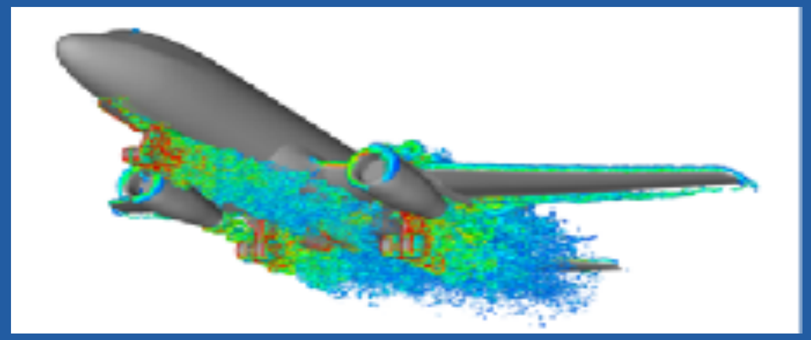
What can AI do for High-Performance Computing?

Corentin Lapeyre
Research Scientist, CERFACS

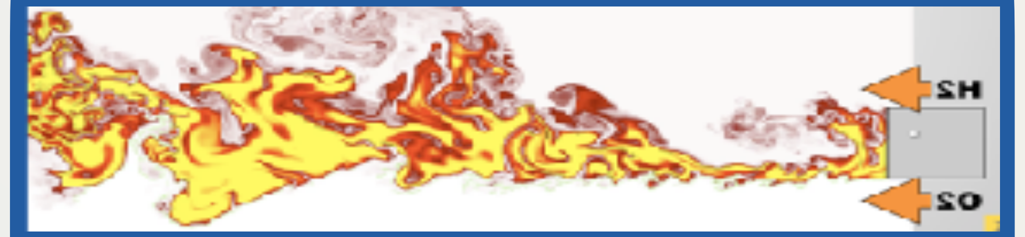
“High performance AI in the industry” Workshop

2022.06.15

Propulsion



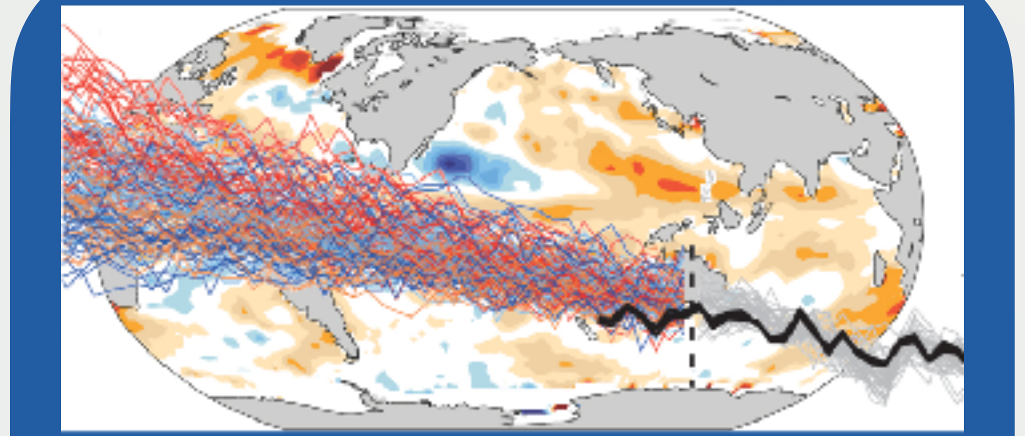
Aerodynamics and Aerocoustics



Hydrogen combustion

Environment and Safety

Climate - air transport interactions



Climate Variability and Predictability

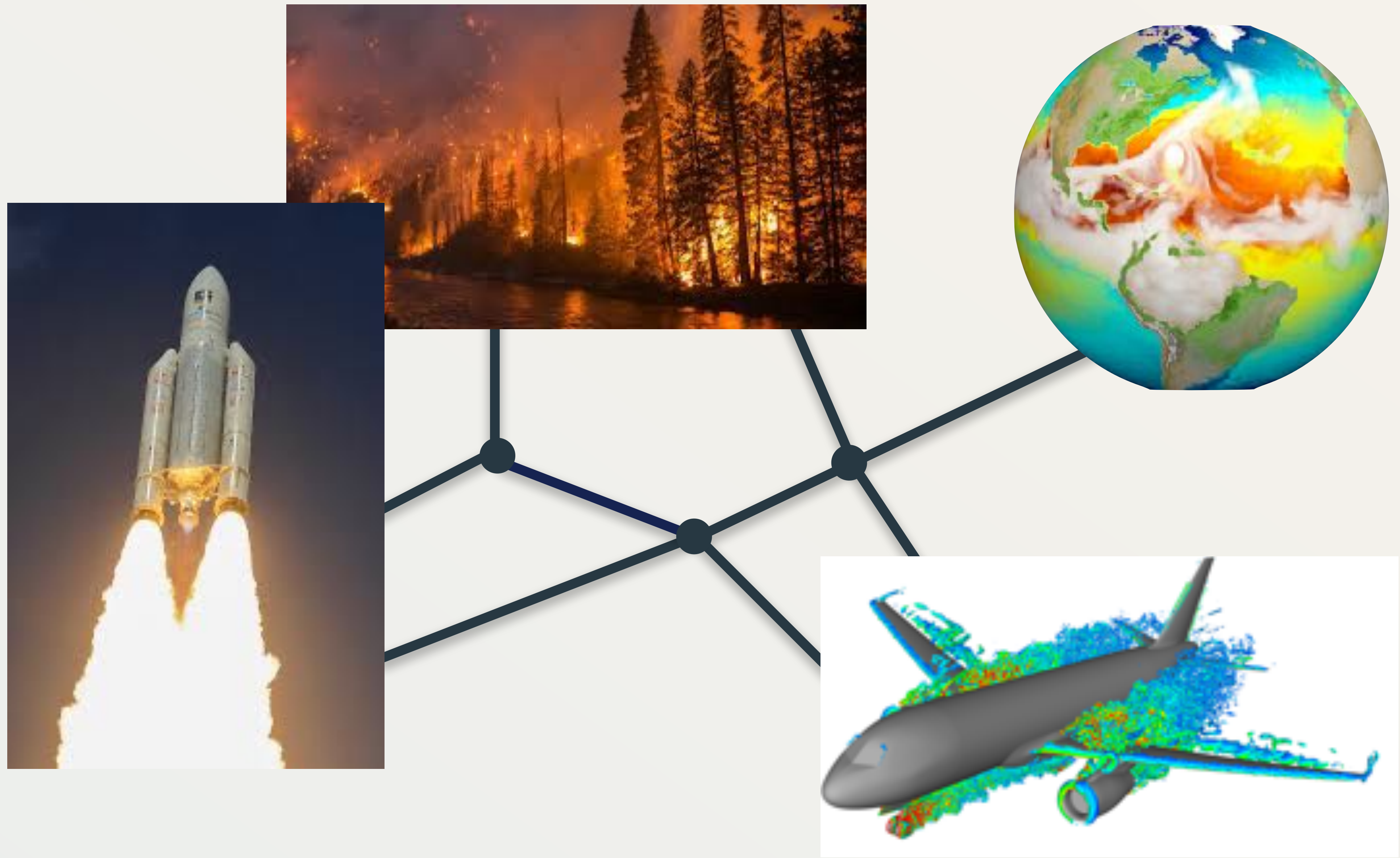
CERFACS

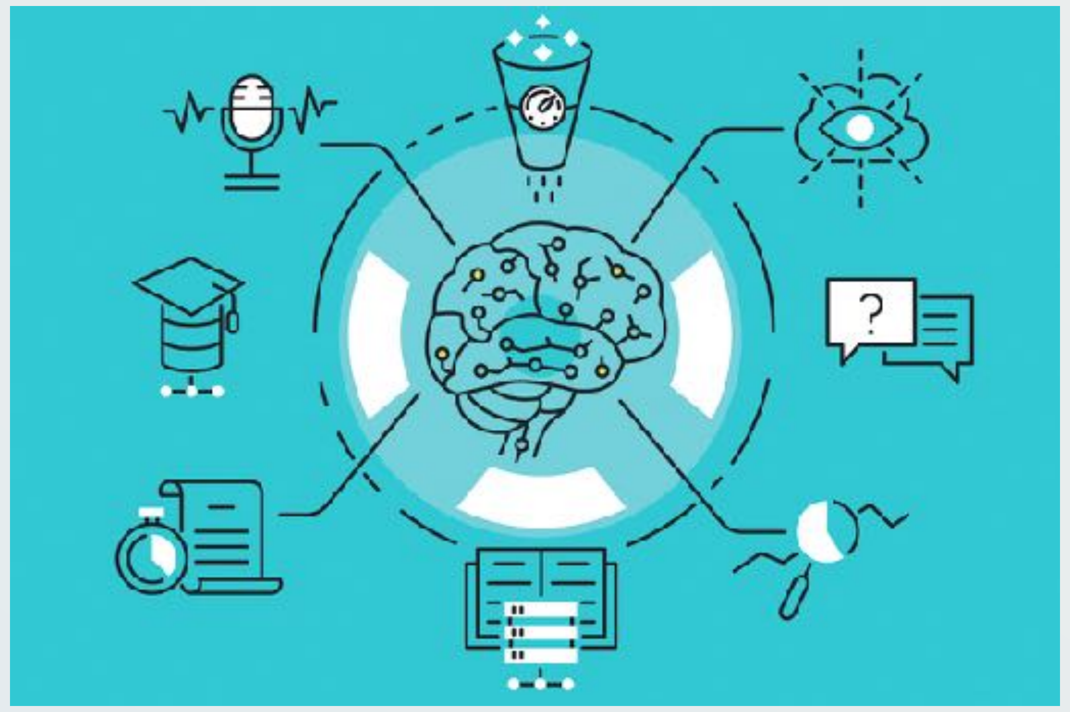
150 researchers

20 training sessions / y

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

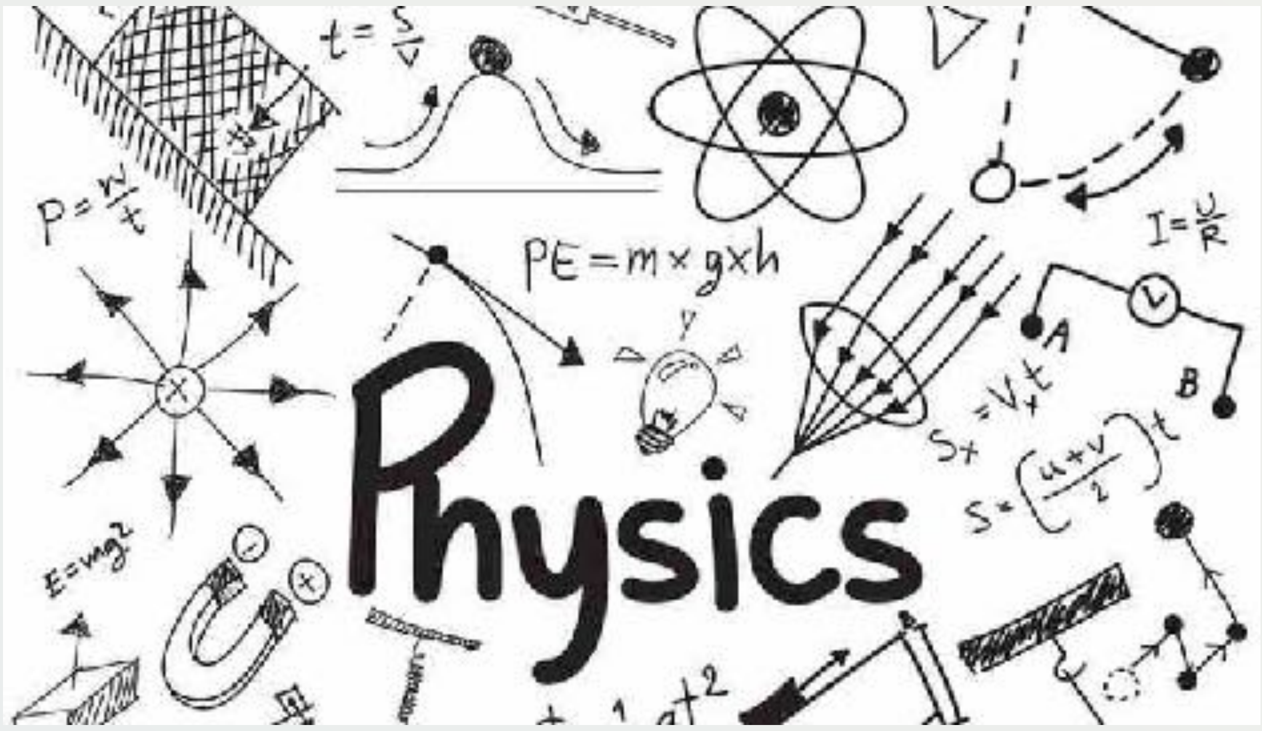
?





Machine Learning

?



A tool for engineers and scientists

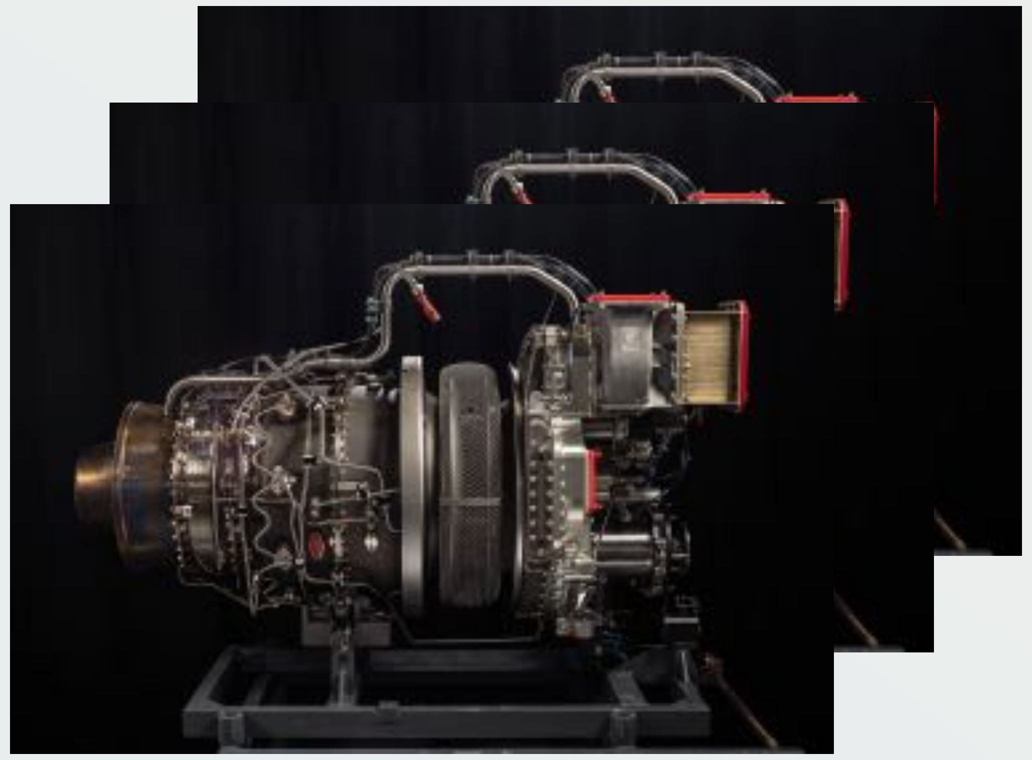
Data Valorization

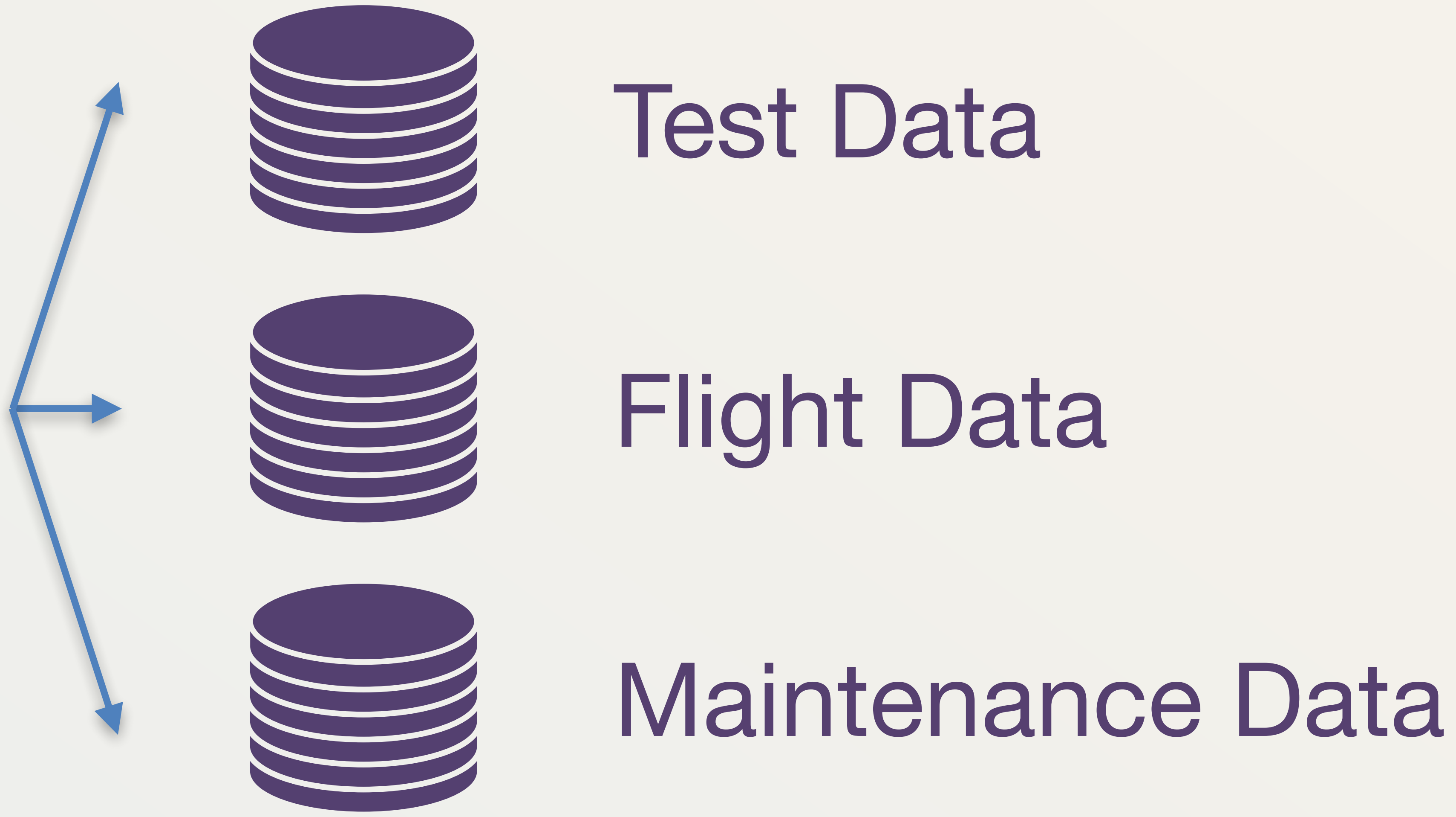
- Predictive Maintenance
- Real time systems

Surrogate models

- From real world data
- From simulations

Data Valorization





Large industrial datasets require **Data Engineering**

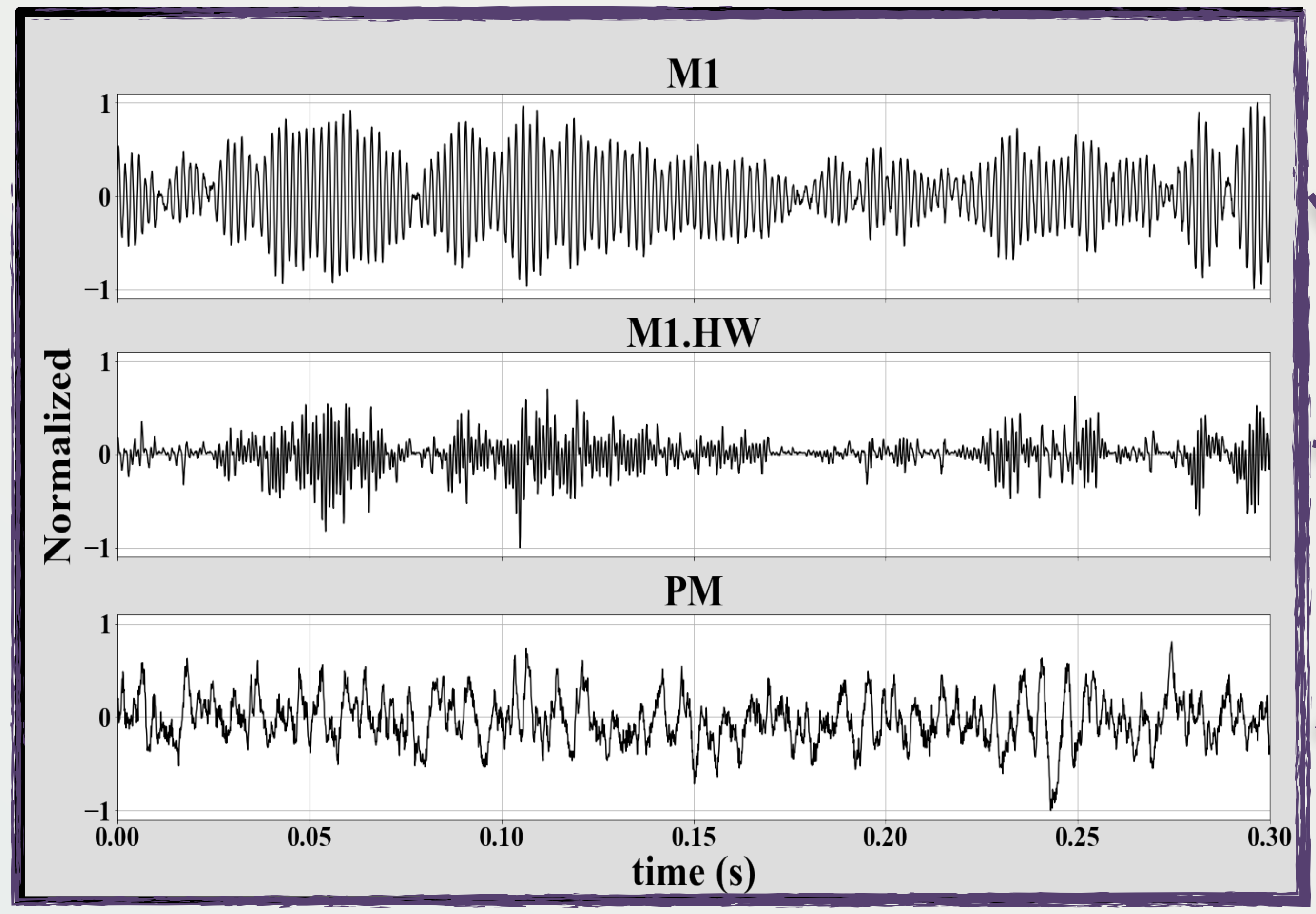
Collection, cleaning & labelling, access

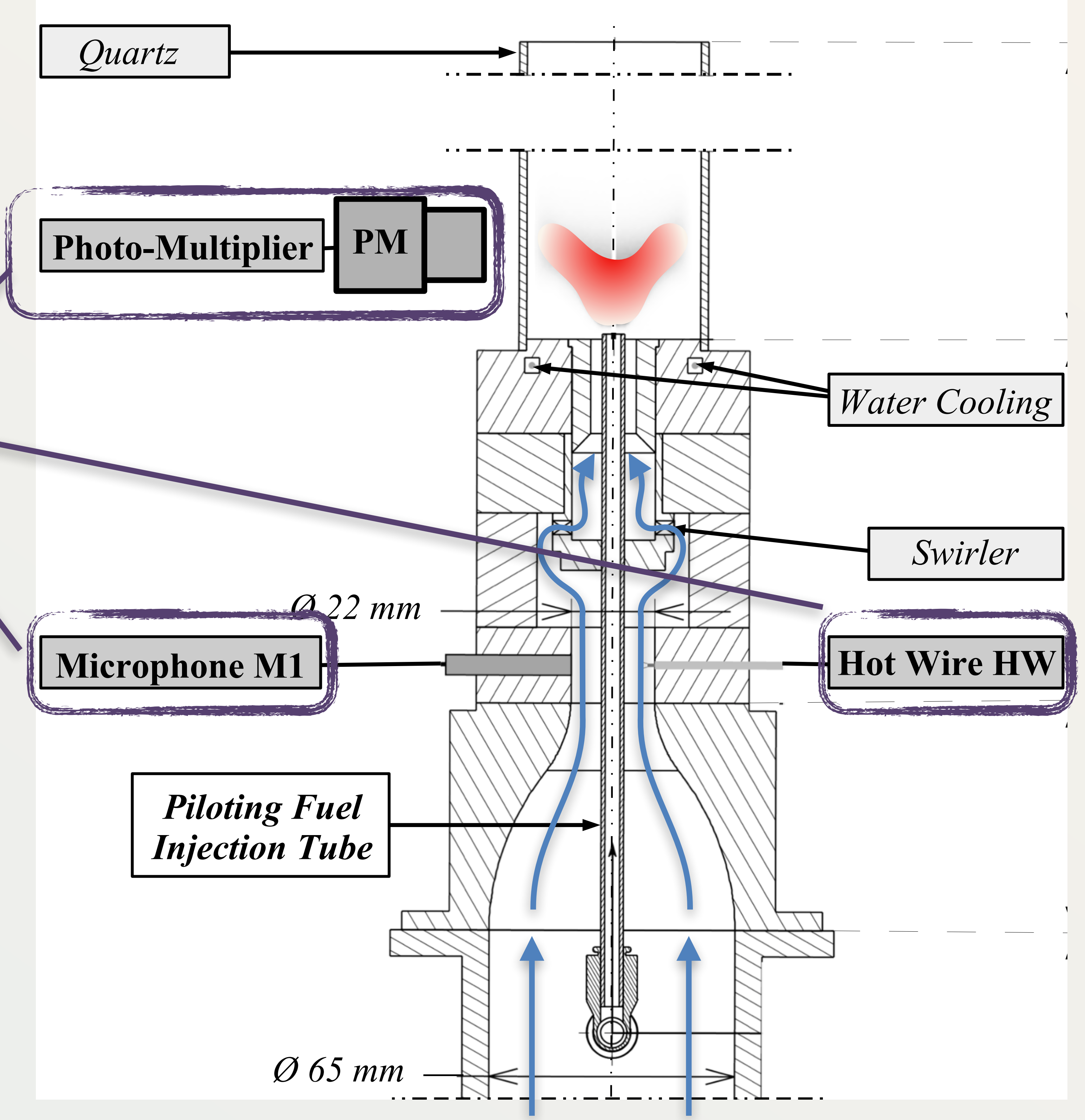
Research Data is often underused

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

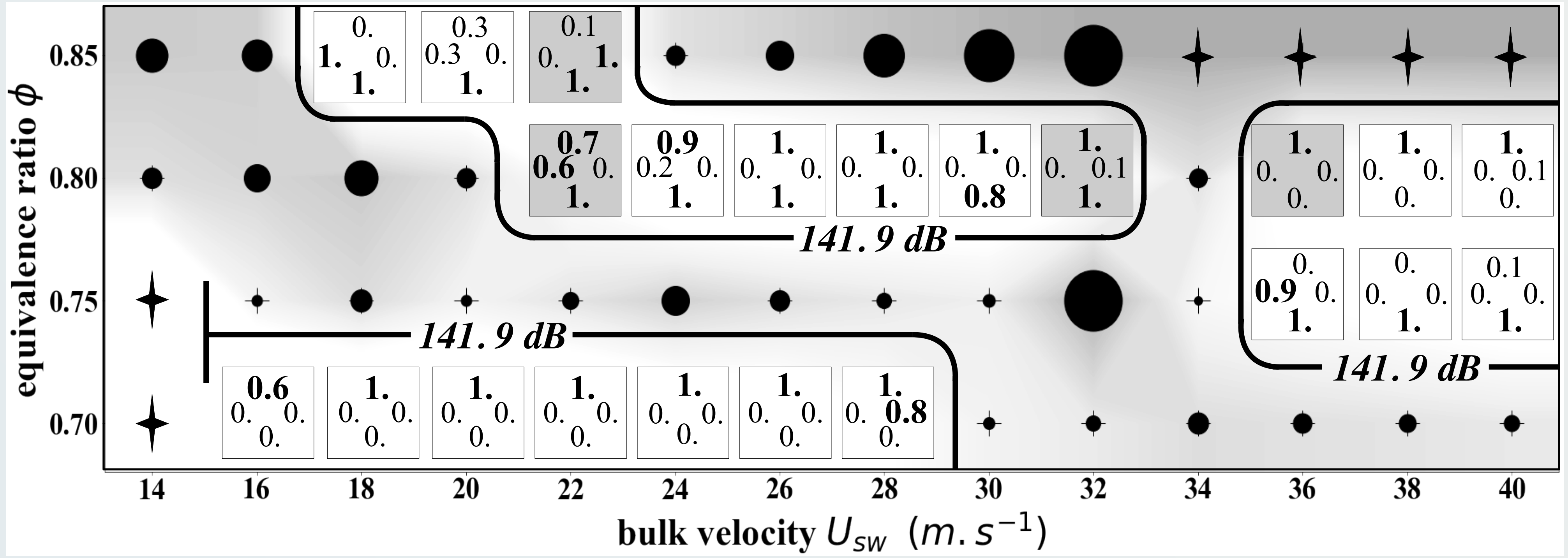
Data Valorization

High-frequency sampling time-series





CNN-LSTM

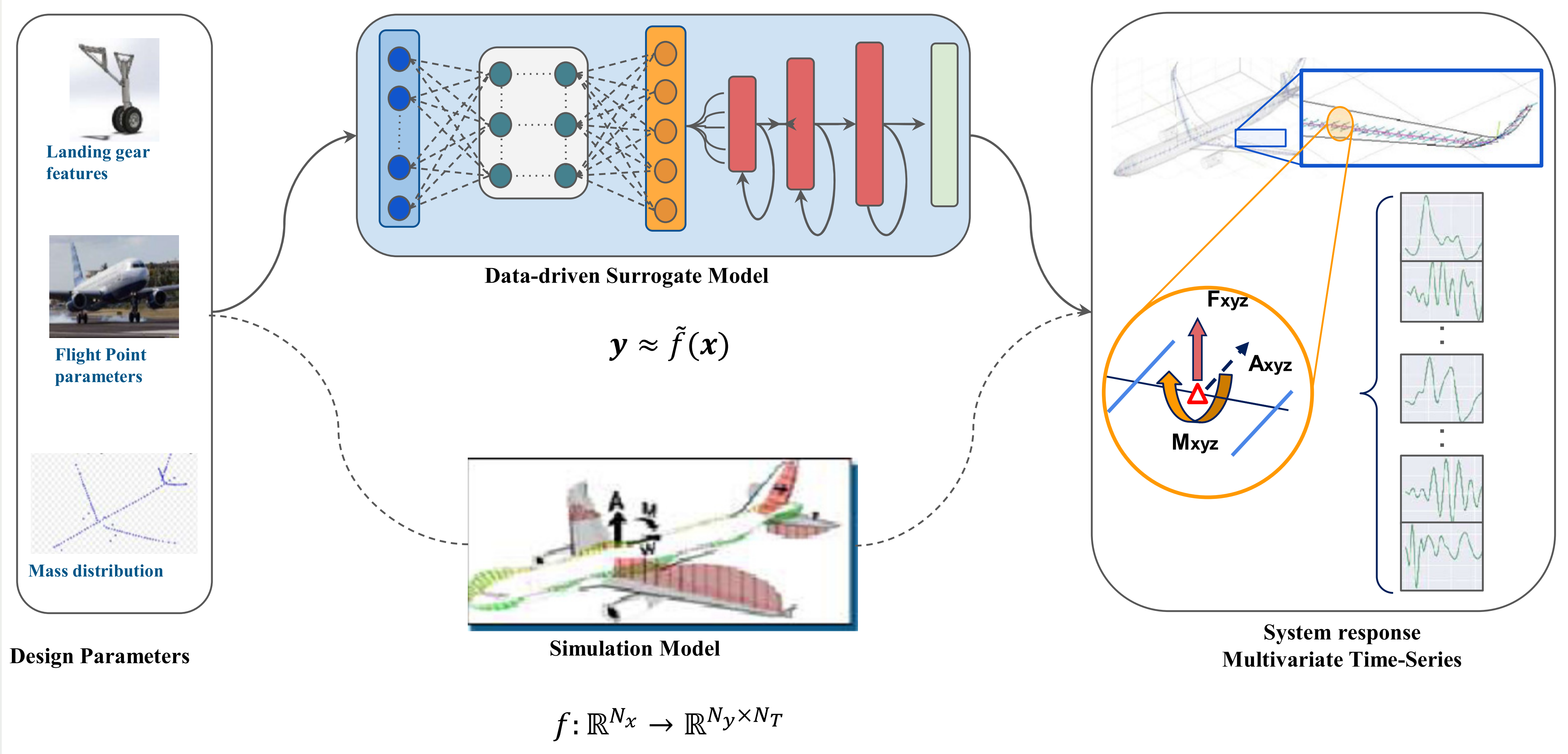


Edge AI

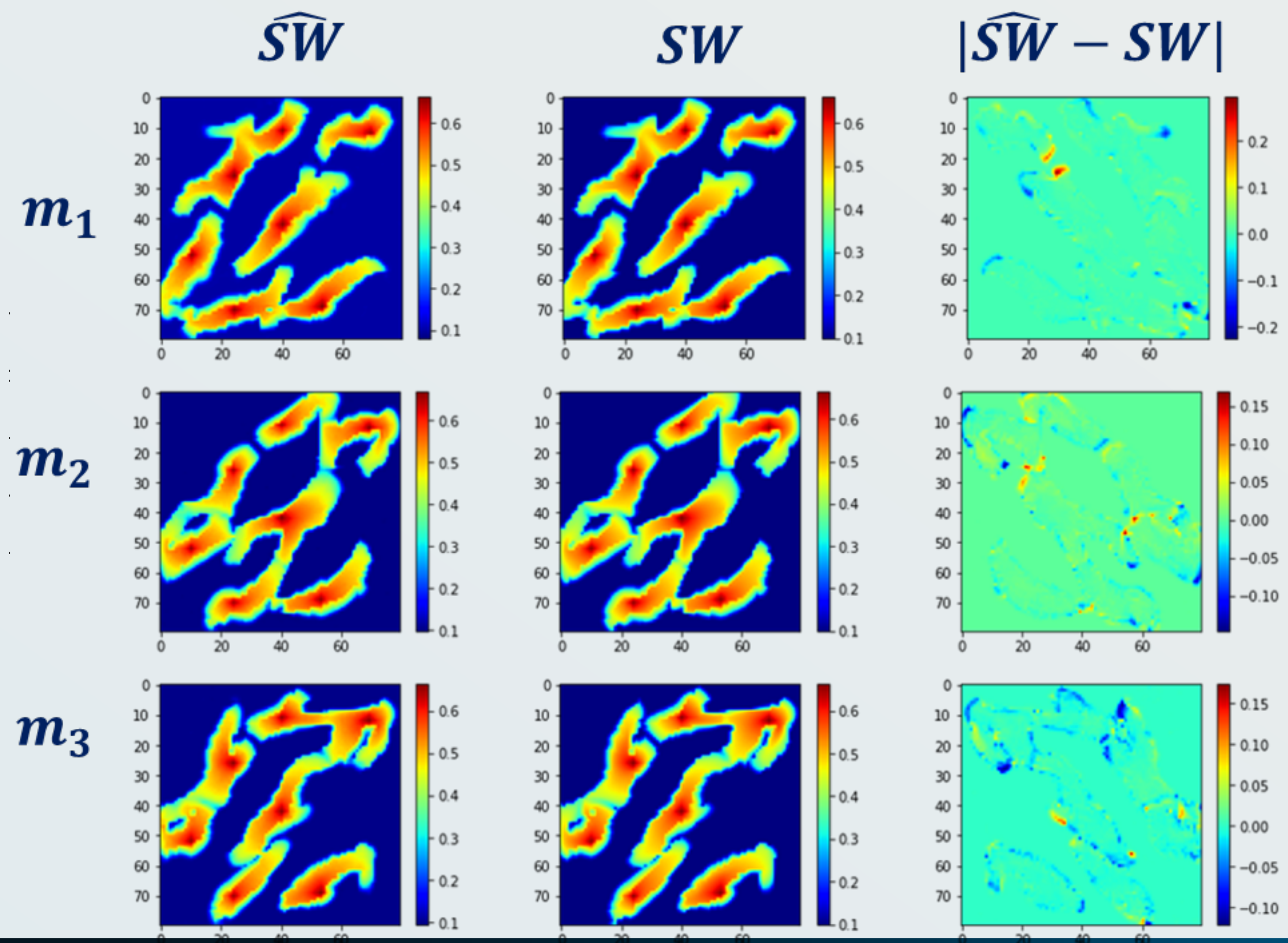
Realtime Predictions (< 100 ms)

Surrogate models

Lapeyre, C. J. *et al.* (2019). Reconstruction of Hydraulic Data by Machine Learning. *SimHydro 2019,* Nice, France, June 12-14, *arXiv:1903.01123*.



Lazzara, M. *et al.* "Surrogate modelling for an aircraft dynamic landing loads simulation using an LSTM AutoEncoder-based dimensionality reduction approach." *Aerospace Science and Technology* (2022): 107629.



Yewgat, A. et *al.* “IMEX-AUNET: Deep Learning proxy for multi-phase subsurface flow”. Submitted to *31st ACM International Conference on Information and Knowledge Management,* Atlanta, Georgia, USA, Oct. 17-22 2022

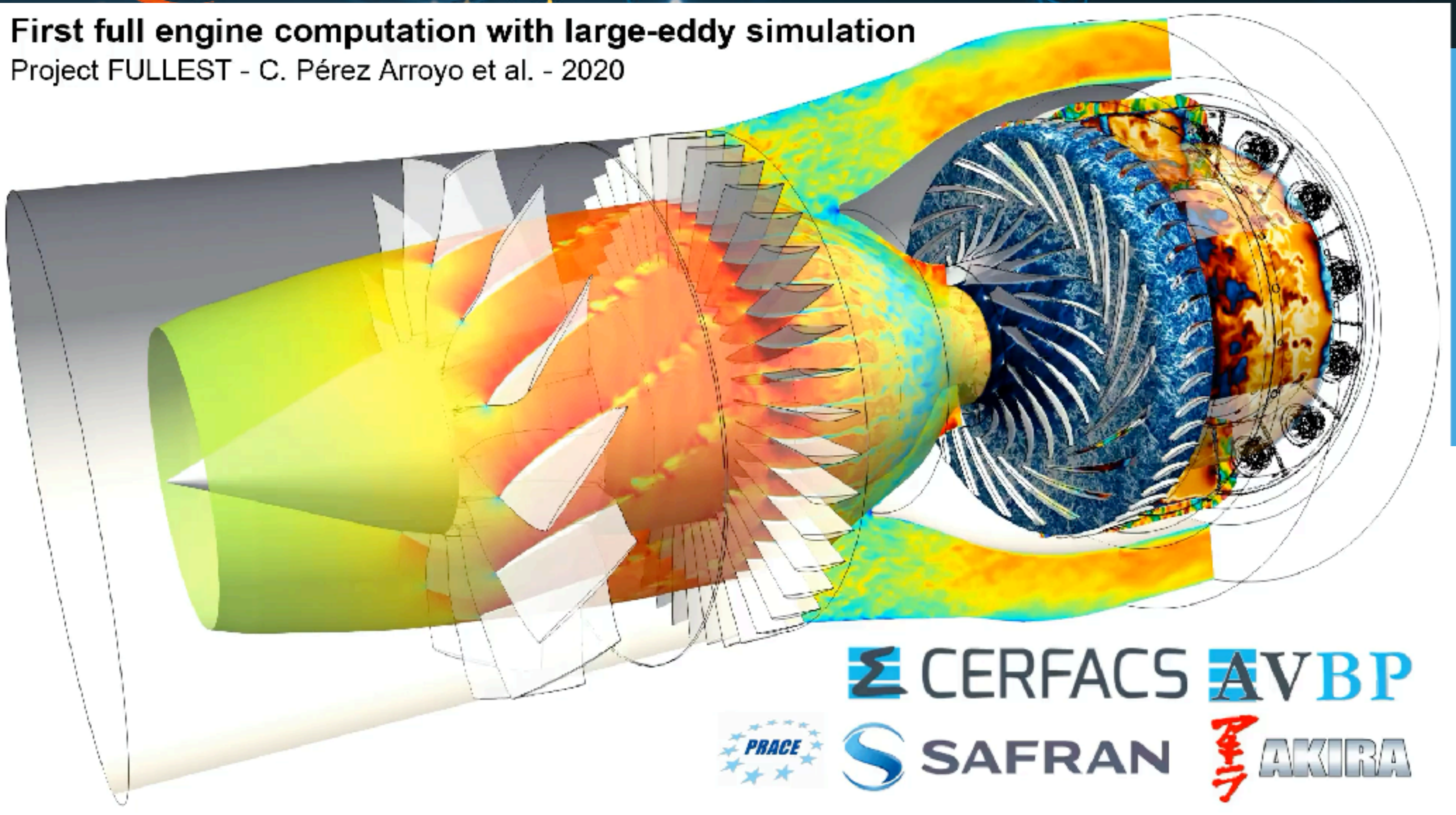
Training (scientists and engineers alike)

Interdisciplinary collaboration

Domain Experts

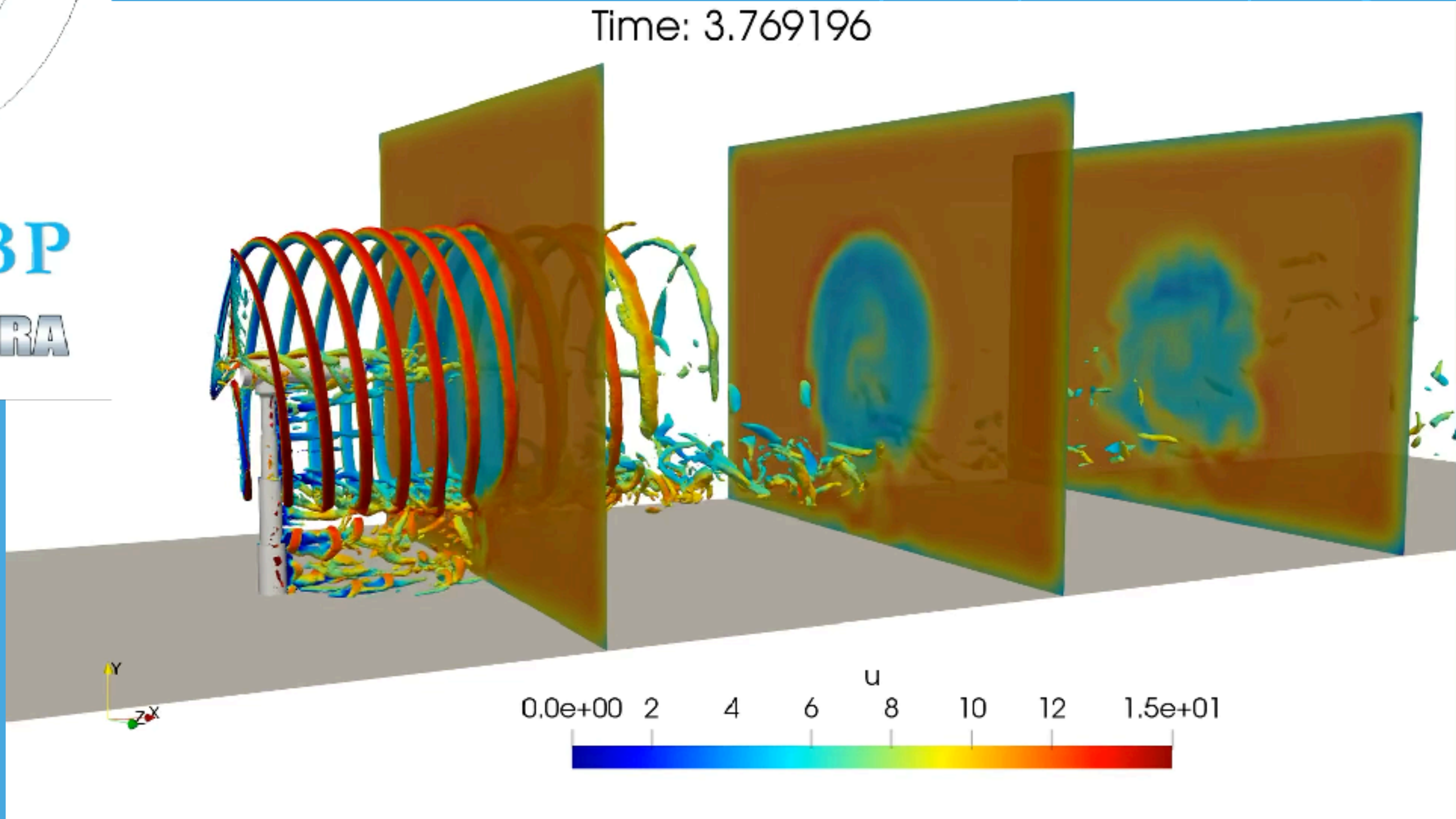
Data Engineers

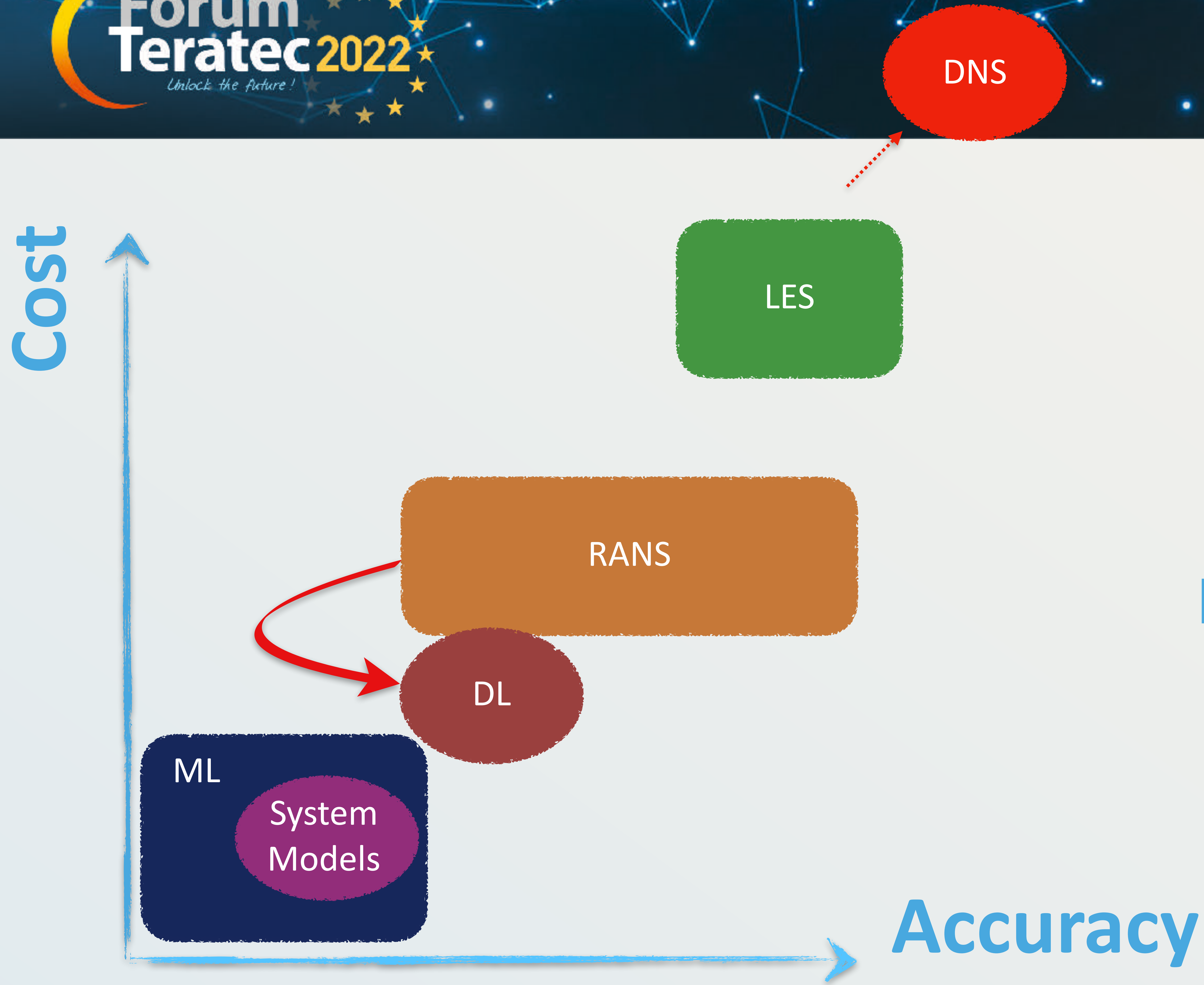
Data Scientists



High Performance

Computational Fluid Dynamics



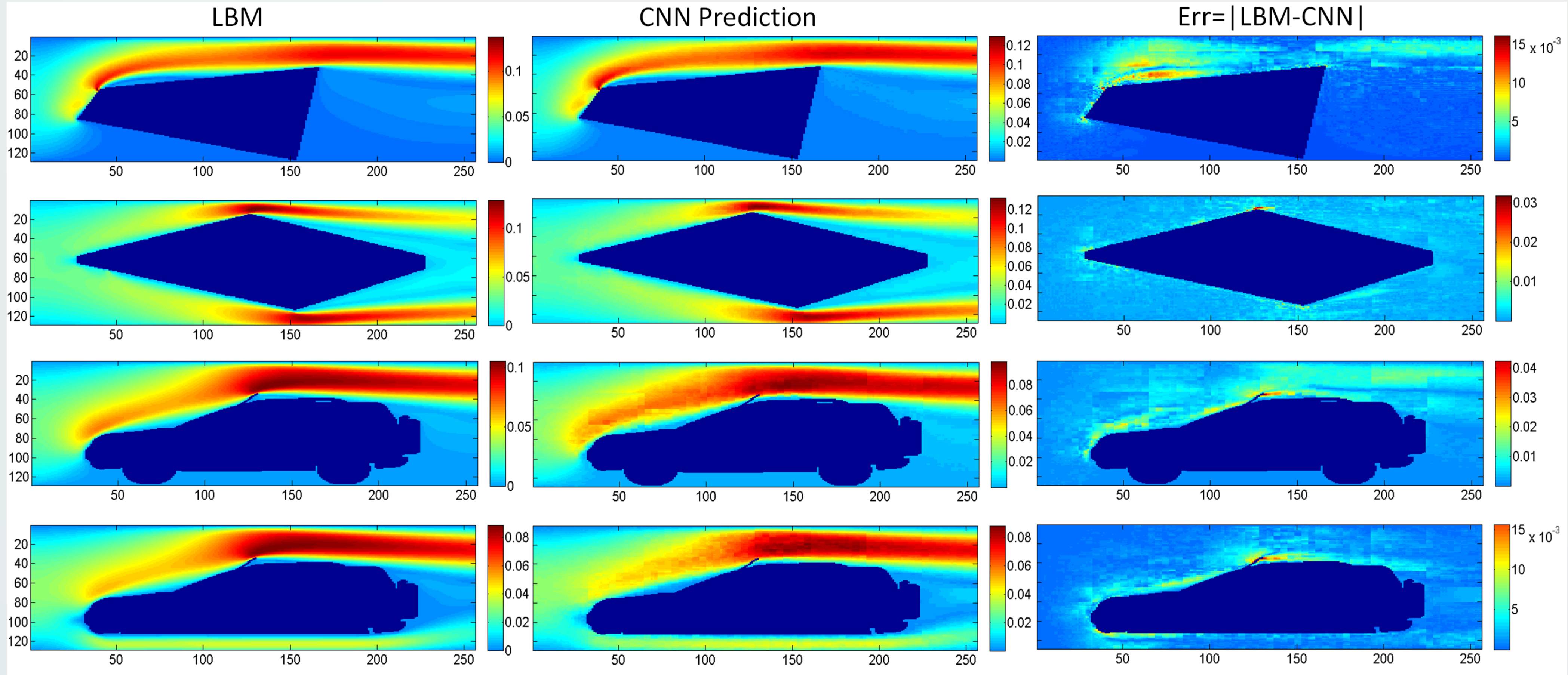


Good tradeoffs

ML for low-cost models

DL as a RANS surrogate

Do we always need CFD?



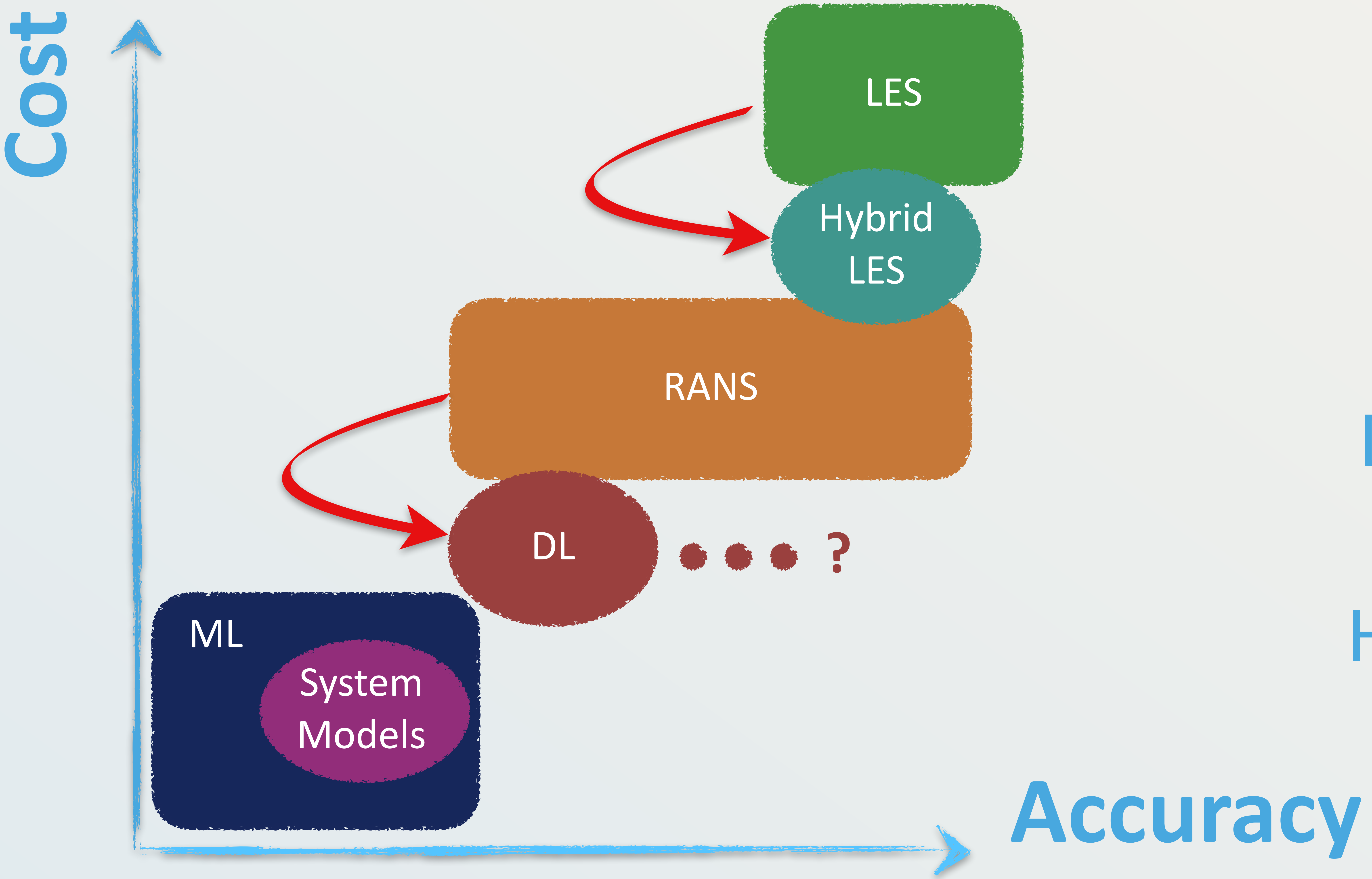
Guo, Xiaoxiao, Wei Li, and Francesco Iorio. "Convolutional neural networks for steady flow approximation." *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*. 2016.

NEURAL CONCEPT

EXTRALITY
Freeing industrial design

CADLM
TRANSFORMING DATA INTO INTELLIGENCE

...



Good tradeoffs

ML for low-cost models

DL as a RANS surrogate

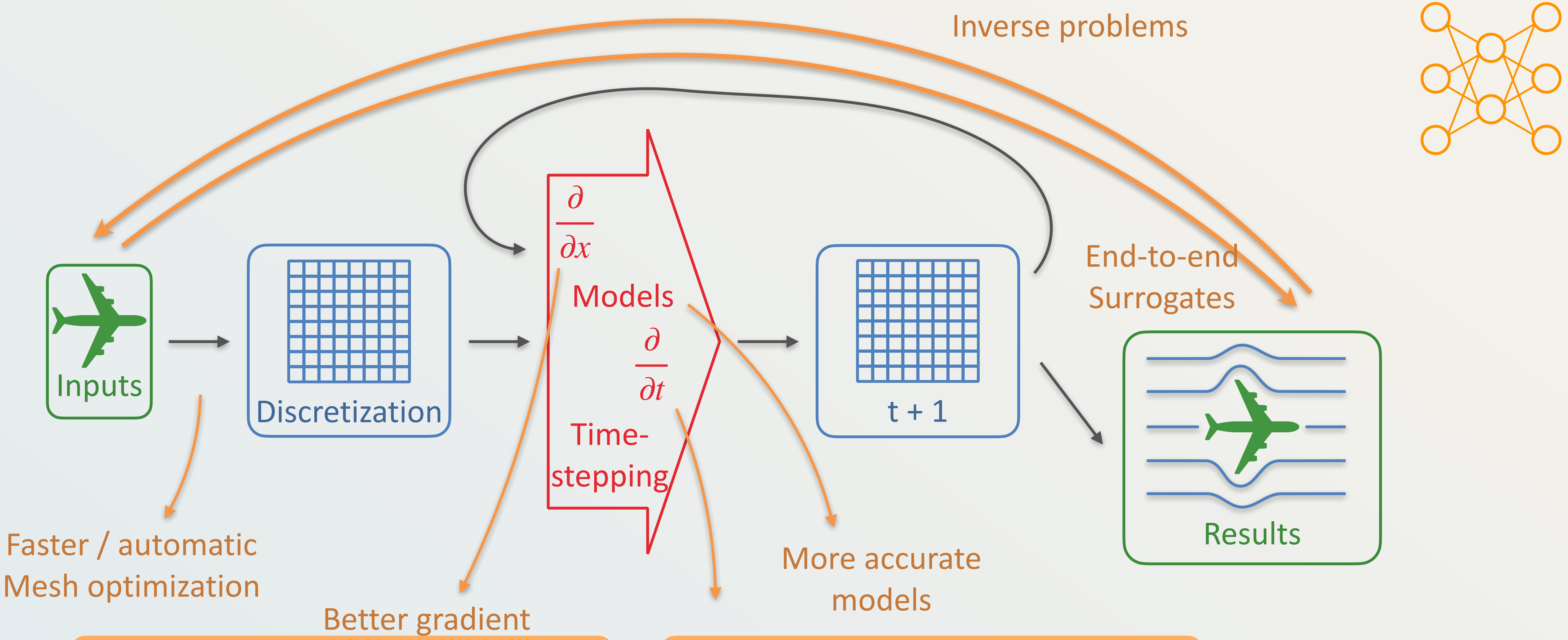
Hybrid LES: faster, better high fidelity?

Hybrid High-Fidelity Simulation

More accurate models

Innovative numerics

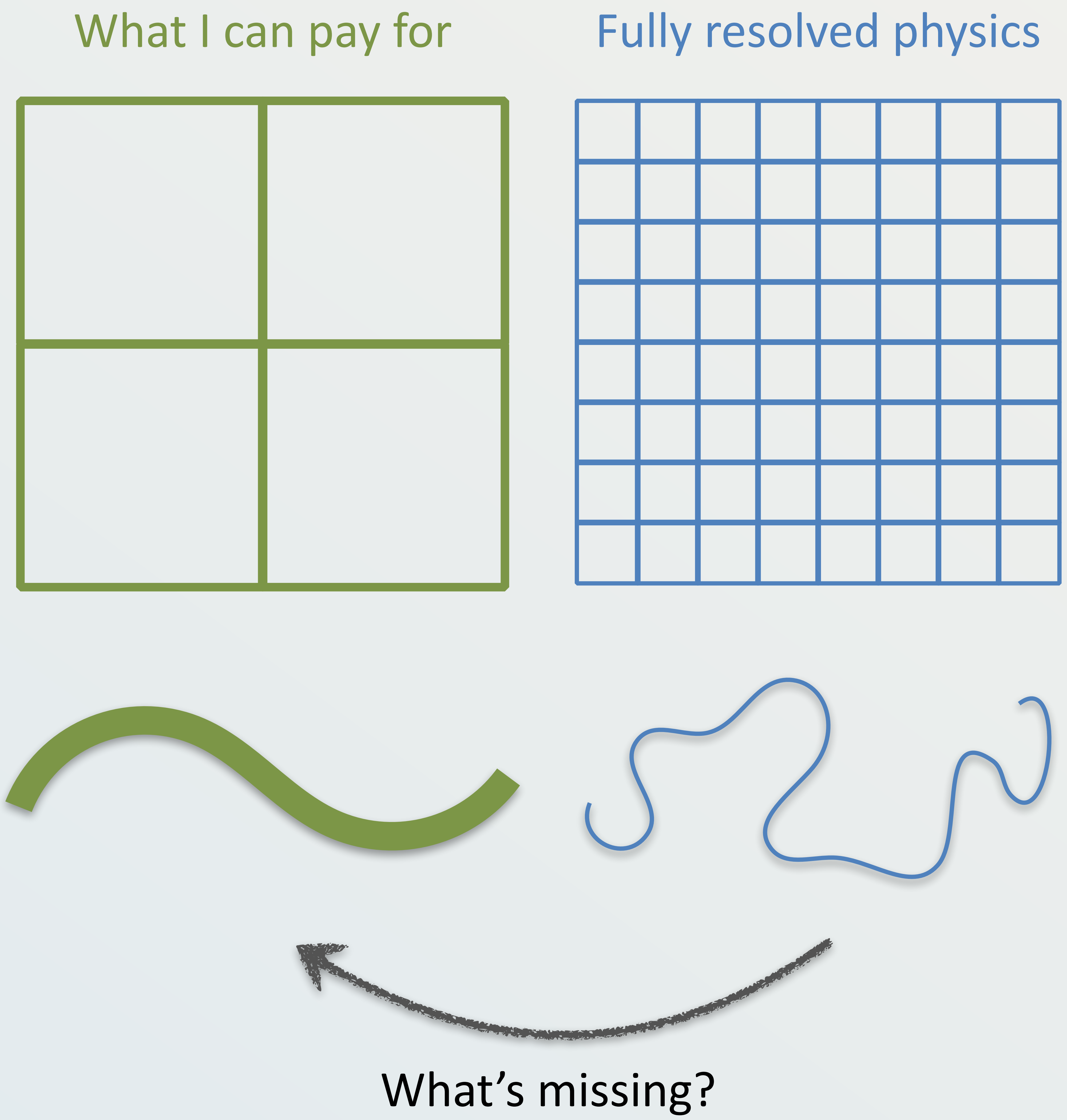
- Better Preconditioners
- New discretisation schemes

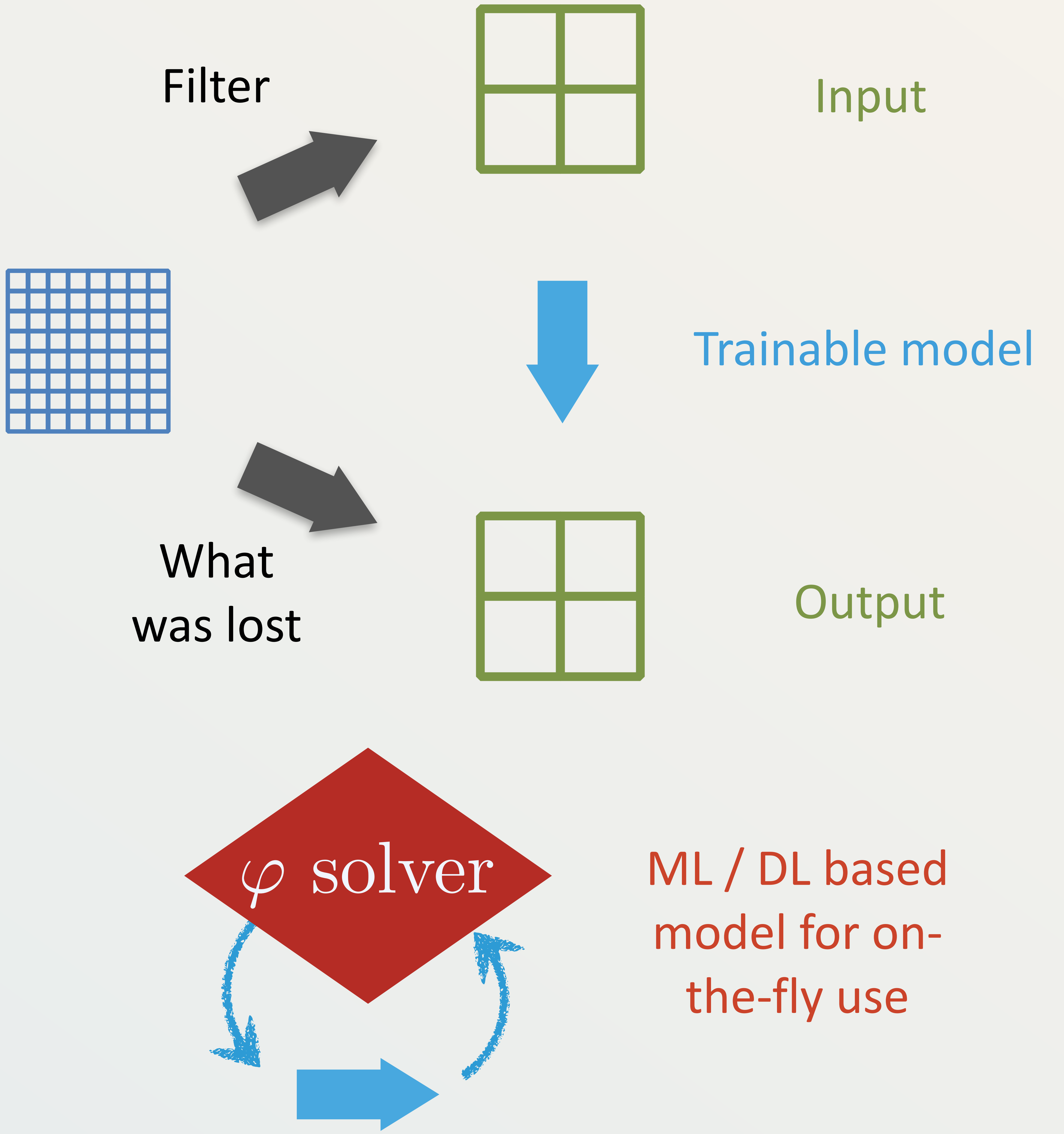


Innovative numerics

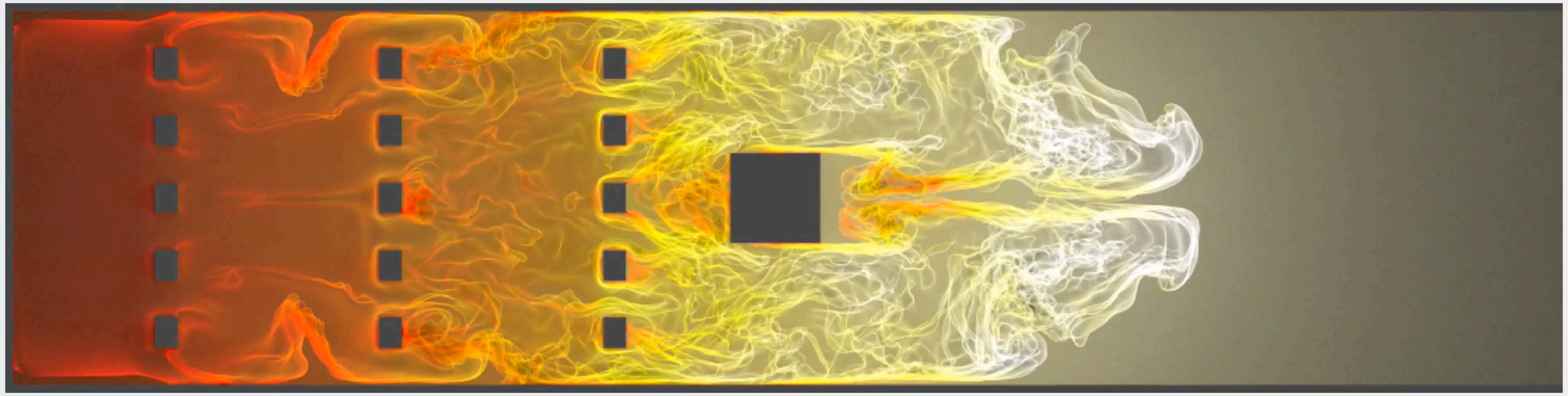
More accurate models

More accurate models

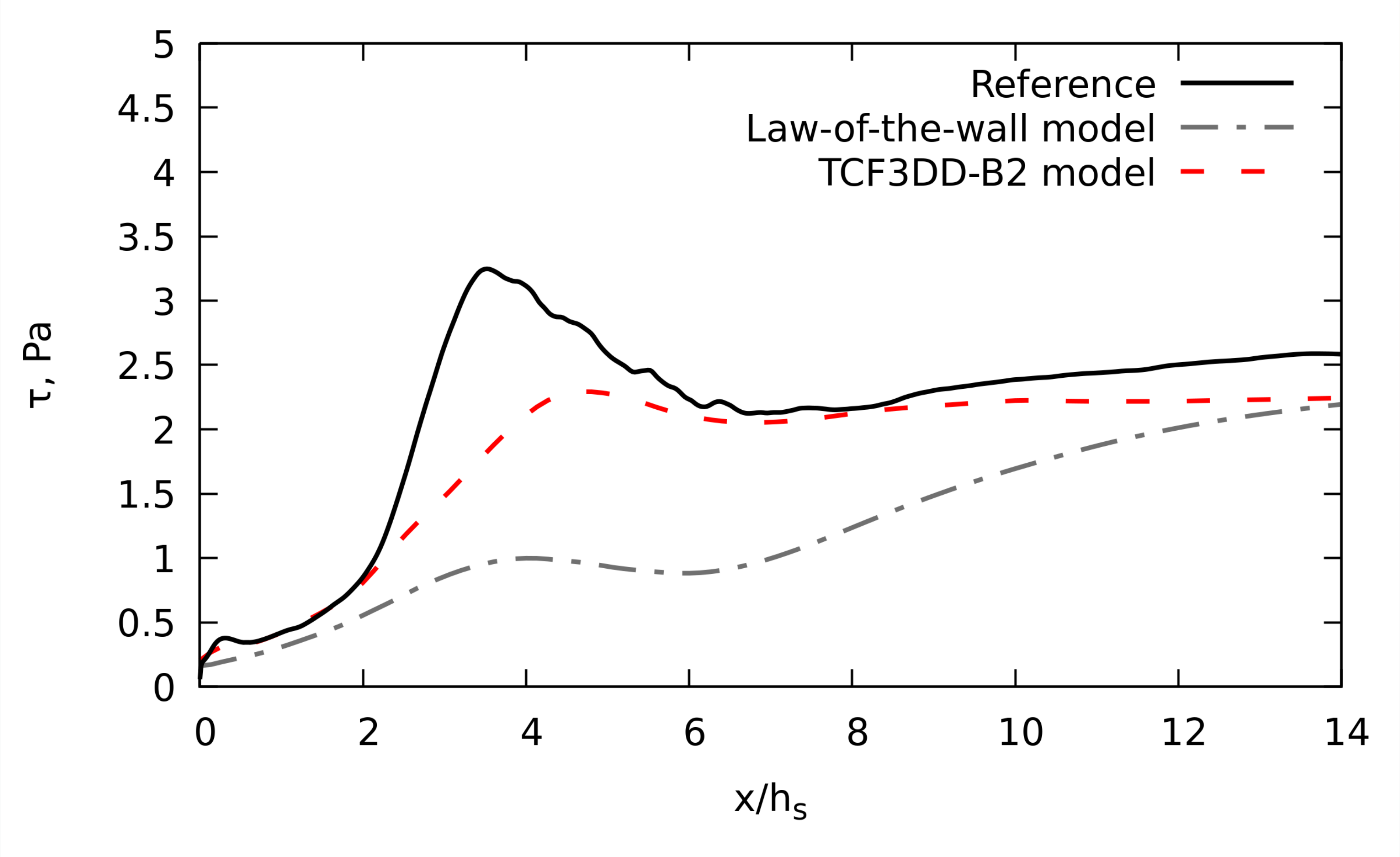




More accurate models



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.



Dupuy, D. *et al*. "Data-driven wall modelling for turbulent separated flows." Submitted to *Physical Review Fluids* (2022).

Preconditioners

x_i

Advection

> fast classical solver

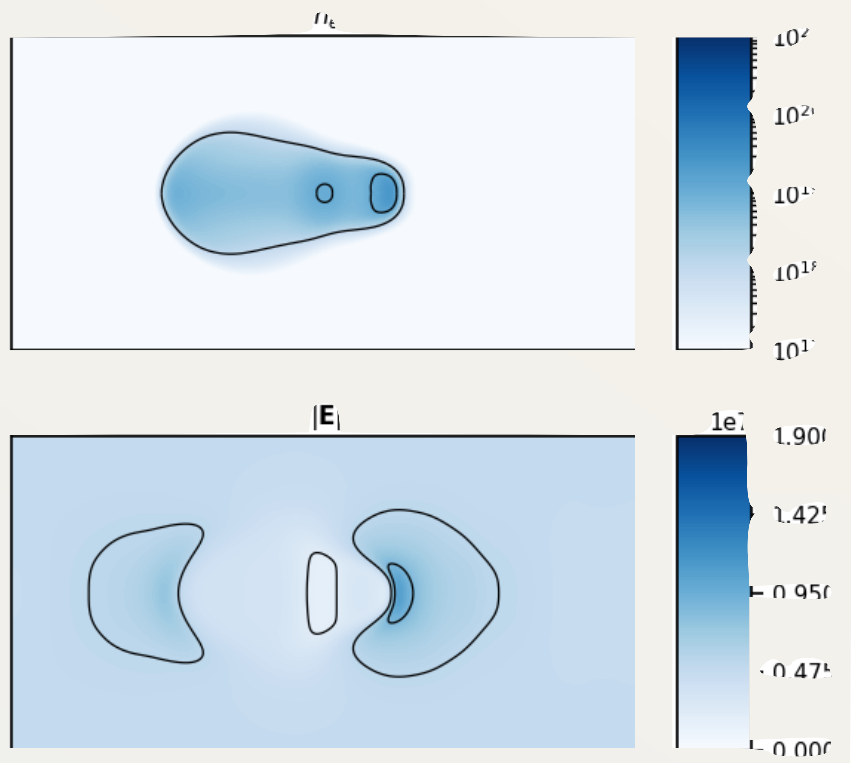
Pressure Correction

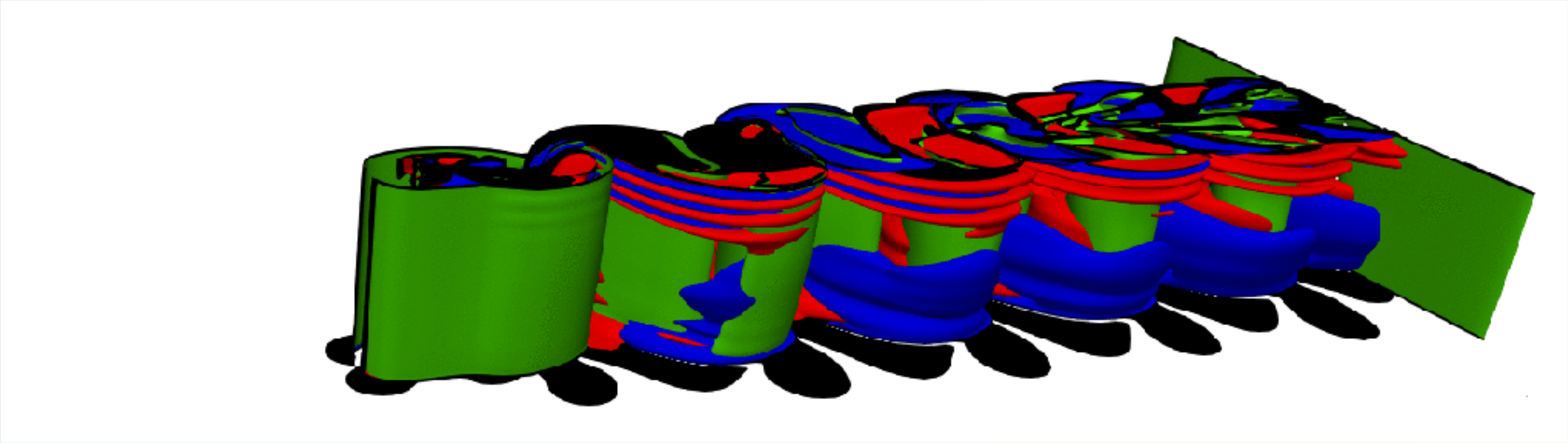
> neural network initial guess

Iterative solver converges to precision if needed

x_{i+1}

Plasma solver



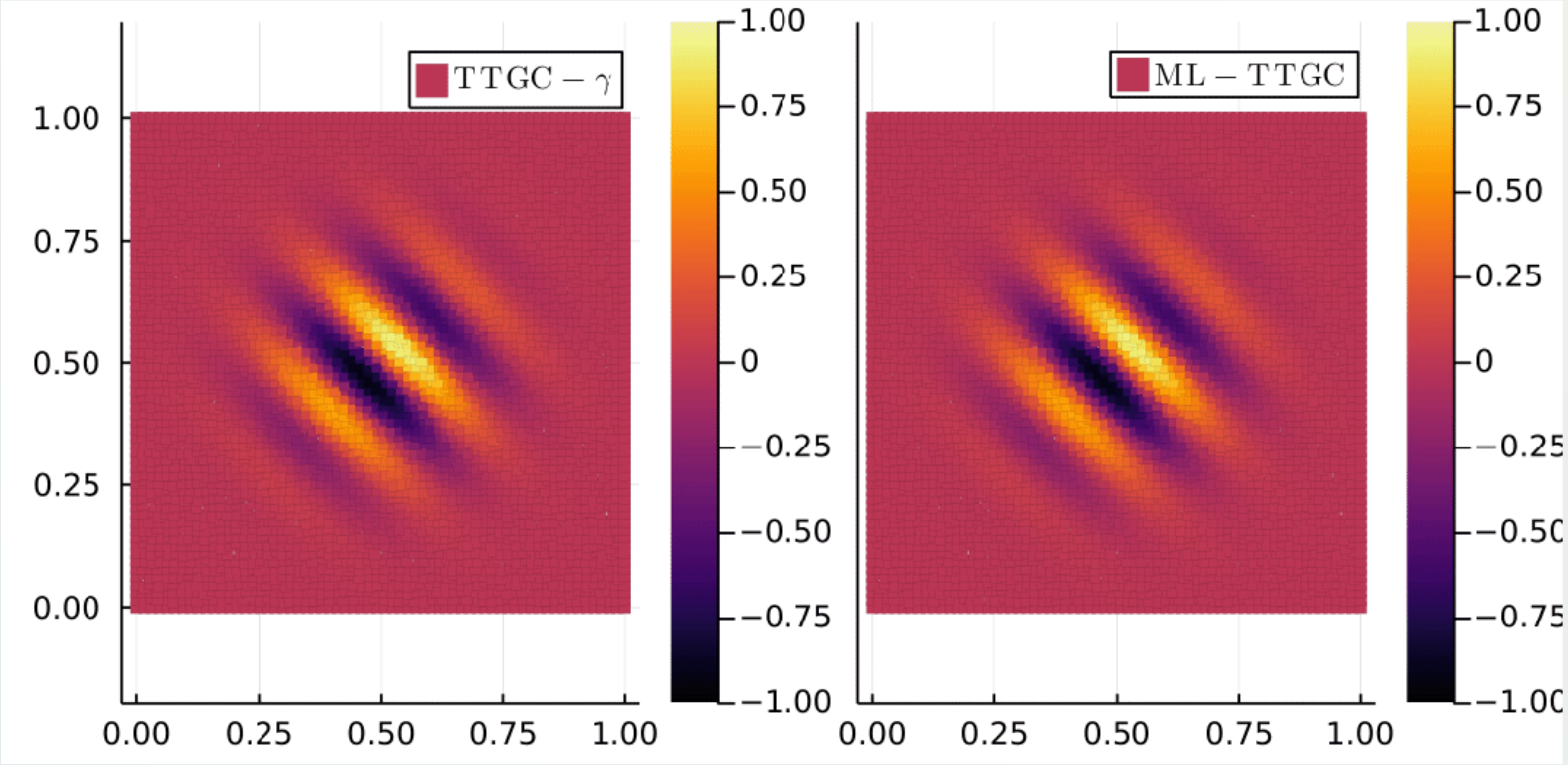


Incompressible flow solver

Cheng, L., Illarramendi, E. A., Bogopolsky, G., Bauerheim, M., & Cuenot, B. (2021). Using neural networks to solve the 2D Poisson equation for electric field computation in plasma fluid simulations. arXiv preprint arXiv:2109.13076.

Ajuria Illarramendi, E., Alguacil, A., Bauerheim, M., Misdariis, A., Cuenot, B., & Benazera, E. (2020). Towards an hybrid computational strategy based on Deep Learning for incompressible flows. In AIAA AVIATION 2020 FORUM (p. 3058).

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



Locally-tuned numerical schemes

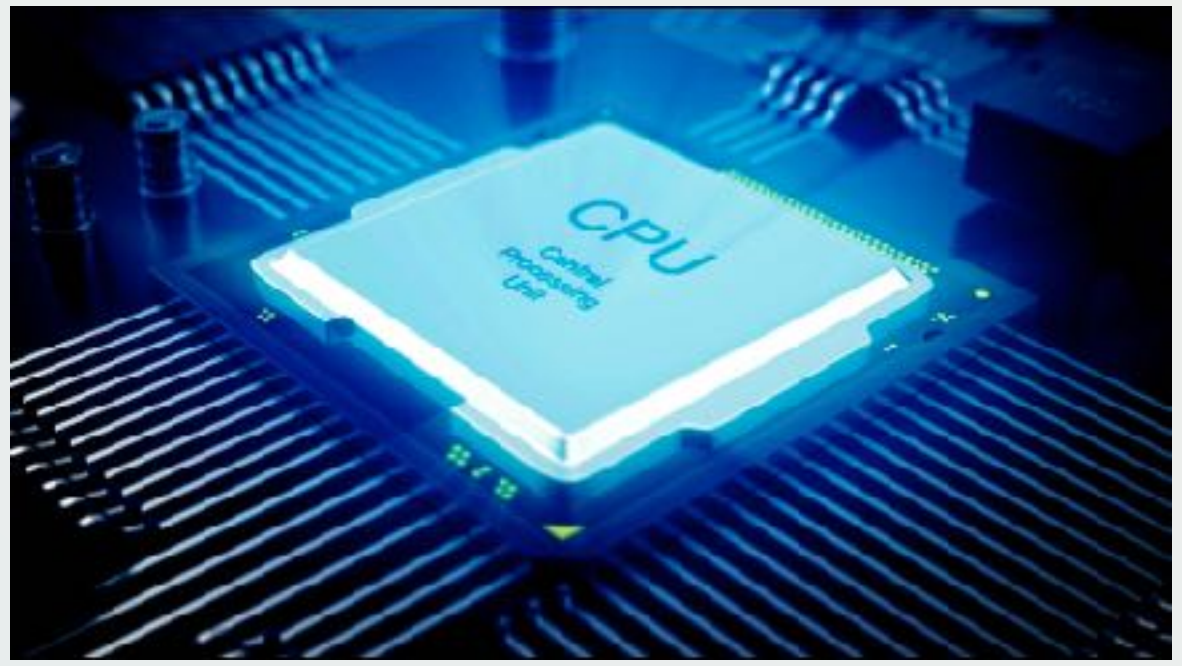
HPC for Hybrid Simulation

CPU/GPU architectures

Mesh issues

- Interpolation strategies
- Innovative network architectures

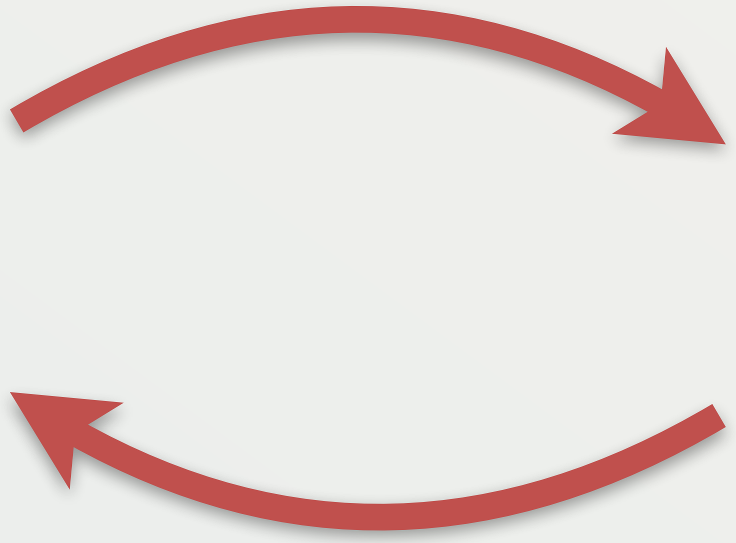
CPU/GPU architectures



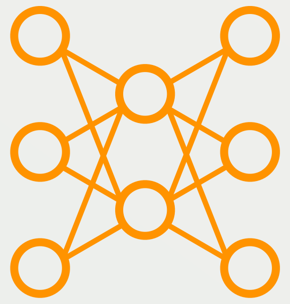
$$\frac{Du}{Dt} = -\nabla p + \mu \nabla^2 u + \varrho F$$

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

Physical fields

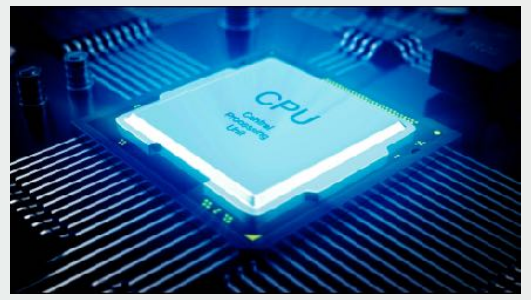


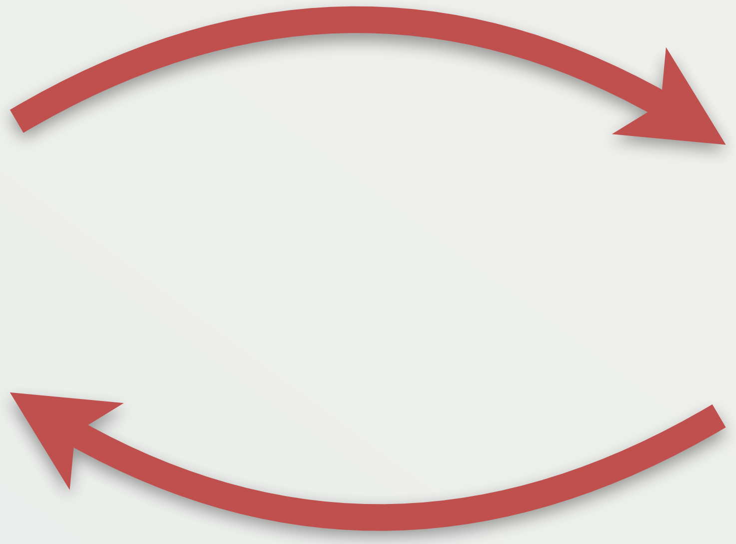
Predictions

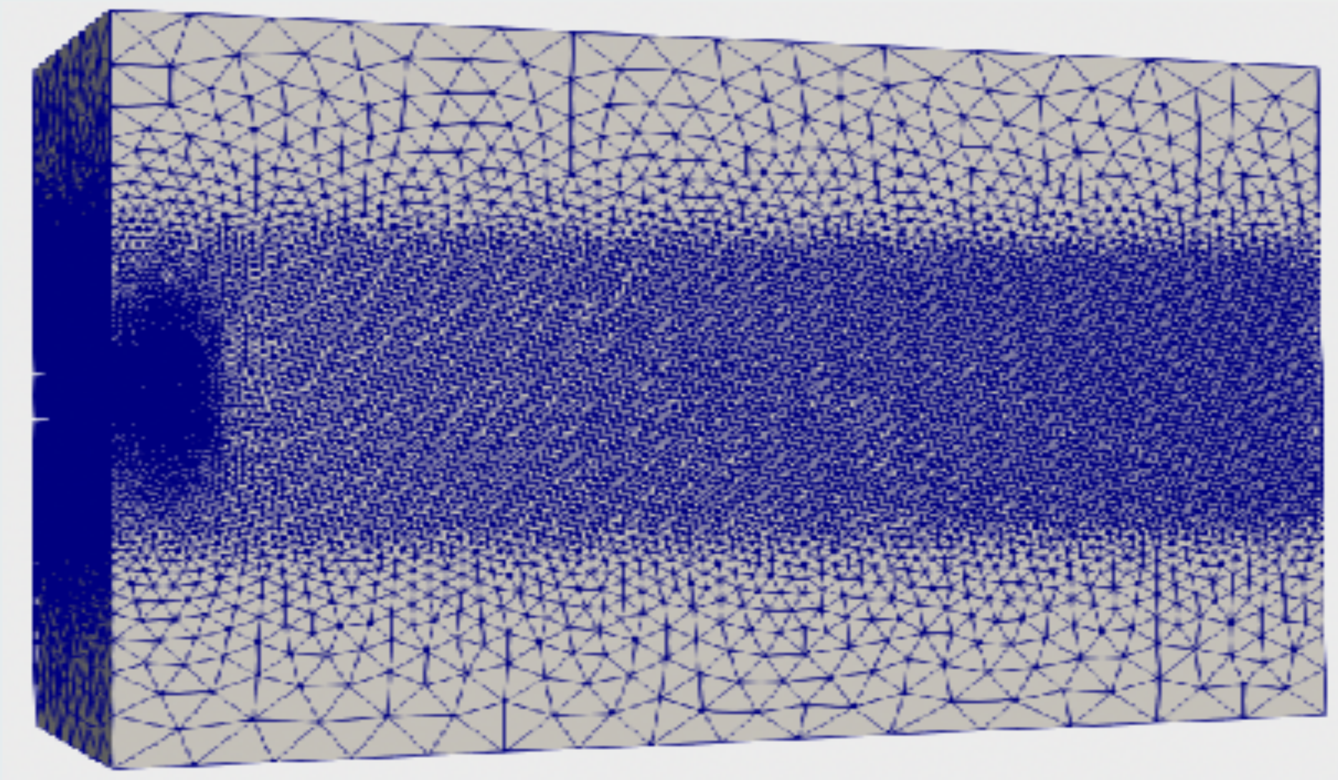


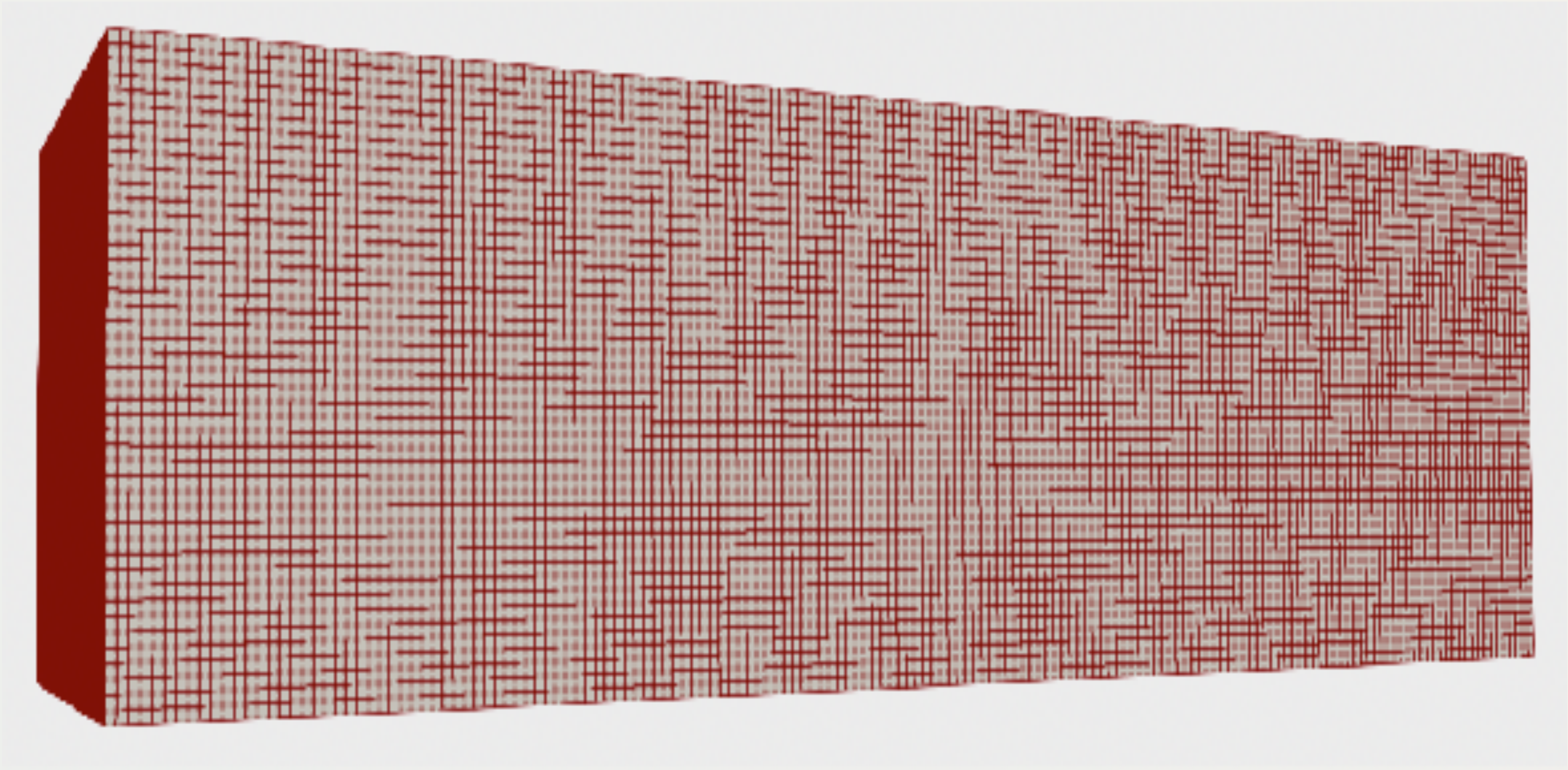
GPU : Neural Net
(TensorFlow)

Mesh issues





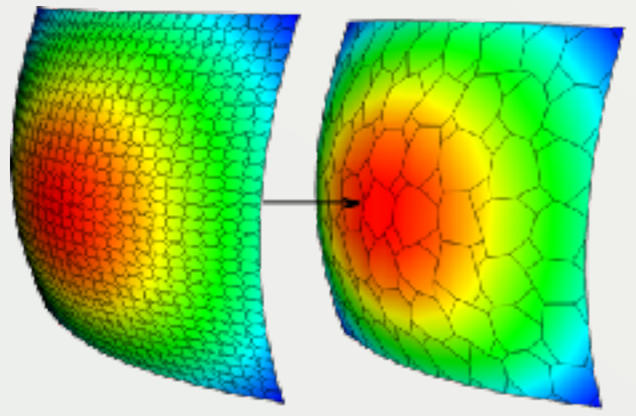




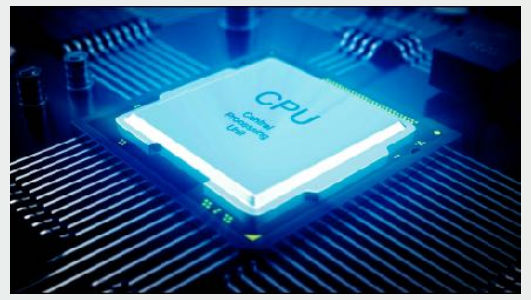
Unstructured mesh

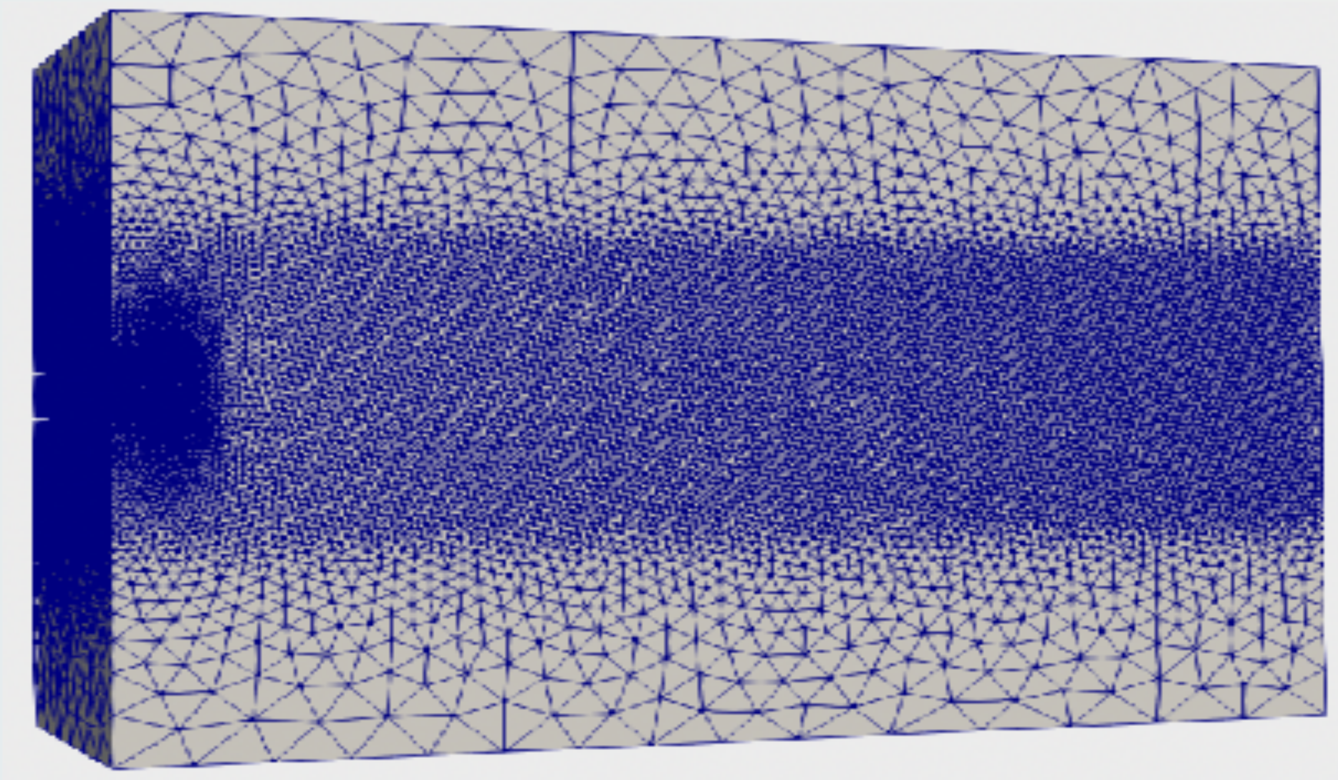
CNN: Pixels / Voxels

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

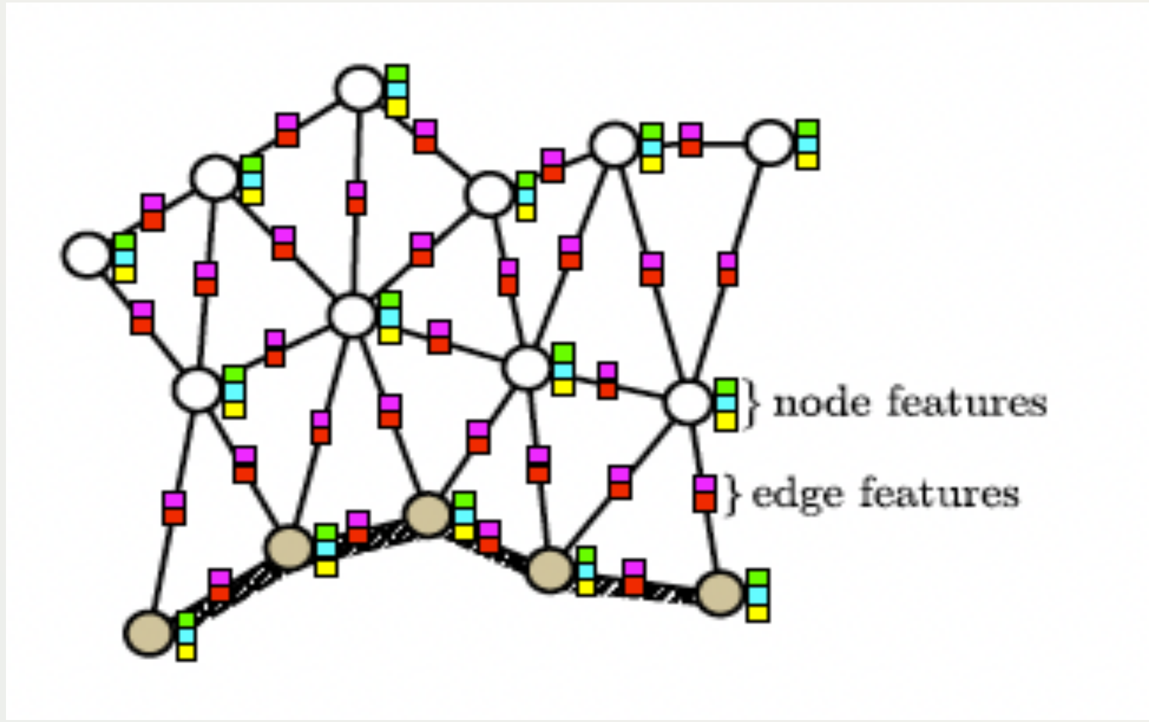


Mesh issues





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.

Training

Interdisciplinary collaboration

Training

Interdisciplinary collaboration

Hybrid simulation:

AI *inside* CFD

Training

Interdisciplinary collaboration

Hybrid simulation:

AI *inside* CFD

Hybrid HPC:

CPUs / GPUs / …?

Recent Papers

- 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, Marseilles, May 2019.