AQTIVATE

Machine Learning for Computational Fluid Dynamics

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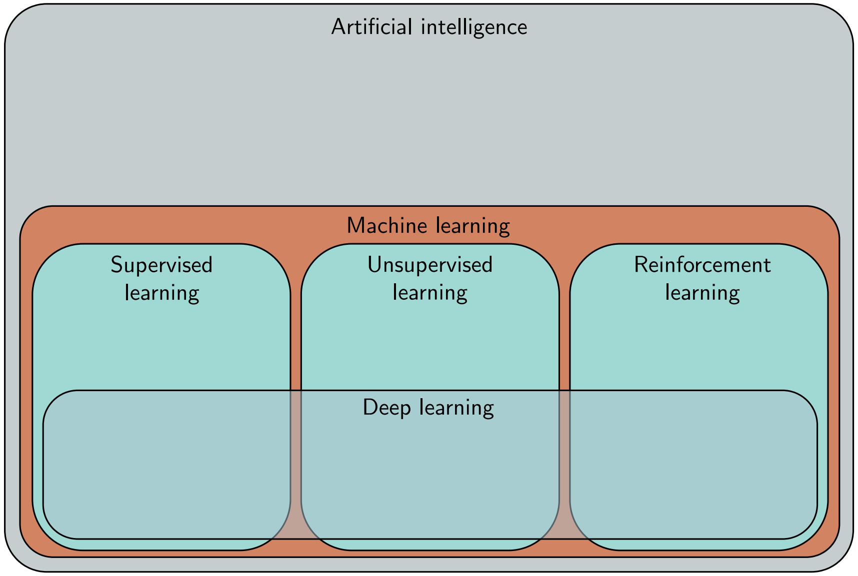
Machine learning

- Artificial intelligence (AI)
  - The use of technologies to realize intelligent behavior
  - Build systems that simulate intelligent behavior

- Machine learning (ML)
  - A subset of AI
  - Enable a machine (or system) to learn from experience (e.g., observed data)

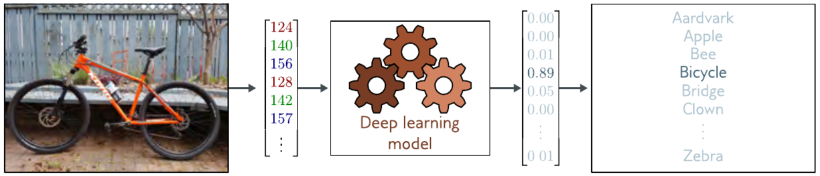
- Deep learning
  - A machine learning technique (a class of algorithms)
  - "Deep" neural network in which multiple layers are used



[Prince, 2023]

Machine learning methods

- Supervised learning
  - Mapping from input data to an output prediction
  - Usually, the output labels are available.

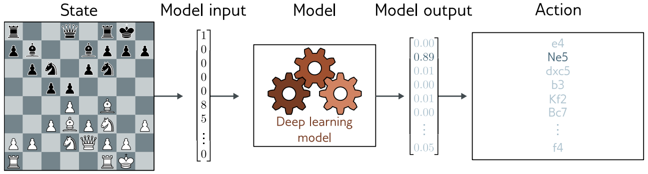


[Prince, 2023]

- Unsupervised learning
  - Constructing a model from input data without corresponding output labels
  - Describe or understand the structure of the data

[Karras et al., 2020]

- Reinforcement learning
  - Modeling an agent that performs certain actions in a given environment
  - Actions change the state and produce rewards
  - Learn to choose actions for high rewards



[Prince, 2023]

Applications

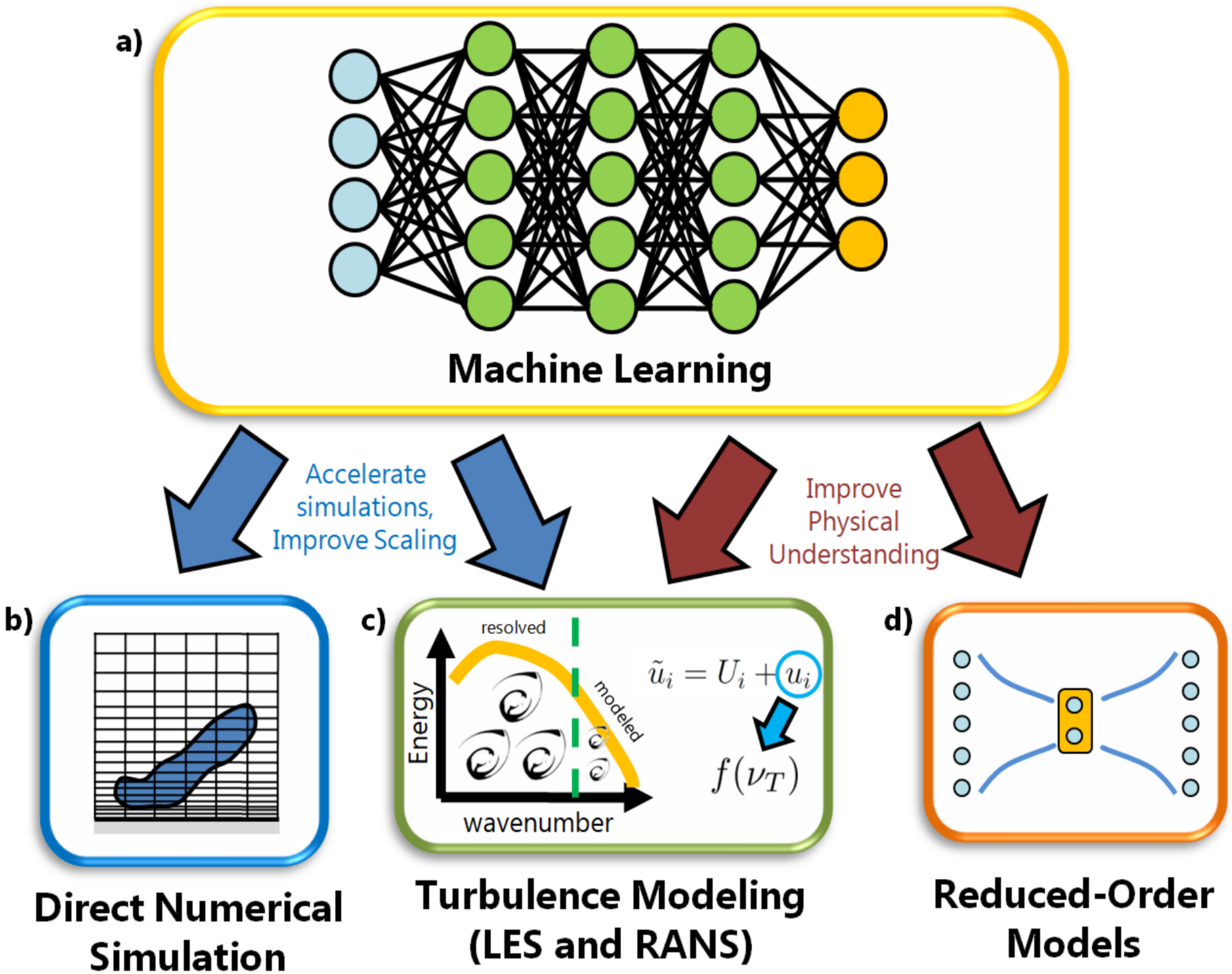
- Computer vision, natural language processing, speech recognition, etc.
- Why not for physics-based simulations?
  Particularly for computational fluid dynamics (CFD)?
  - High-dimensional
  - Nonlinear
  - Non-convex
  - Multi-scale
  - …

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla \cdot (\mathbf{v} \otimes \mathbf{v}) - \frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{g}$$

$$\nabla \cdot \mathbf{v} = 0$$

- Naive (yet straightforward) approach
  - Learn to fit the data for the given objective
- To do better: Enforce prior physical knowledge in learning
  - Conservation of mass, momentum, and energy
  - Symmetries, invariance, and equivariance
  - …

ML for CFD

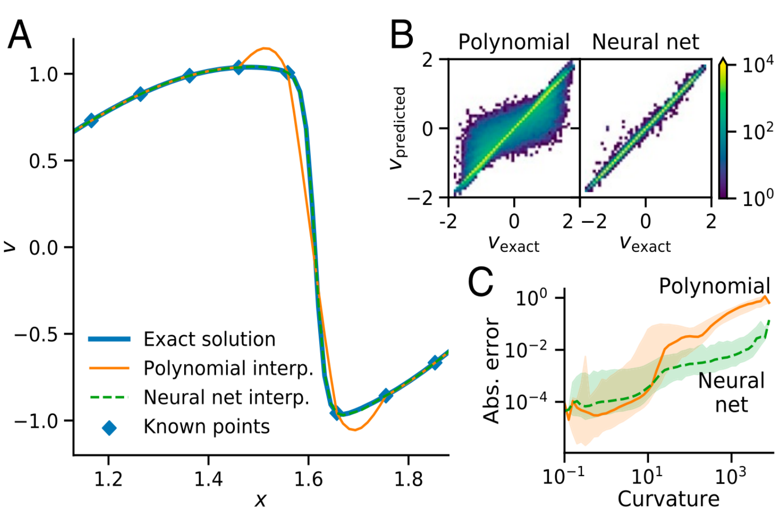


[Vinuesa and Brunton, 2022]

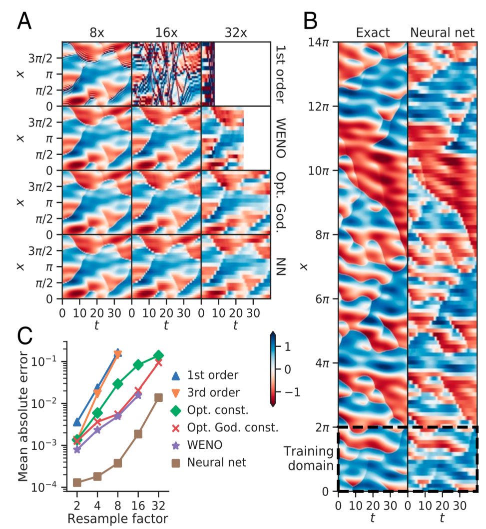
Accurate coarse simulation

- Substantially reduce the computational cost

- *[Bar-Sinai et al., 2019] "Learning data-driven discretizations for partial differential equations," PNAS*
  - Estimate spatial derivatives, $\frac{\partial^n v}{\partial x^n} \approx \sum_i \alpha_i^{(n)} v_i$, in low-resolution grids



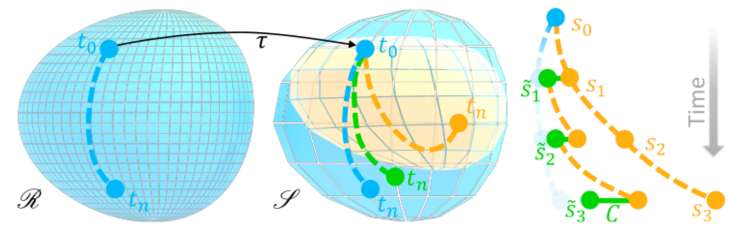
Polynomial vs. neural network

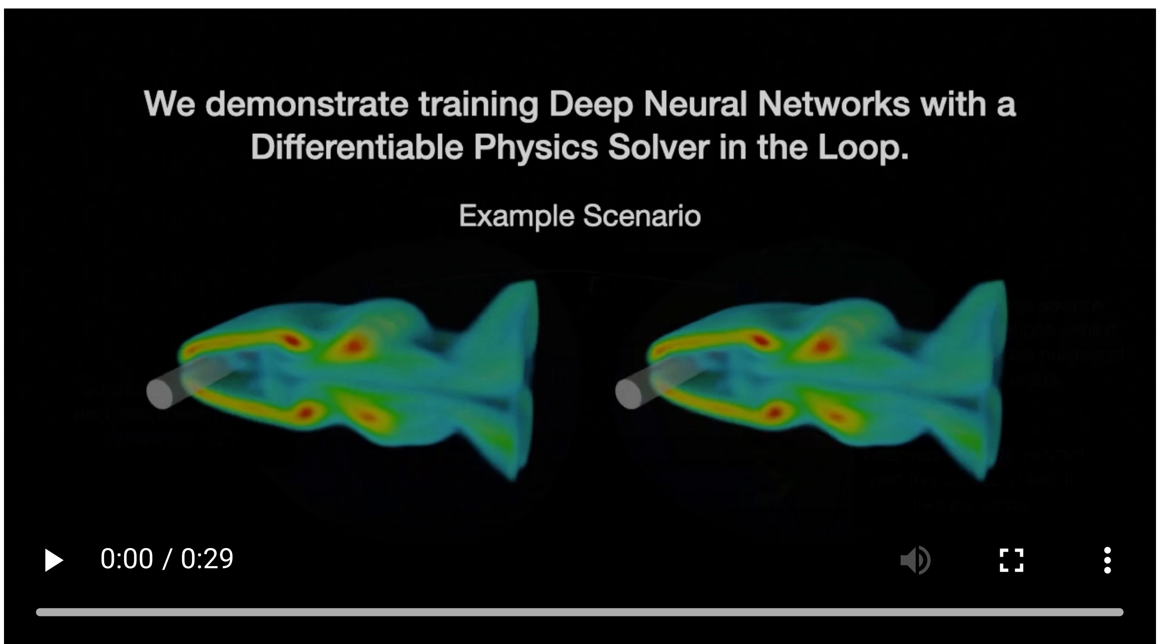


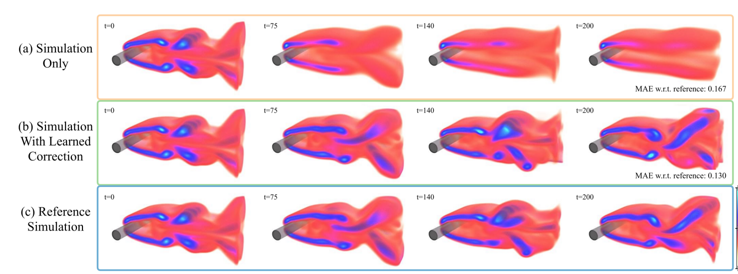
Burgers' equation

Accurate coarse simulation (cont'd)

- *[Um et al., 2020] "Solver-in-the-loop: Learning from differentiable physics to interact with iterative PDE-solvers," NeurIPS*
  - Learn a correction function at coarser simulations
  - Models interact with the solver while learning for the correction
  - Differentiable solver

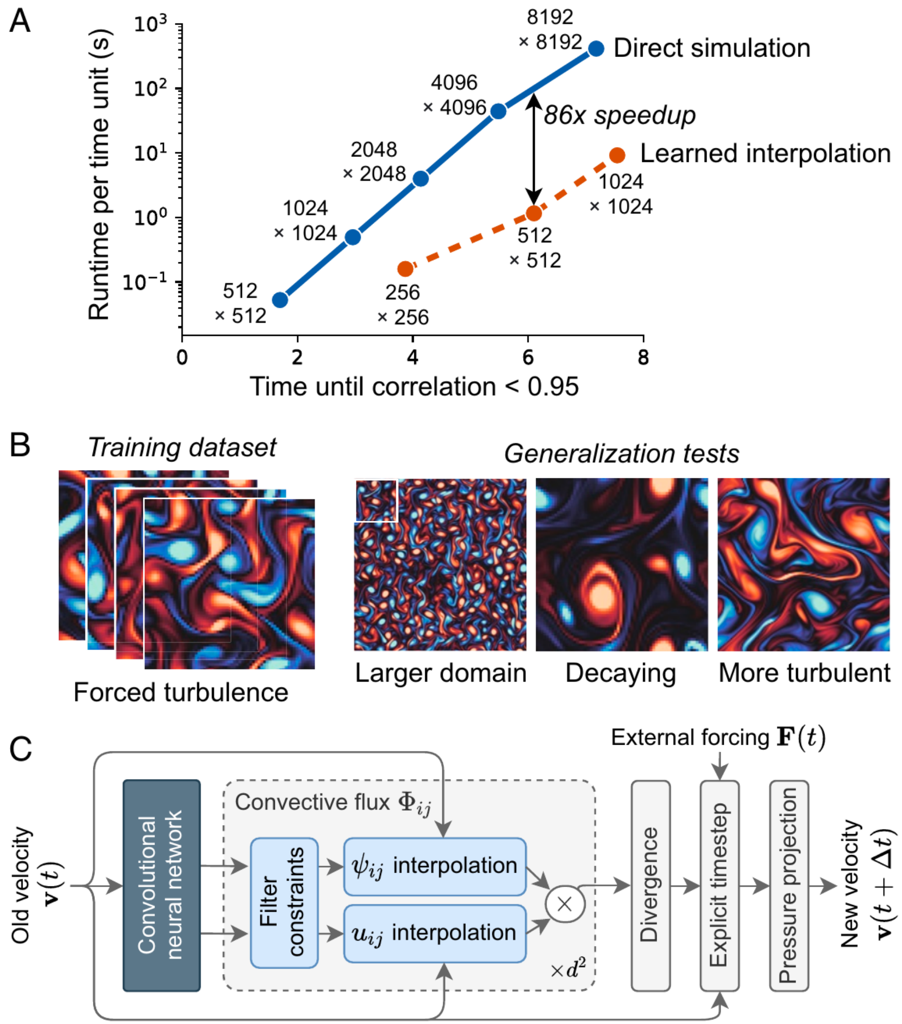






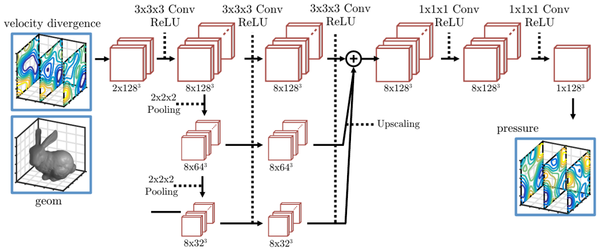
Accurate coarse simulation (cont'd)

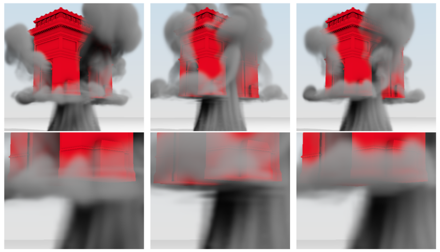
- *[Kochkov et al., 2021] "Machine learning-accelerated computational fluid dynamics," PNAS*
  - Learn the accurate DNS for coarser simulations
    - Learned interpolation
    - Learned correction



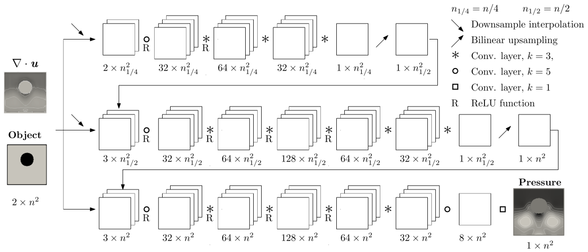
Accelerating numerical simulation

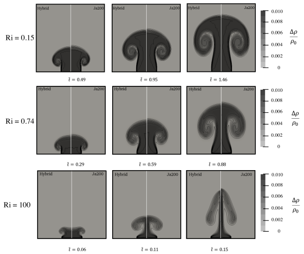
- Replace time-consuming parts with NN
- *[Tompson et al., 2017] "Accelerating Eulerian fluid simulation with convolutional networks," ICML*
  - Use a CNN to solve the Poisson equation, tackling "pressure bottleneck"
  - Outperform a traditional Jacobi solver





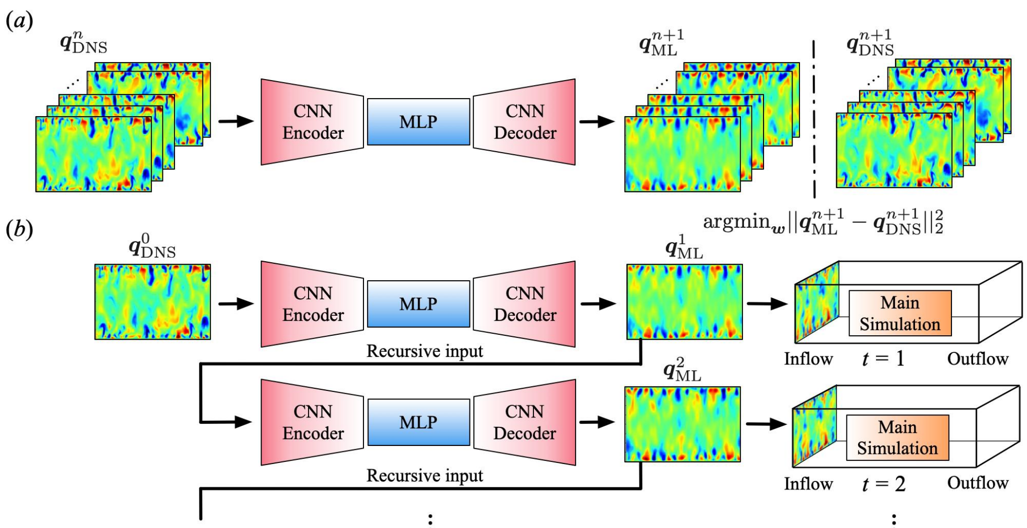
- *[Ajuria et al., 2020] "Towards a hybrid computational strategy based on deep learning for incompressible flows," AIAA AVIATION Forum*
  - Similar to Tompson's with a multi-scale network





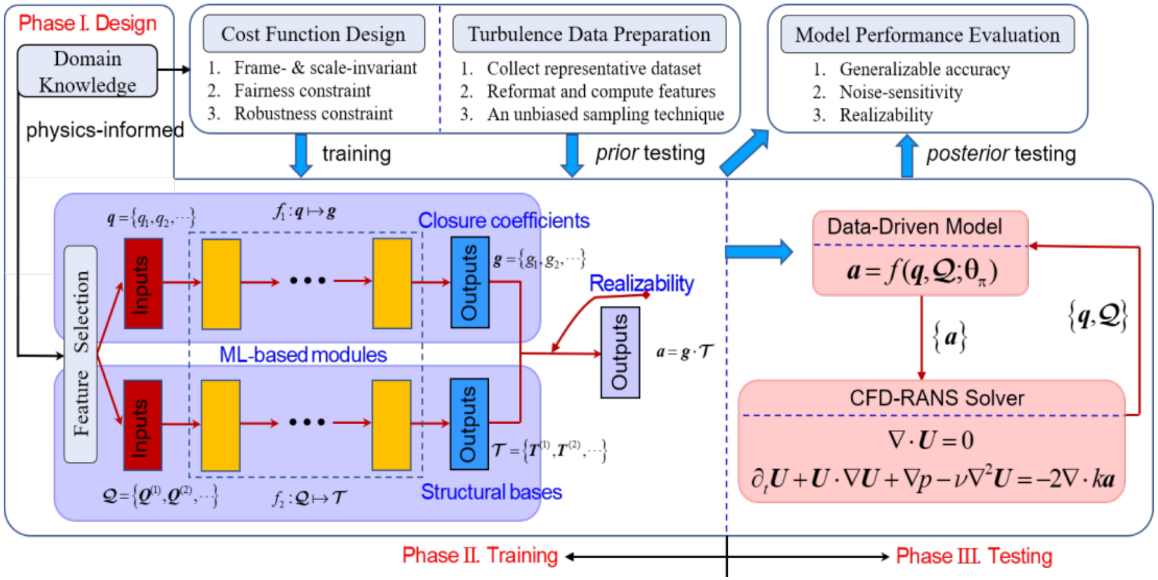
Accelerating numerical simulation (cont'd)

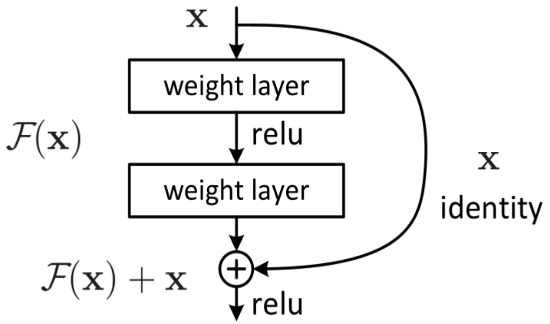
- Decrease the size of the computational domain
  - Replace a section upstream of the domain of interest with an inflow condition
  - Replace part of the far-field region with a suitable boundary condition
- *[Fukami et al., 2019] "Synthetic turbulent inflow generator using machine learning," PRF*
  - Develop a time-dependent inflow generator for wall-bounded turbulence simulations using an autoencoder with MLP



Turbulence modeling

- Better models for turbulence (e.g., Reynolds stress) with RANS
- *[Jiang, 2021] "An interpretable framework of data-driven turbulence modeling using deep neural networks," PRF*
  - Used physics-informed residual network (PiResNet)
    - ***ResNet*** (a.k.a. skip connection)

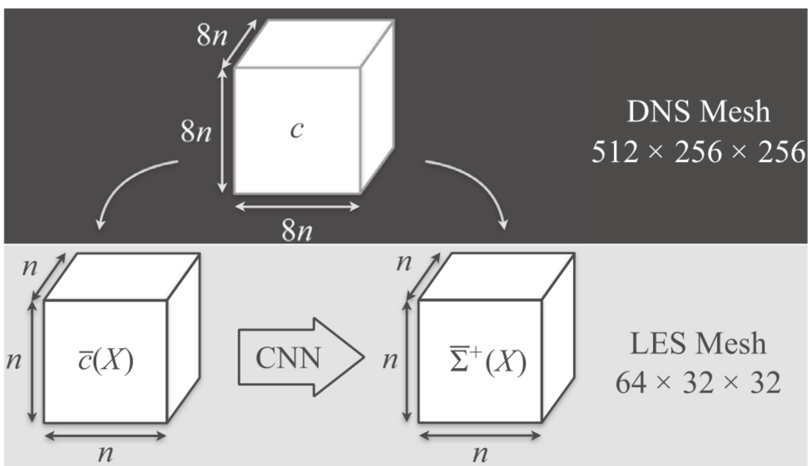


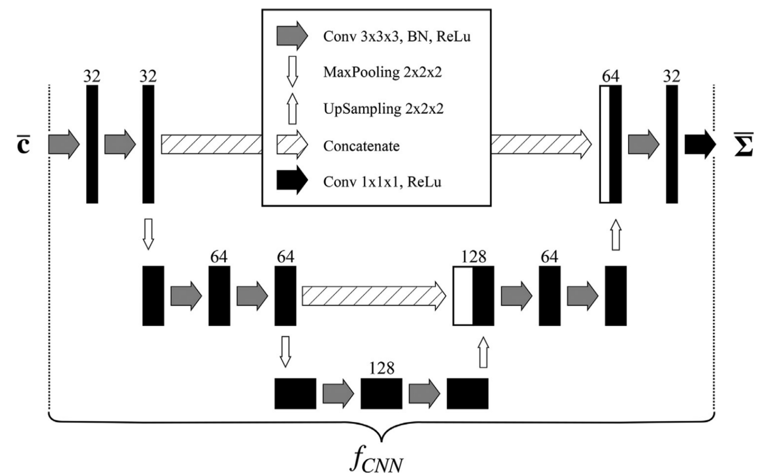


[He et al. 2016]

Subgrid-scale modeling

- *[Lapeyre et al., 2019] "Training convolutional neural networks to estimate turbulent sub-grid scale reaction rates," CaF*
  - Subgrid flame surface density estimation
  - Predict the subgrid-scale wrinkling of the flame surface
    - ***U-net***

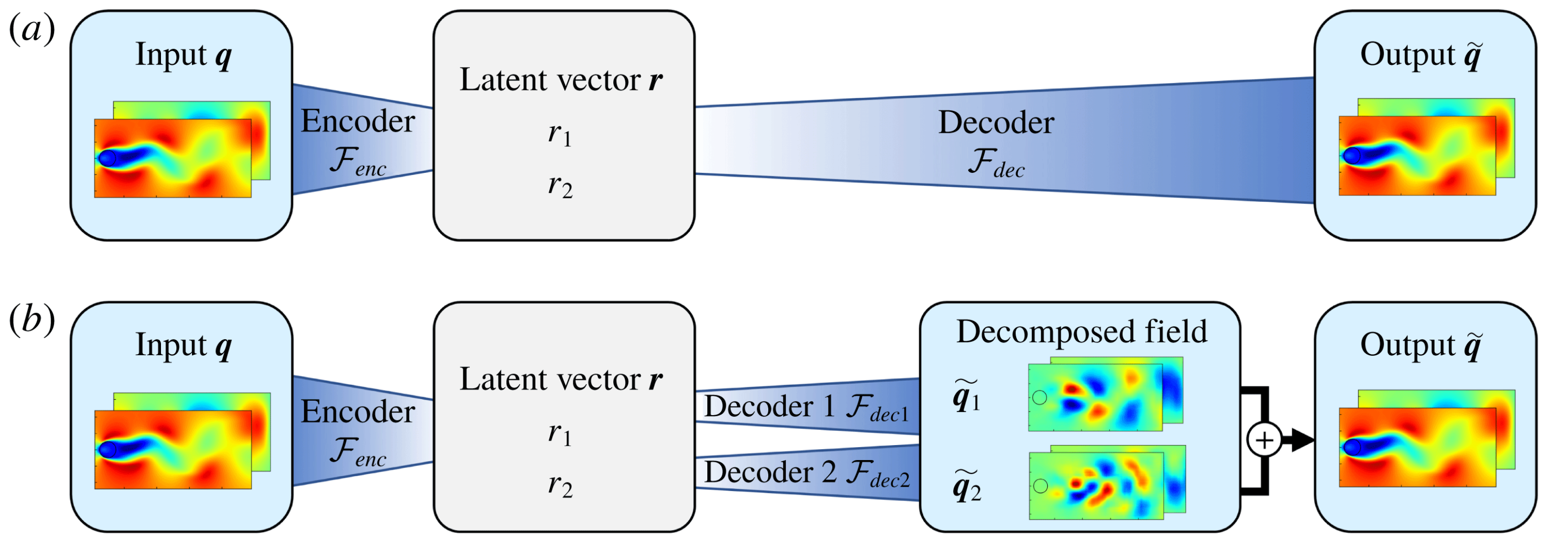




Reduced-order modeling

- Rely on the fact that even complex flows often exhibit a few dominant coherent structures

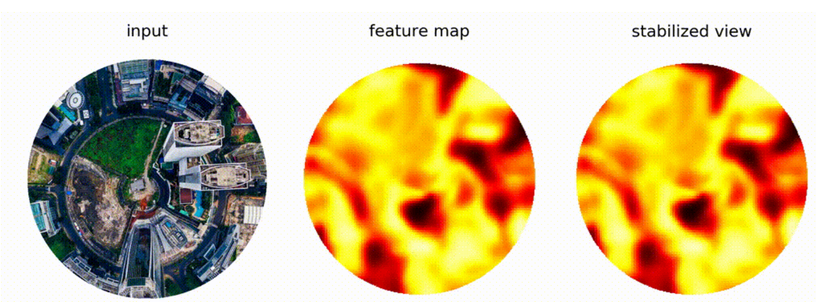
- *[Murata et al., 2020] "Nonlinear mode decomposition with convolutional neural networks for fluid dynamics," JFM*
  - Use an ***autoencoder*** to learn nonlinear manifold coordinates

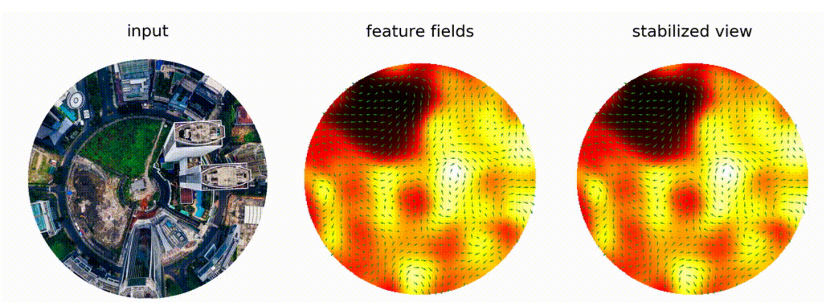


Prior physical knowledge

- *[Frezat et al., 2021] "Physical invariance in neural networks for subgrid-scale scalar flux modeling," PRF*
  - Use hard and soft constraints based on classical transformation invariances and symmetries derived from physical laws
    - Translation invariance: CNN
    - Rotation invariance: Data augmentation
    - Transport linearity: Individual sub-model for the transported scalar
    - Galilean invariance: Standardizing the velocity per sample

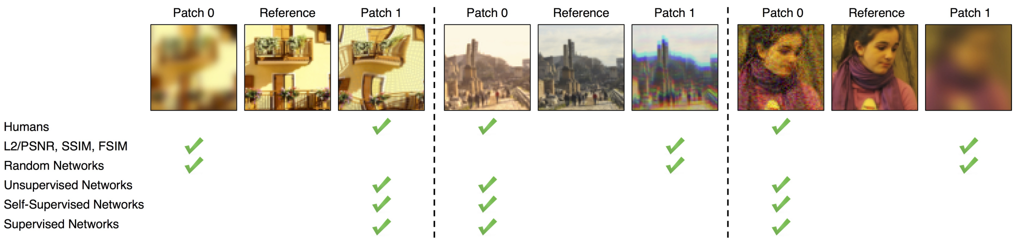
- Rotation invariance
  - *[Cesa et al., 2022] "A program to build E(n)-equivariant steerable CNNs," ICLR*



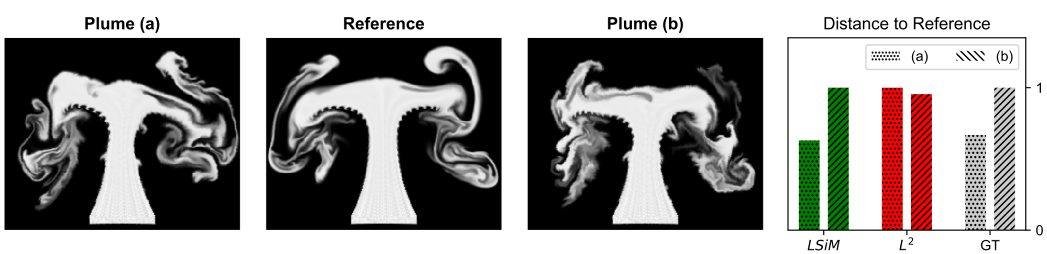


New metrics

- Traditional metrics: L2, PSNR, and SSIM
- *[Zhang et al., 2018] "The unreasonable effectiveness of deep features as a perceptual metric," CVPR*
  - Evaluate deep features across different architectures and tasks
  - Propose the learned perceptual image patch similarity (LPIPS) metric



- *[Kohl et al., 2020] "Learning similarity metrics for numerical simulations," ICML*



What's next?

- We still have far to go ...

- There exist many potential directions
  - For example, *diffusion model* in CFD
    - *[Kohl et al., 2023] "Turbulent flow simulation using autoregressive conditional diffusion models," arXiv*

- Missions
  - ESR 5: Francesco Fossella
    - Deep-data assimilation and deep-feature-based metric for turbulent flows
  - ESR 12: André Freitas
    - Large eddy simulation models in a deep machine learning loop
  - ESR 13: Elisa Bellantoni
    - Complex wetting problems using neural networks



Thank you!