Leveraging AI for better high-fidelity CFD without compromising accuracy and reliability

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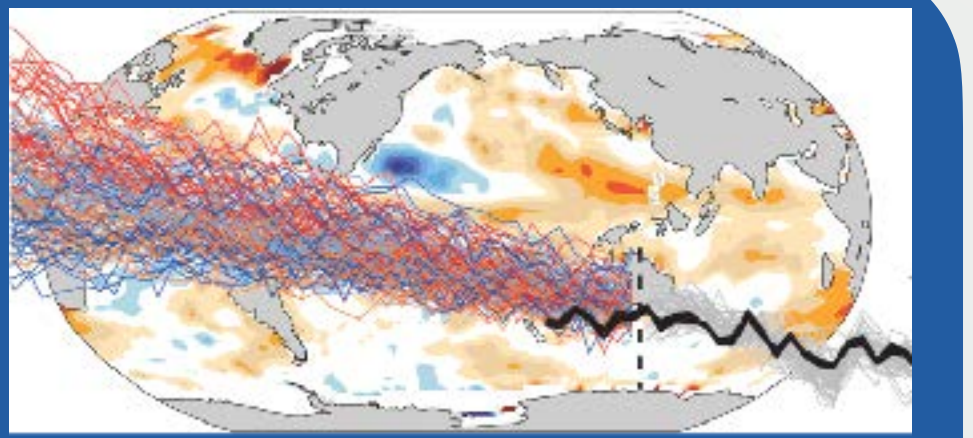
NHR4CES Community Workshop • 2023.03.01
Machine learning in Computational Fluid Dynamics

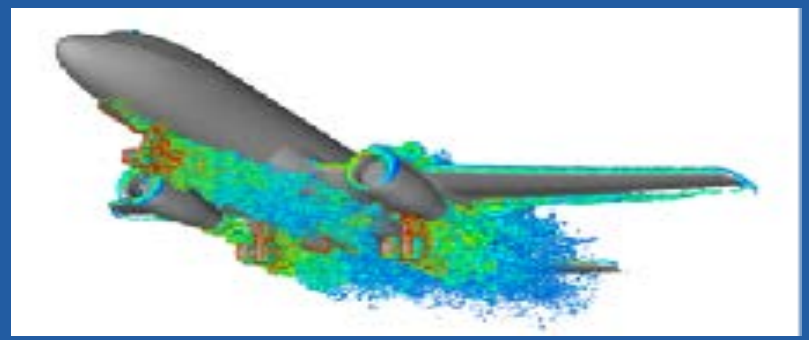


Climate Variability and Predictability

Environment and Safety

Hydrogen combustion

Climate - air transport interactions



Aerodynamics and Aerocoustics

Propulsion

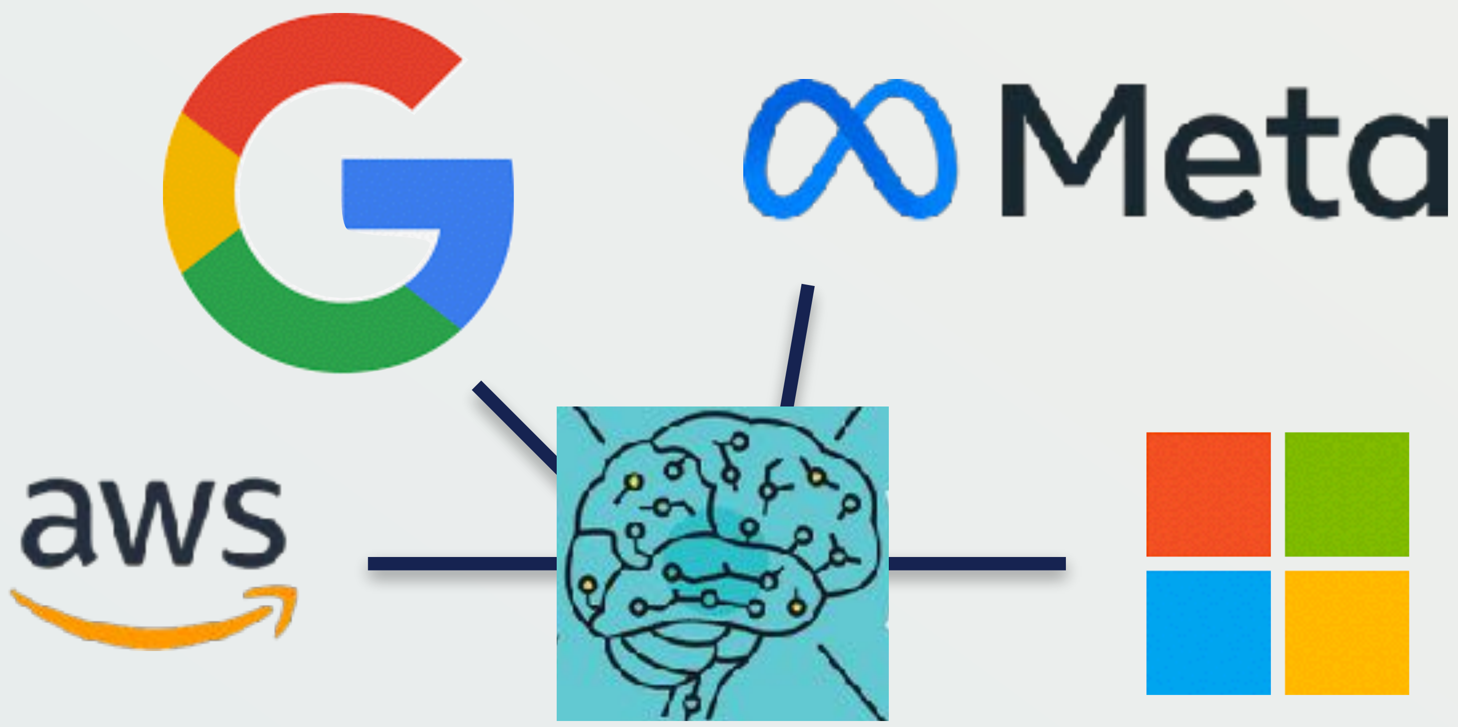
CERFACS

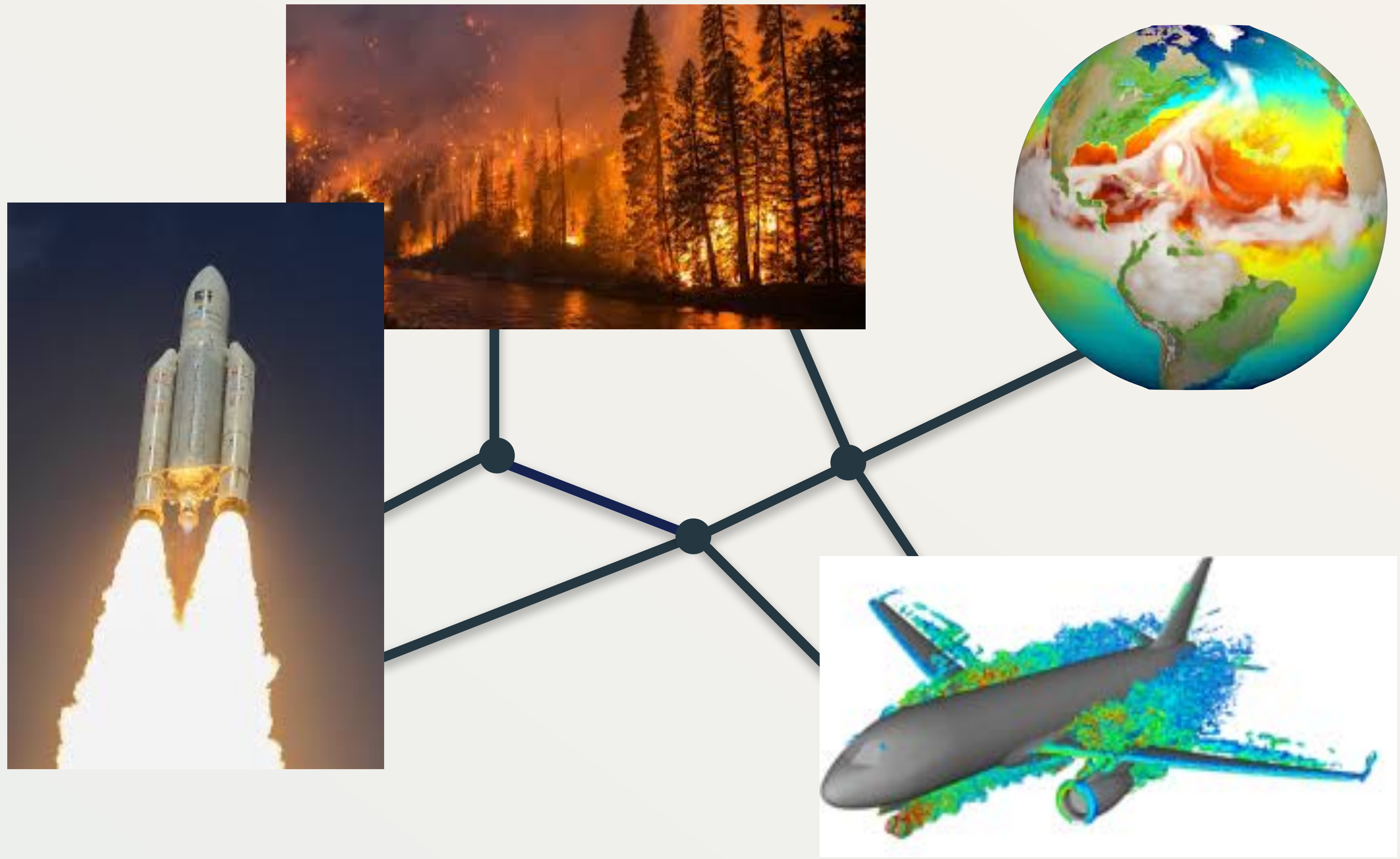
150 researchers

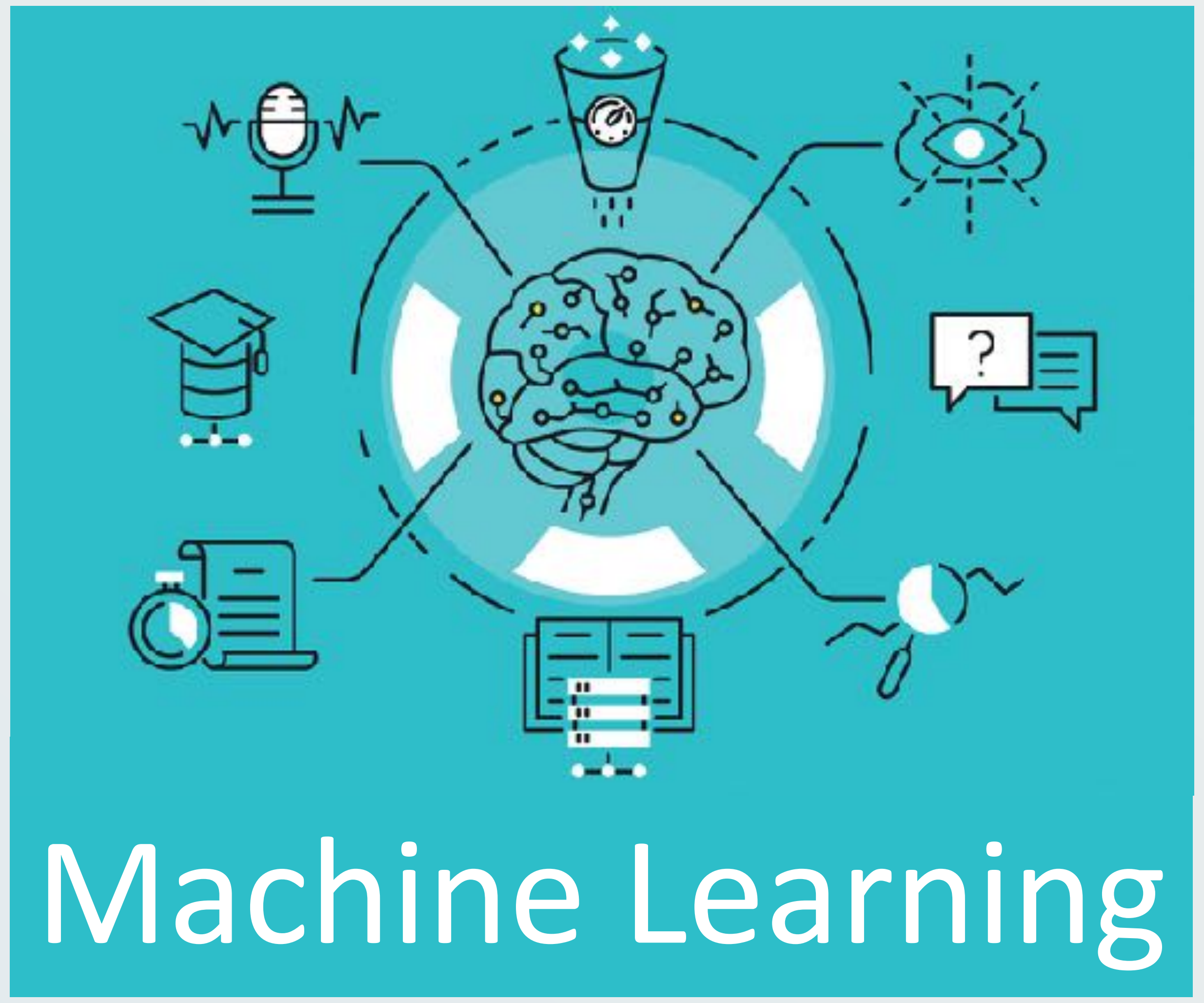
20 training sessions / y

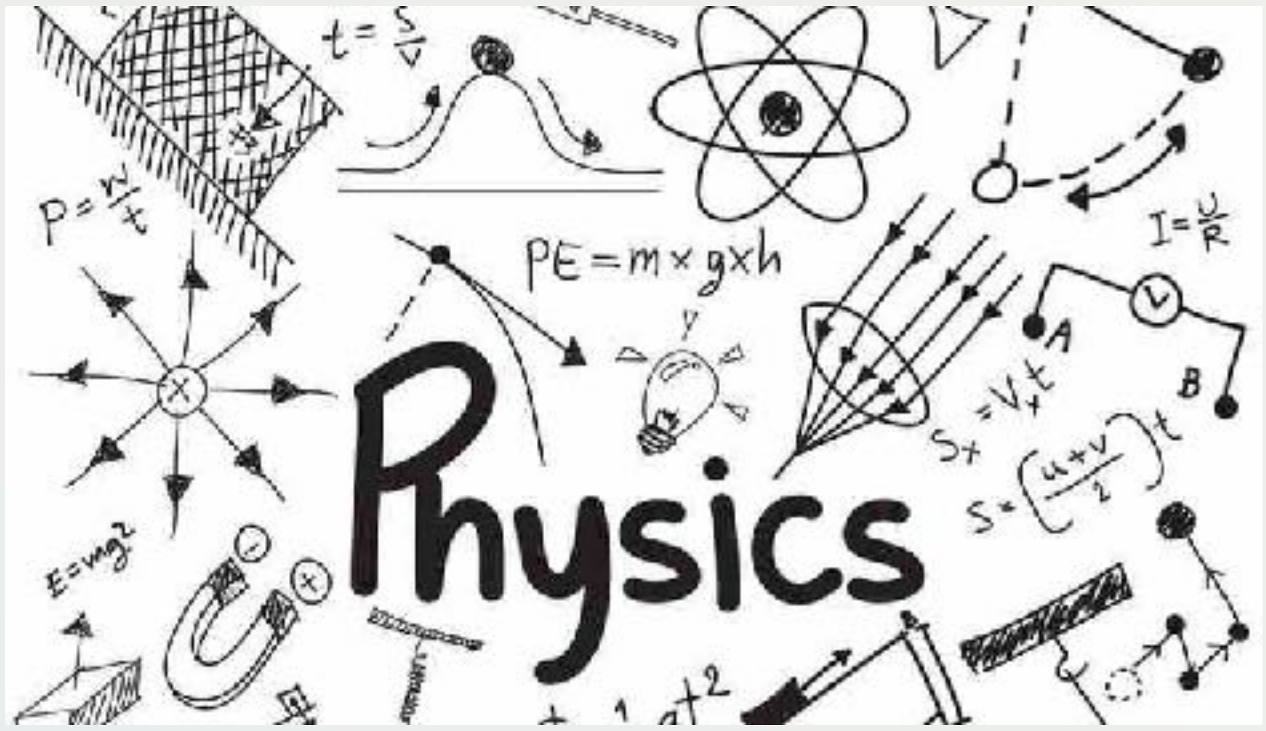
ONERA THE FRENCH AEROSPACE LAB | SAFRAN | cnes | eDF | AIRBUS | METEO FRANCE

AI ?

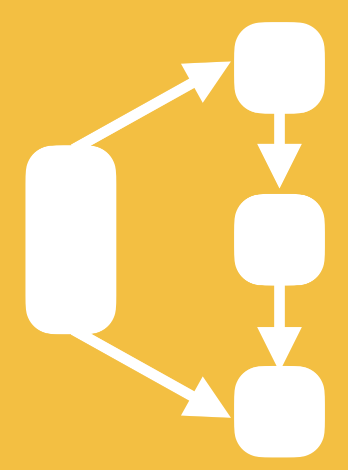




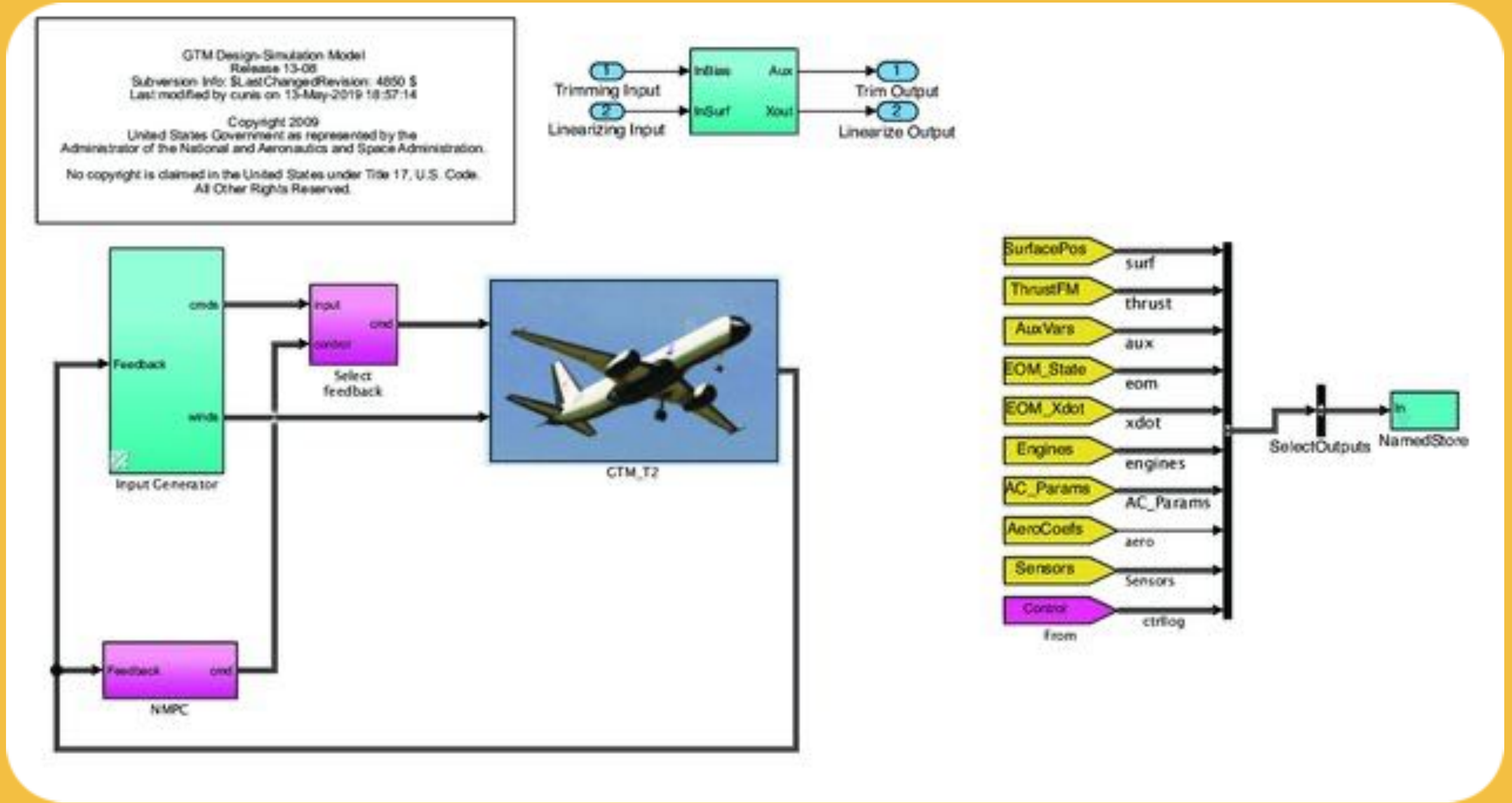




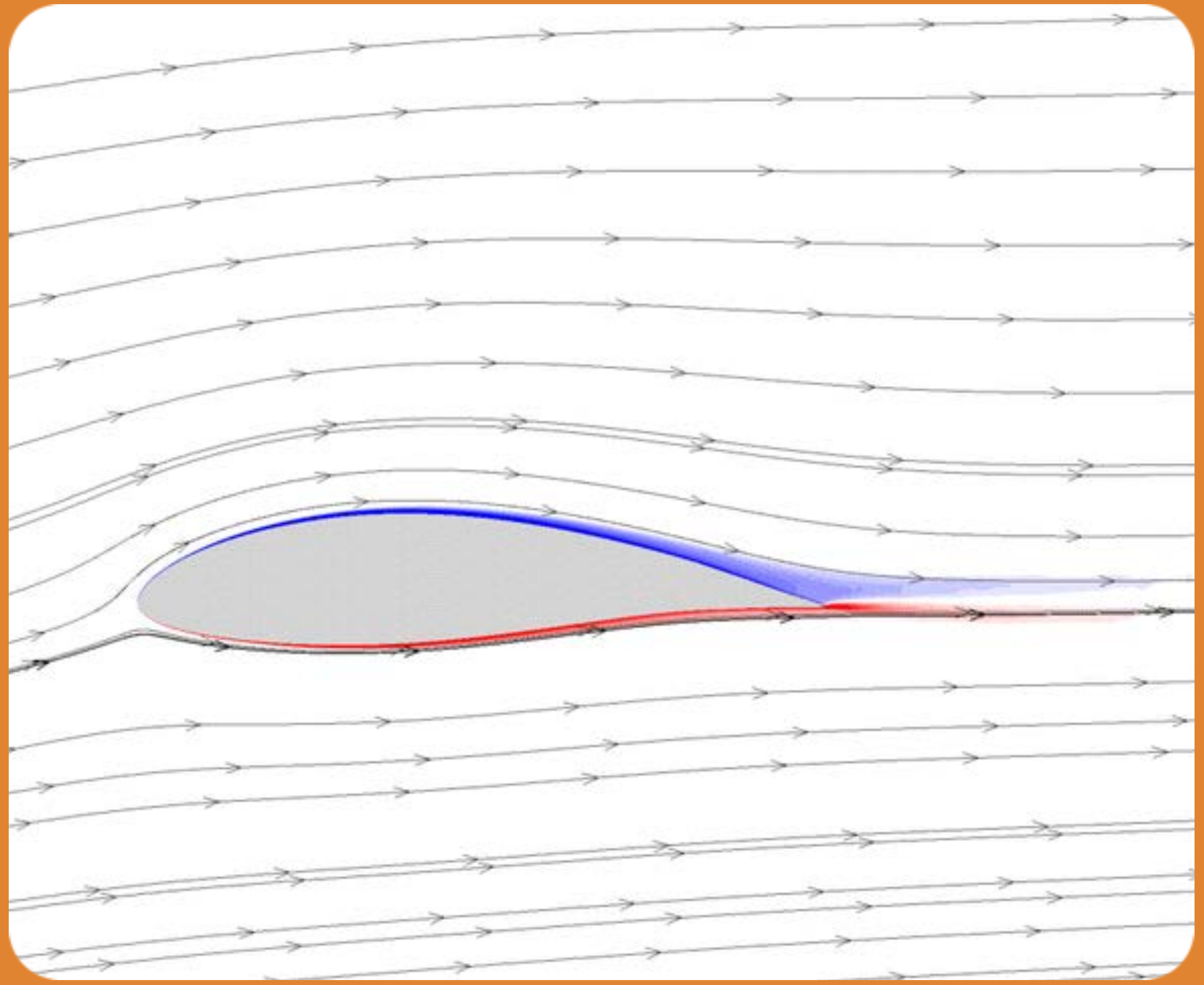
Simulation Tools



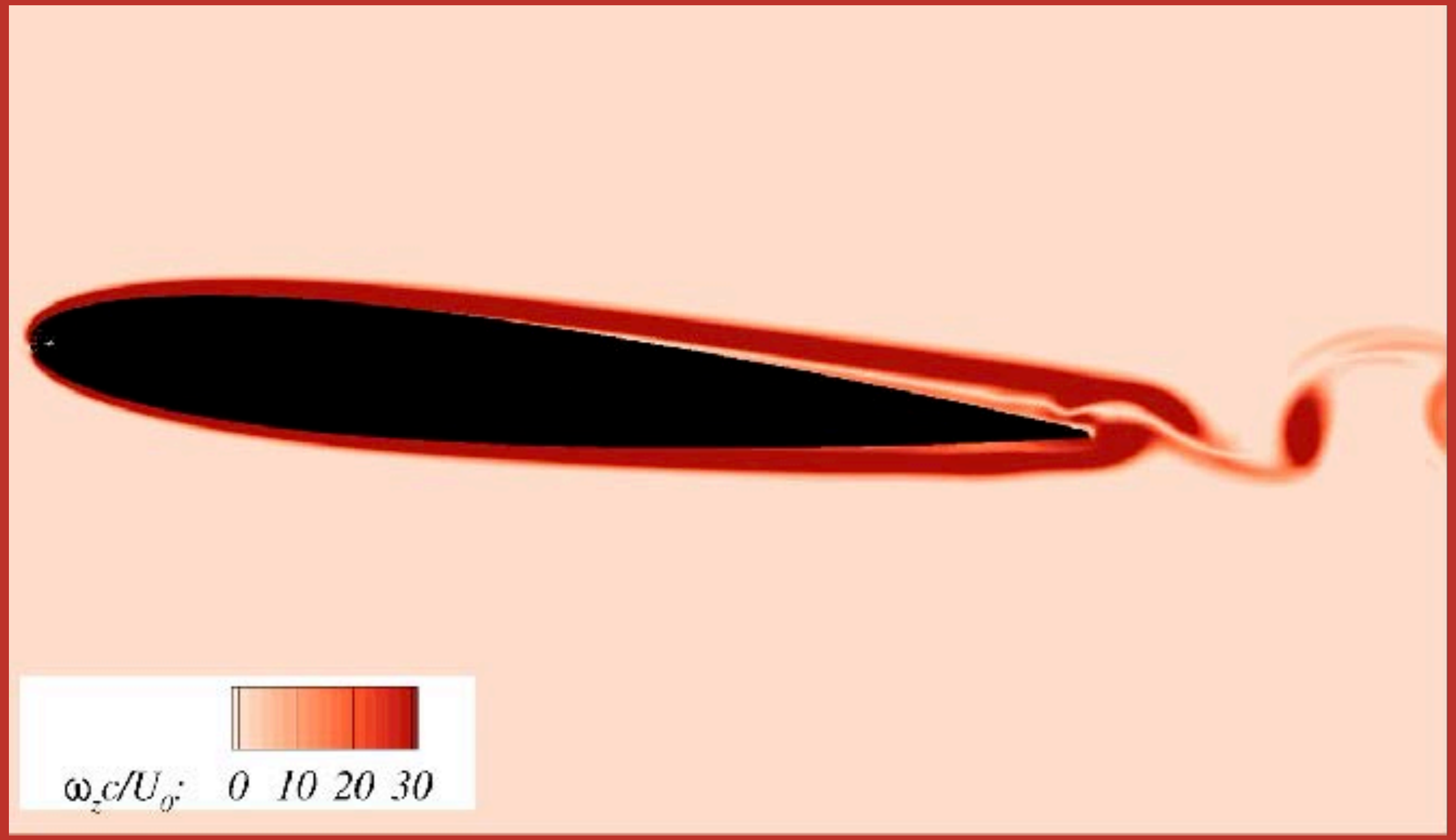
System Models



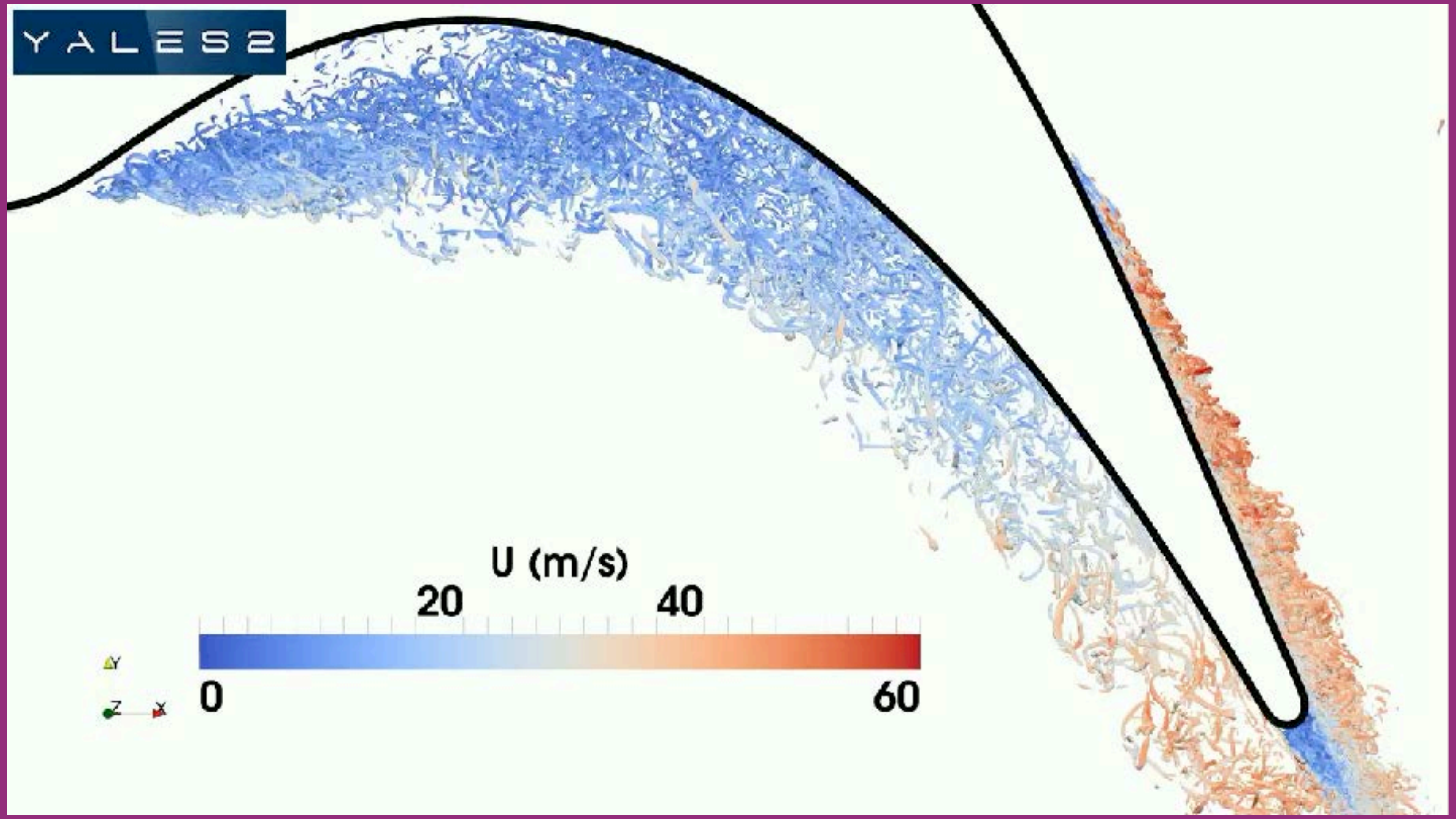
Steady-state simulation



Unsteady simulation (High fidelity)



Direct numerical simulation



Many ML applications

Active research field

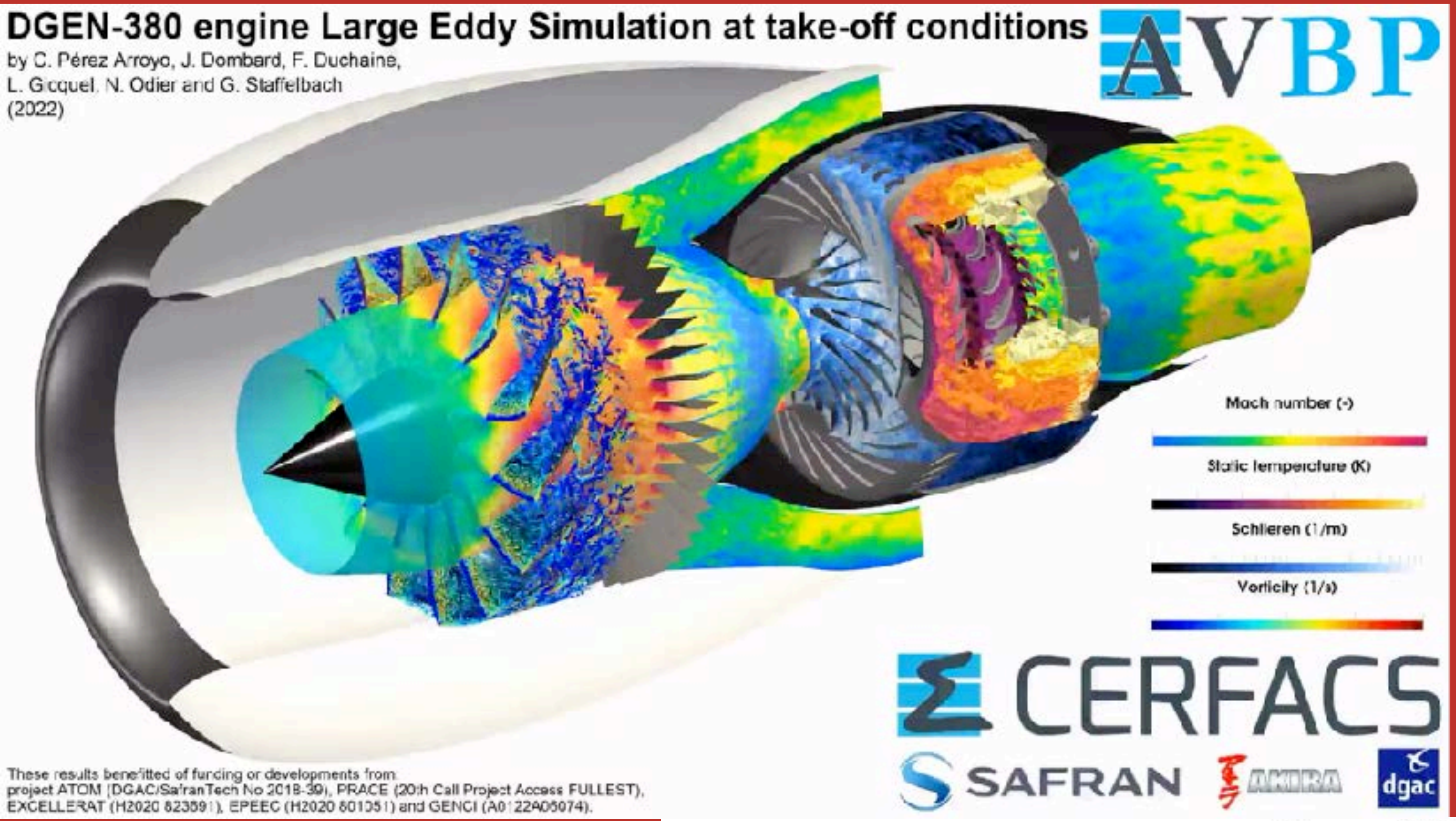
Emerging field

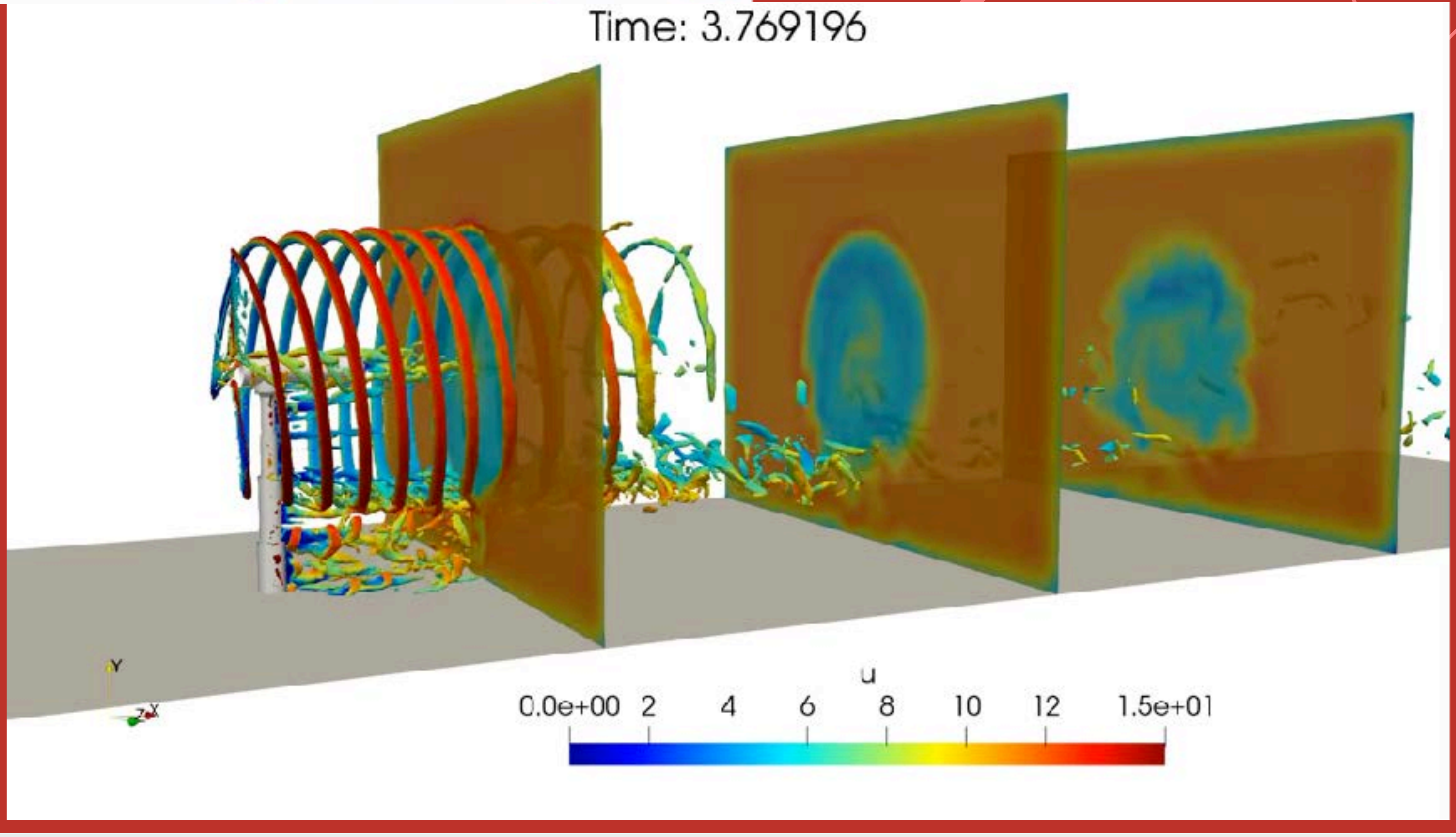
Too expensive

Hybrid High-Fidelity Simulation

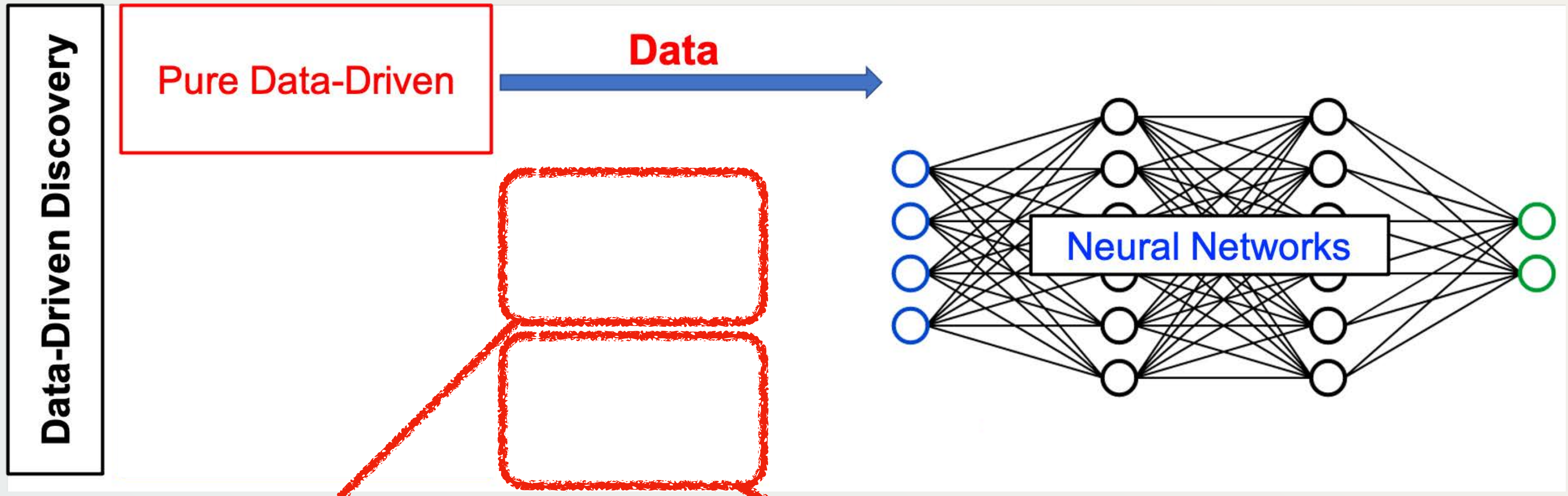
More accurate models

Innovative numerics





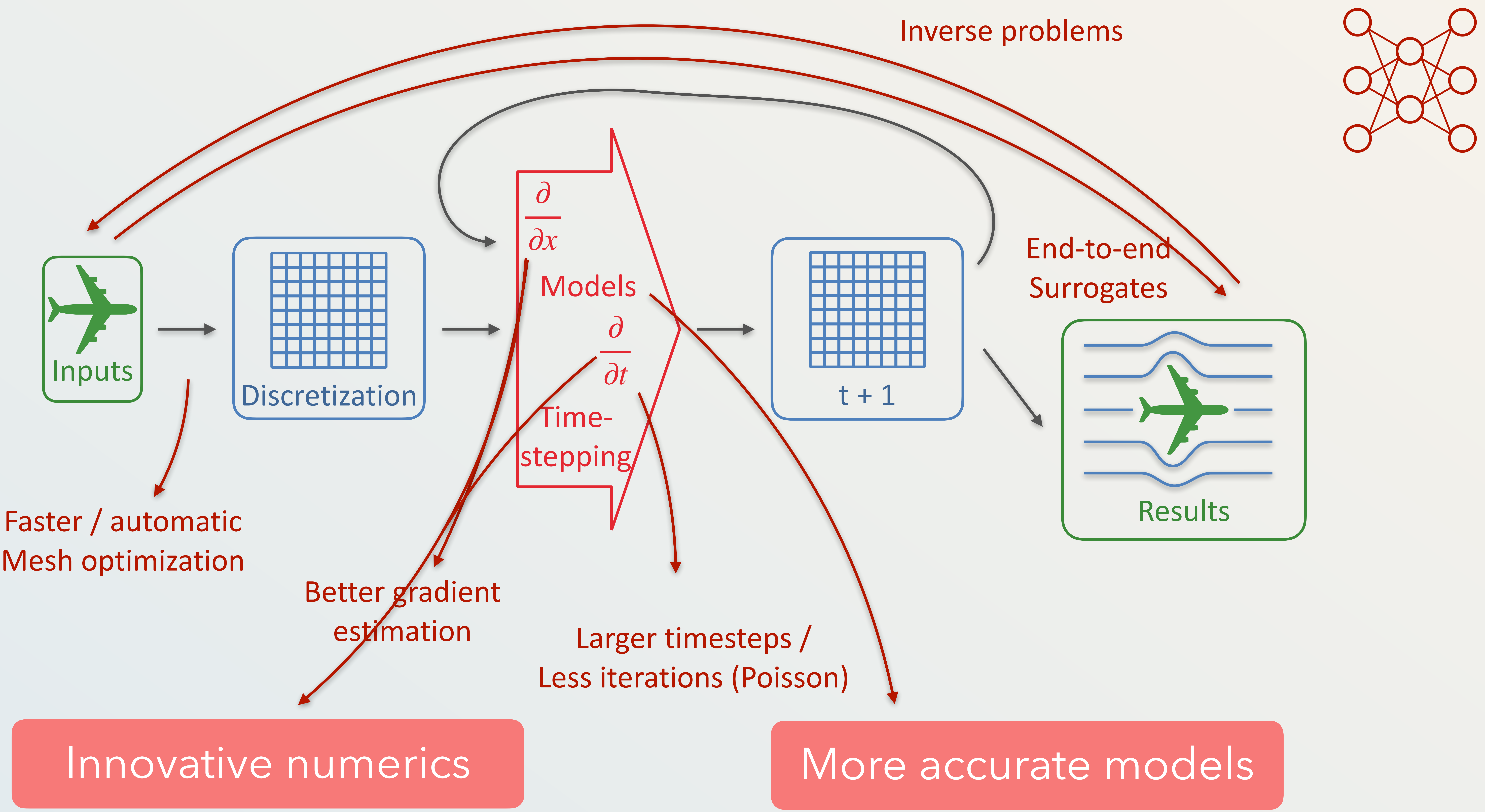
Zhang, Z., Shin, Y., & Em Karniadakis, G. (2022). GFINNs: GENERIC formalism informed neural networks for deterministic and stochastic dynamical systems. *Philosophical Transactions of the Royal Society A*, *380*(2229), 20210207.



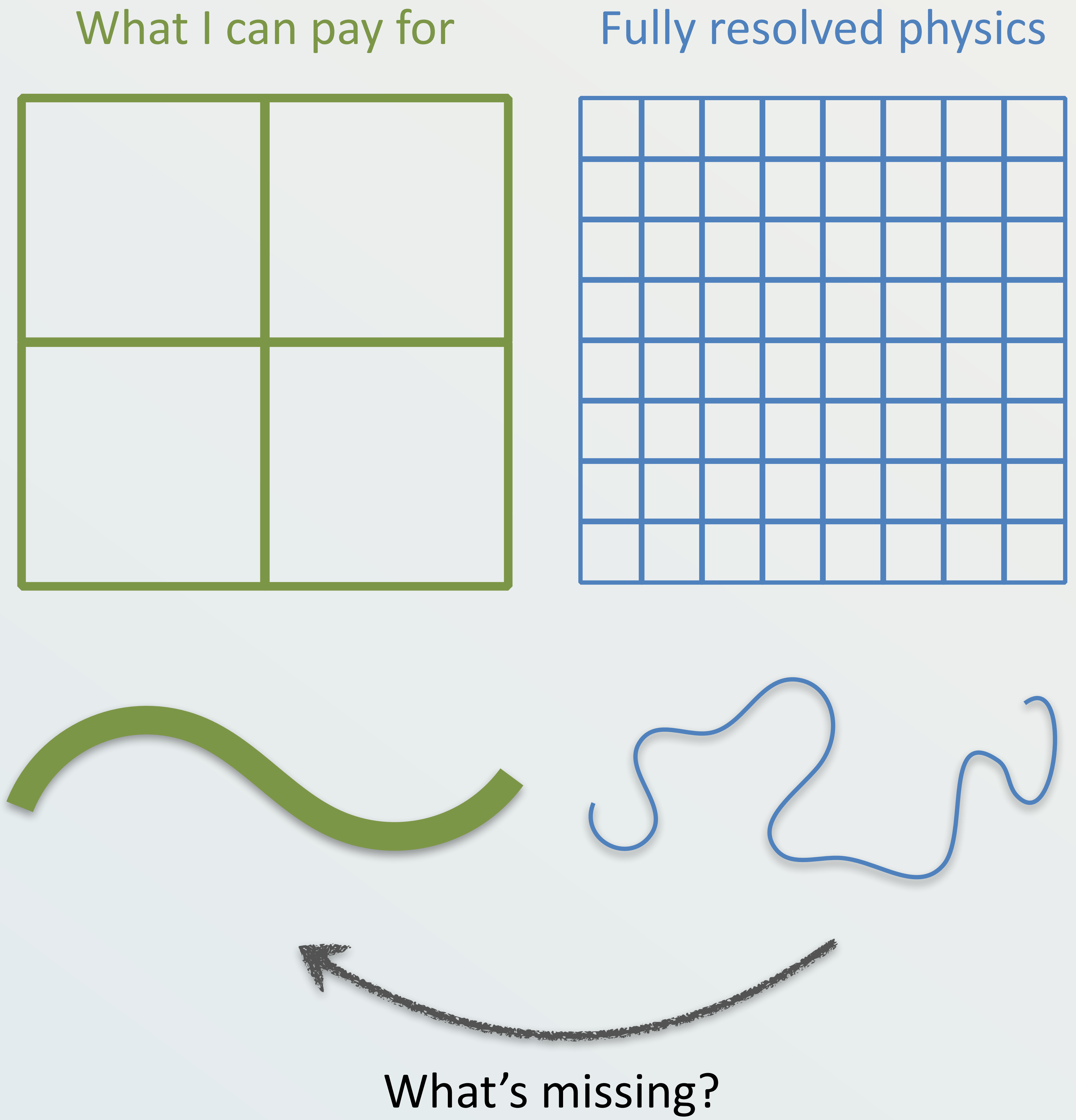
Penalize network with physics constraints through regularisation
Typically: PINNs (Physics-Informed Neural Networks)

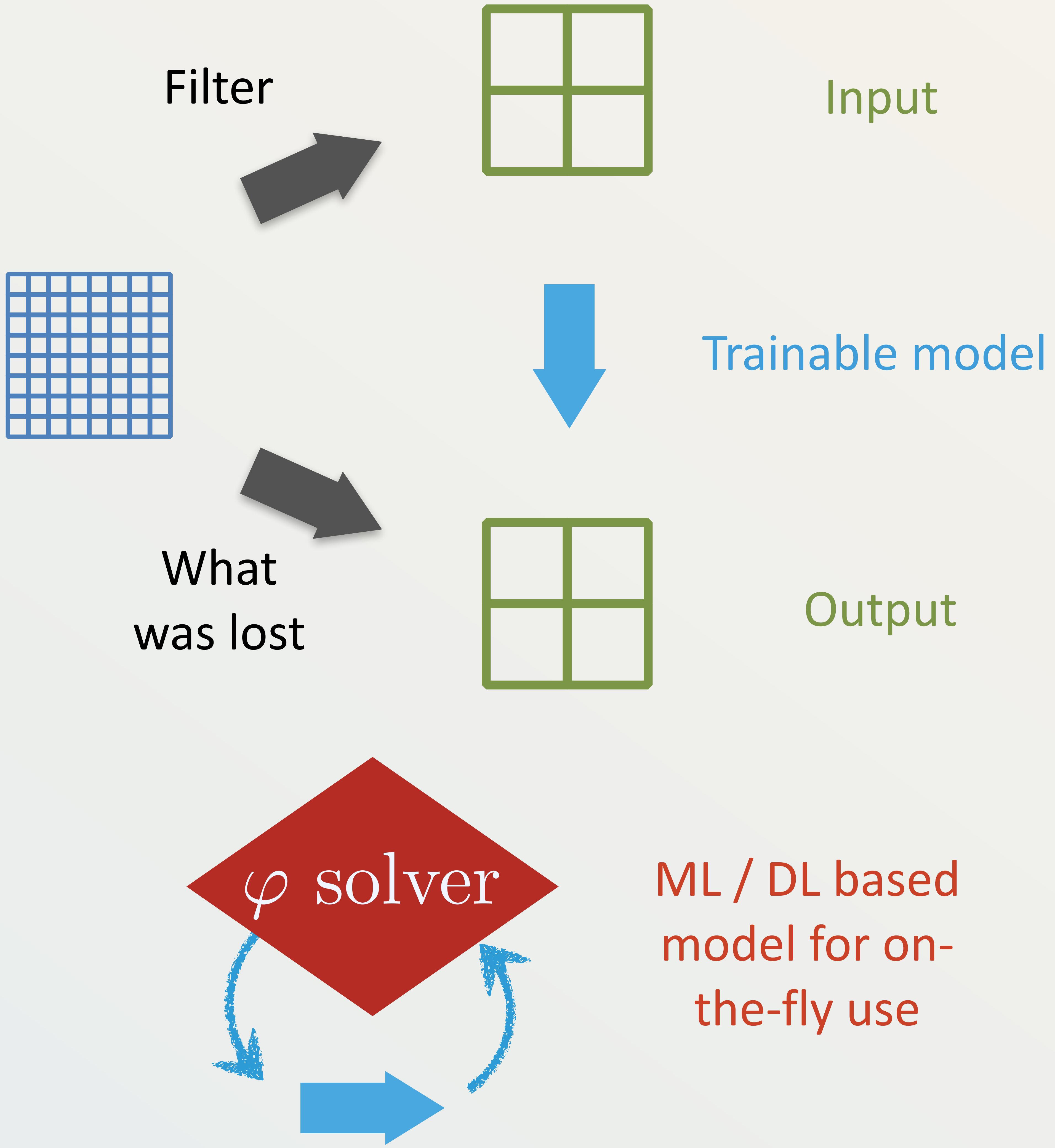
Enforce physics constraints in the network architecture

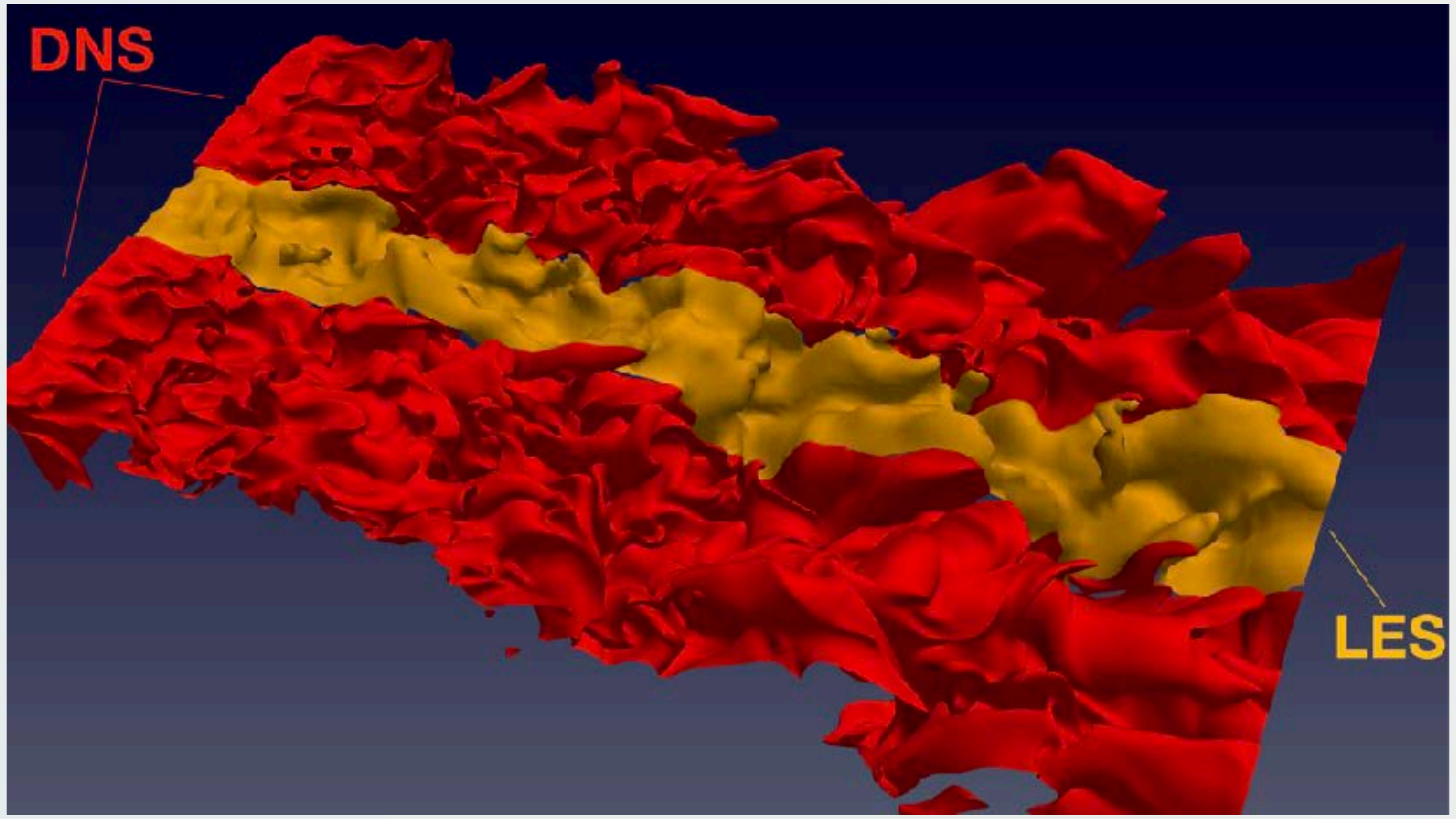
For now, <u>soft</u> constraints tend to under-perform high-fidelity methods
<u>Hard</u> constraints are promising for *accelerated* high-fidelity

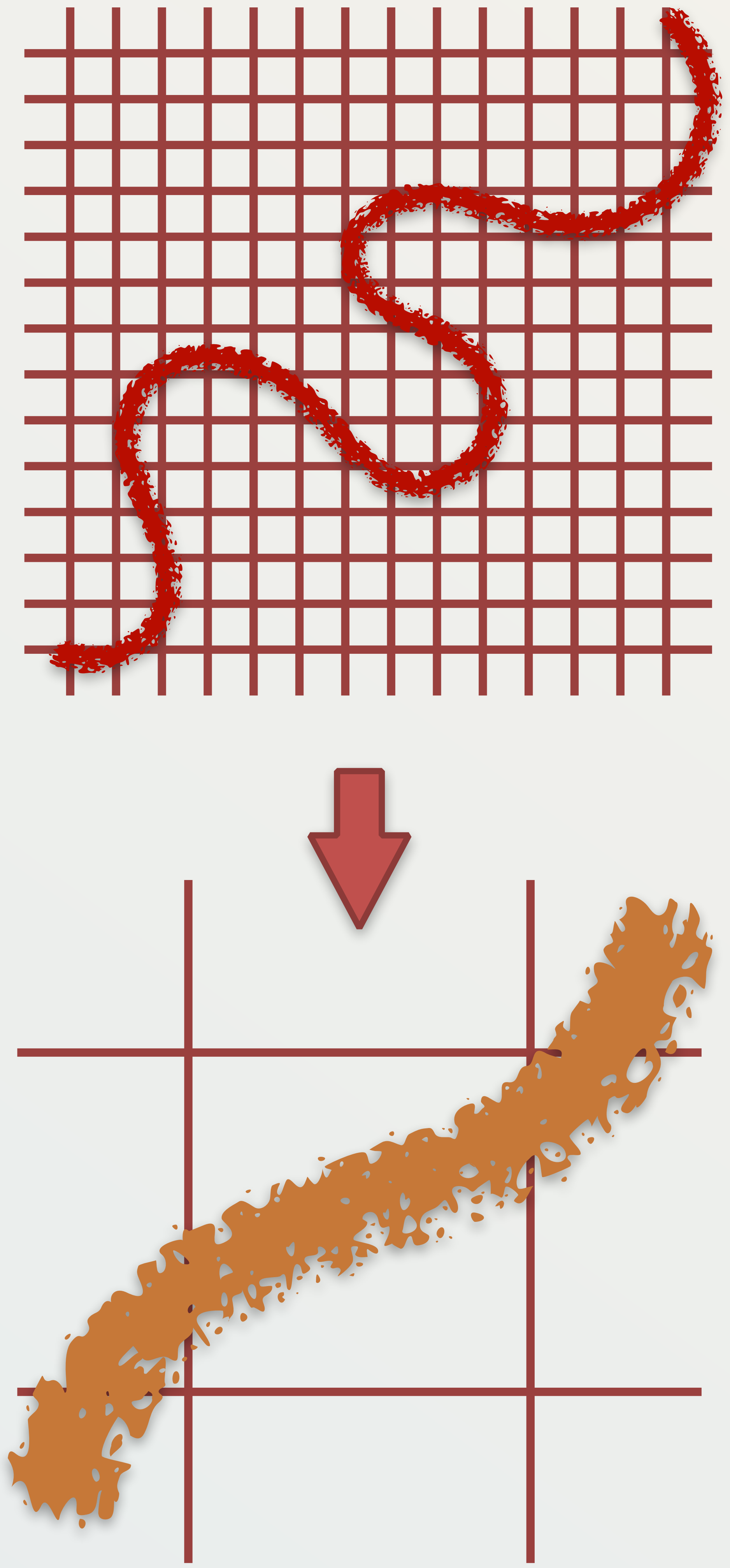

Inverse problems
Inputs
Discretization
$\frac{\partial}{\partial x}$
Models
$\frac{\partial}{\partial t}$
Time-
stepping
t + 1
End-to-end
Surrogates
Results
Faster / automatic
Mesh optimization
Better gradient
estimation
Larger timesteps /
Less iterations (Poisson)
Innovative numerics
More accurate models

More accurate models







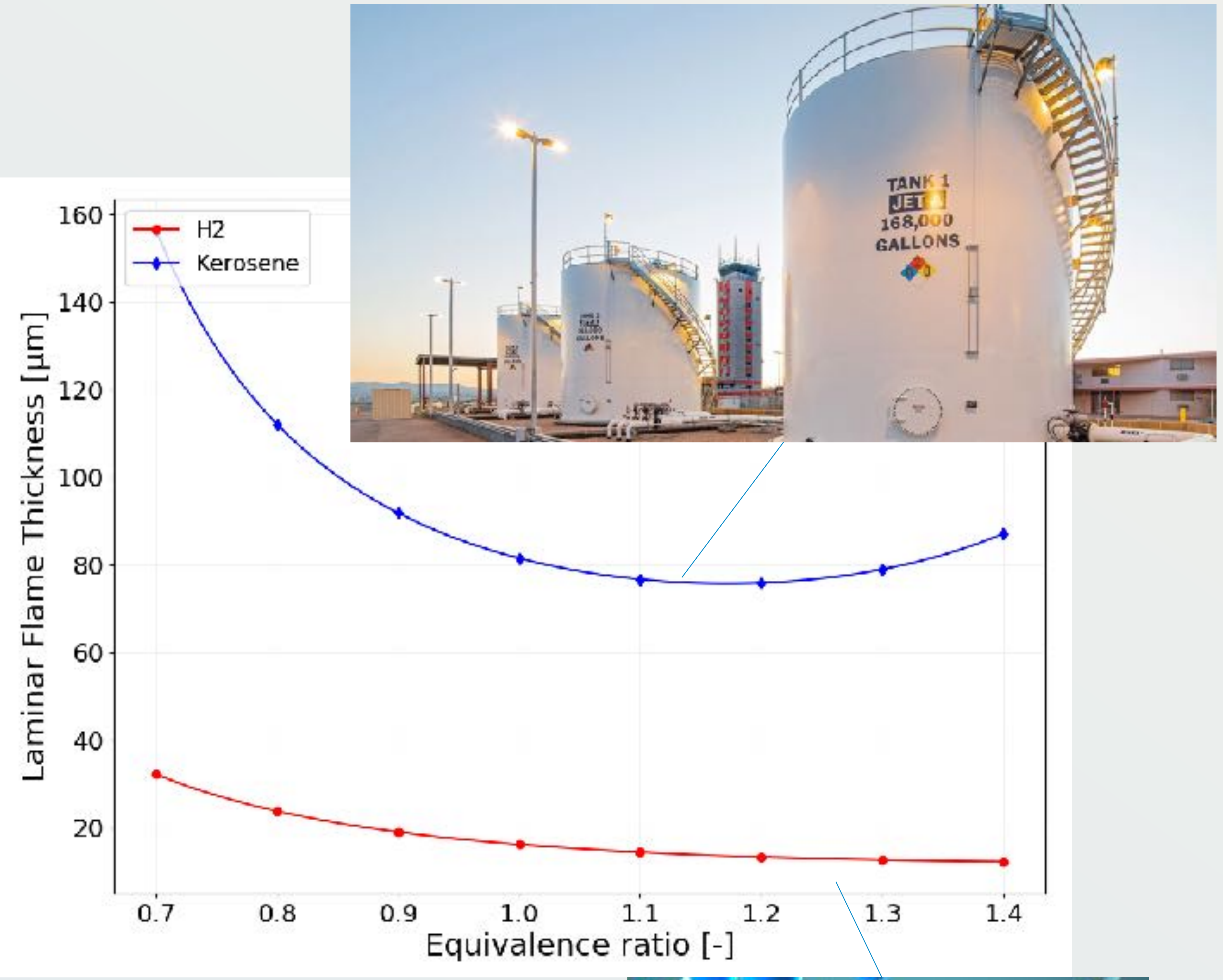


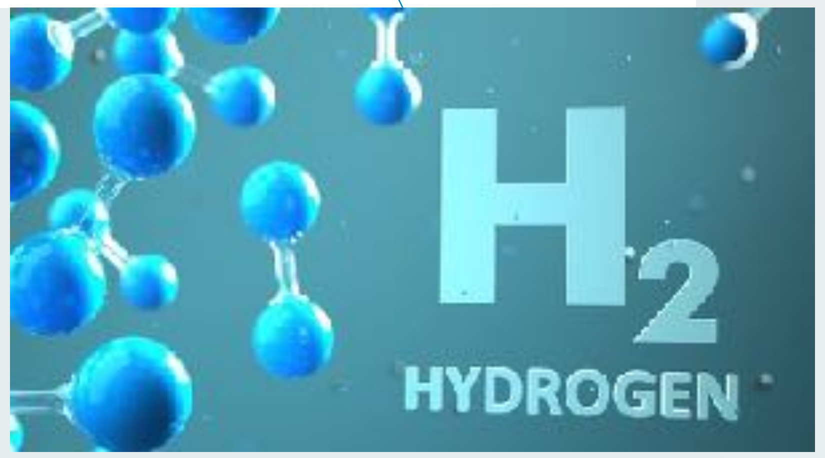
DNS: Resolved flame

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

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

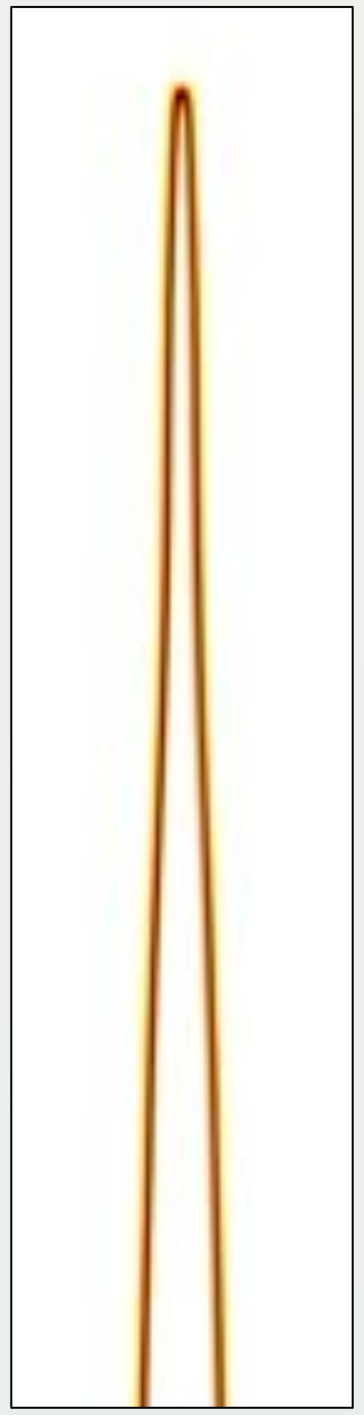
More accurate models



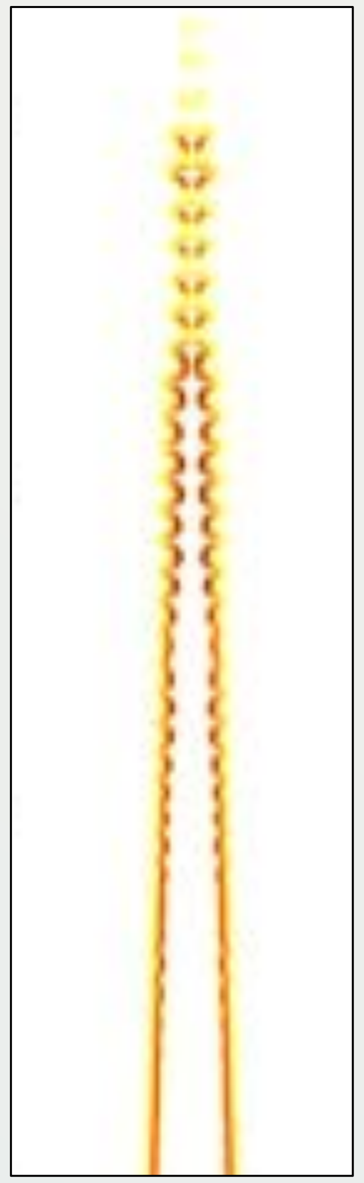


H_2 makes **thin** flames

H_2 makes **complex** flames



CH_4



H_2

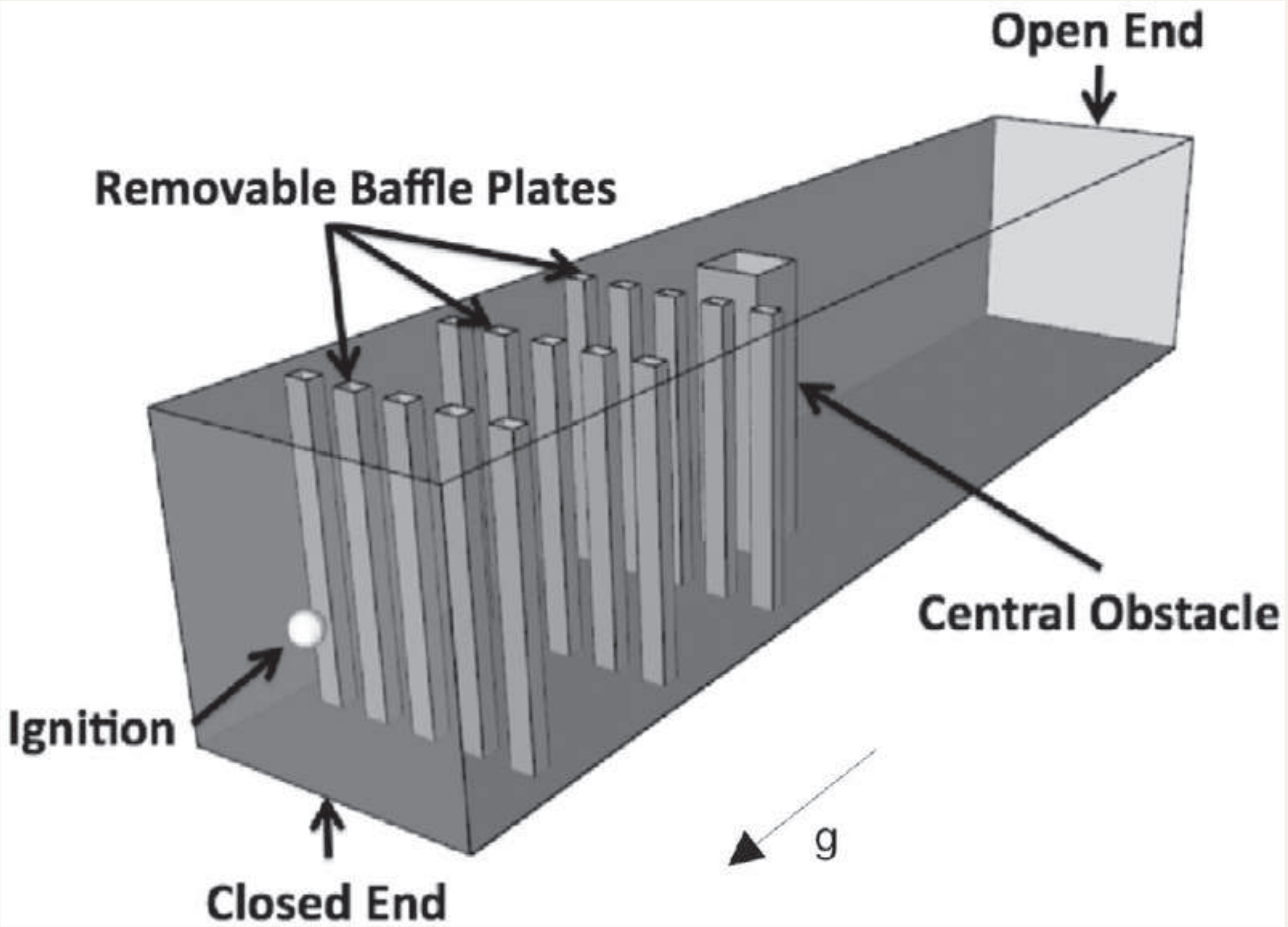
H_2 will stress existing turbulent combustion models.

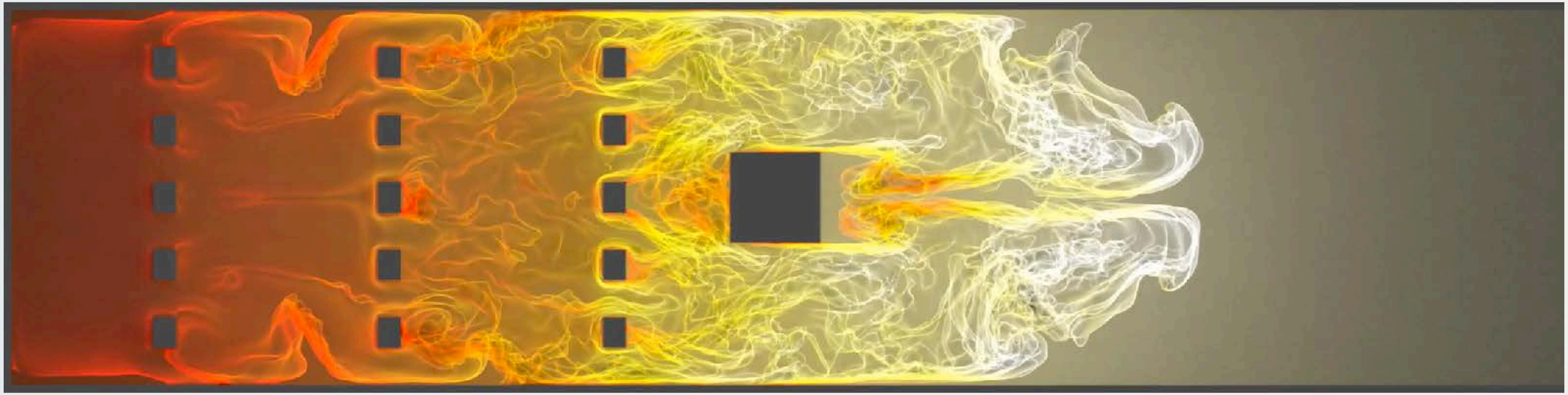
We can't afford to wait 20 years to develop new ones.

More accurate models

- Context: safety of industrial complexes in combustible gas leaks (notably H_2)

- Reactive LES of very large domains





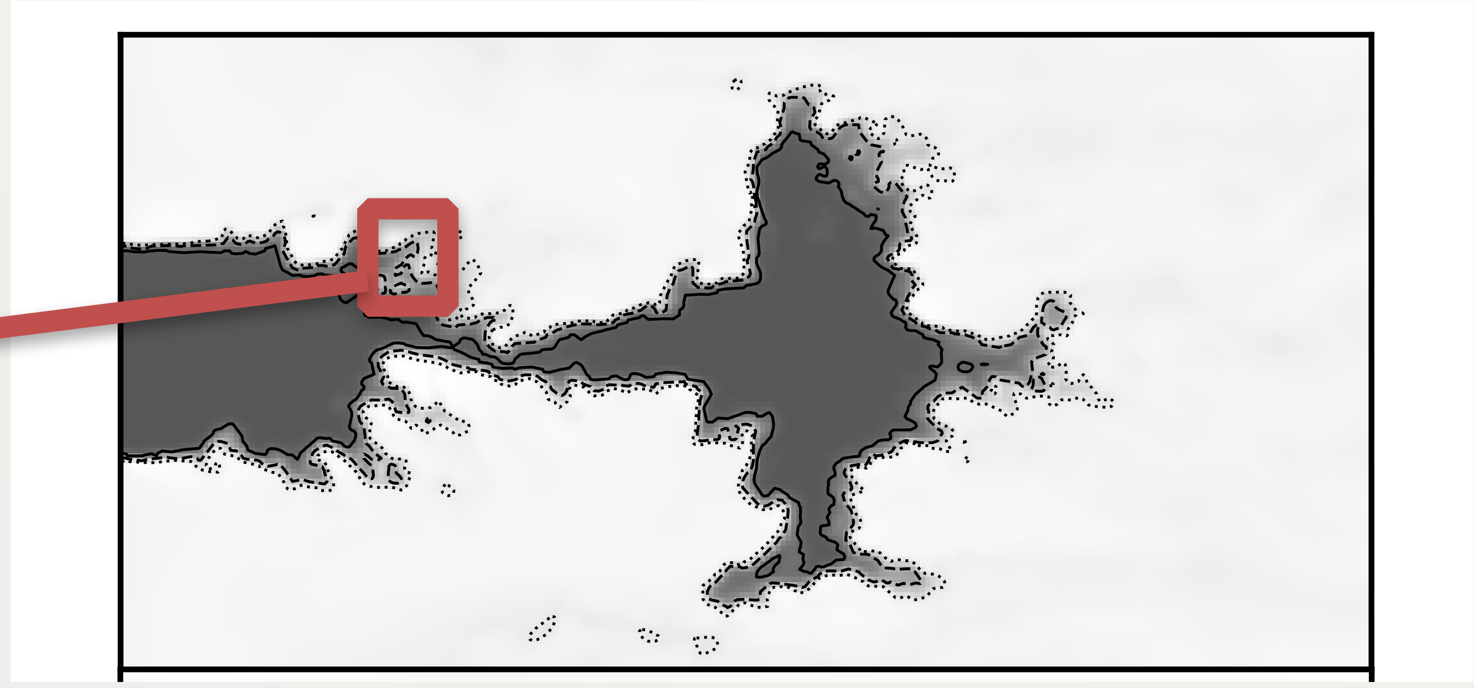
Efficiency functions - local to global

More accurate models

LOCAL FORMULATIONS:

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

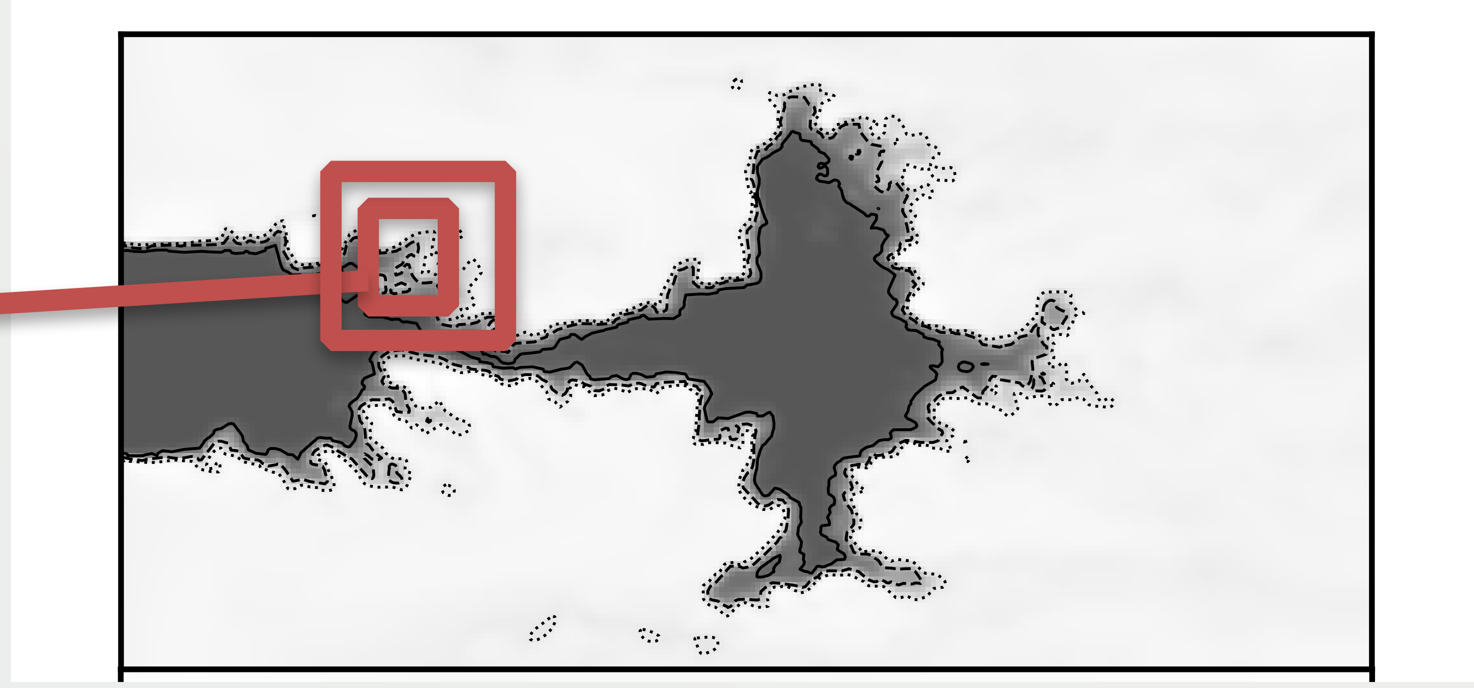
$$\Xi : \mathbb{R}^k \mapsto \mathbb{R}$$



DYNAMIC FORMULATIONS:

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

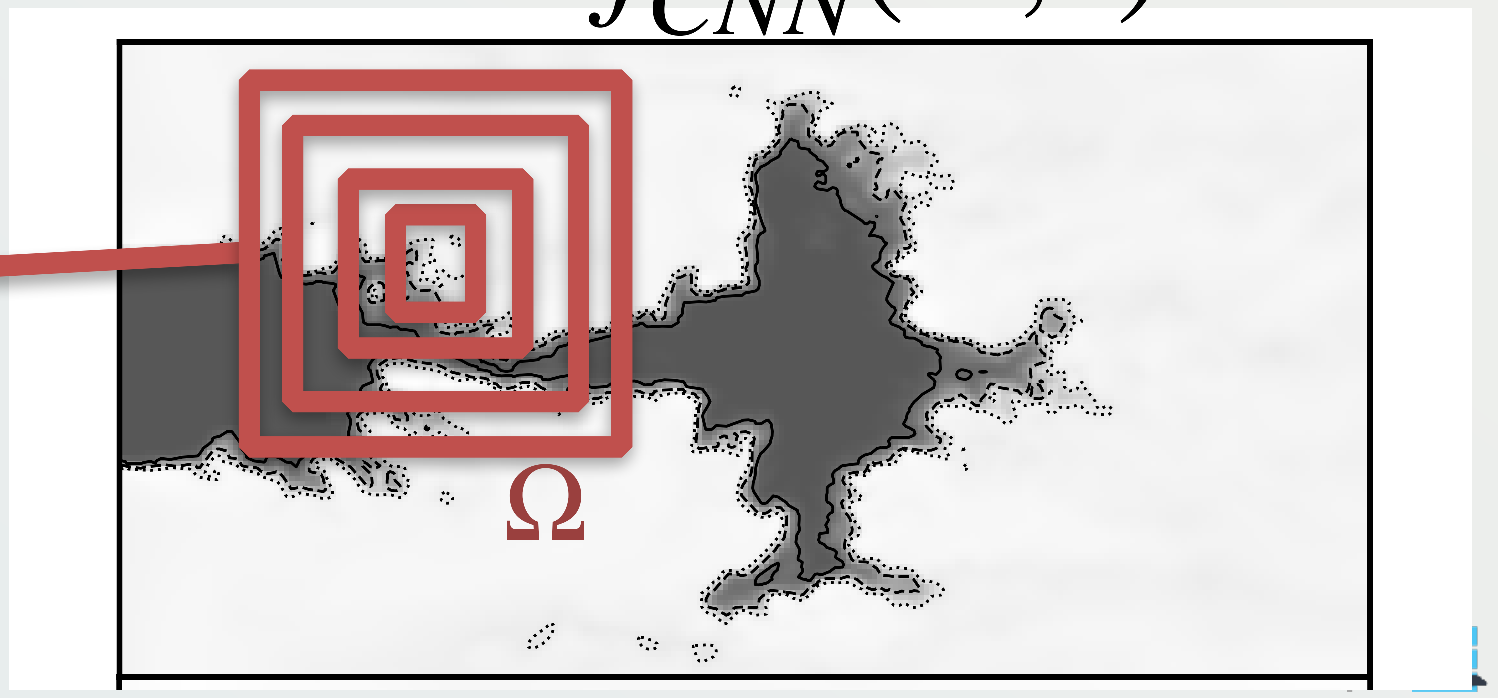
$$\Xi : \mathbb{R}^{2k} \mapsto \mathbb{R}$$



CNN FORMULATION:

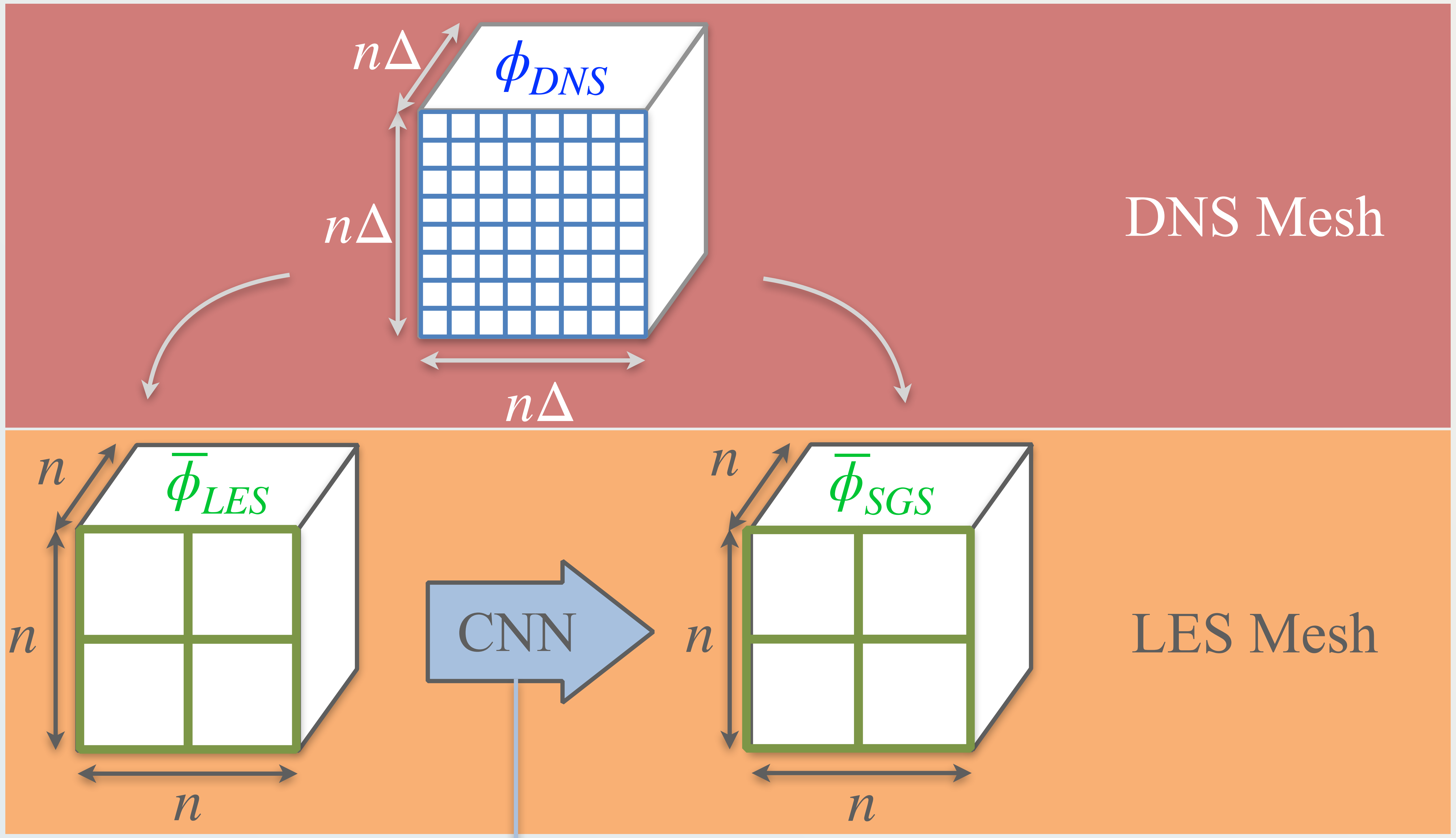
- 2019 - Lapeyre et al.

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



Building the dataset

More accurate models



Convolutional neural network

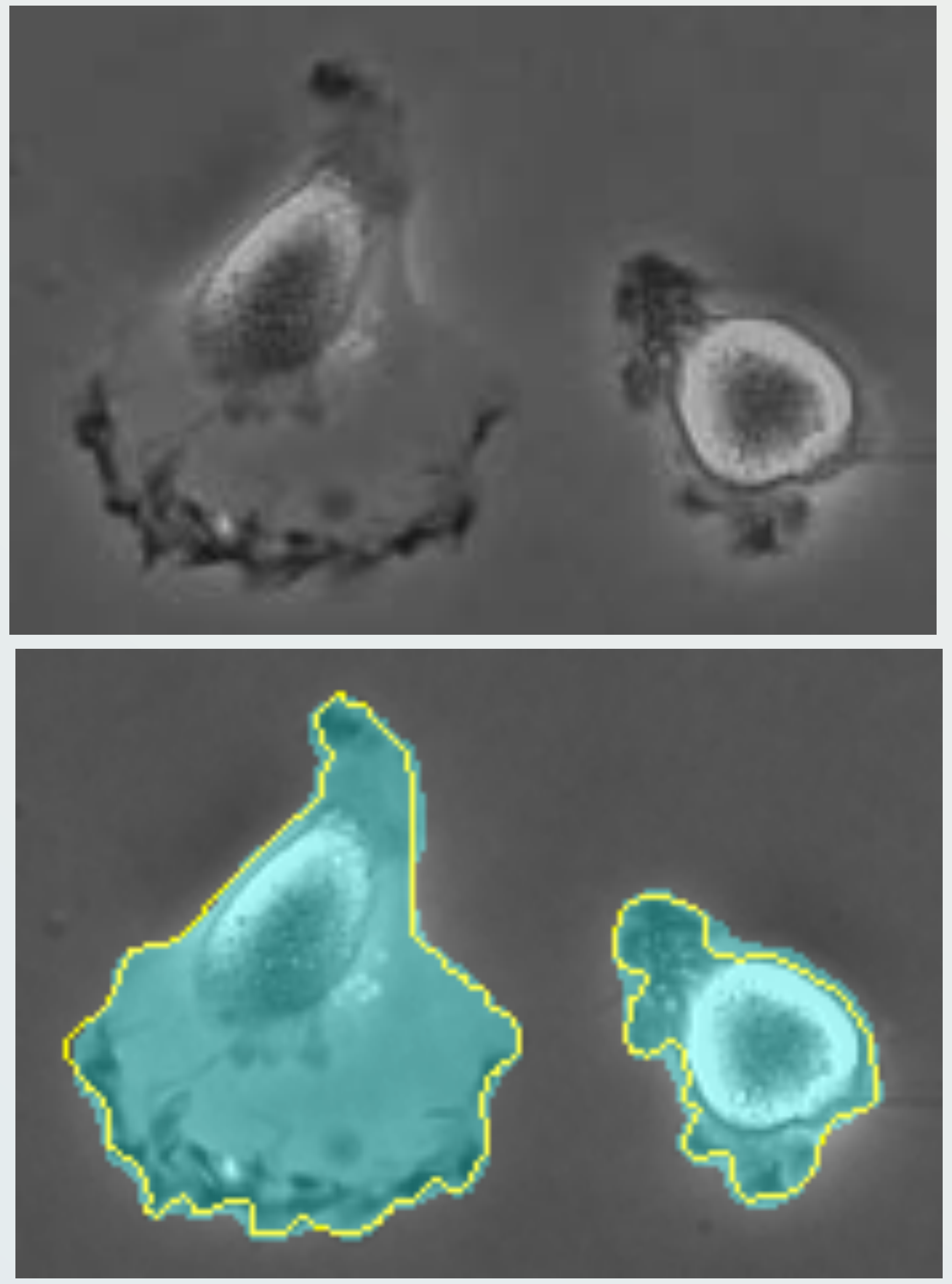
Gaussian filtering equivalent to flame thickening Δ

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

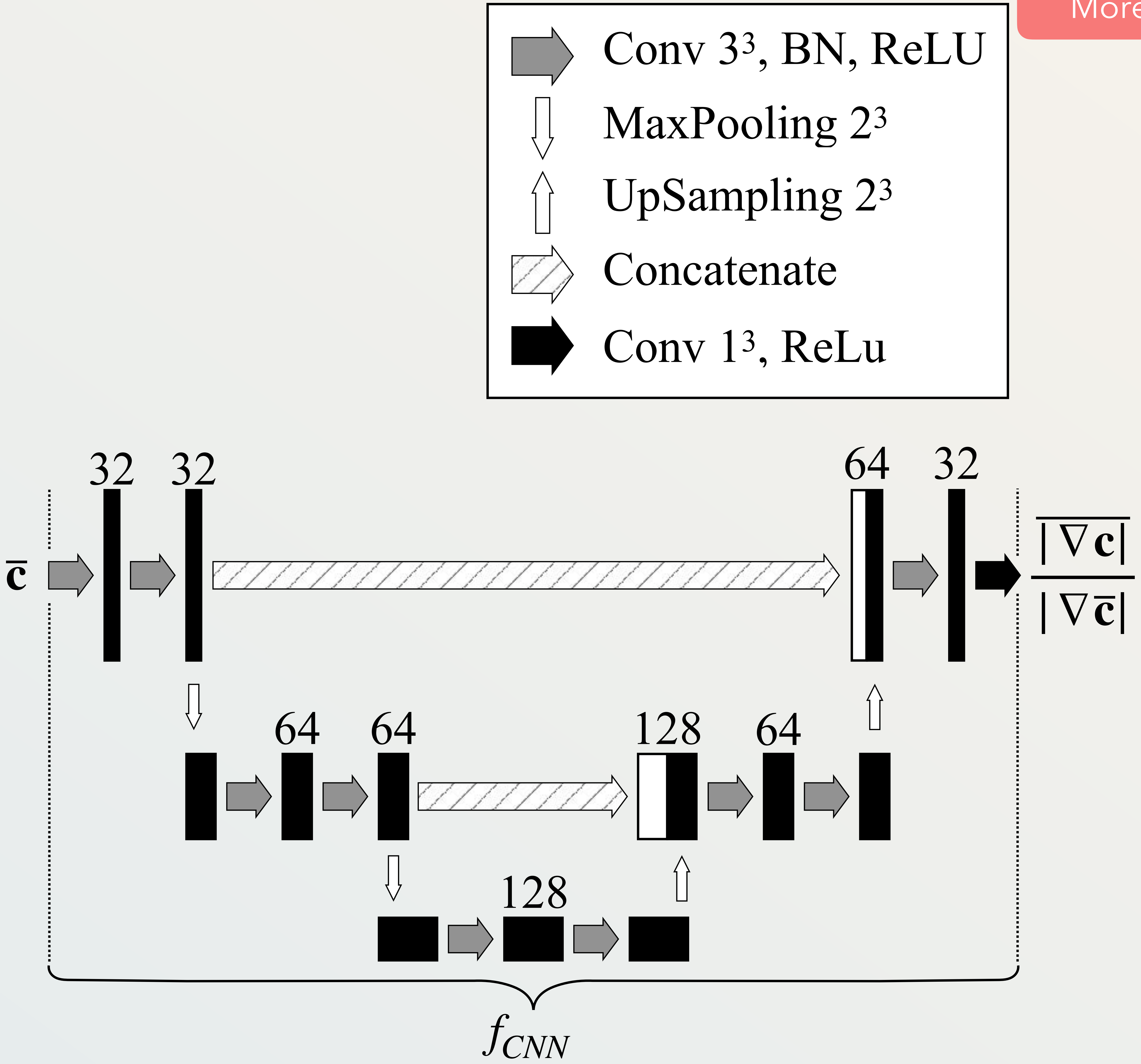
U-Net

More accurate models

Input



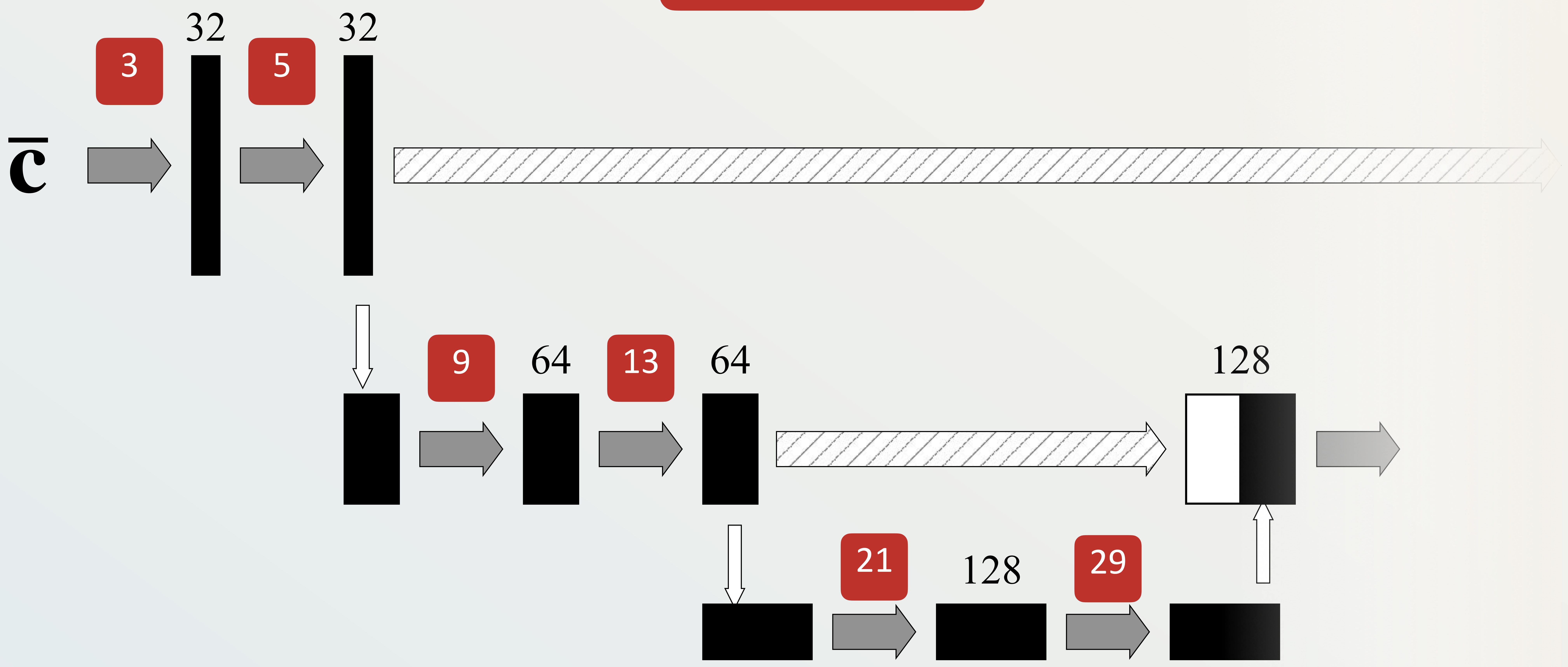
Segmented image



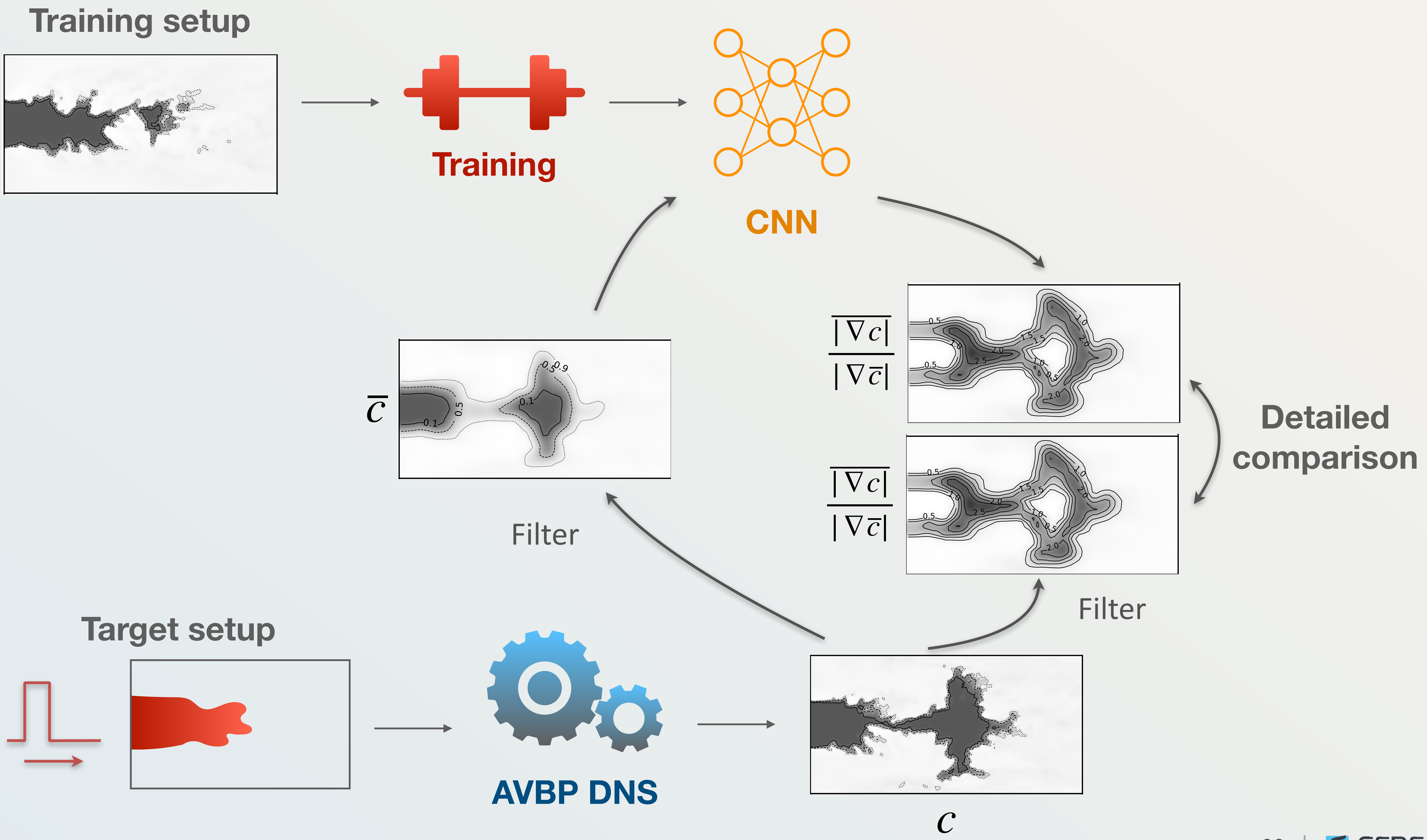
Architecture is adapted from a medical image segmentation network [9]

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.

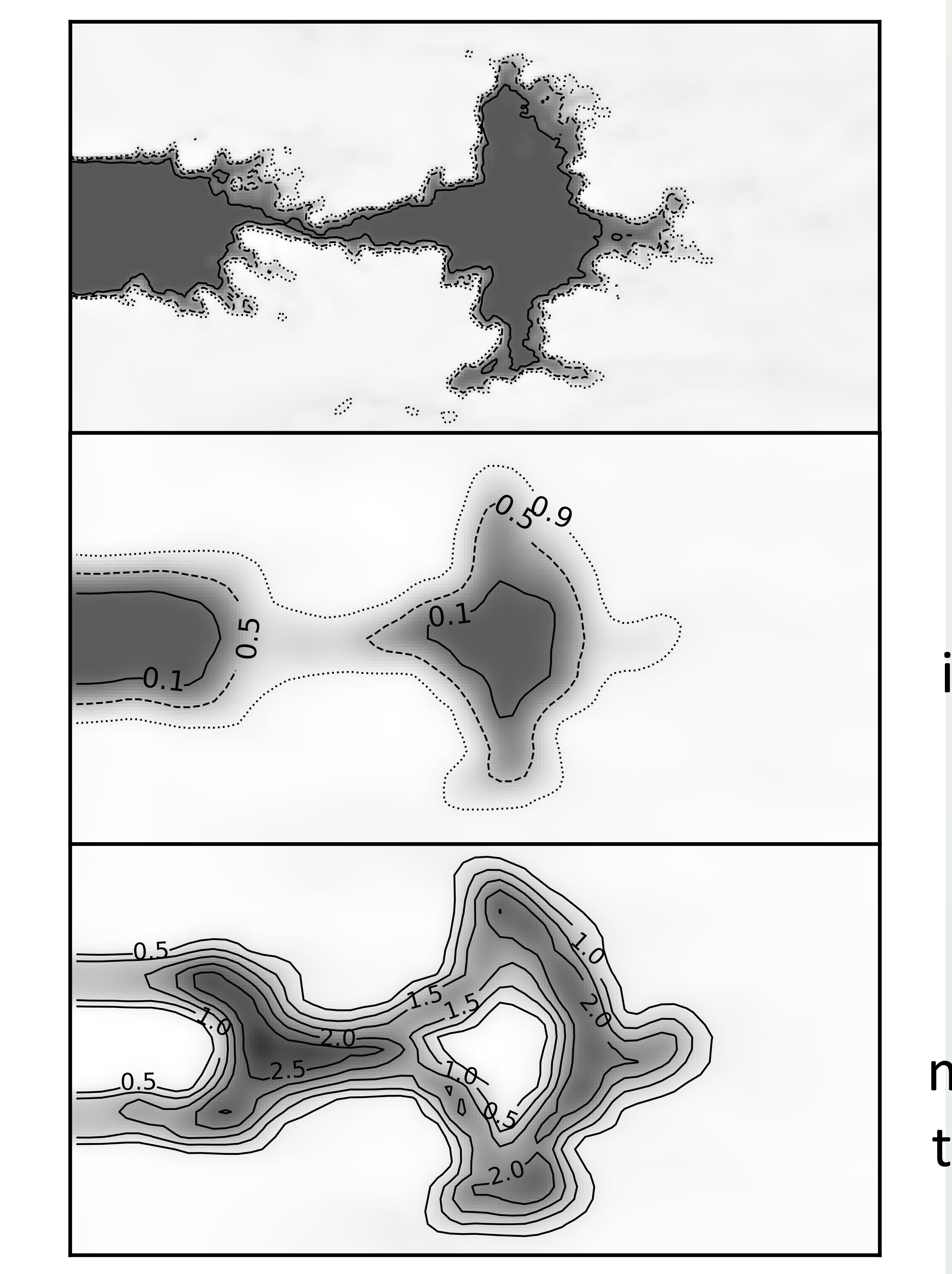
Receptive field



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


Training setup
Training
CNN
$\overline{c}$
Filter
$\frac{\overline{|\nabla c|}}{|\nabla \overline{c}|}$
$\frac{\overline{|\nabla c|}}{|\nabla \overline{c}|}$
Detailed comparison
Filter
Target setup
AVBP DNS
c

More accurate models

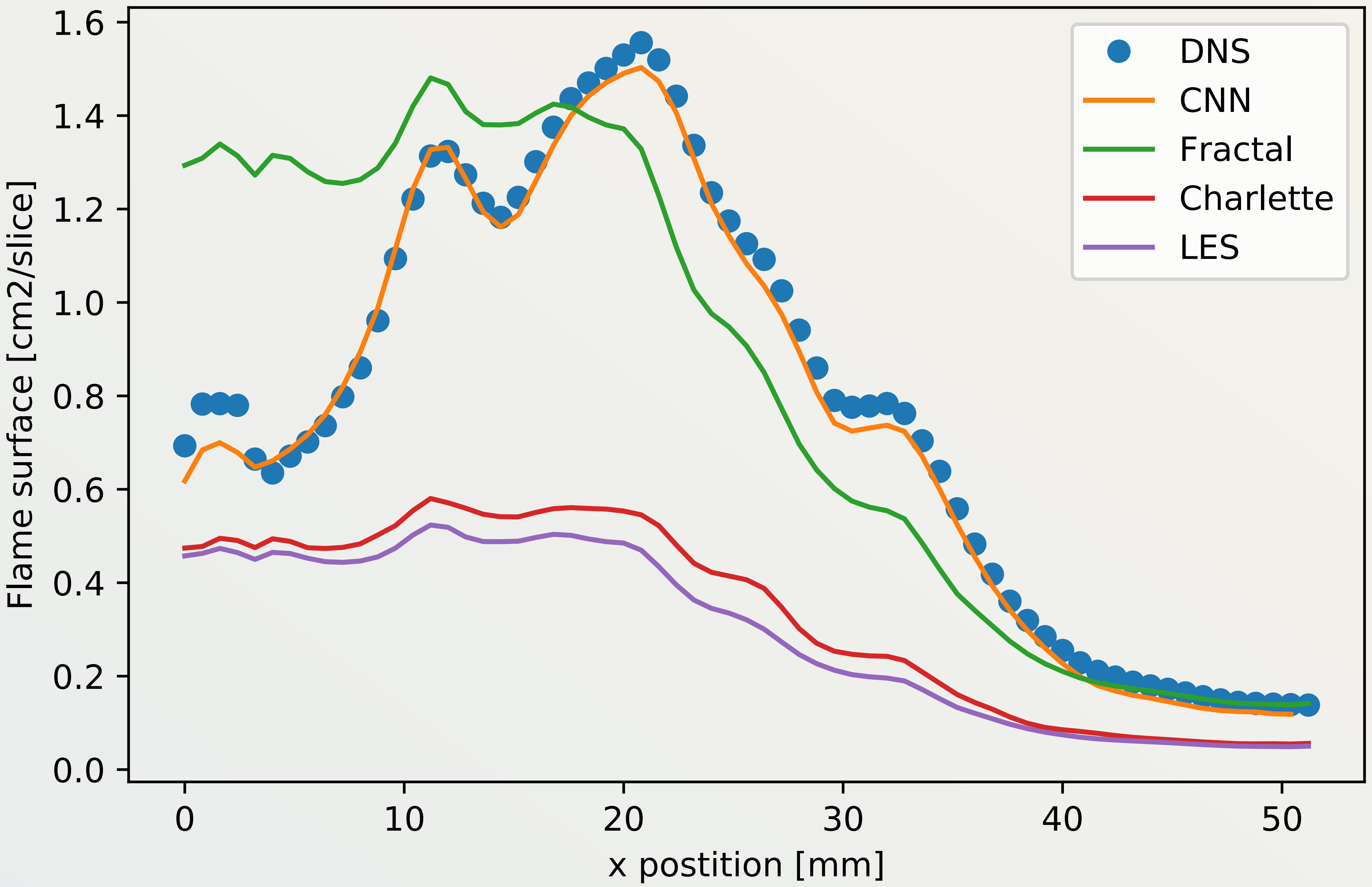


DNS

LES input

LES model target

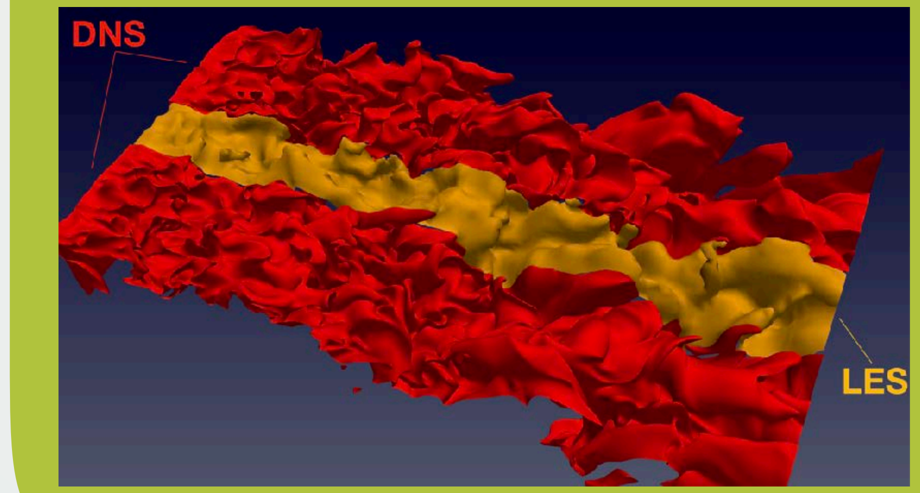
Example snapshot in test set

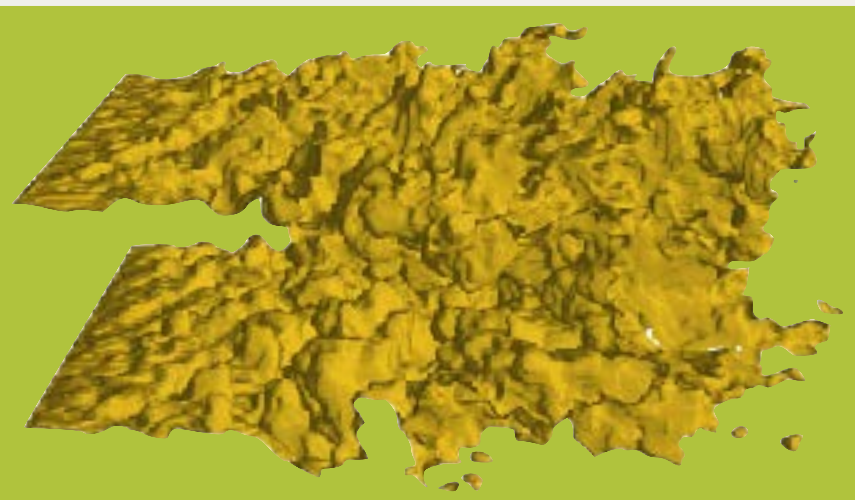


Initial results were promising

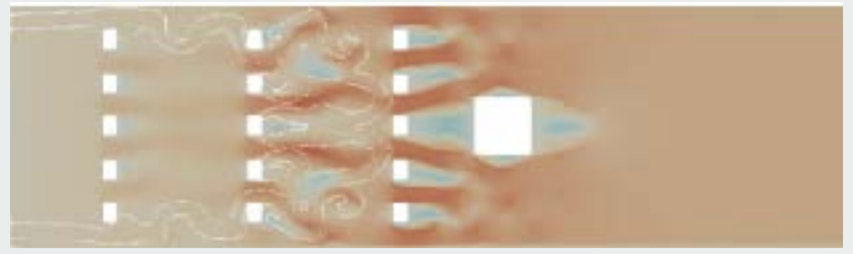
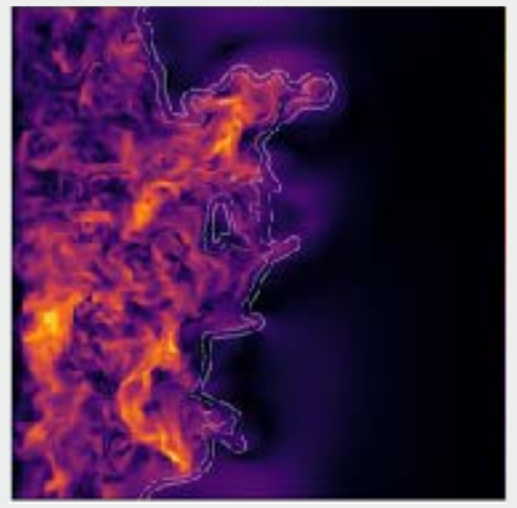
Lapeyre, C.J., Misdariis, A., Cazard, N., Veynante, D. & Poinsot, T. (2019). Training convolutional neural networks to estimate turbulent sub-grid scale reaction rates. Combustion and Flame, 203, 255-264.

More accurate models

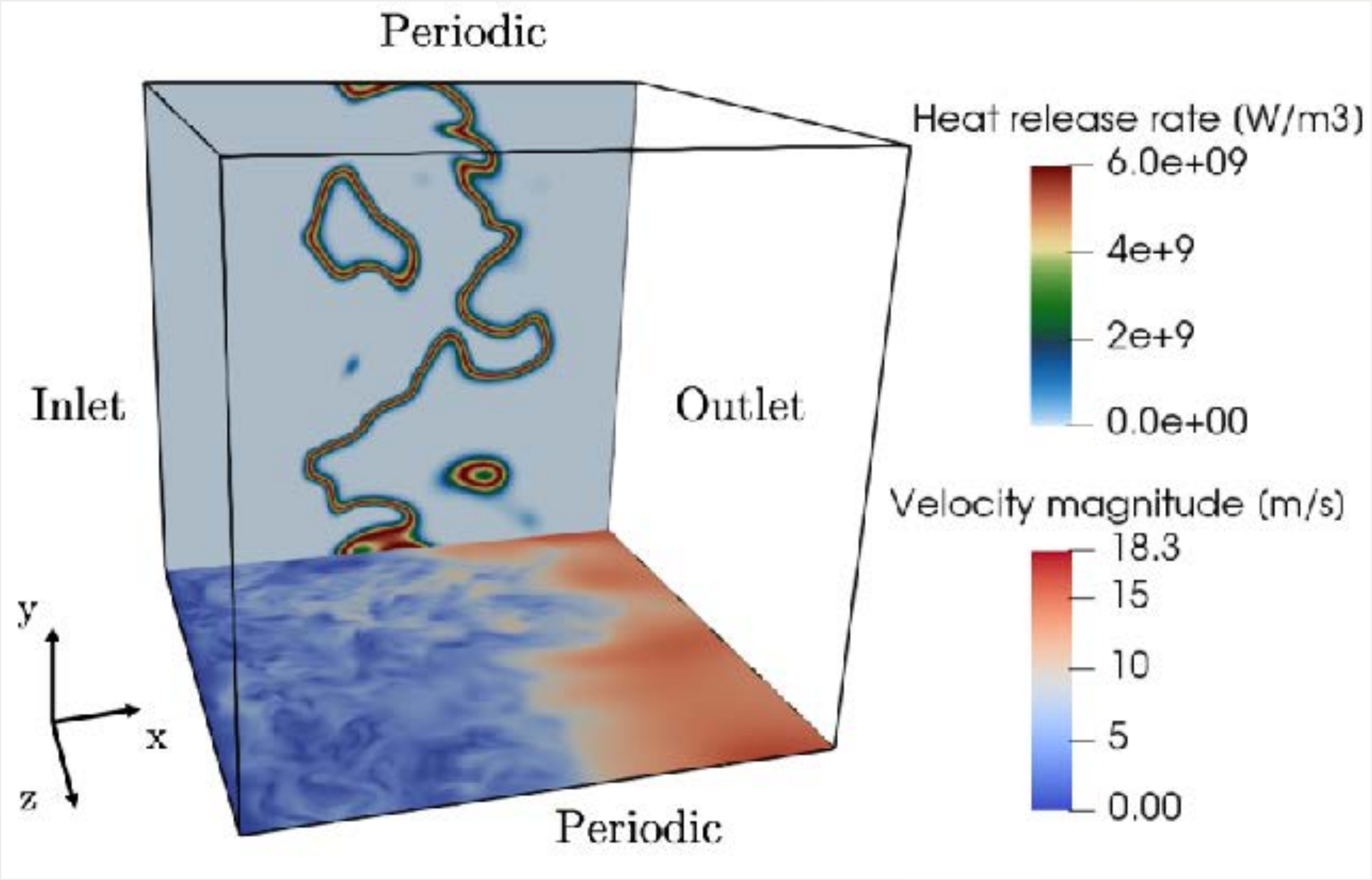




Training Database

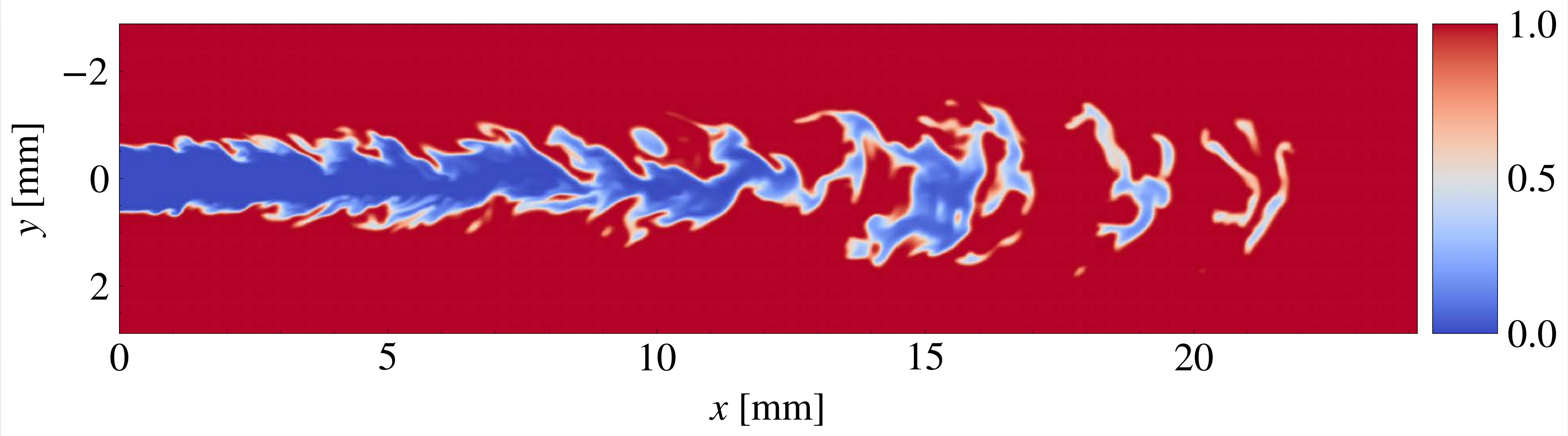
Testing Database	 Similar config	 Different config
Differences	Turbulent realisation Flow dynamics Geometry variations …	Flow regimes Chemistry Geometry Scale …
	Close generalisation	Further generalisation

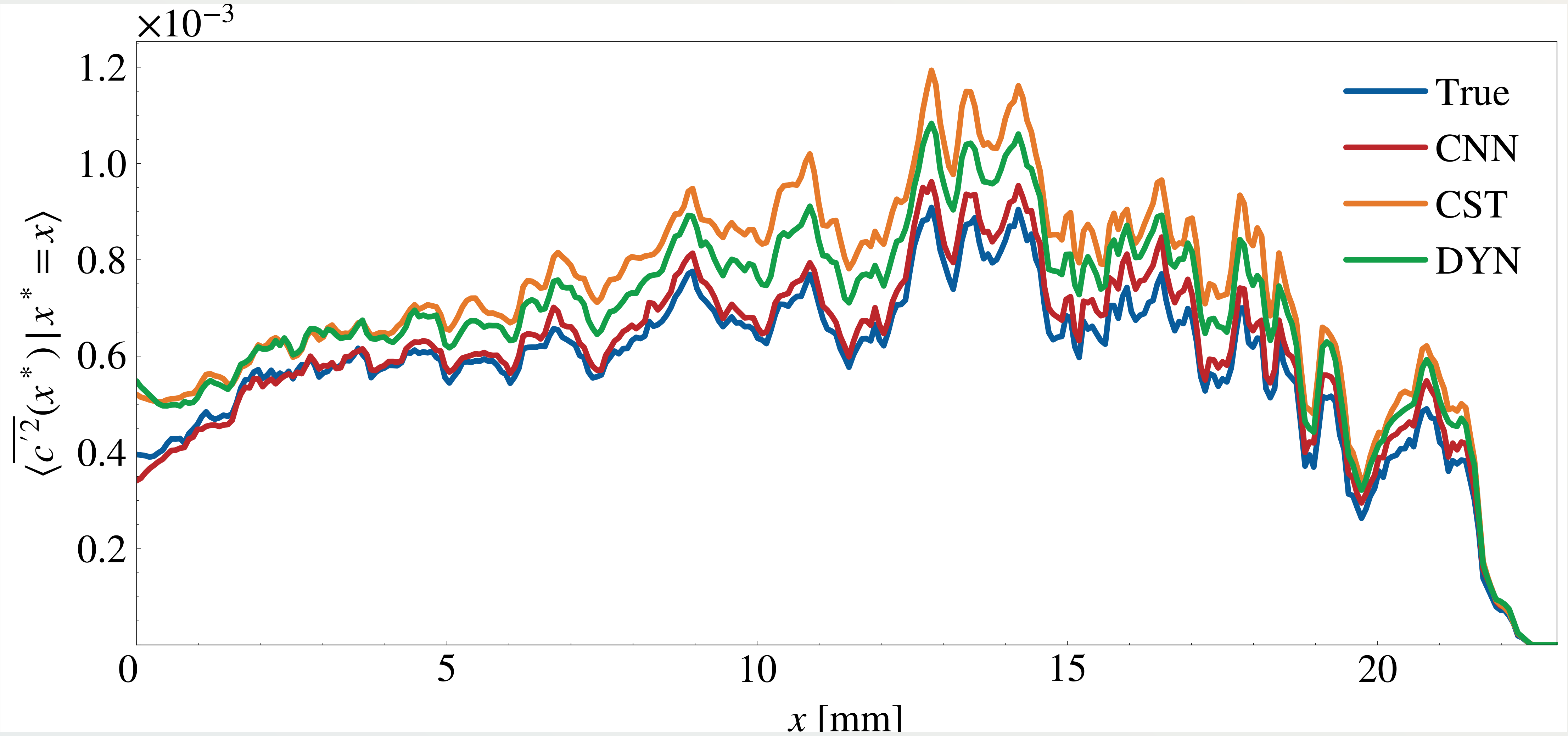
More accurate models



Test

Target [1]



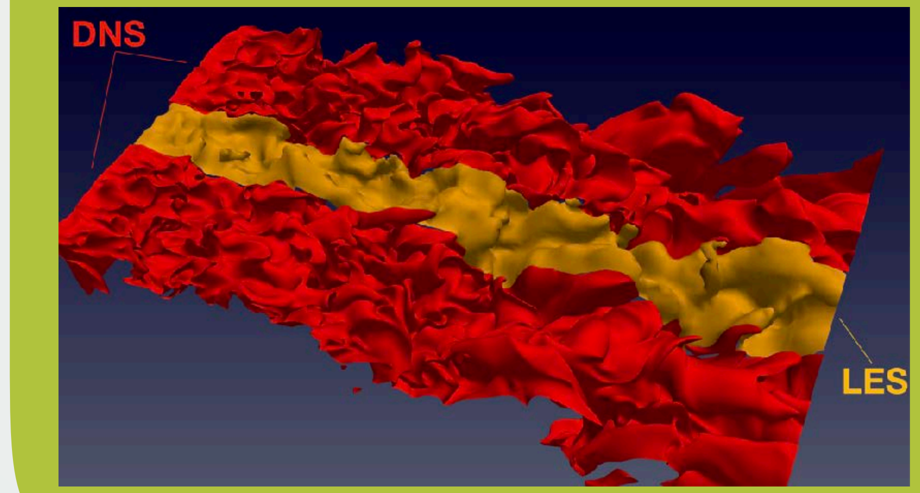


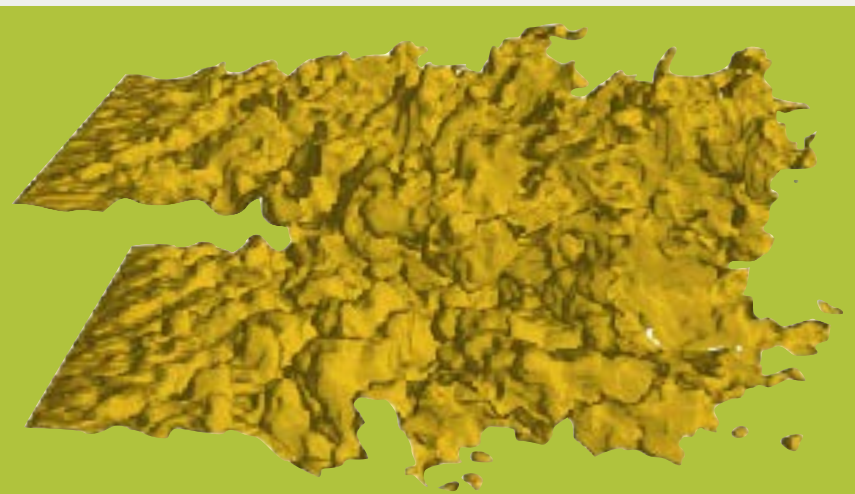
Training: HIT [2]

- Similar turbulence/flame params
- Different fuel
- Different pressure, inlet temperature

[1] Luca, S.; Attili, A.; Bisetti, F. Direct Numerical Simulation of Turbulent Lean Methane-Air Bunsen Flames with Mixture Inhomogeneities. In Proceedings of the 54th AIAA Aerospace Sciences Meeting AIAA, San Diego, CA, USA, 4–8 January 2016
[2] Xing, Victor, et al. "Generalization Capability of Convolutional Neural Networks for Progress Variable Variance and Reaction Rate Subgrid-Scale Modeling." Energies 14.16 (2021): 5096.

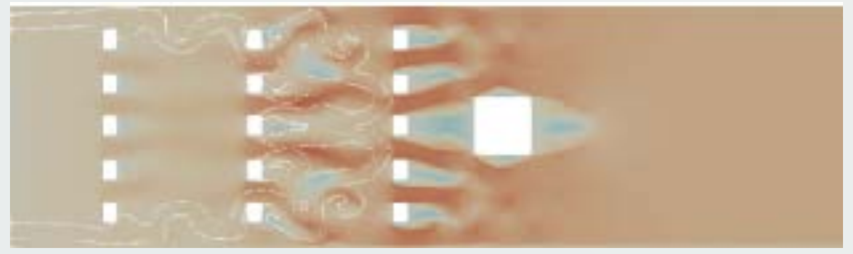
More accurate models



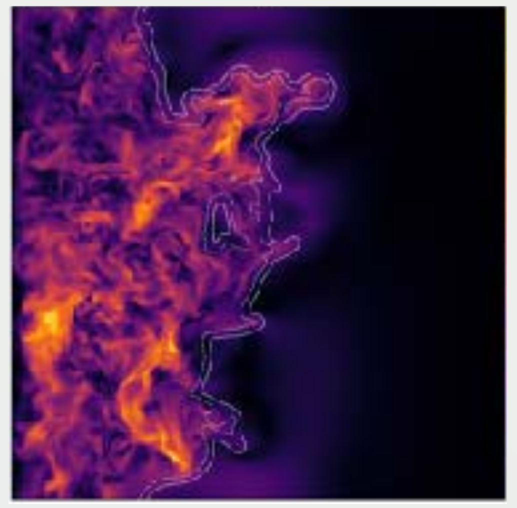


Training Database

Testing Database



Similar config



Different config

In-solver

Differences

Turbulent realisation
Flow dynamics
Geometry variations
…

Close generalisation

Flow regimes
Chemistry
Geometry
Scale
…

Further generalisation

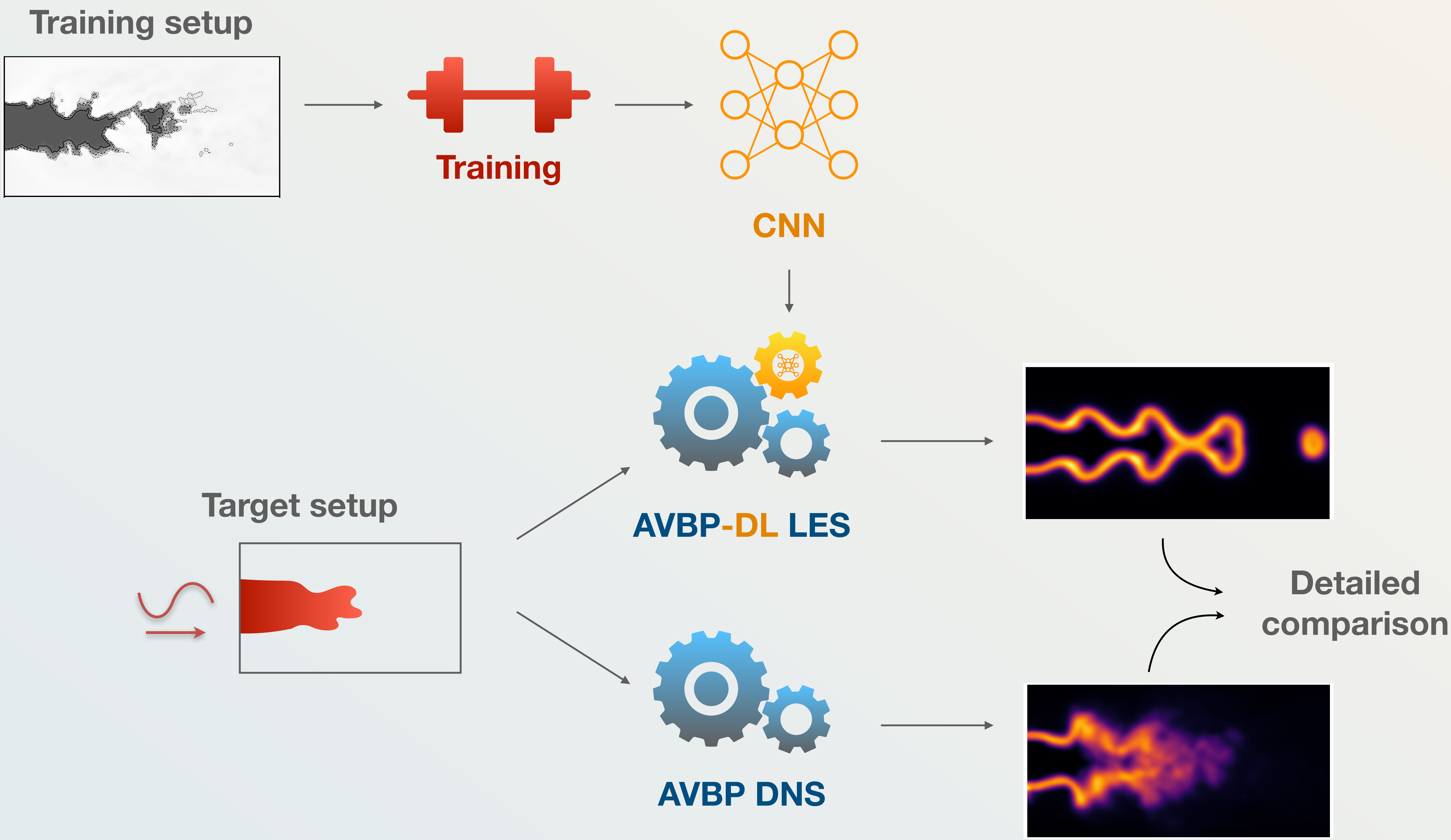
A priori

Does the learning still hold in a feedback loop?

Solver <-> Model

A posteriori

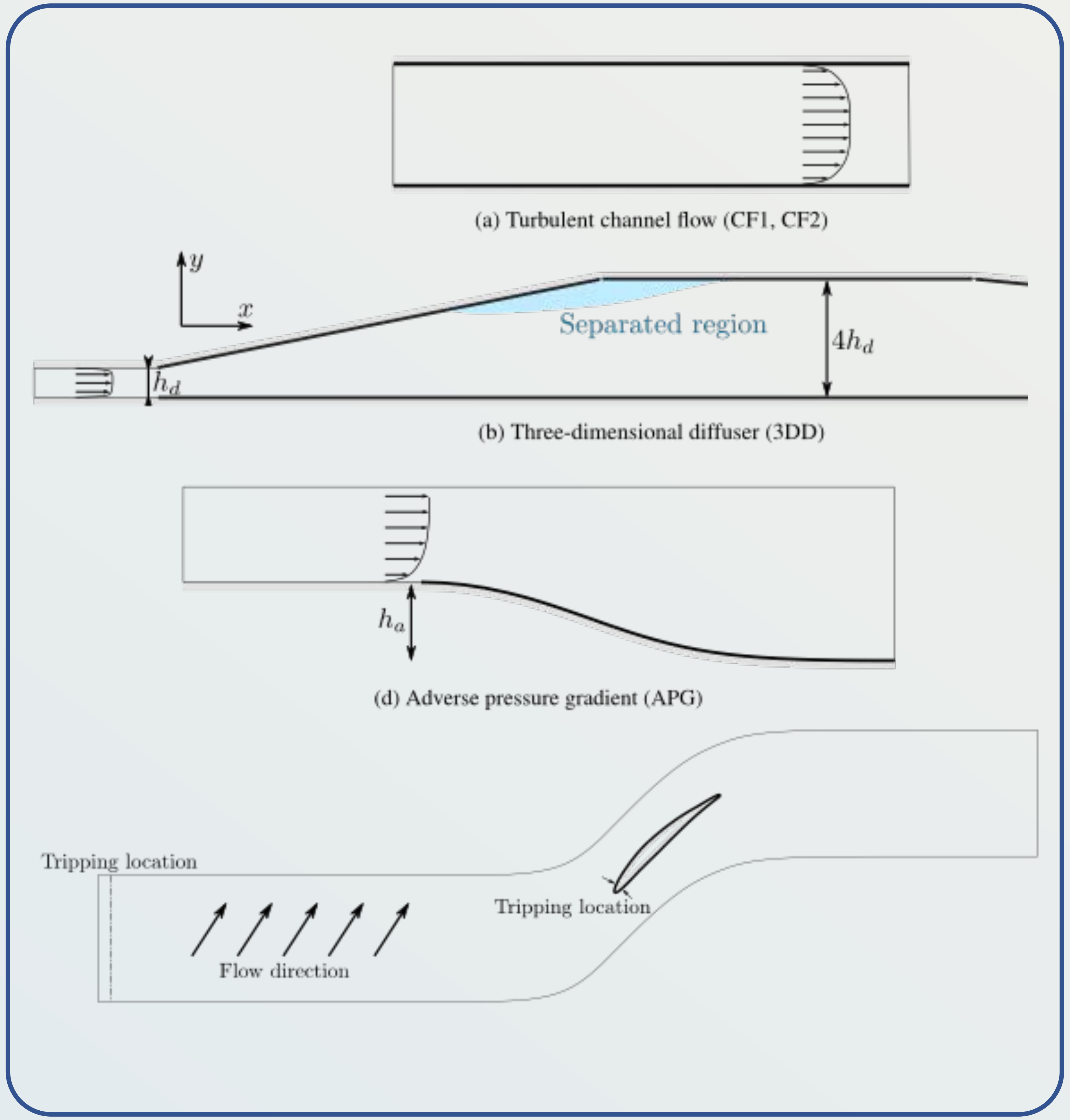
More accurate models



Xing, V, *Deep learning for subgrid-scale modeling in large eddy simulations of turbulent premixed combustion*, PhD thesis (2022)

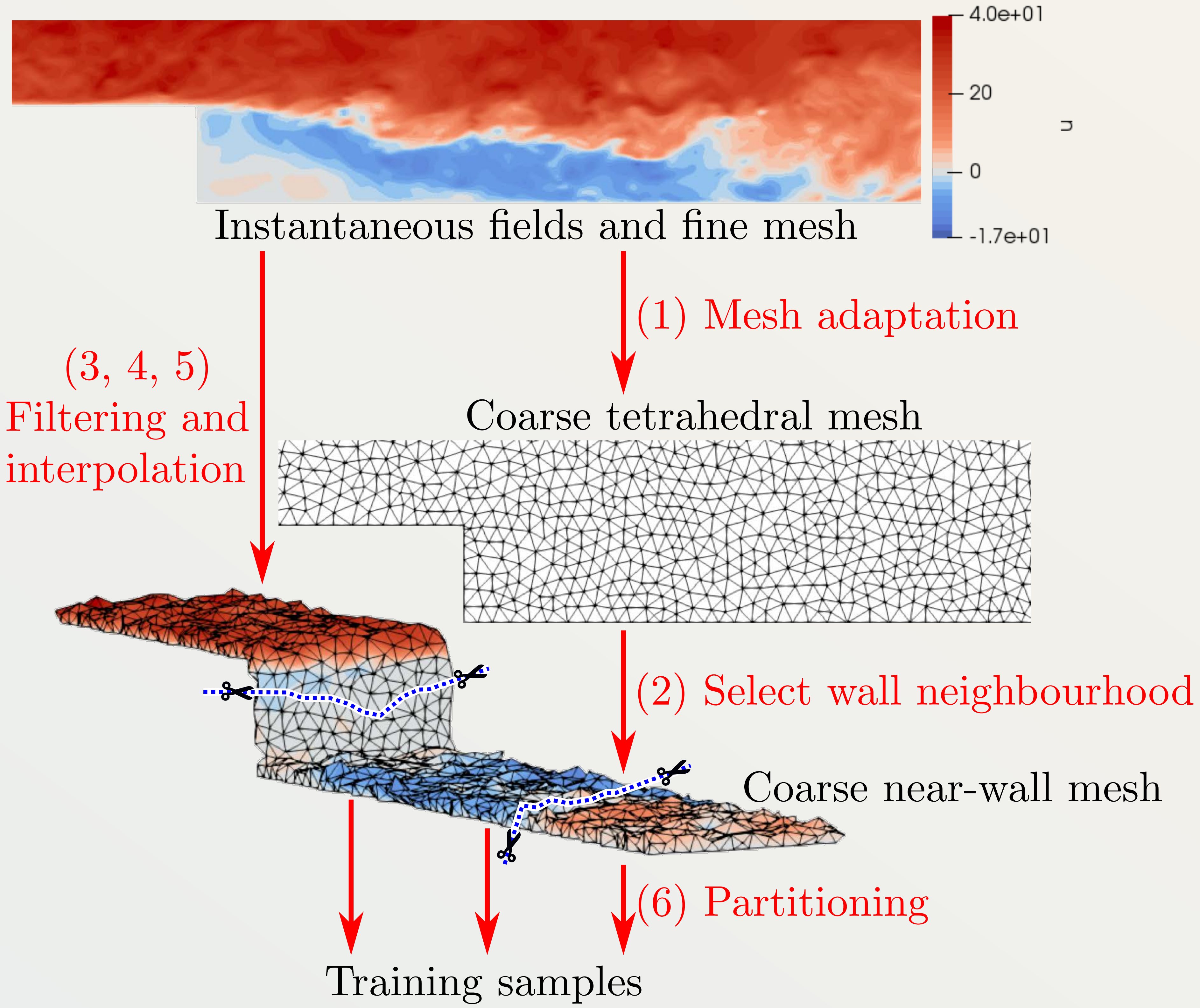
Not just combustion!

A wall modeling application



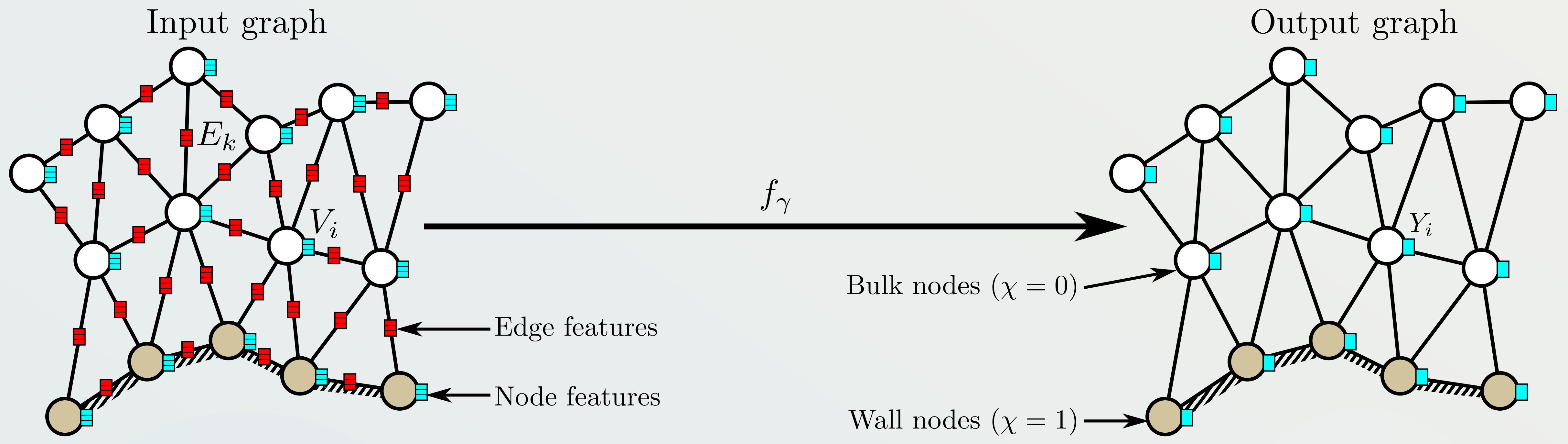
Training data
Multiple Wall-Resolved LES

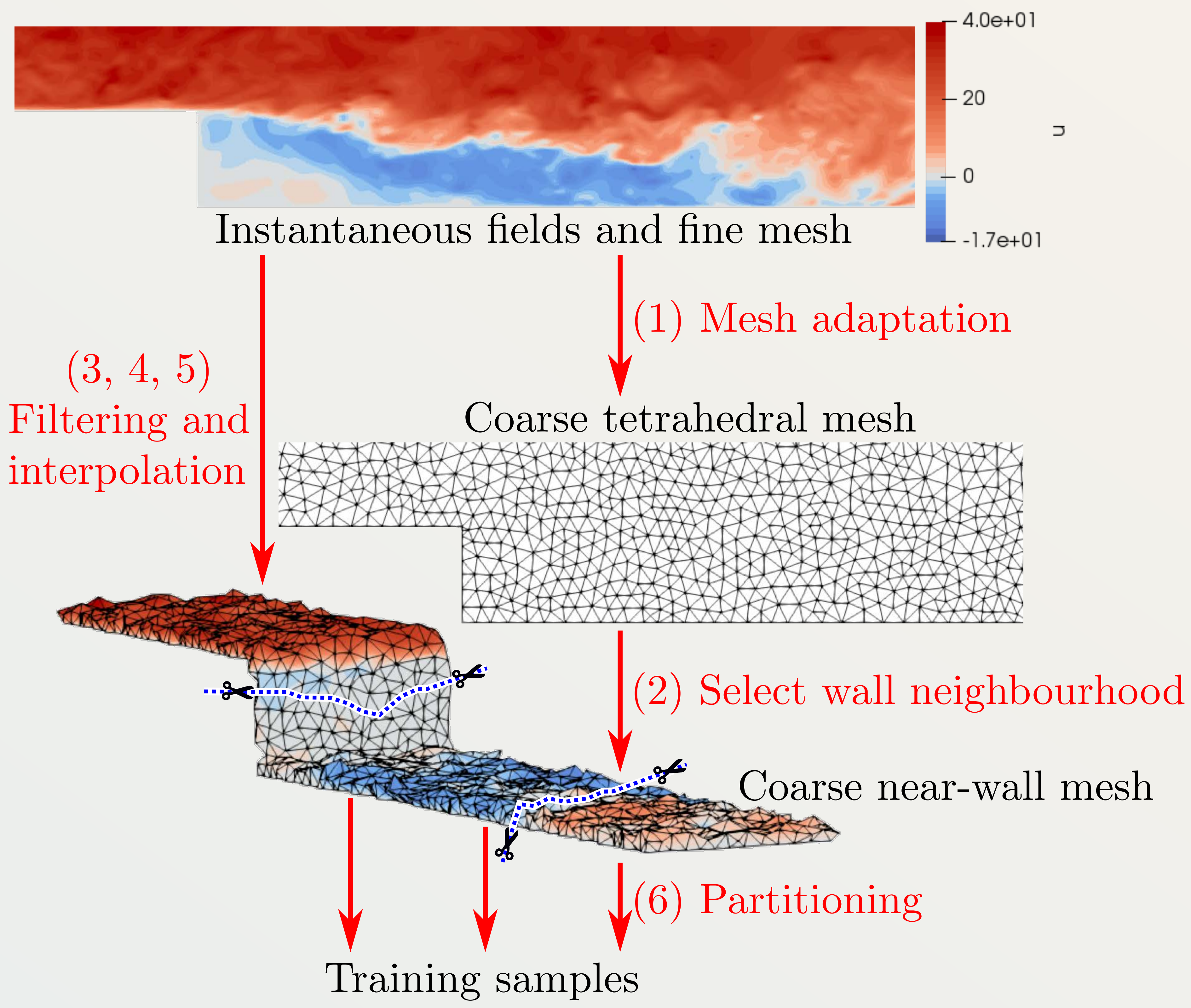
For each:



More accurate models

"MeshGraphNet" [1] architecture operates directly on unstructured mesh nodes





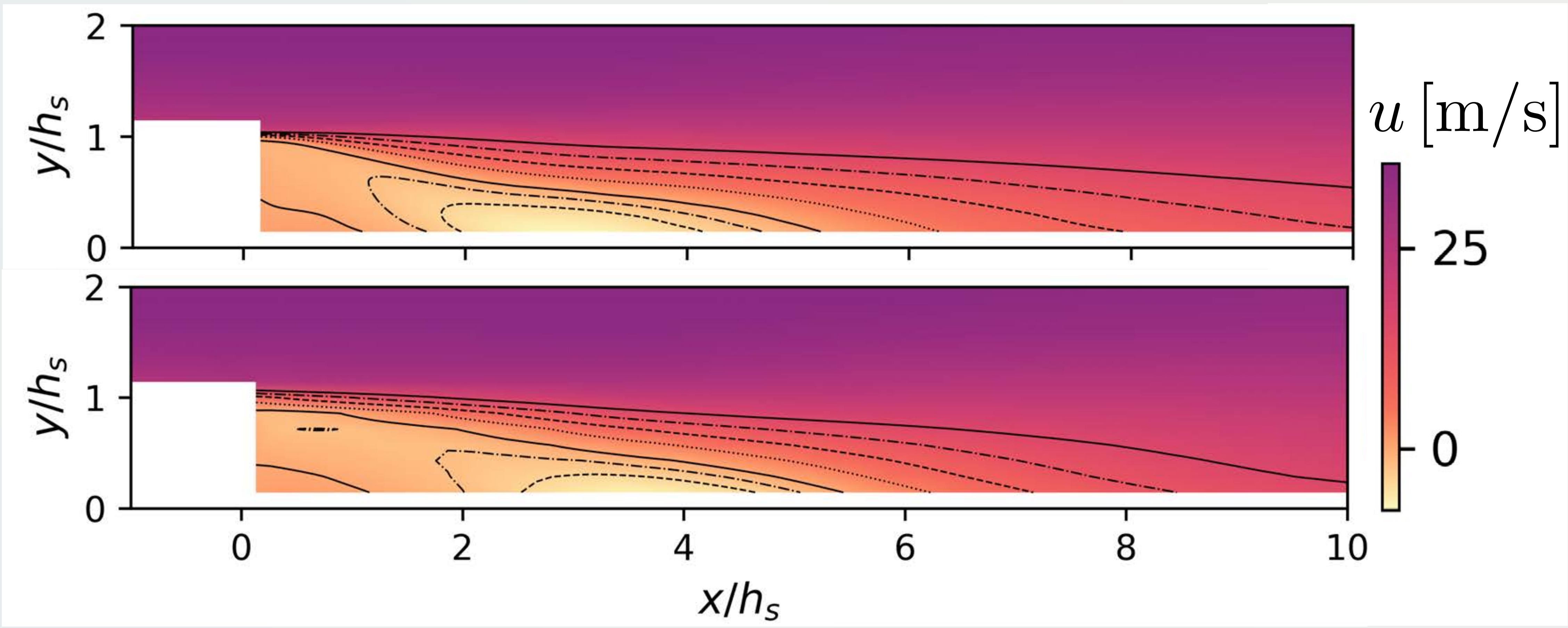
[1] Pfaff, T., Fortunato, M., Sanchez-Gonzalez, A., & Battaglia, P. (2021). Learning Mesh-Based Simulation with Graph Networks. In *International Conference on Learning Representations*.

Validation case: GNN in the LES

Backward facing step LES
with the network as wall model

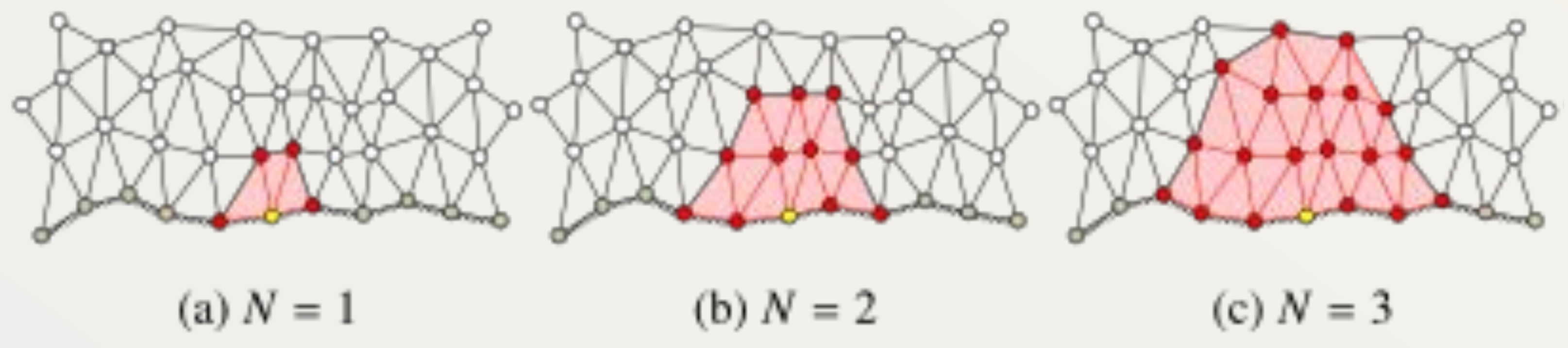
Reference

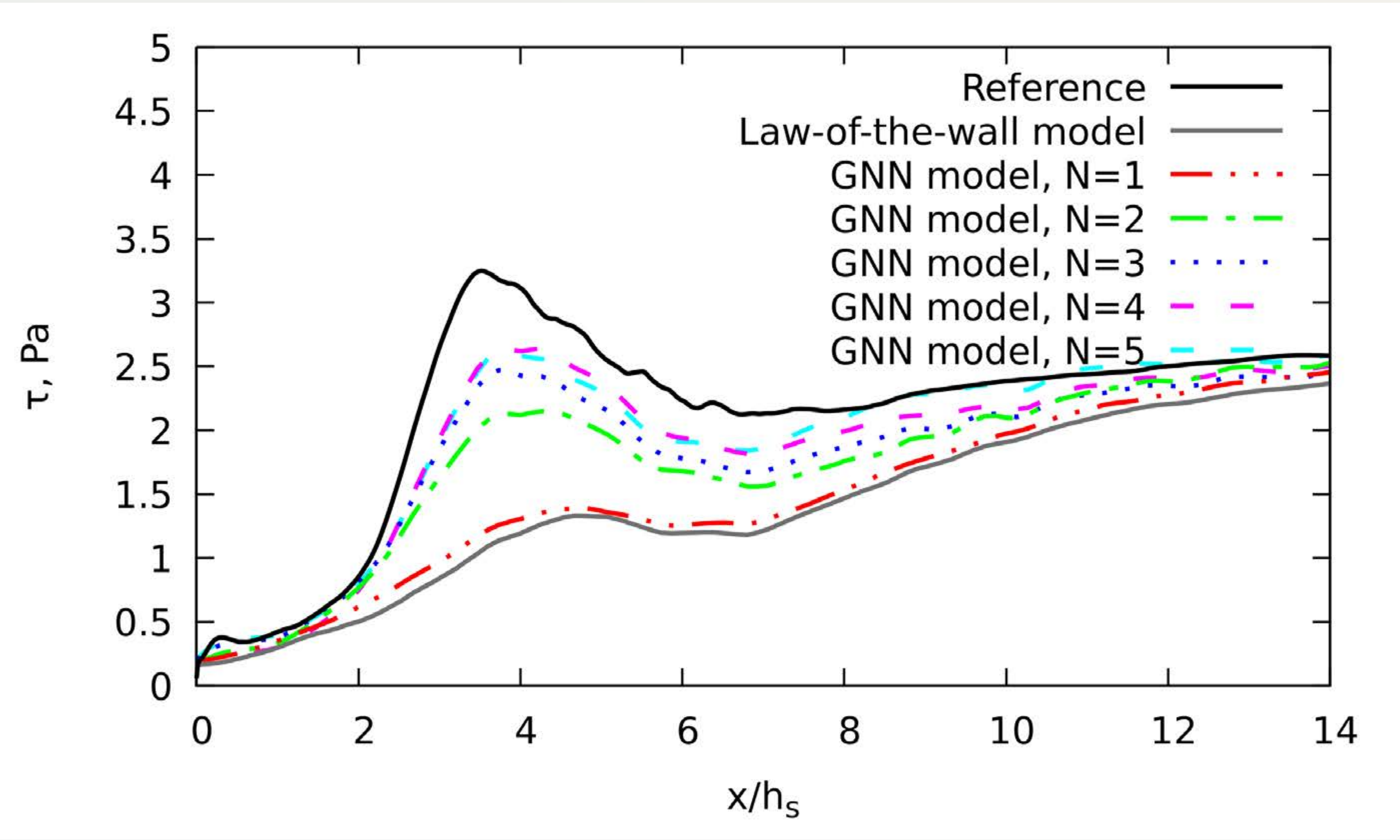
GNN model, $N = 5$



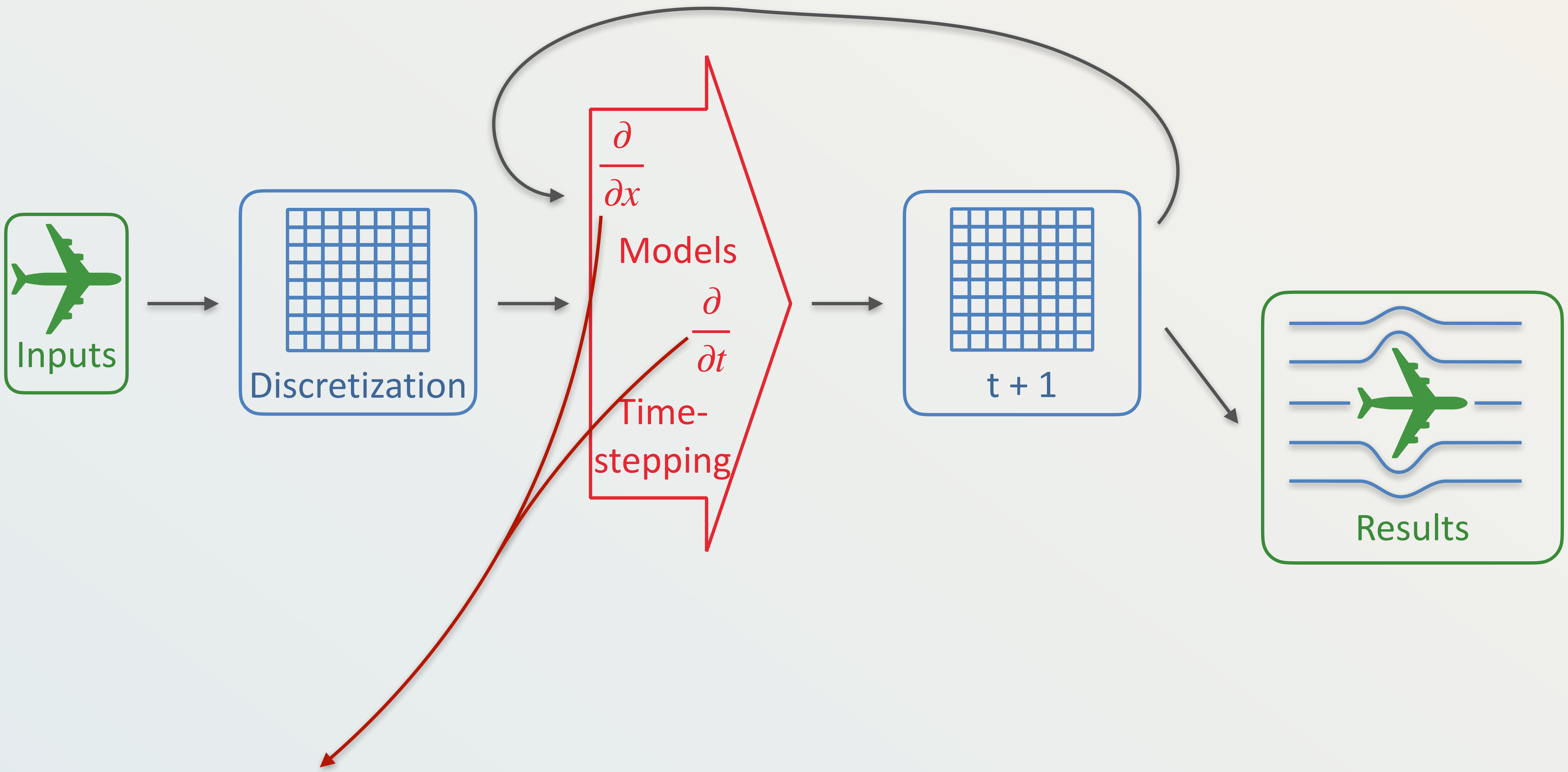
The N parameter controls receptive field:

- N=1 -> similar to log law
- N>1 increases performance (until plateau)





Dupuy, D., Odier, N. and Lapeyre, C. (2023). Modelling the wall shear stress in large-eddy simulation using graph neural networks. *To appear in Data-Centric Engineering*.



Innovative numerics

Precision of numerical methods requires differentiable solvers to train through

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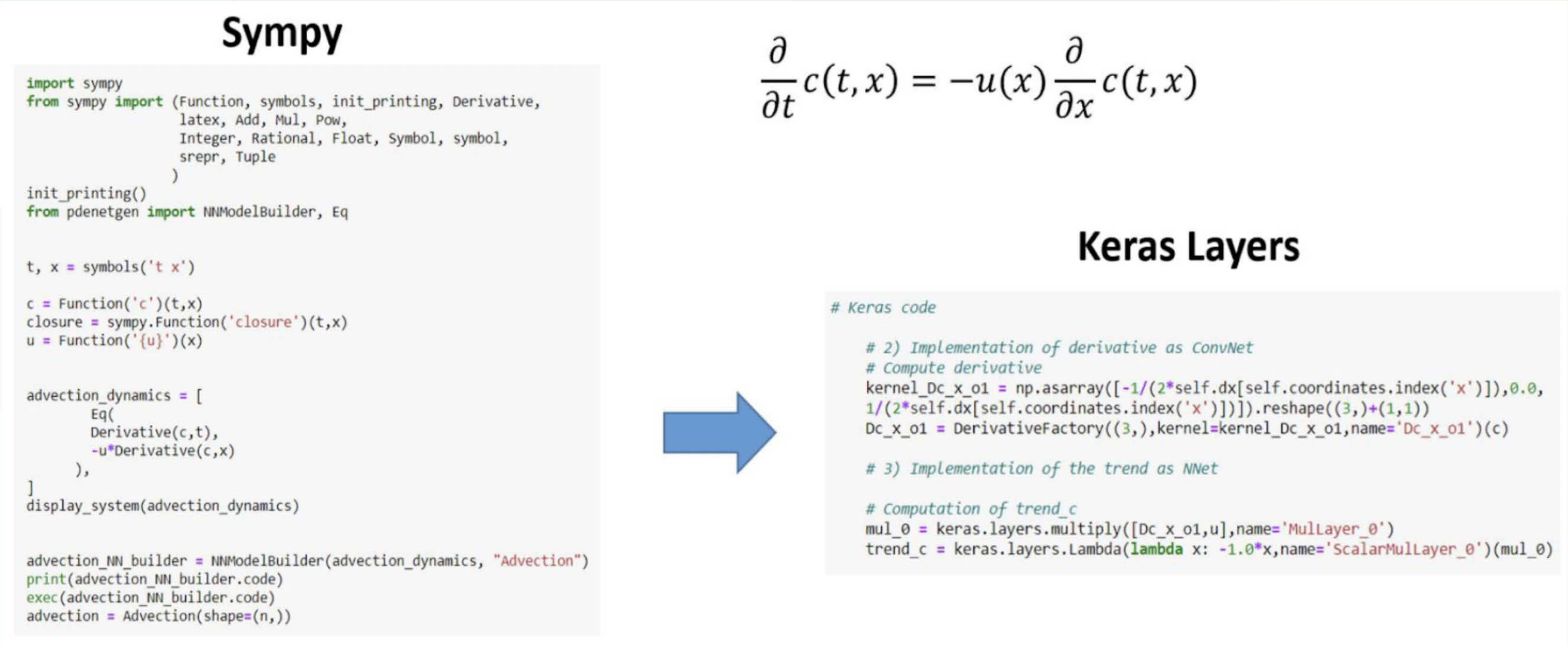
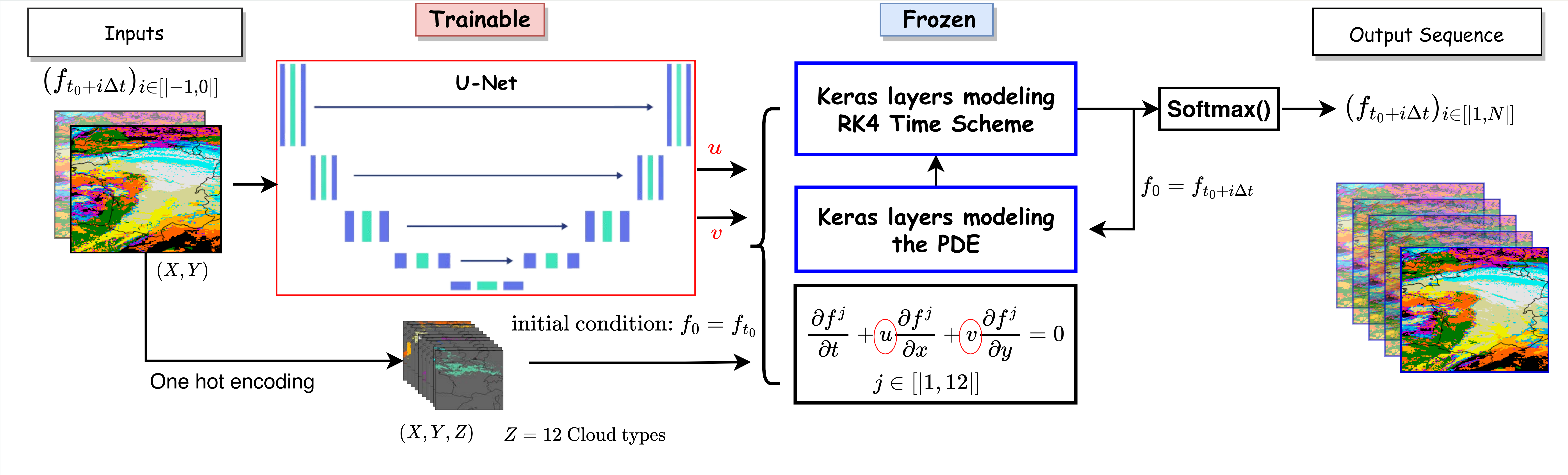
Innovative numerics



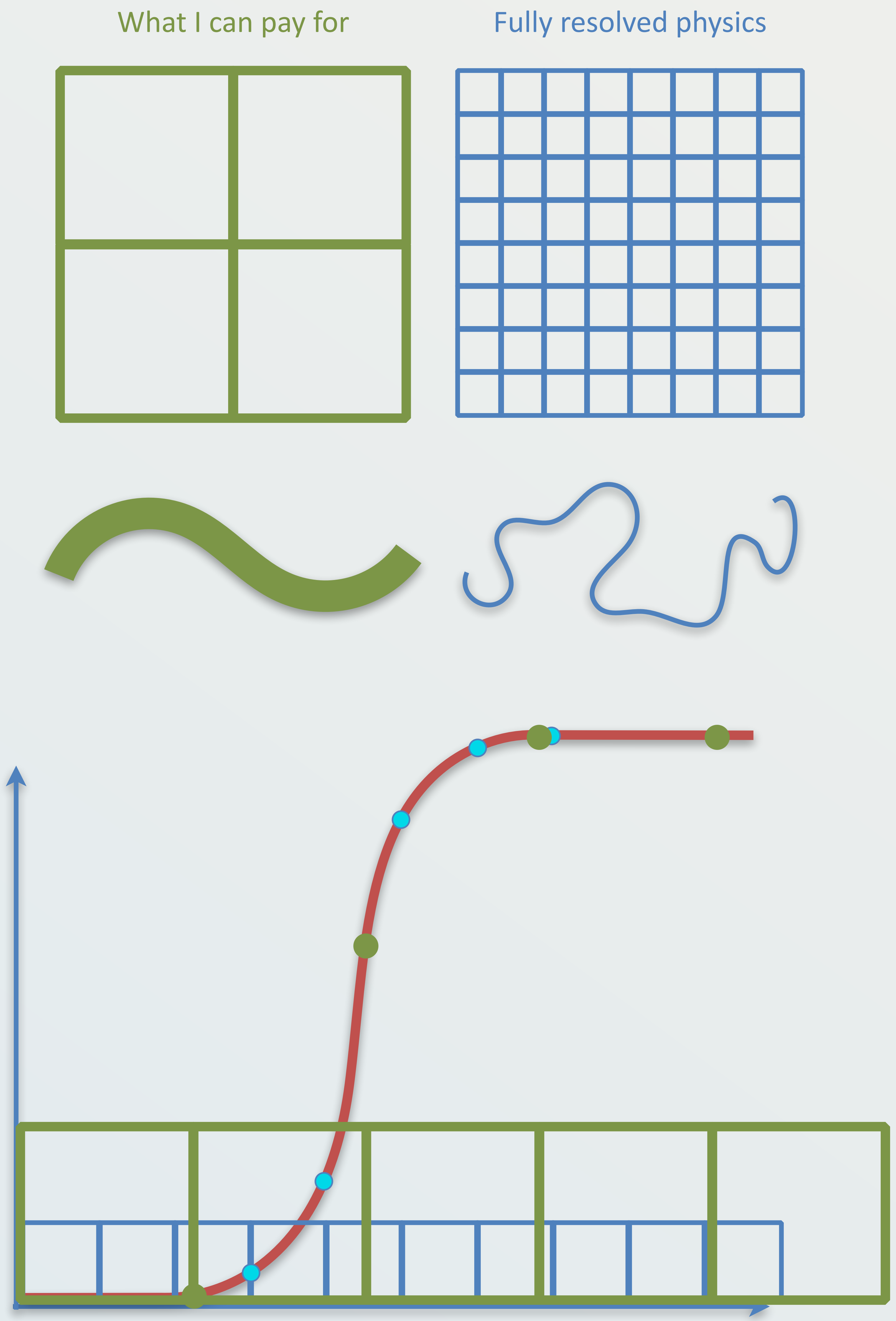
Pannekoucke, O. and Fablet, R. (2020). Pde- netgen 1.0: from symbolic partial differential equation (pde) representations of physical processes to trainable neural network representations. Geoscientific Model Development, 13(7):3373–3382.

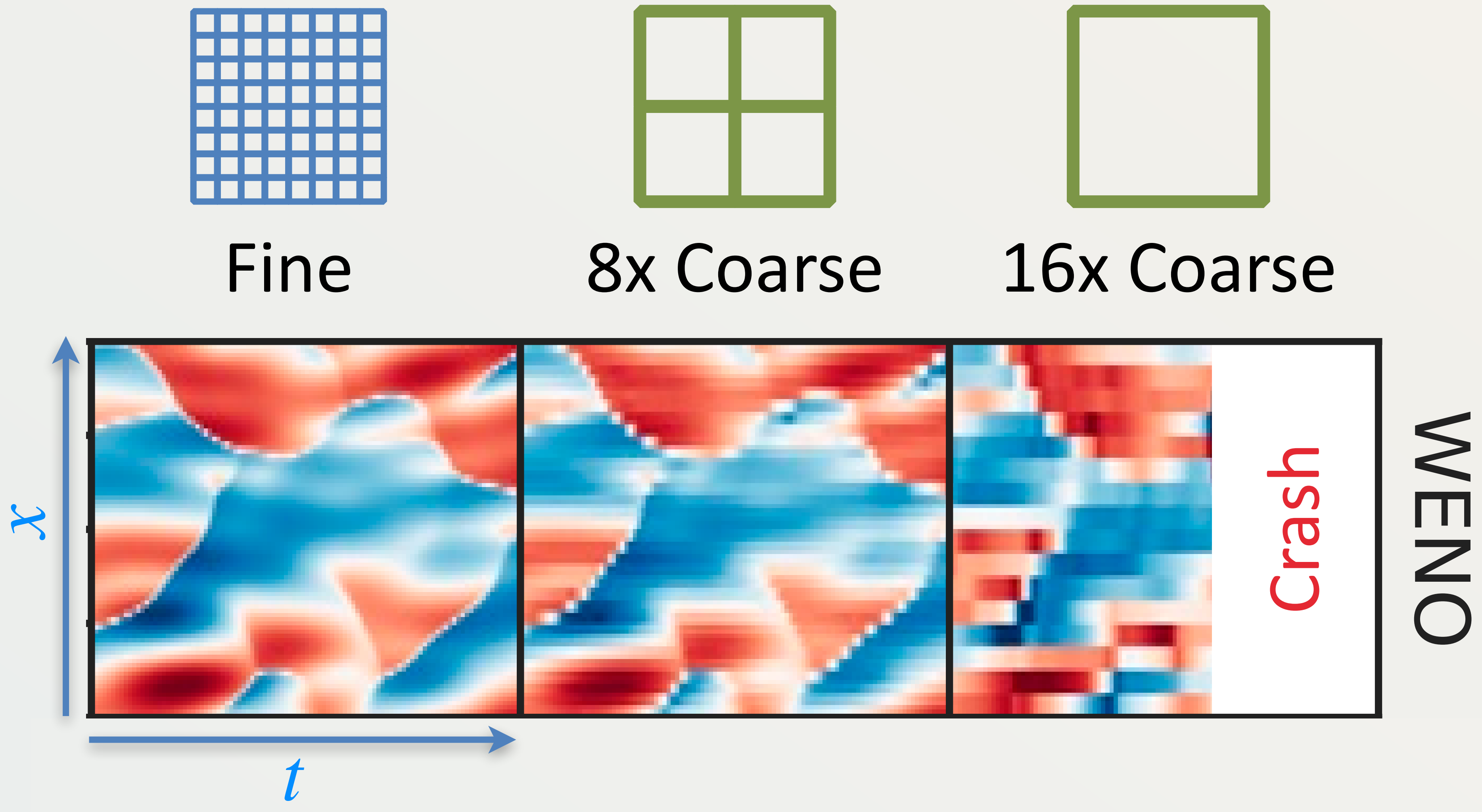
https://github.com/opannekoucke/pdenetgen



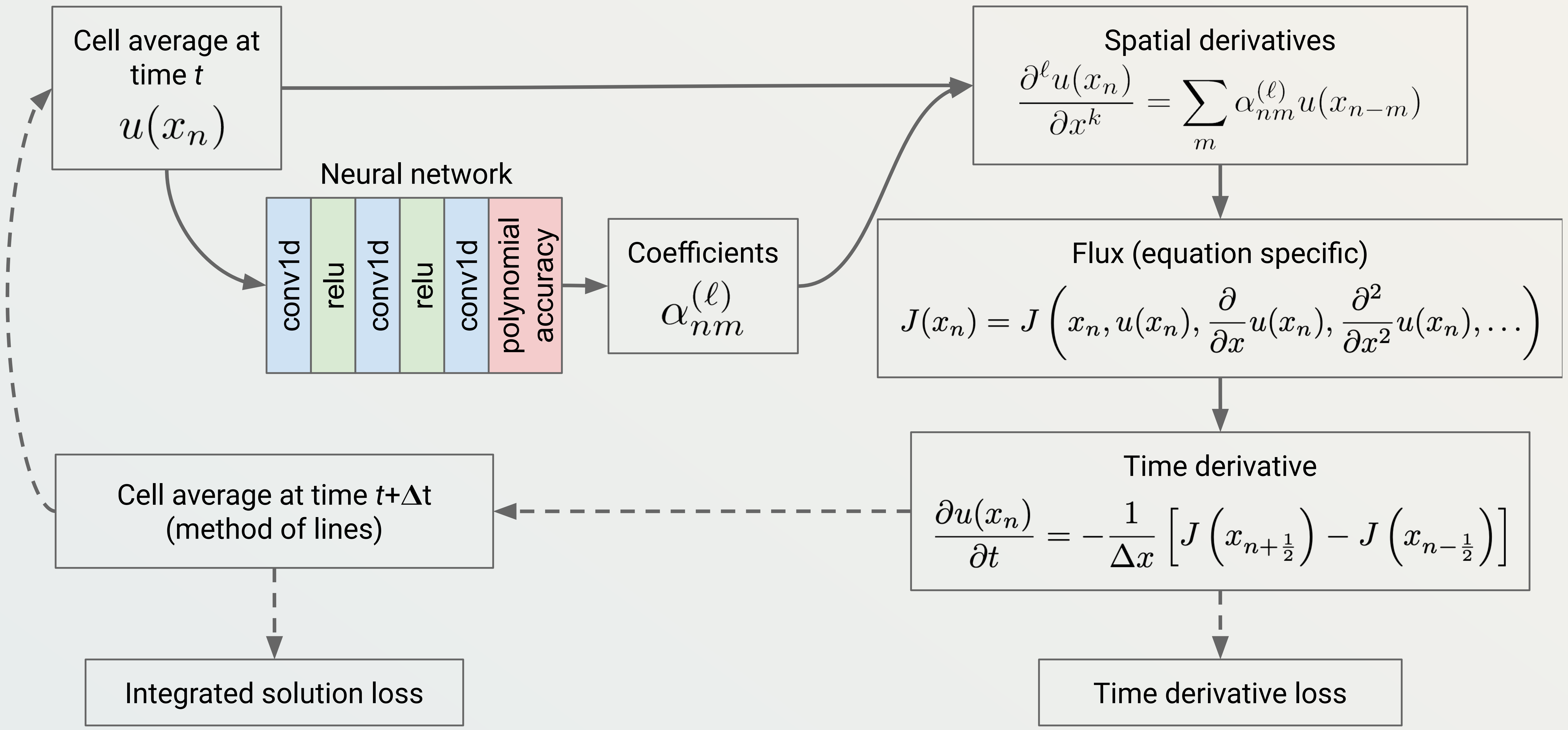
ElMontassir, R., Lapeyre, C., Pannekoucke, O. (2022). Hybrid Physics-AI Approach for Cloud Cover Nowcasting. ECMWF Machine Learning Workshop.

Innovative numerics





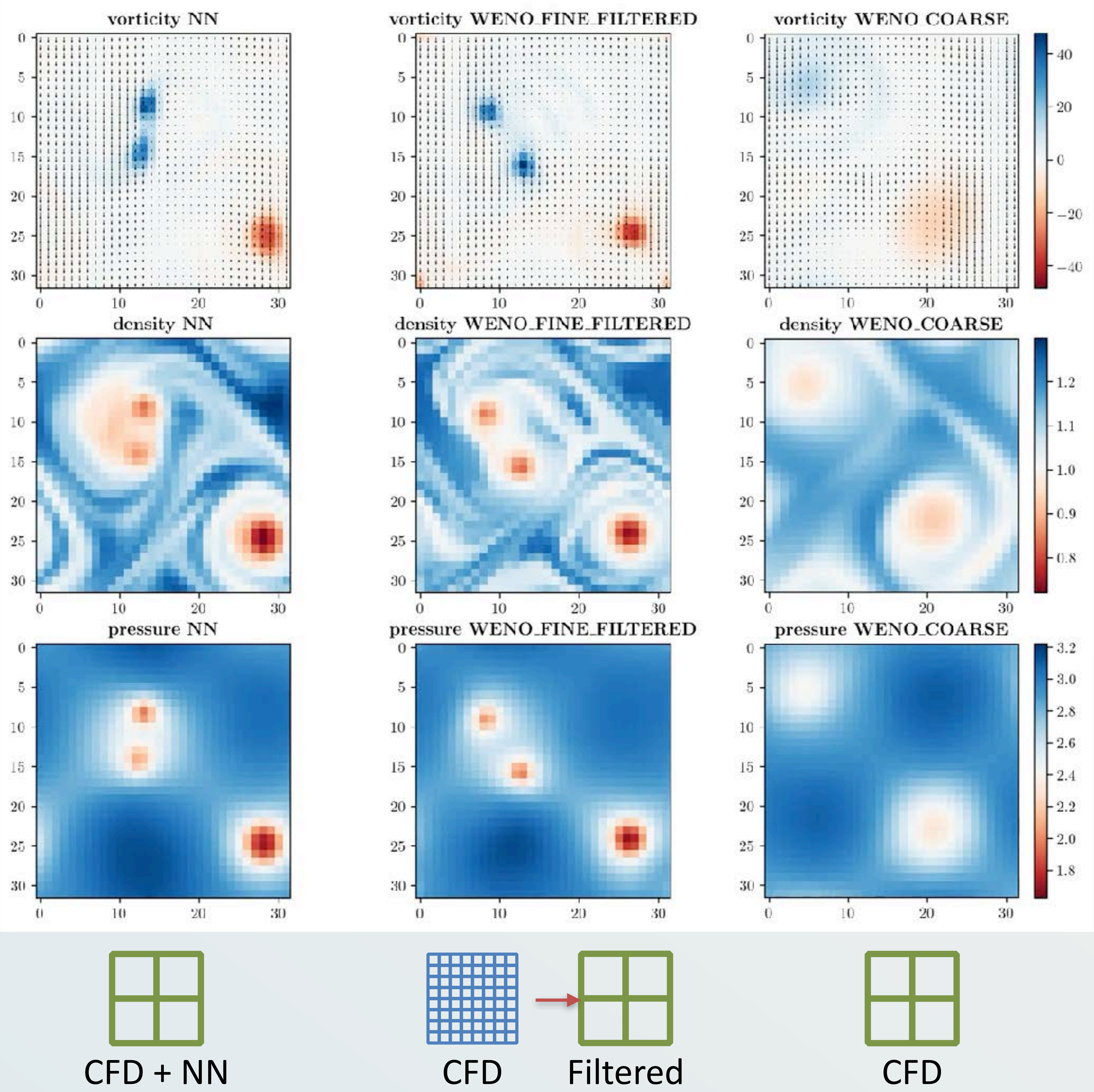
Bar-Sinai, Y., Hoyer, S., Hickey, J., & Brenner, M. P. (2019). Learning data-driven discretizations for partial differential equations. *Proceedings of the National Academy of Sciences*, *116*(31), 15344-15349.



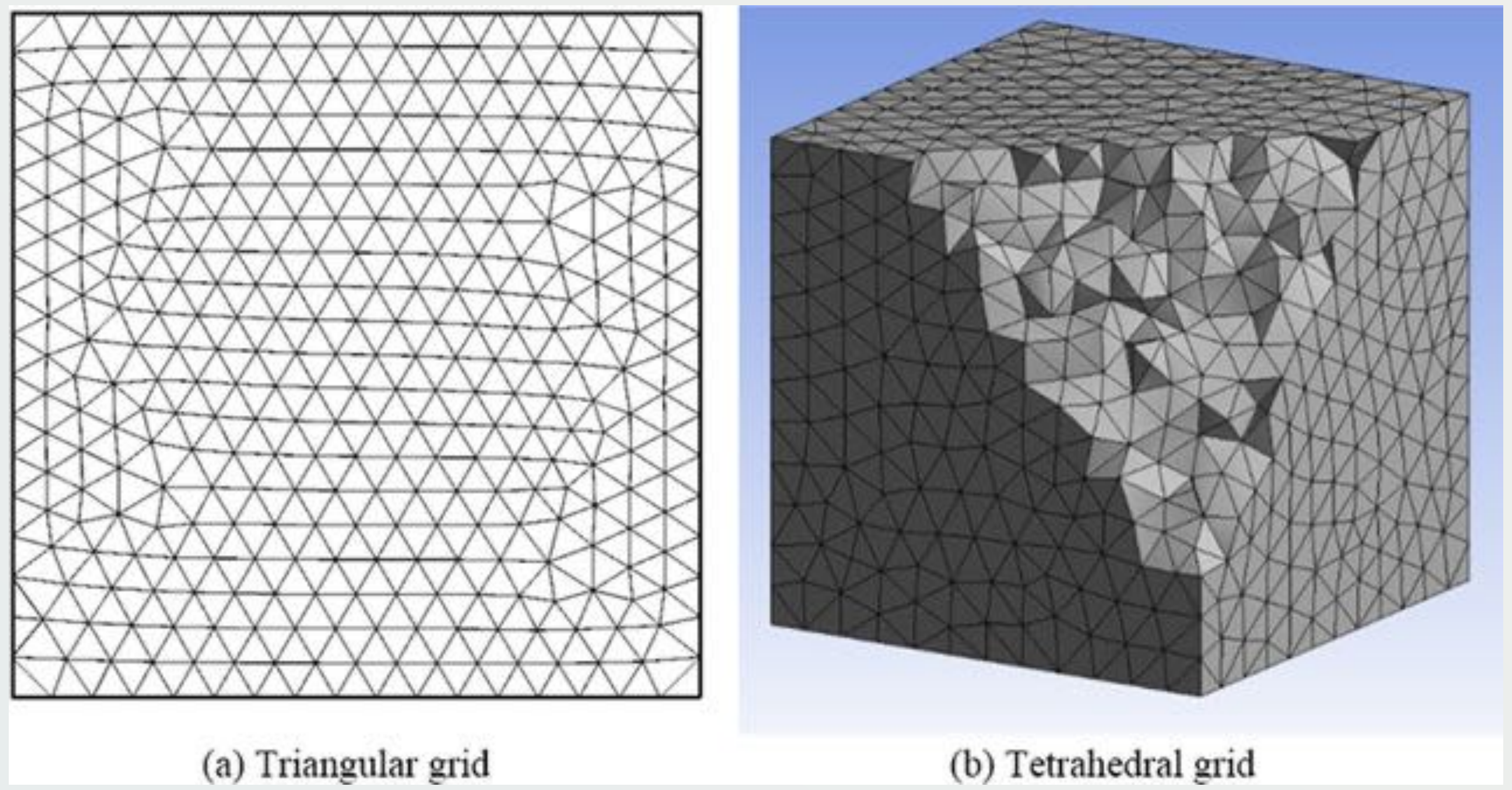
To train *through* the solver,
it must be *differentiable.*

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.

Innovative numerics



CFD solver rewritten in Julia (fully differentiable framework)



Unstructured numerical scheme
(popular at CERFACS):

Two-step Taylor-Galerkin type C

TTGC

$$\tilde{u}^n = u^n + (0.5 - \gamma)\, \Delta t\, u_t^n + (1/6)\, \Delta t^2\, u_{tt}^n$$

$$u^{n+1} = u^n + \Delta t\, \tilde{u}_t^n + \gamma\, \Delta t^2\, u_{tt}^n$$

Innovative numerics

TTGC: typical unstructured numerical scheme

Usually optimised <u>globally</u>

$$\tilde{u}^n = u^n + (0.5 - \gamma)\ \Delta t\ u_t^n + (1/6)\ \Delta t^2\ u_{tt}^n$$

$$u^{n+1} = u^n + \Delta t\ \tilde{u}_t^n + \gamma\ \Delta t^2\ u_{tt}^n \qquad \boxed{\gamma = 0.01}$$

Equally spaced mesh

Irregular mesh

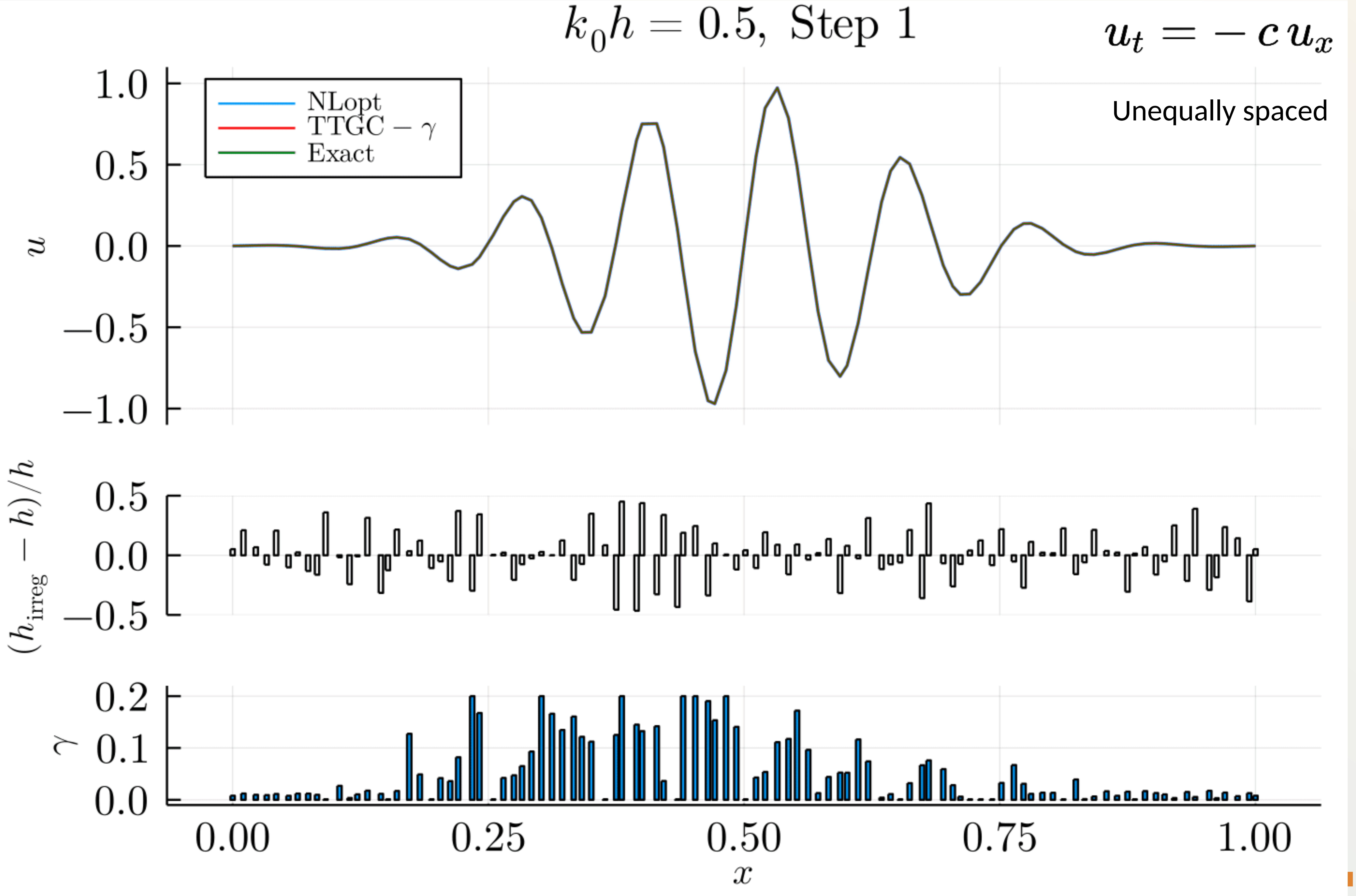
Global optimal is **not** a *local* optimal!

$$\boxed{\gamma = 0.01}$$

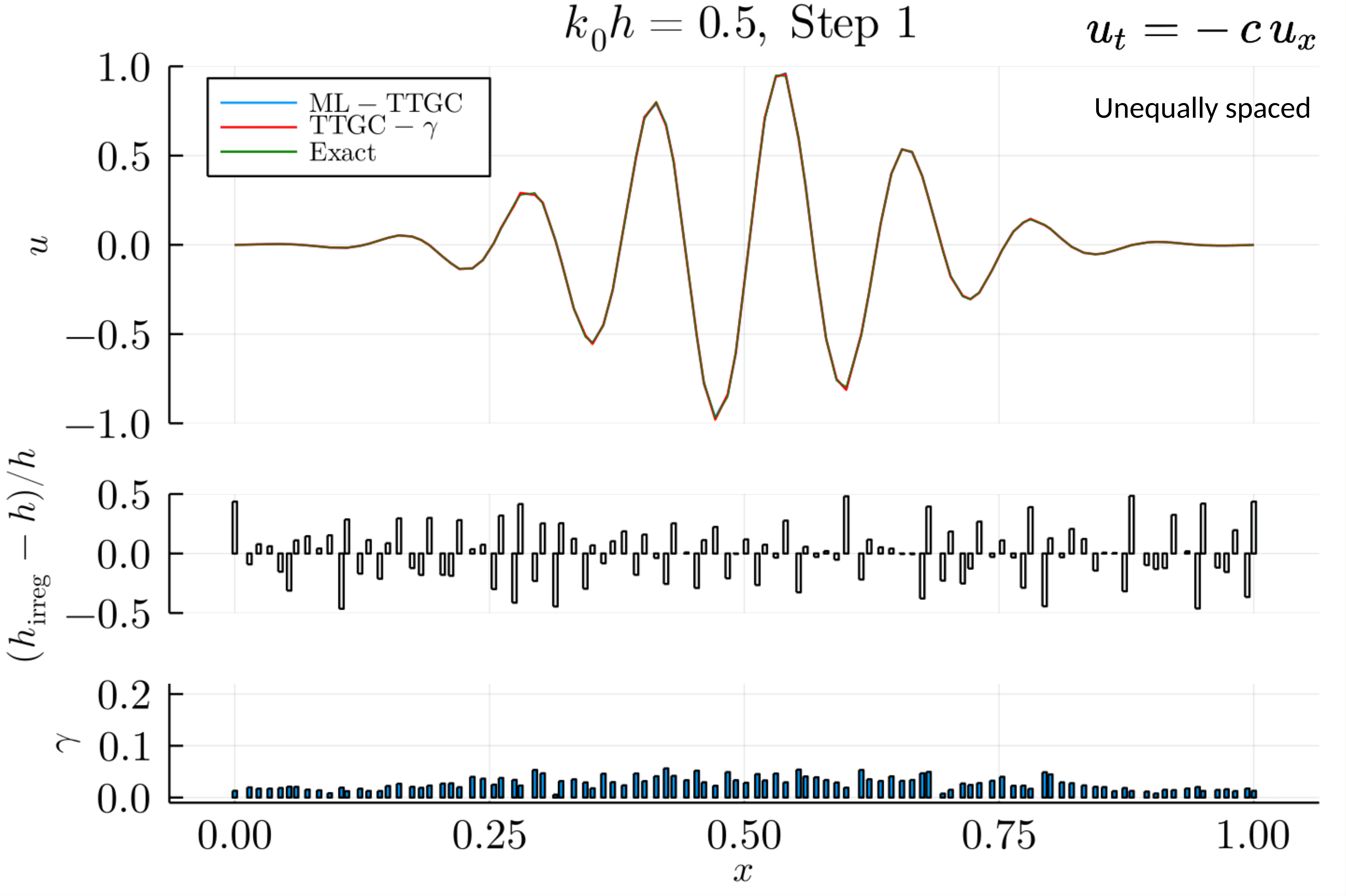
Allow γ to change **locally** in the mesh

Differentiate TTGC solver

Supply gradients to **NLopt** (optimizer)



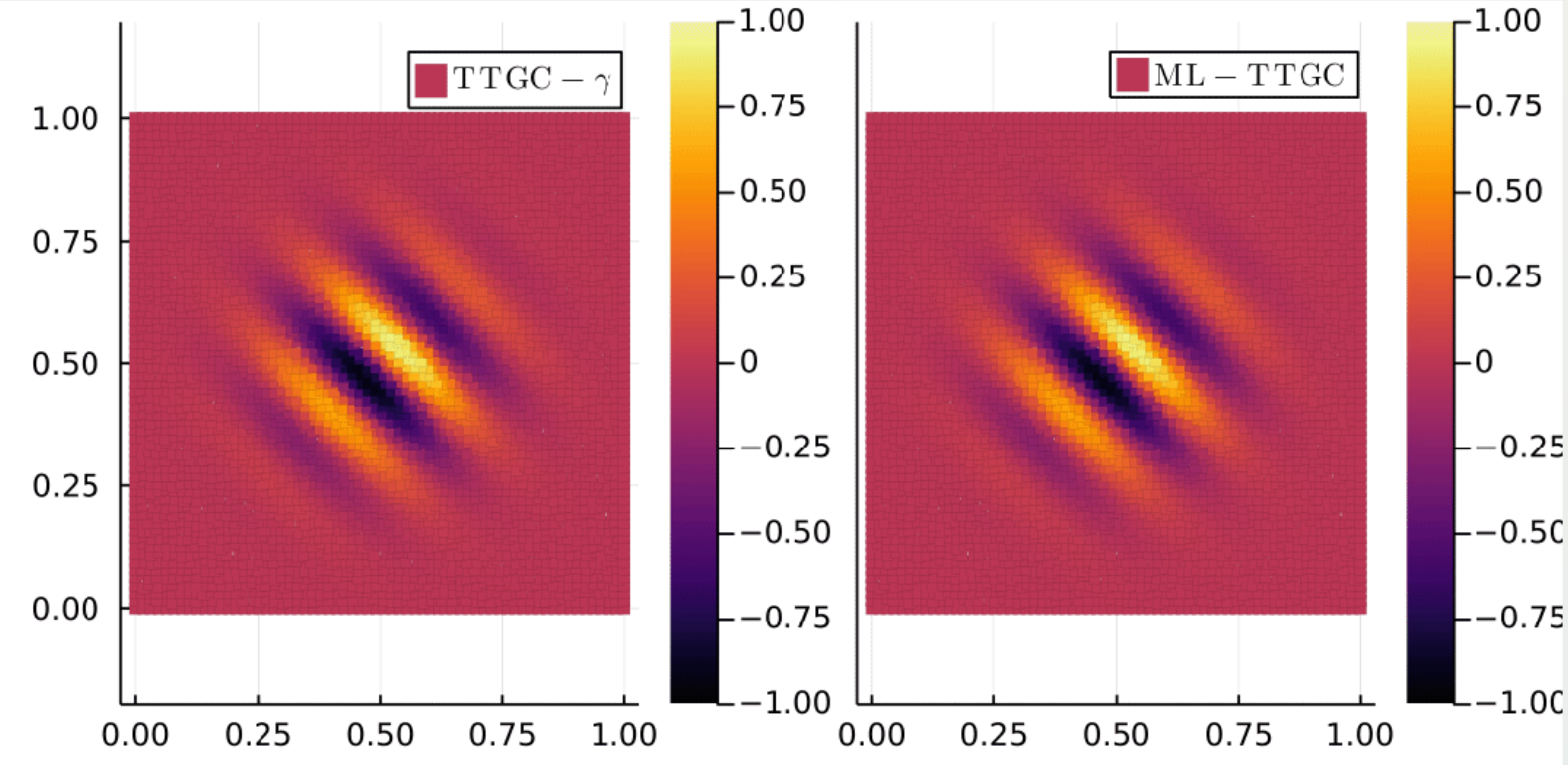
$k_0 h = 0.5$, Step 1
$u_t = -c\,u_x$
Unequally spaced
NLopt
TTGC − γ
Exact
u
$(h_{\mathrm{irreg}} - h)/h$
γ
x
1.0
0.5
0.0
−0.5
−1.0
0.2
0.1
0.00
0.25
0.50
0.75
1.00


$k_0 h = 0.5,\ \text{Step } 1$
$u_t = -c\, u_x$
Unequally spaced
ML − TTGC
TTGC − γ
Exact
u
$(h_{\text{irreg}} - h)/h$
γ
x
1.0
0.5
0.0
−0.5
−1.0
0.2
0.1
0.00
0.25
0.50
0.75
1.00

Locally-adaptive numerical schemes for unstructured solvers

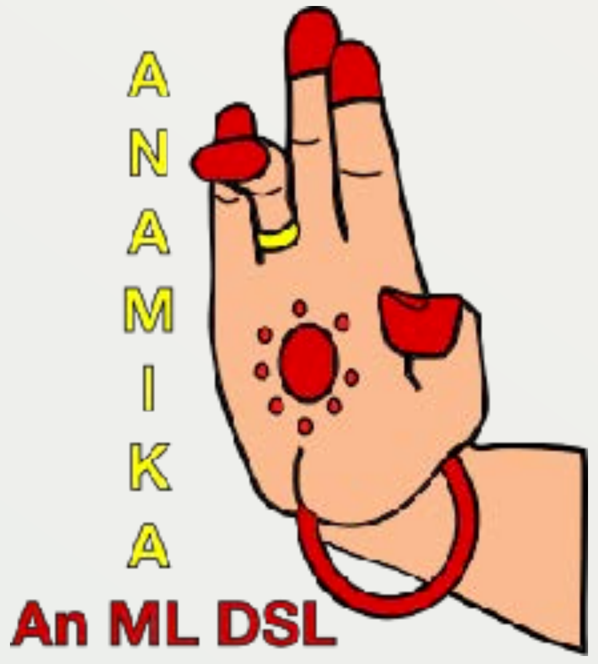
Innovative numerics

Drozda, L. *et al.* (2021). Data-driven Taylor-Galerkin finite-element scheme for convection problems.
The Symbiosis of Deep Learning and Differential Equations - Neurips 2021 Workshop



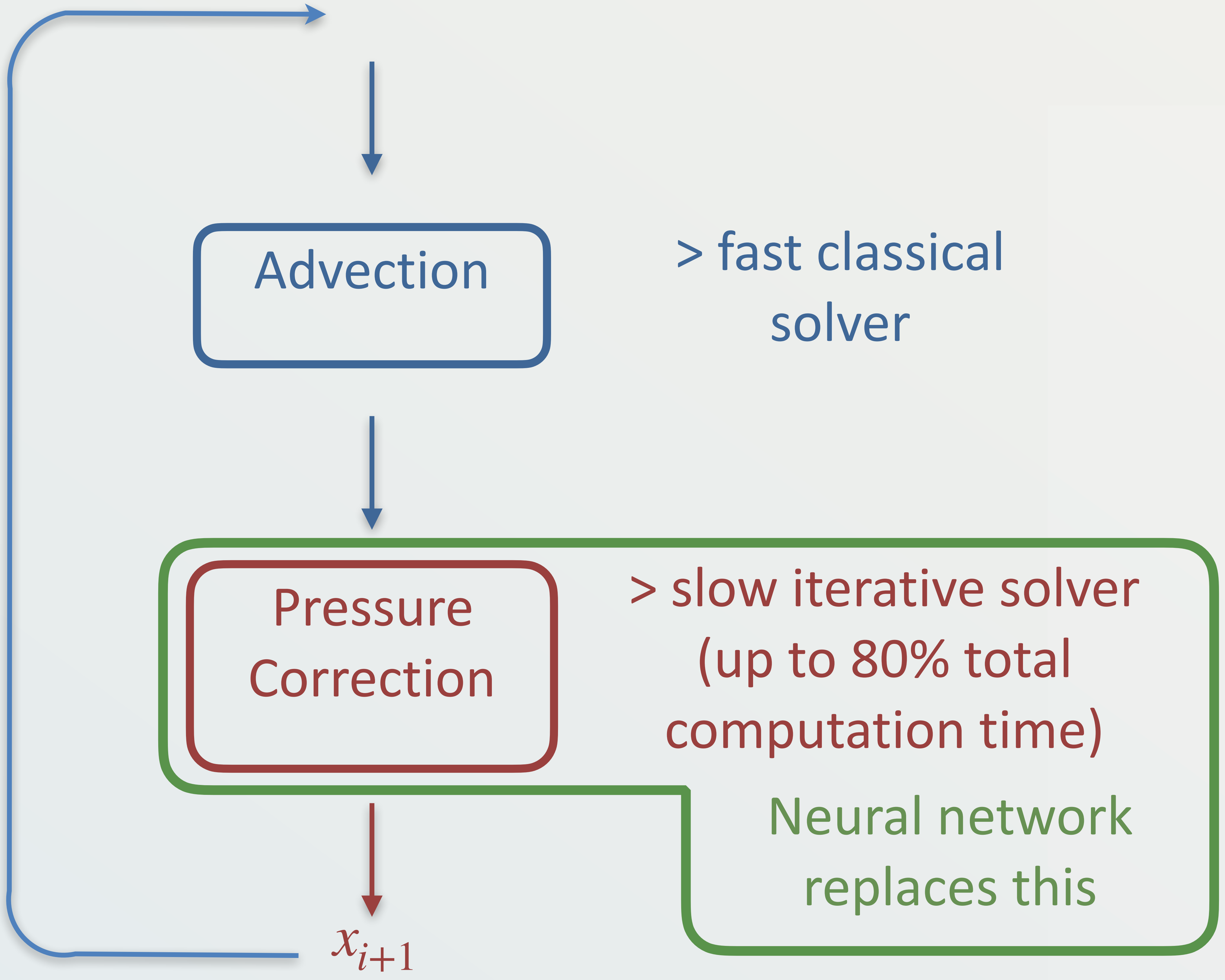
Differentiable Euler Solver in Julia (Zygote)

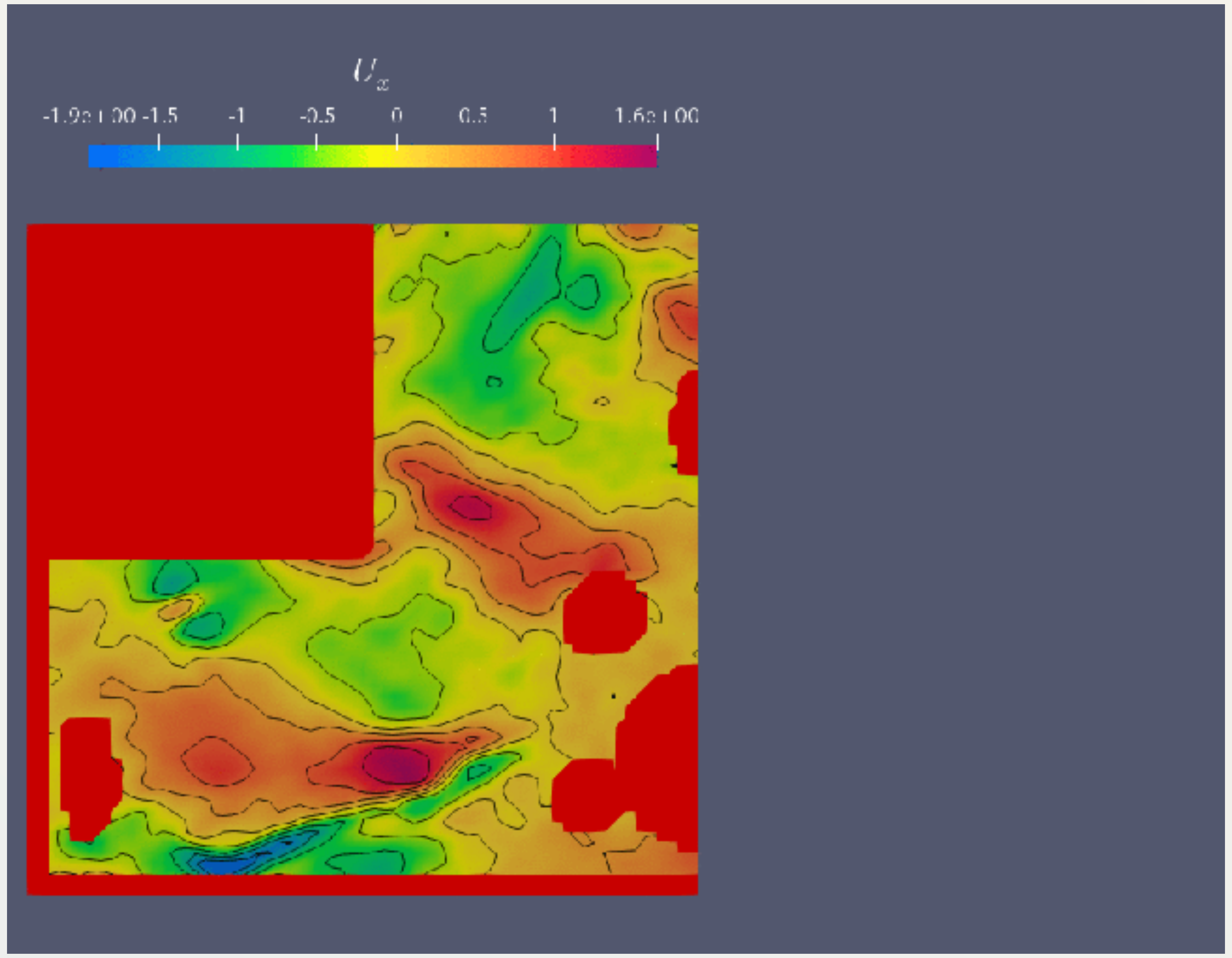
-> Too many limitations with mutability
Development of dedicated open-source
C++ / Tapenade solver: Anamika



https://cerfacs.fr/coop/DSL

Poisson solvers



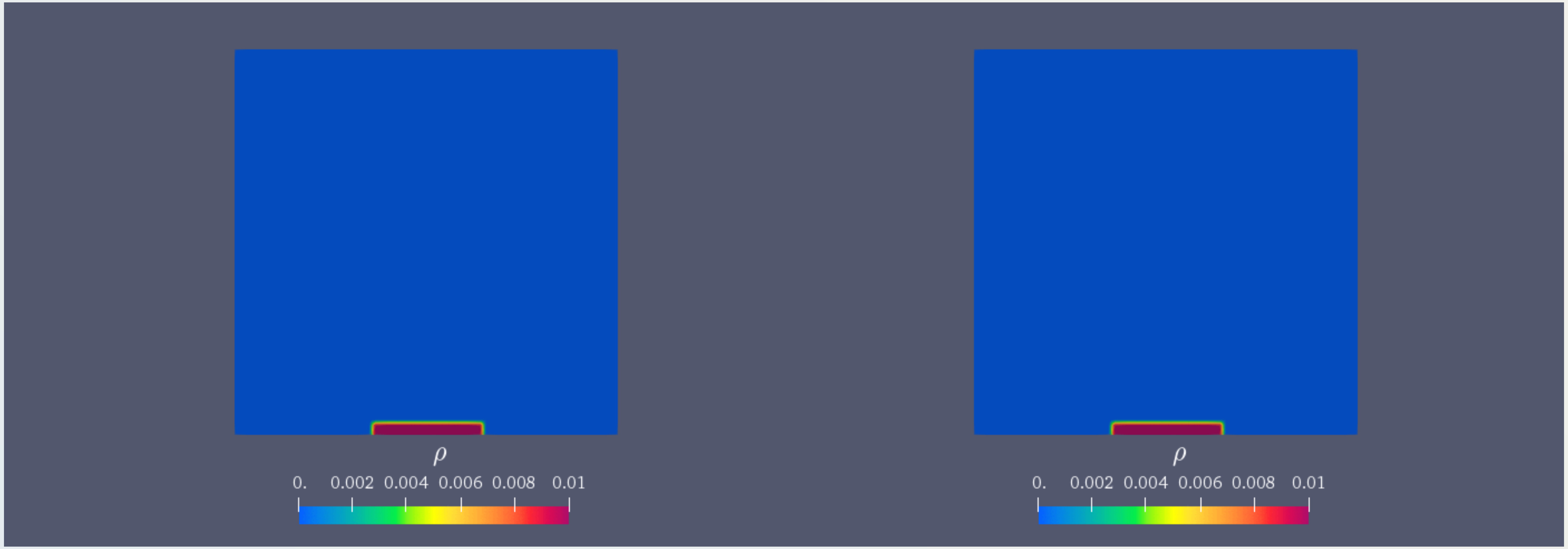


Strategy originally proposed as « FluidNet » [1]

[1] Tompson, Jonathan, et al. "Accelerating eulerian fluid simulation with convolutional networks." *Proceedings of the 34th International Conference on Machine Learning-Volume 70*. JMLR. org, 2017.

Full network approach

Innovative numerics



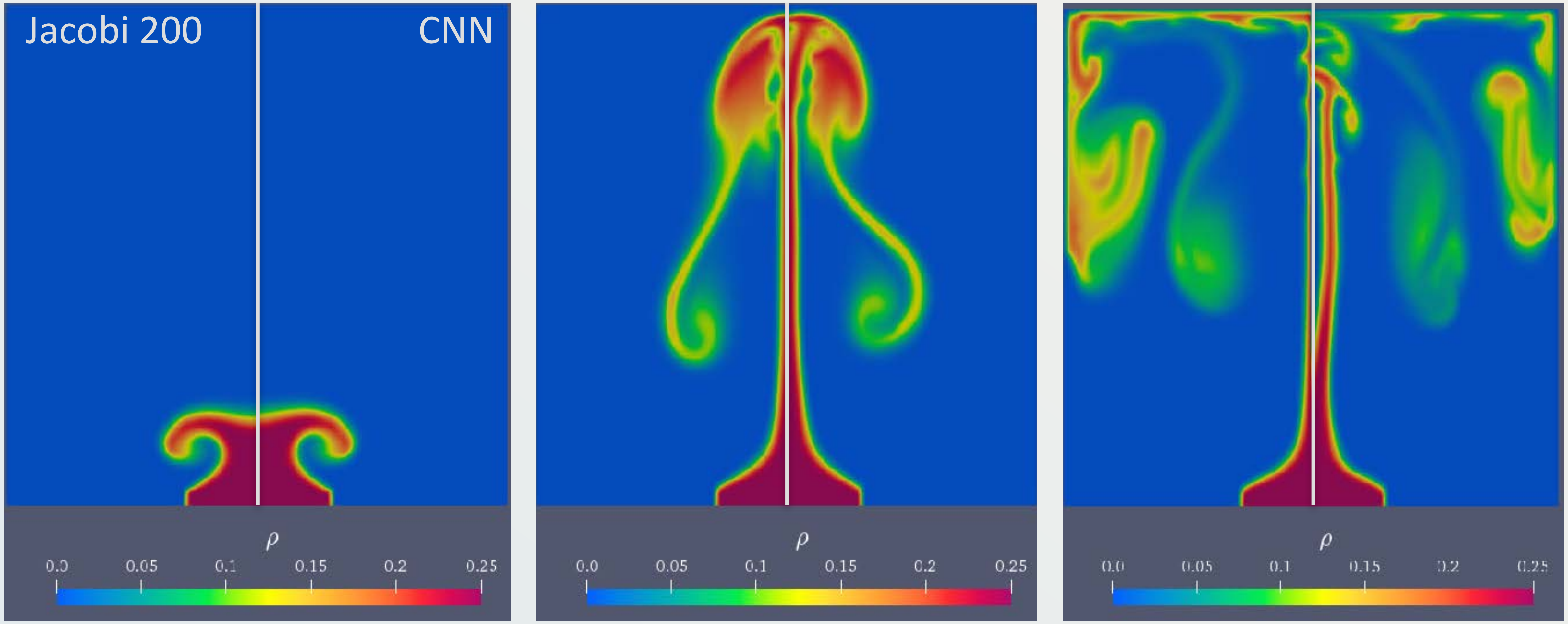
CNN

Jacobi 200

Full network approach

Innovative numerics

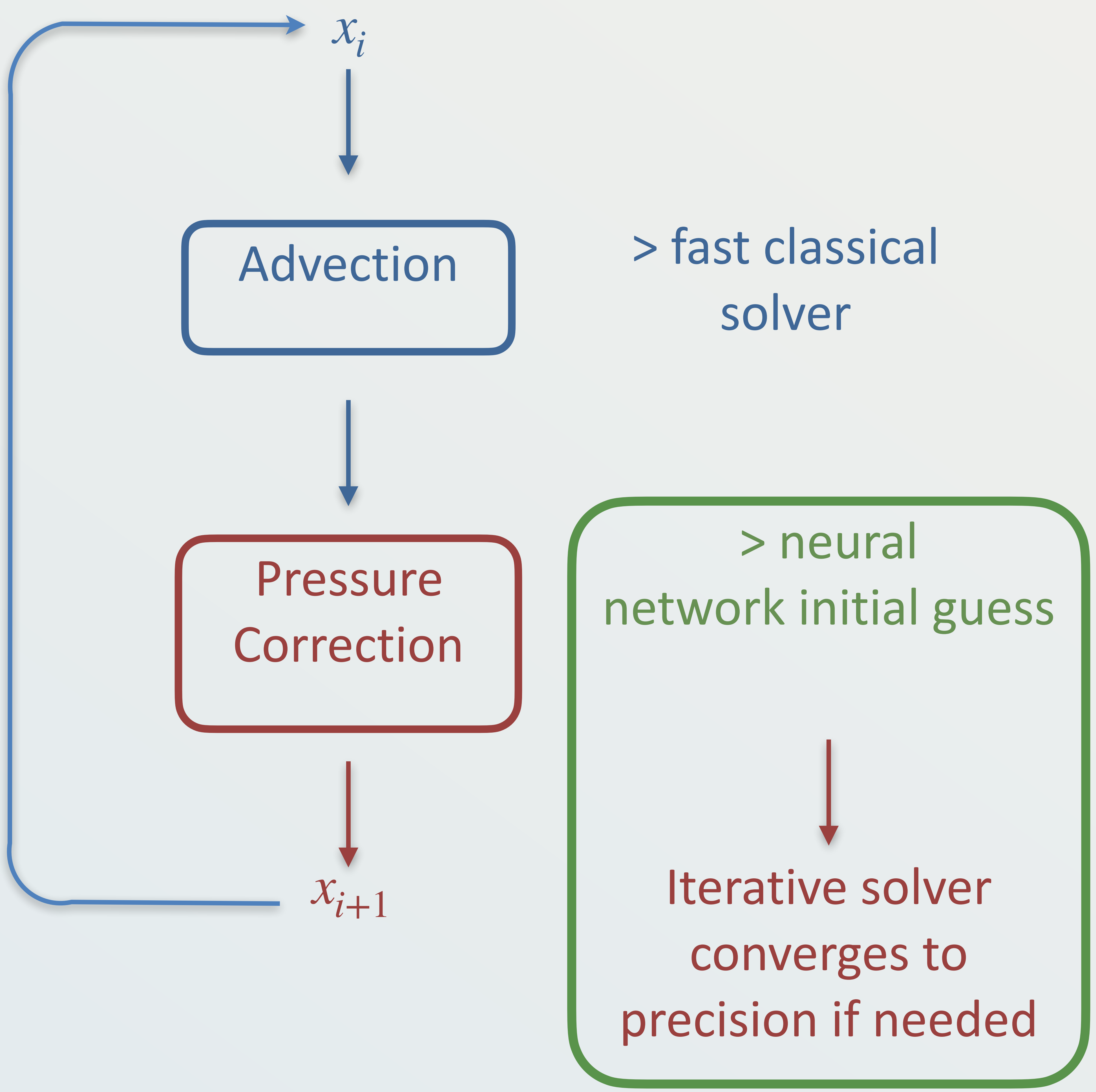
- Interesting results but robustness problems

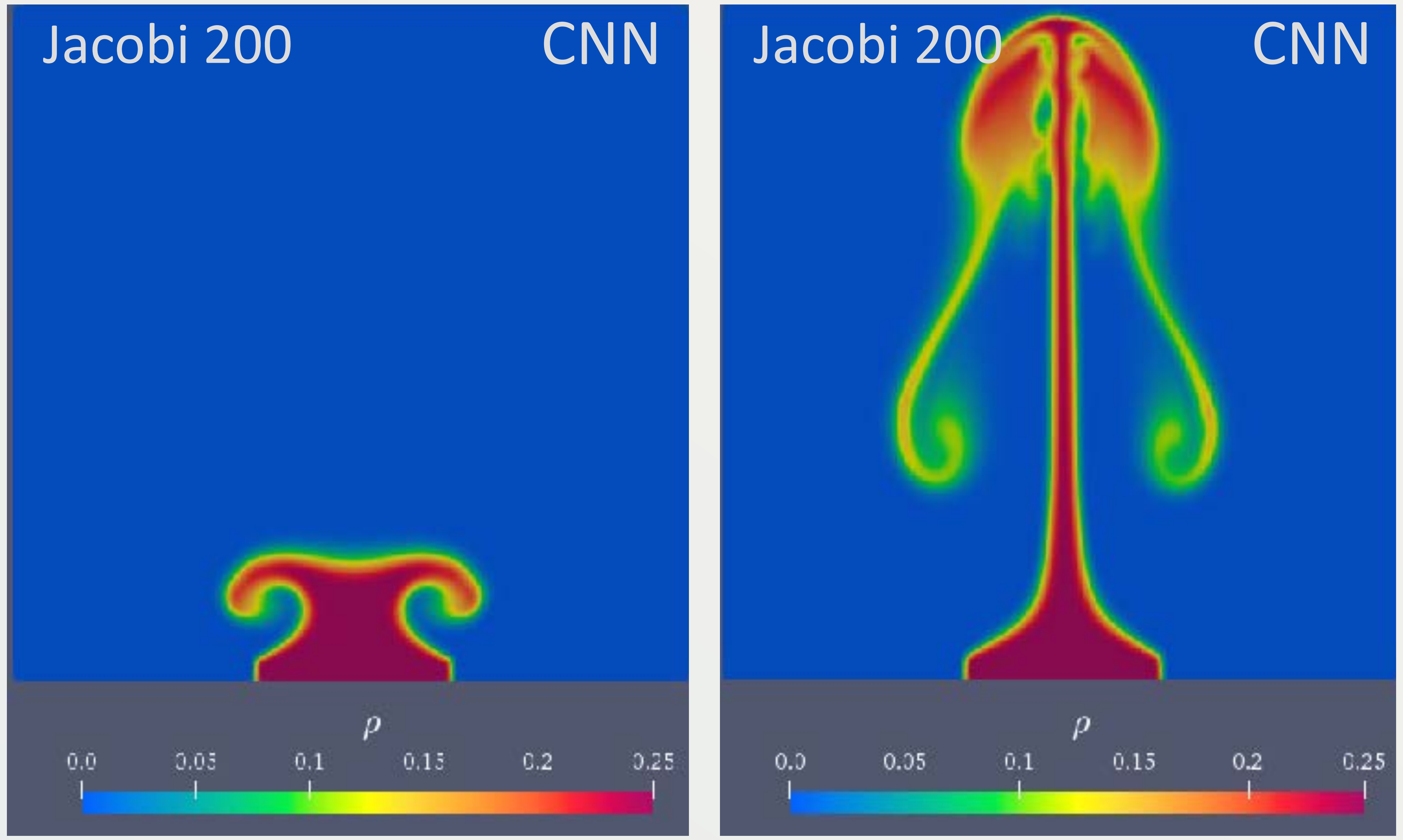


- How could we guarantee the accuracy of the pressure correction? => Hybrid

Hybrid approach

Innovative numerics

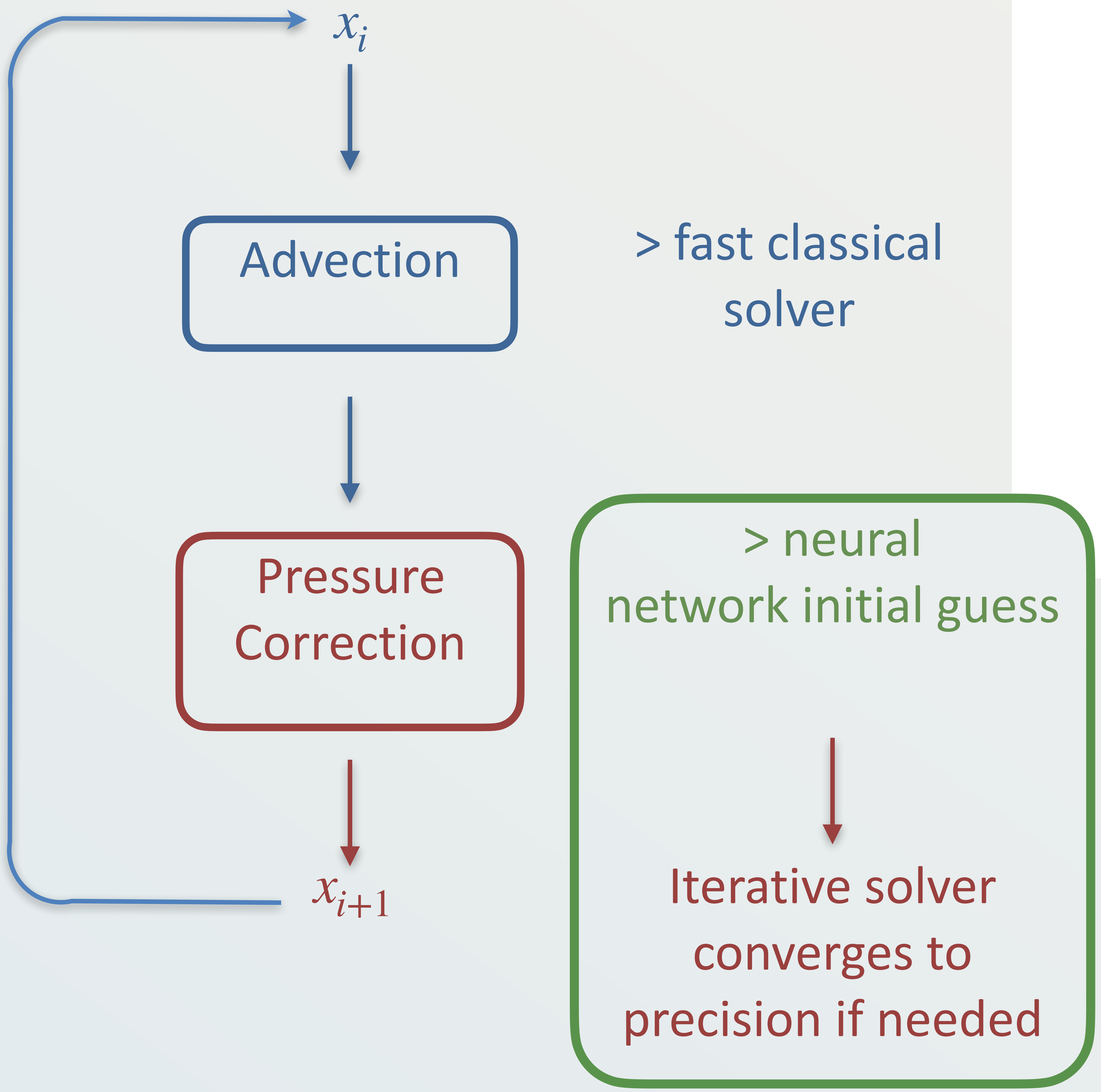




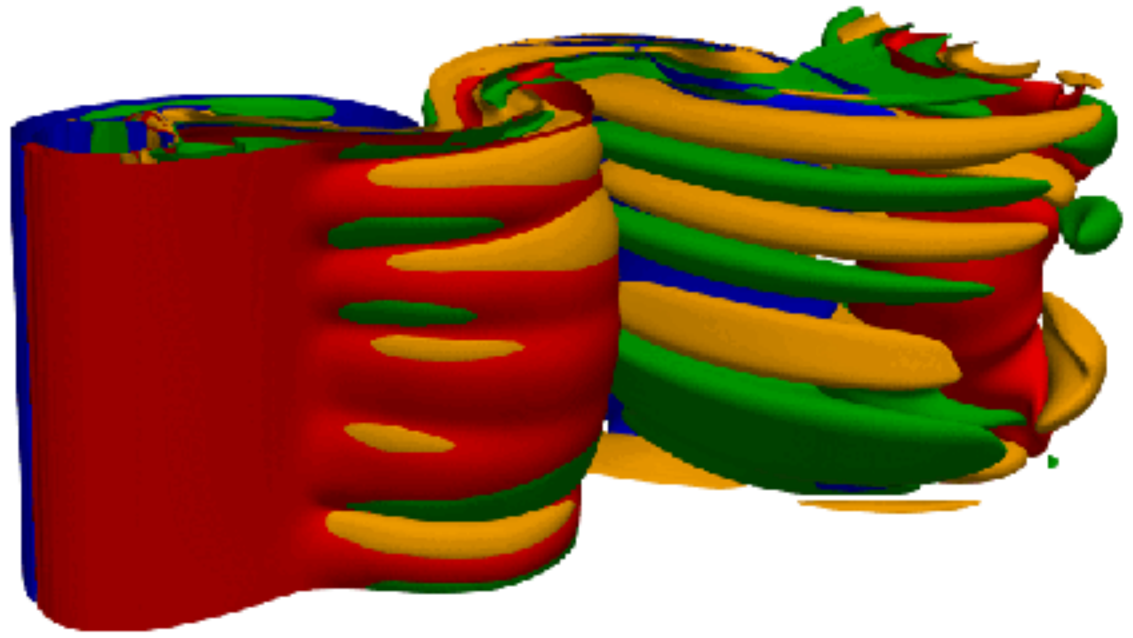
Ajuria Illarramendi, Ekhi, et al. "Towards an hybrid computational strategy based on deep learning for incompressible flows." AIAA Aviation 2020 forum. 2020.

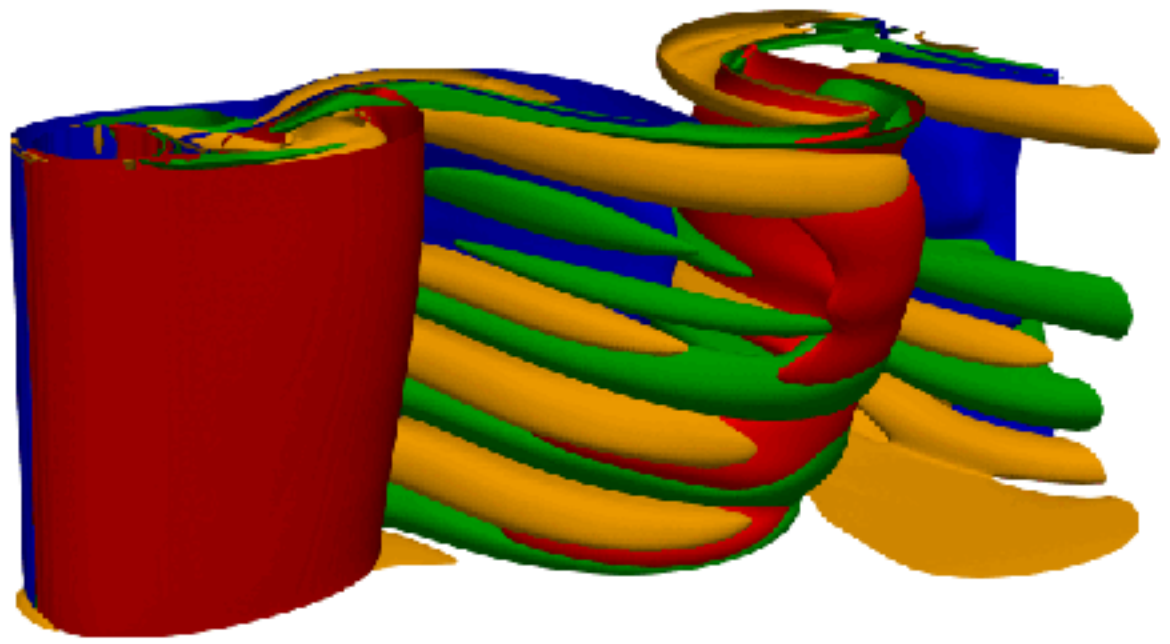
Hybrid approach

Innovative numerics



Traditional method





AI-based method: 1.5x faster

Ajuria Illarramendi, Ekhi, et al. "Towards an hybrid computational strategy based on deep learning for incompressible flows." AIAA Aviation 2020 forum. 2020.

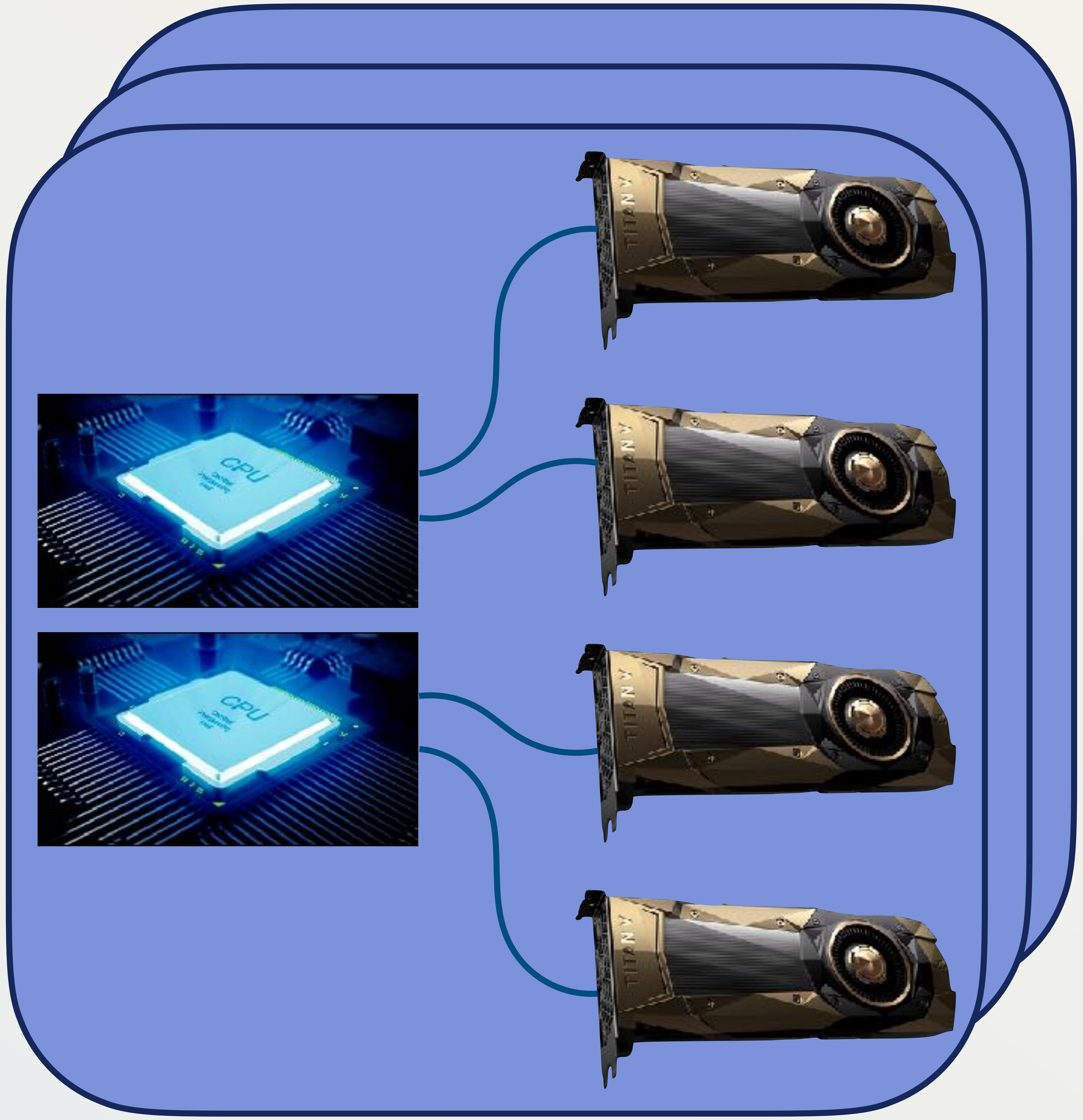
HPC for Hybrid Simulation

CPU/GPU architectures

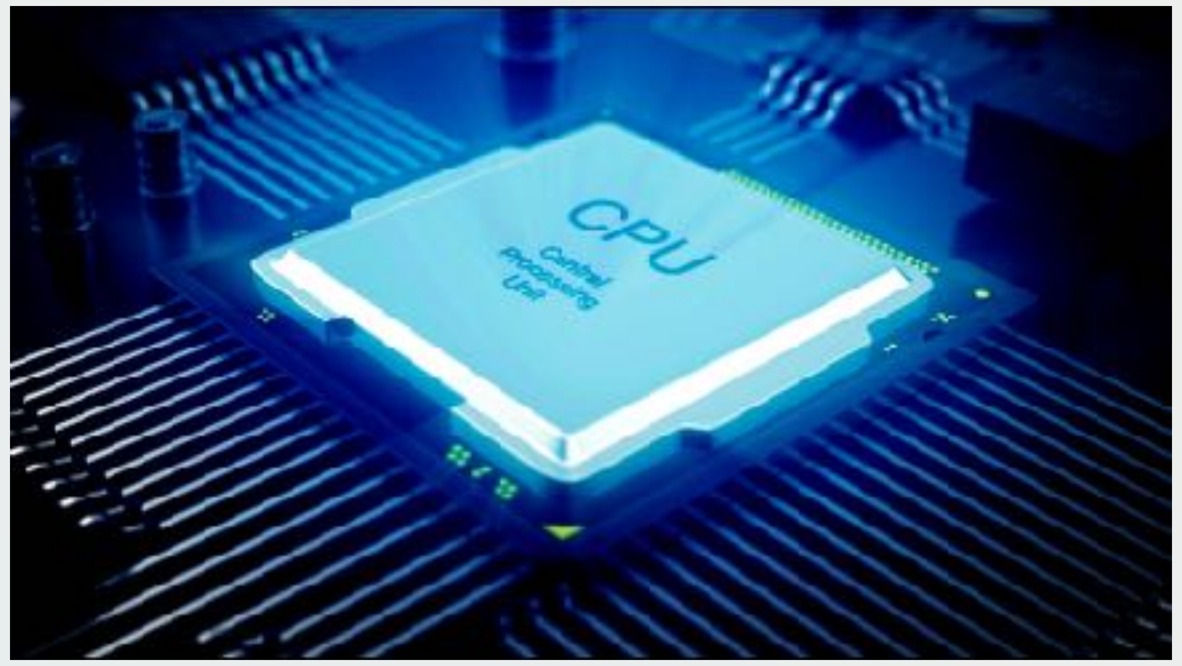
Mesh issues

- Interpolation strategies
- Innovative network architectures

Jean Zay Supercomputer
CNRS - IDRIS, France



CPU/GPU architectures



Physical fields

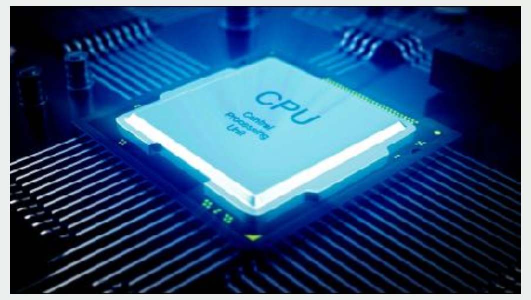
Predictions

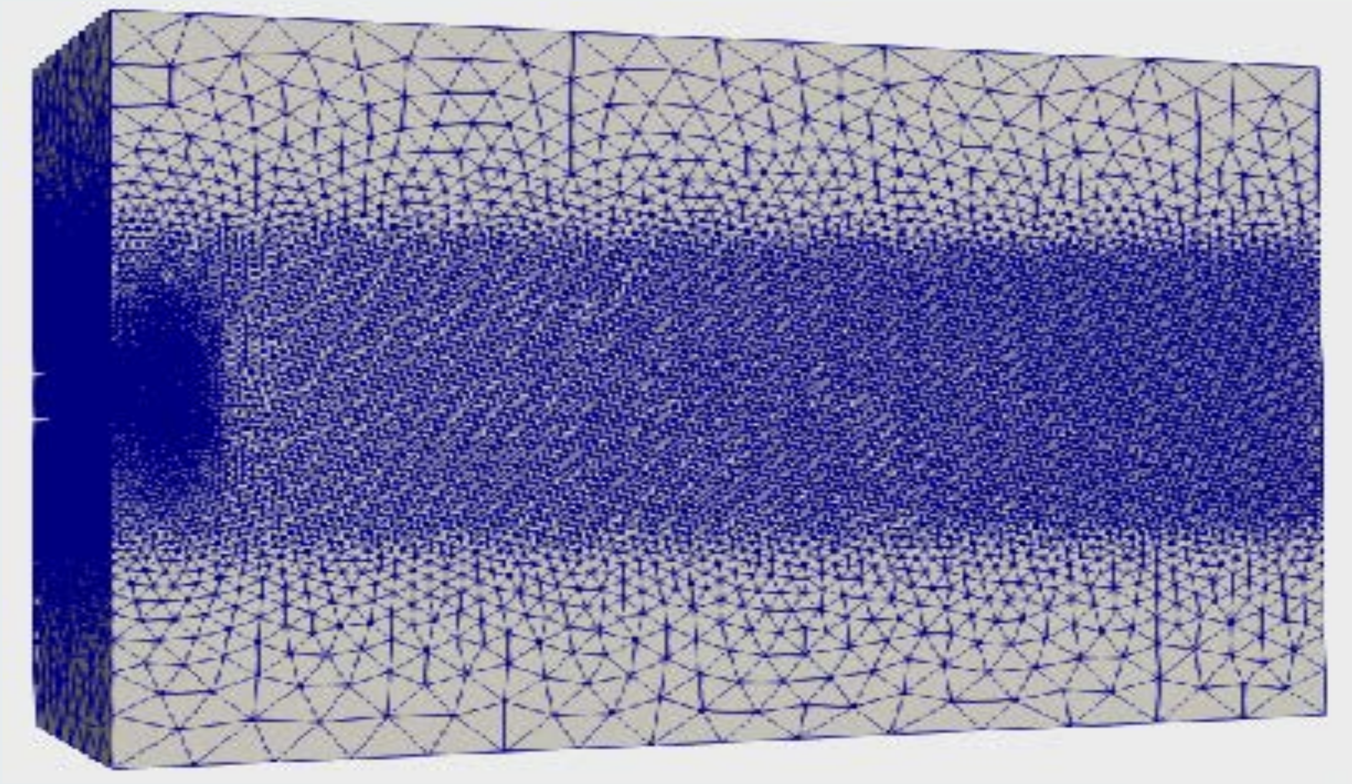
$$\frac{Du}{Dt} = -\nabla p + \mu \nabla^2 u + \varrho F$$

CPU : Navier-Stokes solver
(e.g. AVBP)

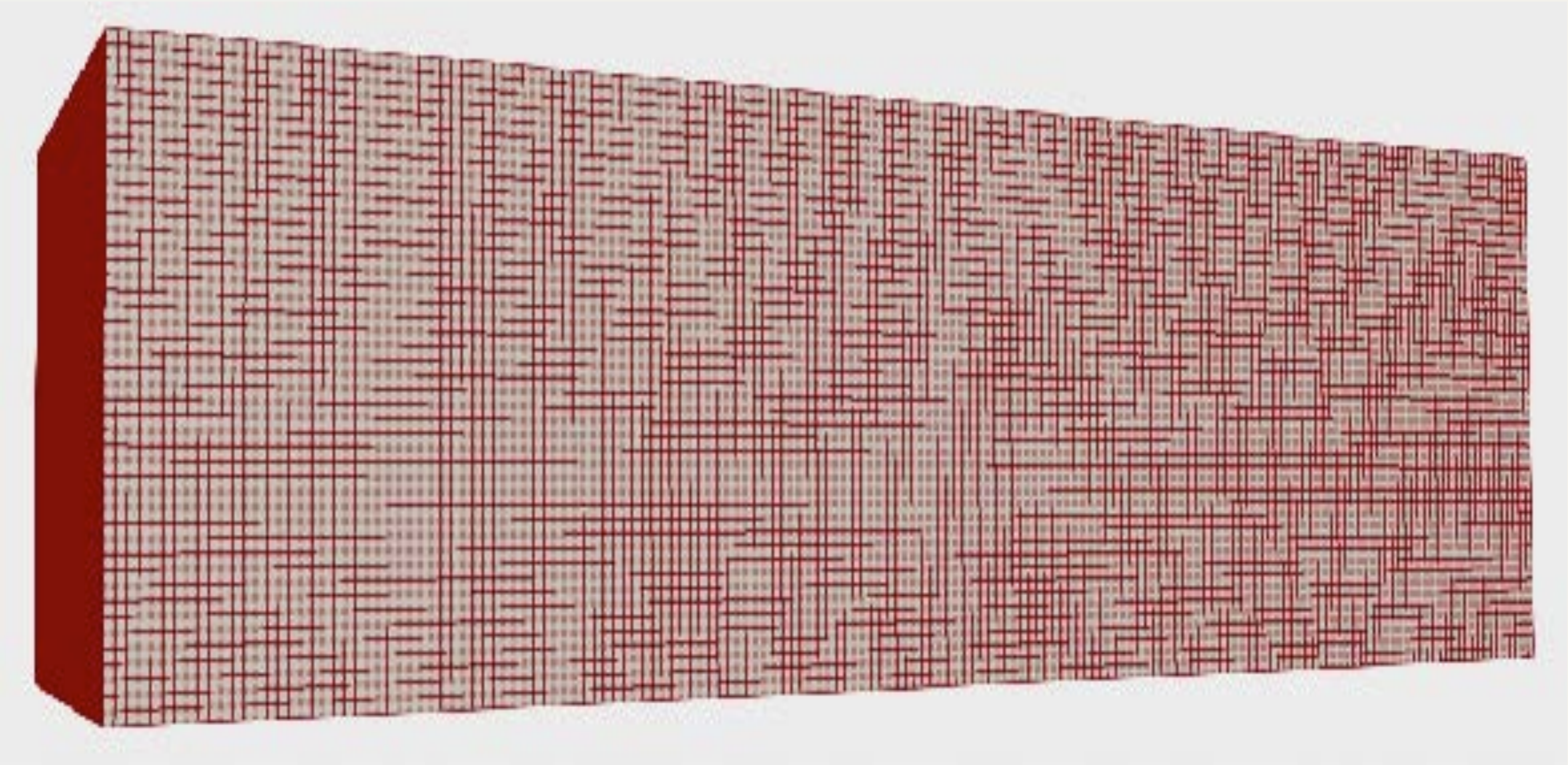
GPU : Neural Net
(TensorFlow)

Mesh issues



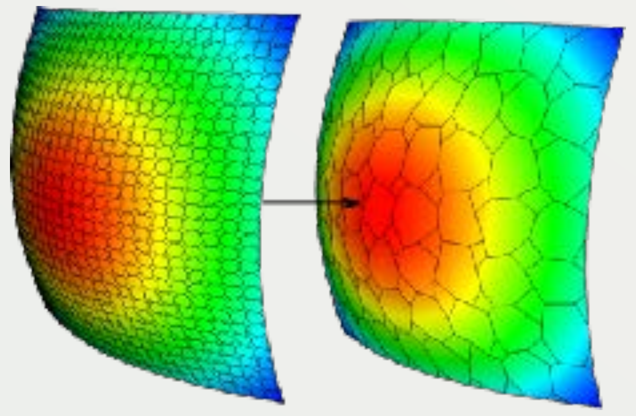


Unstructured mesh

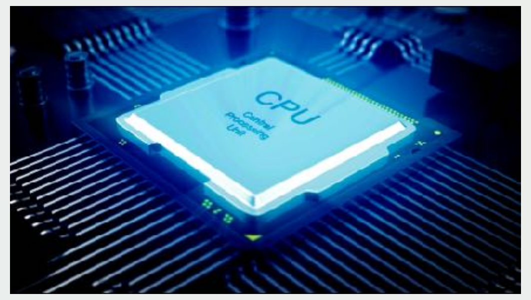


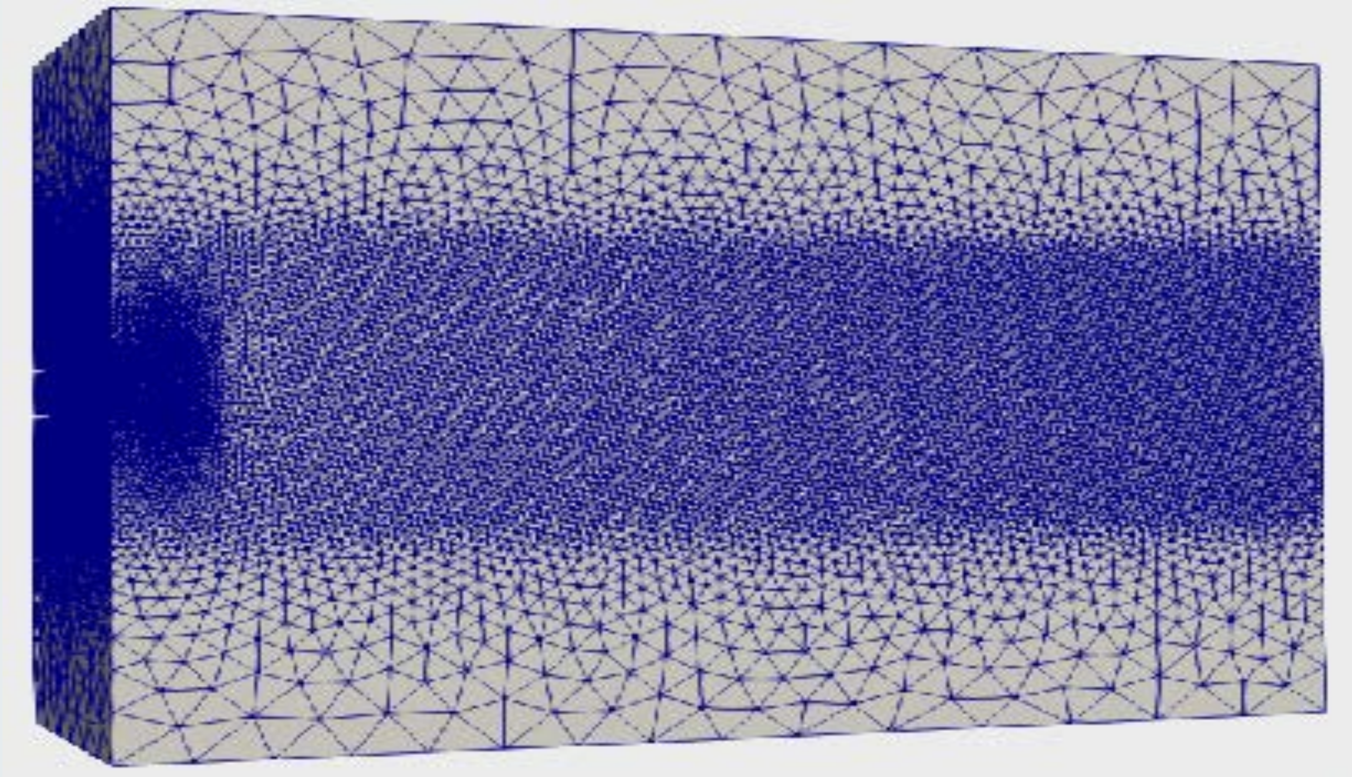
CNN: Pixels / Voxels

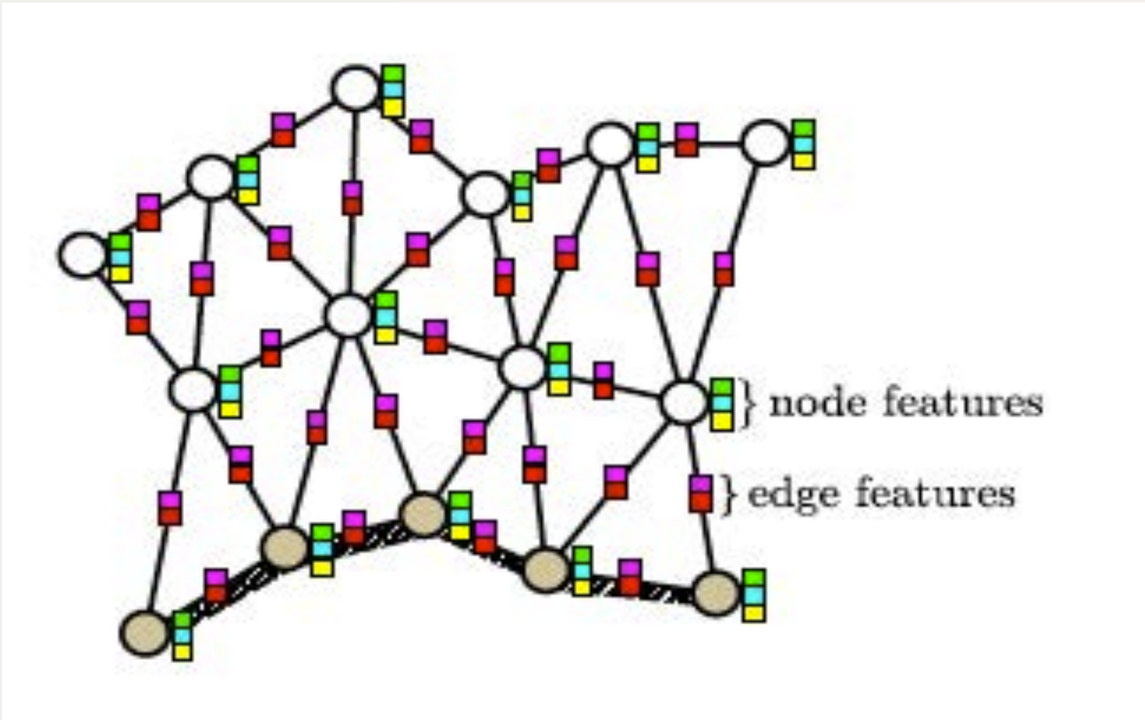
Mesh mismatch => on-the-fly interpolation (CWIPI library)



Mesh issues







Unstructured mesh

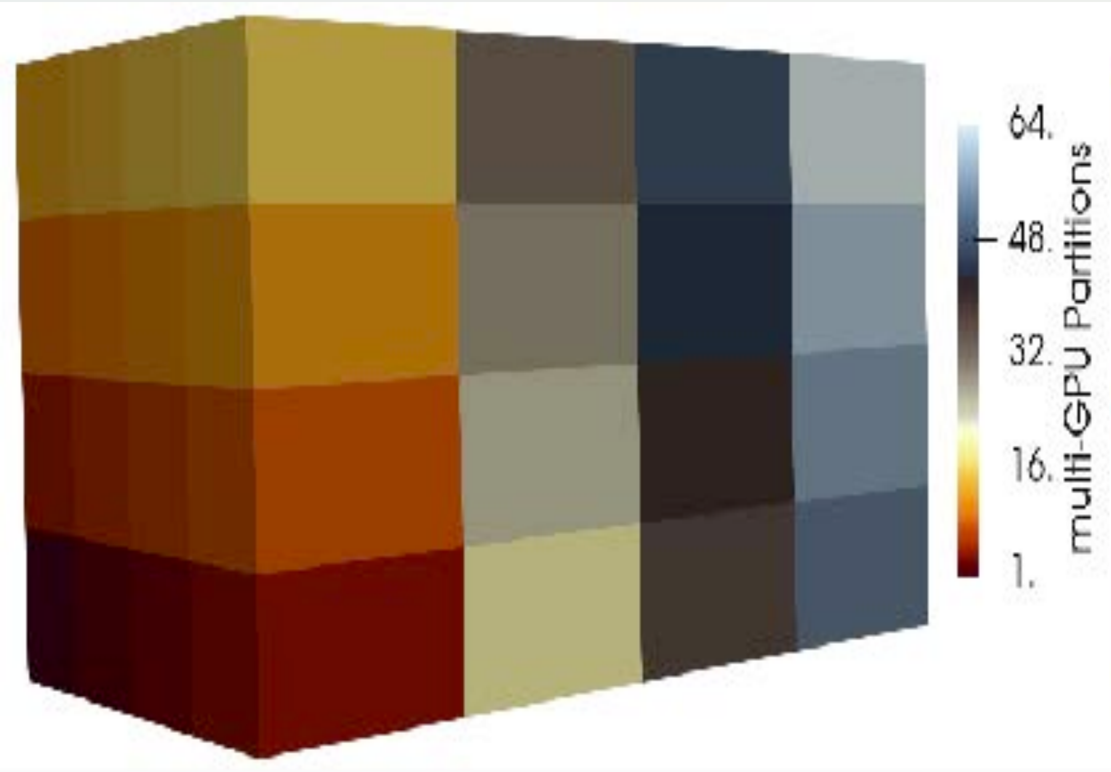
GNN: Same mesh

Direct use of *Mesh Graph Networks* can alleviate interpolation

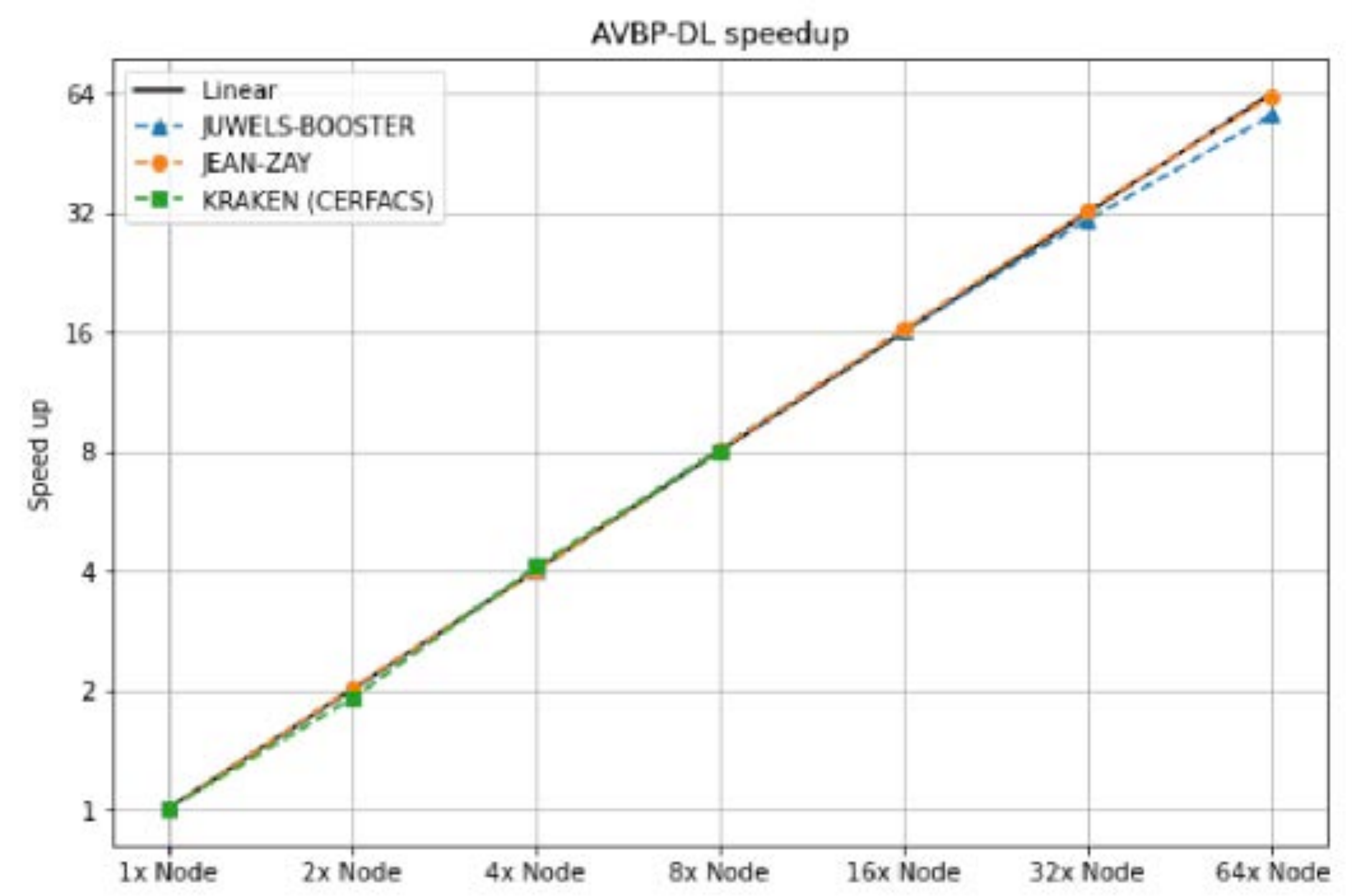
Serhani, A., Xing, V., Dupuy, D., Lapeyre, C., Staffelbach, G. (2022). High-performance hybrid coupling of a CFD solver to deep neural networks. 33rd Parallel CFD International Conference, May 25-27, Alba, Italy.

This shouldn't happen…

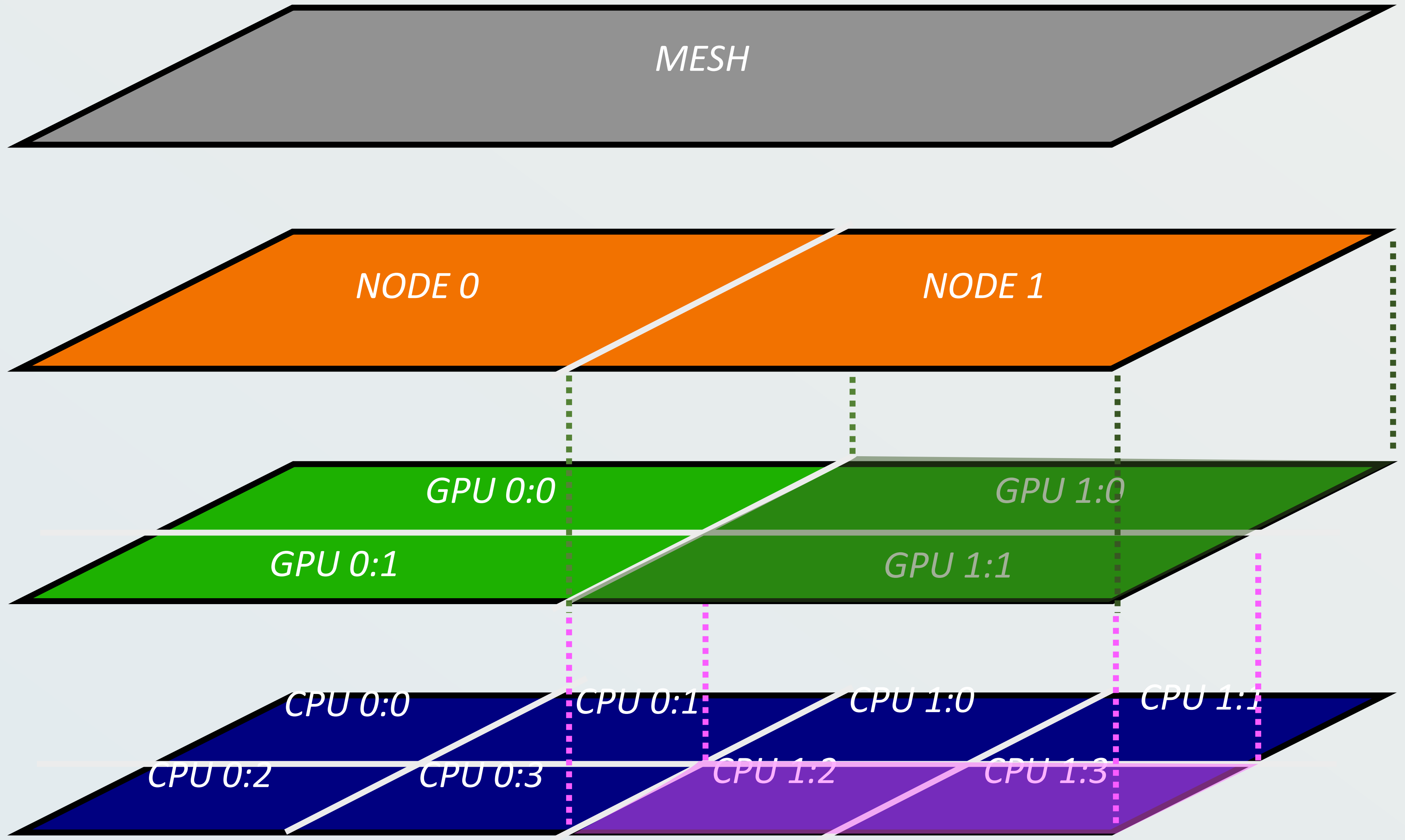
/



GPU Partitions



Parallel scaling



Domain Mesh

Node-level partitioning

GPU-level partitioning
(nb of Python processes)

CPU-level partitioning
(nb of AVBP processes)

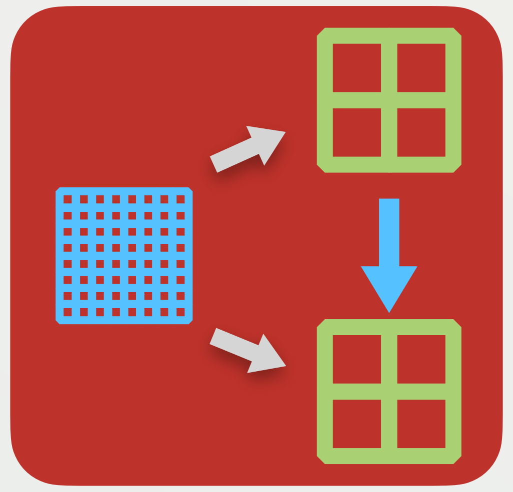
Hierarchical domain discretization with treepart

PhyDLL :

the **Phy**sics - **D**eep **L**earning Coup**L**er

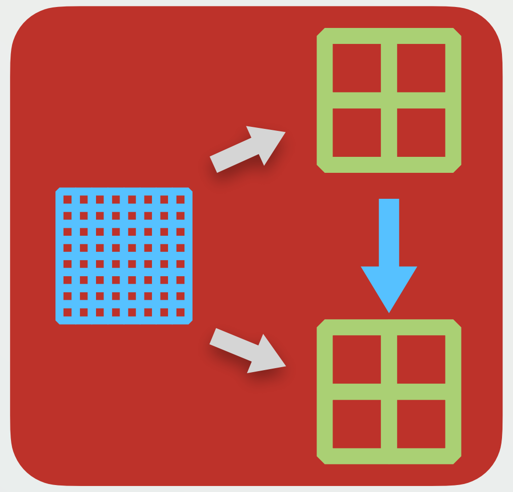
(open-source software)

https://phydll.readthedocs.io



Hybrid-simulation:

More accurate models

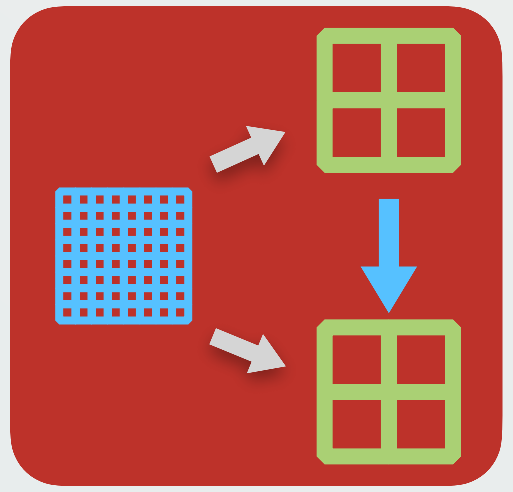


Hybrid-simulation:

More accurate models

Hybrid simulation:

Innovative numerics



Hybrid-simulation:

More accurate models

Hybrid simulation:

Innovative numerics

Hybrid HPC:

CPUs / GPUs / …?

Recent Papers

- Dupuy, D., Odier, N. and Lapeyre, C. (2023). Modelling the wall shear stress in large-eddy simulation using graph neural networks. To appear in *Data-Centric Engineering.*
- Lazzara, M., Chevalier, M., Colombo, M., Garay Garcia, J., Lapeyre, C., Teste, O. (2022). Surrogate modelling for an aircraft dynamic landing loads simulation using an LSTM AutoEncoder-based dimensionality reduction approach. *Aerospace Science and Technology*, 126, 107629.
- Yewgat, A., Busby, D., Chevalier, M. et al. (2022). Physics-constrained deep learning forecasting: an application with capacitance resistive model. Comput Geosci.
- 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.

Recent Conferences

- Serhani, A., Xing, V., Dupuy, D., Lapeyre, C., Staffelbach, G. (2022). High-performance hybrid coupling of a CFD solver to deep neural networks. 33rd Parallel CFD International Conference, May 25-27, Alba, Italy.
- ElMontassir, R., Lapeyre, C., Pannekoucke, O. (2022). Hybrid Physics-AI Approach for Cloud Cover Nowcasting. ECMWF Machine Learning Workshop.
- Drozda, L., Mohanamuraly, P., Realpe, Y., Lapeyre, C., Adler, A., Daviller, G., & Poinsot, T. (2021). Data-driven Taylor-Galerkin finite-element scheme for convection problems. The Symbiosis of Deep Learning and Differential Equations - Neurips 2021 Workshop
- 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.
- 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, Marseille, May 2019.