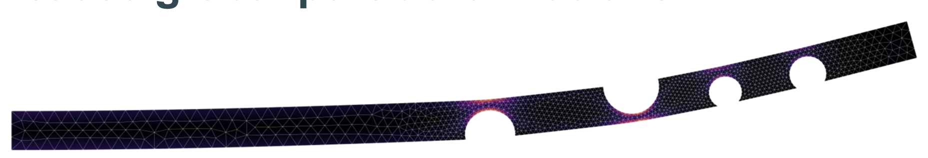
Diffusion-Based Hierarchical Graph Neural Networks for Simulating Nonlinear Solid Mechanics

Challenges

Message Passing Bottleneck

- **Local boundary conditions**…

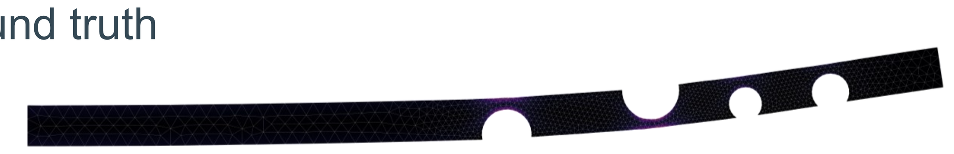
- … cause **global part deformations**



- Local Information has to be propagated globally
- However, Message Passing Layer act locally
- Infeasible for large (mesh-) graphs / graph diameters

Spectral bias of MSE-trained Model

- Ground truth



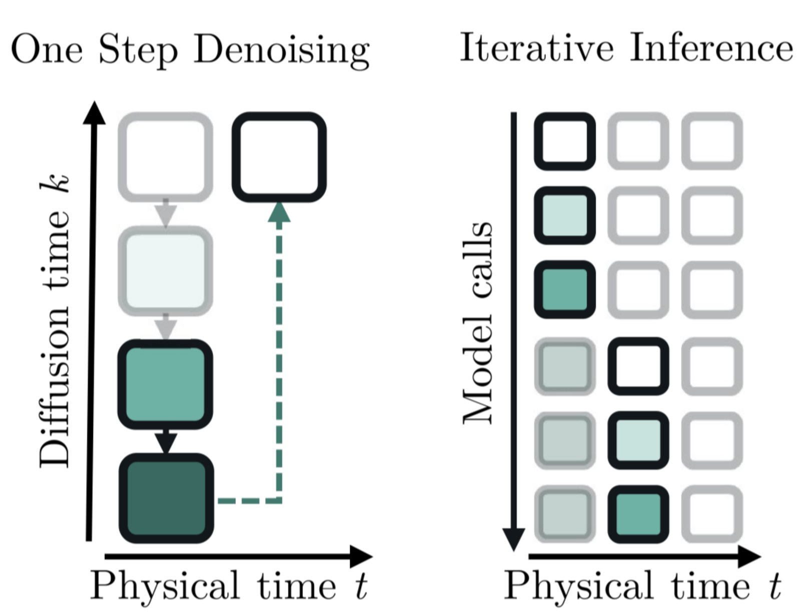
- Prediction with **low frequency bias**

- Prediction with **high frequency bias**

- Conventional MSE-based training is **more sensitive to global deformation deviations** than to local mesh distortions (**spectral bias**)

Conventional Denoising

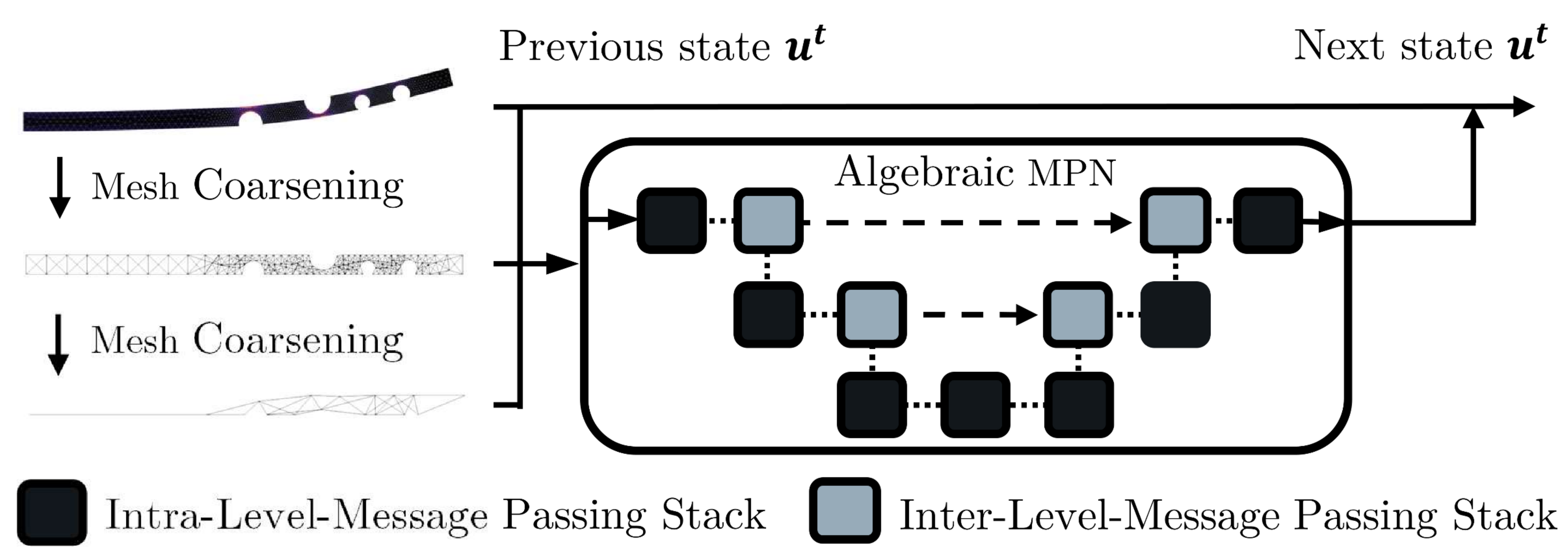
- Conventional diffusion-based simulators denoise step-wise
  → $\mathcal{O}(KT)$ for K diffusion and T physical steps



ROBIN: Rolling diffusion-Batched Inference Network

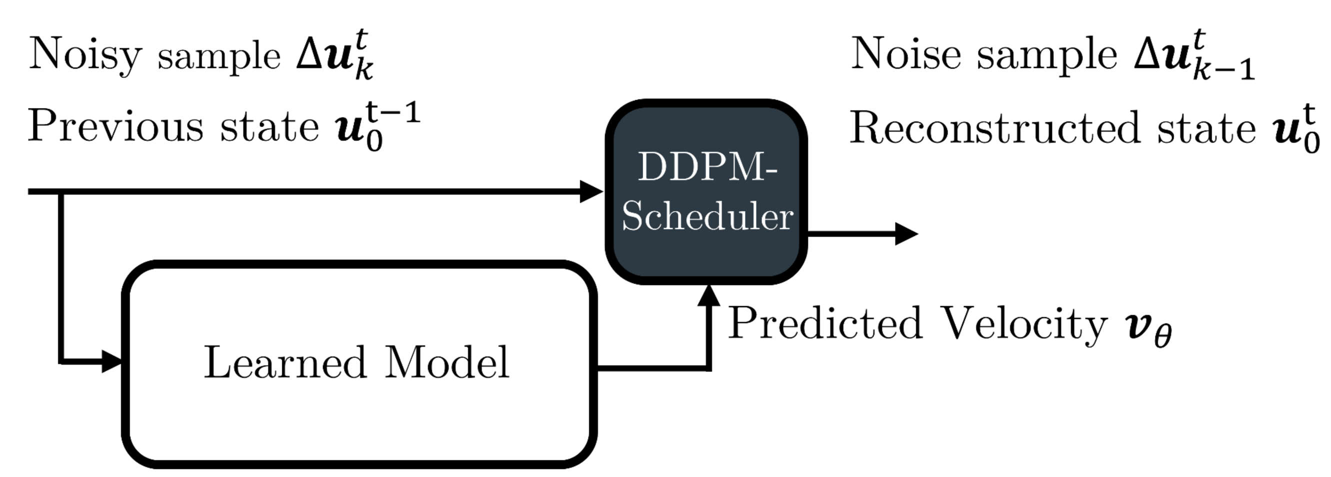
Algebraic hierarchical Message Passing Networks

- **Maximized receptive field** – One cycle propagates information across the entire mesh
- Increase **prediction fidelity** by multiscale message passing
- Algebraic Multigrid (AMG)-based Mesh **Coarsening that preserves the geometry**
- **Mesh-size independent architecture** by shared blocks



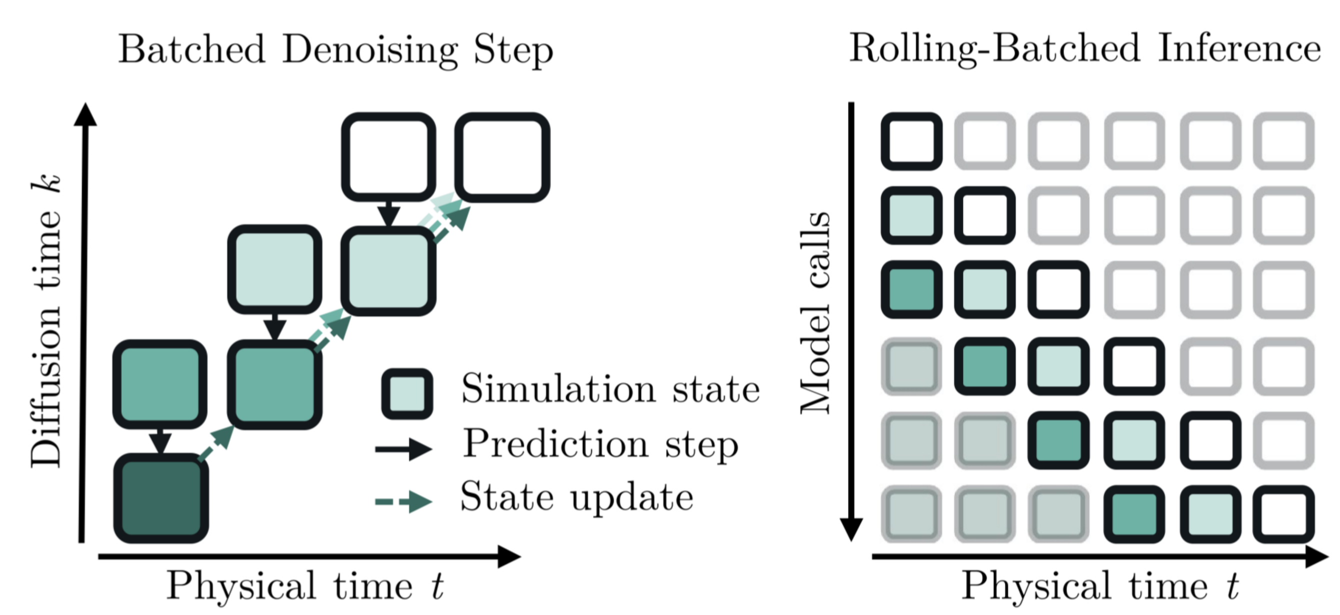
Denoising diffusion probabilistic models

- DDPMs and AMPNs allow for **rich, high-fidelity predictions across frequencies**
- Early denoising steps focus on global frequencies, and the later on local frequencies

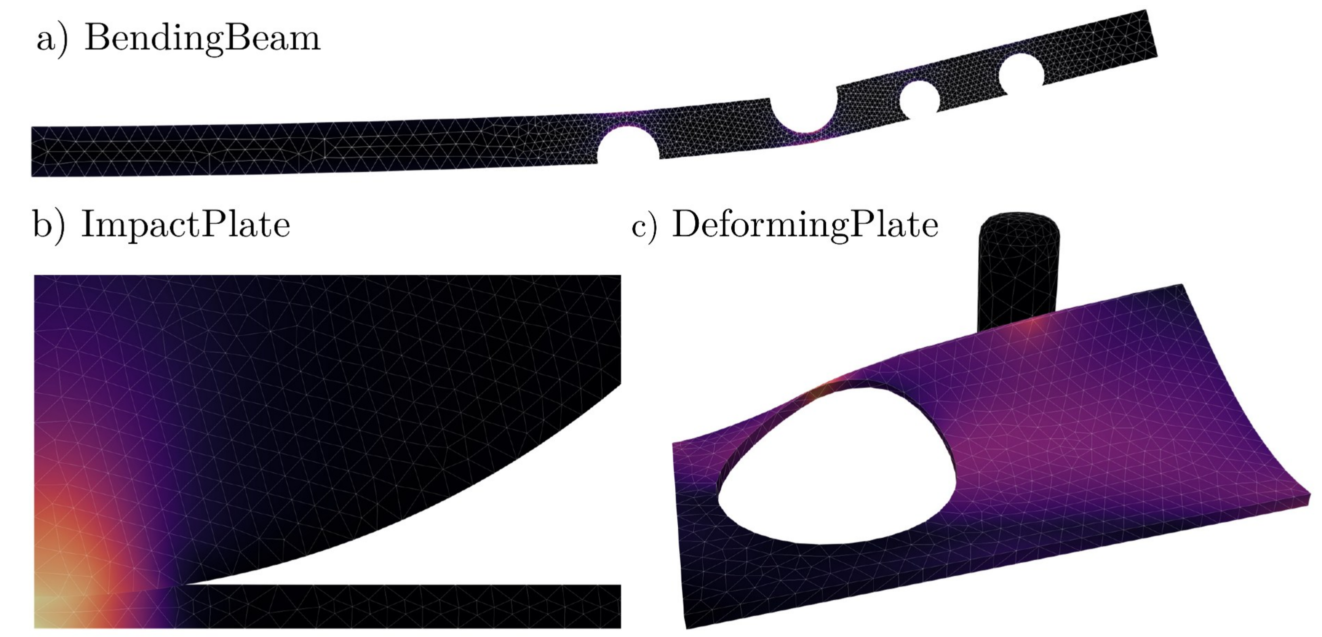


ROBI: Rolling diffusion-Batched Inference

- ROBI **parallelize the denoising** of consecutive time steps → $\approx \mathcal{O}(T)$
- The model prediction still only depends on the previous physical state, **preserving training efficiency and time-shift equivariance**
- Denoising stride and truncation step **enable the trade-off of accuracy for speed**



Datasets

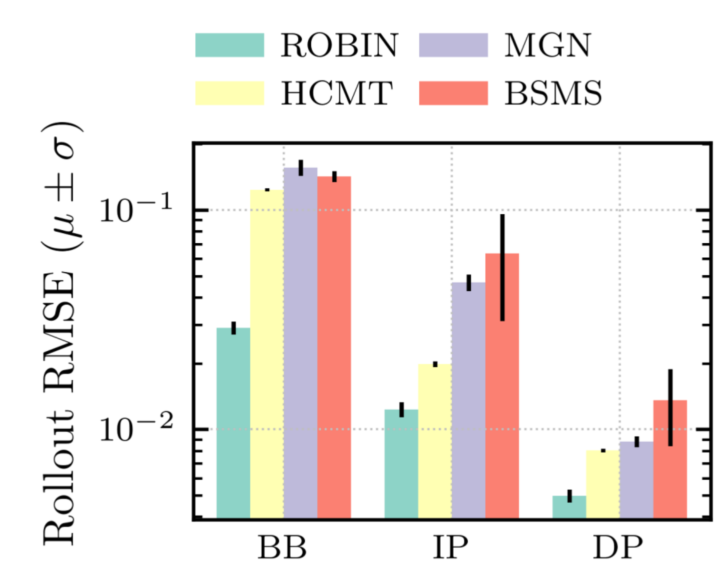


Tobias Würth[1*], Niklas Freymuth[2], Gerhard Neumann[2], Luise Kärger[1]

[1]Institute of Vehicle System Technology
[2]Autonomous Learning Robots
*tobias.wuerth@kit.edu

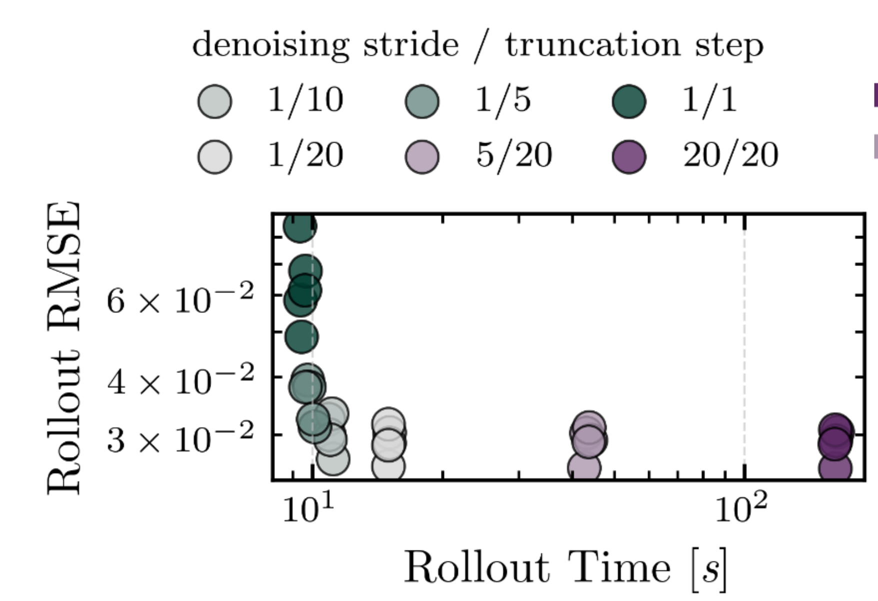
Results

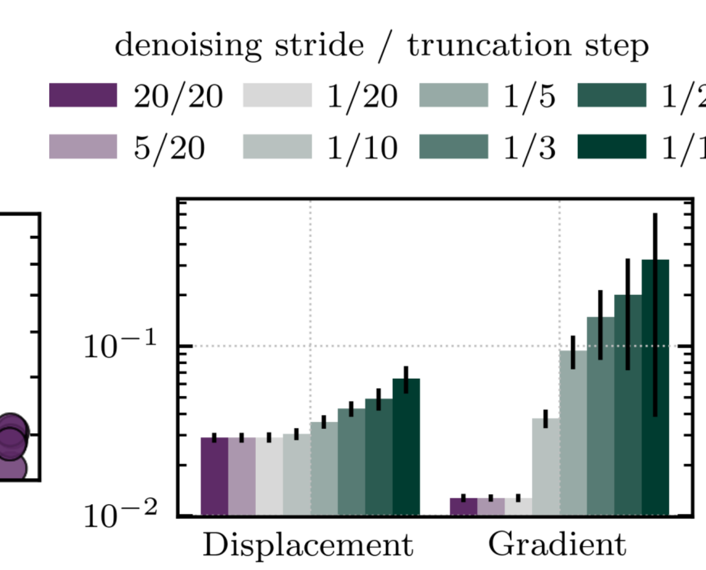
High-fidelity physical simulations



Variable Inference with ROBI

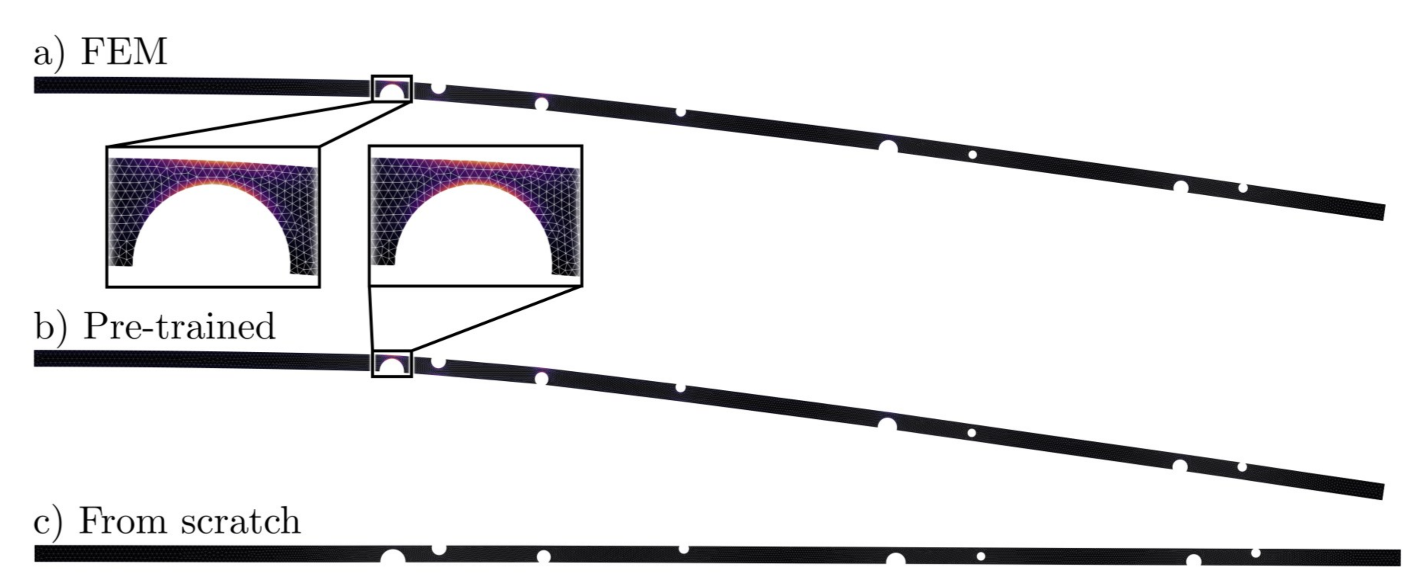
- ROBI enables **faster yet equally accurate** inferences **as conventional inference** (20/20).
- Early denoising steps reduce displacement error (global), later displacement gradient error (local)





Generalization to large meshes

- The AMPN architecture enables quick transfers to much larger meshes



Project website