Physics-Aware Deep Learning for Reduced Order Modeling

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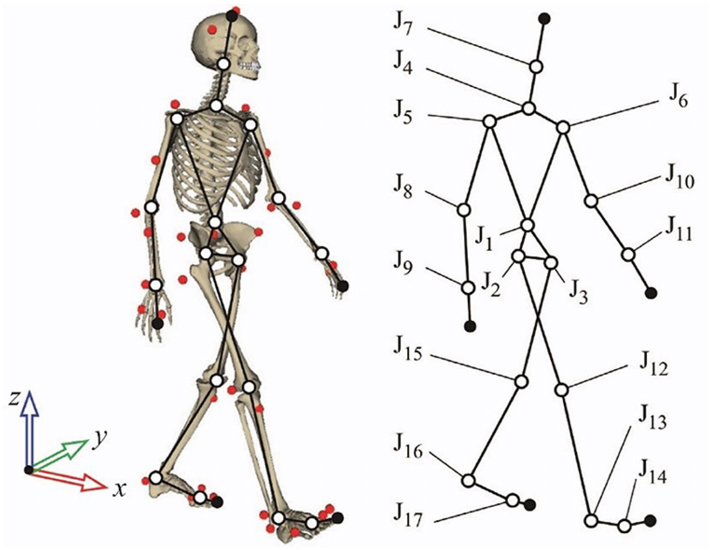
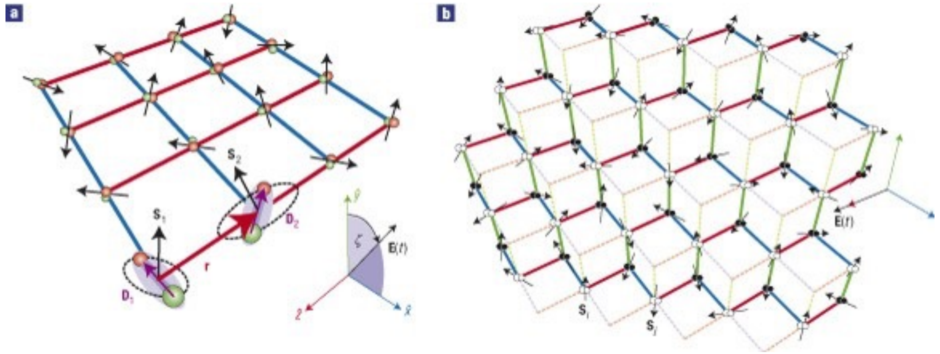
High Dimensional Data

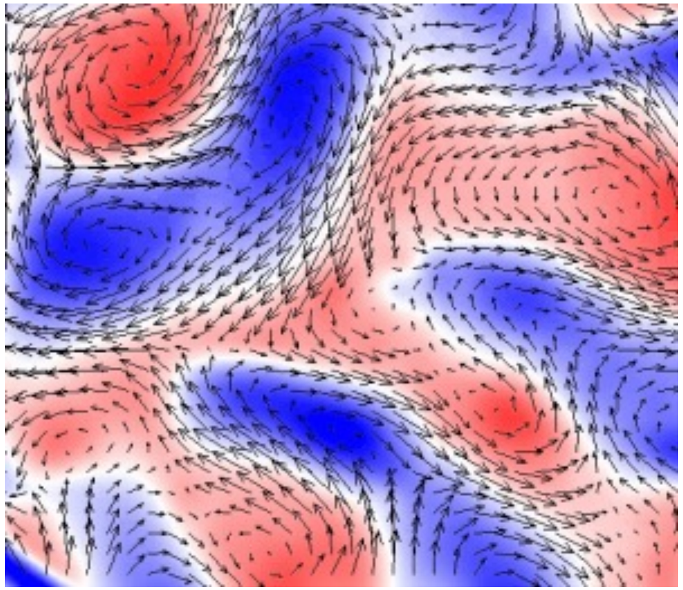
- The data representing the behavior of physical systems is usually high dimensional with complex patterns and modalities.



Human body motion



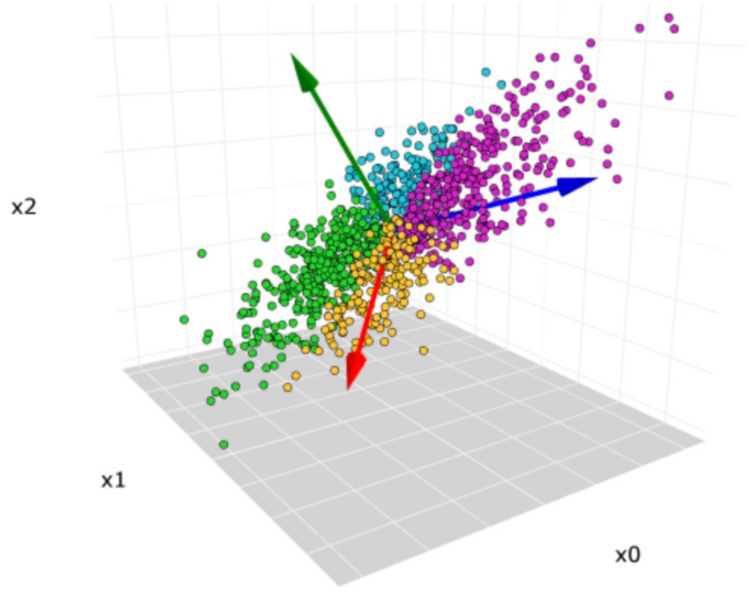
Lattice of electrons in a crystalline material



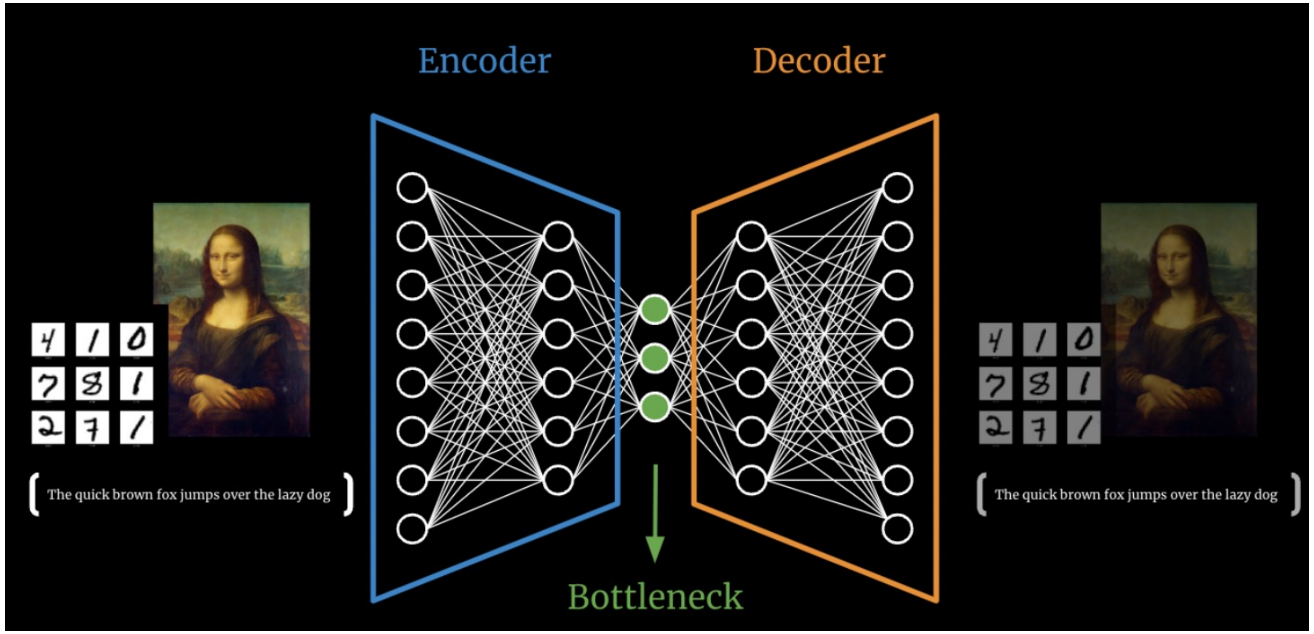
Velocity field of a fluid flow

Model Reduction

- One needs lower dimensional projections of the experimental/simulation data for many optimization and design applications in engineering.



Principal Component Analysis (PCA)



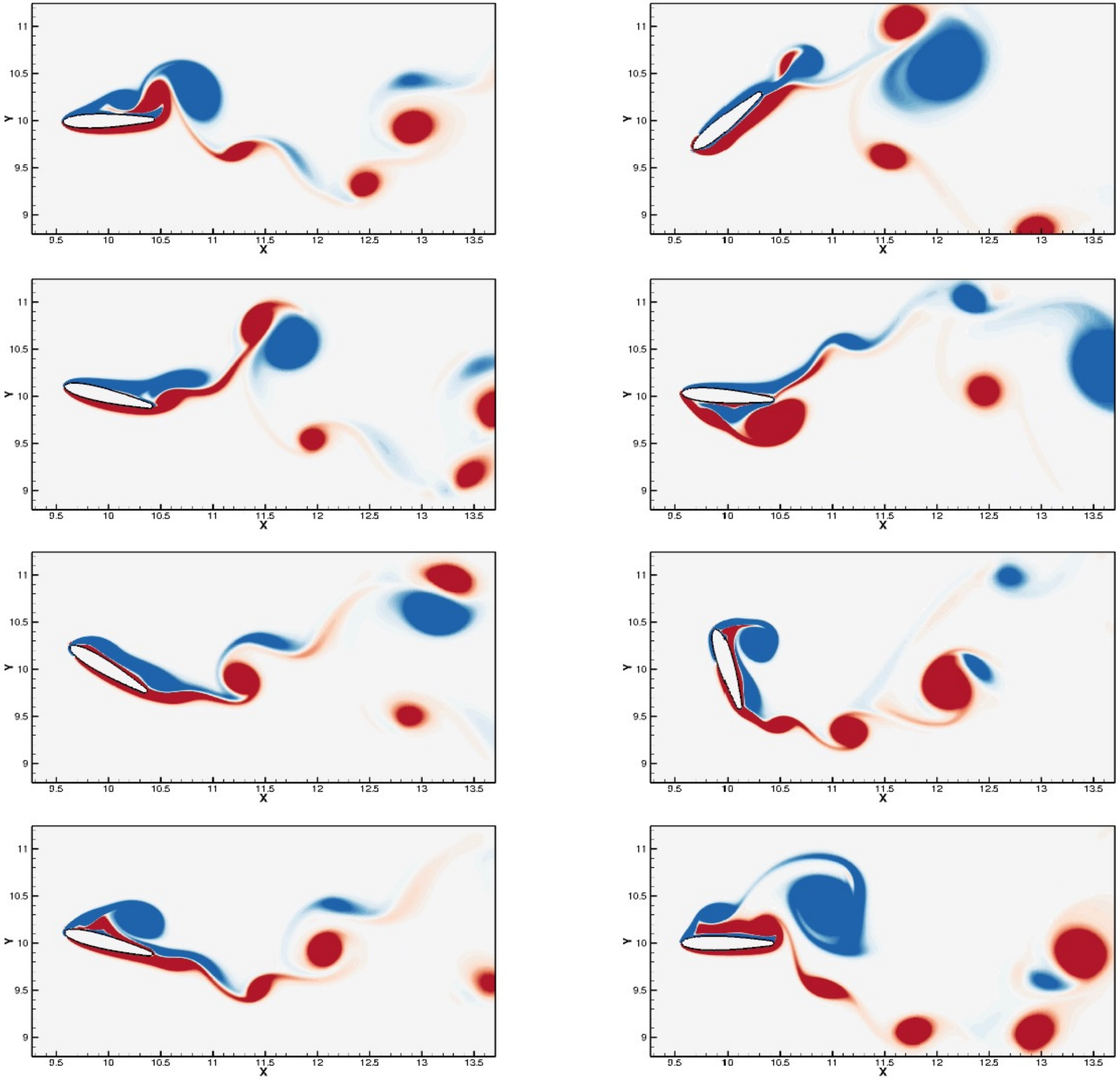
Deep neural network-based Autoencoder (AE)

Deficiency of Classical Autoencoders

- The reconstruction loss for training classical autoencoders does not incorporate:

  1) The temporal and spatial correlation between consecutive snapshots of the physical system's evolution

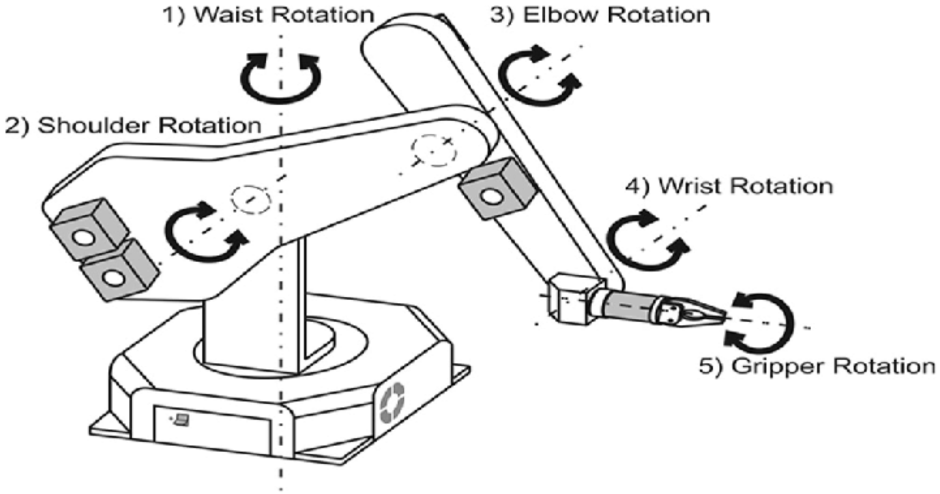
  2) The underlying physical laws governing the dynamics of the system

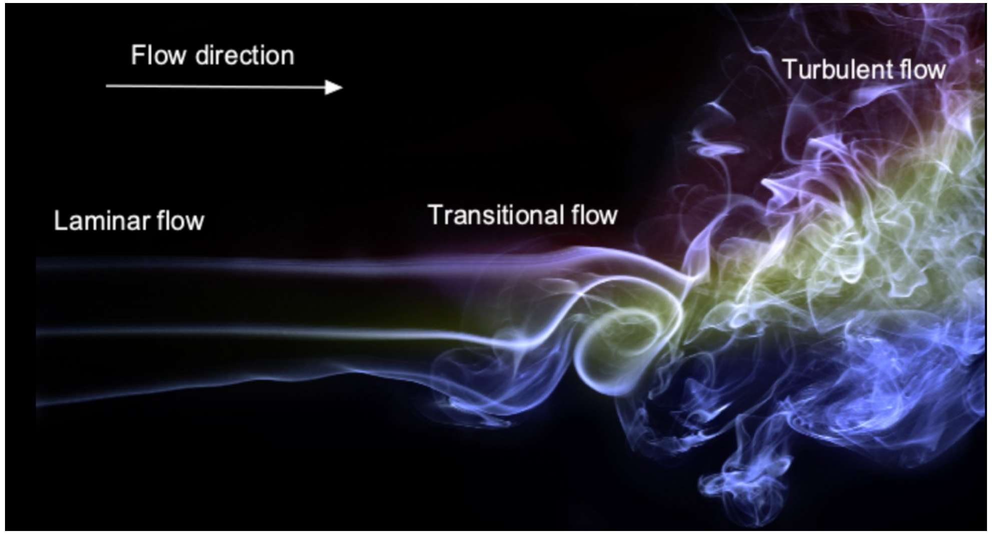


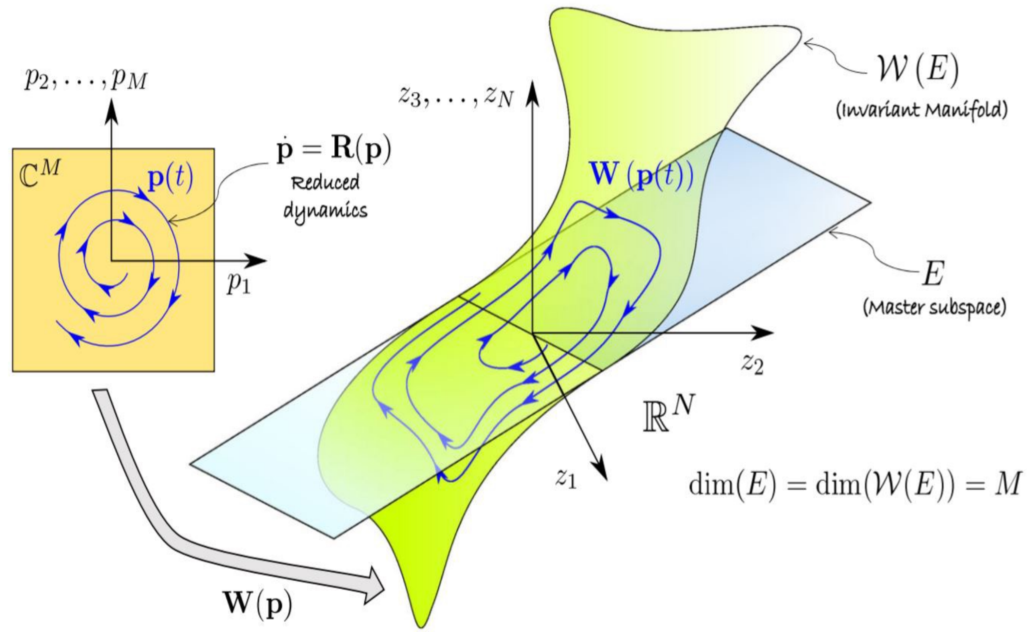
Menon et al., Computational modelling and analysis of aeroelastic flutter, 2018

Encoding Physical Evolution (Dynamics) into Latent Space

- Hypothesis: the effective evolution of the system happens over a lower dimensional space (dynamics manifold) embedded into the high dimensional pixel space.







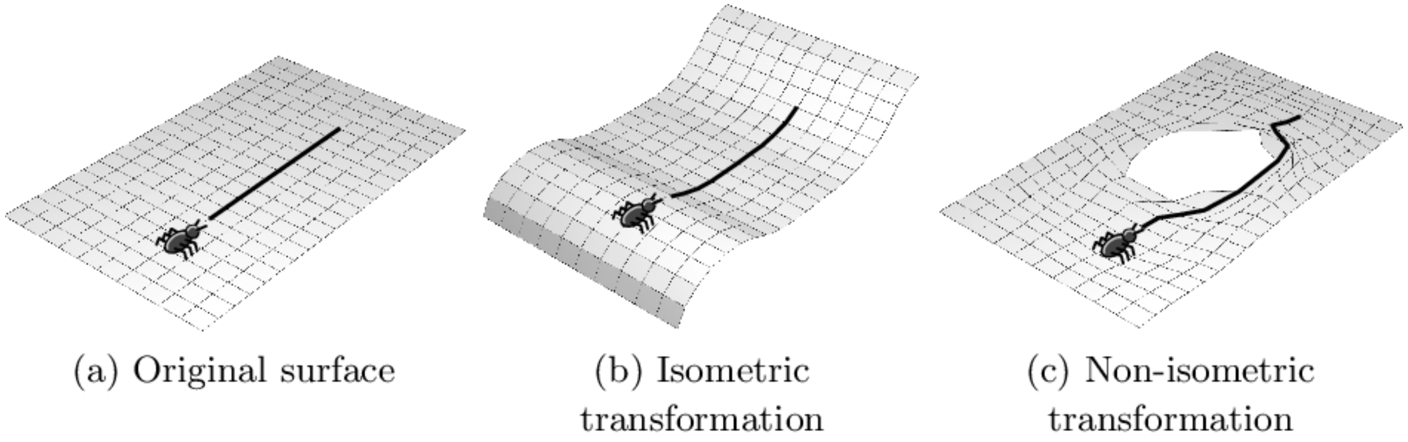
Low dimensional representation of the effective dynamics

Jain e al., How to compute invariant manifolds and their reduced dynamics in high dimensional finite element models, 2021

Autoencoder equipped with Isometric Loss

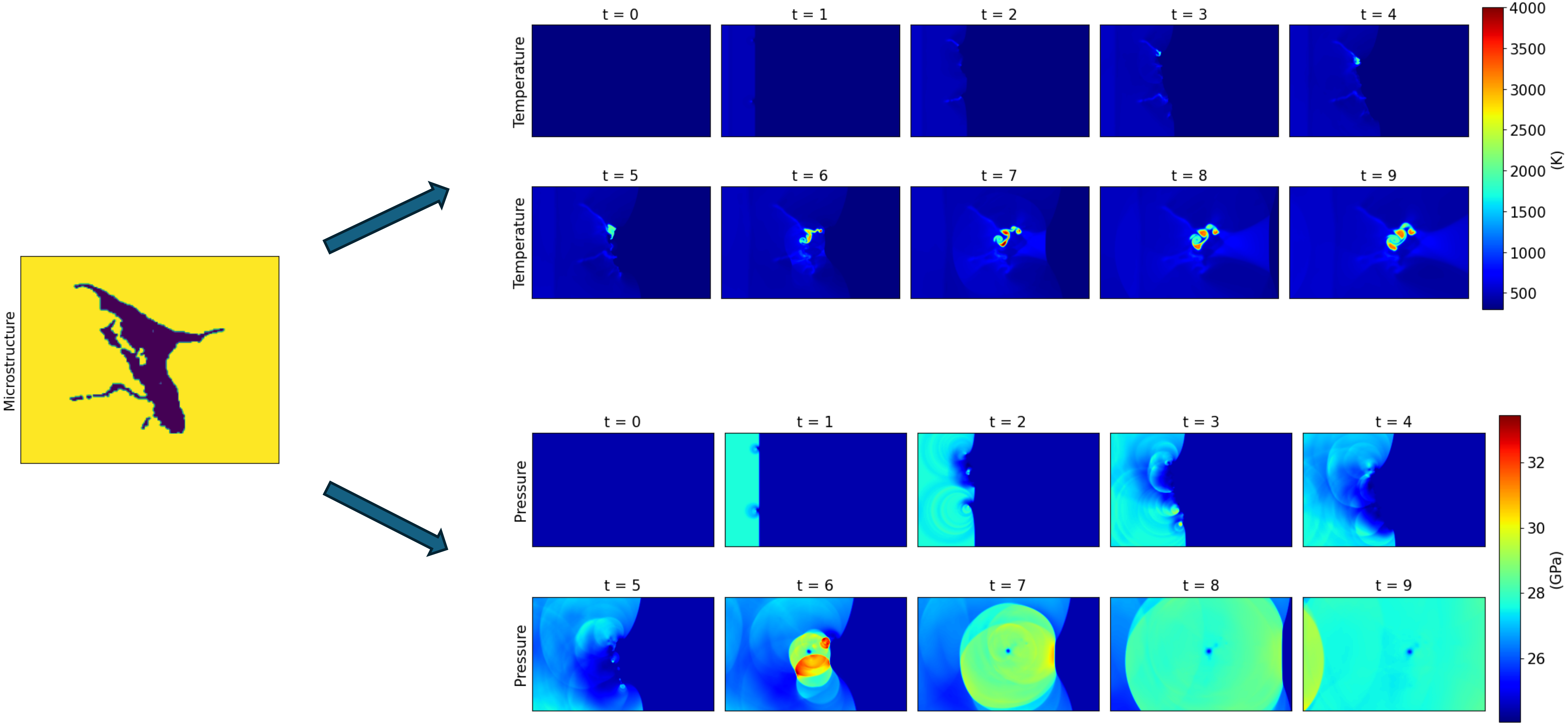
- The shape and geometry of the dynamics manifold incorporate important information about the underlying physics.

Distortion of different areas of the earth under the stereographic projection



Lee et al., Regularized Autoencoder for Isometric Representation Learning (2022)
Bronstein et al., Isometric embedding of facial surfaces into S3, 2004

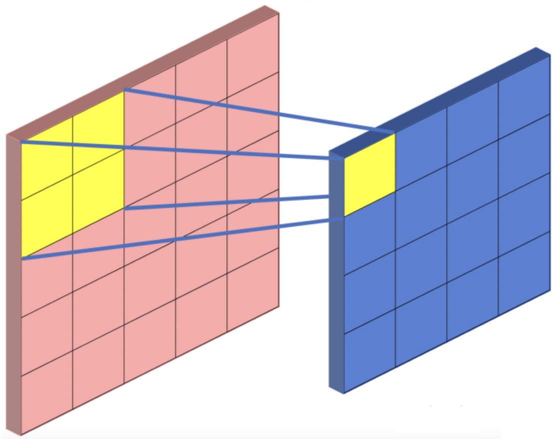
Energy Localization due to Chemical Reaction



Latent-PARC Model

- Three independent variational autoencoders (VAE) for encoding the three fields (T, P, μ)

- For each field snapshot X, the VAE associates a field Z of i.i.d. multivariate Gaussians $P(Z|X)$ with:
  - mean field $\bar{Z}$
  - log-variance field Z^{σ}



- The time evolution of the latent field Z is encapsulated in the evolution of the corresponding $\bar{Z}$ and Z^{σ}.

Latent-PARC Model

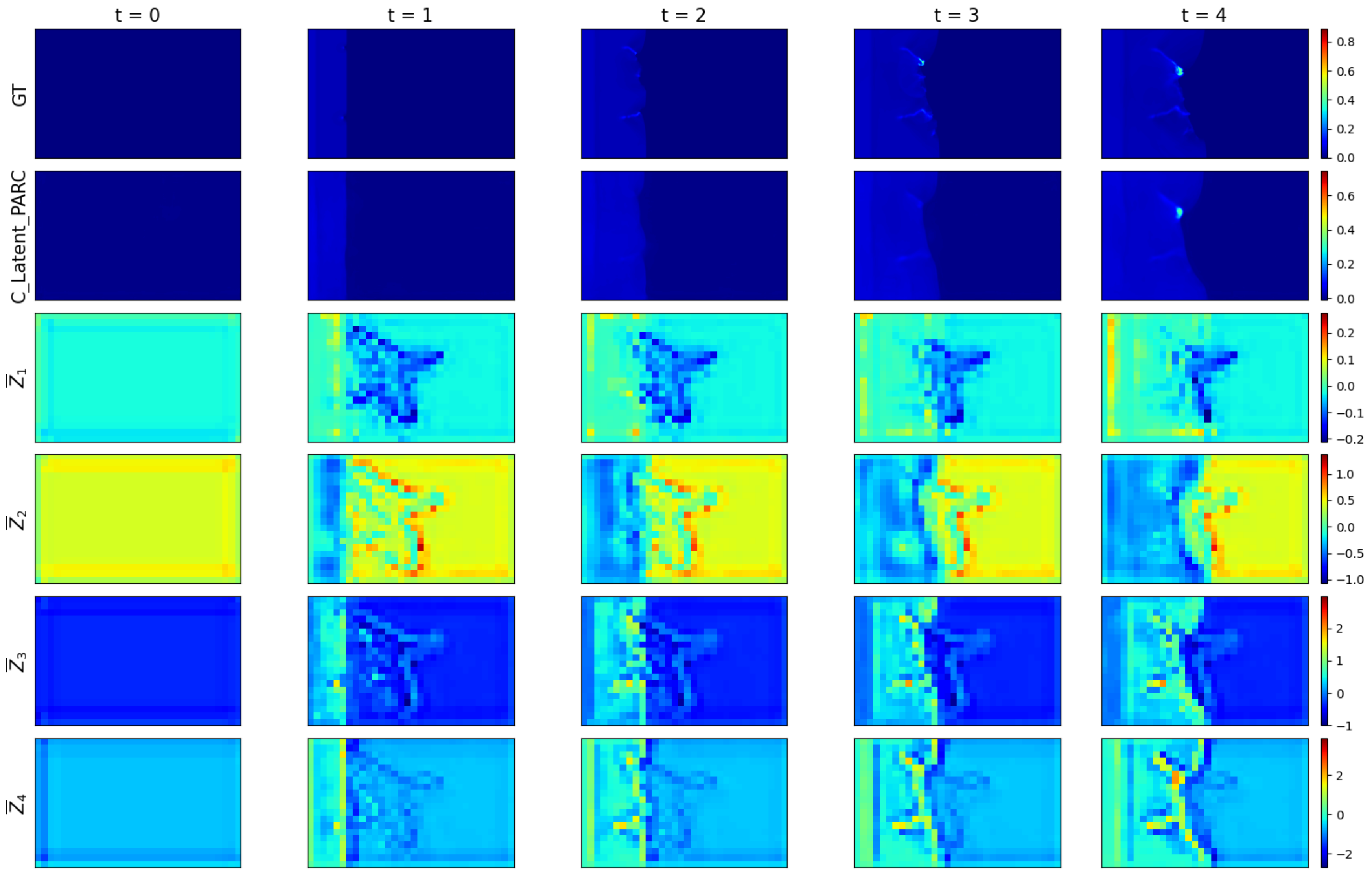
- Deterministic part of the latent dynamics:

$$\begin{bmatrix} \bar{Z}_T \\ \bar{Z}_P \\ \bar{Z}_\mu \end{bmatrix}_{|t+1} = \bar{F} \begin{bmatrix} \bar{Z}_T \\ \bar{Z}_P \\ \bar{Z}_\mu \end{bmatrix}_{|t} \tag{1}$$

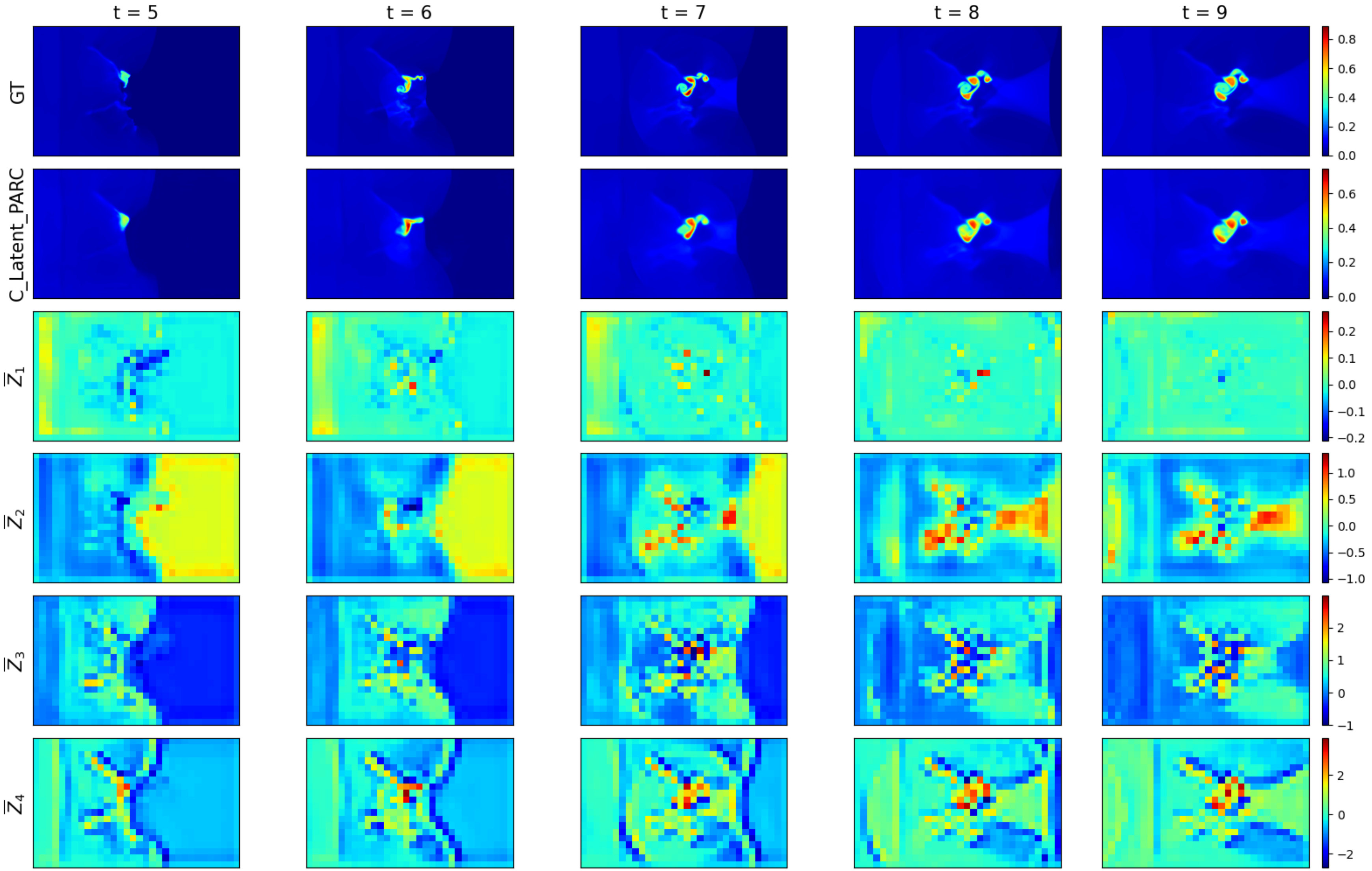
- Stochastic part of the latent dynamics:

$$\begin{bmatrix} Z_T^\sigma \\ Z_P^\sigma \\ Z_\mu^\sigma \end{bmatrix}_{|t+1} = F^\sigma \begin{bmatrix} (\bar{Z}_T\,,\, Z_T^\sigma) \\ (\bar{Z}_P\,,\, Z_P^\sigma) \\ (\bar{Z}_\mu\,,\, Z_\mu^\sigma) \end{bmatrix}_{|t} \tag{2}$$

Latent-PARC Prediction of Temperature Evolution



Latent-PARC Prediction of Temperature Evolution



Conclusion / Next Steps

- In order to get a faithful compressed representation of a physical system, one needs to take into account:

1) The underlying physical laws
2) The geometric structure of the system's state space

- In order to improve the prediction accuracy of the Latent-PARC model, we plan to consider the following architectures for the latent dynamics model:

1) A recurrent neural network architecture (e.g. Convolutional LSTM)
2) A differentiator – integrator architecture (similar to PARCv2)

Shi et al., Convolutional LSTM Network: A Machine Learning Approach for Precipitation Nowcasting (2015)
Nguyen et al., PARCv2: Physics-aware Recurrent Convolutional Neural Networks for Spatiotemporal Dynamics Modeling (2024)

Thank You!