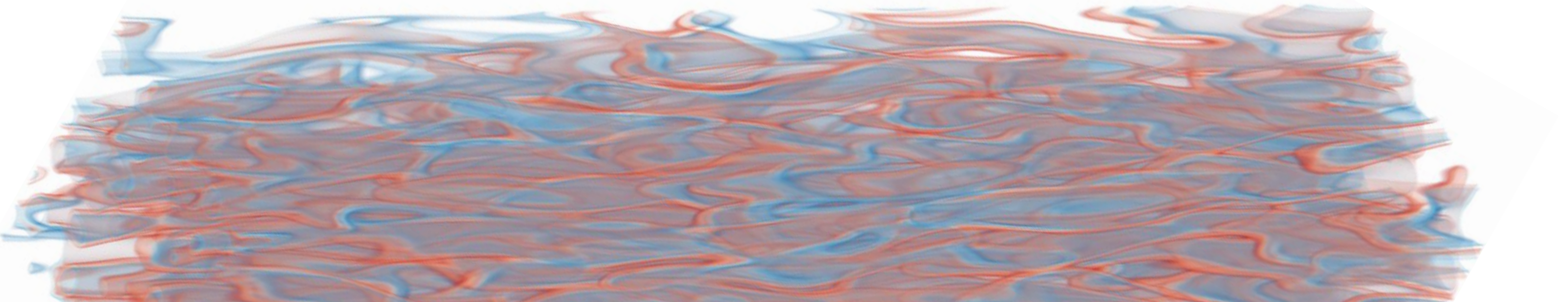
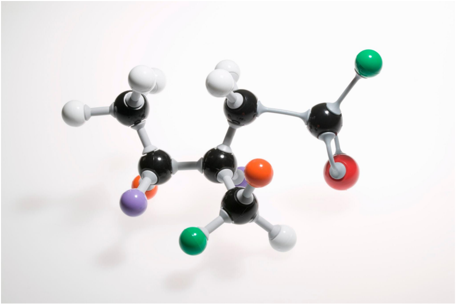
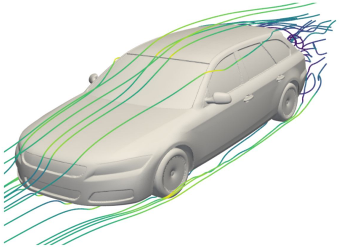
From Numerical Simulators of PDEs to Neural Emulators and Back

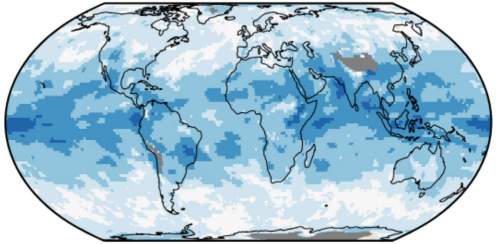
Felix Koehler | PhD Defense | 29 July 2026



The Simulation of Natural Phenomena is Important!







Molecular/Quantum Simulations

⇩

Material & Drug Discovery

Visual Effects & Game Physics

⇩

Plausibility, Immersion, Entertainment

Engineering Simulations

⇩

Saver & more efficient designs

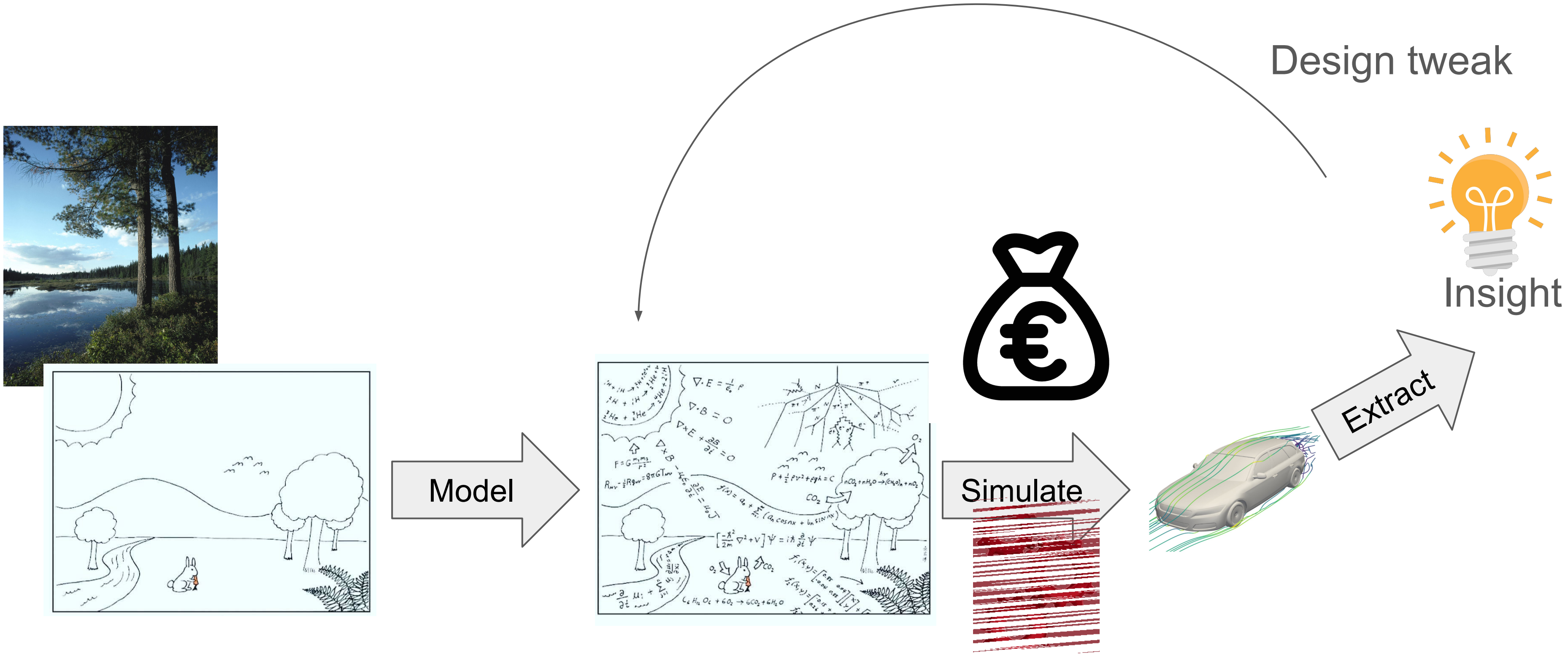
Weather & Climate

⇩

Weather Prediction, Understanding Climate Change

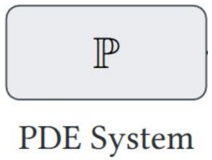
The Path of Simulation

Loop back, don't only run once



Can we approximate Simulations with Neural Networks?

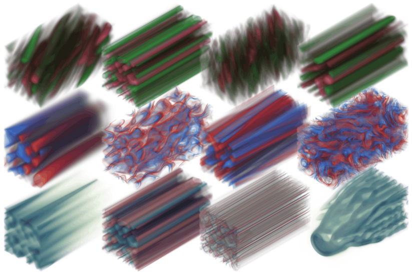
Yes, we can! - Data-Driven Surrogates/Emulators



Exposes the neural emulator to concrete simulations

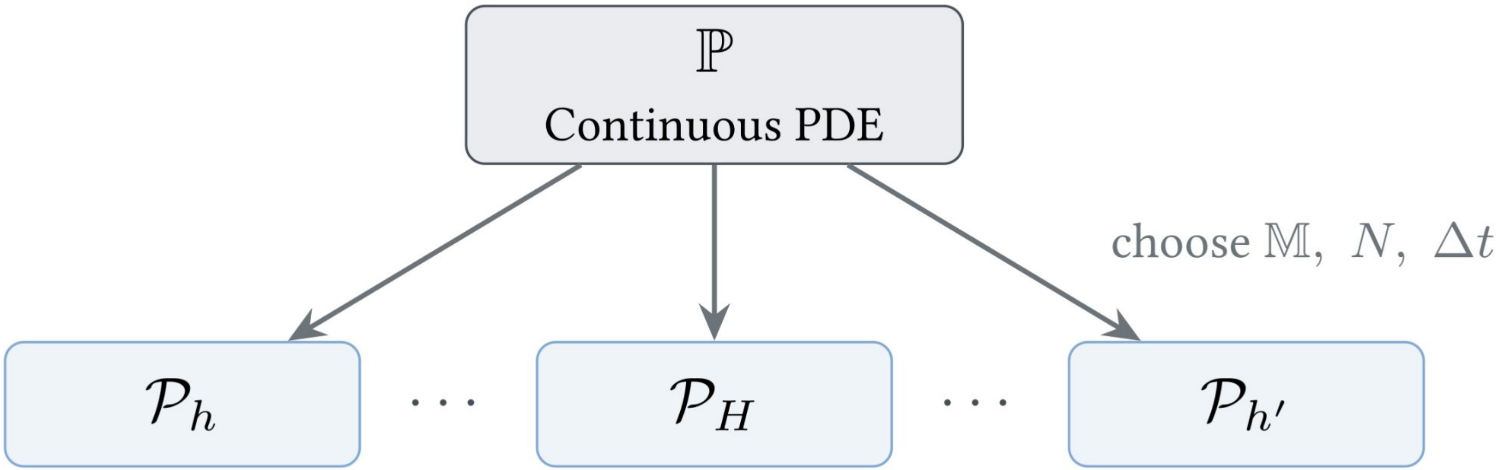
Builds upon the pattern-matching abilities of machine learning and the fast inference of NNs on GPUs

This is different from other fields of ML!



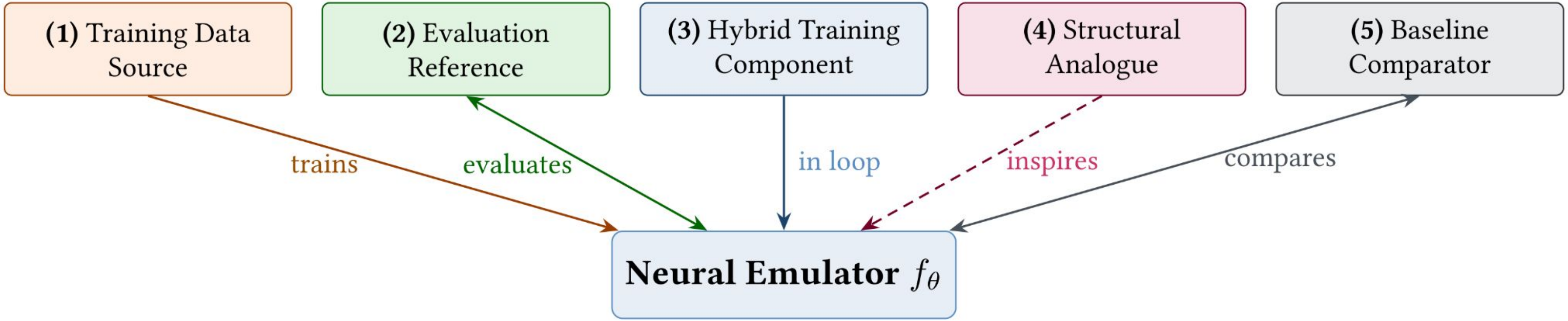
Focus of this talk: The interaction between the data generating solver and the neural surrogate

There is not "this solver" for one PDE



By selecting different schemes and discretization choices we reach different solvers that can be order alongside their "fidelity" (but also their cost)

… and multiple solvers can appear as different roles



39th Conference on Neural Information Processing Systems (NeurIPS 2025).

Neural Emulator Superiority: When Machine Learning for PDEs Surpasses its Training Data

Felix Koehler & Nils Thuerey
Technical University of Munich
Munich Center for Machine Learning (MCML)
{f.koehler,nils.thuerey}@tum.de

Three Numerical Simulators

PDE

Highly Accurate/Exact Solver

Good Solver

Okay-ish Solver

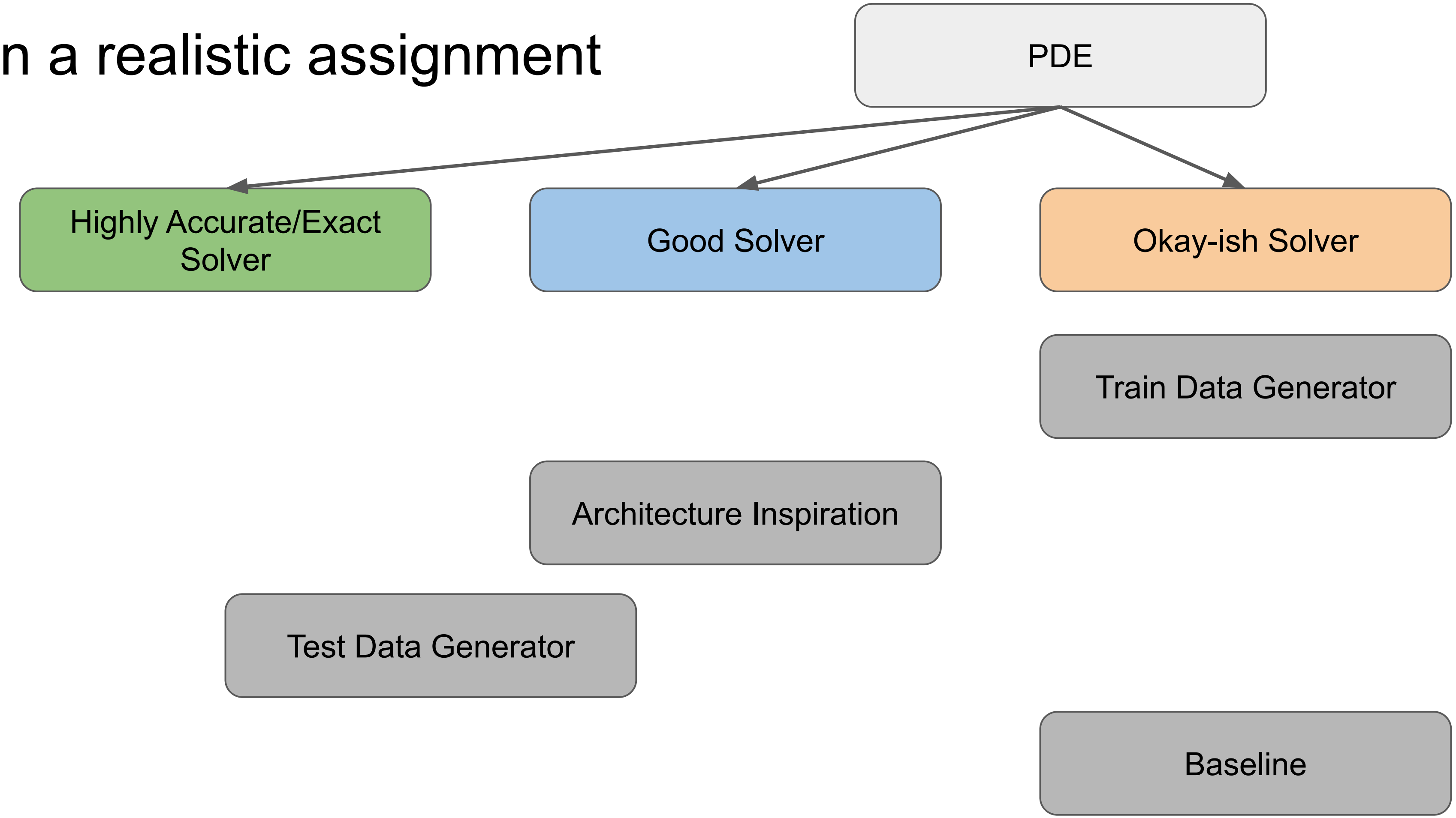
Train Data Generator

Architecture Inspiration

Test Data Generator

Baseline

In a realistic assignment



Understanding Difference Between Training and Testing

One-Step Training

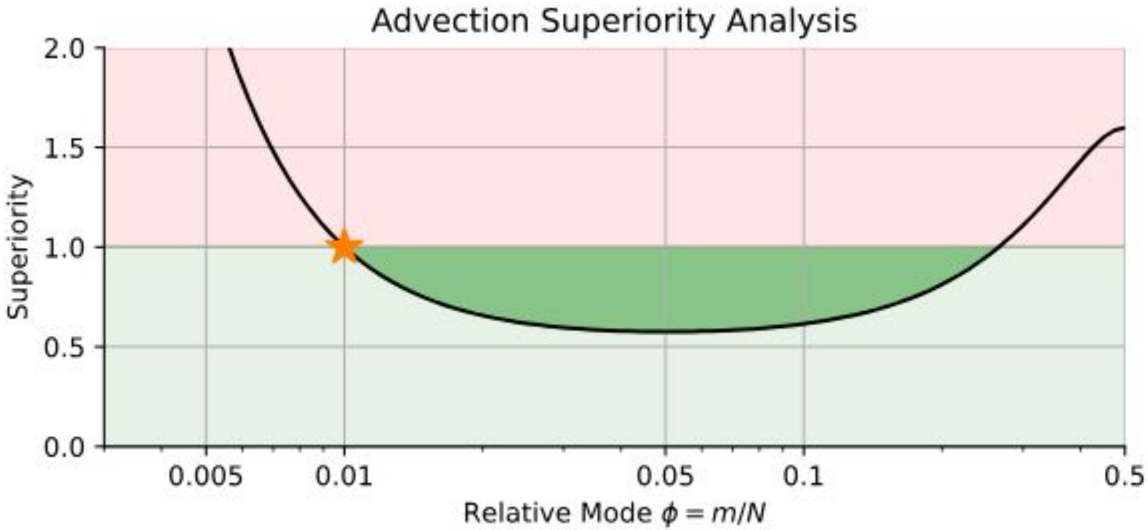
$$L(\theta) = \mathbb{E}_{\{\mathbf{u}_h^{[t]}, \mathbf{u}_h^{[t+1]}\} \sim \mathcal{T}_{\mathcal{P}_h}(\mathbf{u}_h^{[0]}),\ \mathbf{u}_h^{[0]} \sim \mathcal{I}_h} \left[\zeta \left(f_\theta(\mathbf{u}_h^{[t]}), \mathbf{u}_h^{[t+1]} \right) \right]$$

Autoregressive Testing

$$e^{[t]} = \mathbb{E}_{\mathbf{u}_h^{[0]} \sim \tilde{\mathcal{I}}_h} \left[\tilde{\zeta} \left(f_\theta^t(\mathbf{u}_h^{[0]}), \tilde{\mathcal{P}}_h^t(\mathbf{u}_h^{[0]}) \right) \right]$$

Leads to provable Emulator Superiority

$$\xi^{[t]} = \frac{\mathbb{E}_{\mathbf{u}_h^{[0]} \sim \tilde{\mathcal{I}}_h} \left[\tilde{\zeta} \left(f_\theta^t(\mathbf{u}_h^{[0]}), \tilde{\mathcal{P}}_h^t(\mathbf{u}_h^{[0]}) \right) \right]}{\mathbb{E}_{\mathbf{u}_h^{[0]} \sim \tilde{\mathcal{I}}_h} \left[\tilde{\zeta} \left(\mathcal{P}_h^t(\mathbf{u}_h^{[0]}), \tilde{\mathcal{P}}_h^t(\mathbf{u}_h^{[0]}) \right) \right]}$$



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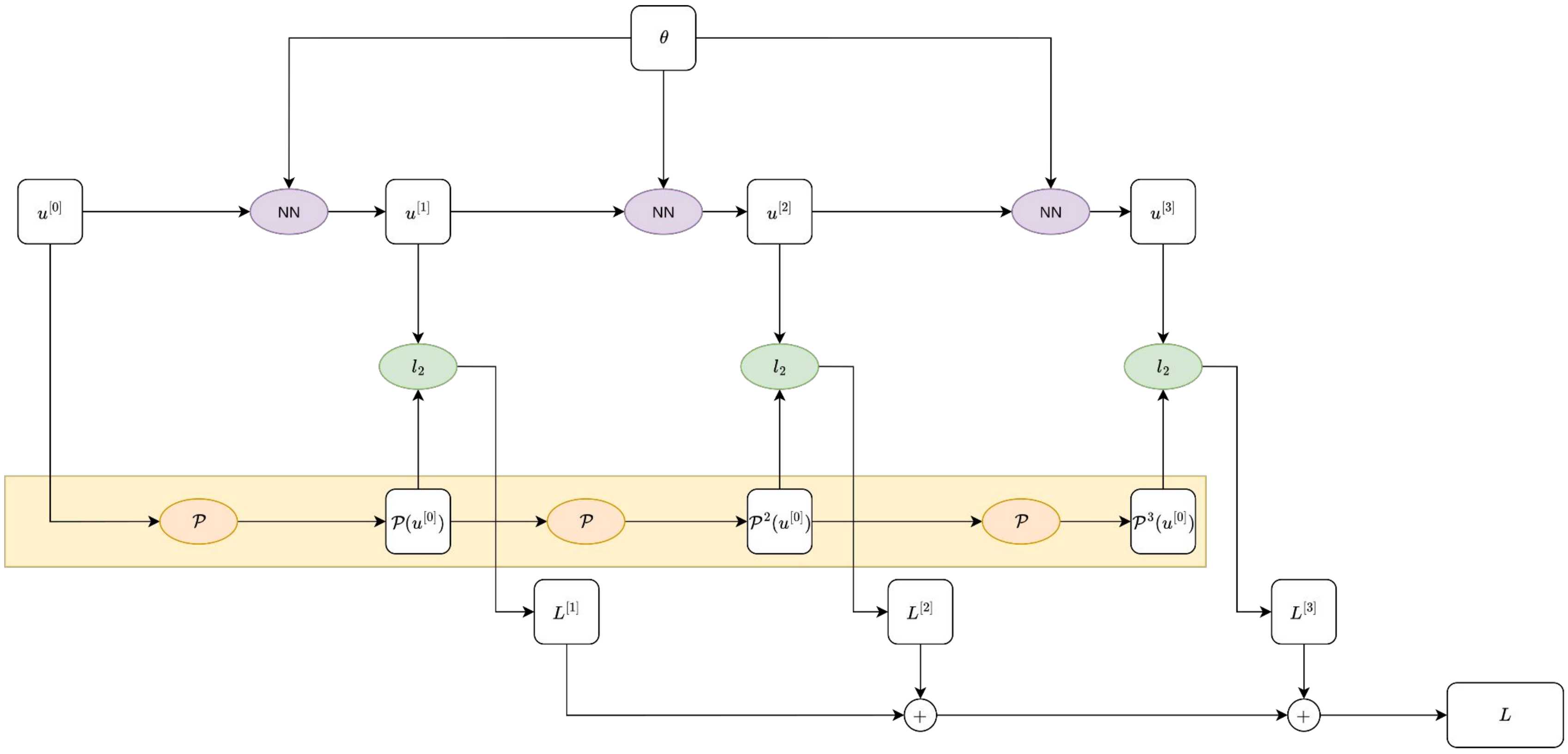
PRDP: Progressively Refined Differentiable Physics

Kanishk Bhatia[*], Felix Koehler[*1], Nils Thuerey
Technical University of Munich
{kanishk.bhatia,f.koehler,nils.thuerey}@tum.de
[*]Equal contribution



θ
$u^{[0]}$
NN
$u^{[1]}$
NN
$u^{[2]}$
NN
$u^{[3]}$
l_2
l_2
l_2
$\mathcal{P}$
$\mathcal{P}(u^{[0]})$
$\mathcal{P}$
$\mathcal{P}^2(u^{[0]})$
$\mathcal{P}$
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$L^{[1]}$
$L^{[2]}$
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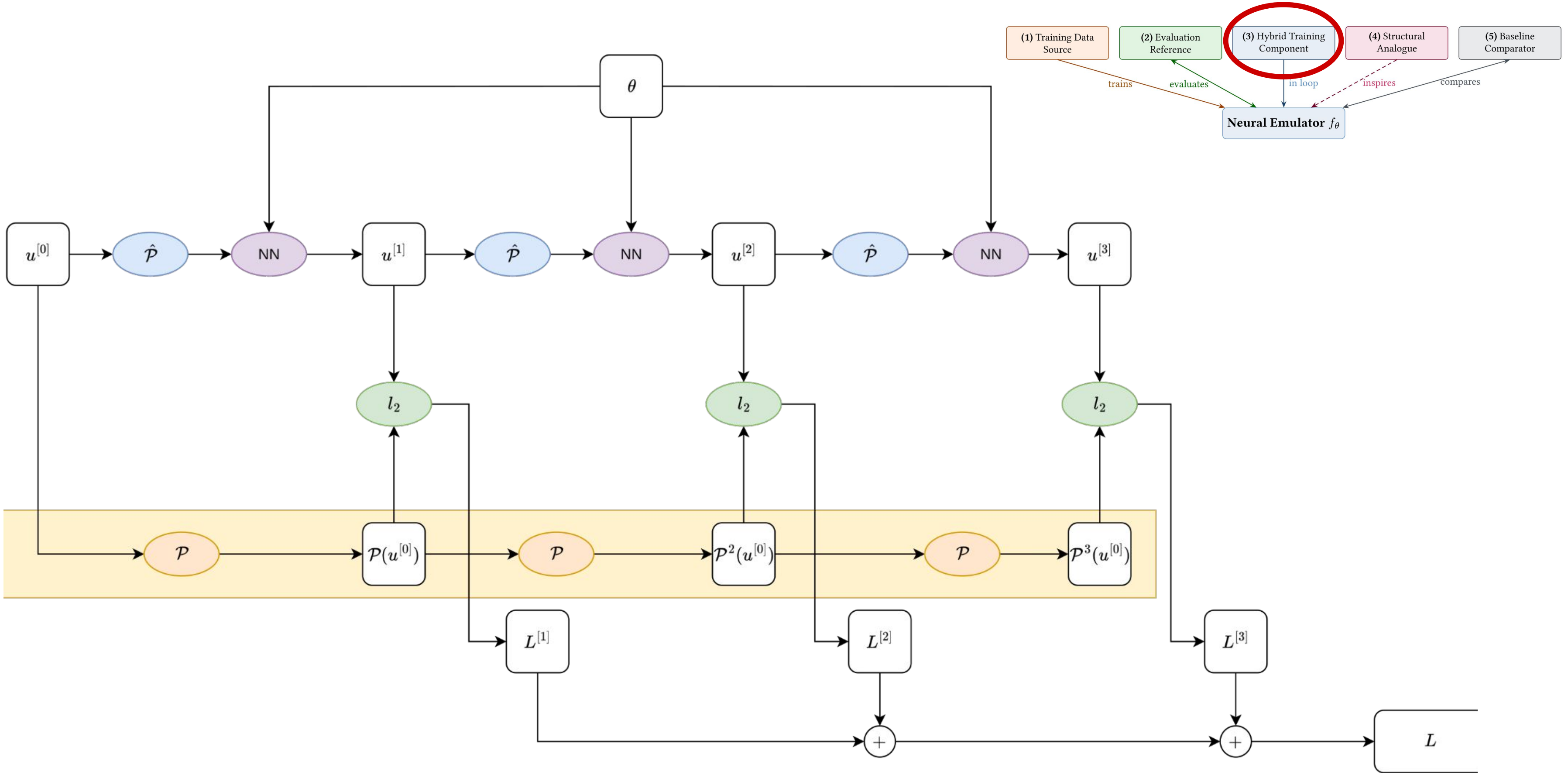
$+$
$+$
L


(1) Training Data Source
(2) Evaluation Reference
(3) Hybrid Training Component
(4) Structural Analogue
(5) Baseline Comparator
trains
evaluates
in loop
inspires
compares
Neural Emulator f_θ
θ
$u^{[0]}$
$\hat{\mathcal{P}}$
NN
$u^{[1]}$
$u^{[2]}$
$u^{[3]}$
l_2
$\mathcal{P}$
$\mathcal{P}(u^{[0]})$
$\mathcal{P}^2(u^{[0]})$
$\mathcal{P}^3(u^{[0]})$
$L^{[1]}$
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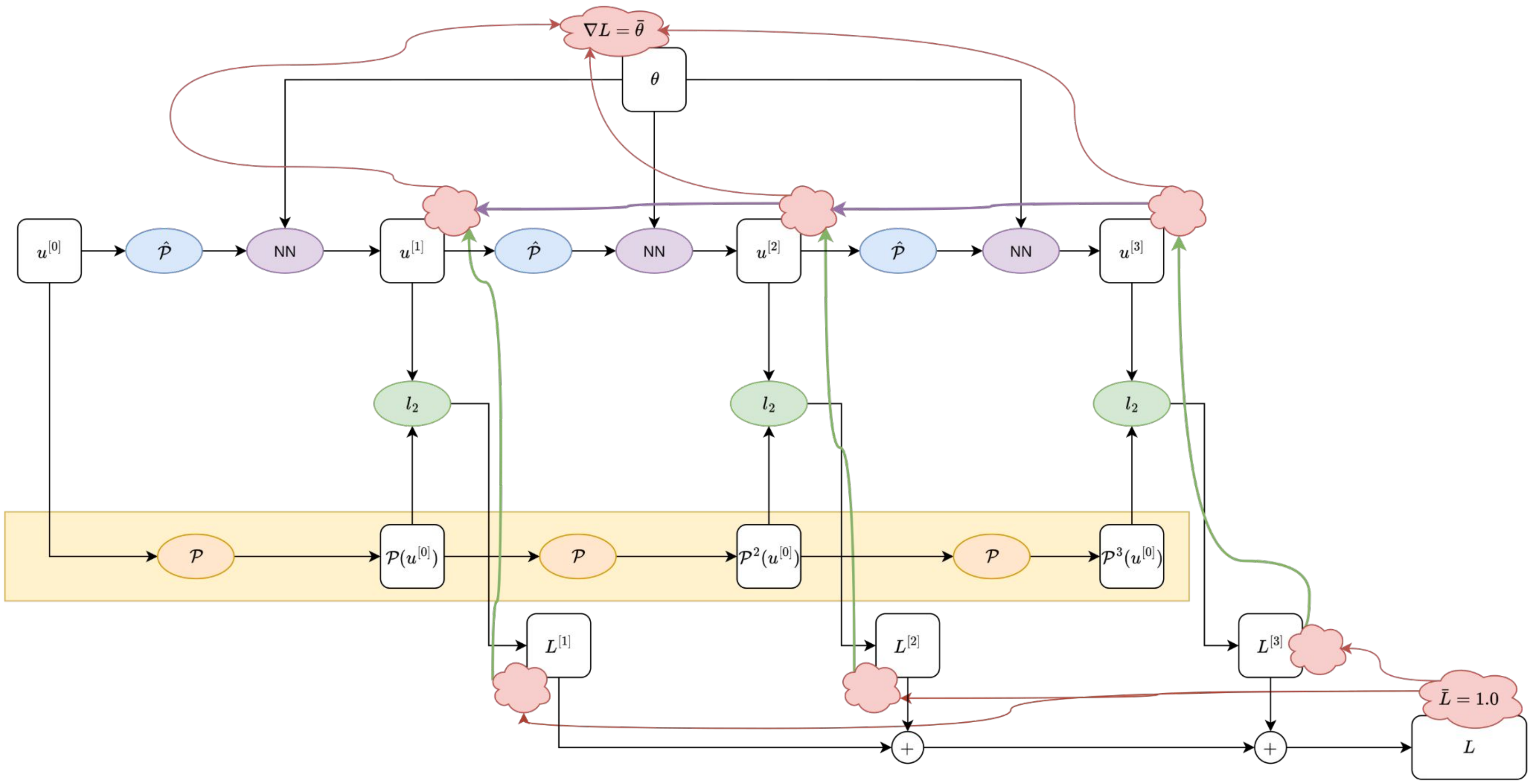
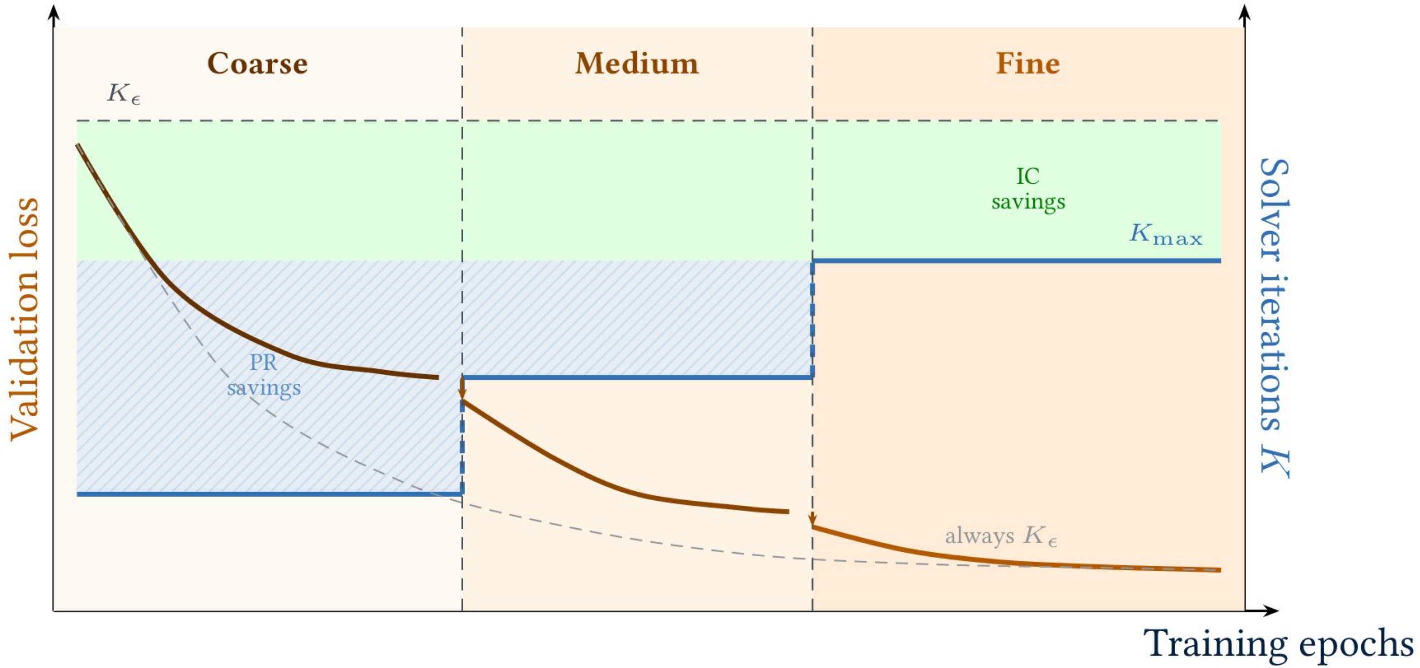
$+$
L

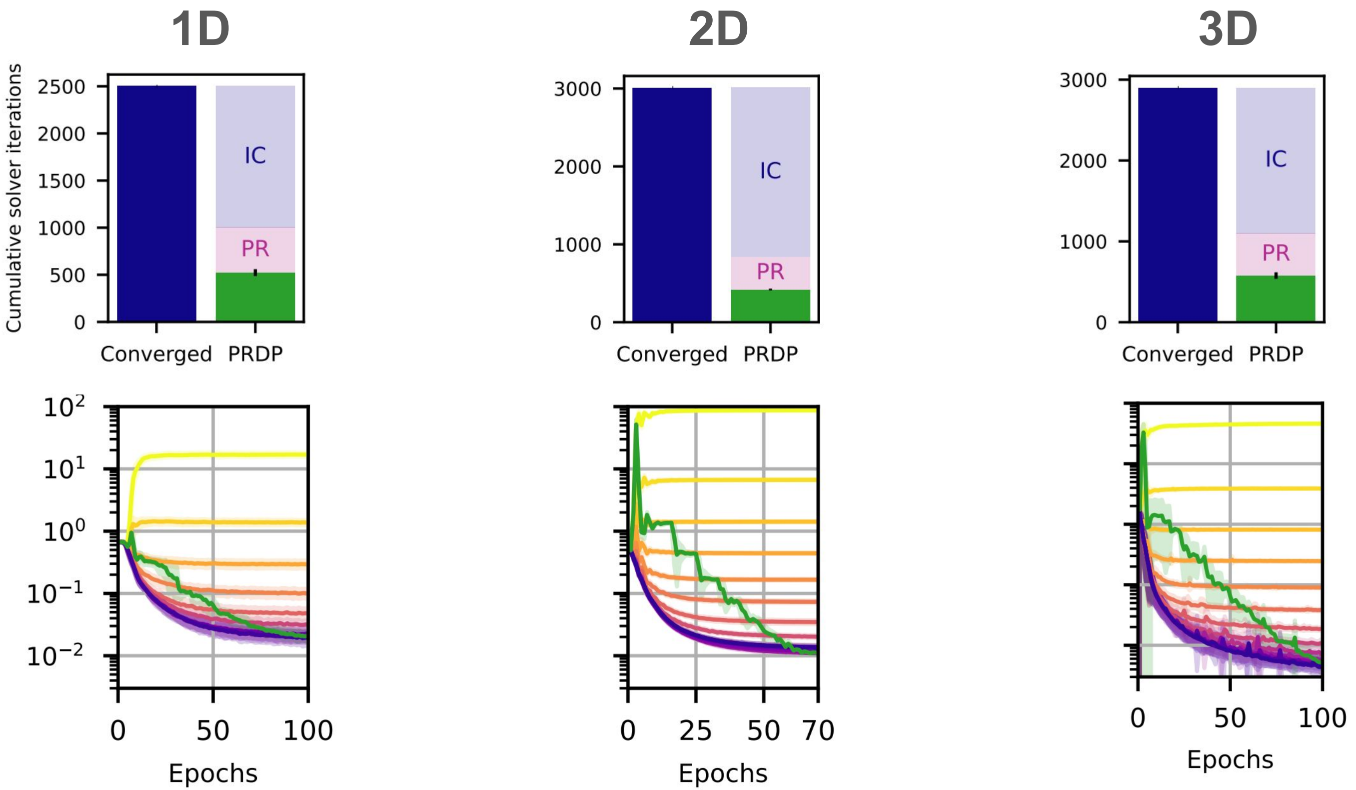


$\nabla L = \bar{\theta}$
θ
$u^{[0]}$
$\hat{\mathcal{P}}$
NN
$u^{[1]}$
$\hat{\mathcal{P}}$
NN
$u^{[2]}$
$\hat{\mathcal{P}}$
NN
$u^{[3]}$
l_2
l_2
l_2
$\mathcal{P}$
$\mathcal{P}(u^{[0]})$
$\mathcal{P}$
$\mathcal{P}^2(u^{[0]})$
$\mathcal{P}$
$\mathcal{P}^3(u^{[0]})$
$L^{[1]}$
$L^{[2]}$
$L^{[3]}$
$\bar{L} = 1.0$
$+$
$+$
L

A fidelity-scheduling heuristic



An example of the heat equation



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APEBench: A Benchmark for Autoregressive Neural Emulators of PDEs

Felix Koehler
Technical University of Munich
Munich Center for Machine Learning
f.koehler@tum.de

Simon Niedermayr
Technical University of Munich
simon.niedermayr@tum.de

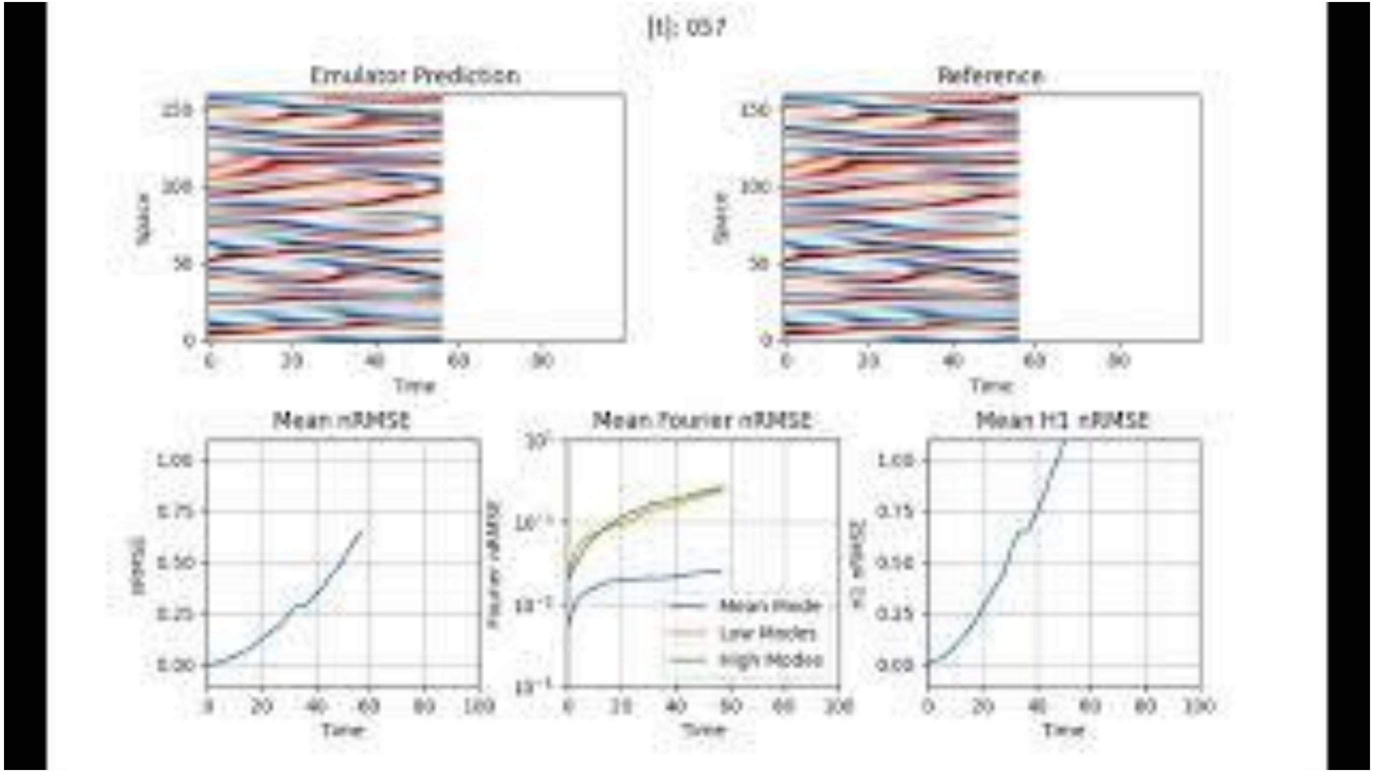
Rüdiger Westermann
Technical University of Munich
westermann@tum.de

Nils Thuerey
Technical University of Munich
nils.thuerey@tum.de

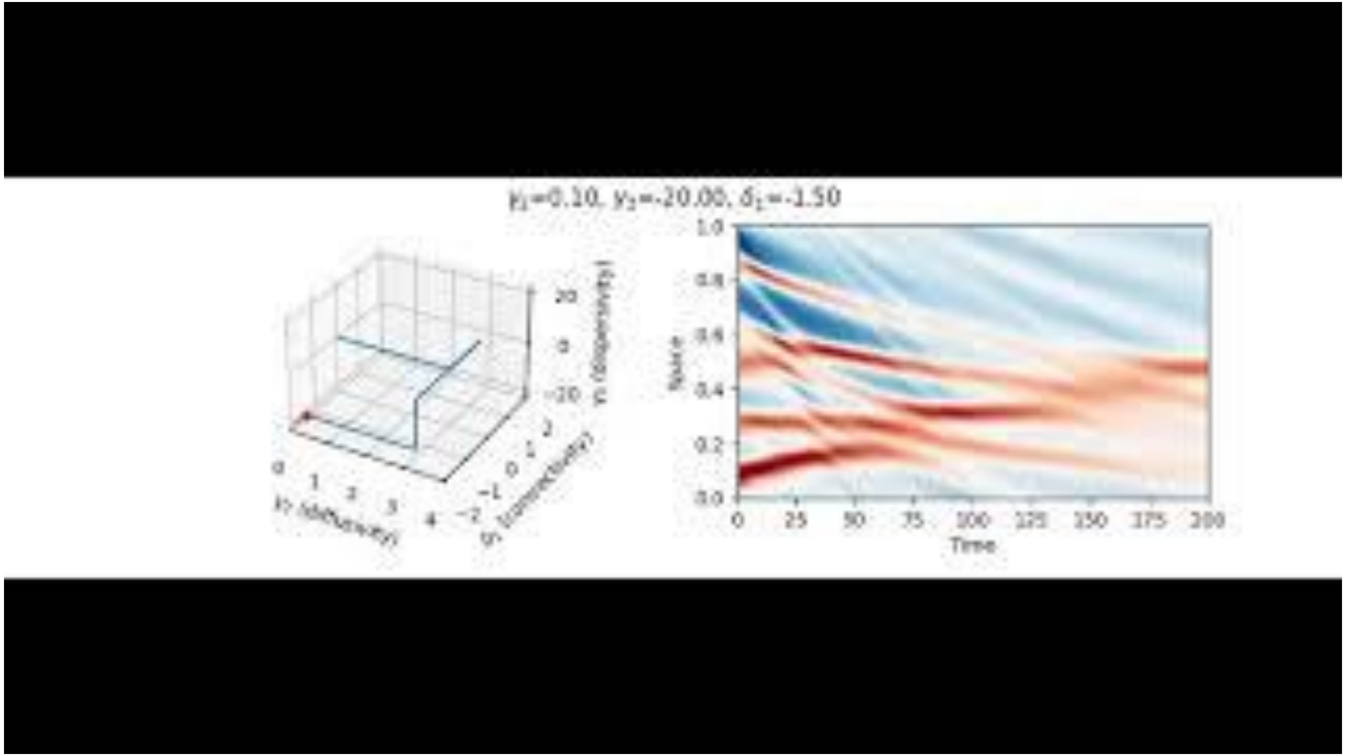
Implications of what we’ve seen for Benchmarking

1. Need of High-Fidelity Reference Solutions (in particular for testing!) ✅
2. Flexible Data Generators over Fixed Datasets ✅
3. Include options for neural-hybrid correctors ✅
4. Rollout Metrics over One-Step Accuracy
5. Precise Specification of the Emulated System

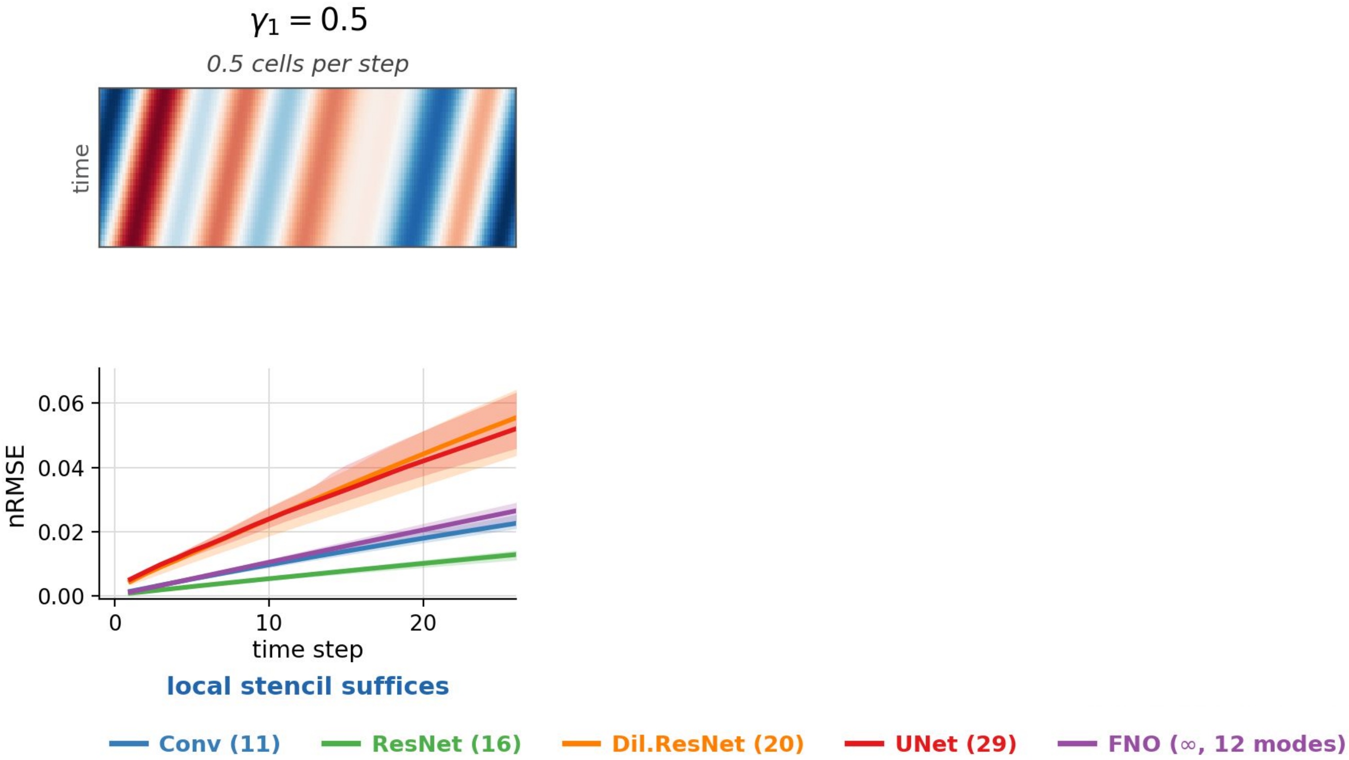
Focusing on rollouts with APEBench



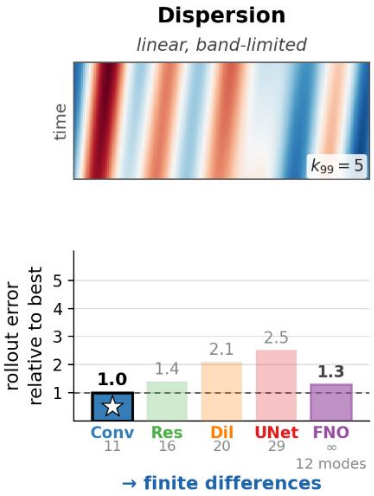
A better emulator exchange protocol



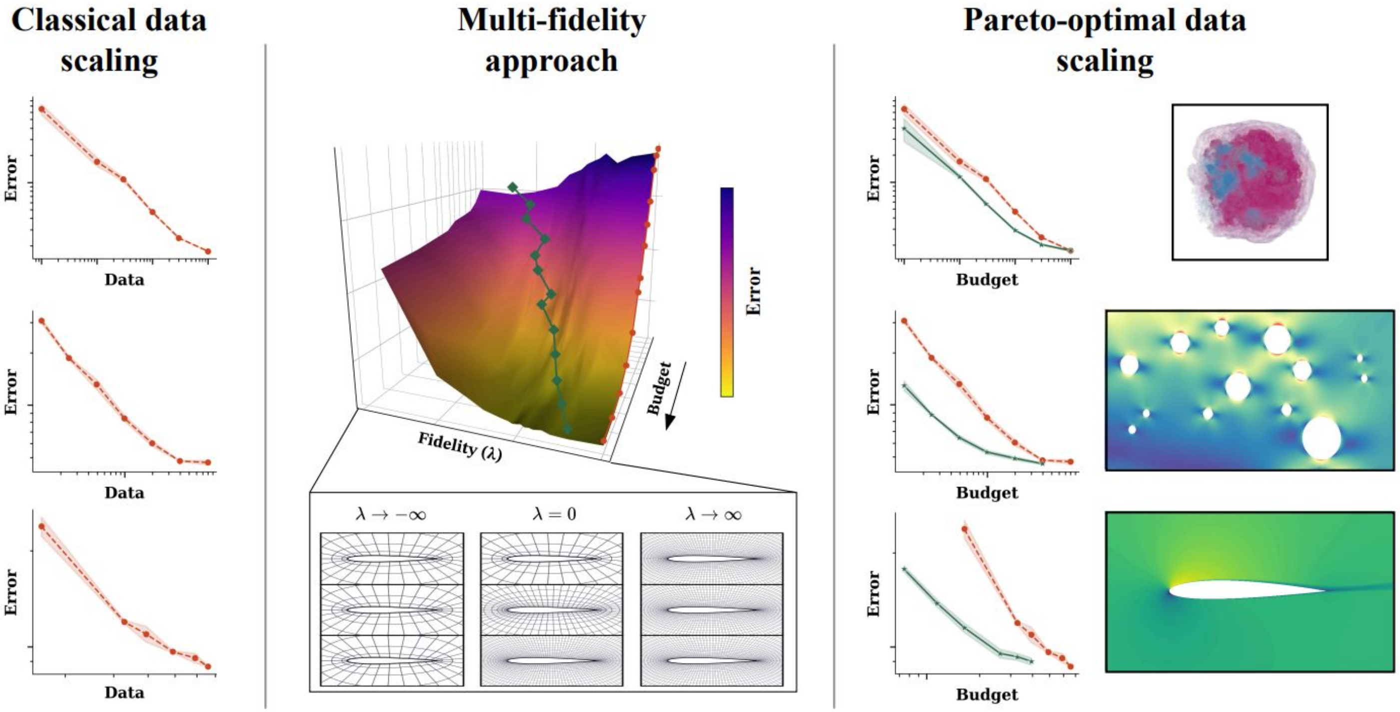
Core Finding: Receptive Fields have to match Physics



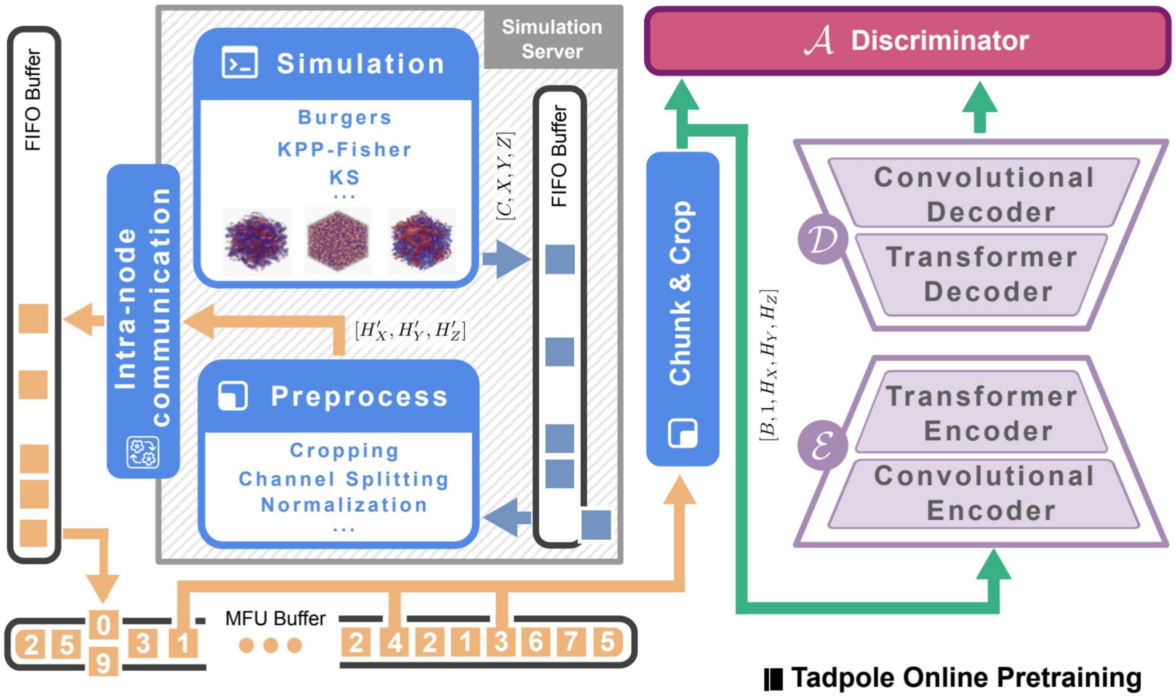
Core Finding: Match Architecture and Physics Properties



Outlook: Compute-Optimal Data Generation



Outlook: Online Data Generation for FM Pretraining



Thank you!

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Simon Niedermayr
Technical University of Munich
simon.niedermayr@tum.de

Rüdiger Westermann
Technical University of Munich
westermann@tum.de

Nils Thuerey
Technical University of Munich
nils.thuerey@tum.de

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PRDP: PROGRESSIVELY REFINED DIFFERENTIABLE PHYSICS

Kanishk Bhatia[*], Felix Koehler[*1], Nils Thuerey
Technical University of Munich
{kanishk.bhatia,f.koehler,nils.thuerey}@tum.de
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