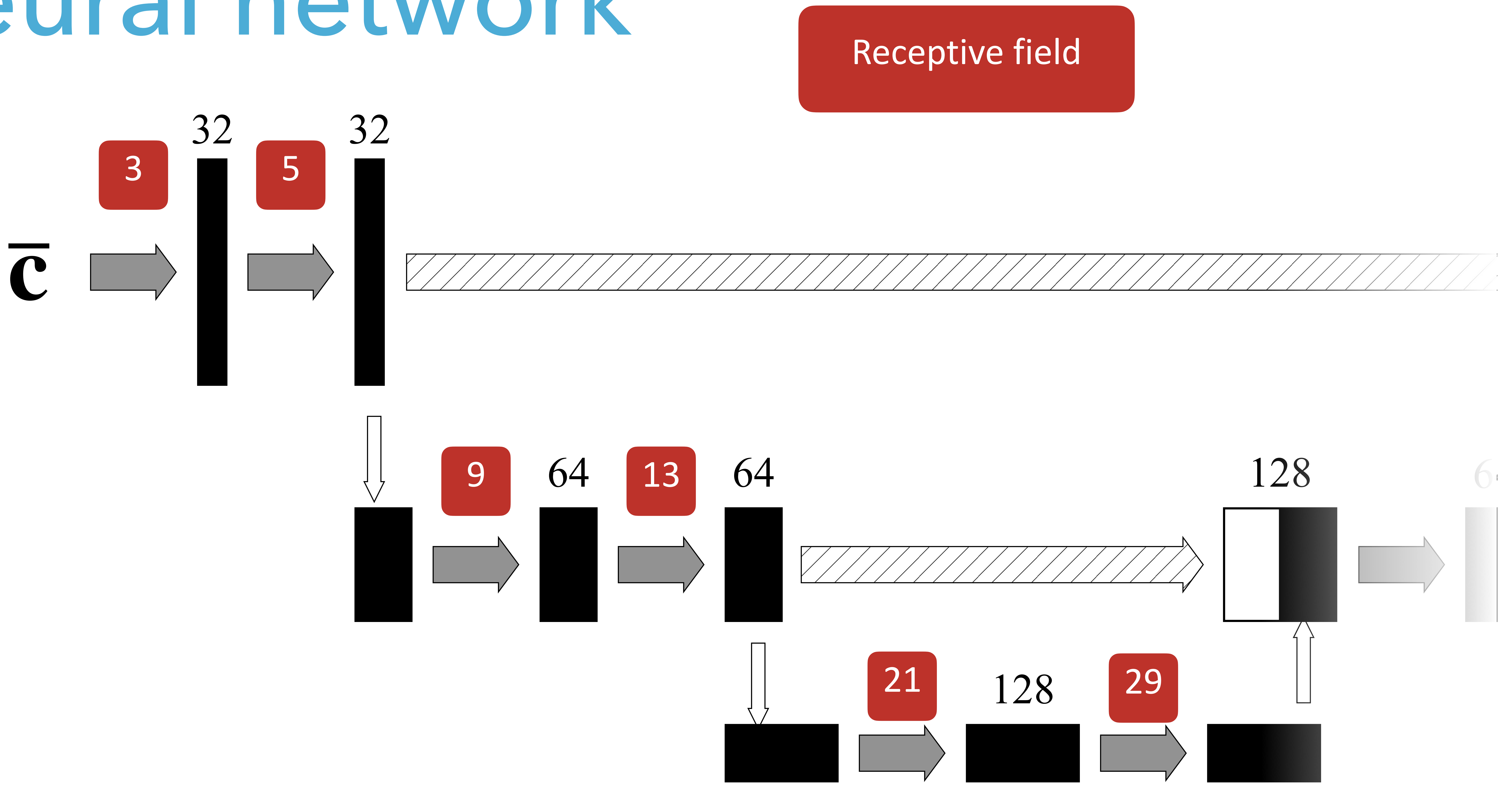
Neural network



Neural network



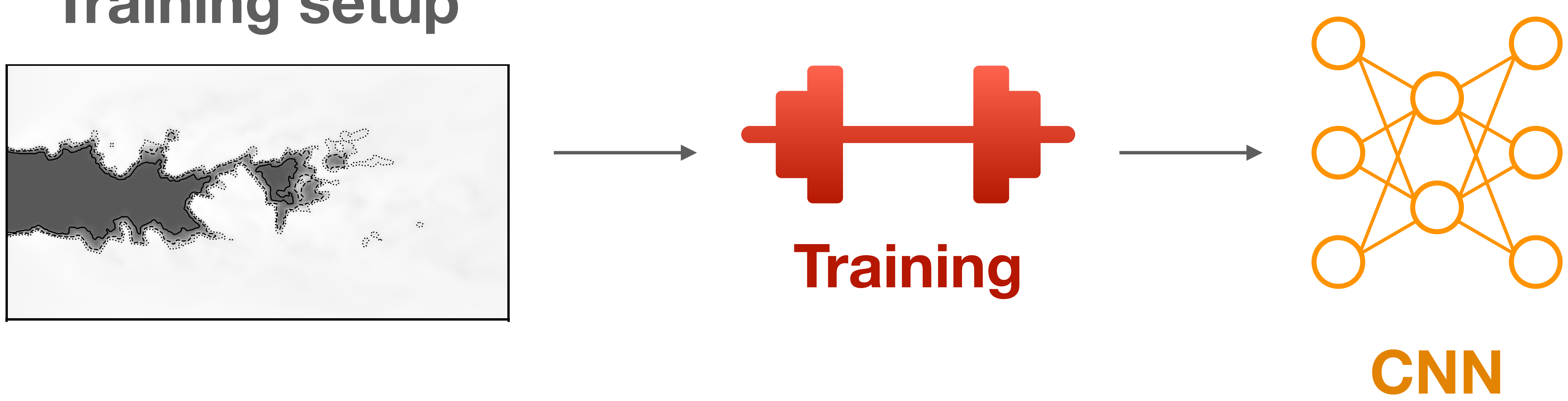
Neural network



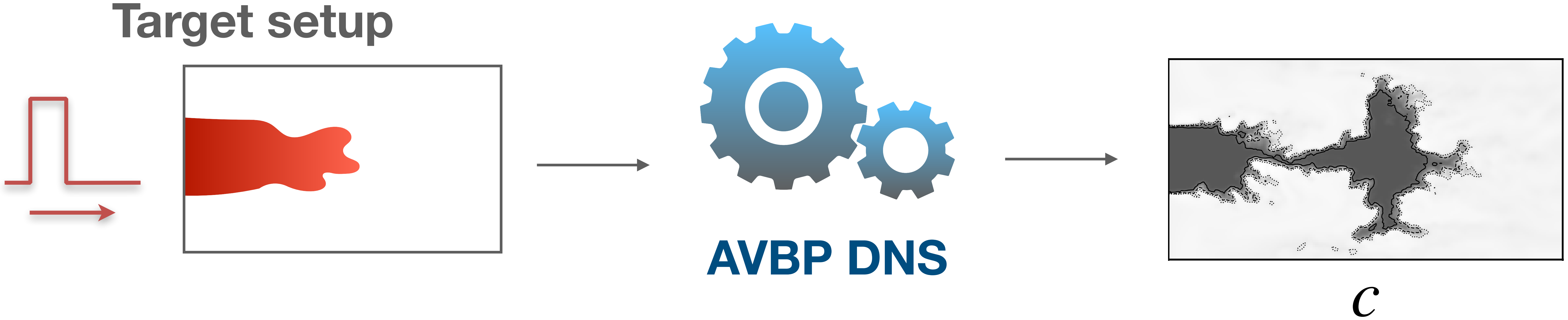
- Network is trained on increasing size inputs: 8^3, then 16^3, and finally 32^3.

A priori strategy

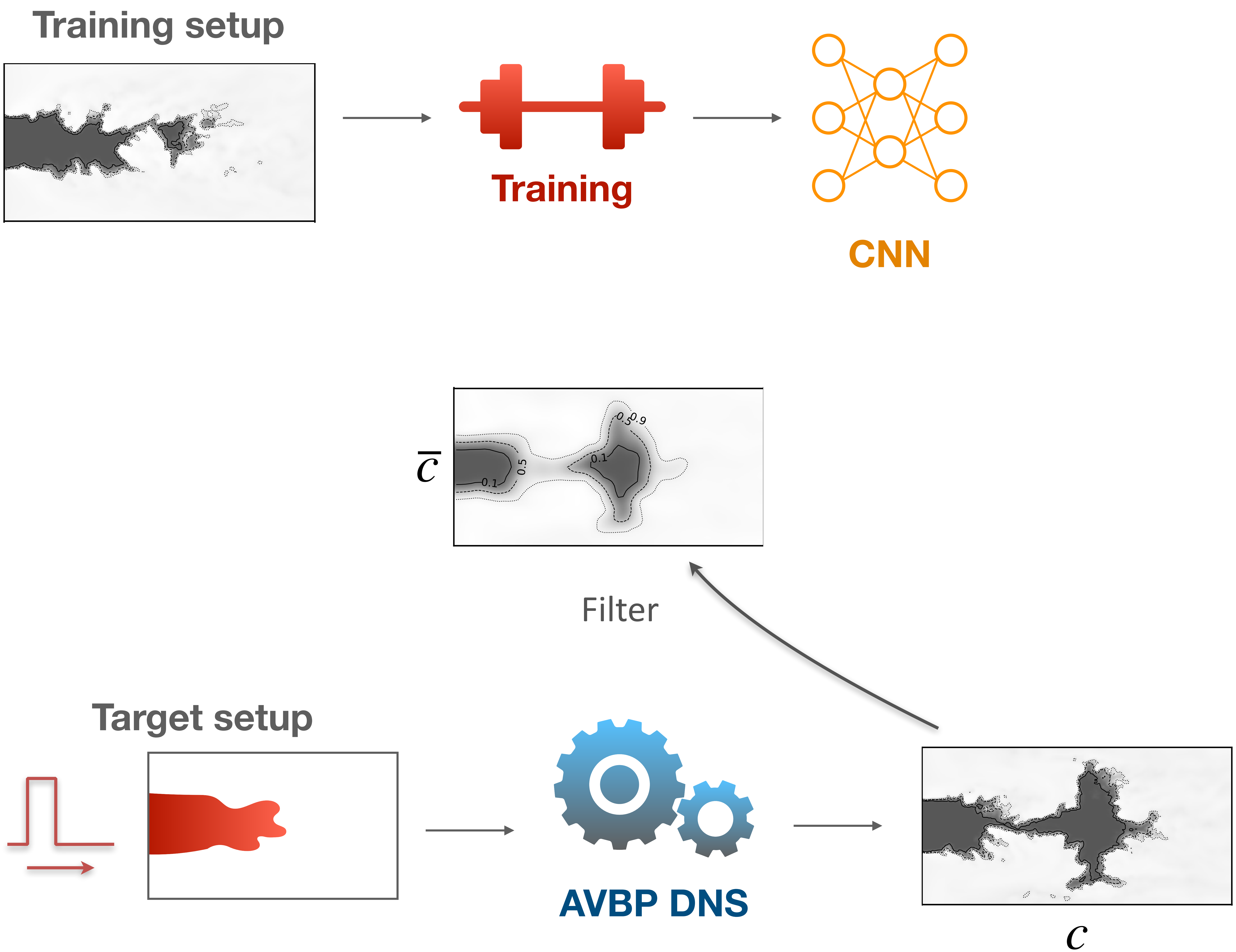
Training setup



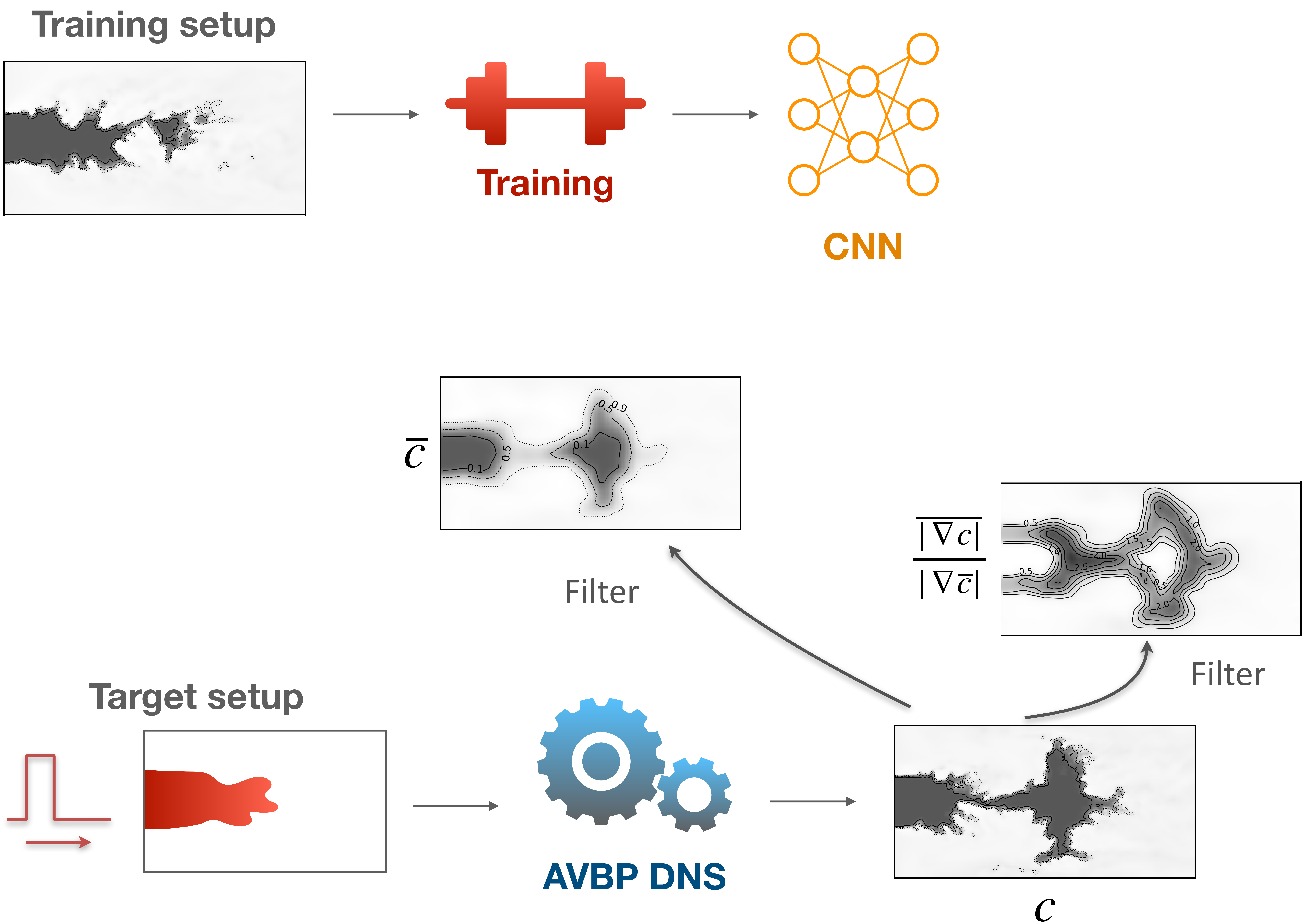
Target setup



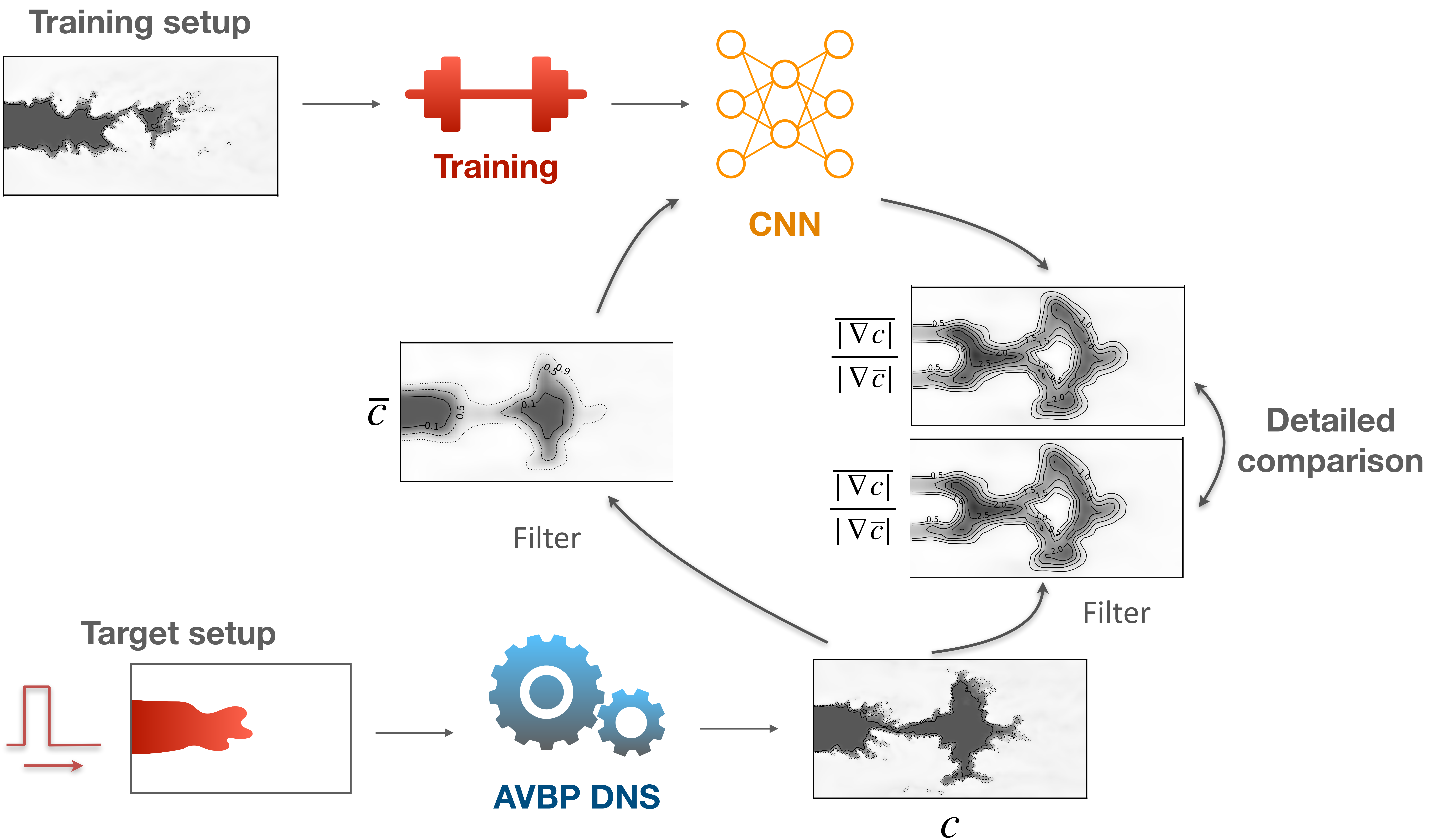
A priori strategy



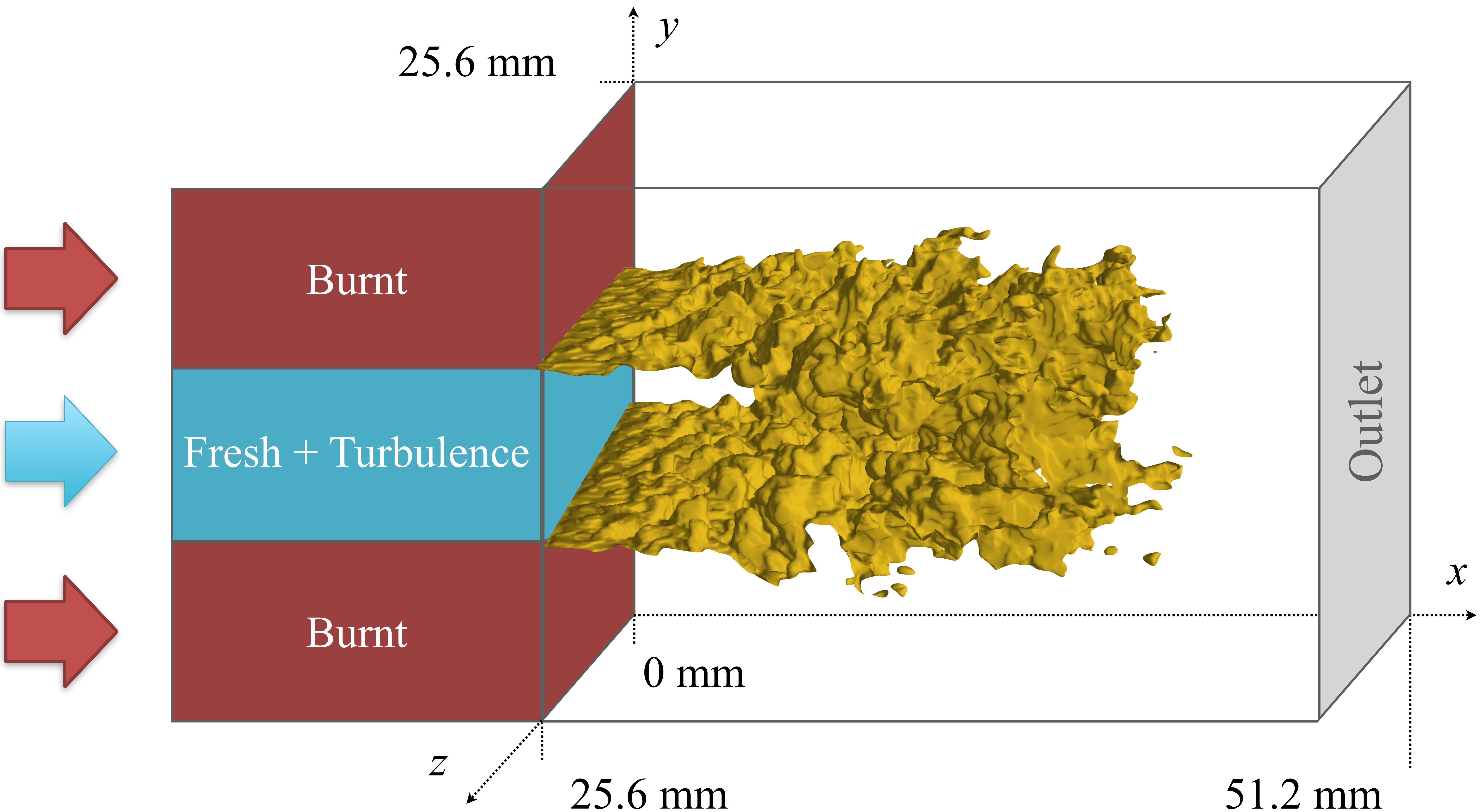
A priori strategy



A priori strategy



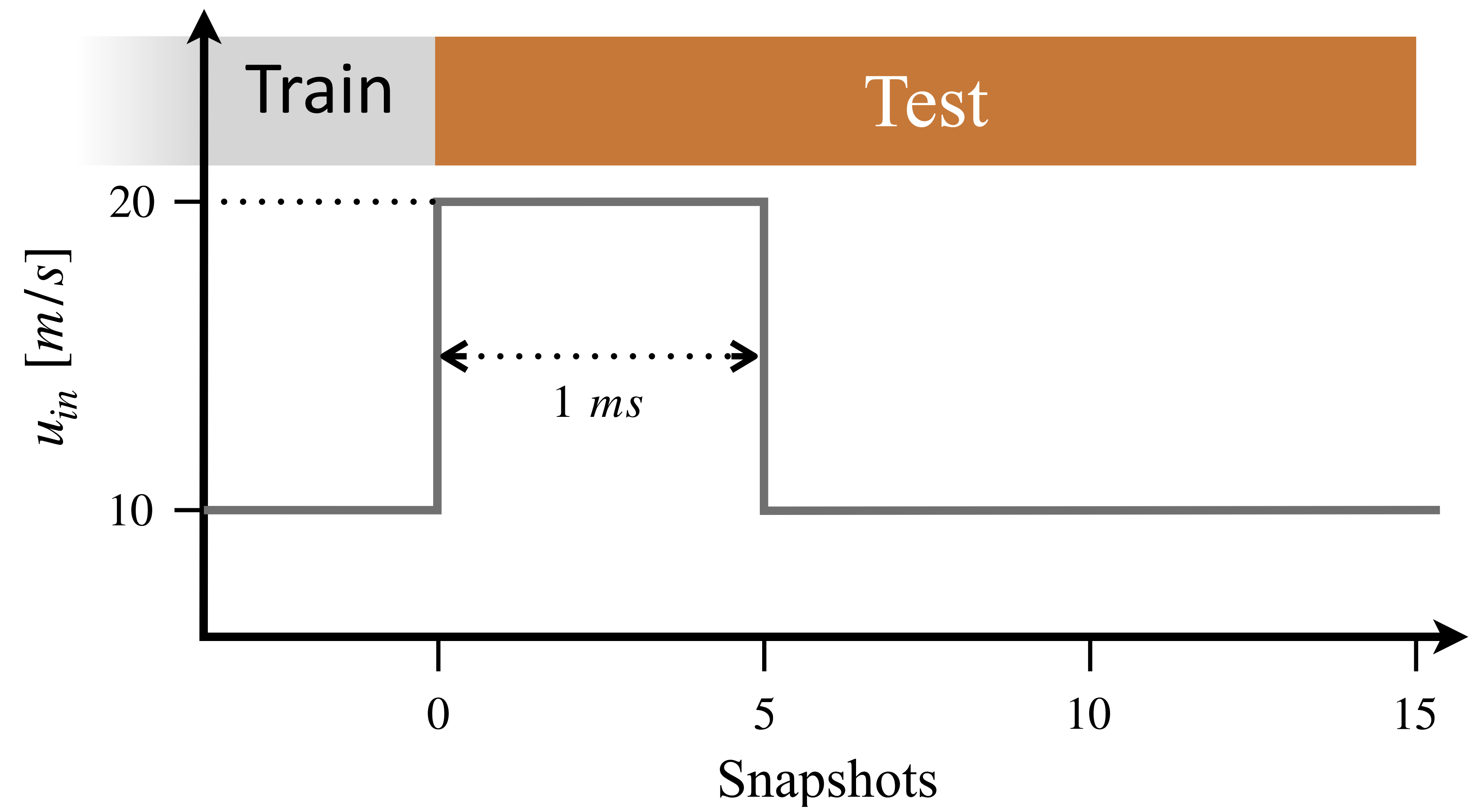
DNS for training

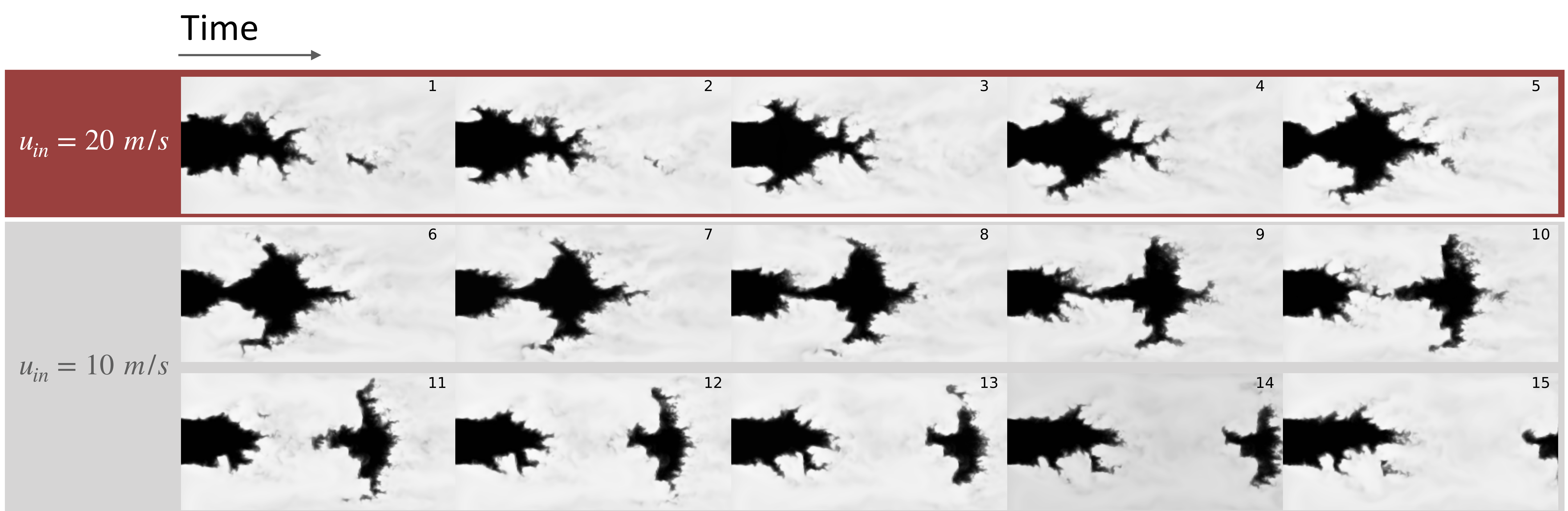


Similar to: Bell, J. B., Day, M. S., Grcar, J. F., Lijewski, M. J., Driscoll, J. F., & Filatyev, S. A. (2007). Numerical simulation of a laboratory-scale turbulent slot flame. *Proceedings of the combustion institute*, *31*(1), 1299-1307.

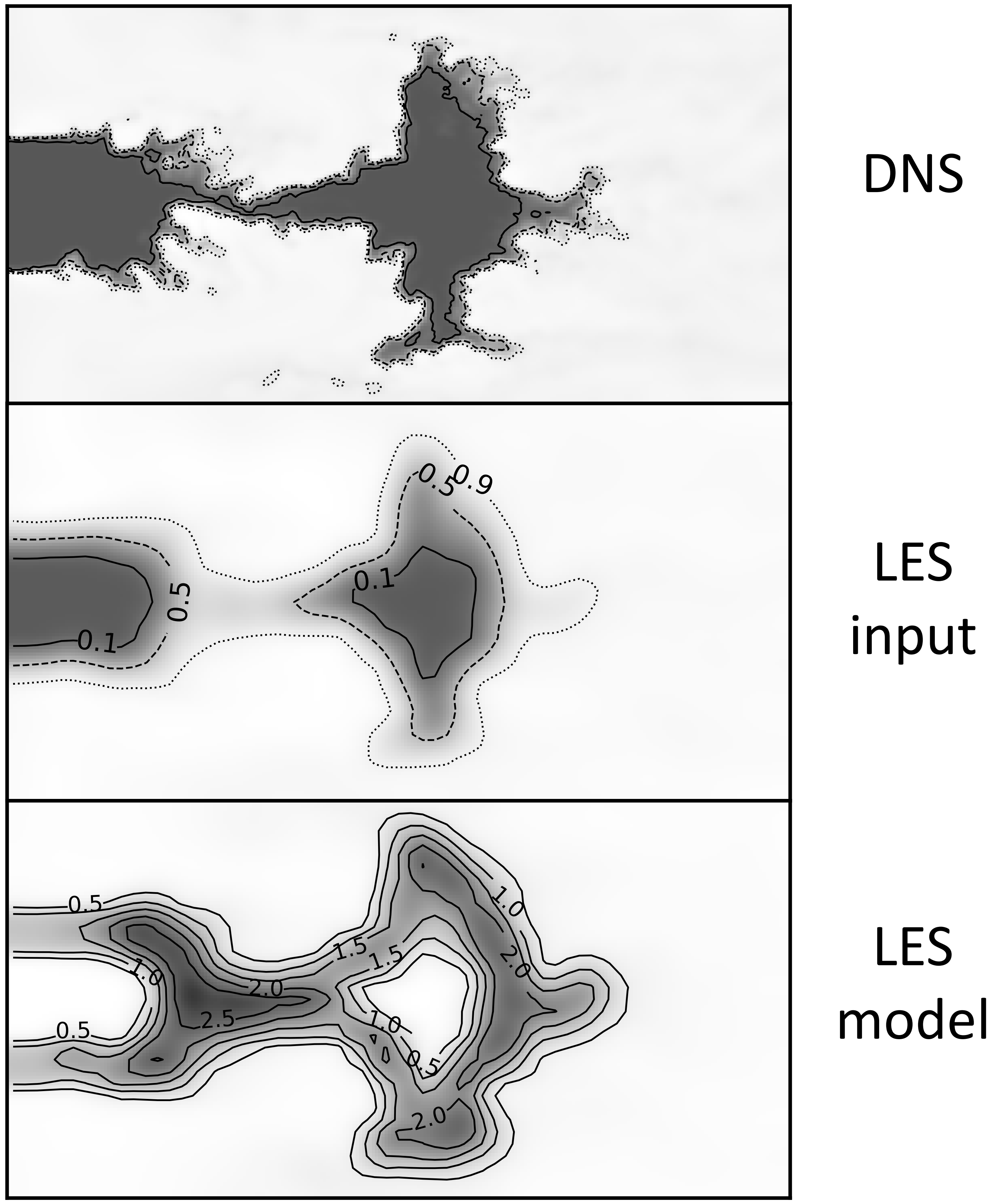
A priori test

- Test case: unsteady flow dynamics

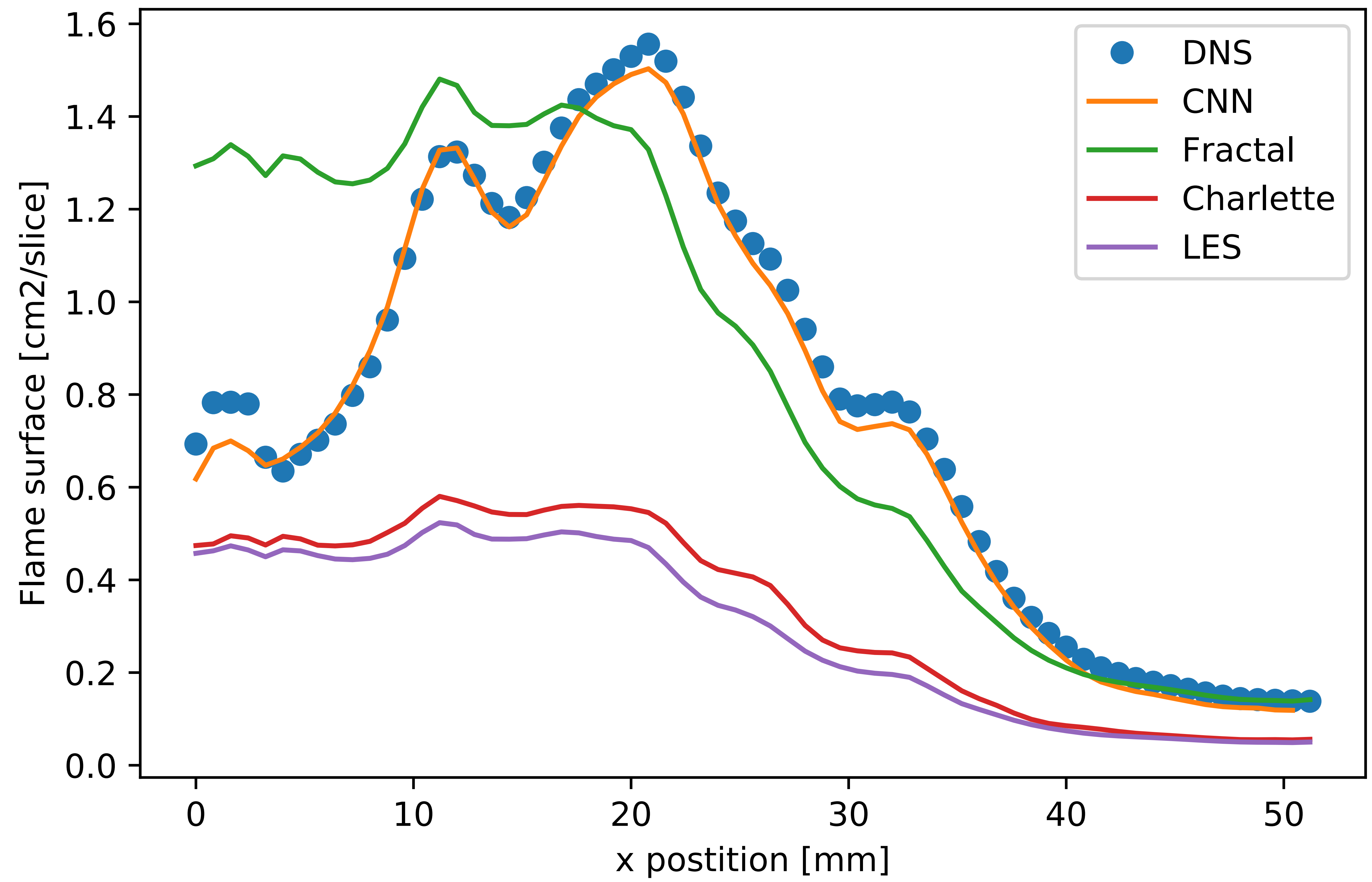




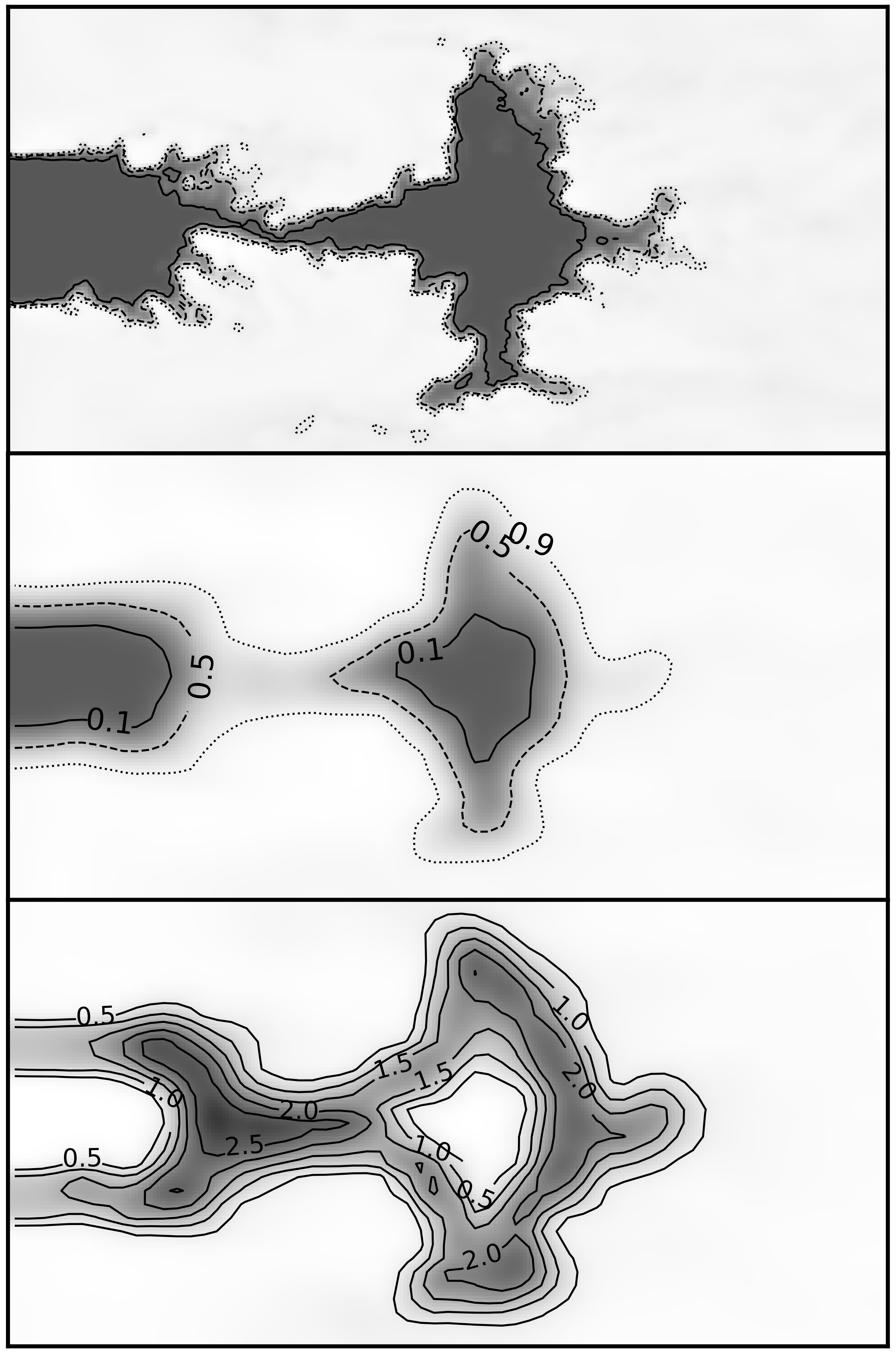
A priori results



Example snapshot during test



A priori results

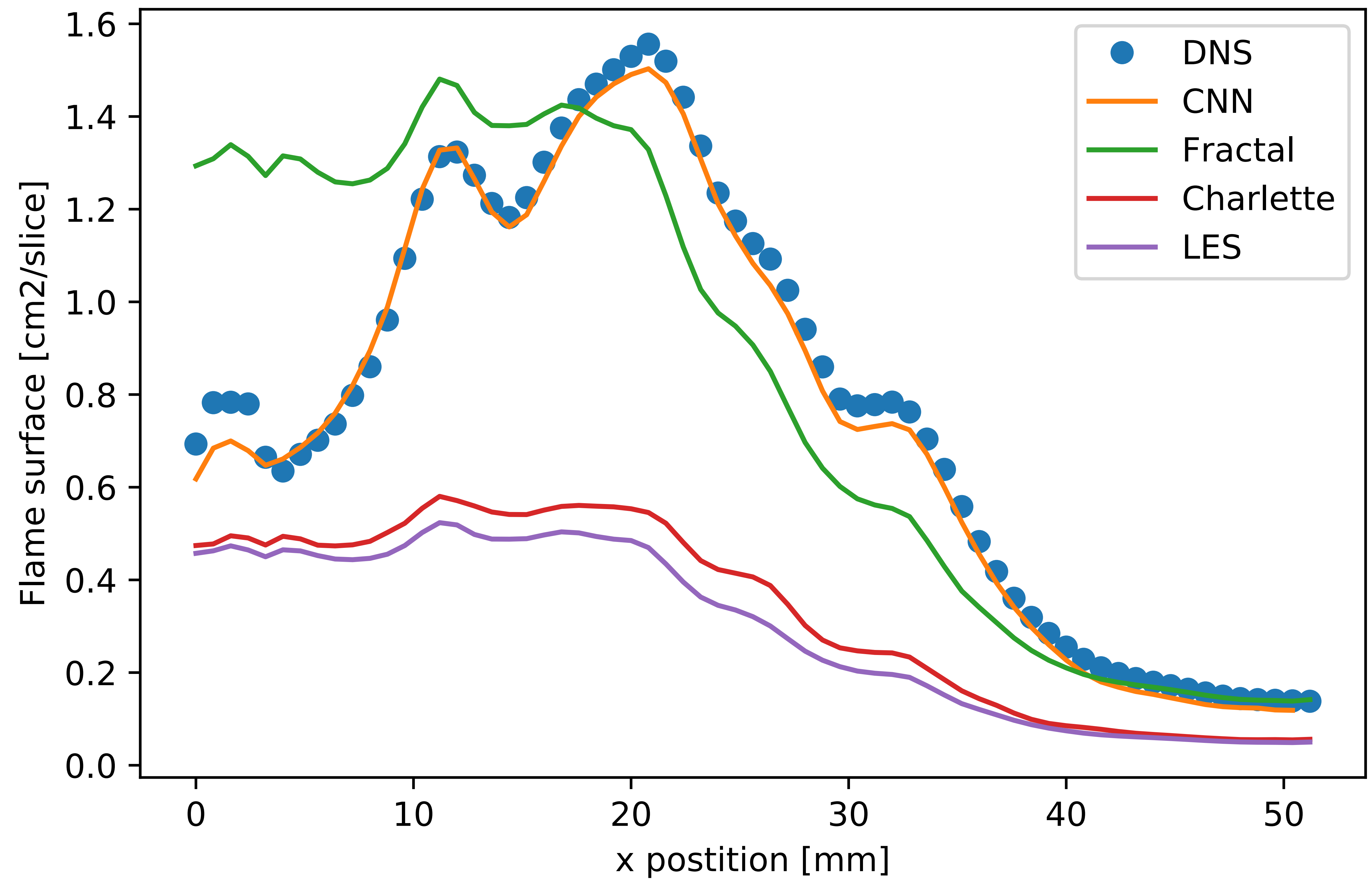


DNS

LES input

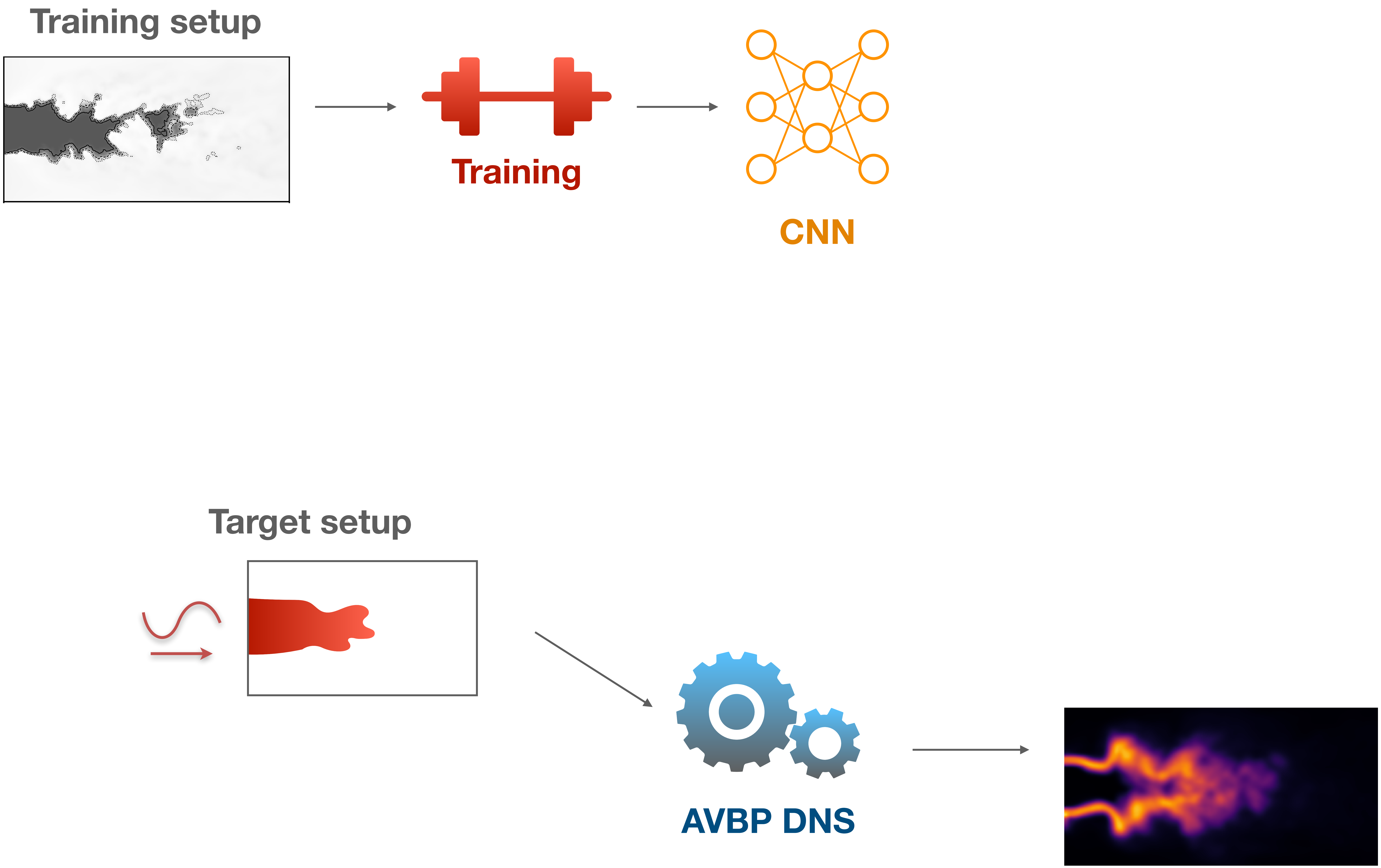
LES model

Example snapshot during test

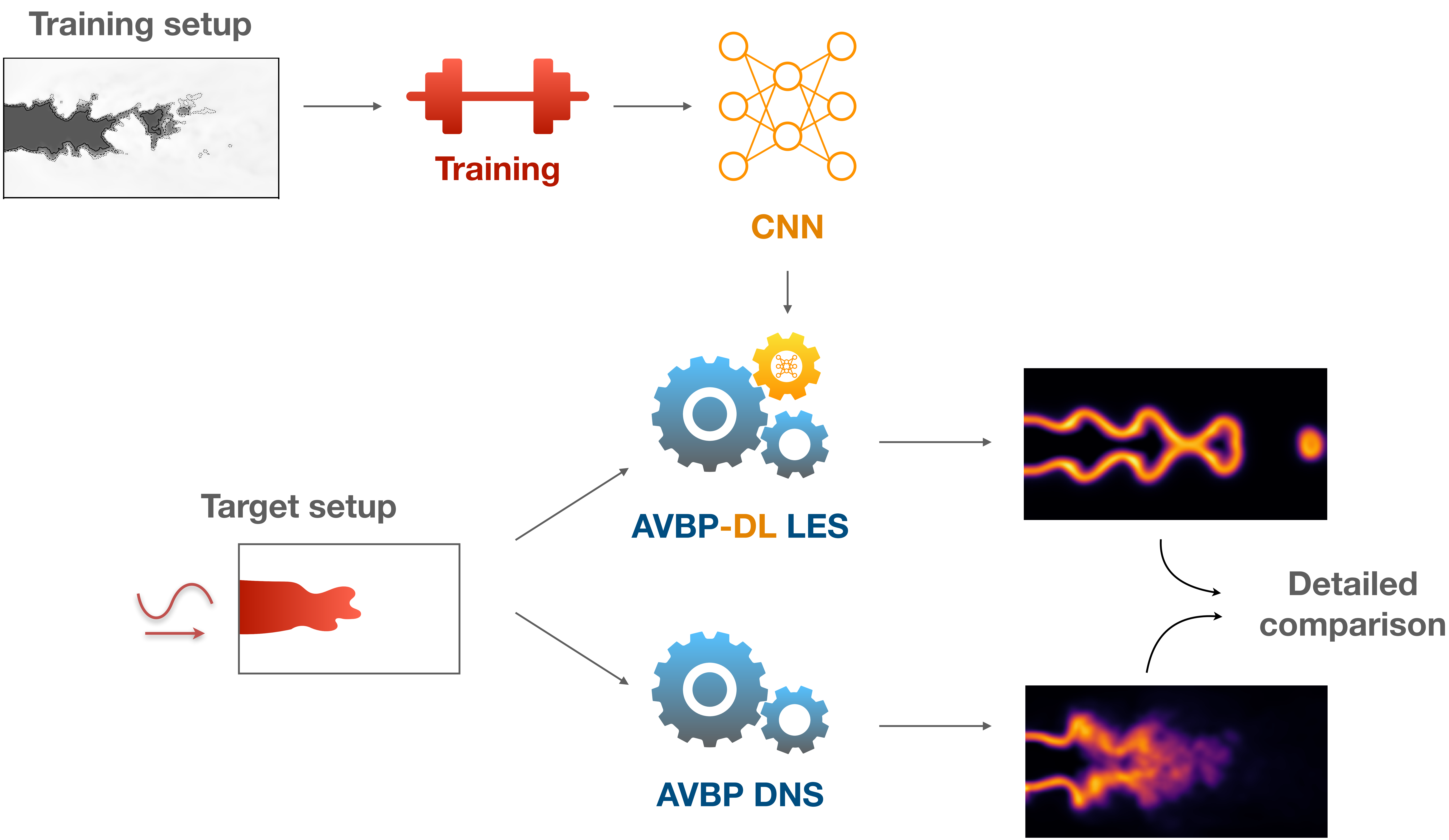


Excellent agreement compared to litterature.

A posteriori strategy



A posteriori strategy



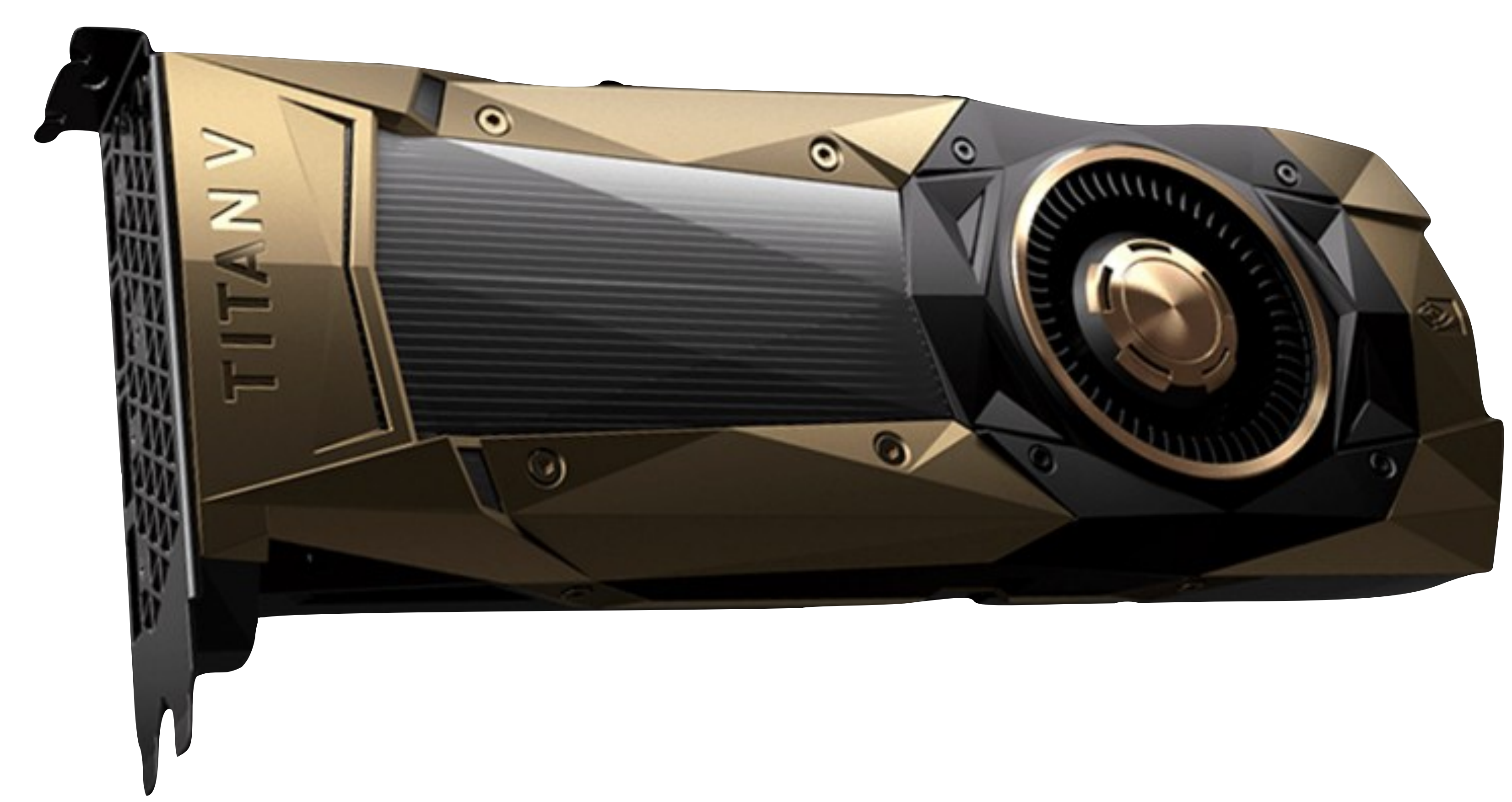
Tests a posteriori in LES:

- The CNN can be integrated in AVBP code to compute flame wrinkling but the inference time (evaluation of f_{CNN}) becomes too long on CPU: GPUs are much better
- -> hybrid architecture is needed

CPU : Navier-Stokes solver
(AVBP)

$\overline{c}$

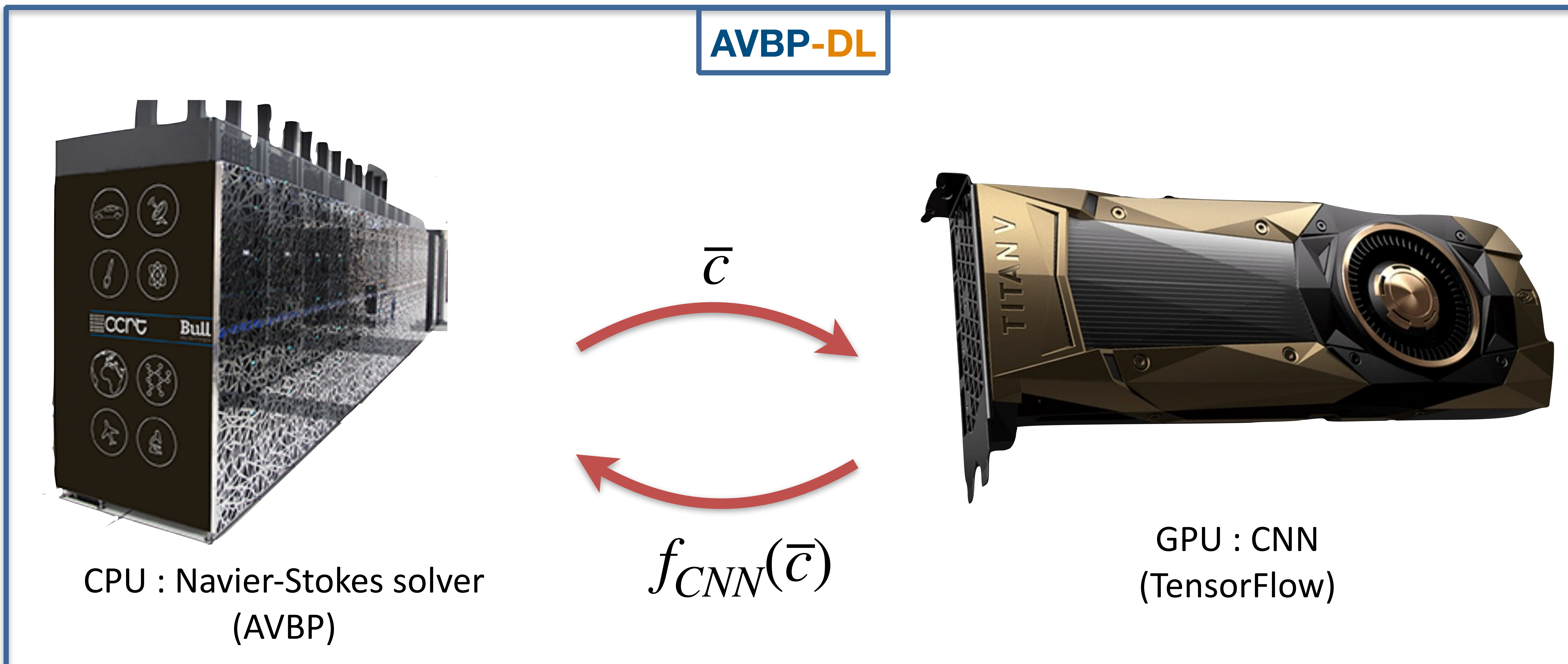
$f_{CNN}(\overline{c})$



GPU : CNN
(TensorFlow)

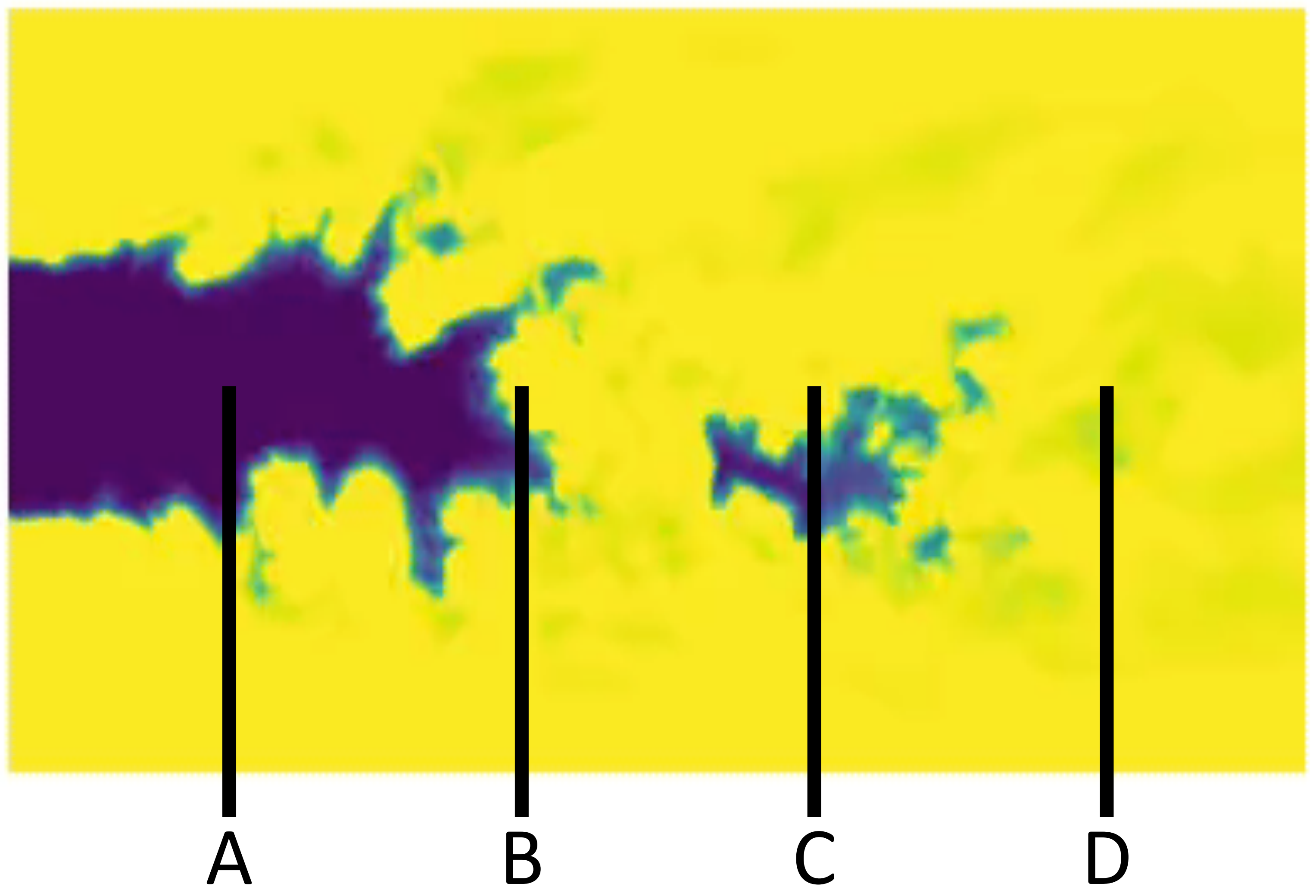
Tests a posteriori in LES:

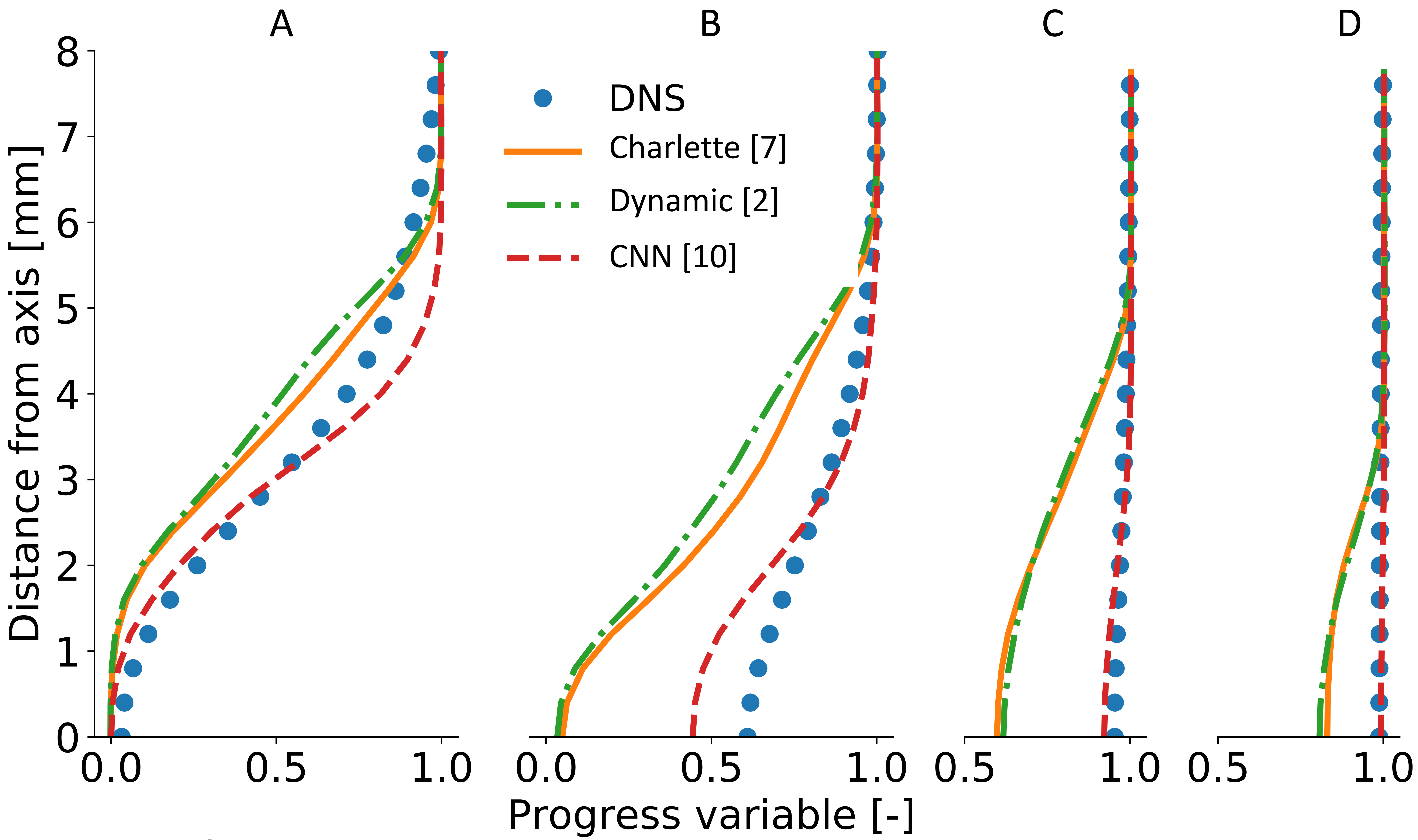
- The CNN can be integrated in AVBP code to compute flame wrinkling but the inference time (evaluation of f_{CNN}) becomes too long on CPU: GPUs are much better
- -> hybrid architecture is needed



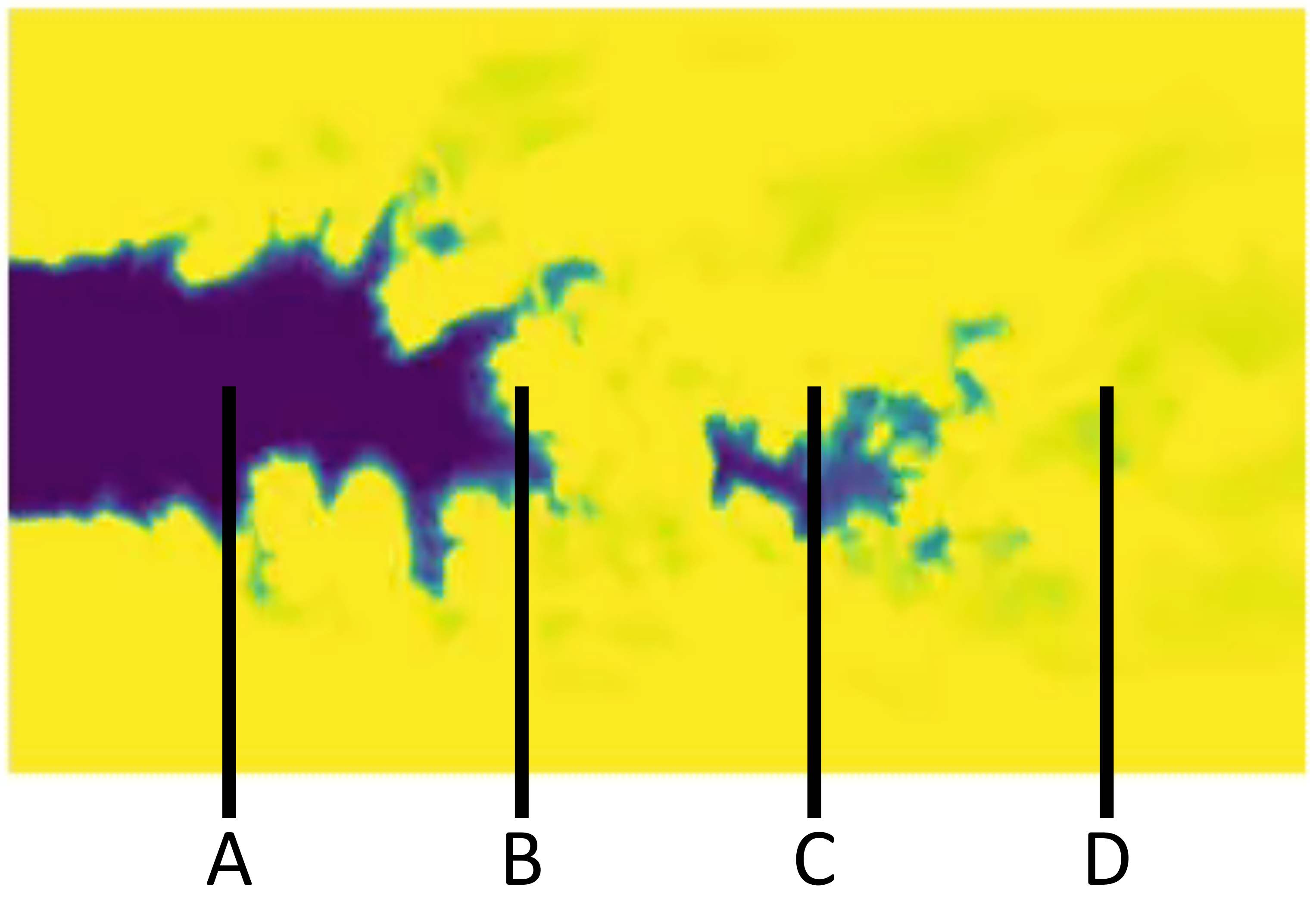
A posteriori results

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





A posteriori results



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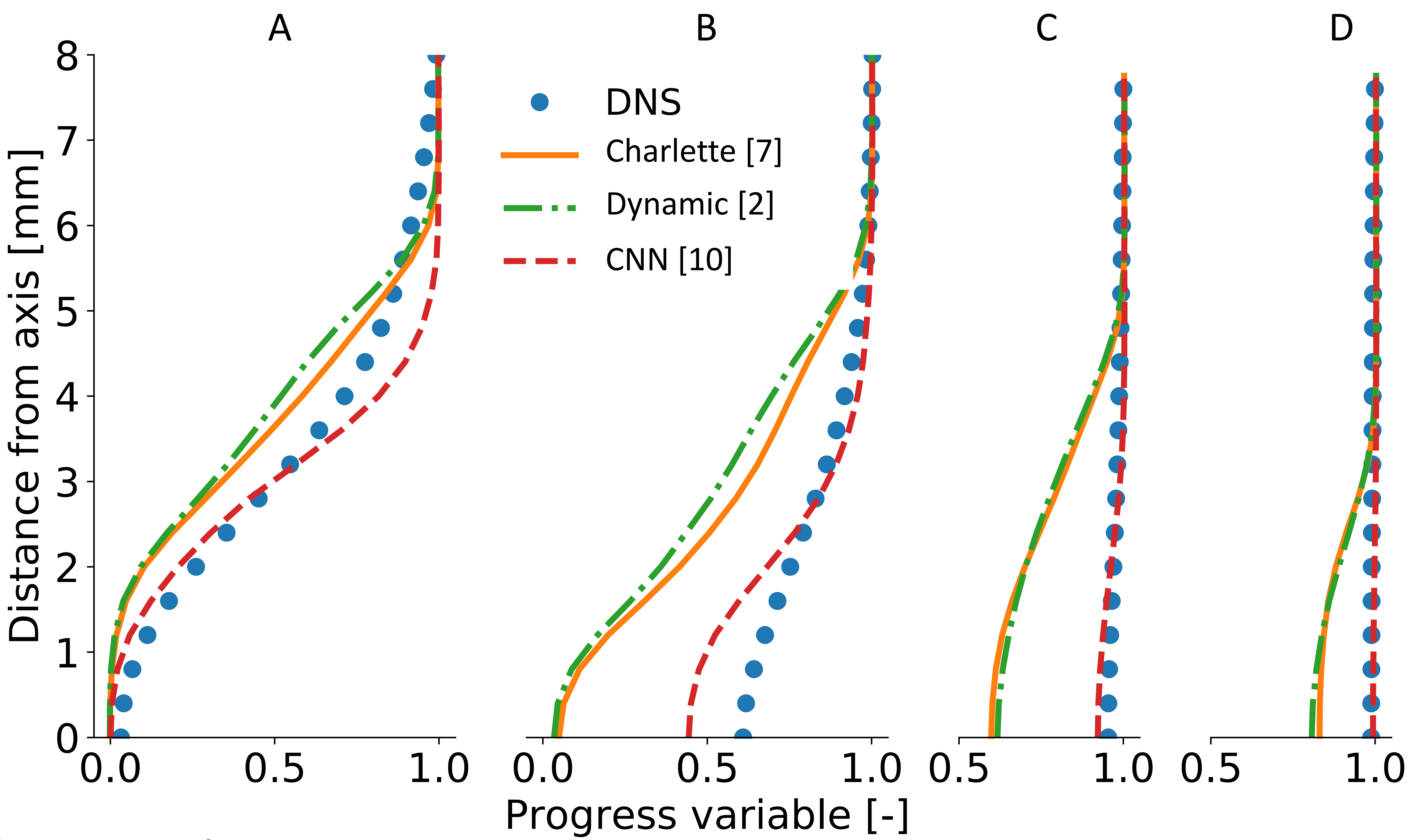
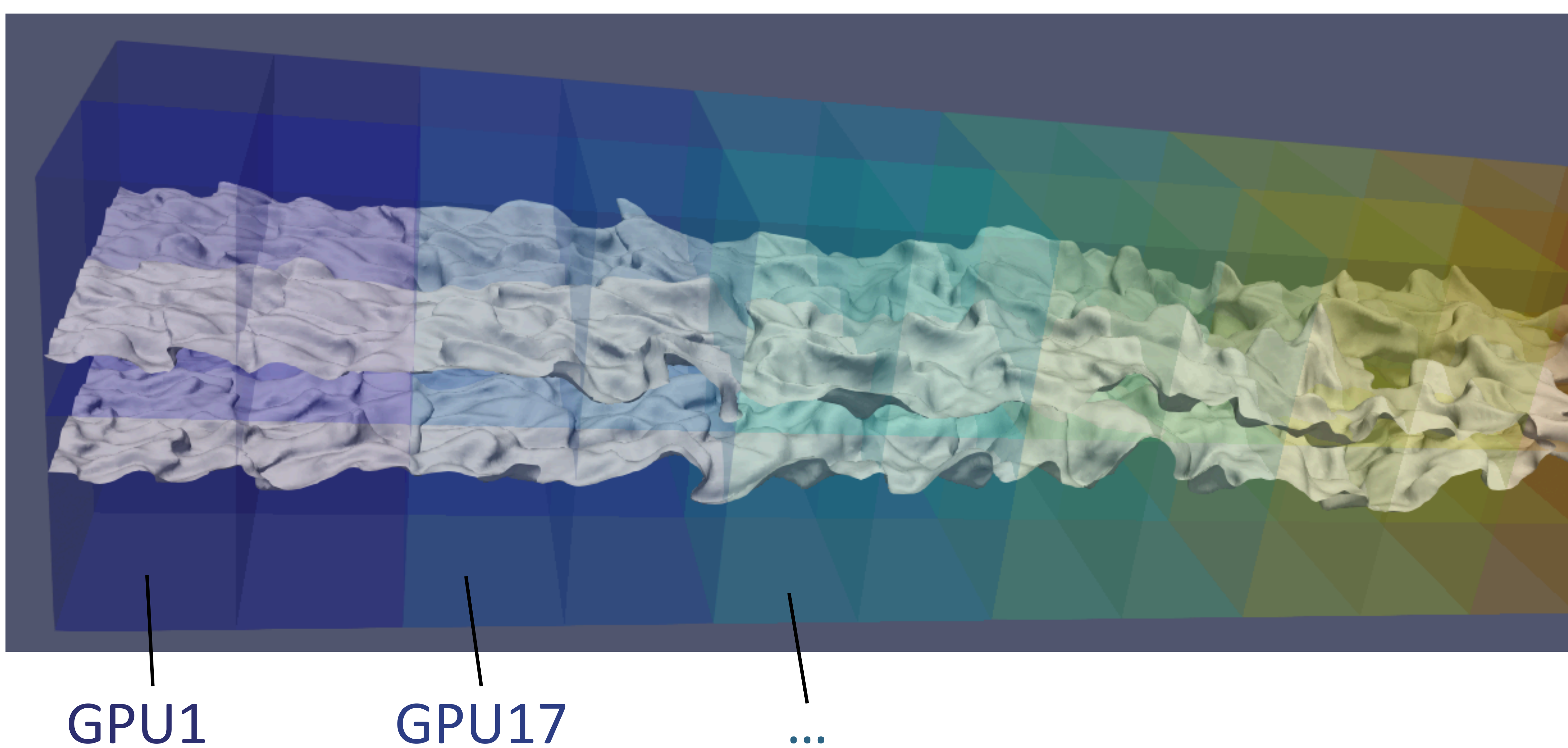


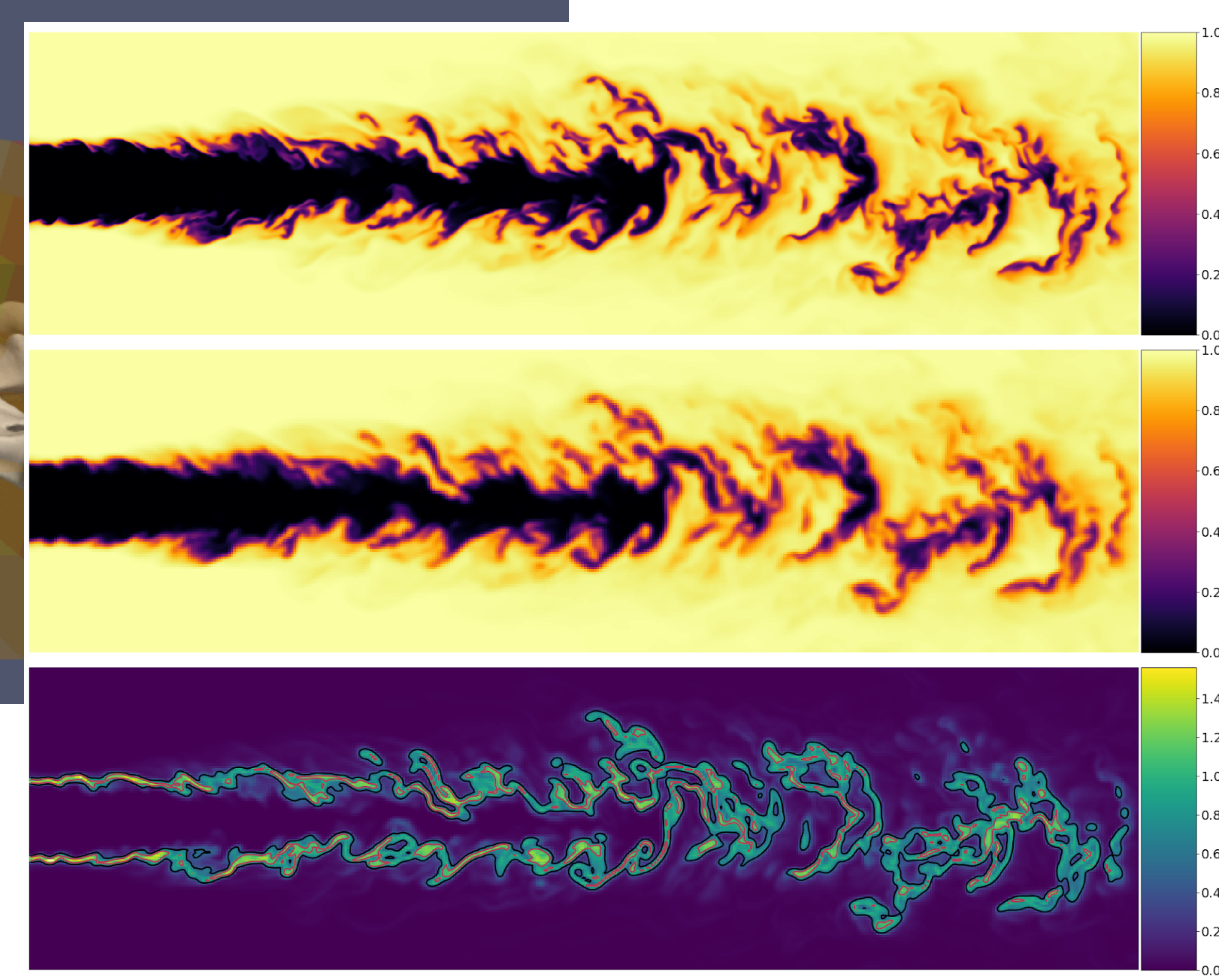
JZ Grand Challenge

- We target large scale LES => hybrid CPU/GPU and solver/neural network approach must scale to HPC
- 2019-2020: Jean Zay Grand Challenge

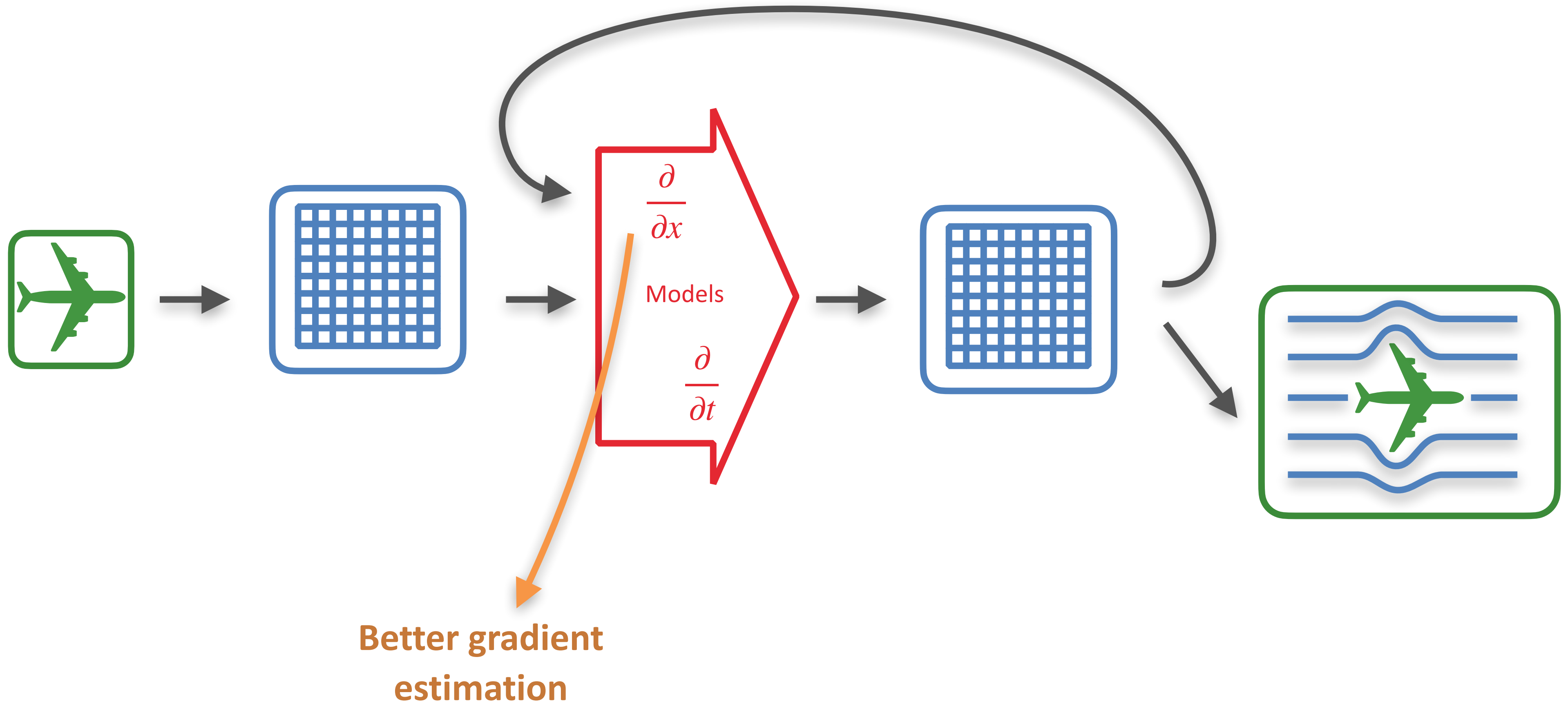
AVBP-DL: 2000 CPU + 64 GPU simulation on Jean Zay

V. Xing, A. Misdariis, G. Staffelbach, C. Lapeyre





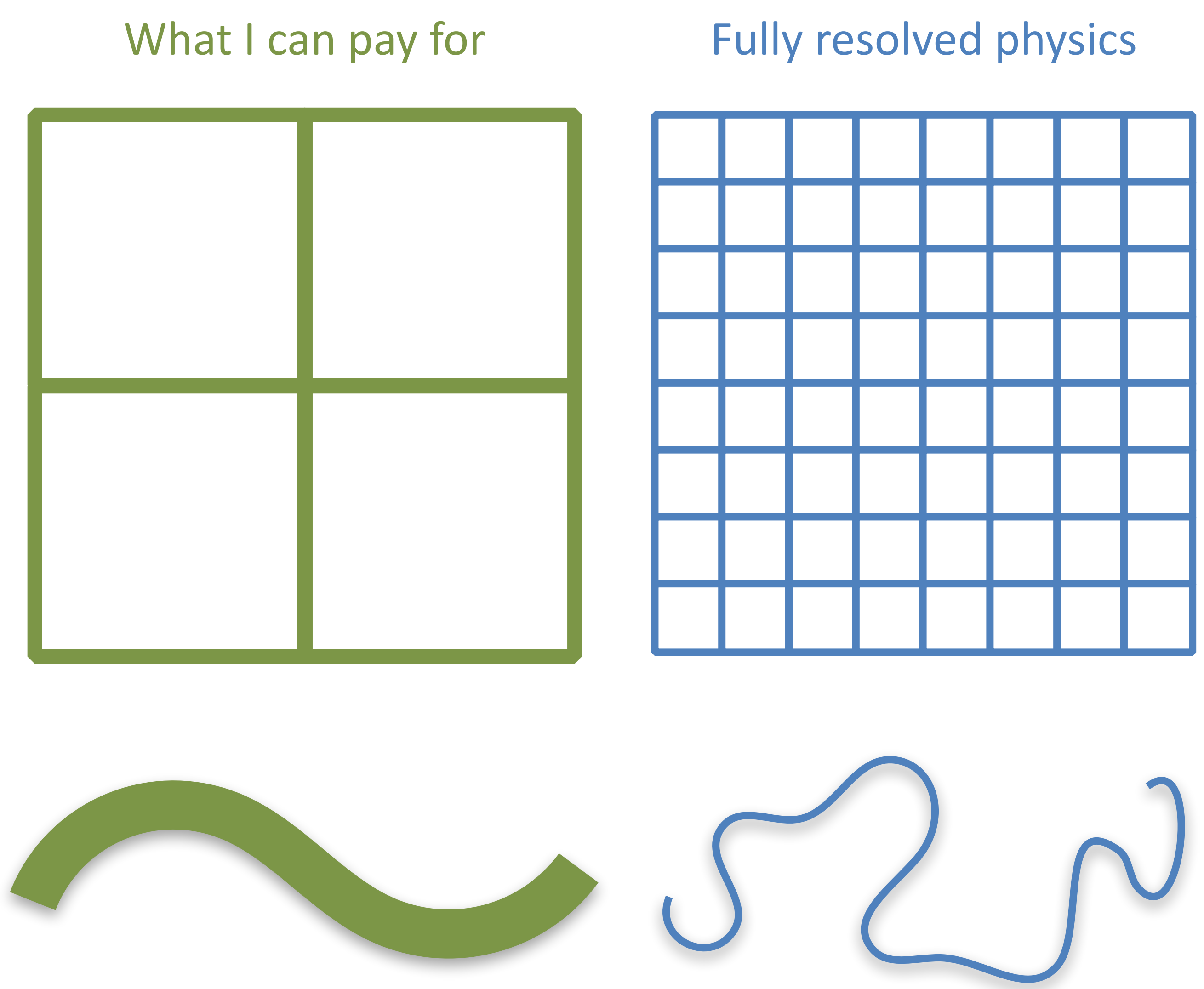
V. Xing (Ph.D. started 2019), supervised by C. Lapeyre, A. Misdariis, O. Vermorel & T. Poinsot



2. Data-driven discretization

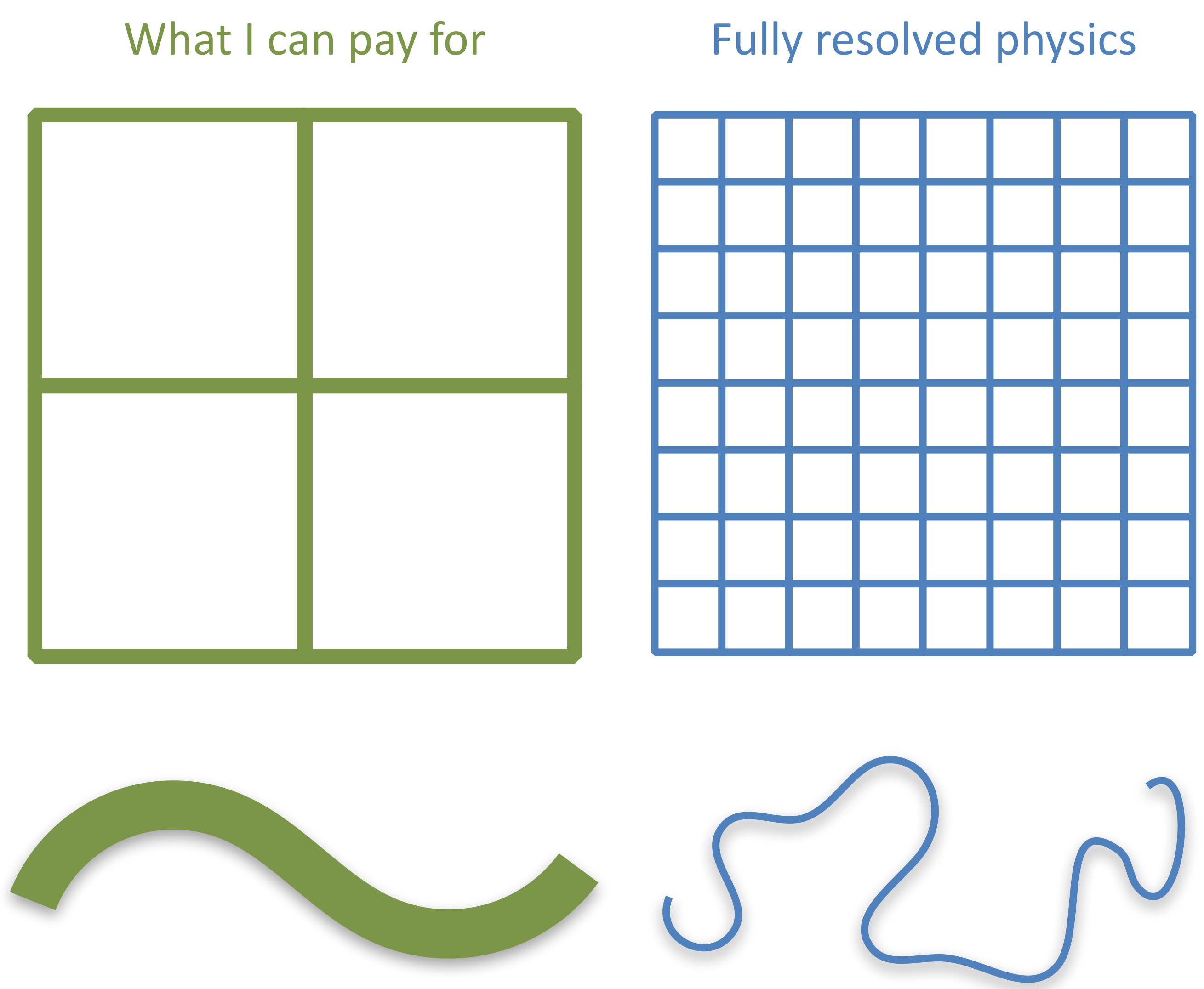
Ongoing PhD of Luciano Drozda, Cerfacs

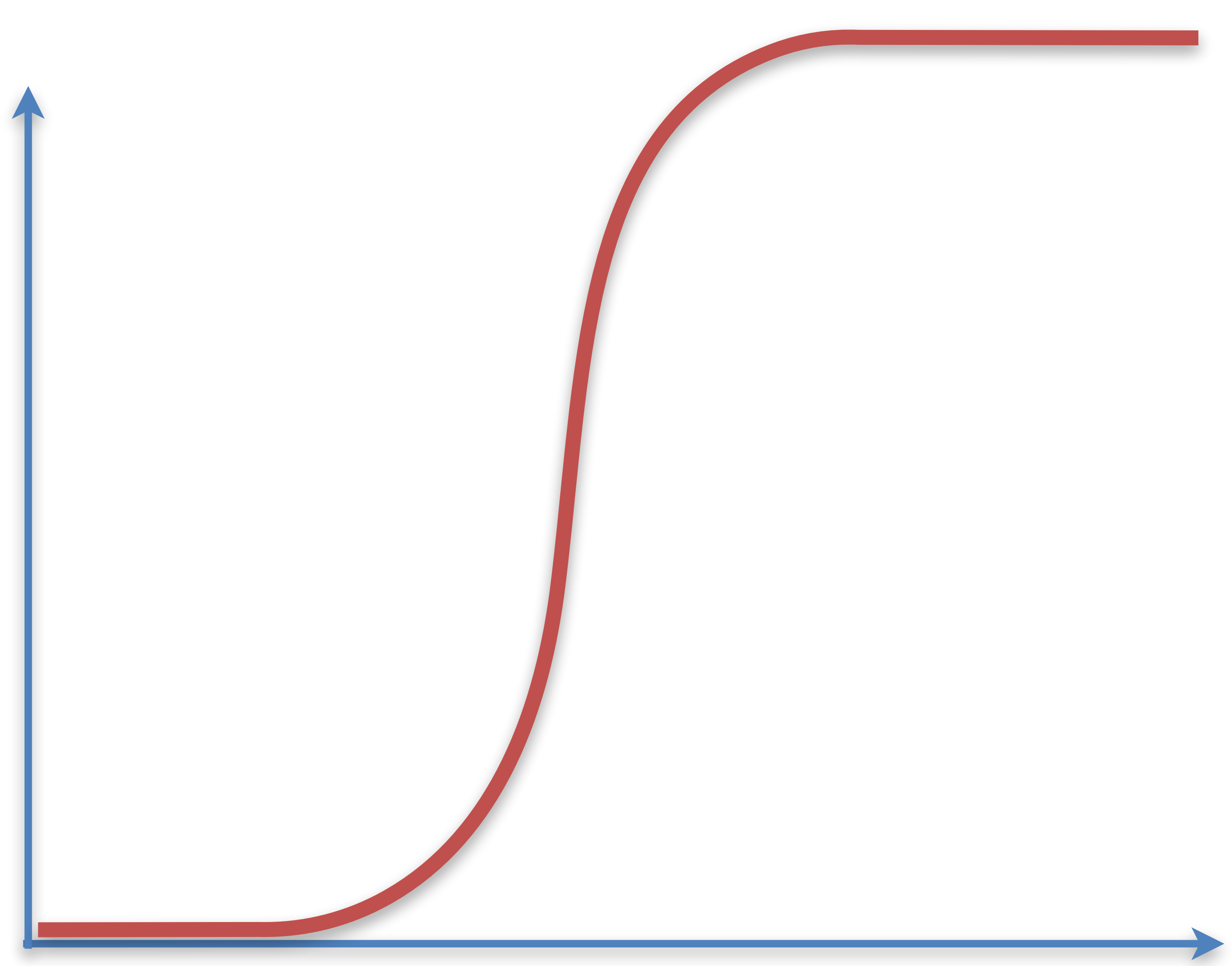
Solving fine structures



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.

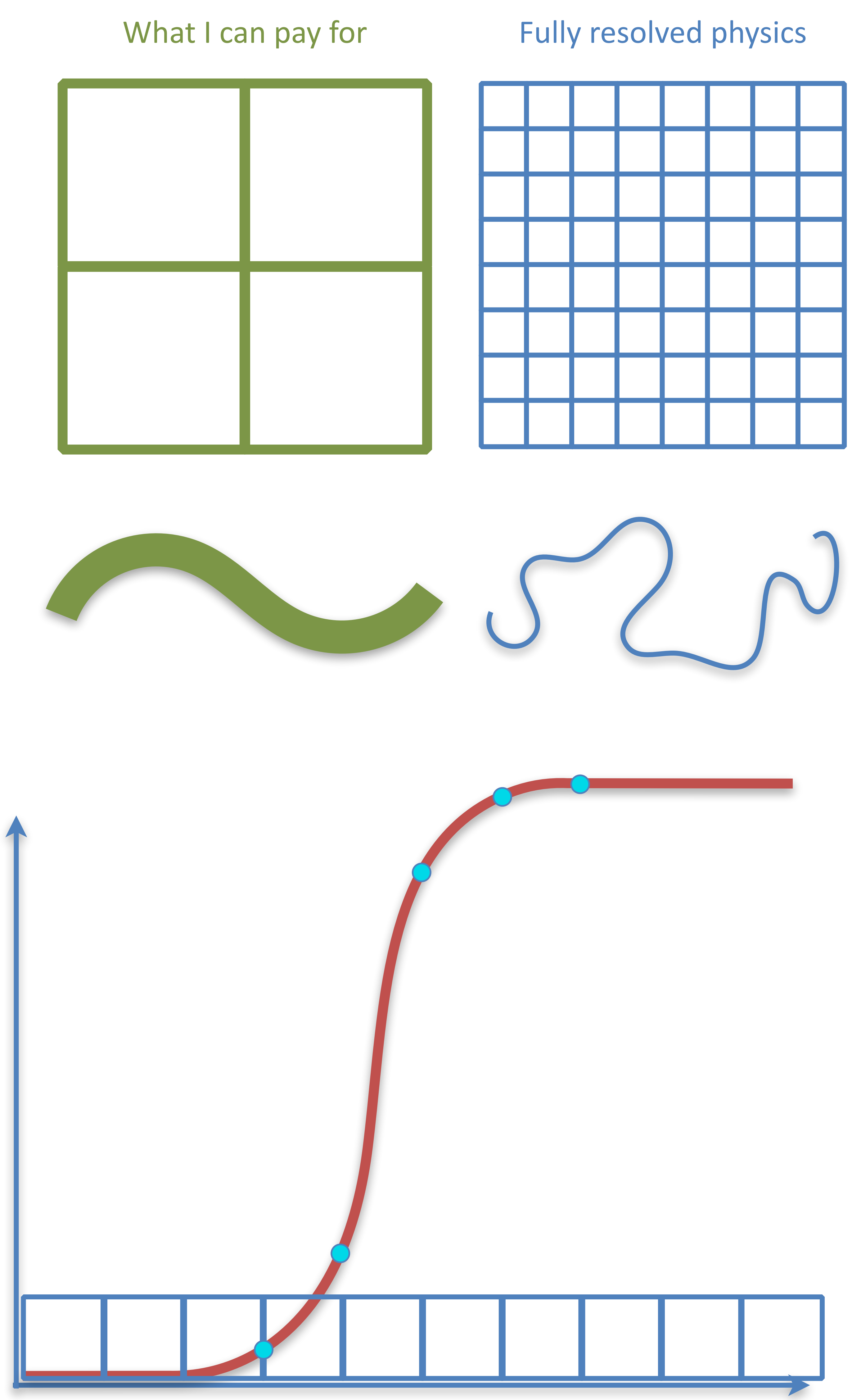
Solving fine structures





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.

Solving fine structures



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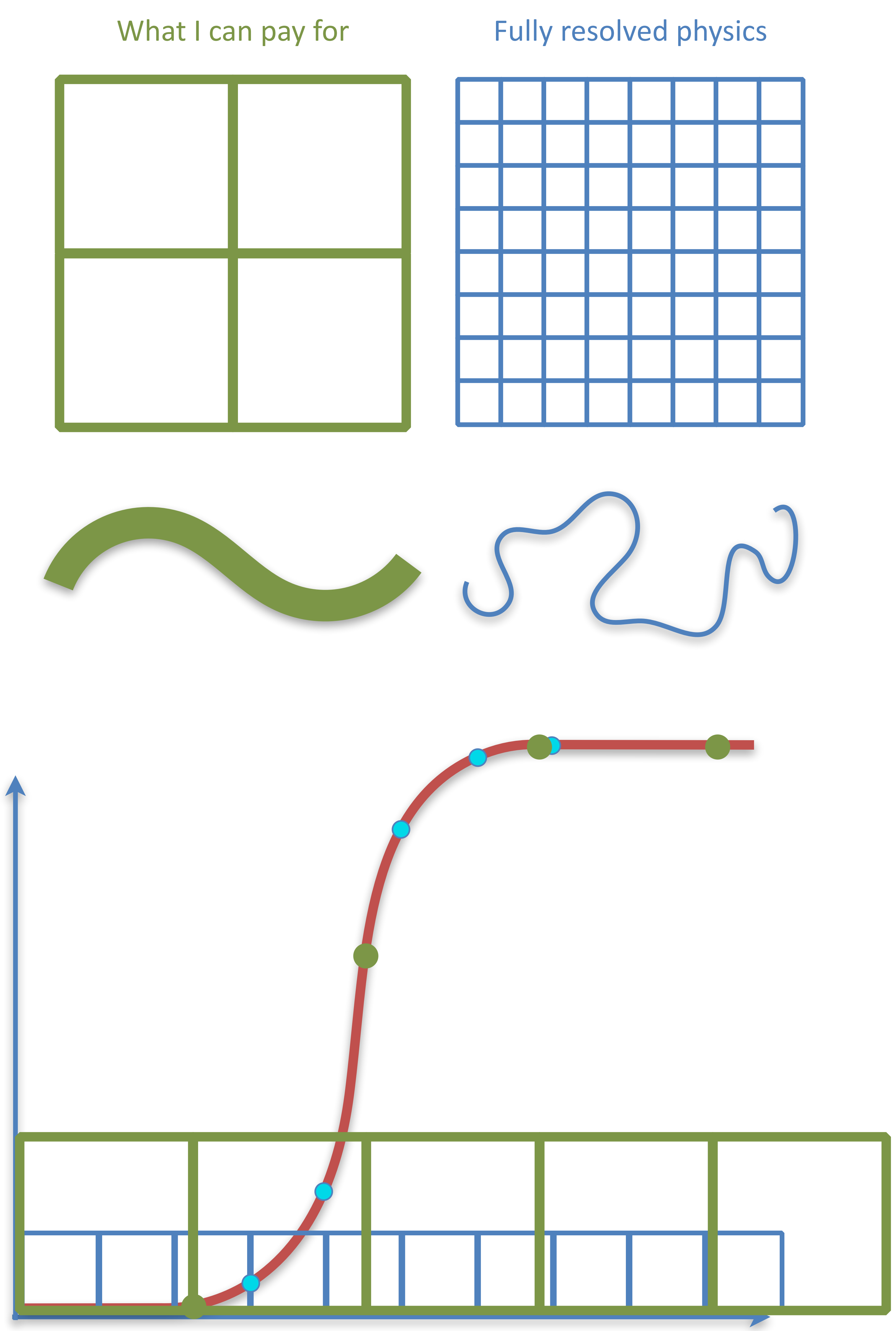

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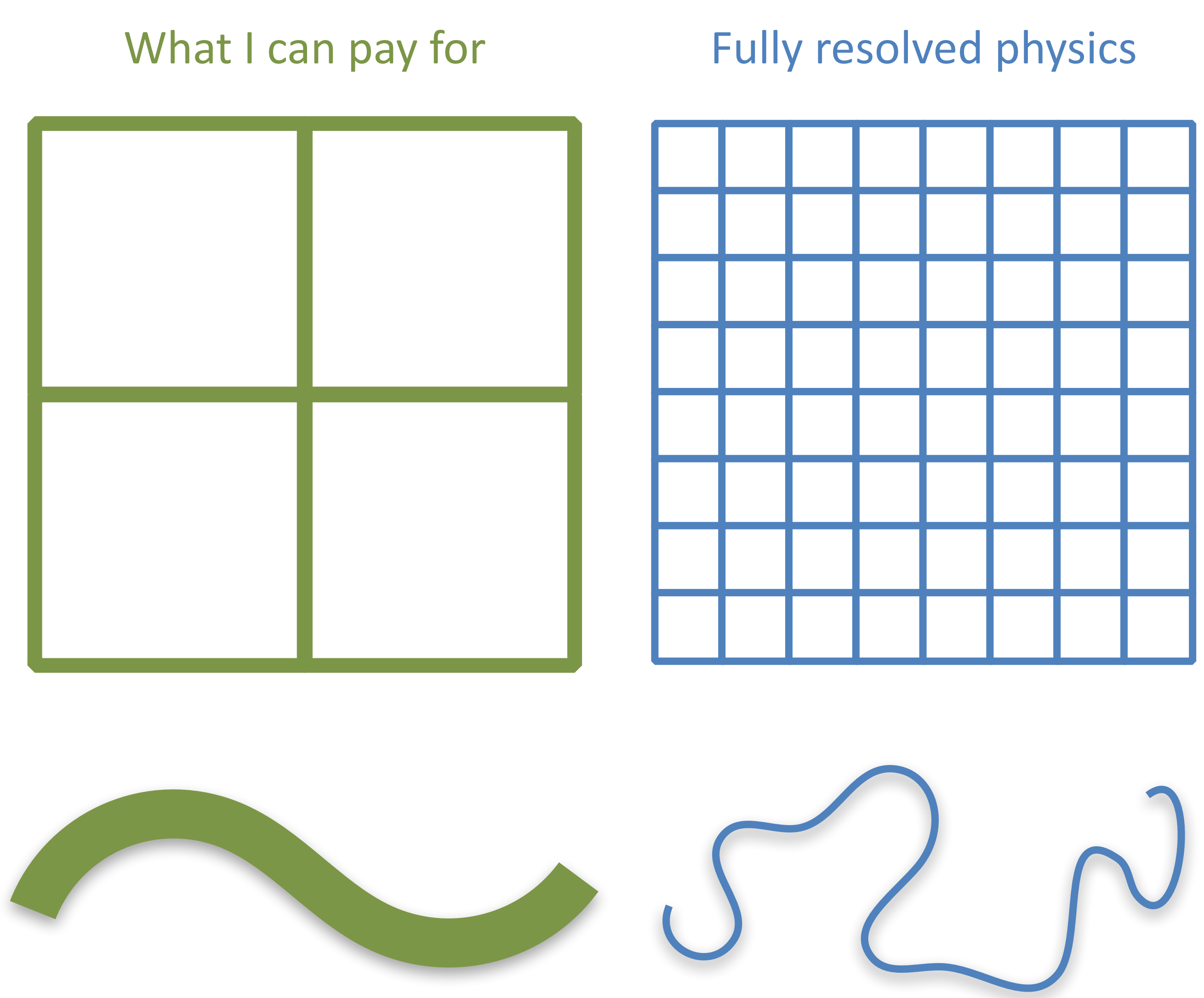

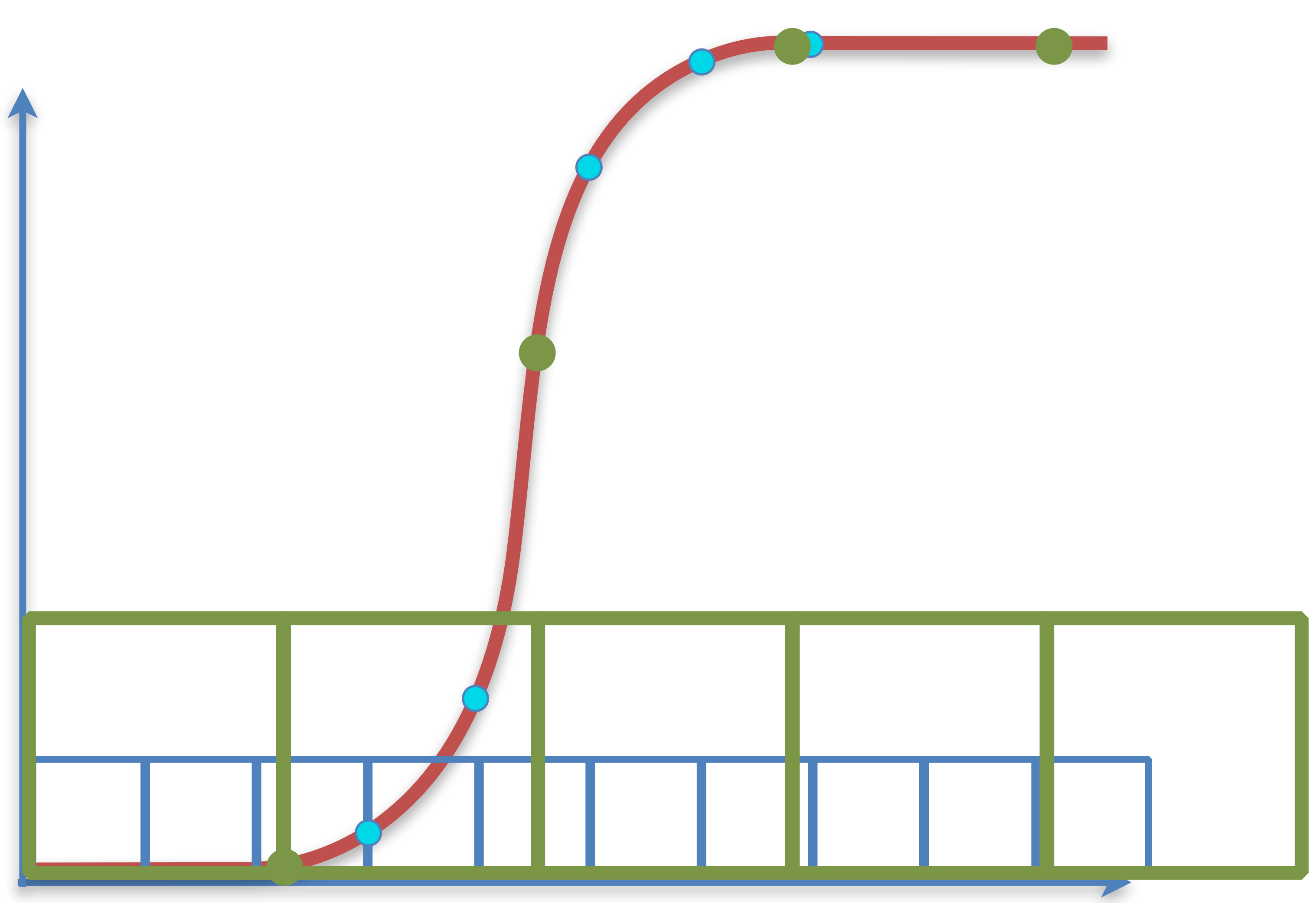

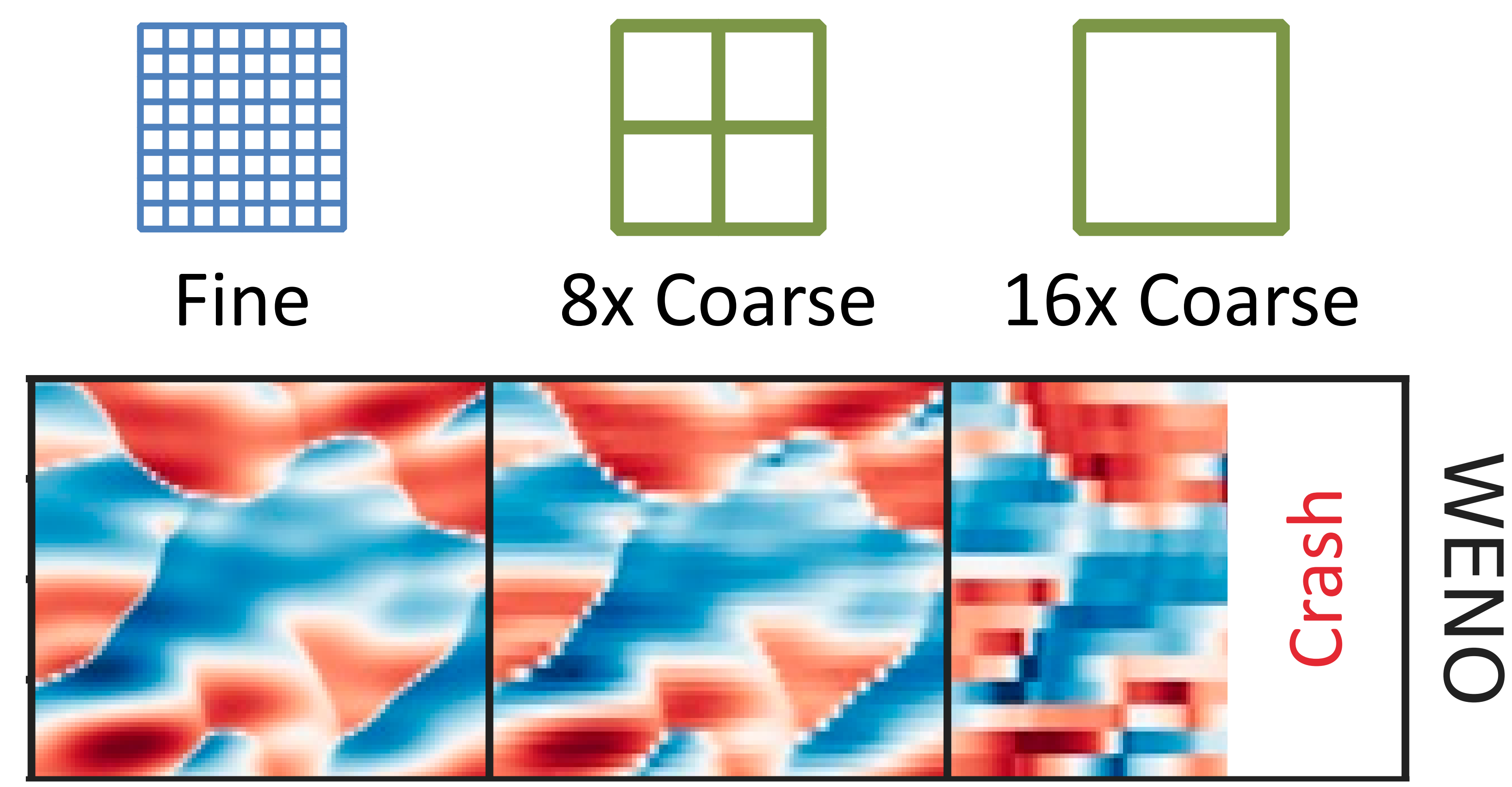

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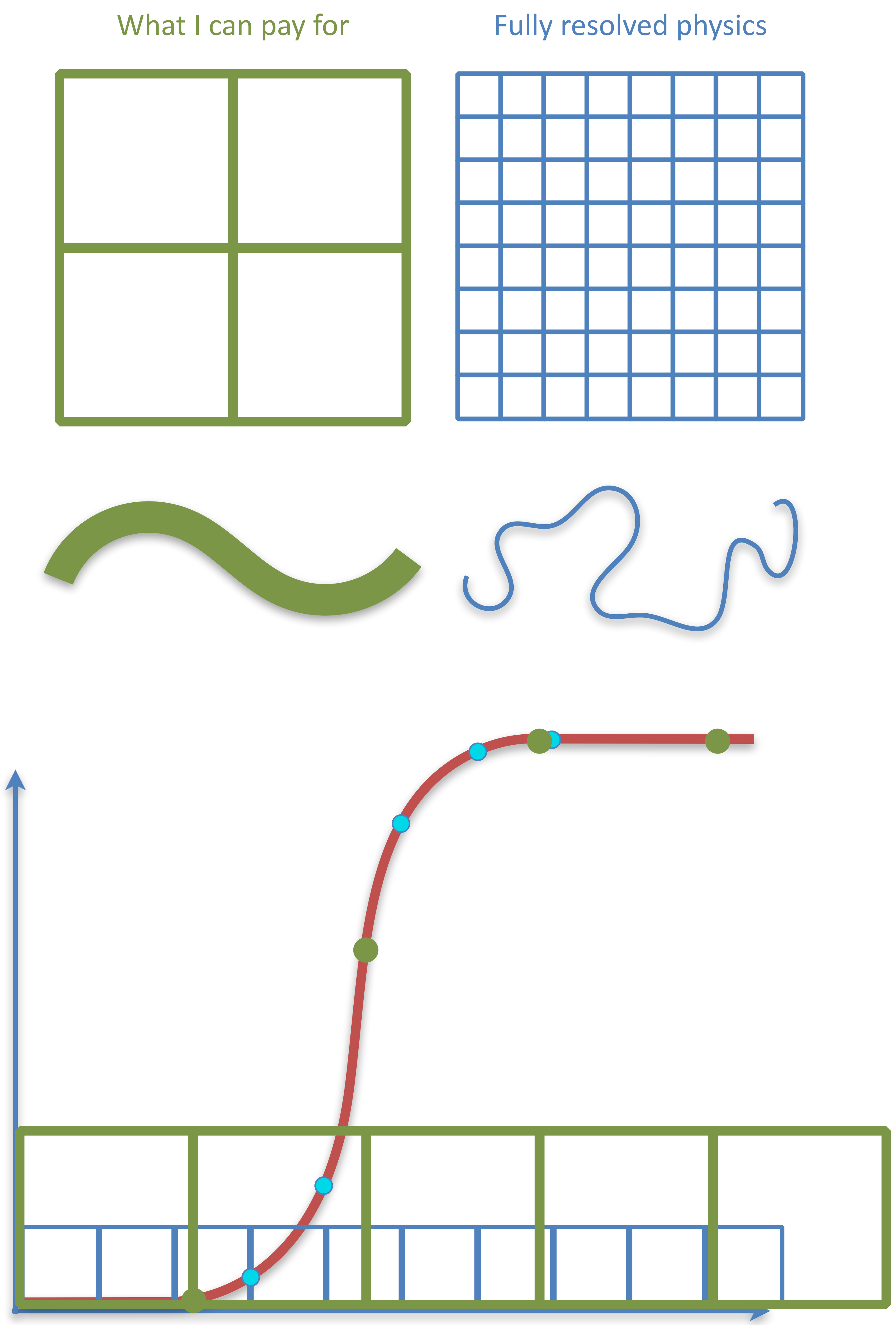

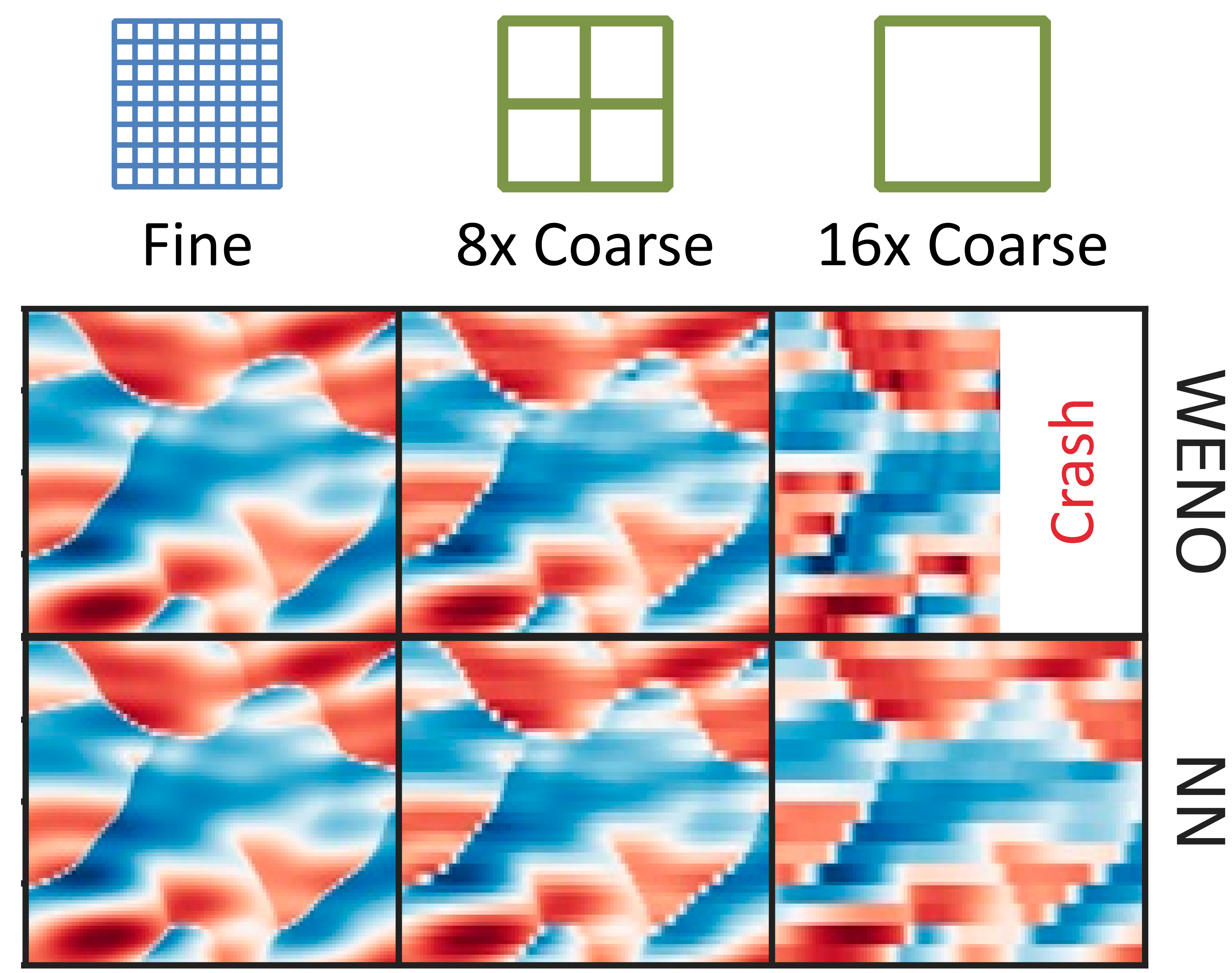

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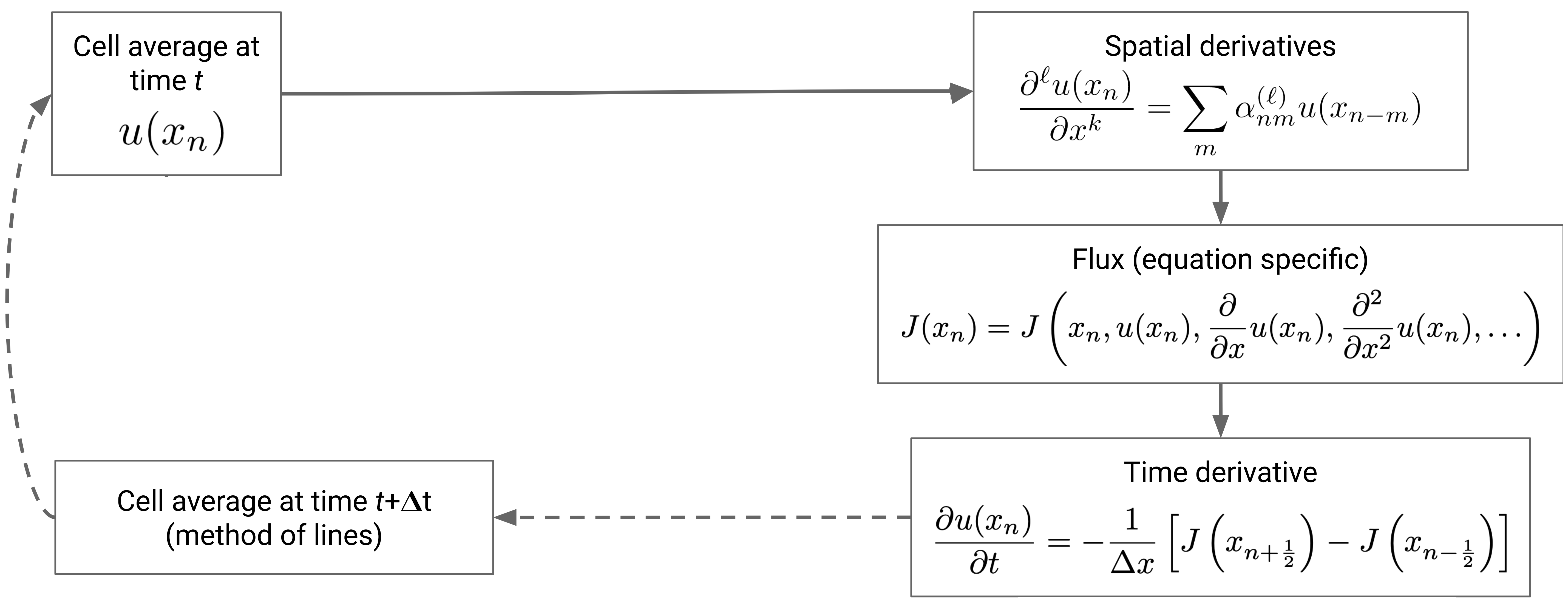
Data Driven Discretization



- One of the less intrusive approaches

- Objective: achieve better gradient estimation on coarse meshes <=> run same simulation on coarser mesh

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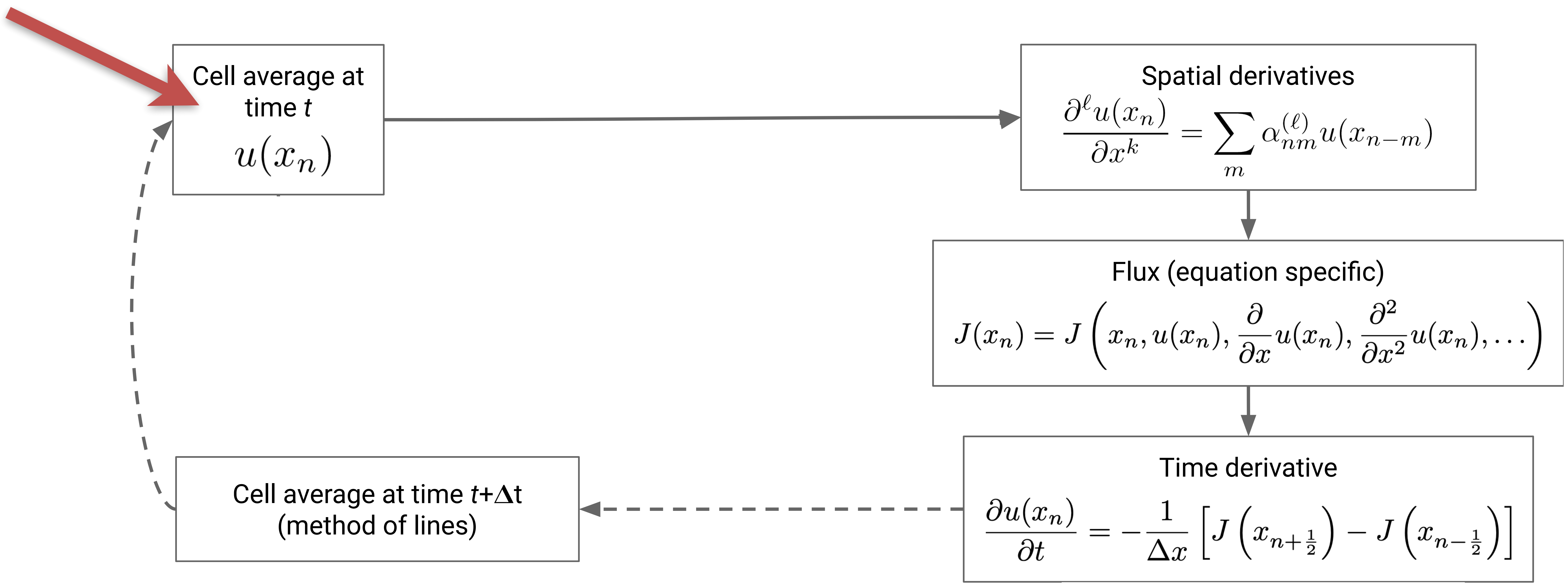

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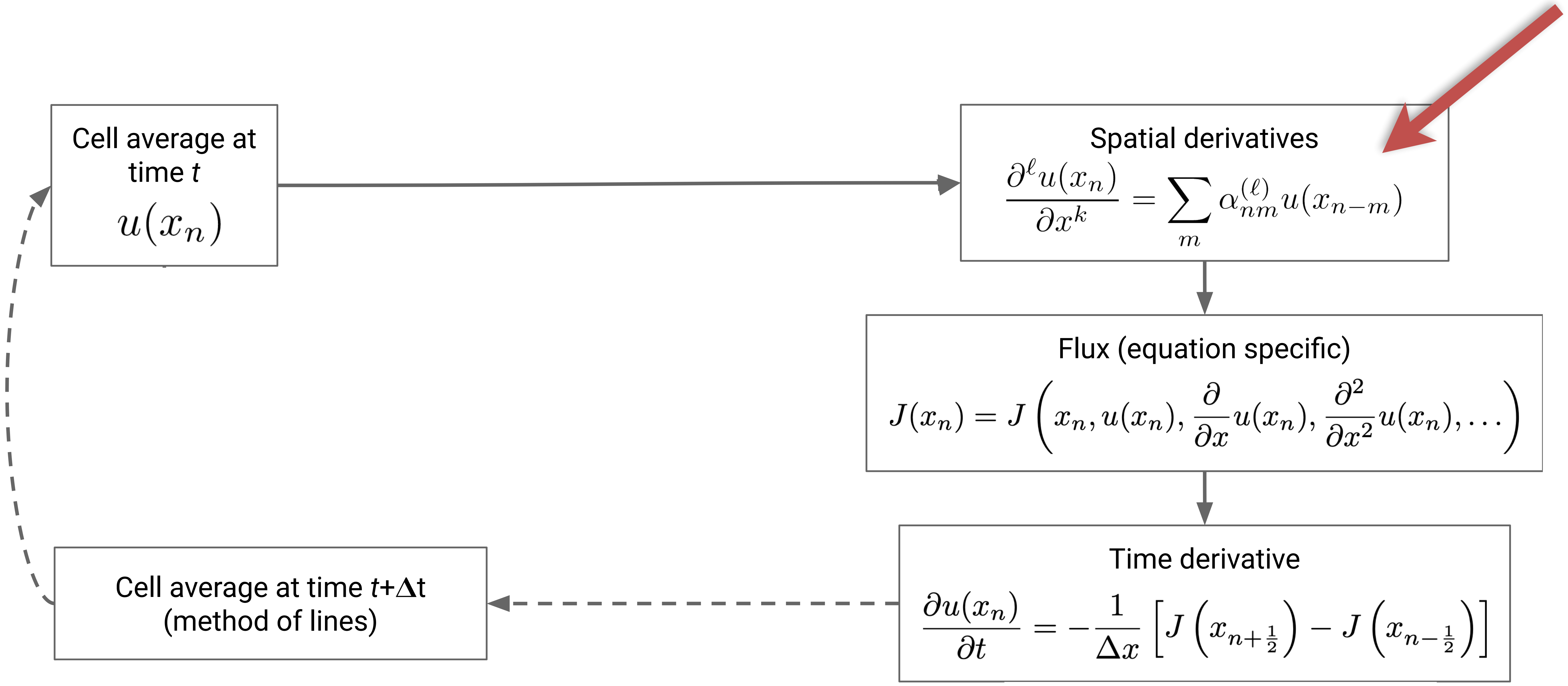

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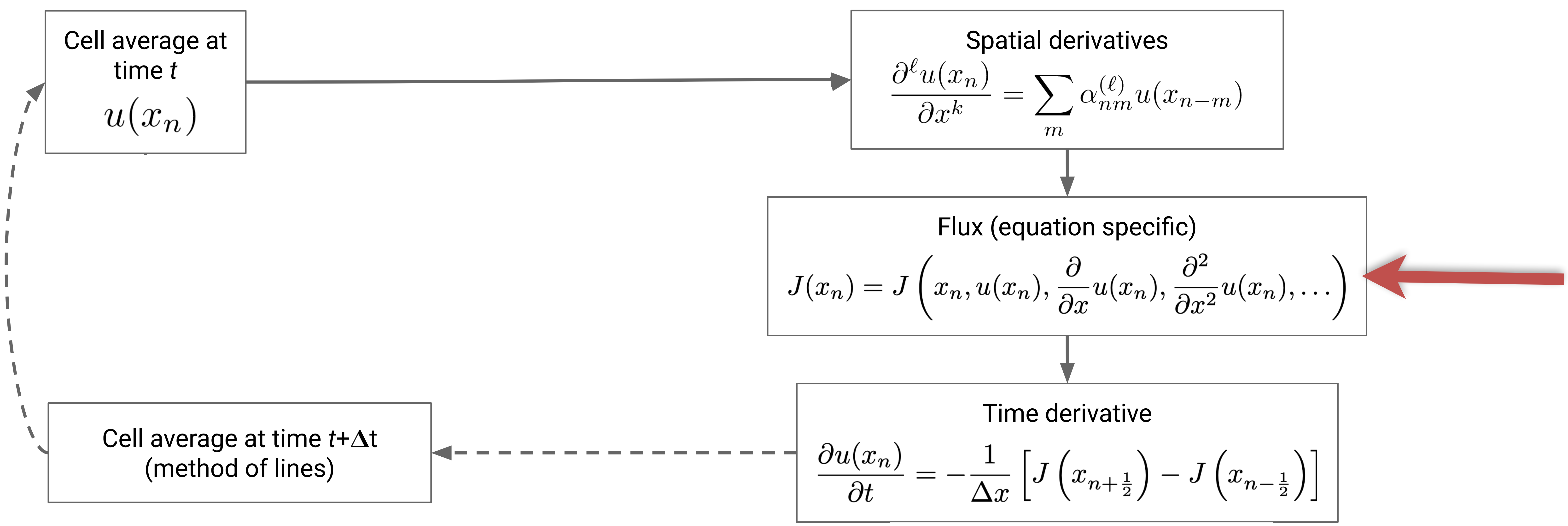

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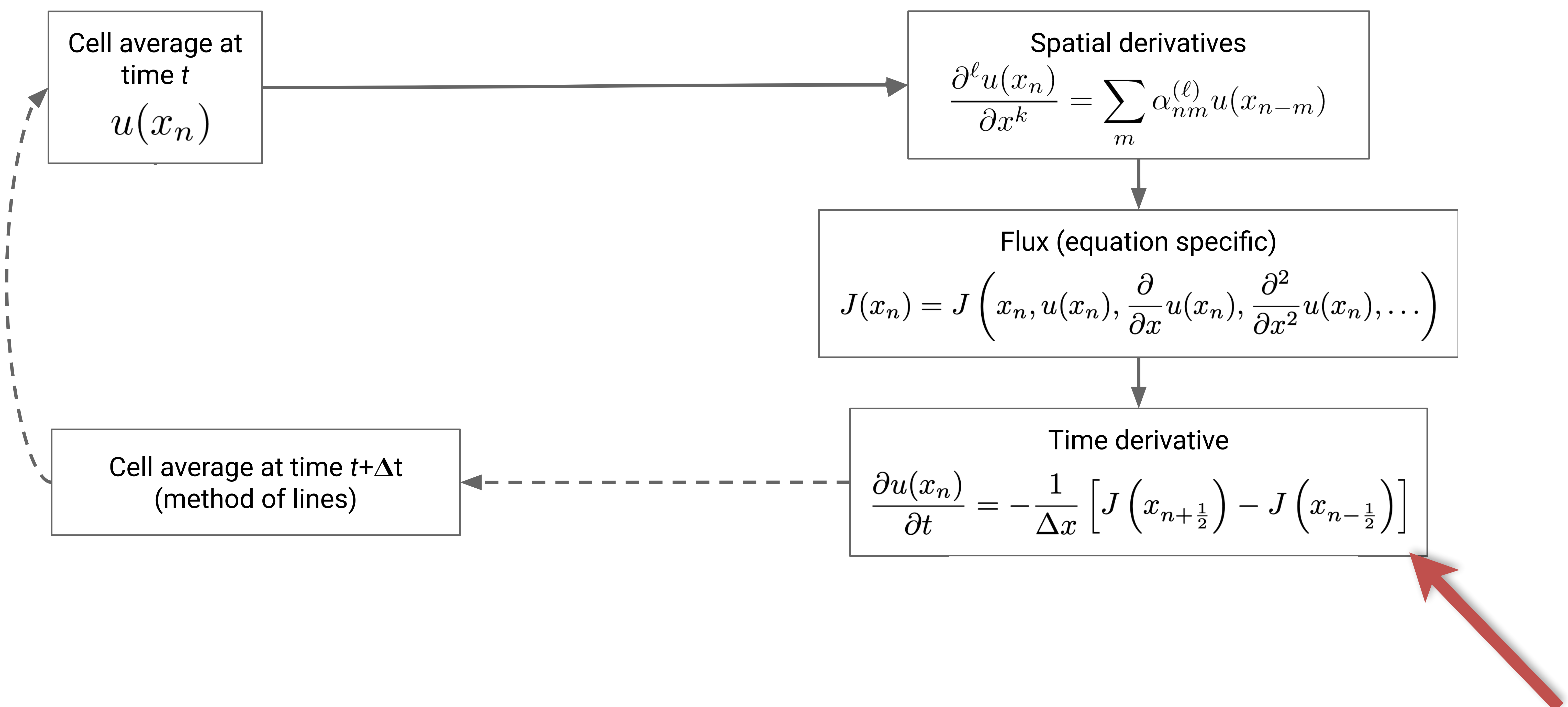

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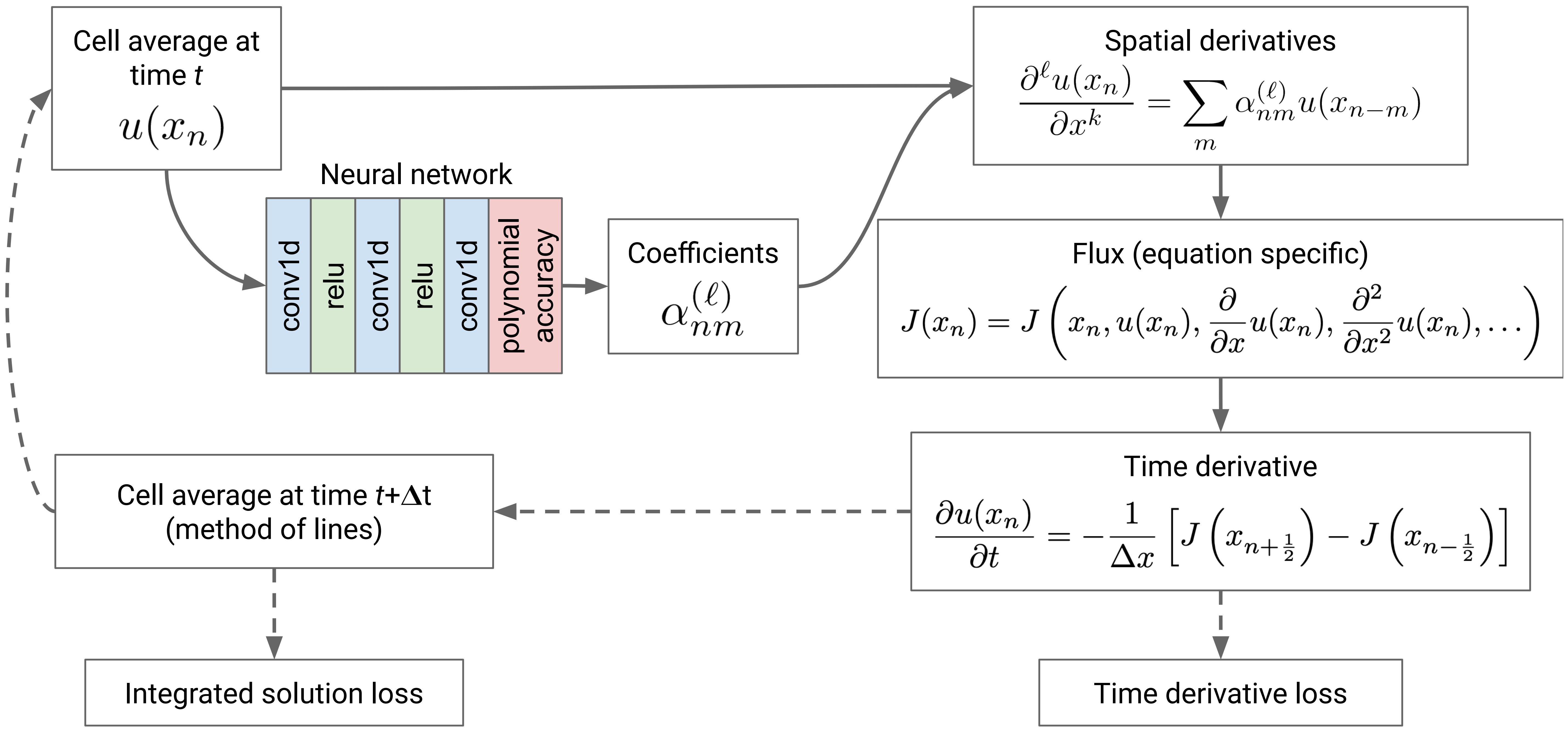

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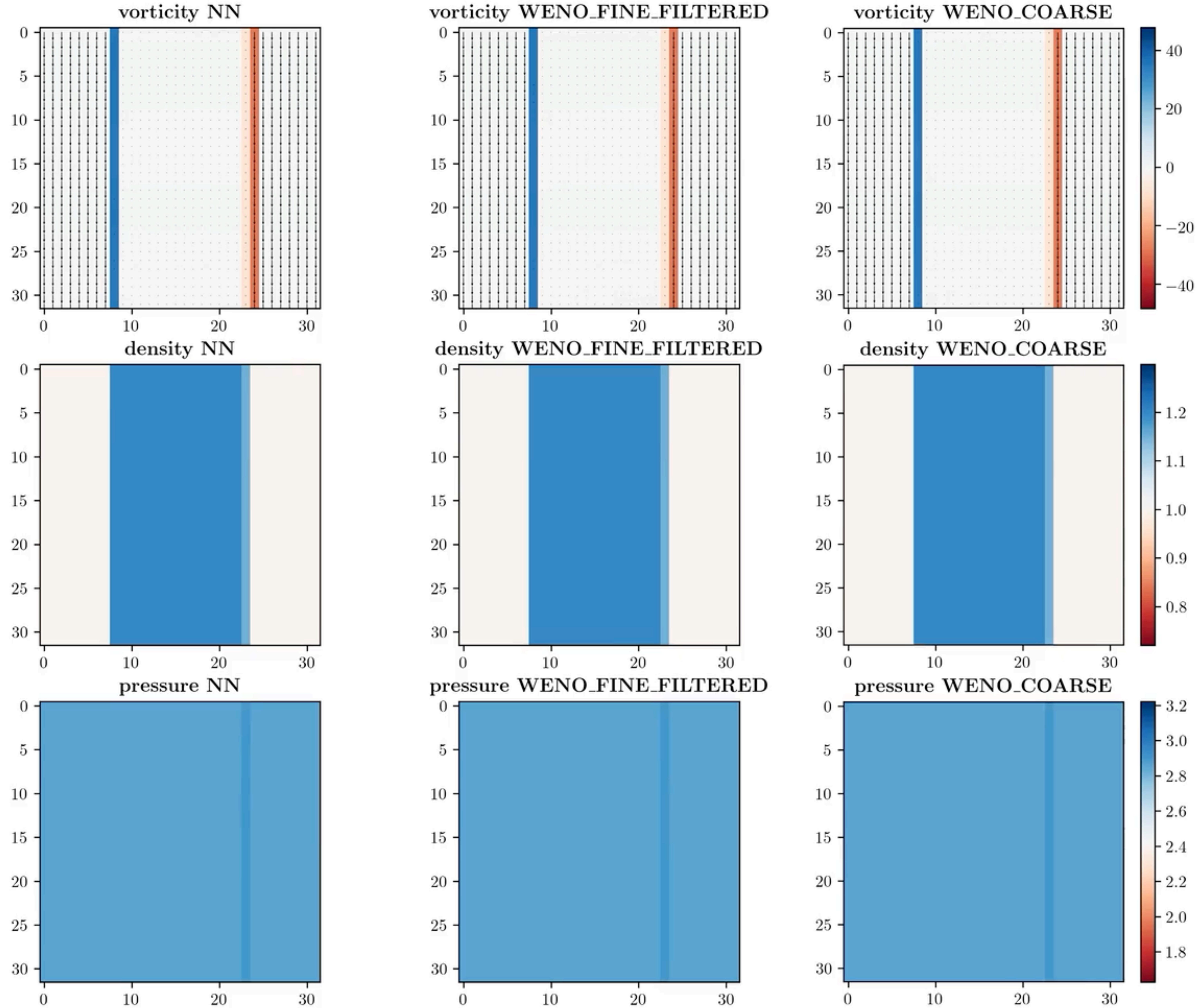
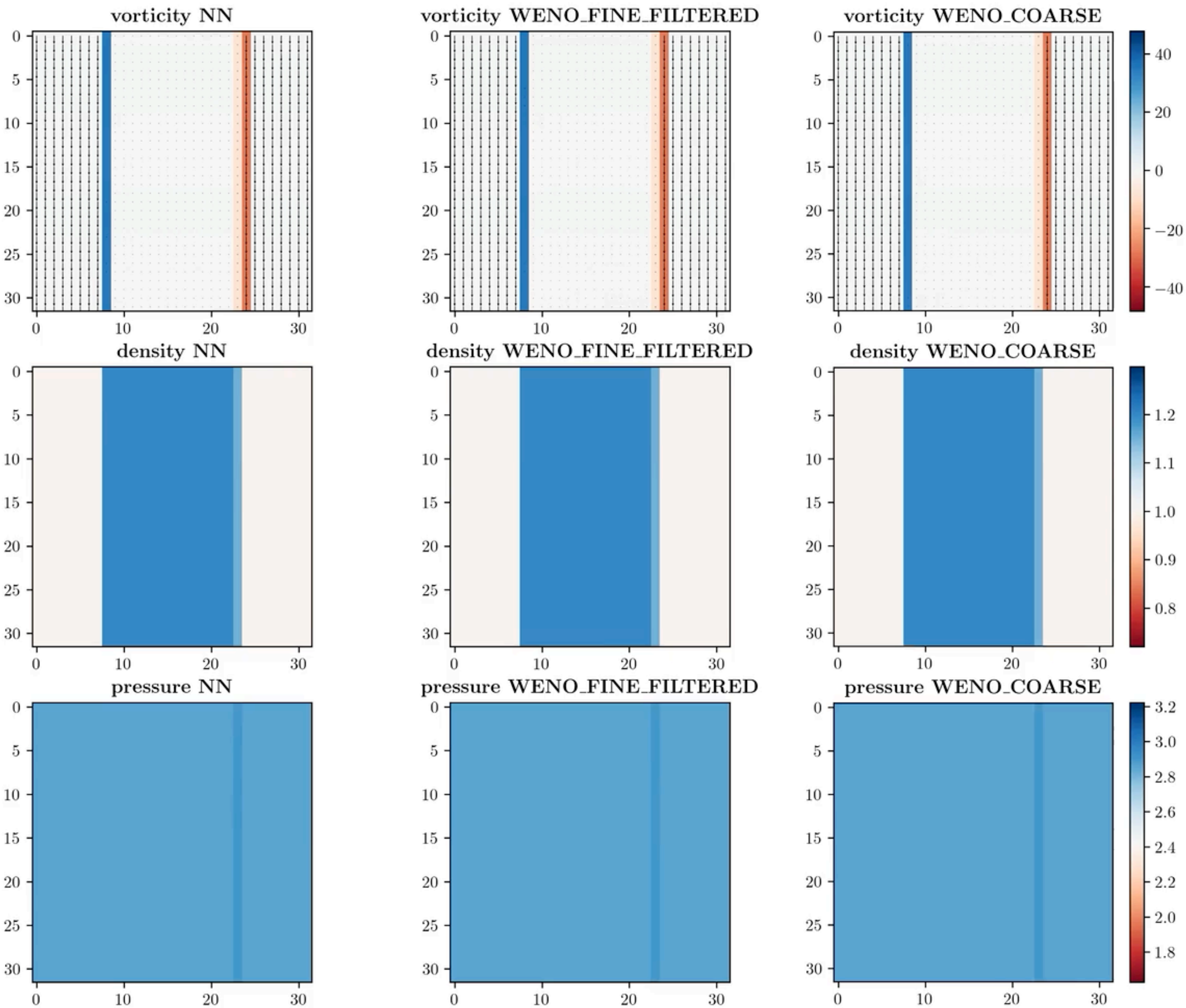


Coarse LES with NN

« Truth » (DNS)

Coarse LES

Ongoing PhD of Luciano Drozda, Cerfacs



Coarse LES with NN « Truth » (DNS) Coarse LES

Ongoing PhD of Luciano Drozda, Cerfacs

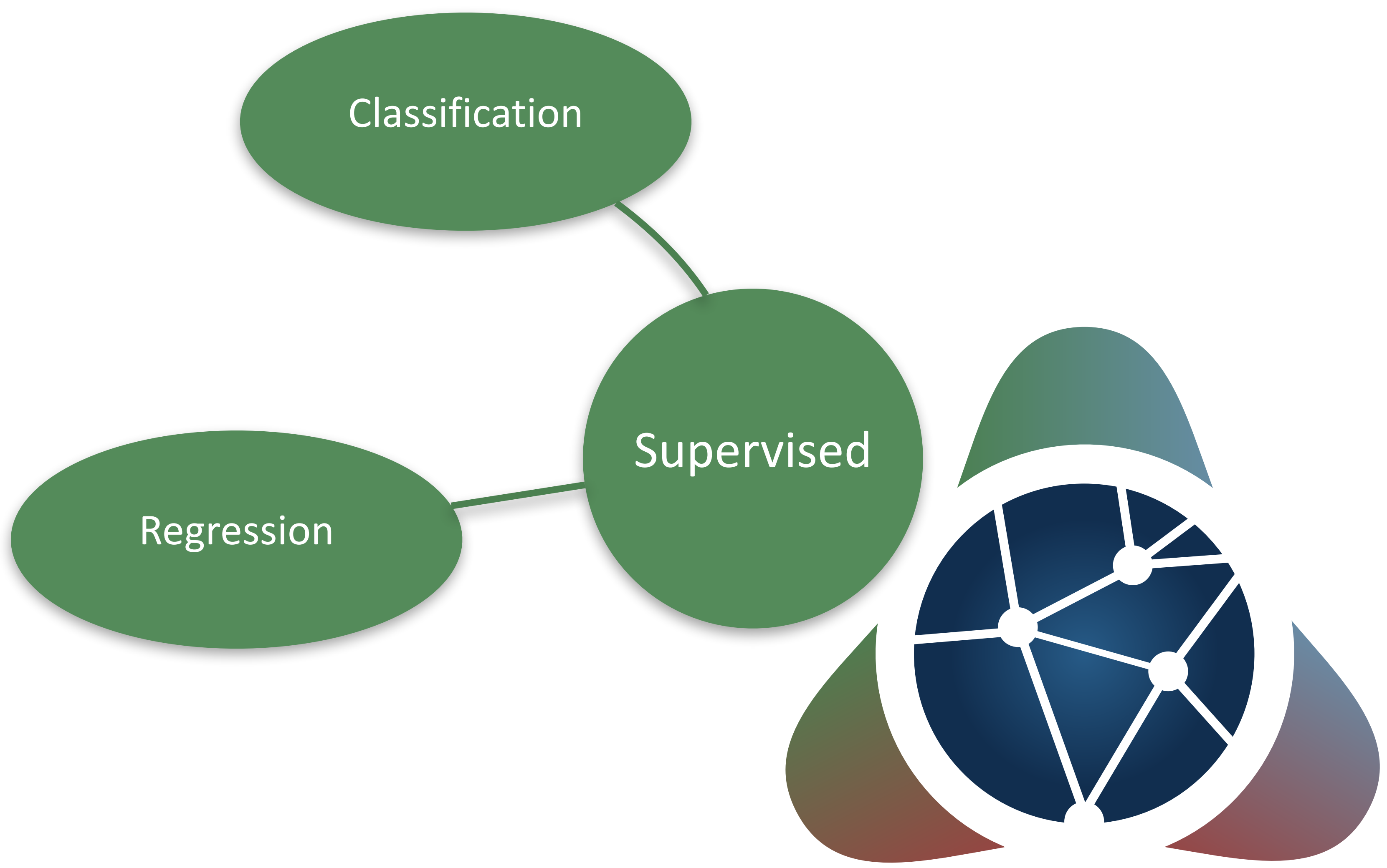
Great idea, difficult execution

- Challenge #1: differentiability
  - NN require the chain to be differentiable *i.e.* <u>you must rewrite your CFD solver in a deep learning framework</u>
  - Several solvers with this tech under development (*e.g.* PhiFlow [1] at TUM)

- Challenge #2: time stability
  - Supervised learning (error wrt next iteration) leaves room for small errors that accumulate => divergence
  - *BUT* training in a supervised manner long term doesn't seem to work: turbulent paths differ, and punishing the network for difference to DNS doesn't work anymore

[1] https://ge.in.tum.de/research/phiflow/

Concluding remarks


Classification
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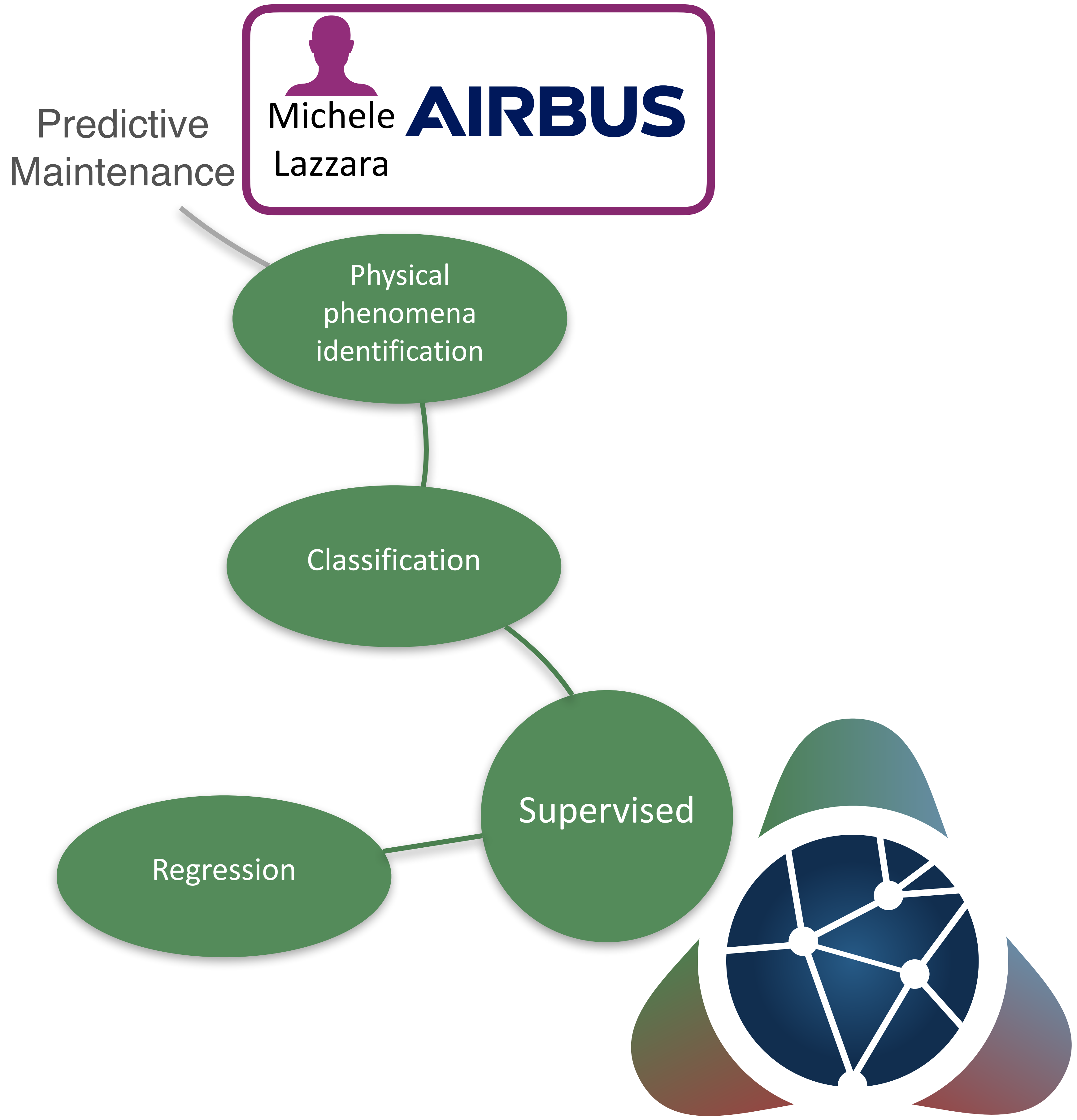
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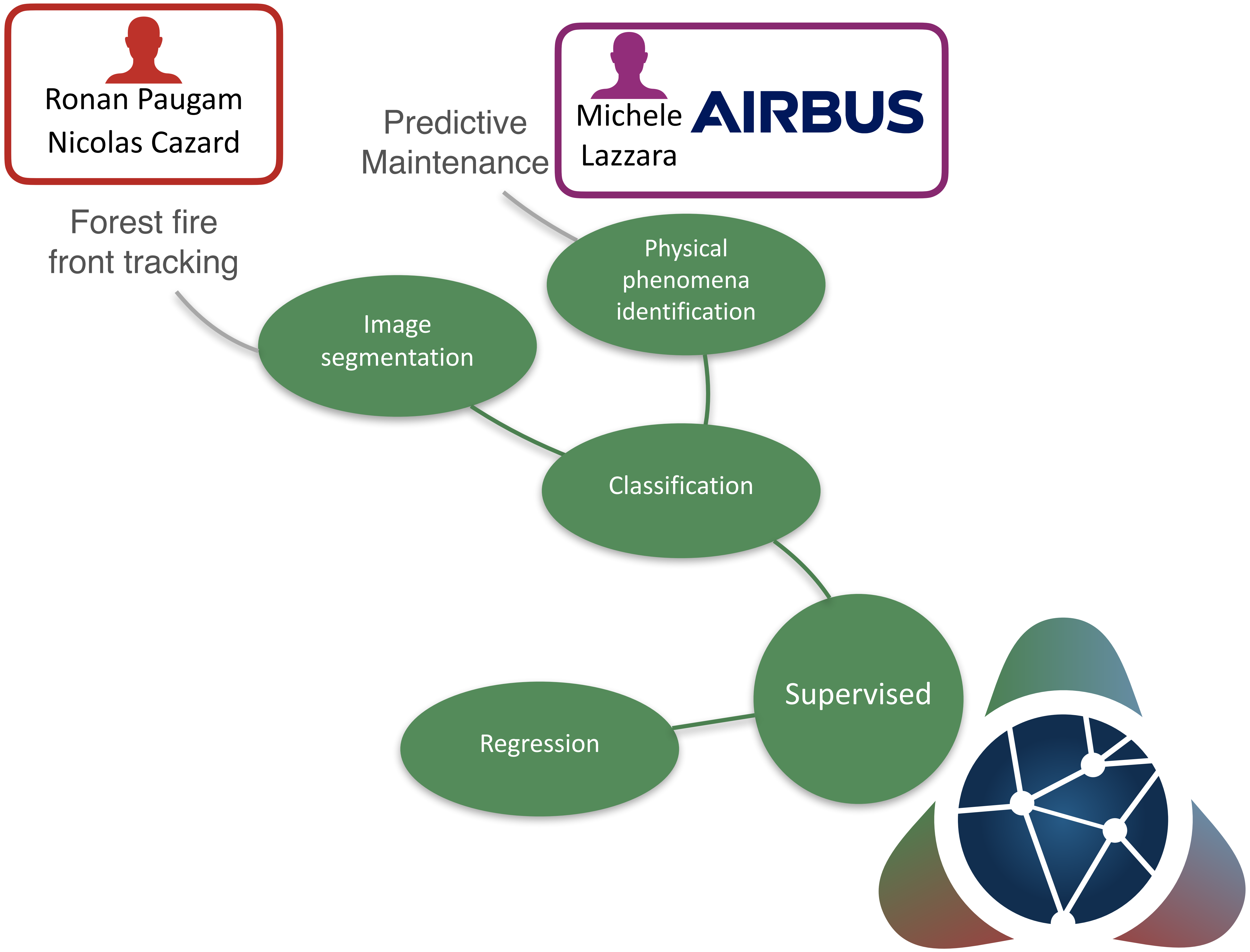

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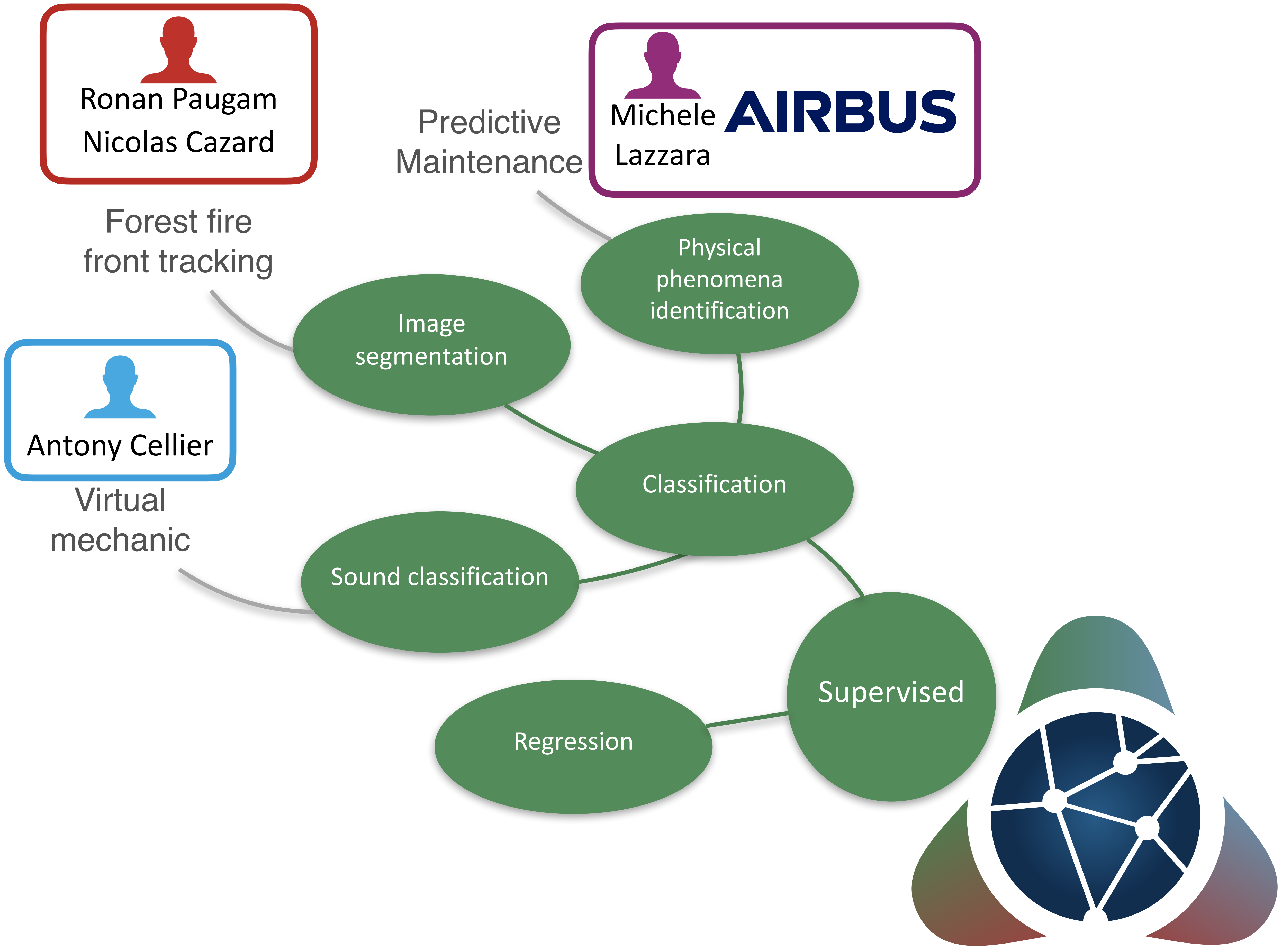
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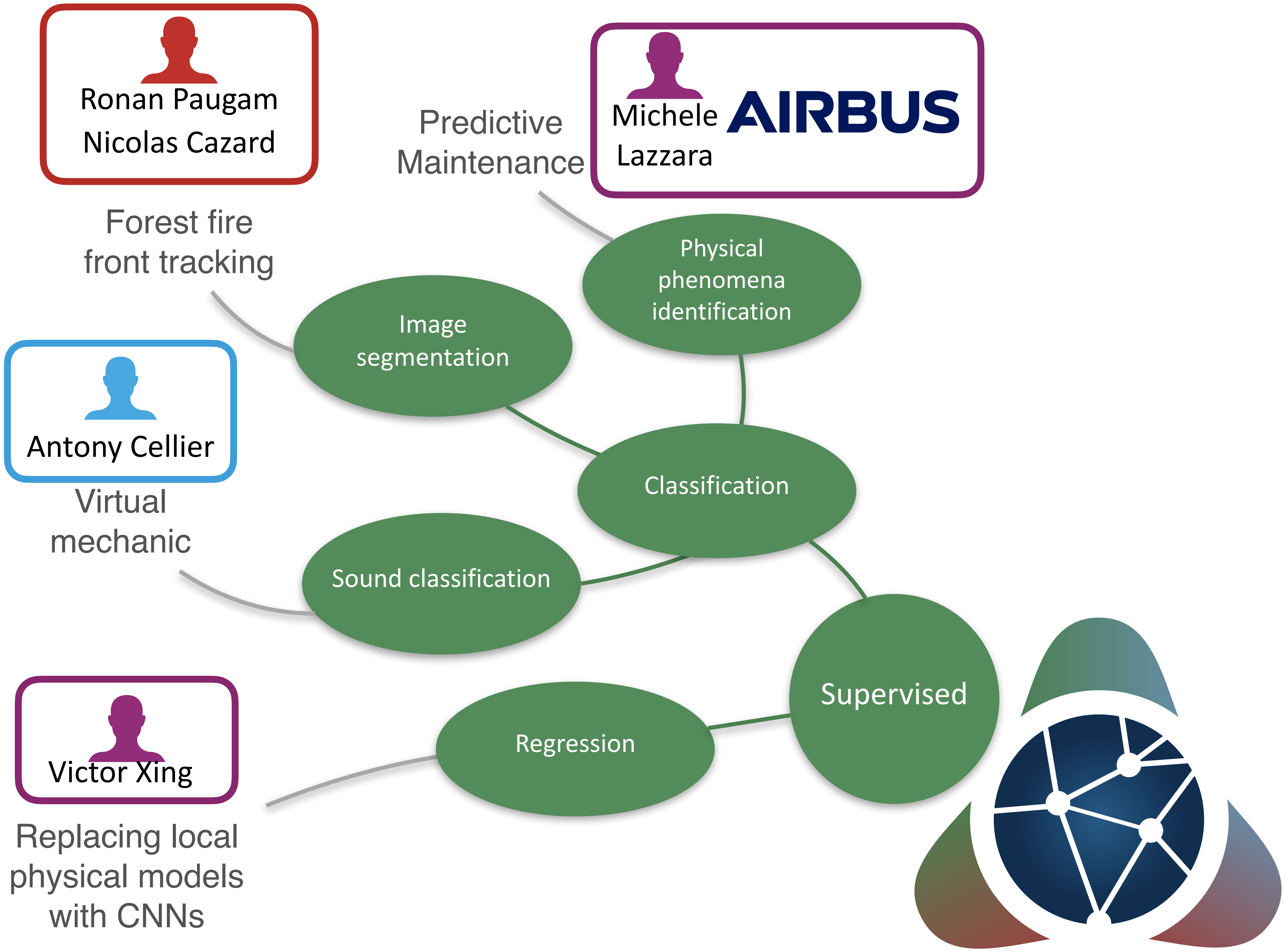
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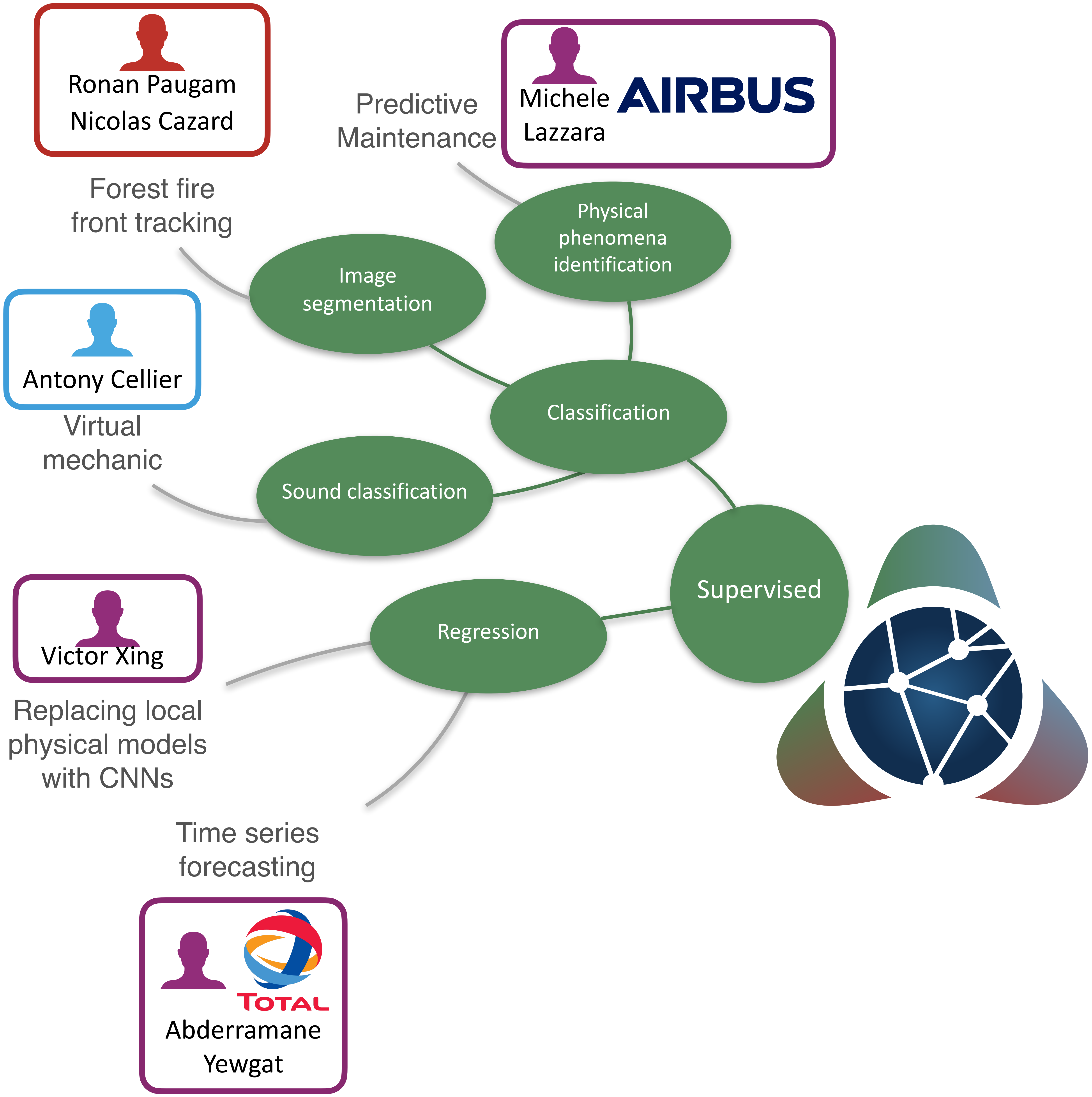
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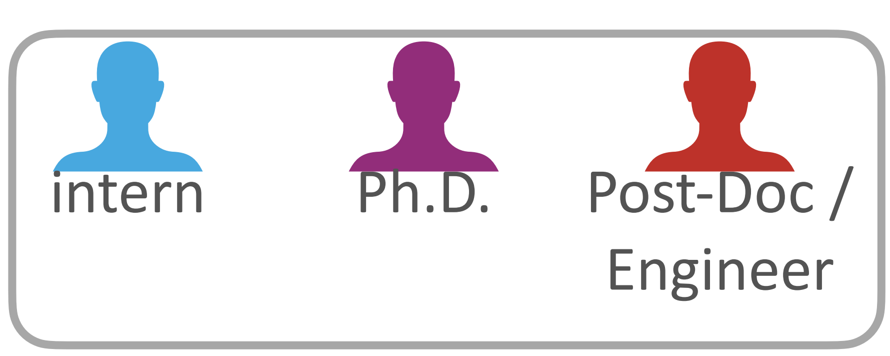
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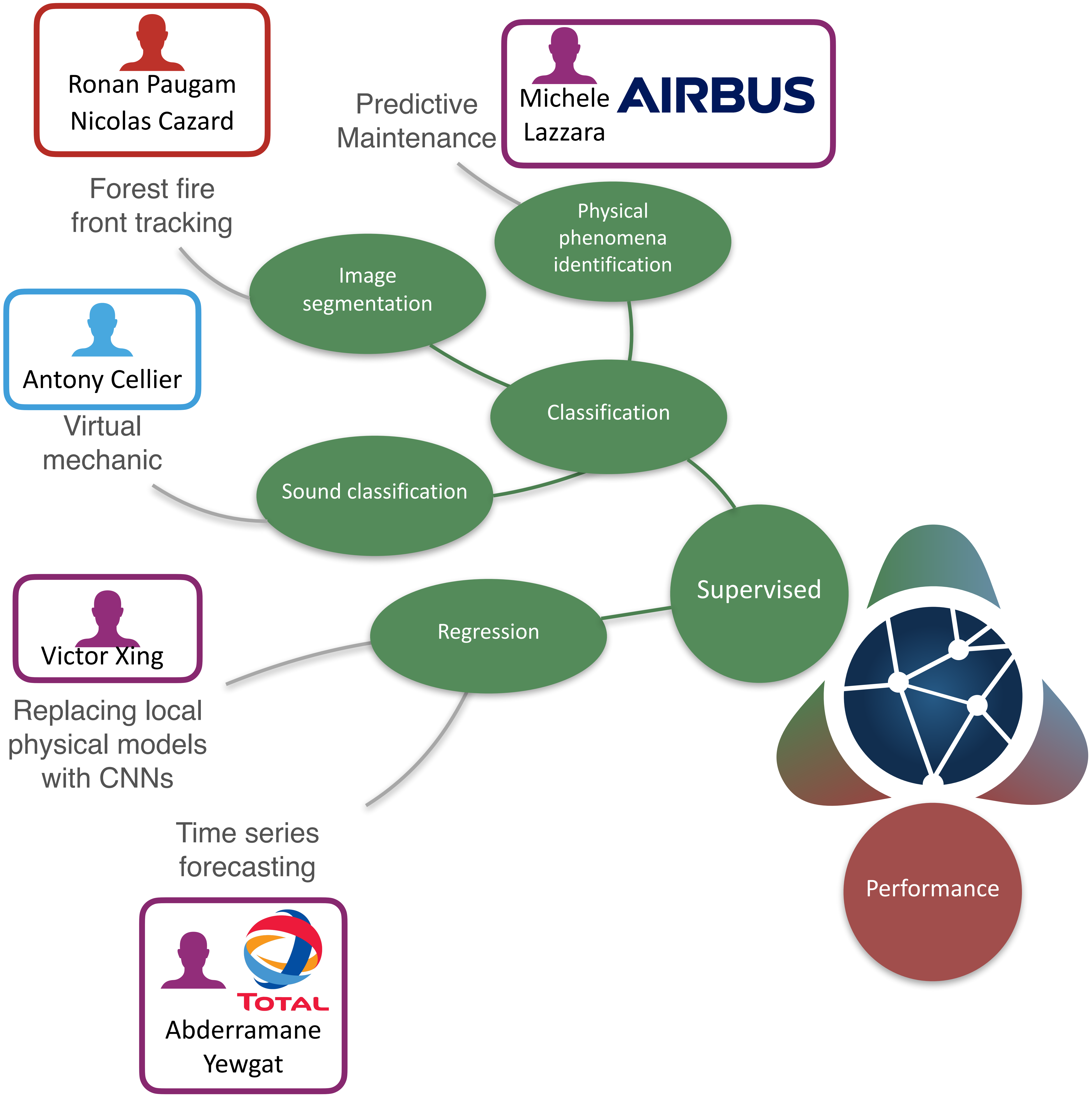
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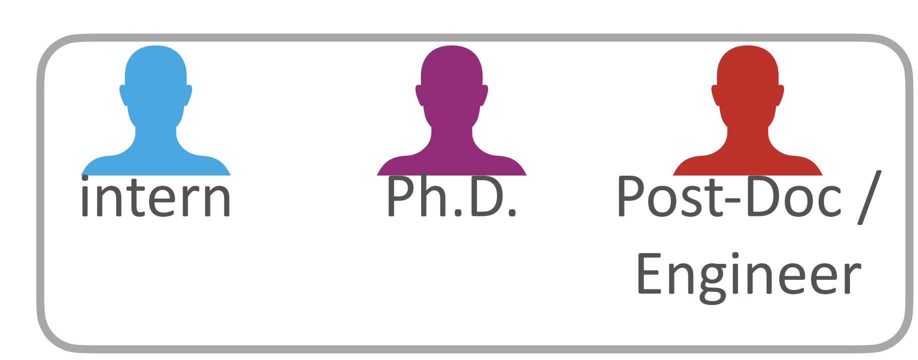
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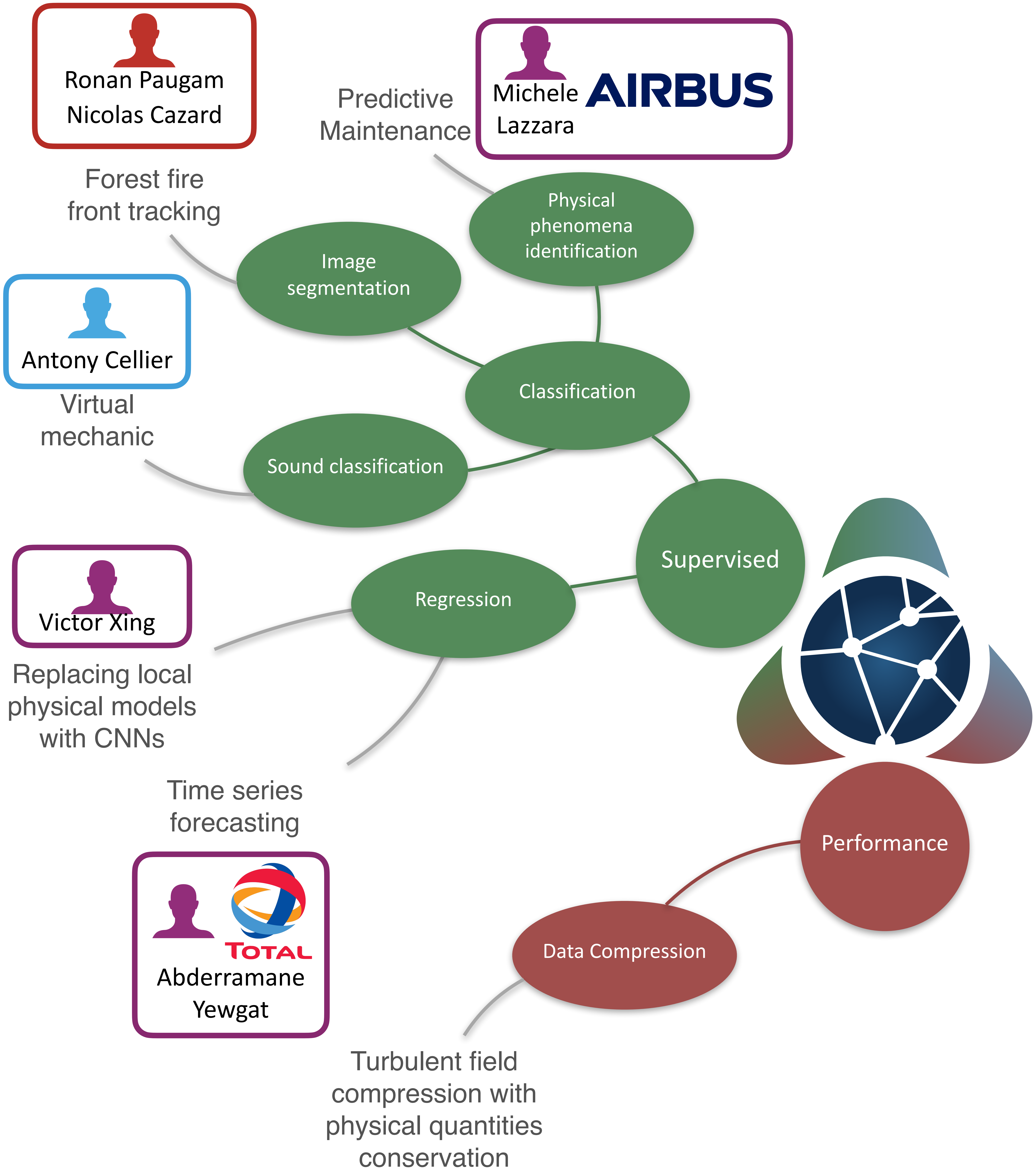

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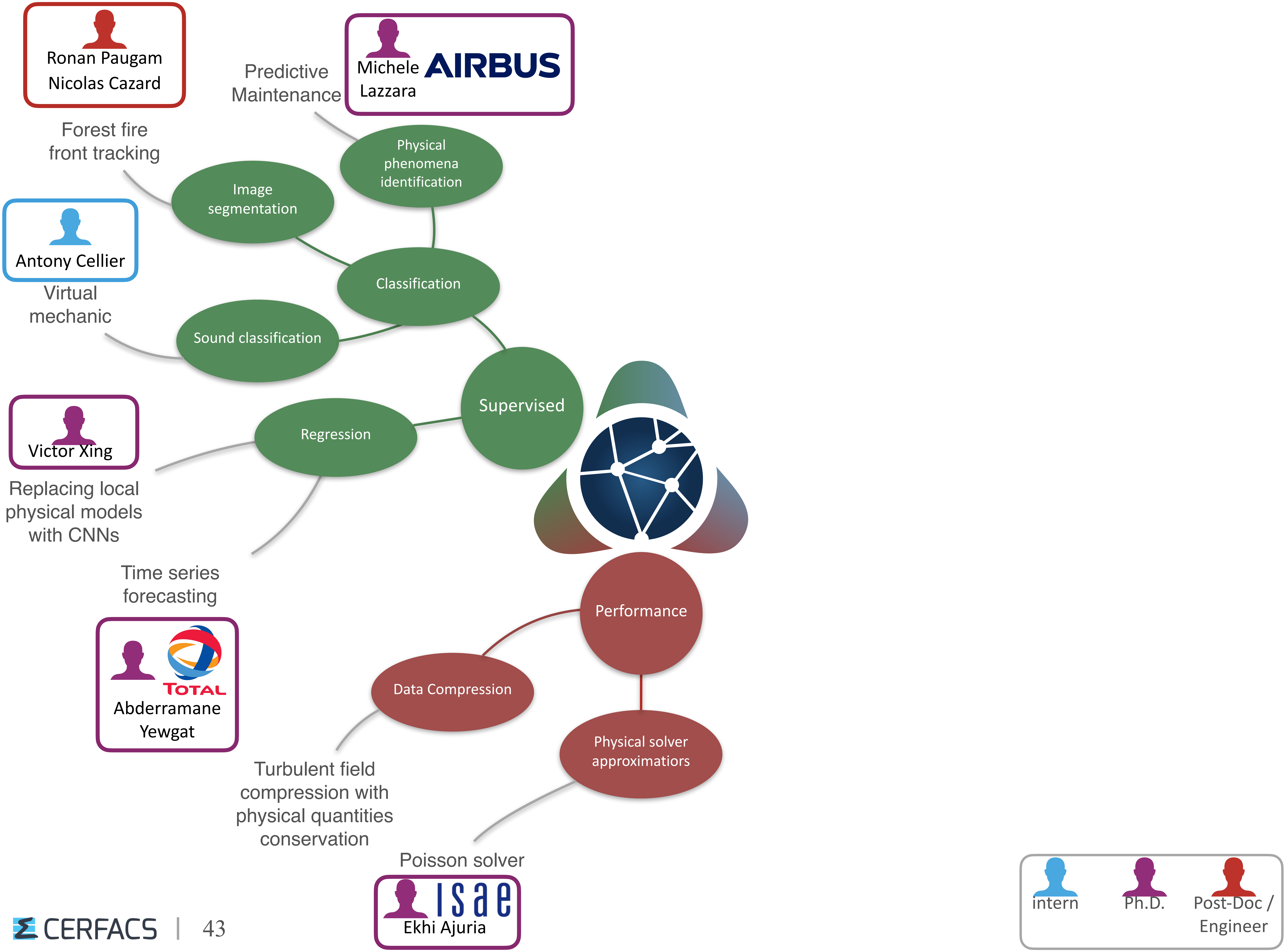

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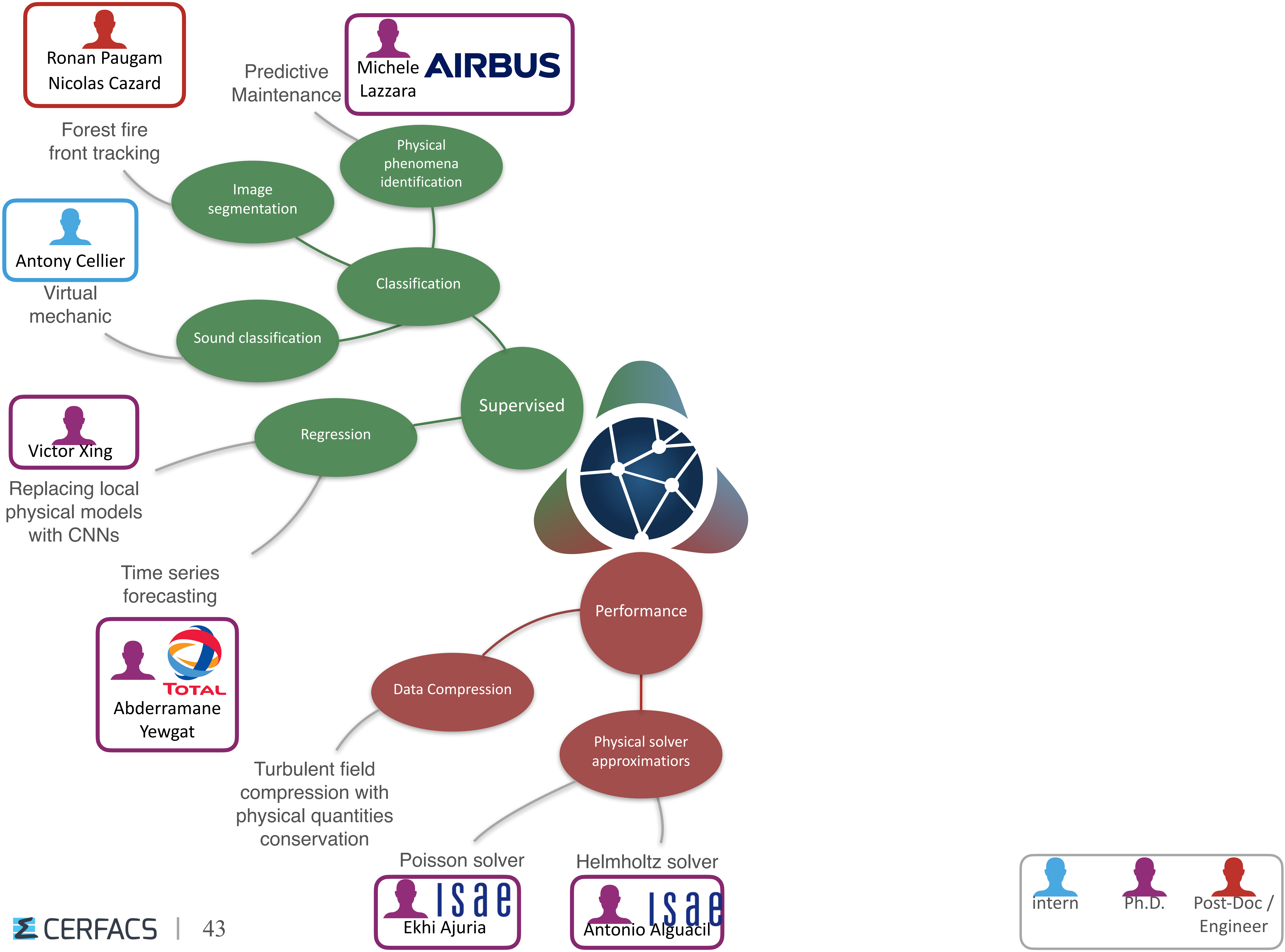
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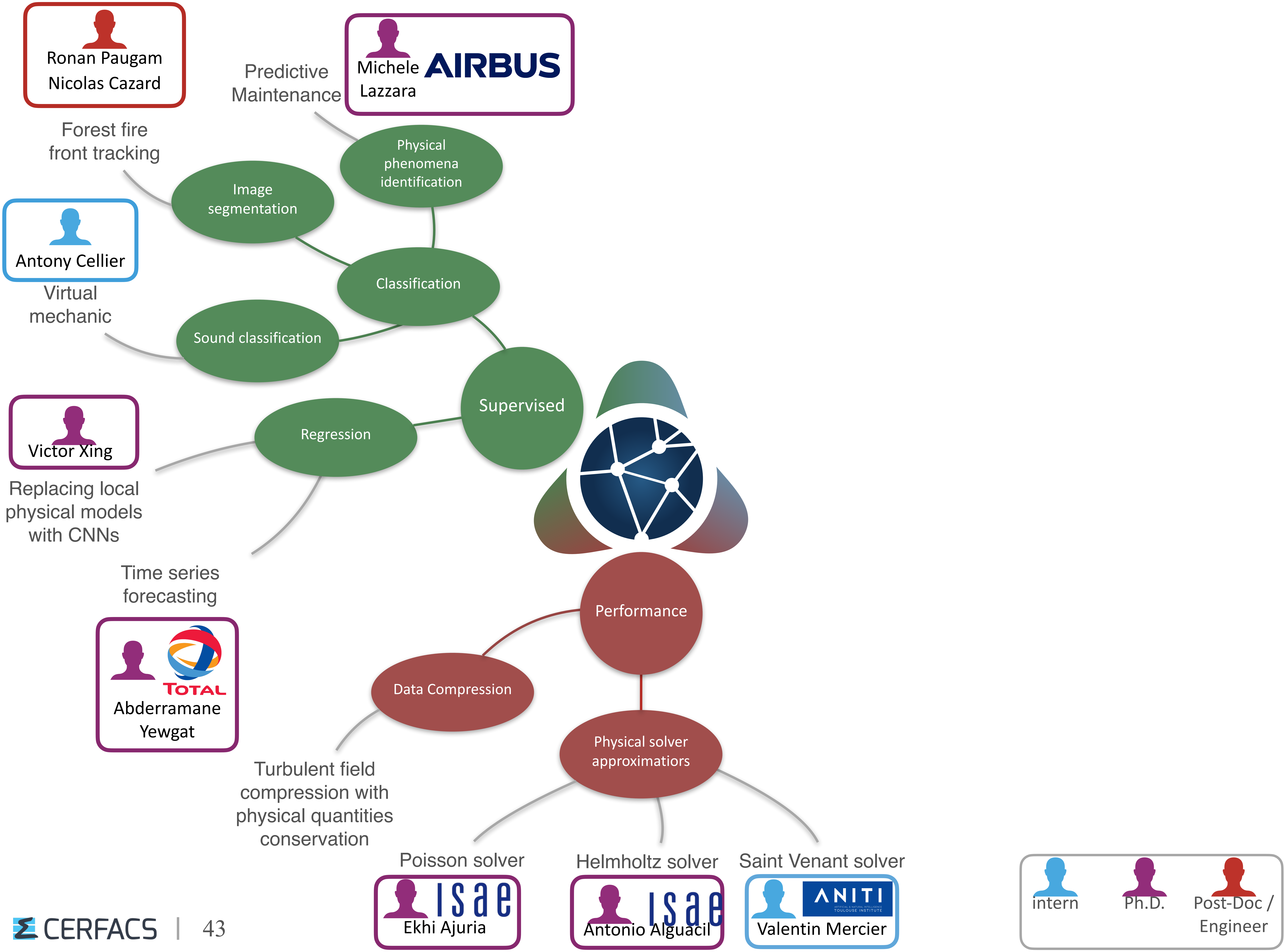
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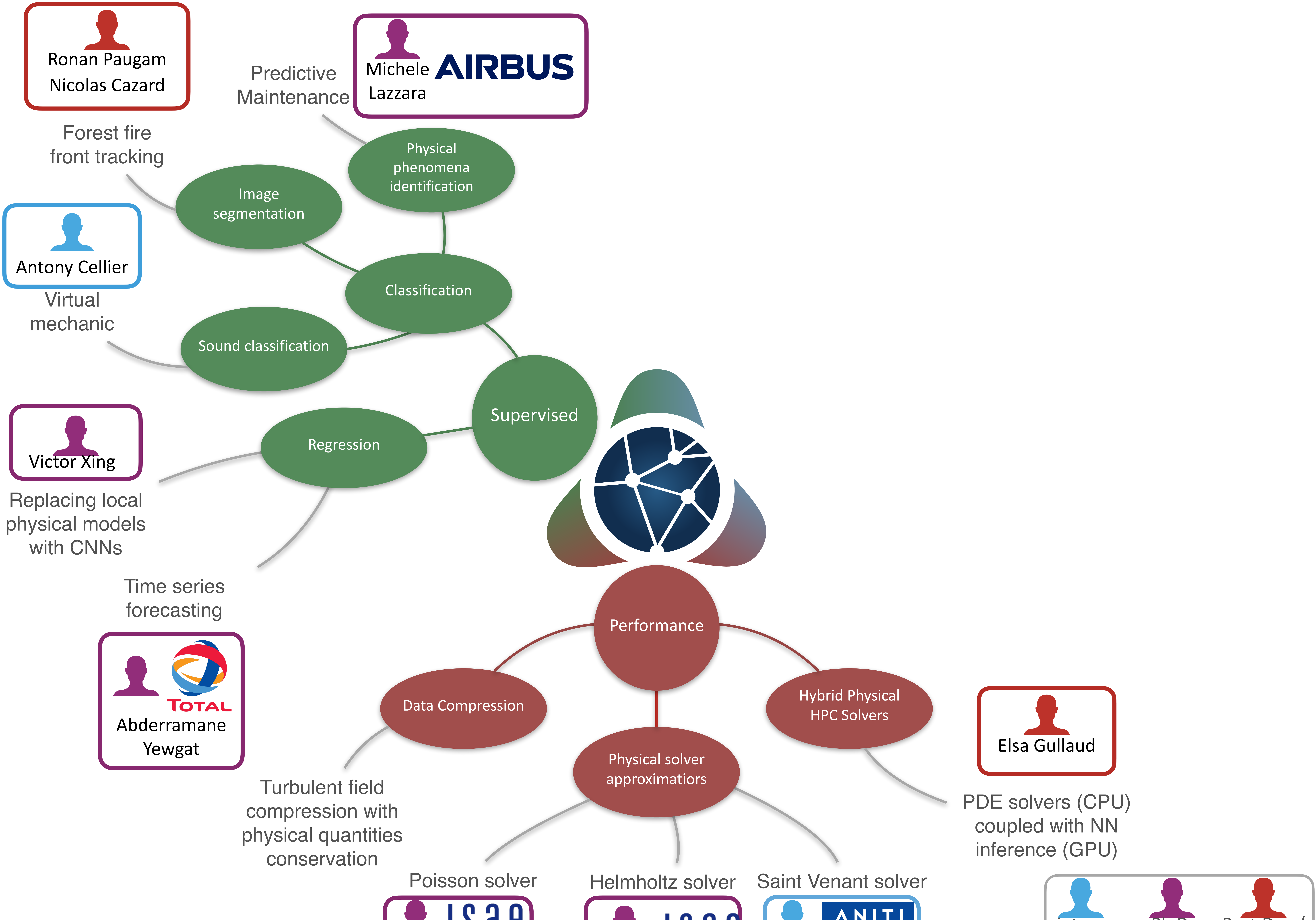

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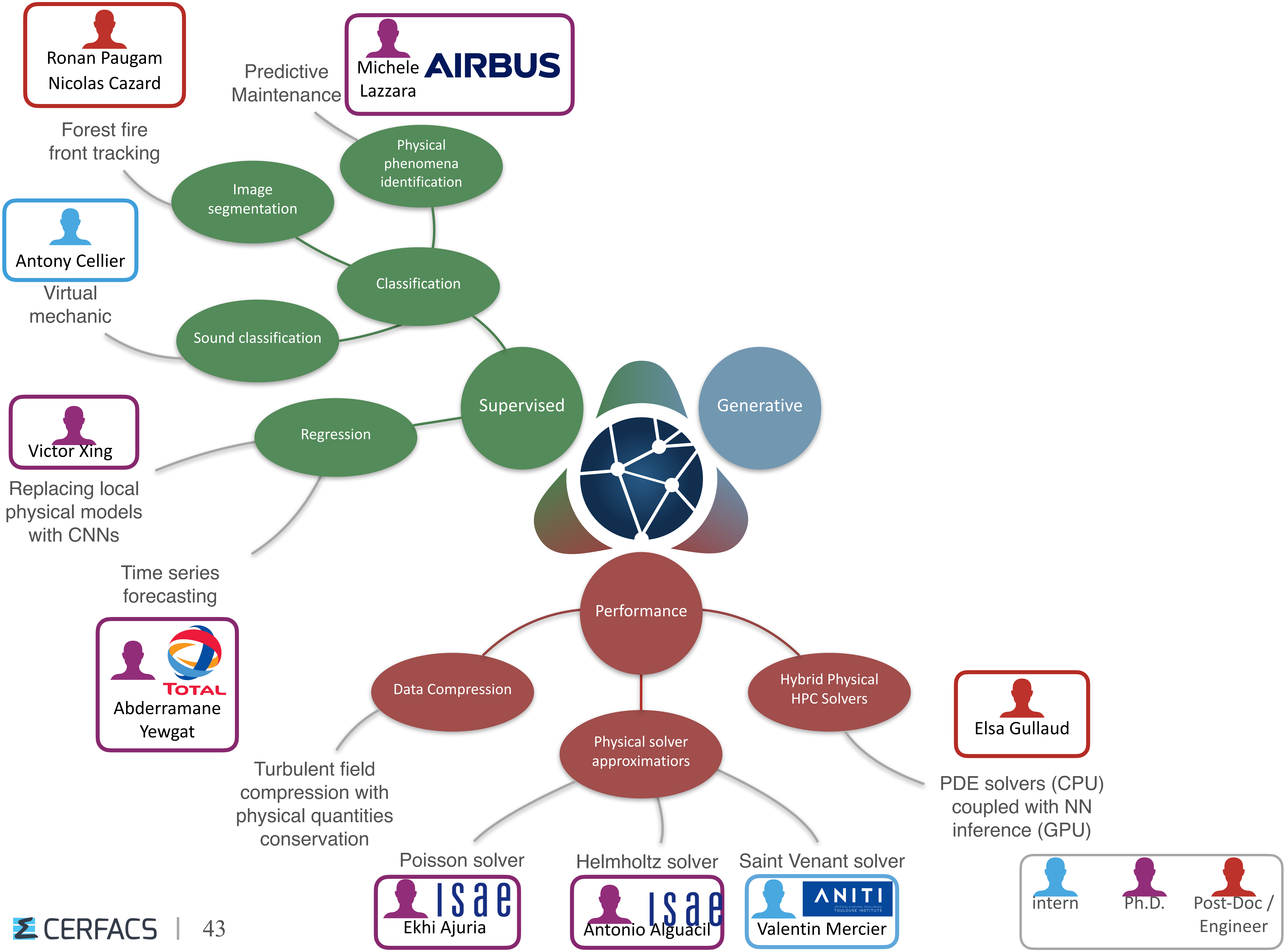
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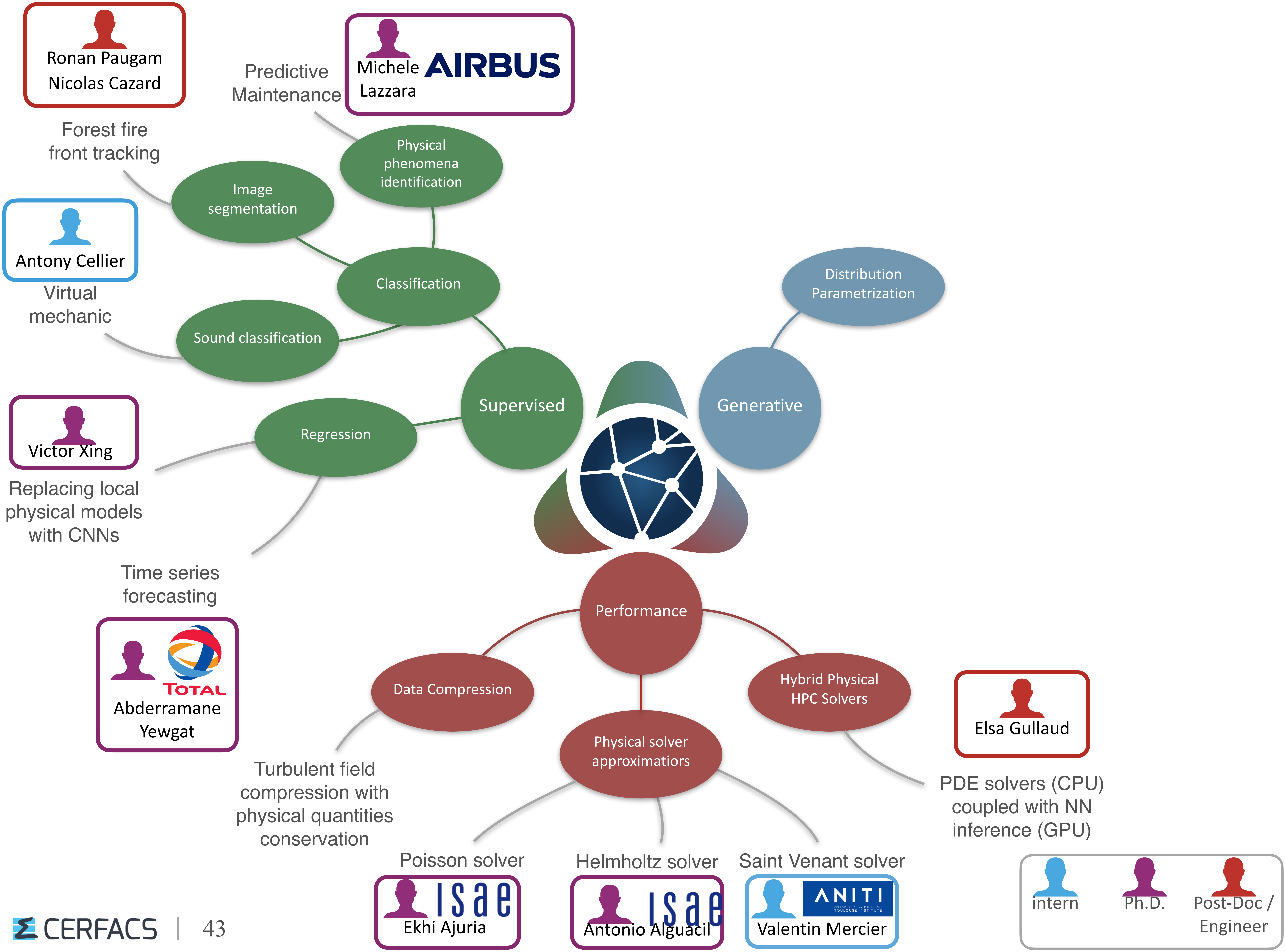

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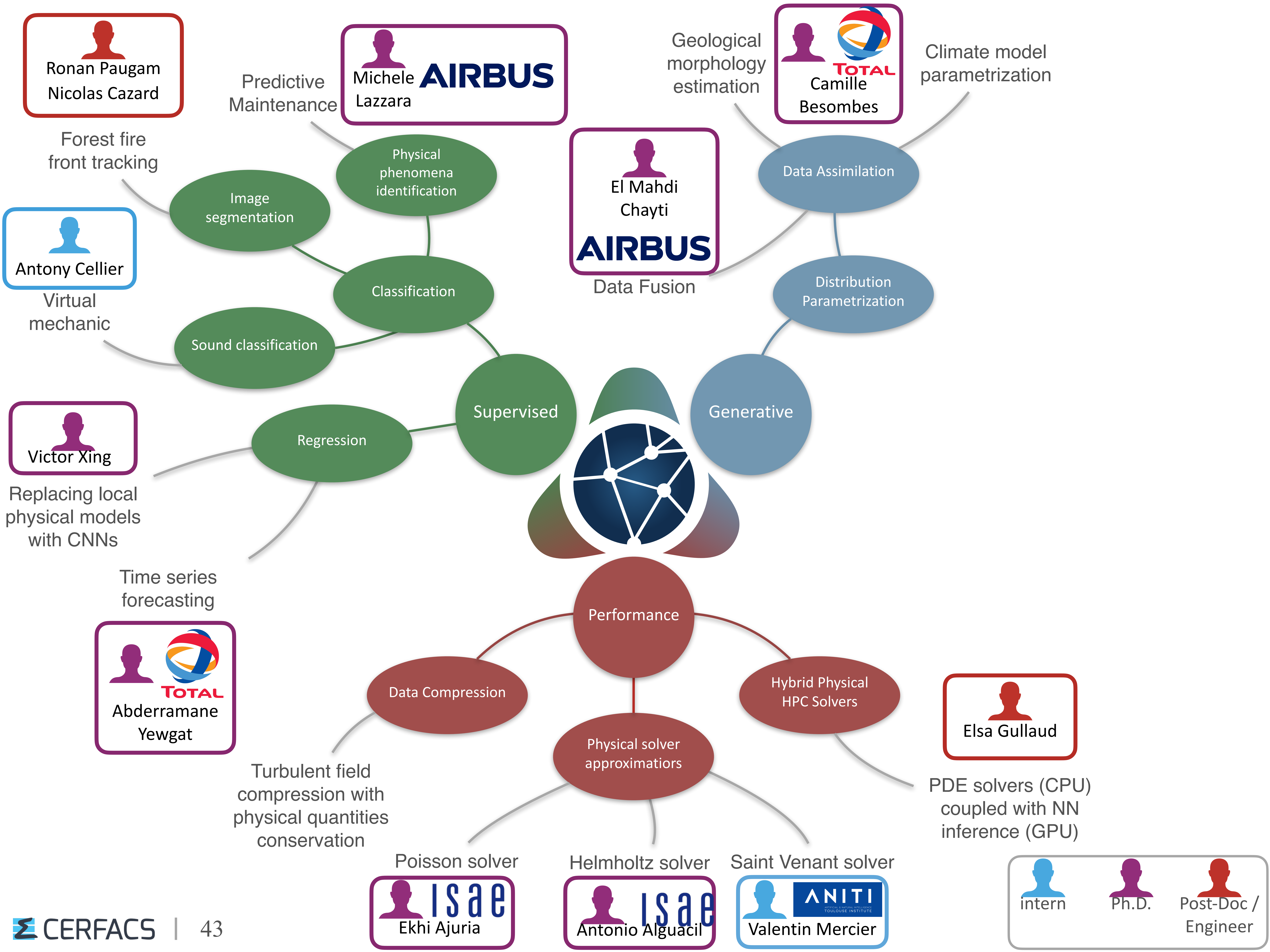
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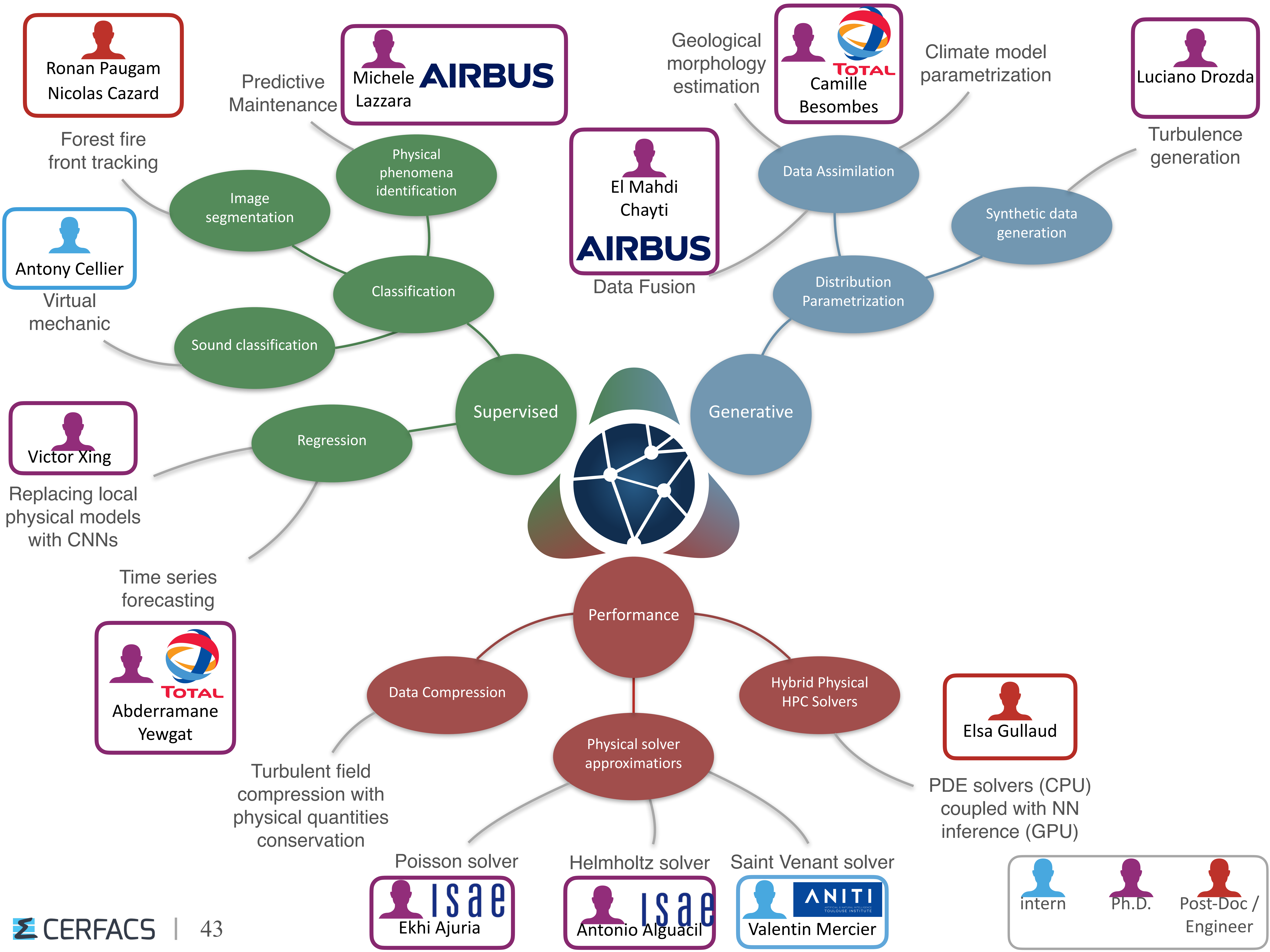

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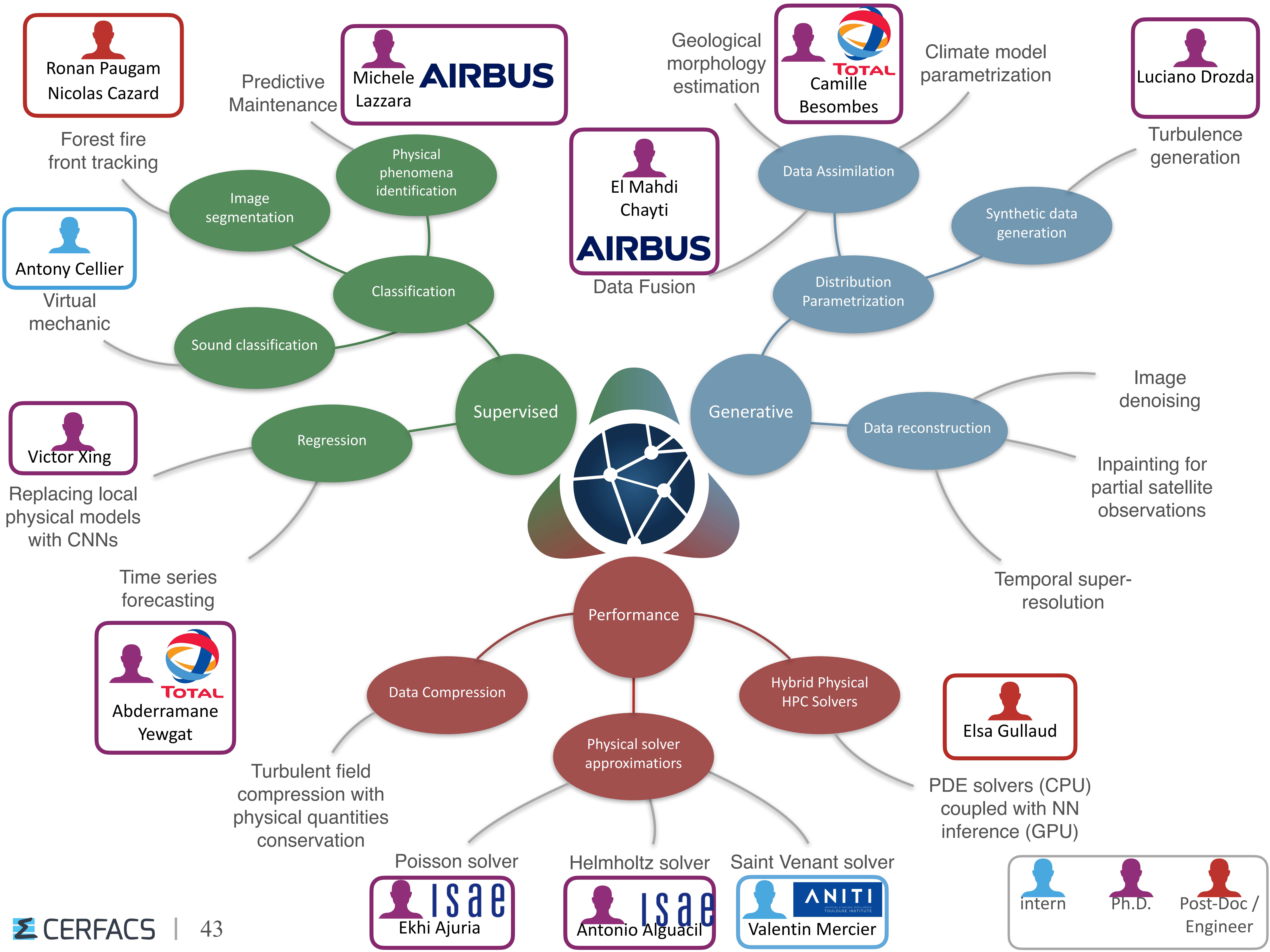

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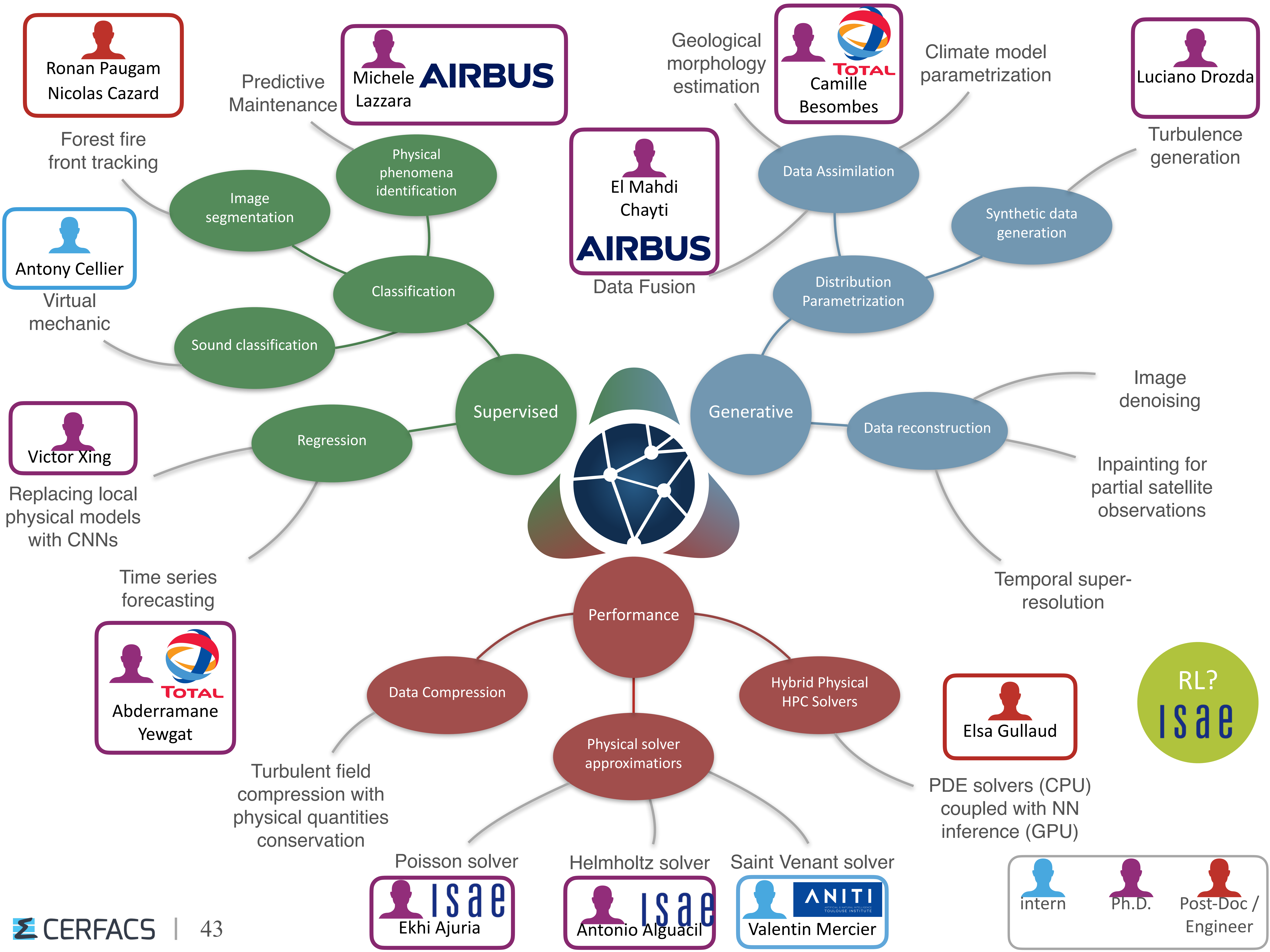
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Thank you

- Papers:
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- Conferences:
  - 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.