Physics-Informed Machine Learning

-in a nutshell-

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About me …

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Founder @tensorDynamic GmbH

tensor Dynamic

Data analytics for physical systems.

Turning dark data into value.

www.tensordynamic.com

Feel free to get in contact!

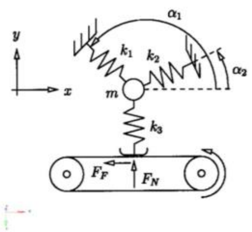
Our mission

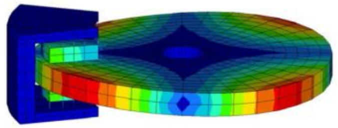
Physics

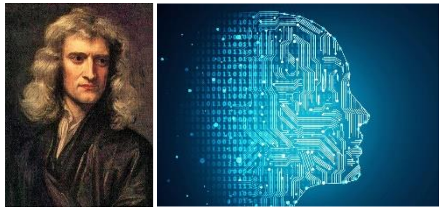
- Waves and vibrations
- Analytical modeling
- Numerical simulations

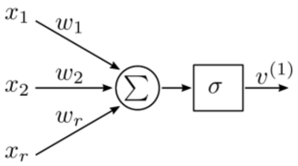
Data Science

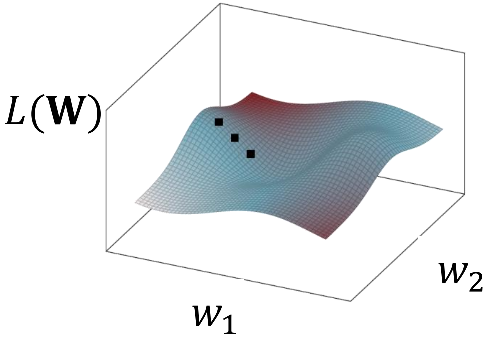
- Data management and analytics
- Machine Learning, Deep Learning
- Explainable Artificial Intelligence







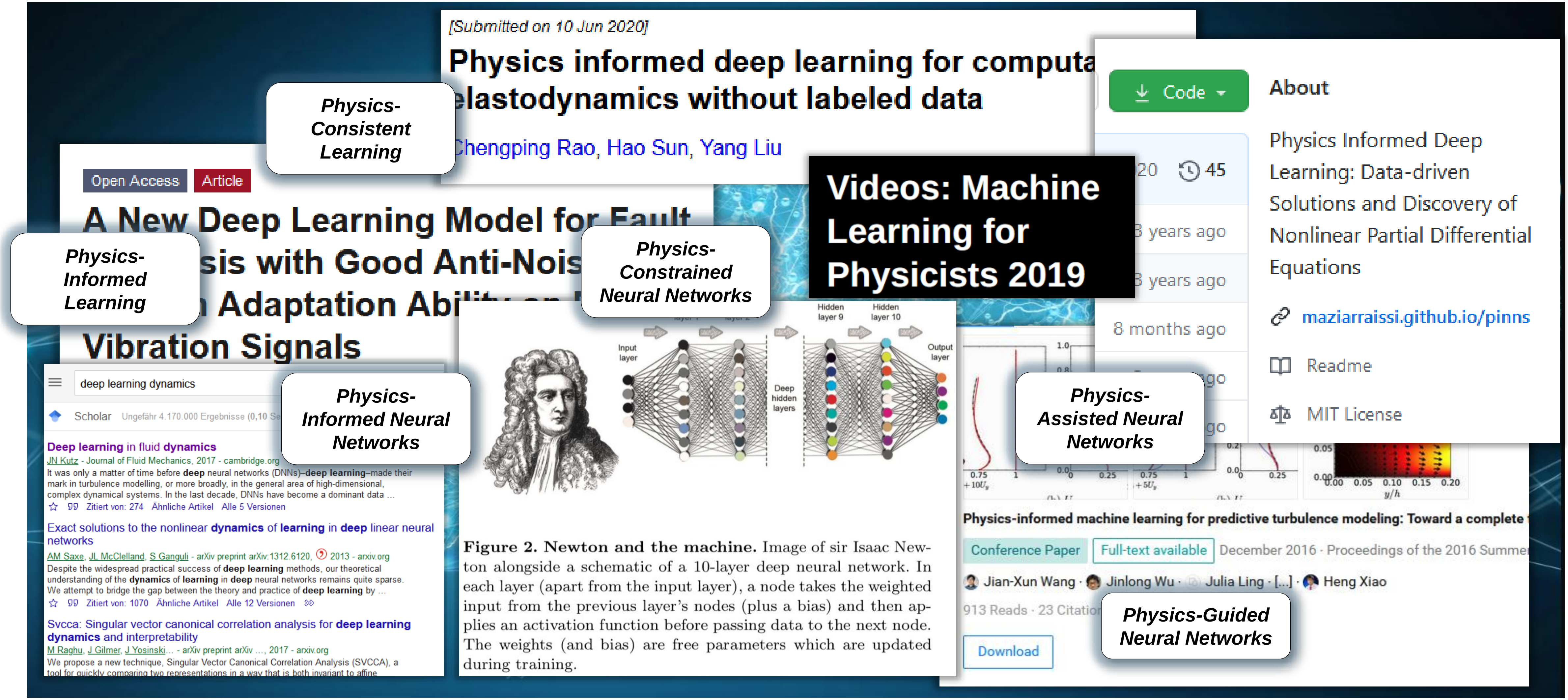




Physics-Informed Machine Learning

Digital Twins

Today: more than buzz-words …



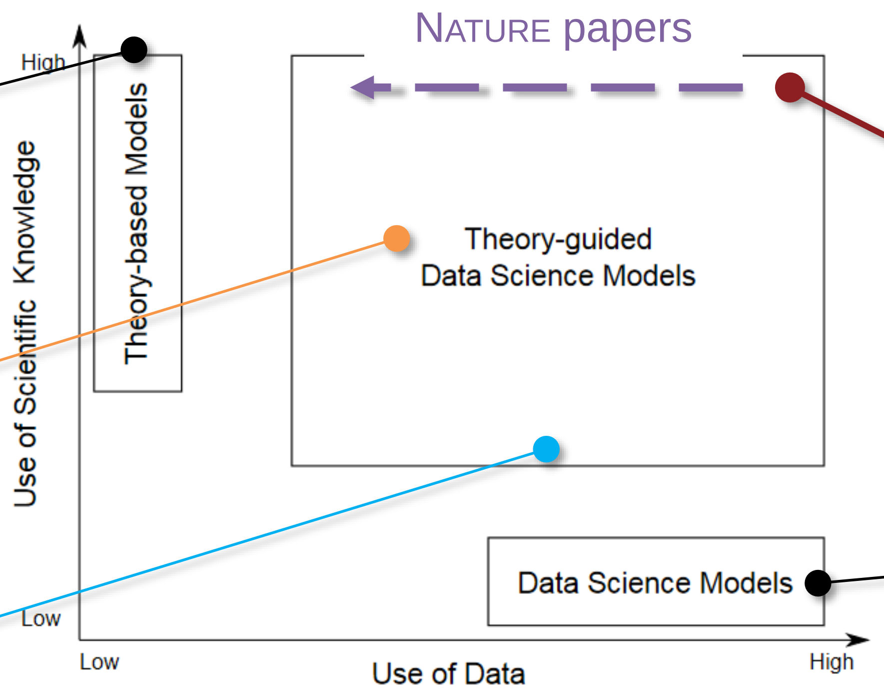
Data and Scientific Knowlege: the big picture

How to achieve **knowledge conservation *and* data-driven discovery**?

$$\ddot{x} \cdot m = \sum F$$

- Conservation laws,
- First principles
- Engineering mathematics,
- Numerical simulations

„we know the relation, let‘s see if ML can figure it out“



Holy grail

„let‘s try this ML API“

```
import tensorflow
model.add()
```

- Brute force data mining
- Lack of models and equations

Karpatne et al. (NIPS 2017): How Can Physics Inform Deep Learning Methods in Scientific Problems?

Challenges in physical data
(opposed to www data streams)

1. **Availability** & cost of acquisition

2. **Sparsity**
   a) Time
   b) Space
   c) Hidden variables

3. **Labels**

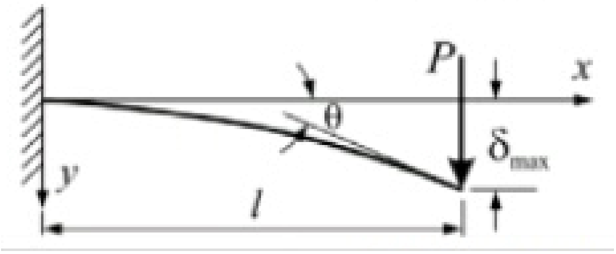
4. **Non-stationarity**

First principles vs. universal function approximators

- Foundation of (deep) neural networks: ***Universal function approximation theorem*** Cybenko, G. (1989)

“Given a sufficiently complex architecture, a neural network with sigmoid activations can approximate any function”
(a non-mathematical summary)

- **Learning the bending beam problem** $f_\theta(P) = \hat{\delta}$
  - Provide many load-deflection pairs $[P, \delta]$
  - Train a NN $f_\theta(P) = \hat{\delta}$ optimizing weights θ
  - Be happy if $|\hat{\delta} - \delta| < \mathrm{tol}$ ☺



- **But …**
  - *How to ensure generalization for out-of-sample predictions?*
  - *How to make predictions for a beam of different material / length / cross-section?*

$$\boldsymbol{y = \frac{px^2}{6EI}(3l - x)}$$

How to constrain universal function approximators to learn solely physically correct relations?

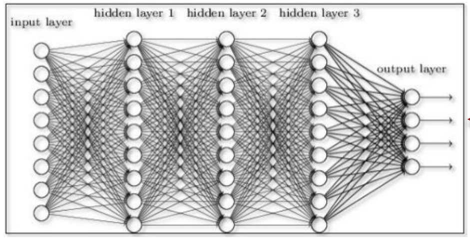
Physics-Informed Machine Learning

- Complex pattern recognition
- Highly nonlinear relationships
- High dimensionality
- Generality, adaptivity

- Mass/energy/… conservation
- Determinism, continuity
- Structure, symmetries
- Underlying principles

Models featuring millions of parameters for learning some correlations

(mostly) Simplistic equations explaining highly complex processes



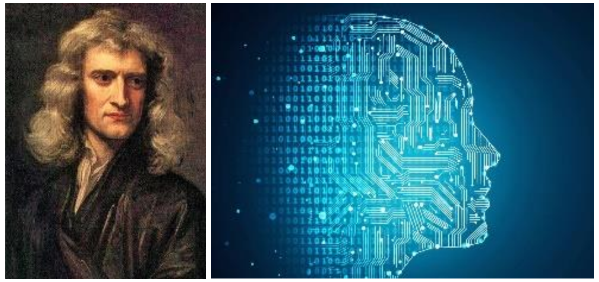
?

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\nabla)\,\vec{v}\right) = -\nabla p + \mu\Delta\vec{v} + \vec{f}$$

How can we even dream about finding physics-constrained models?

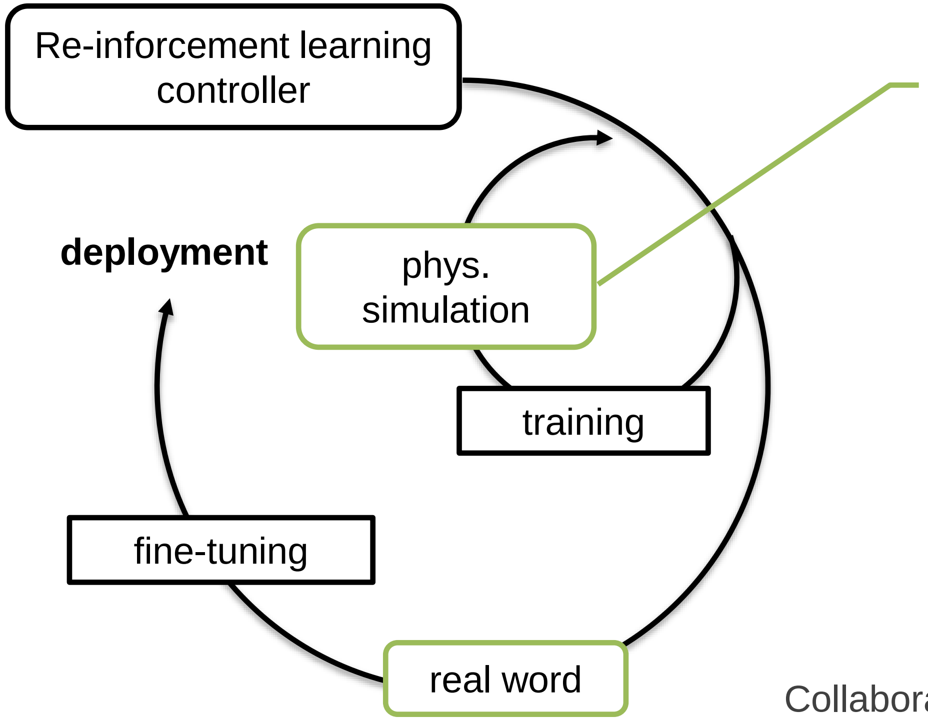
Some ideas to encode physics into NNs

- **Light** (*Physics-assisted learning, physics-guided NNs*)
  - Training data from well-controlled physical process / numerical simulation with minimal noise corruption
  - Discrepancy models
- **Medium** (*Physics-informed learning*)
  - Physical NN regularizers
- **Deep** (*Physics-constrained learning*)
  - Physics-conform activation functions?
  - Completely new neural architectures / models?
  - ???

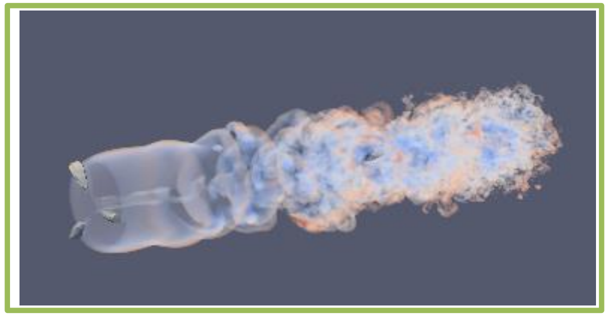


Physics-guided learning

- **Training data from simulations**
  - Pre-training using handcrafted data (many)
  - Transfer learning / fine tuning on real/experimental data (few!)



High-fidelity simulations (Lattice-Boltzmann)

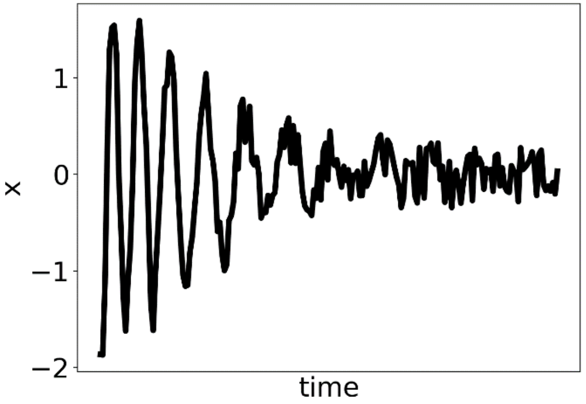


Collaboration with Uppsala Universitet
Wind Energy Group (Stefan Ivanell)
Henrik Asmuth, Henry Korb

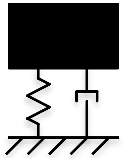
UPPSALA UNIVERSITET

Physics-assisted learning: Discrepancy models

https://github.com/TUHH-DYN/DigitalTwin_Tutorial



$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{t})$

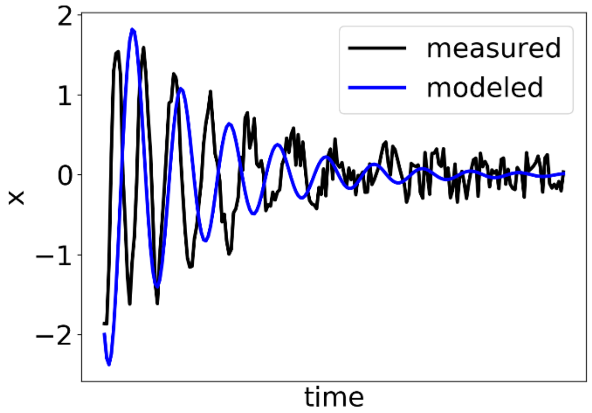


Fourier transf. → $\omega_n = 3$
Hilbert transf. → $\delta = 0.25$

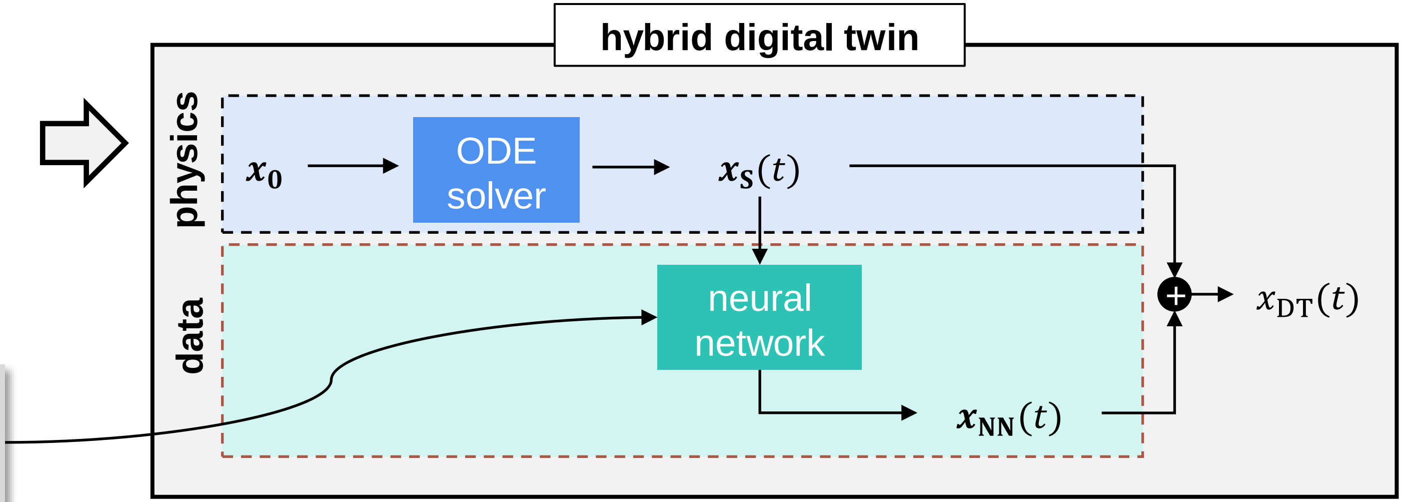
$\ddot{\boldsymbol{x}} + \mathbf{2}\boldsymbol{\delta}\dot{\boldsymbol{x}} + \boldsymbol{\omega}_n^2\boldsymbol{x} = \mathbf{0}$

time integration

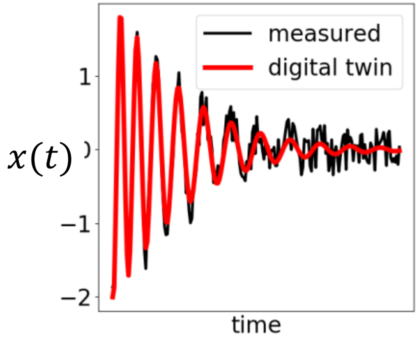
$\boldsymbol{x}(t) = f(\boldsymbol{x}_0)$



Initial value $\mathbf{x_0}$



- Uncertainty
- Modeling errors
- …



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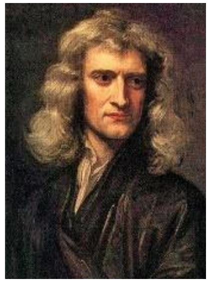


Physics-informed learning (1)

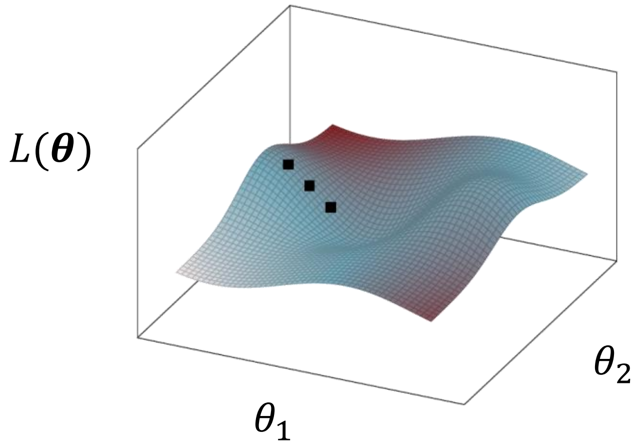
Conventional formulation of the loss function:

$L(\theta, x, \hat{y}) = \|\hat{y} - y\|$ (some norm) → MAE, MSE, …

- **Soft regularization**:
  - Loss function $L(\theta, x, \hat{y})$ formulated with respect to physical quantities derived from predictions $\hat{y}$ and ground truth y
  - e.g. emphasizing spectral properties $L(\theta, x, \hat{y}) = |\mathrm{FFT}(\hat{y}) - \mathrm{FFT}(y)|$
  - Can be tricky! Non-convex / non-smooth loss functionals, … !

<u>Overall goal:</u>

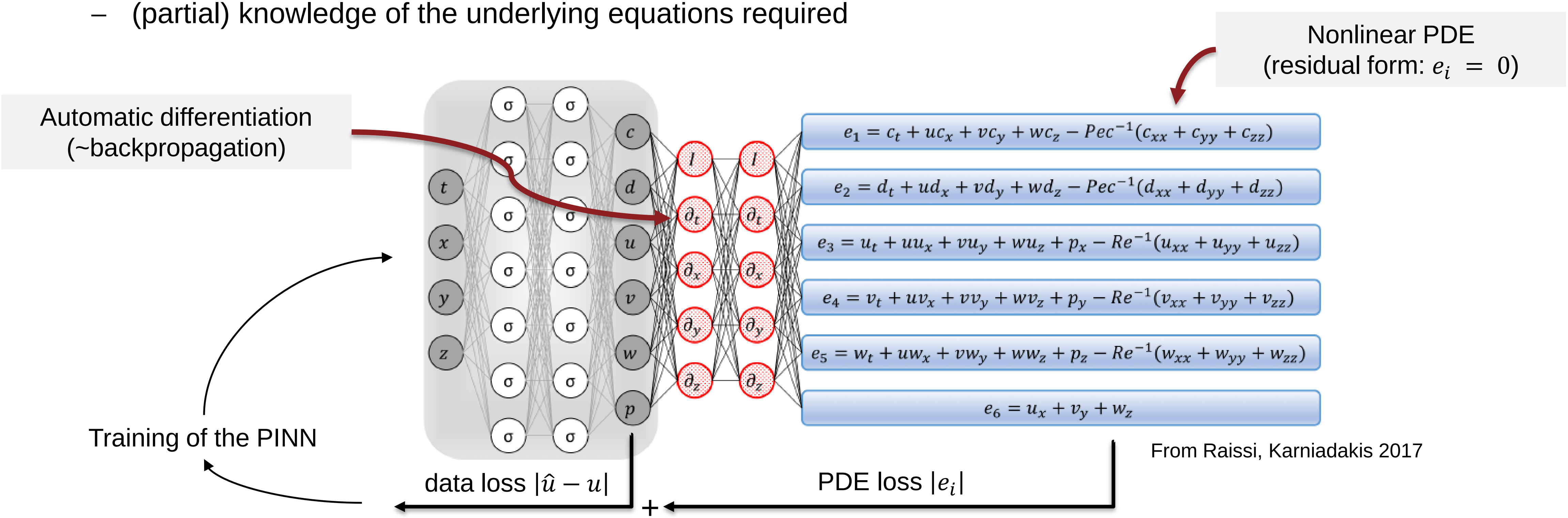
Engineer gradients that point into directions that promote function approximators with minimal prediction error w.r.t. physical aspects



Physics-informed learning (2)

Data-driven solution of nonlinear PDEs

- **Strict regularization**: PINNs [Raissi, Karniadakis 2017]
  - Loss function $L(\theta, x, \hat{y})$ formulated with respect to governing equations
  - Governing equations ~exactly fulfilled at sample points
  - (partial) knowledge of the underlying equations required



From Raissi, Karniadakis 2017

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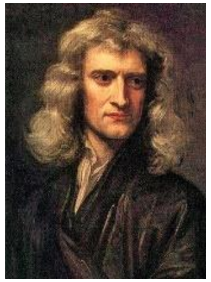
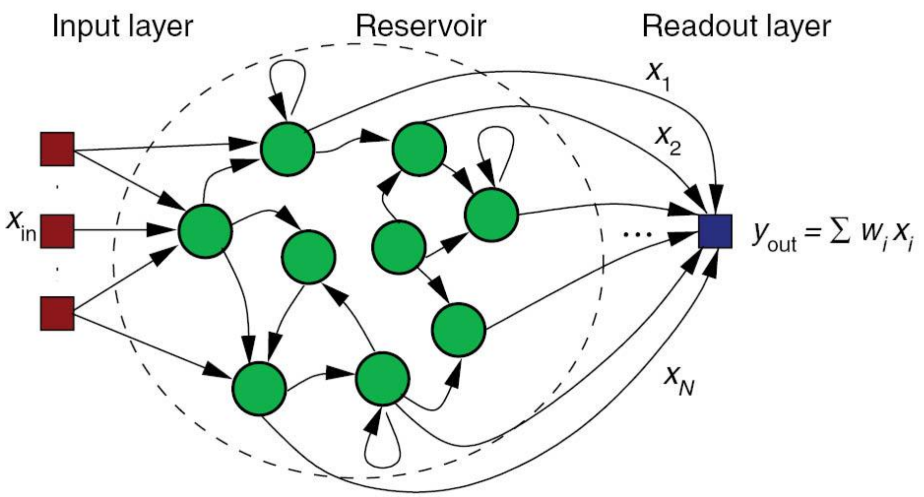
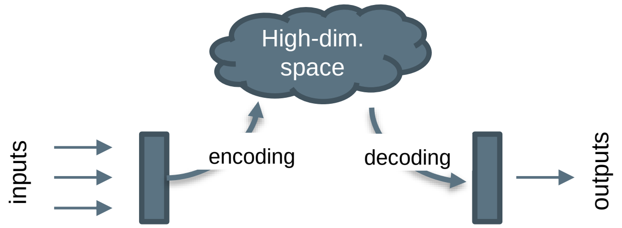


Physical reservoir computing

Reservoir computing



https://julien-vitay.net/project/reservoircomputing/



- Nonlinear mapping in high-dim. feature space
- Read observations from that space
- Fixed weights in reservoir! → hardware design

Physical reservoirs

Tanaka, Gouhei, et al. "Recent advances in physical reservoir computing: A review." *Neural Networks* 115 (2019): 100-123.

Reservoir: water basin

Input: droplets falling into the water

Decoding: surface elevation measurement

References

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Outlook

- Interested in collaborations / networking / discussing?
- Methods / application cases for Physics-Informed Learning?

Thank you!

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