Mathematical and Applied Aspects of Complexity Reduction Methods, Collège de France

From Latent Space Representations to Practical Surrogate Models for Structural Dynamical Systems

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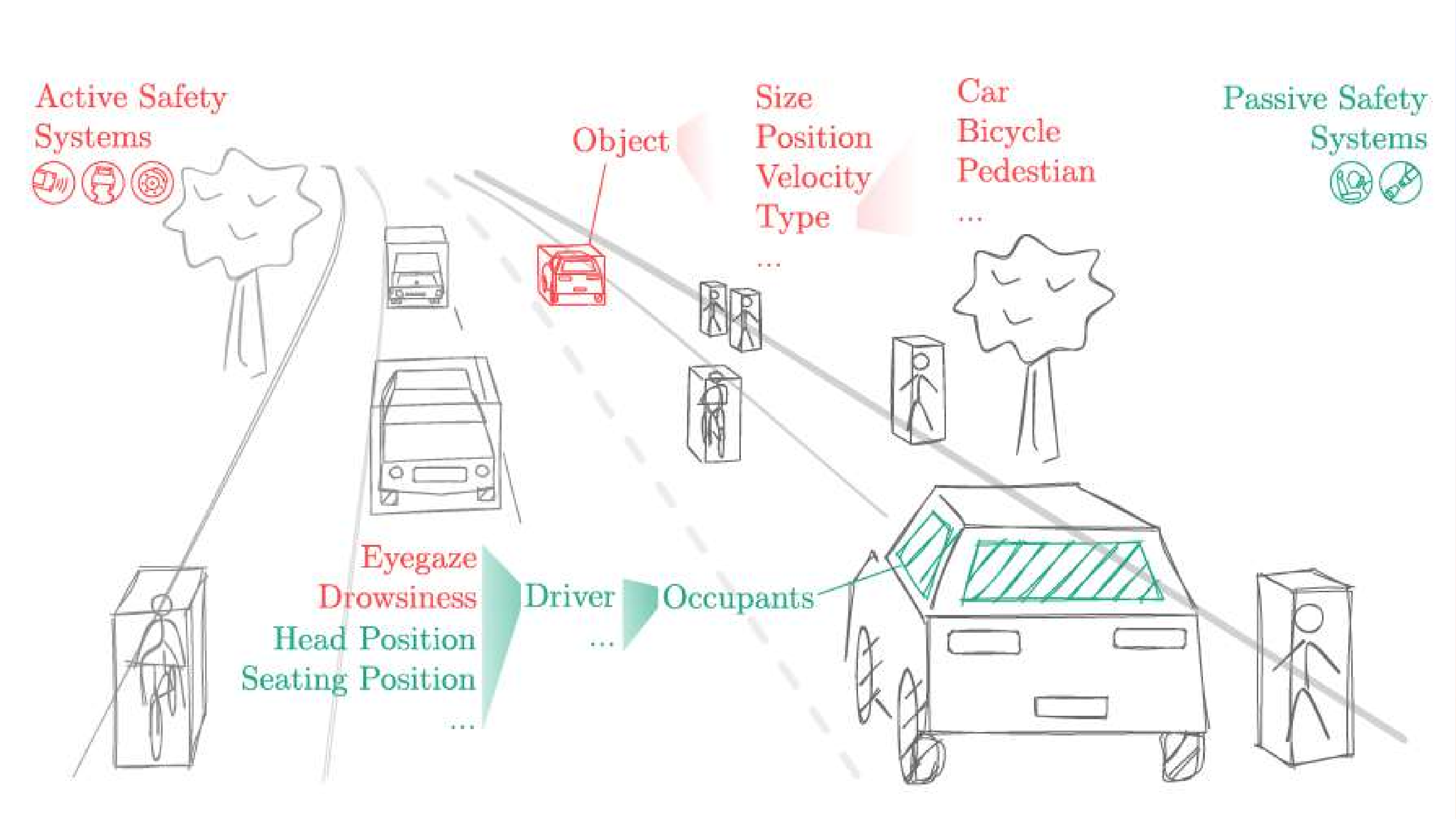
SimTech
Cluster of Excellence

- What makes today's car the "most advanced" (and affordable) technical system most of us own?"

The Car as a Complex Mechatronic System

- **Integration of disciplines:** mechanics ⚙️ electronics 🔋 software 💻
- **Tightly coupled systems:** drivetrain, chassis, interior, infotainment, sensors
- **Autonomy is growing:** cars increasingly sense, decide, act in real time
- **Result:** modern vehicle behaves like a “computer on wheels”

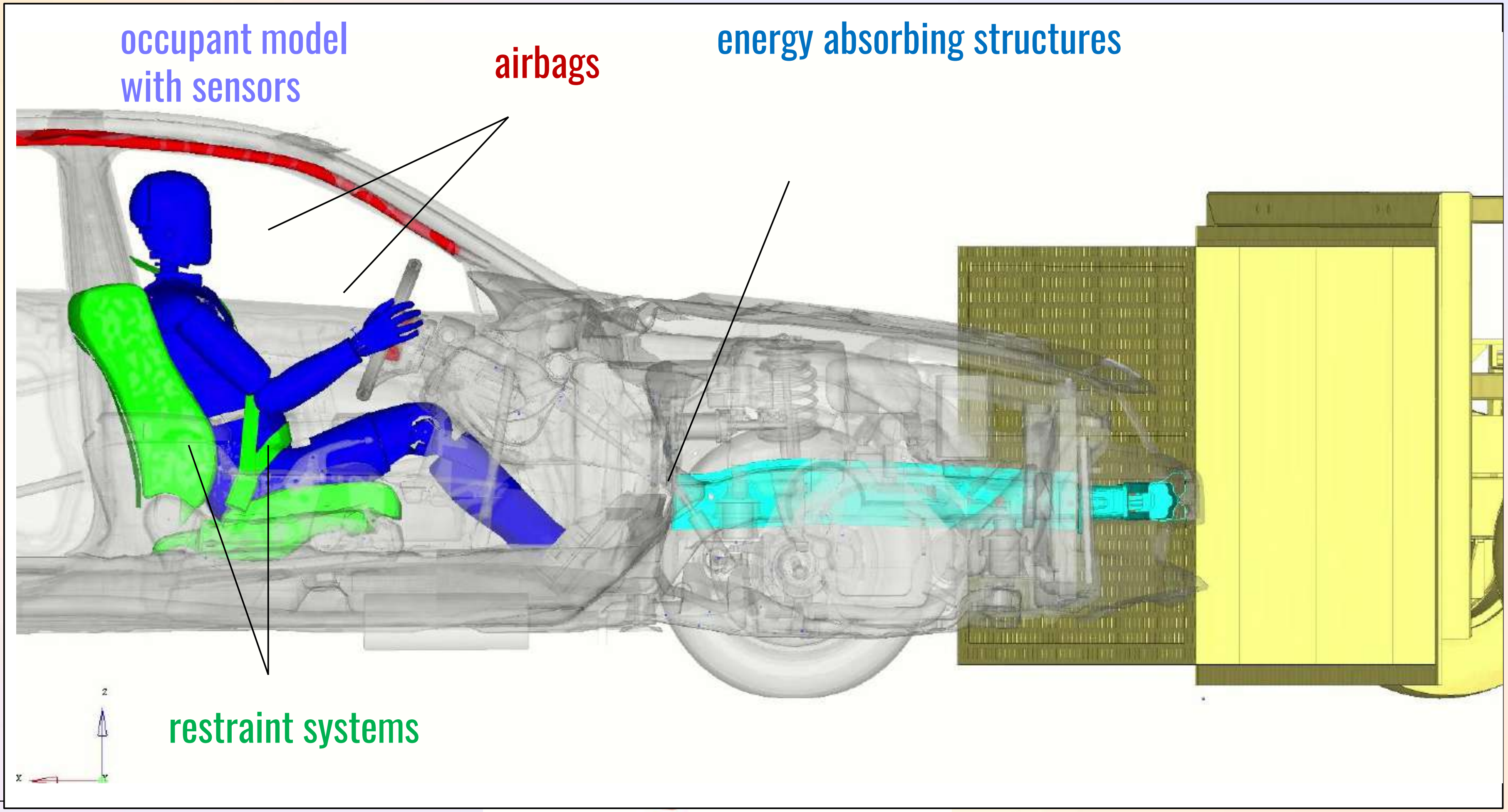


What Do You Get for Your Money?

- **Complex technical sub-systems inside every car:**
  - Safety & comfort → **seats, airbags, steering systems**
  - Electronics & monitoring → **sensors, measurement instruments, interior monitoring**
  - Power & infrastructure → **motors, charging systems**
- **Thousands of components** integrated into a single product
- A car = **the most complex and value-for-money technical system most people ever own**

2,89 € per day
8,4 Cent per kilometer
(no gas, insurances and reparis)

Example of High-Fidelity Simulations



Crash Simulations
Honda Accord plus two THOR dummies
5 200 000 elements
96 nodes,
17 hours calculation
for **120 ms** sim. time

High-fidelity Simulations – CAE Process

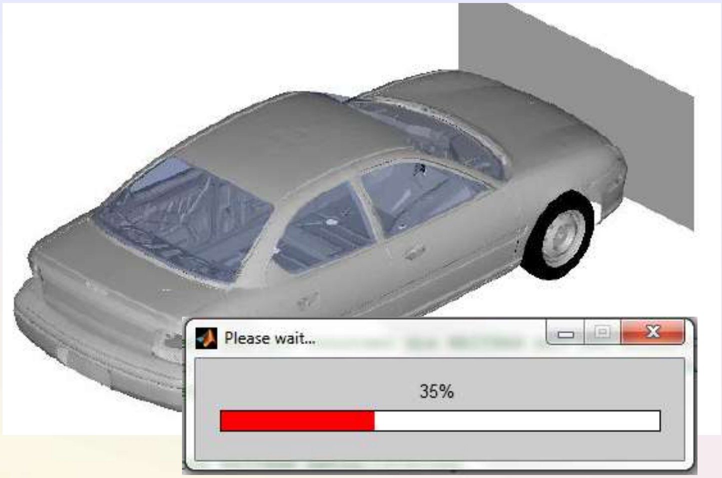
- crash simulations → large computational effort
- Honda Accord plus two THOR dummies 5 200 000 elements

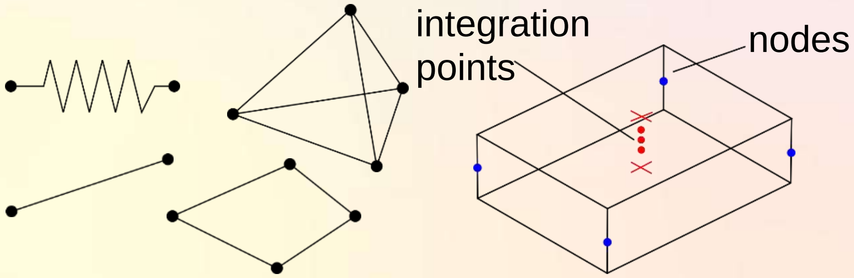
  96 nodes, 17 hours calculation time for 120 ms sim. time
- nonlinear FE equation

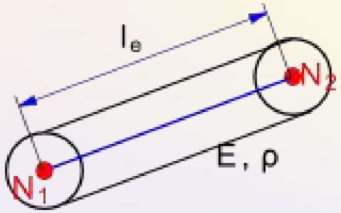
  $$\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{f}^{\text{int}}\,(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \boldsymbol{f}^{\text{ext}}$$
- explicit time integration in **LS-Dyna**
- three basic sources of nonlinearities in mechanics

  geometry, physics (material laws), boundary conditions
- multiple element types, element definitions, etc.
- maximum time step limited by Courant-Friedrichs-Lewy condition

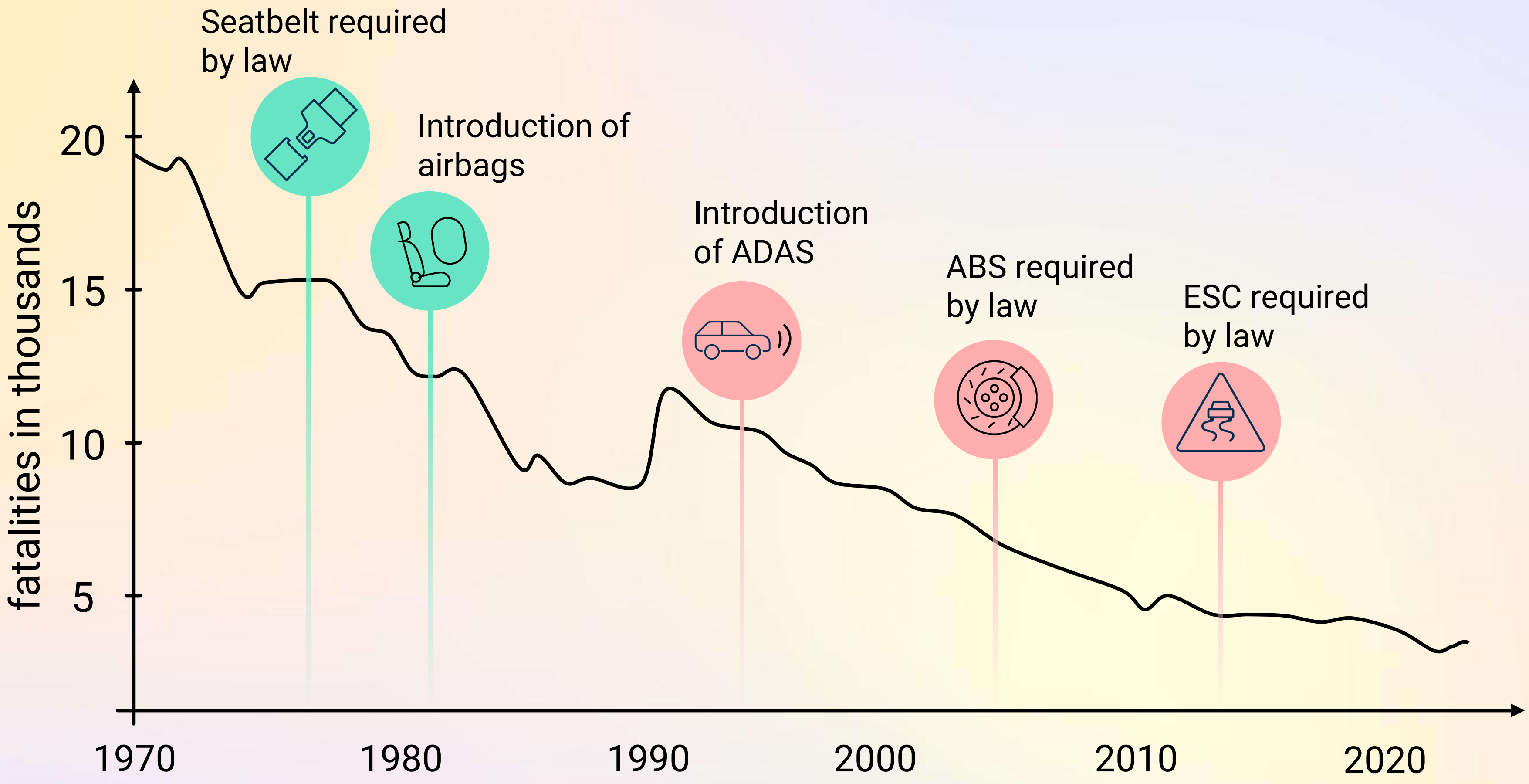
  $$\Delta T_{CFL} = l_e / c_w$$
  $$c_w = \sqrt{E/\rho}$$







Current State of Vehicle Safety



[Destatis: Traffic Accidents and Fatalities Over Time in Germany, 2022]

Germany Automotive Industry

Employment

- **870,000 direct employees** in motor vehicle and parts manufacturing (BA)
- **2.2 million total jobs** across the value chain (suppliers, dealers, logistics, R&D, testing)

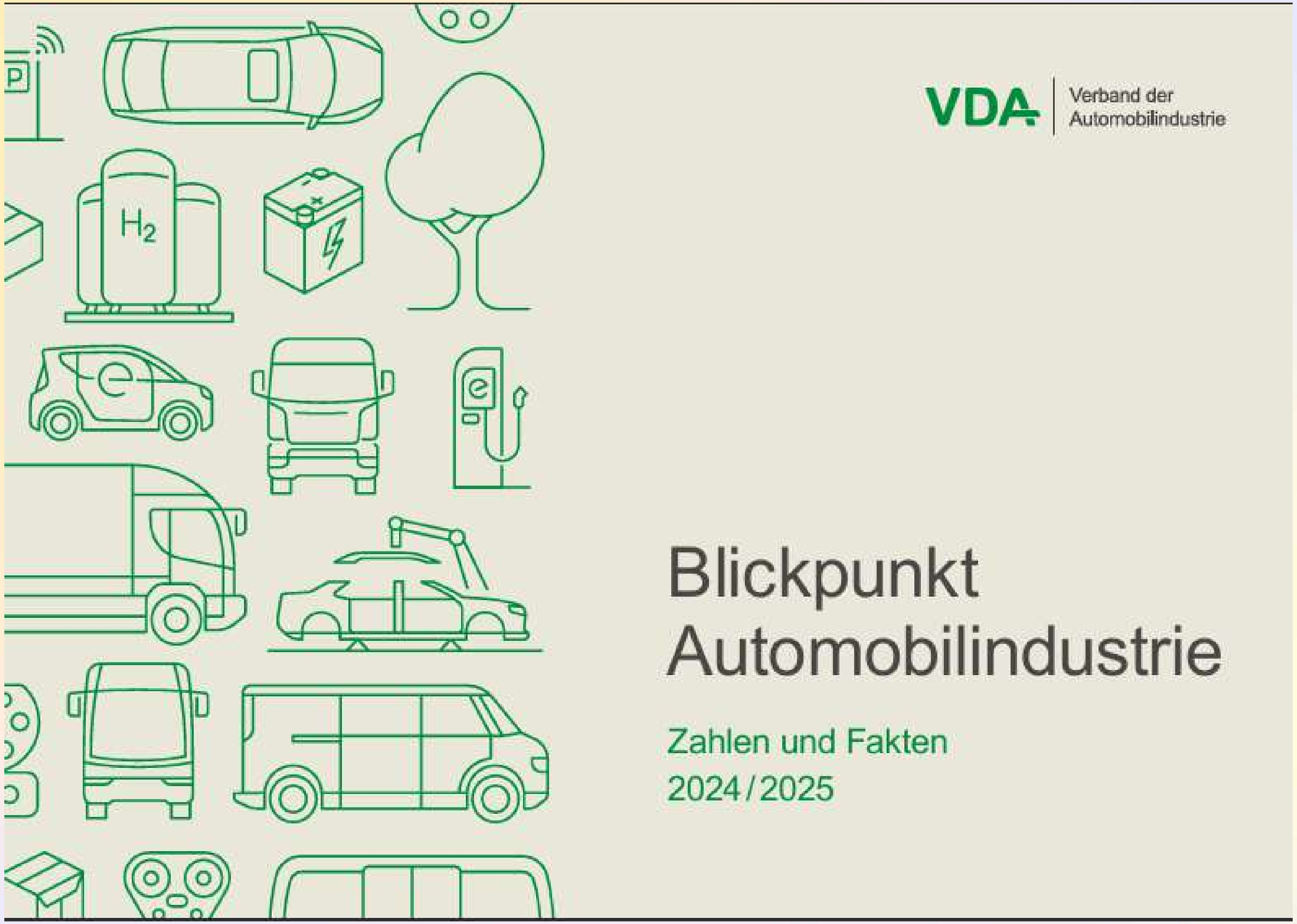
Economic Weight

- **~20% of total industrial revenue** comes from automotive sector
- **~€30 billion annually** in R&D spending → Innovation driver

Exports & Trade (data from 2024)

- **3.18 million passenger cars**
  – export value €135.0 billion
- **€112.7 billion trade surplus**
- **17% of all German exports** = vehicles & parts

BLICKPUNKT AUTOMOBILINDUSTRIE VDA



Blickpunkt Automobilindustrie_Zahlen und Fakten_2024-2025.pdf

What Happens if the Motor is Stuttering?

30

Die Automobil-
industrie:
Ein **flächendeck-
ender Jobmotor**

2,5 von 100 Beschäftigten in Deutschland arbeiten für die Automobilindustrie

- >4,0 %
- 4,0 – 2,5 %
- 2,5 – 1,0 %
- 1,0 – 0,5 %
- 0,5 – 0,0 %
- nicht vorhanden

Hamburg
nicht vorhanden

Bremen
nicht vorhanden

Niedersachsen
134.100 Beschäftigte

Nordrhein-Westfalen
76.600 Beschäftigte

Rheinland-Pfalz
28.100 Beschäftigte

Hessen
52.400 Beschäftigte

Saarland
20.900 Beschäftigte

Baden-Württemberg
222.400 Beschäftigte

Schleswig-Holstein
3.500 Beschäftigte

Mecklenburg-Vorpommern
2.900 Beschäftigte

Berlin
4.900 Beschäftigte

Brandenburg
14.200 Beschäftigte

Sachsen-Anhalt
4.300 Beschäftigte

Sachsen
44.200 Beschäftigte

Thüringen
14.700 Beschäftigte

Bayern
251.600 Beschäftigte

Stand: September 2024

Quelle: Bundesagentur für Arbeit

Imagine this: I am in the middle of a doctoral exam when suddenly the phone rings.

Why

Problem definition

Analyze the structure's behavior in a *frontal crash scenario*

We don't want to drive *the actual* kart against a wall

Modeling

Import geometry

Spatial discretization

Assign material properties

…

Cur
Situ

High-fideli

Pre

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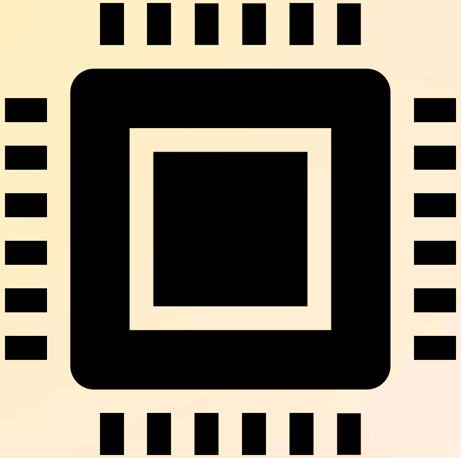
Par
impact velocity ρ_1, ...)

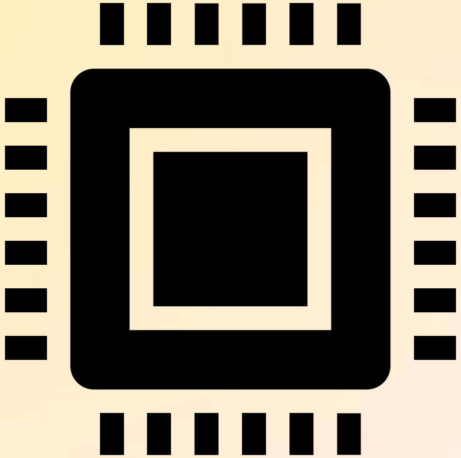
Complexity

Prohibitive Computational Effort



Weak Hardware

Prohibitive Computational Effort



Weak Hardware

Real-time Capabality

Prohibitive Computational Effort

Data-driven

Surrogate Modeling

Hardware

Capabality

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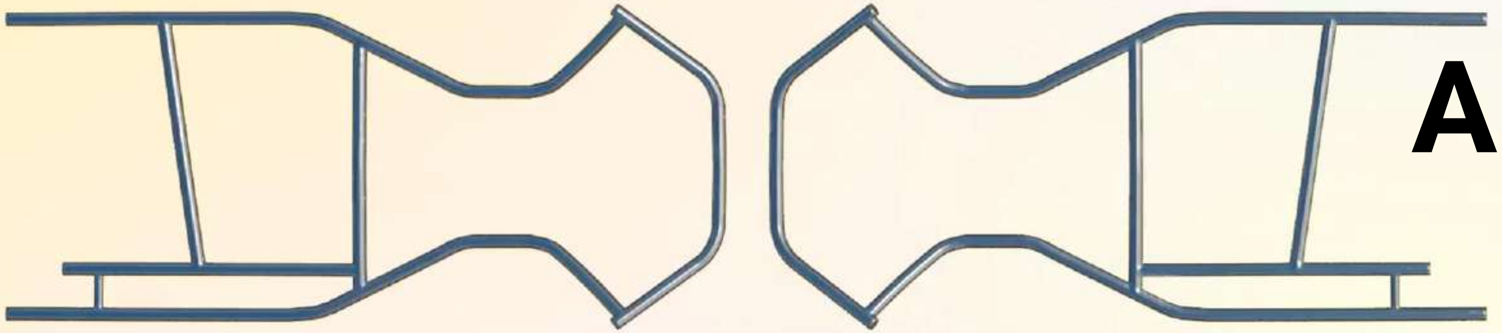
Problems

What is a Surrogate Model?



Efficient Approximator

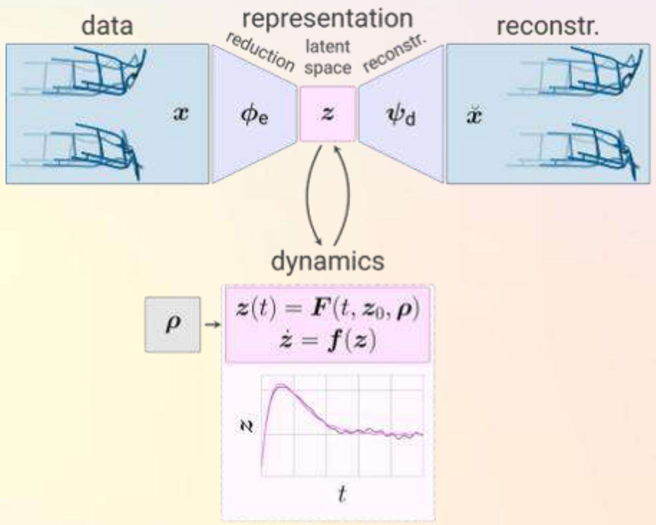
emulate the *essential behavior*

drastically *reduce* computational effort

Challenges

Challenges

Dimension | **Representation** | **Accessibility** | **Data Quality** | **Physicality** | **Multi-X**



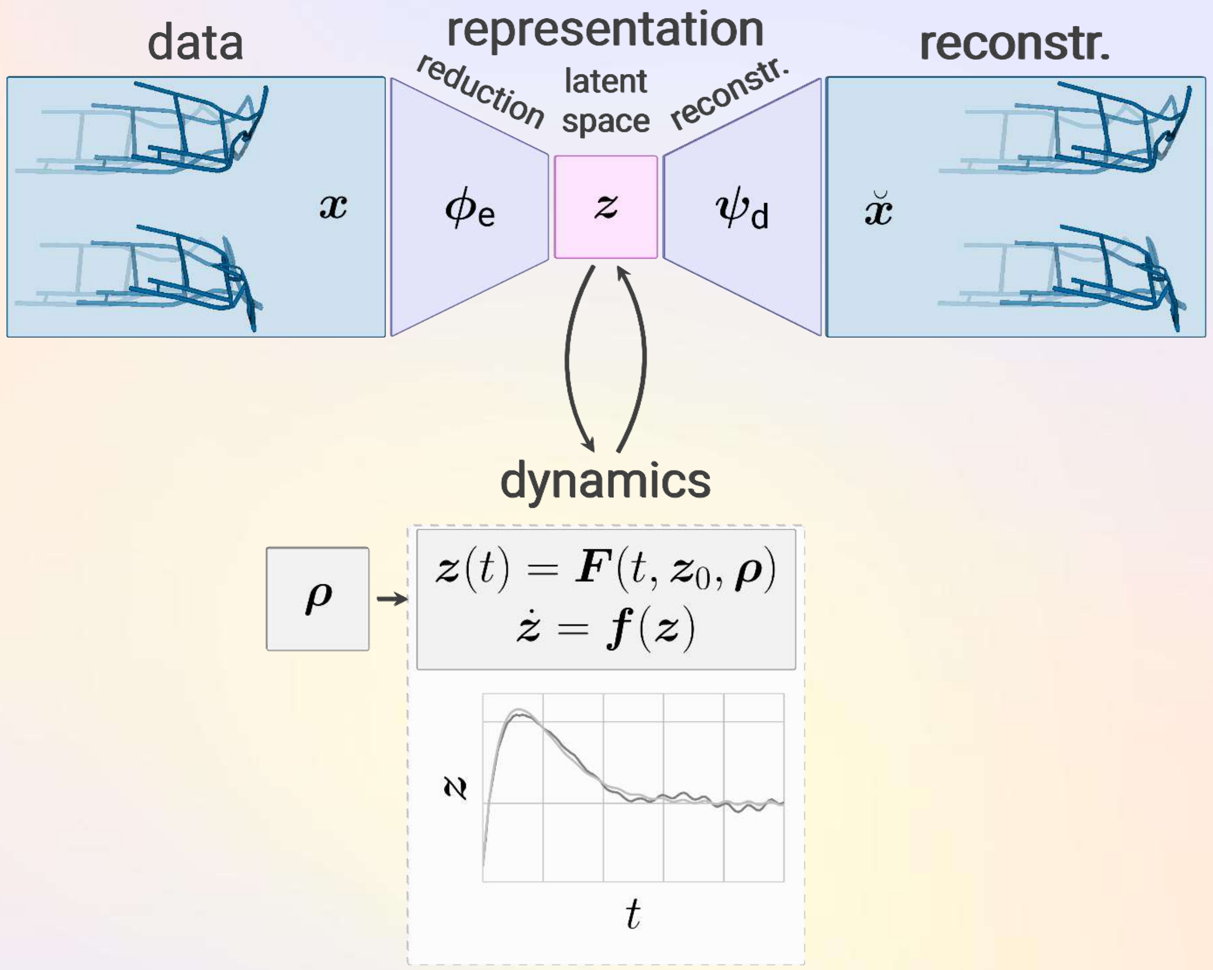
General Approach

Non-intrusive data-driven model order reduction

- Approximate high-fidelity model solution $\boldsymbol{x}$

Use data $\boldsymbol{x}$ to ...

- identify suitable low-dimensional coordinates
- approximate reduced dynamics



Linear Dimensionality Reduction

Projection-based reduction

- Galerkin projection

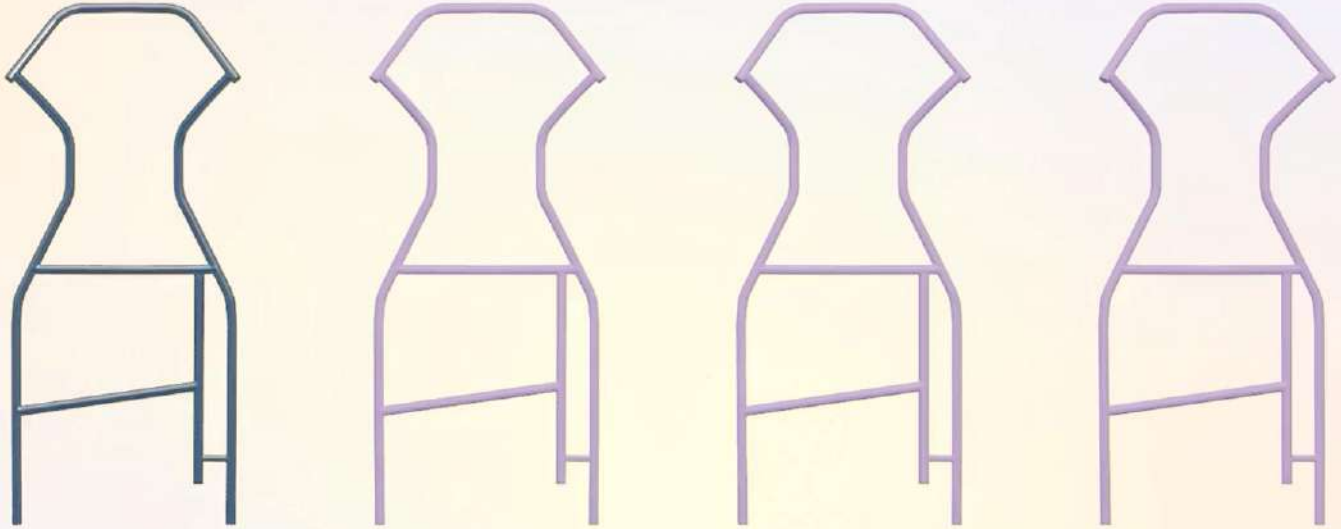
$$\boldsymbol{x} \approx \breve{\boldsymbol{x}} = \boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}\boldsymbol{x} = \boldsymbol{V}\boldsymbol{z}$$

  - *Linear combination* of *reduced basis vectors*

***Principal Component Analysis* (PCA)**

- Applying a truncated SVD

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{W}^{T}$$
$$\boldsymbol{V} = \boldsymbol{U}_{1:r}$$

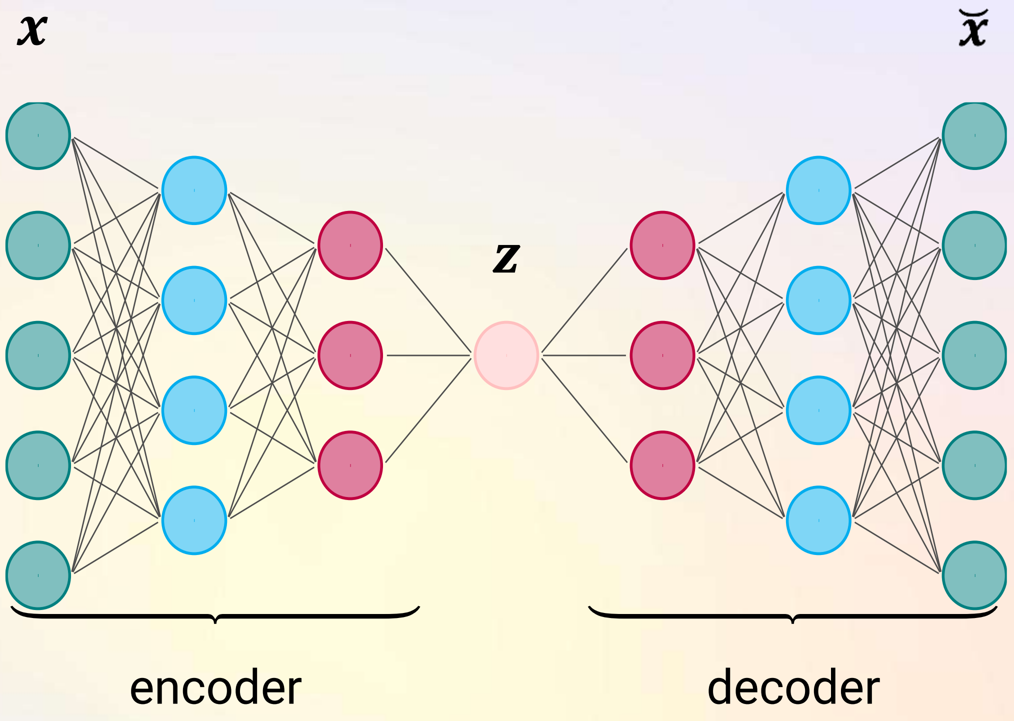


Nonlinear Dimensionality Reduction

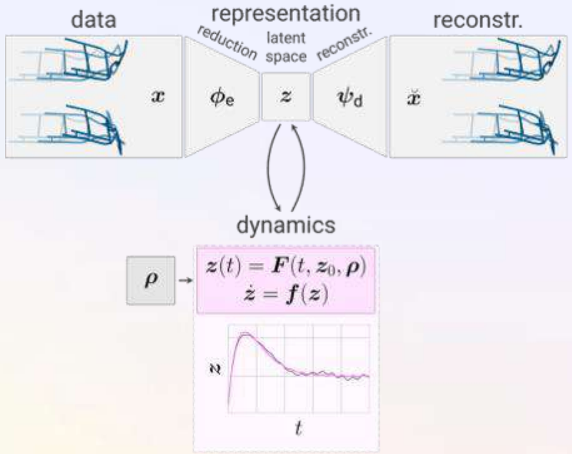
Autoencoder

Neural network with bottleneck architecture

- **Variational autoencoder**
  - Regularize reduced/latent space
- **Convolutional autoencoder**
  - Convolution operations
- **Graph convolutional autoencoder**
  - Convolution operations on irregular non-Euclidean structured data



Compact



Information dense

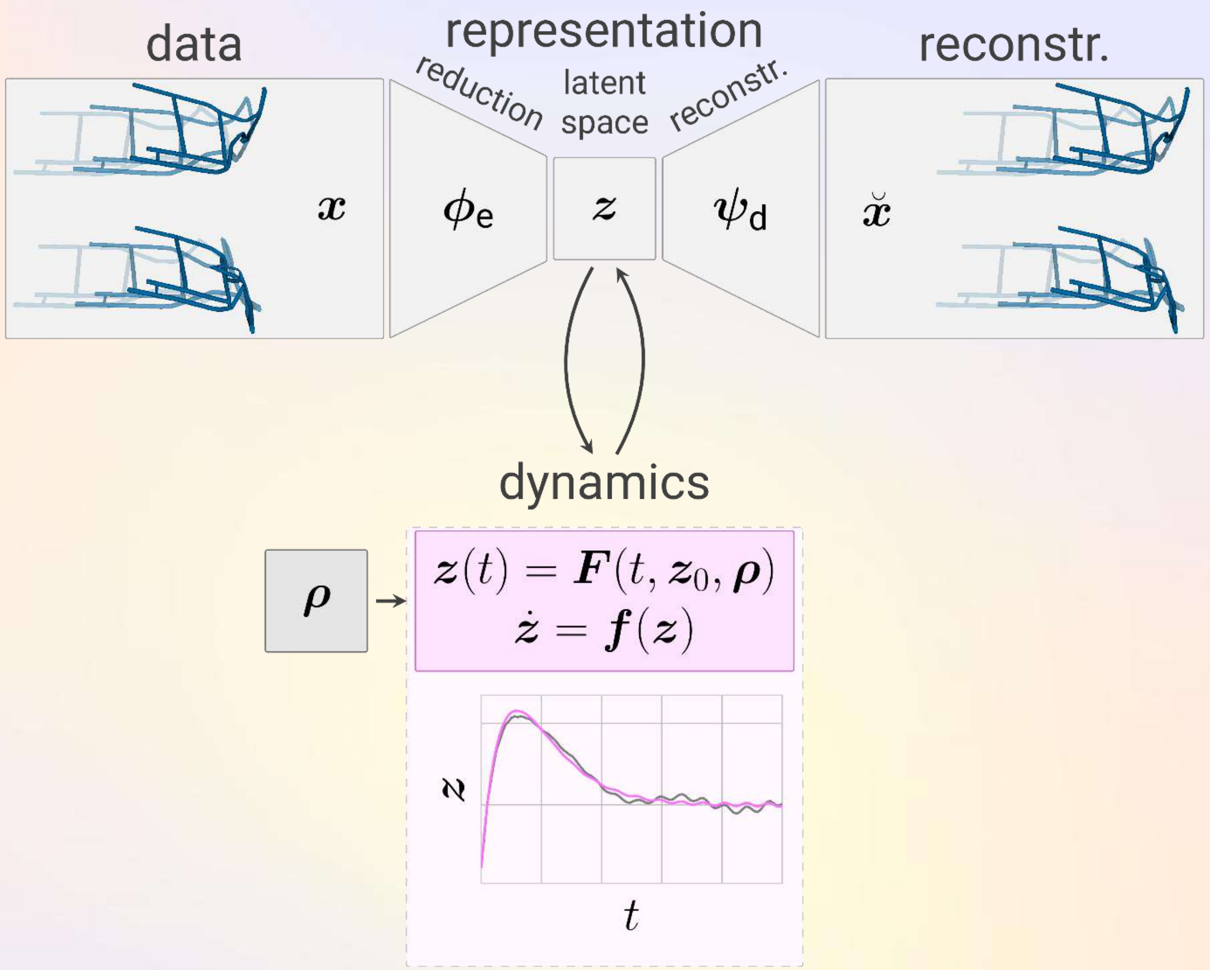
Feature extraction

Simpler Dynamics

Approximate solution $z(t, \boldsymbol{\rho})$ directly

- Map time and parameter to latent state:

$$t, \boldsymbol{\rho} \xrightarrow{\text{regression}} \boldsymbol{z}(t, \boldsymbol{\rho})$$



General Approach

Approximate solution $z(t, \boldsymbol{\rho})$ directly

- Map time and parameter to latent state:

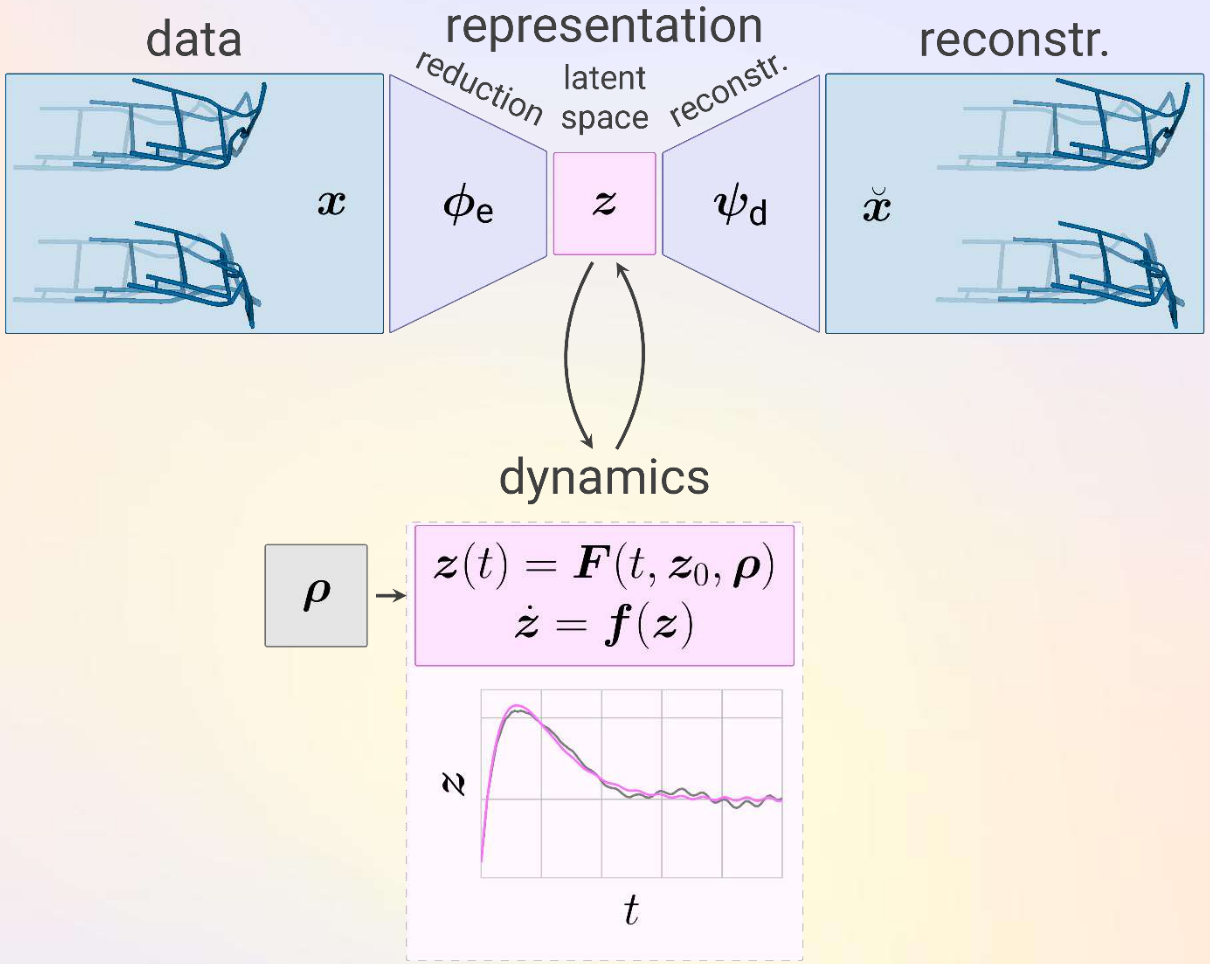
$$t, \boldsymbol{\rho} \xrightarrow{\text{regression}} \boldsymbol{z}(t, \boldsymbol{\rho})$$

Combined Optimization goal

$$\mathcal{L} = \underbrace{\lambda_1 \left| \boldsymbol{x} - \boldsymbol{\psi}_{\boldsymbol{d}}\left(\boldsymbol{\phi}_{\boldsymbol{e}}(\boldsymbol{x})\right) \right|^2}_{\text{reconstruction}}$$
$$+ \underbrace{\lambda_2 \left| \boldsymbol{\phi}_{\boldsymbol{e}}(\boldsymbol{x}) - \mathbf{mlp}(\boldsymbol{\rho}, t) \right|^2}_{\text{latent approximation}}$$

Surrogates

- Representation: PCA / Autoencoder
- Dynamics: Multi-layer Perceptron



Can we do better ?
It would be great if the error is below 2 %.

Finite Element

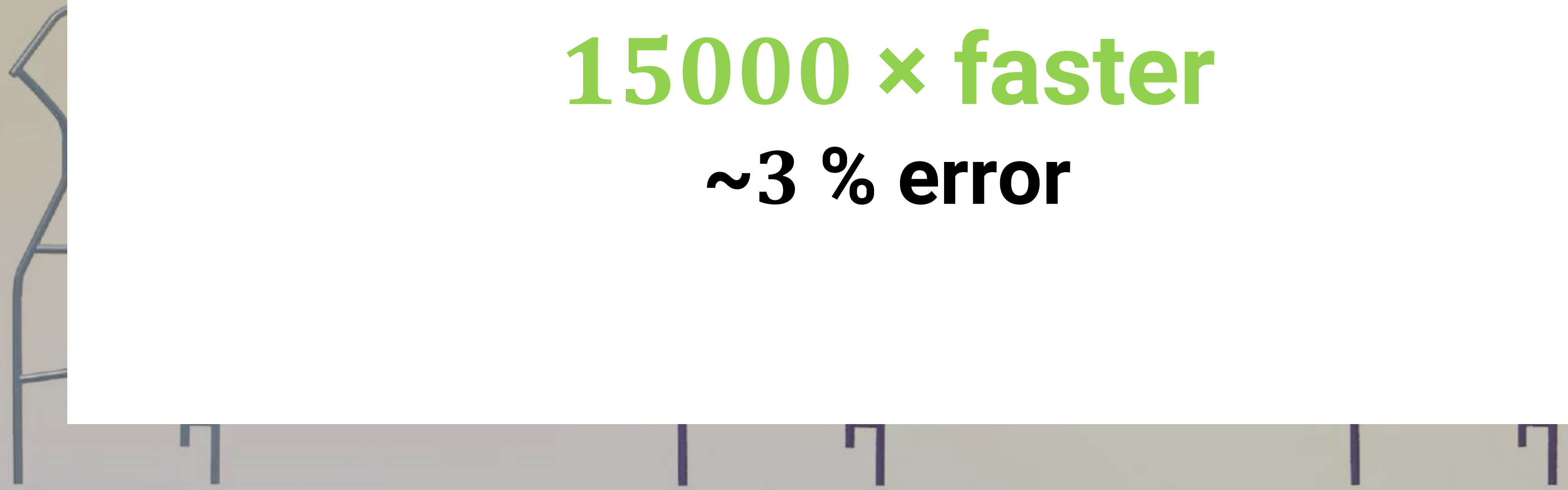
Evaluation: ~15 – 20 min

PCANN

Evaluation: ~75 ms

AENN

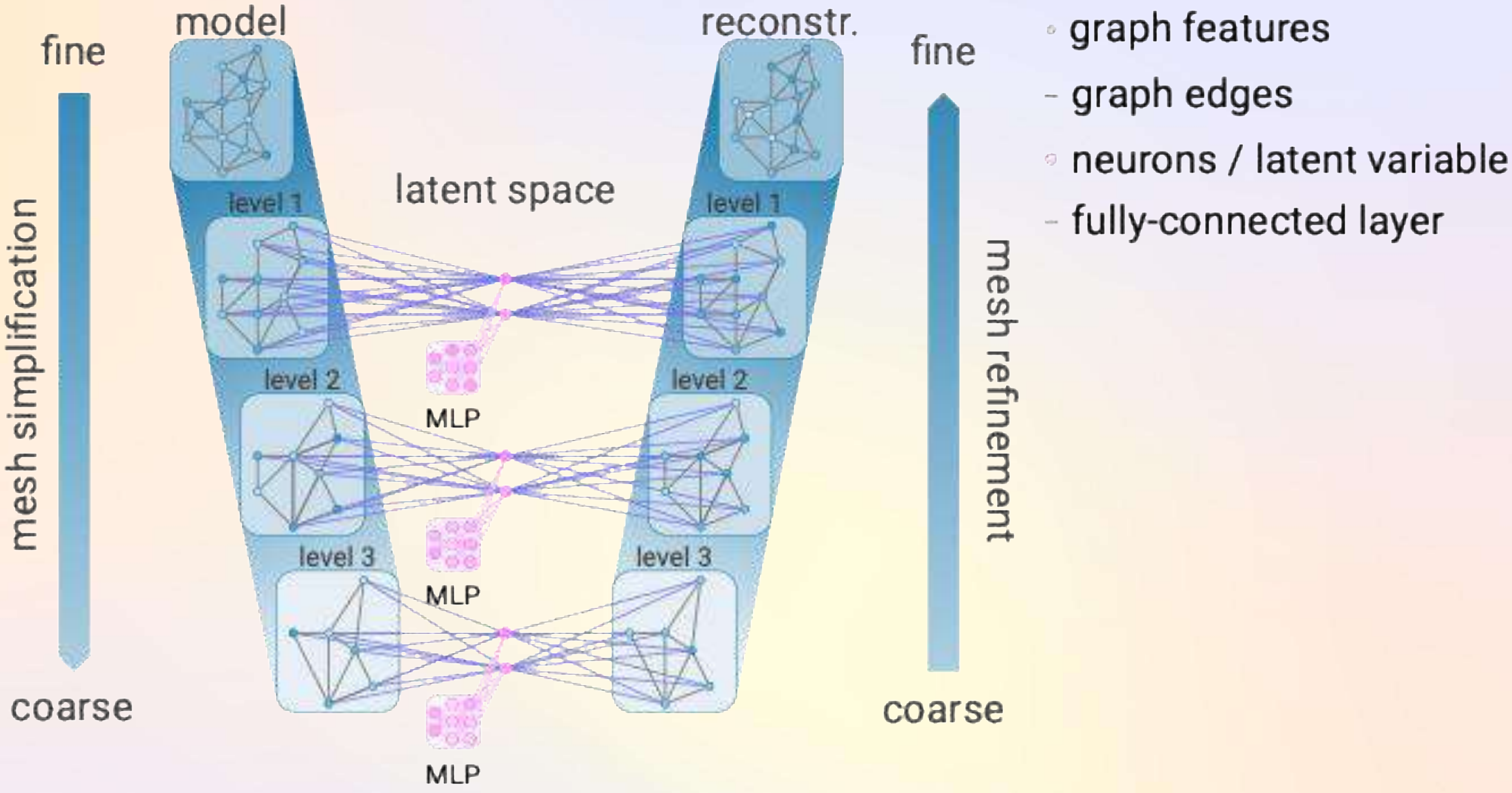
Evaluation: ~78 ms



15000 × faster

~3 % error

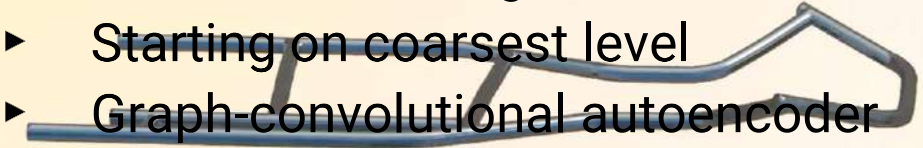
Multi-Hierarchic Surrogate Modeling Scheme [KneiflEtAl24]



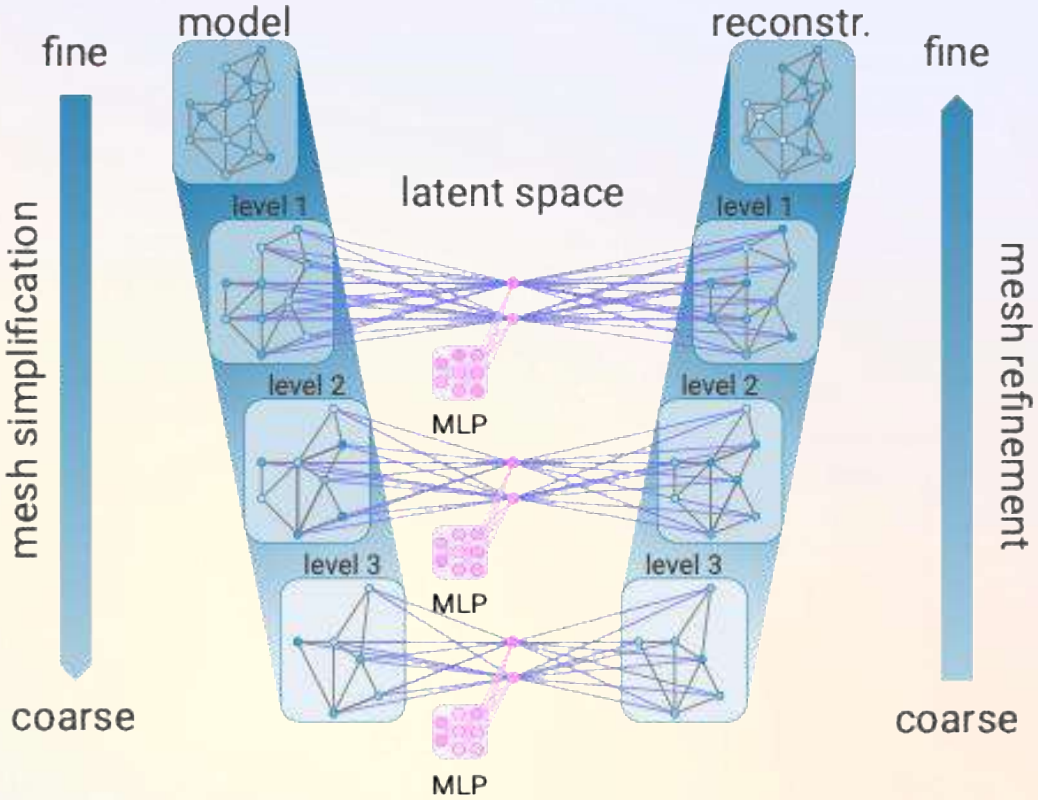
Multi-Hierarchic Surrogate Modeling Scheme

1. Creation of coarser models
   - Down- and upsampling of the graph

2. Generation of surrogate model
   - Starting on coarsest level
   - Graph-convolutional autoencoder based surrogates



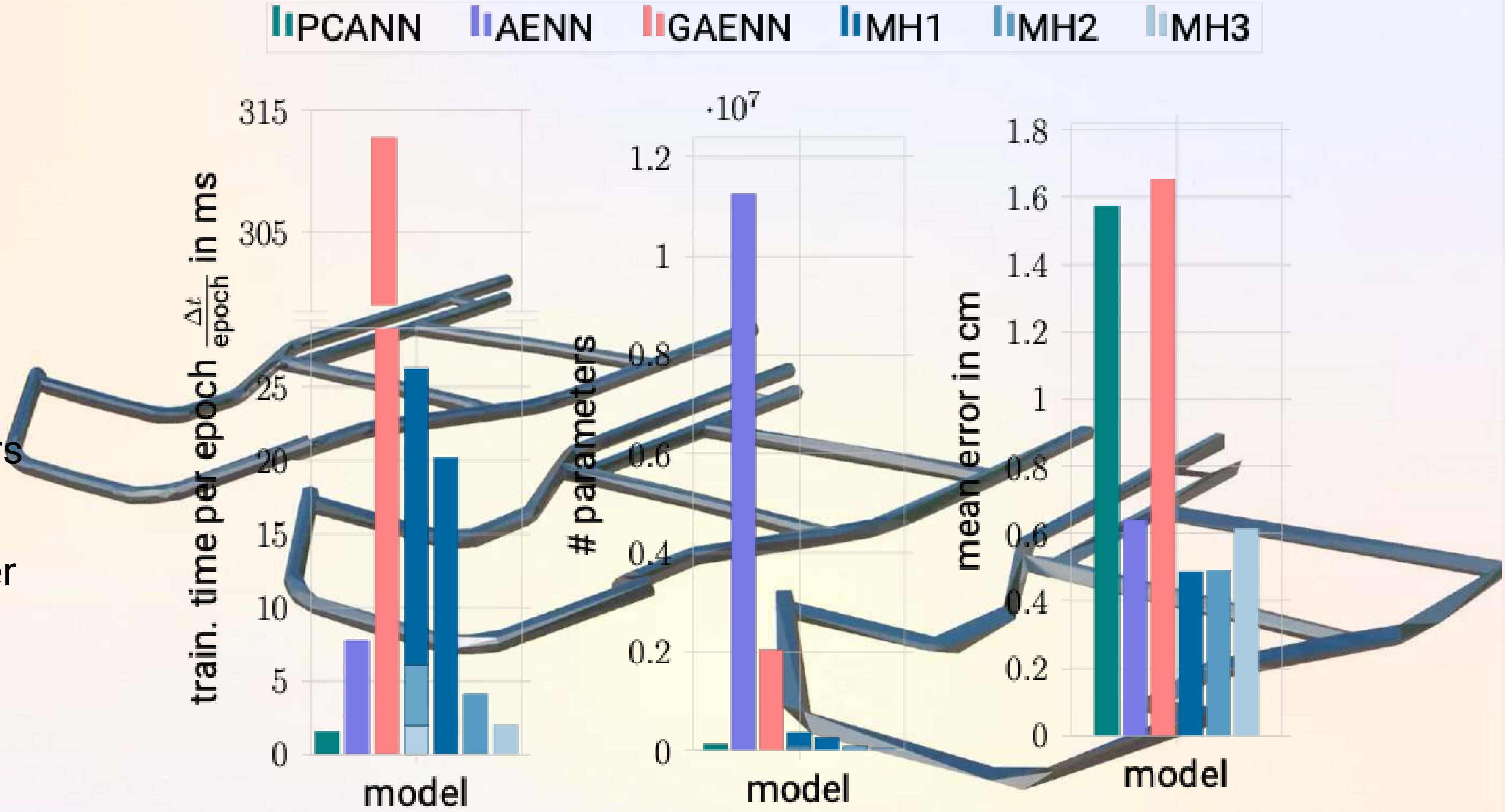
3. Model Refinement
   - Transfer learning



Numerical Results

Multi-hierarchic (MH) Model Properties

- Macroscale features are learned on coarse level
- Training time significantly reduced
- Low amount of parameters
- Approximation Quality
  - Outperforms the other approaches
  - Relative error below 1.5%



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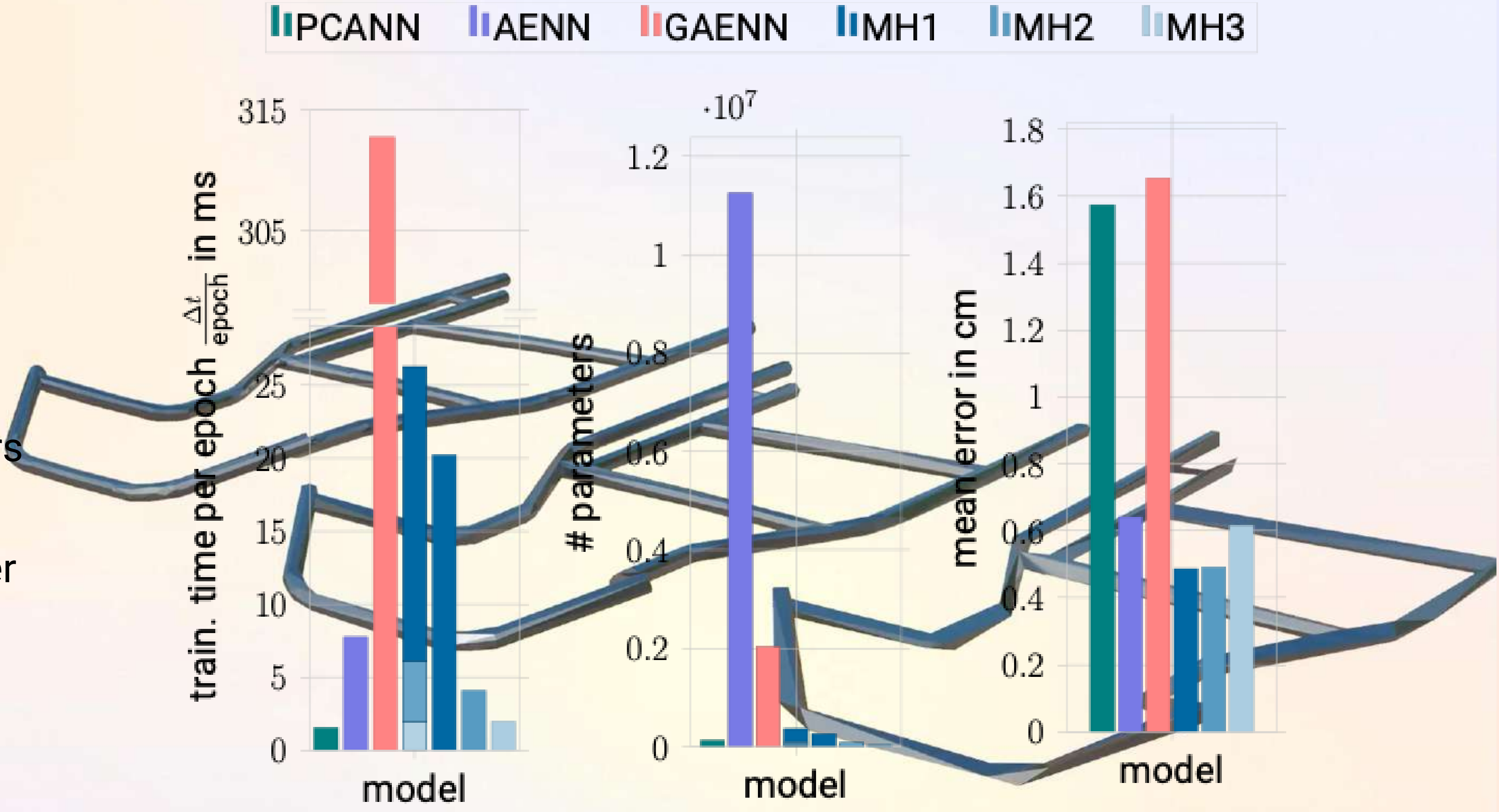


Agenda

- Introduction
  - Why does Simulation Matter
- Dimensionality Reduction of Dynamical Systems
  - Multi-Hierarchic Surrogate
- **Multiphysics Problems**
  - **Interpretable Surrogate for a Disc-Brake Model**

Model Setup

- Fully-coupled linear thermo-mechanical system
- *Stable* and *passive*

Port-Hamiltonian System Description

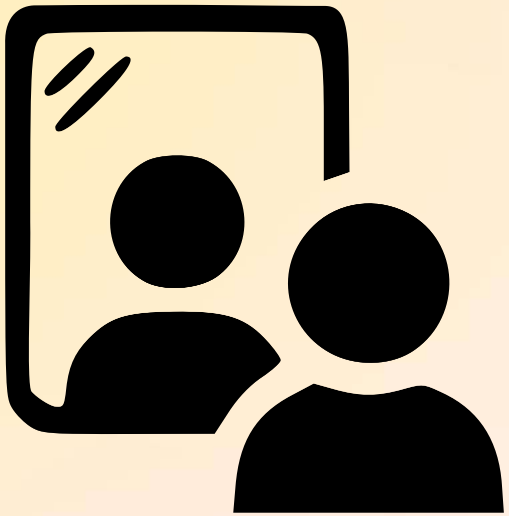
$$\dot{\boldsymbol{x}} = (\boldsymbol{J} - \boldsymbol{R})\mathbf{Q}\mathbf{x} + \boldsymbol{B}\boldsymbol{u}$$
$$\boldsymbol{y} = \boldsymbol{B}^T\mathbf{Q}\mathbf{x}$$

with properties:

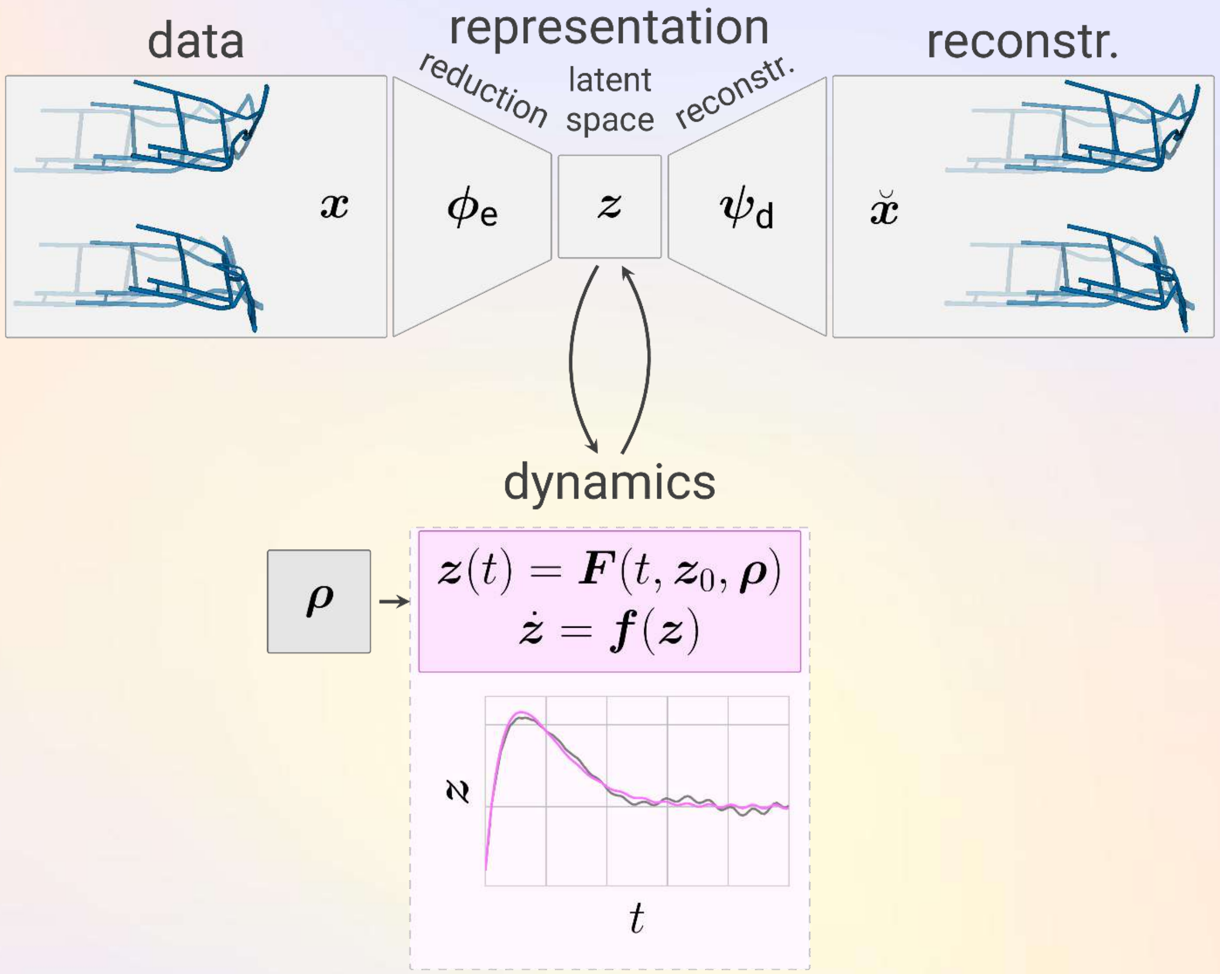
- $\mathbf{Q} = \mathbf{Q}^{\mathrm{T}} > 0$
- $\boldsymbol{J} = -\boldsymbol{J}^T$
- $\boldsymbol{R} = \boldsymbol{R}^T \geq 0$

*Expansion scaled by 500000

Latent Discovery of Dynamical Systems



~~Replicate Behavior~~



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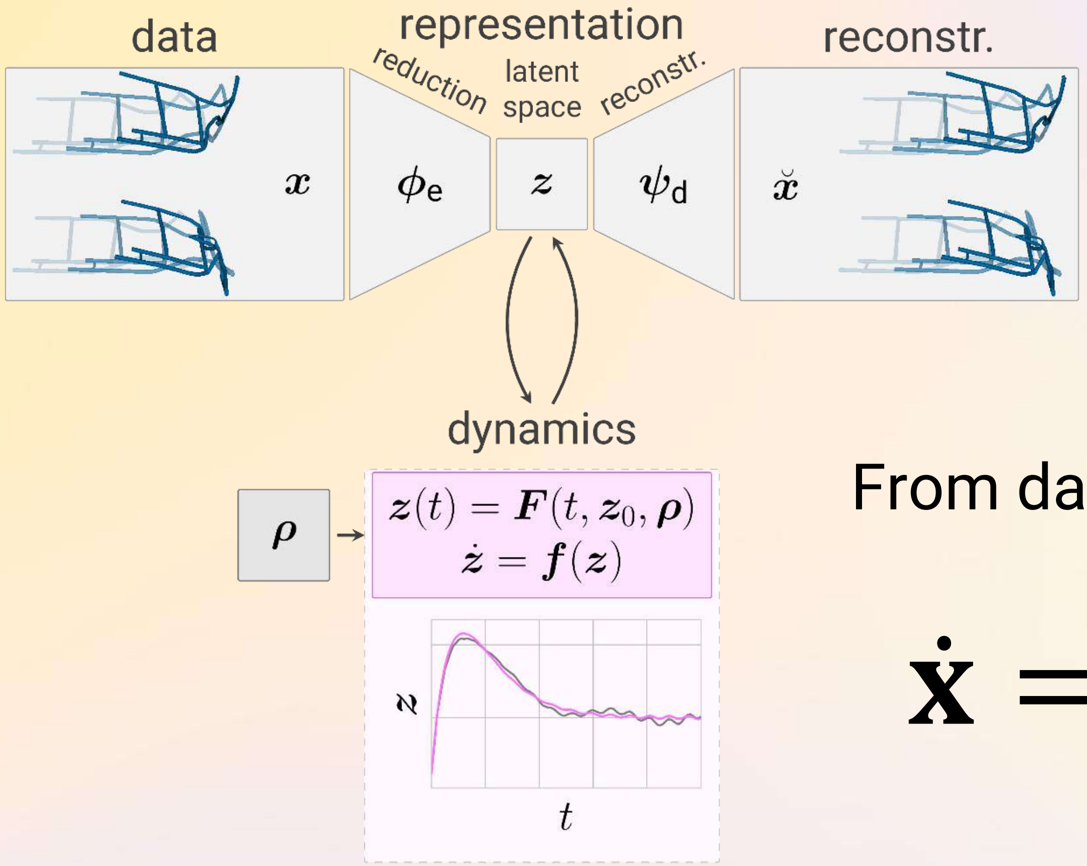
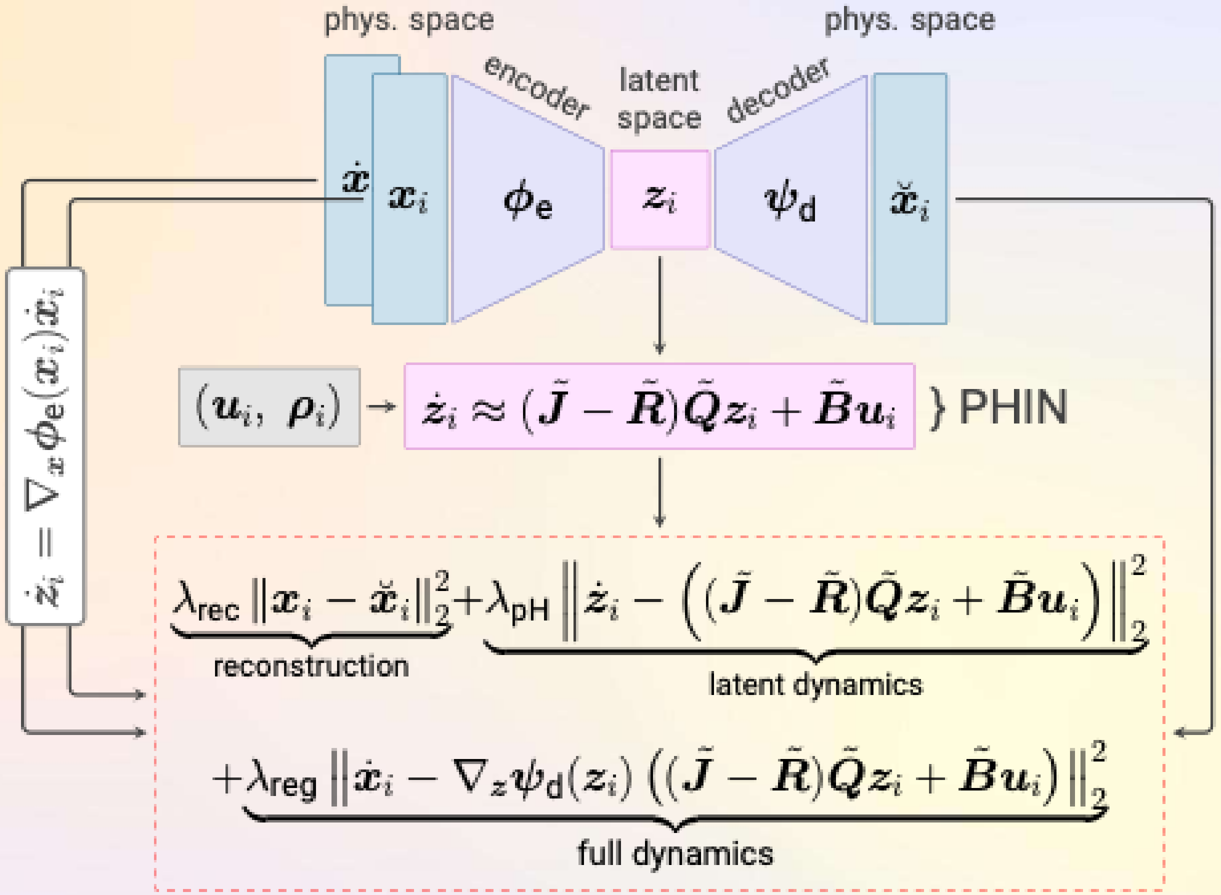


From data $\mathbf{x}$, $\dot{\mathbf{x}}$ find $\mathbf{f}$
s.t.

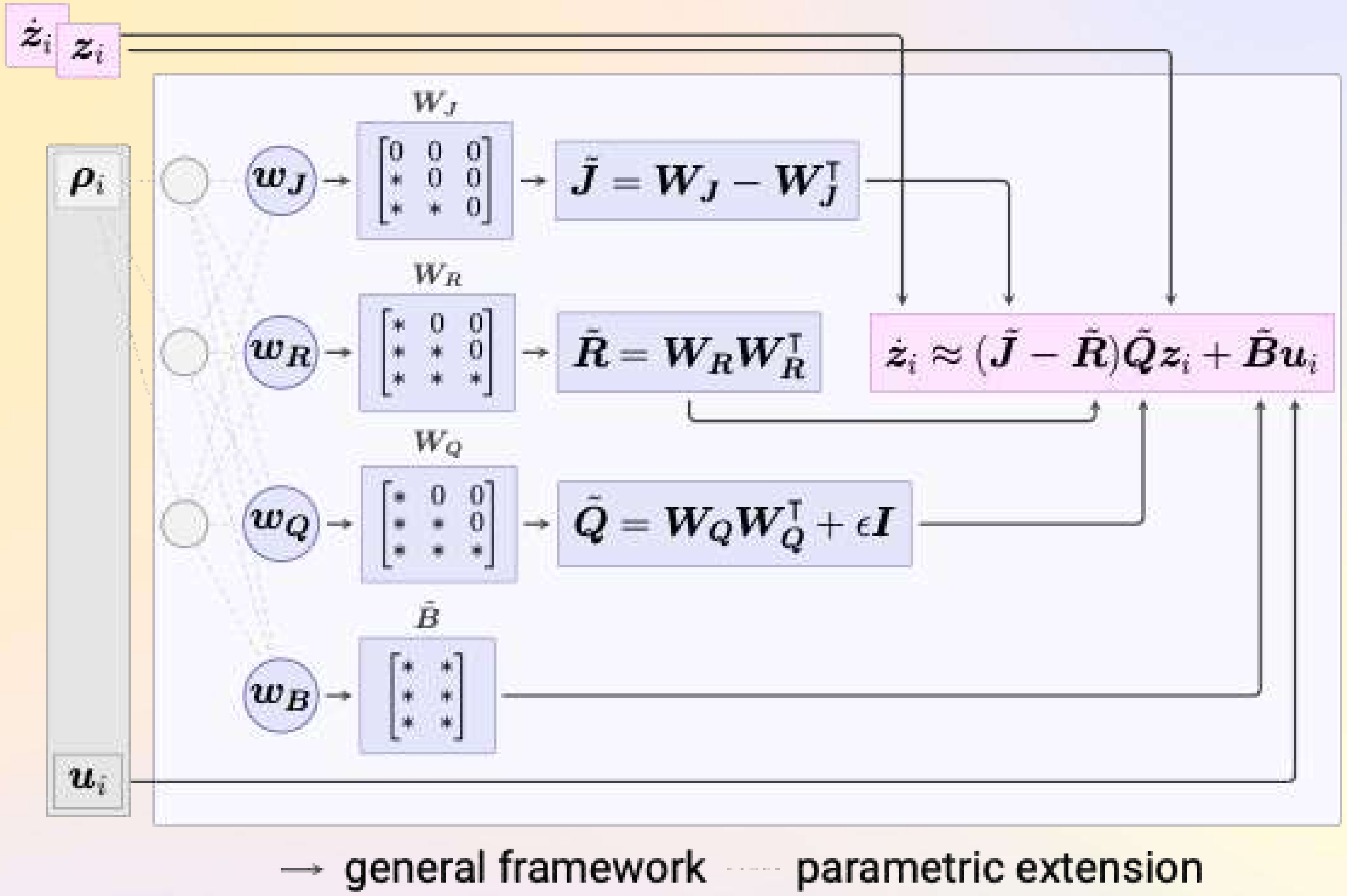
$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$$

Uncover Governing Equations

Structure-preserving Latent Discovery [RettbergEtAl24]



Port-Hamiltonian Identification Layer



Identified pH-system

$$\dot{z} = (J - R)\mathbf{Q}\mathbf{z} + Bu$$

with *guaranteed* properties:

- $\mathbf{Q} = \mathbf{Q}^\mathrm{T} > 0$
- $J = -J^T$
- $R = R^T \geq 0$

Discbrake – Numerical Results

Test case

Predictions for unseen

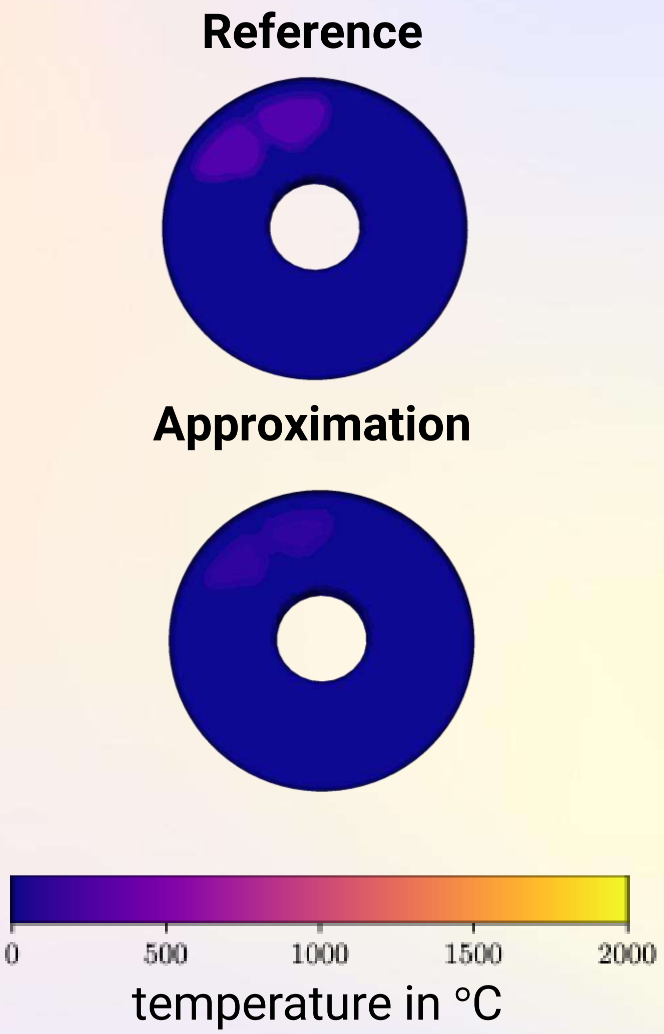
- Material properties
- Heat Flux

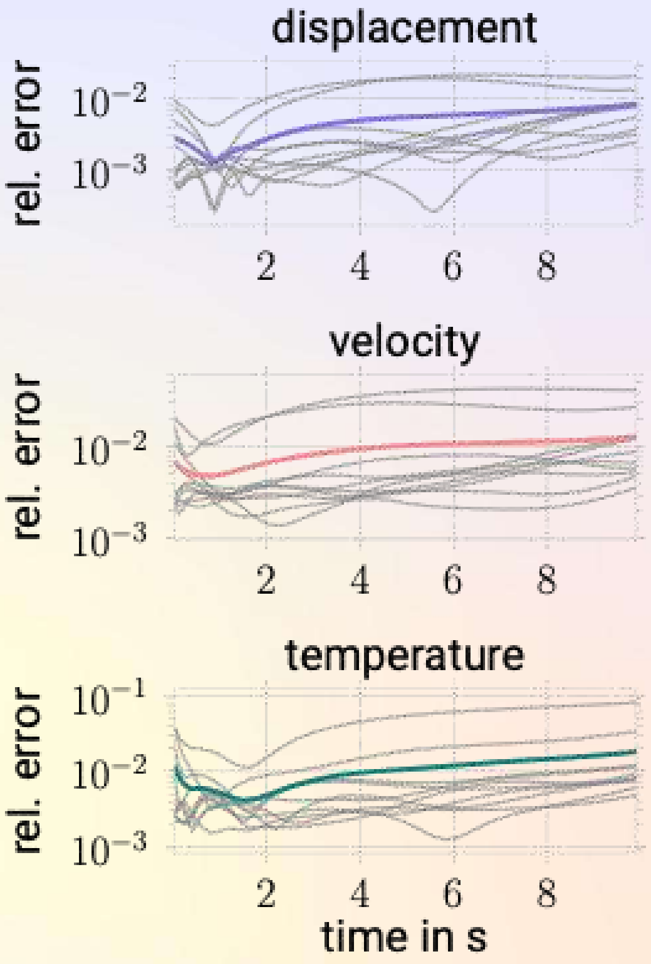
Model Properties

- Real-time capable
- Stable and passive

Approximation Quality

- Mean error stays below
  - 2 % for the temperature
  - 1.5 % for the velocity
  - 1% for the displacement





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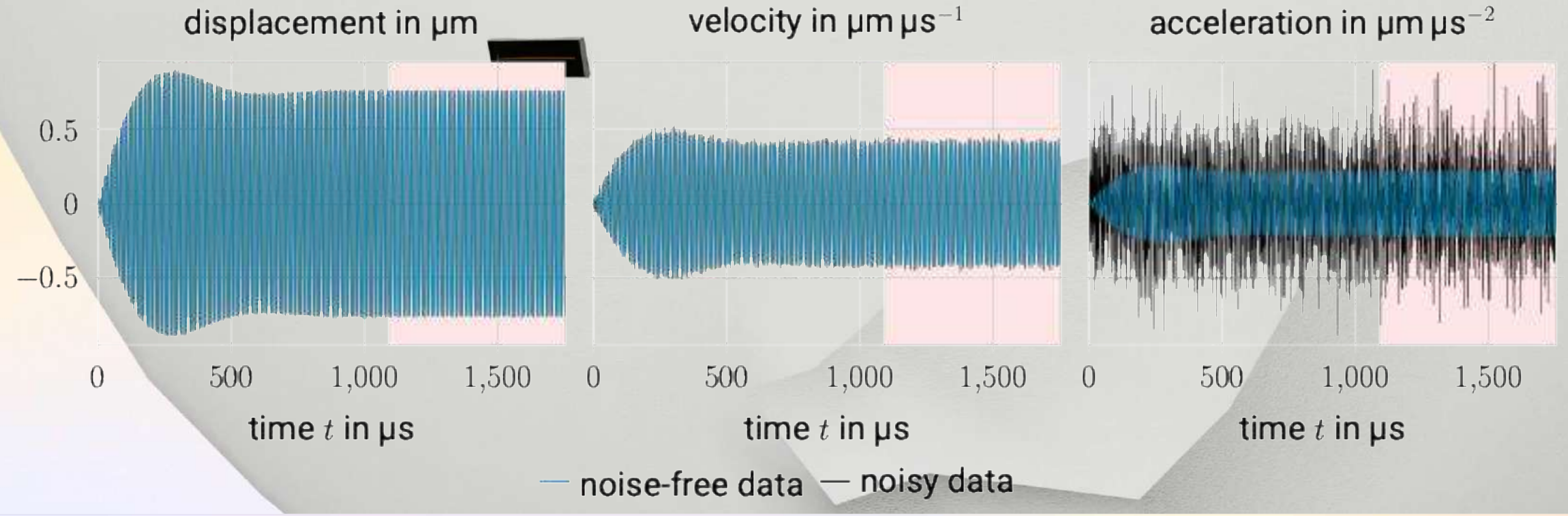
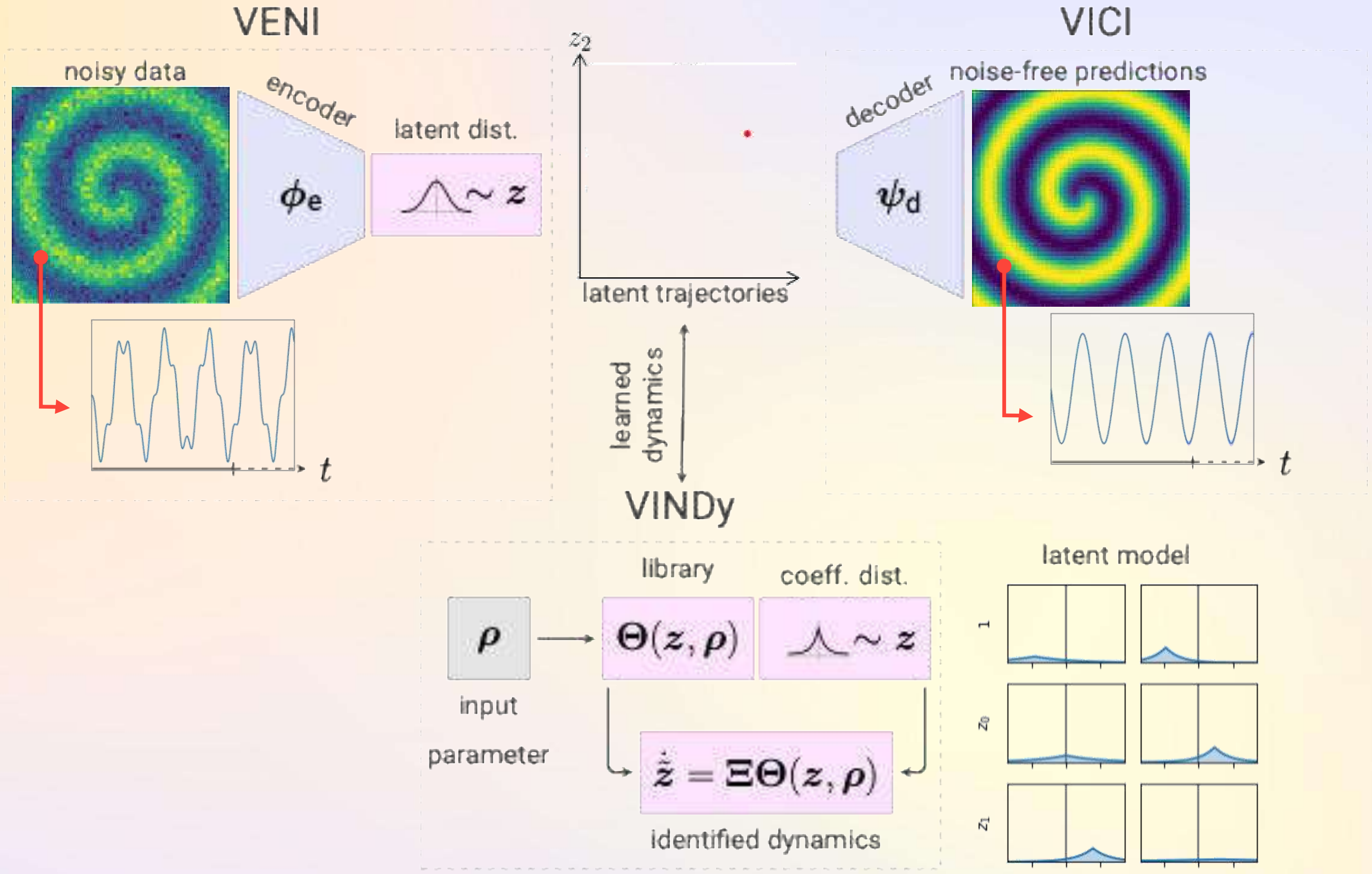
- Multiphysics Problems
  - Interpretable Surrogate for a Disc-Brake Model
  - Structure-preserving Latent Discovery
- **Uncertainty and Noise Data**
  - **MEMS Resonator (Beam) i.e. Sensor for an Airbag**
  - **VENI, VINDY, VICI**

MEMS Resonator (Beam)



VENI, VINDy, VICI [ContiEtAl24]

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JONAS KNEIFL

Offline Training: VENI

VENI

Variational **E**ncoding of **N**oisy **I**nputs

- **Probabilistic Autoencoder**: Learns a distribution over the latent space instead of fixed codes
- **Encoder**: Maps input to parameters of a latent distribution (mean & variance)
- **Latent Space**: Encodes uncertainty via sampling $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\mu}, \mathrm{diag}(\boldsymbol{\sigma}^2))$
- **Decoder**: Reconstructs data from sampled latent vectors

Offline Training: VINDy

VENI

Variational **E**ncoding of **N**oisy **I**nputs

VINDy

Variational **I**dentification of **N**onlinear **Dy**namics

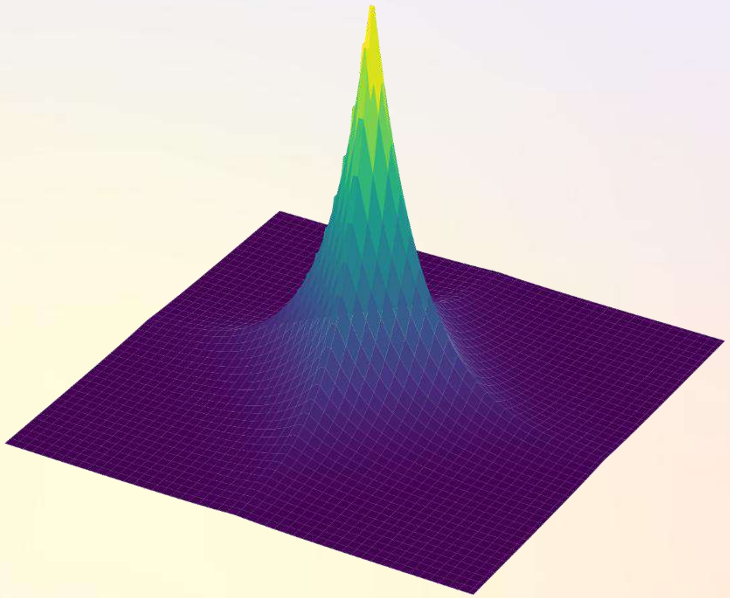
From data $\mathbf{z}, \dot{\boldsymbol{z}}$ find $\boldsymbol{f}$ s. t.

$$\dot{\boldsymbol{z}} = \boldsymbol{f}(\mathbf{z}) \approx \boldsymbol{\Xi}\boldsymbol{\Theta}(\boldsymbol{z})$$

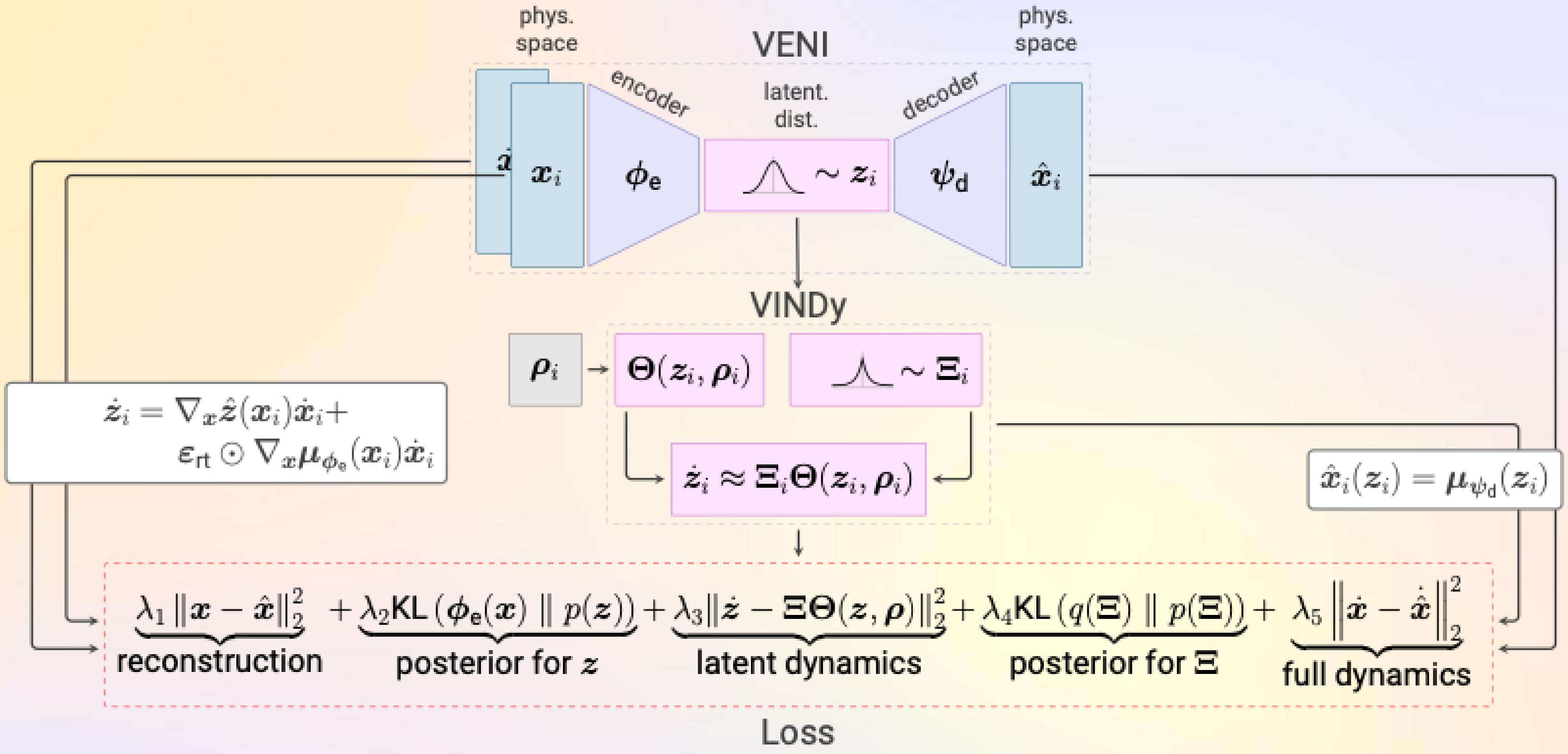
- Set of candidate features $\boldsymbol{\Theta}(\mathbf{z}) = [\mathbf{1}, \mathbf{z}, \mathbf{z}^2, \dots]^{\mathrm{T}}$
- Unknown coefficients $\boldsymbol{\Xi}$

Obtain a **probabilistic model** with $\boldsymbol{\Xi} \sim \mathcal{L}(\boldsymbol{w}_\mu, \boldsymbol{w}_\delta)$

$$\dot{\boldsymbol{z}} = \boldsymbol{f}(\boldsymbol{z}) = \xi_0 + \xi_1 z + \cdots + \xi_m z^m + \cdots = \boldsymbol{\theta}(z)\boldsymbol{\Xi}$$



Offline Training: VENI, VINDy



Inference: VICI

VENI

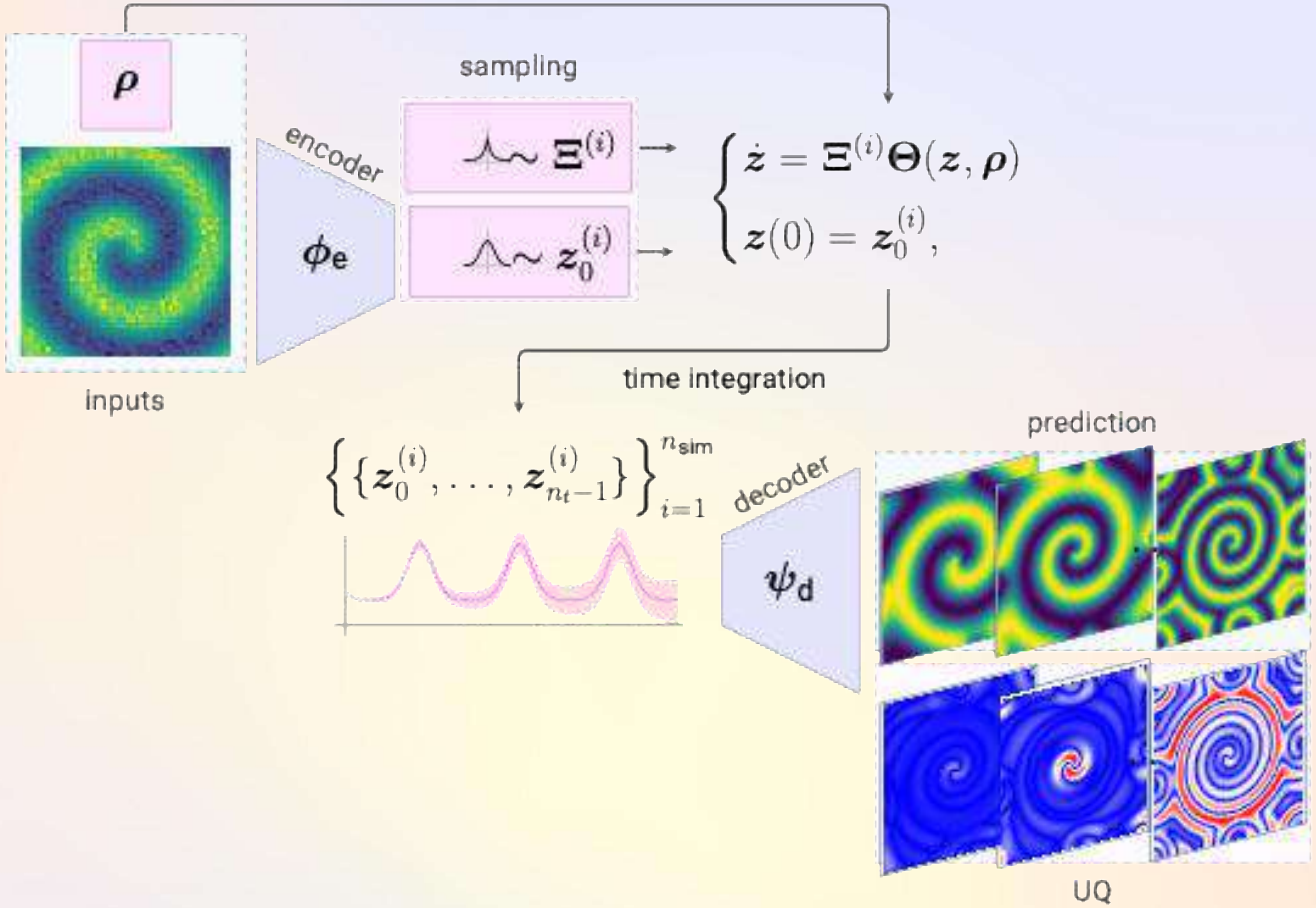
Variational Encoding of Noisy Inputs

VINDy

Variational Identification of Nonlinear Dynamics

VICI

Variational Inference with Certainty Intervals



MEMS Resonator (Beam) – Numerical Results

Scenario

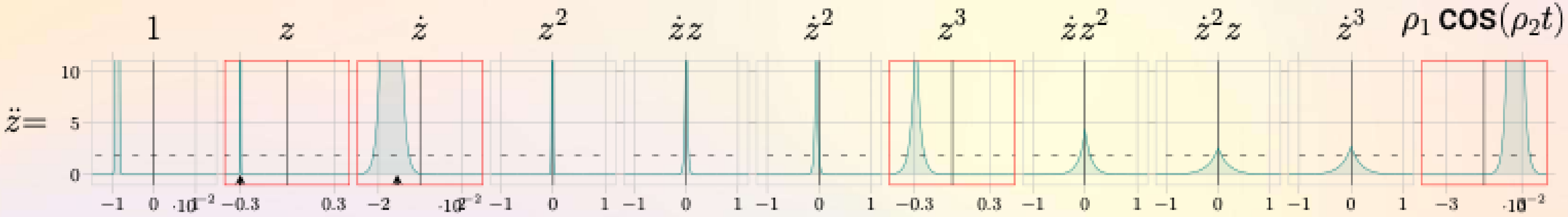
- Noisy data
- Identify physical-consistent model

Comparison

- Analytic equation in normal form

$$\ddot{z} = -\omega_0^2 z - 2\xi\omega_0\dot{z} - \gamma z^3 - \alpha F\cos(\omega t)$$

Identified model terms and coefficients



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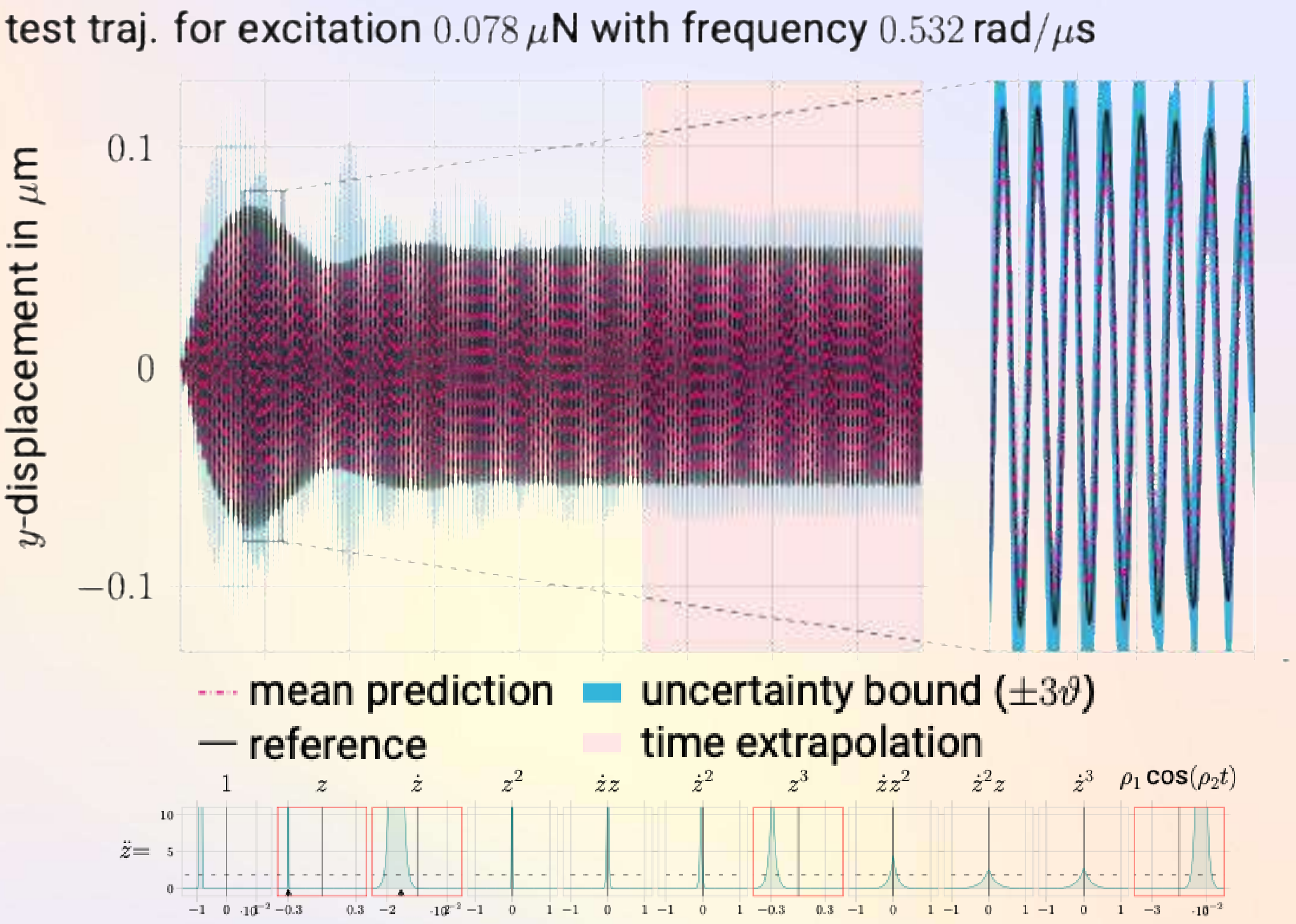
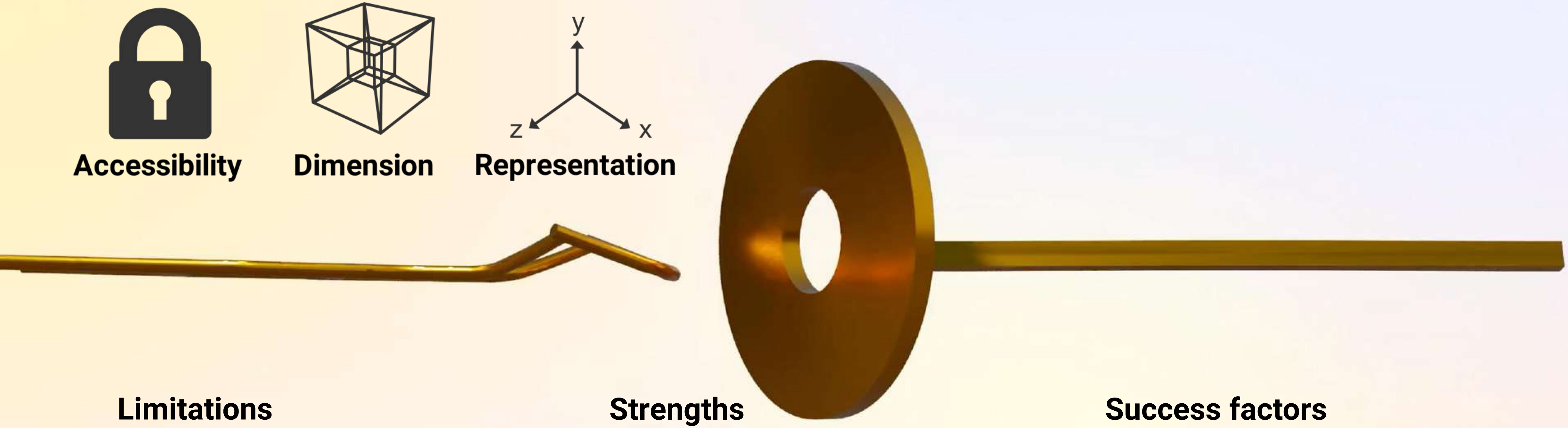
$$\ddot{z} = -\omega_0^2 z - 2\xi\omega_0\dot{z} \\ -\gamma z^3 - \alpha F\cos(\omega t)$$

- Time extrapolation



Conclusion Data-driven Surrogate Modeling



Limitations

- Expensive offline phase
- Hyperparameter tuning
- Scope of validity
- Extrapolation

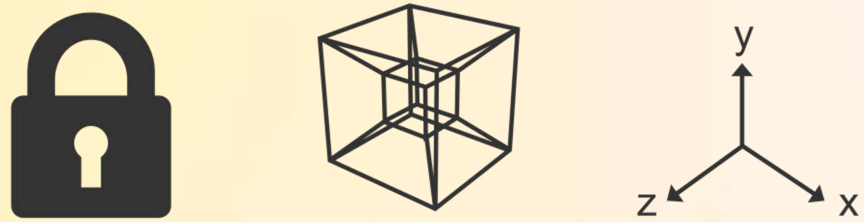
Strengths

- Non-intrusive
- Nonlinearity
- Efficient

Success factors

- Latent embedding
- Latent dynamics
  - Approximation
  - Identification

Conclusion Data-driven Surrogate Modeling



Accessibility **Dimension** **Representation**

Multi-X **Physicality** **Data Quality**

Multi-hierarchic approach

- Black-box: ease of implementation + comp. speed
- Capture macro- and microscale features

PH approach

- Multi-domain
- Structure-preservation

VENI, VINDy, VICI

- Physically consistent
- Uncertainty quantification

Thank You!

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https://www.itm.uni-stuttgart.de/en/institute/team/Fehr/

SimTech
Cluster of Excellence

Literature

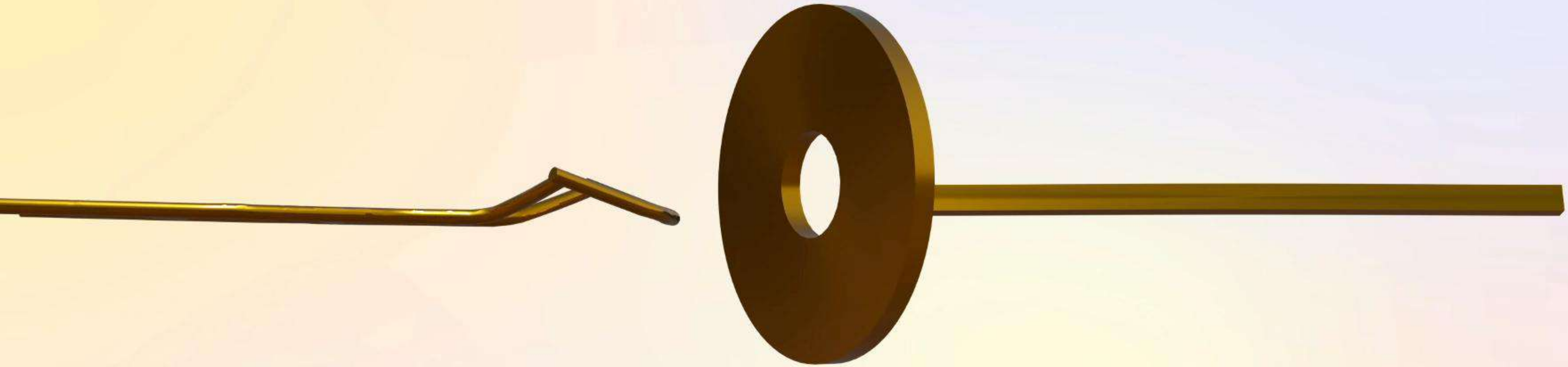
[KneiflEtAl24] Kneifl, J.; Fehr, J.; Brunton, S.L.; Kutz, J.N.: Multi-hierarchical Surrogate Learning for Explicit Structural Dynamical Systems using Graph Convolutional Neural Networks. Computational Mechanics, Bd. 75, Nr. 3, S. 1115–1135, 2024. http://dx.doi.org/10.1007/s00466-024-02553-6

[RettbergEtAl24] Rettberg, J.; Kneifl, J.; Herb, J.; Buchfink, P.; Fehr, J.; Haasdonk, B.: Data-driven identification of latent port-Hamiltonian systems., 2024. https://doi.org/10.48550/arXiv.2408.08185

[ContiEtAl24] Conti, P.; Kneifl, J.; Manzoni, A.; Frangi, A.; Fehr, J.; Brunton, S.L.; Kutz, J.N.: VENI, VINDy, VICI: a Variational Reduced-order Modeling Framework with Uncertainty Quantification, 2024. https://arxiv.org/abs/2405.20905https://arxiv.org/abs/2405.20905

Conclusion Data-driven Surrogate Modeling

Multi-scale Hierarchy | **Structure-preservation** | **Uncertainty Quantification**



Friedrich Merz (Chancellor)
Thanks! XOXO

Thanks! 😘