

A novel gauge-equivariant neural network architecture for preconditioners in lattice QCD

Daniel Knüttel, Christoph Lehner, **Simon Pfahler**, Tilo Wettig

University of Regensburg

October 28, 2025

The image features a white background with several abstract, hand-drawn shapes. A large, irregular purple shape is centered, containing the word "Background" in a black, sans-serif font. This purple shape is outlined with a dark blue line. In the top-left corner, there is a teal shape. In the top-right corner, there is a pink shape. In the bottom-left corner, there is an orange shape. In the bottom-right corner, there is a smaller purple shape. All these peripheral shapes are also outlined with dark blue lines.

Background

Problem statement

Bigger picture

- ▶ Lattice QCD calculations are expensive
- ▶ One of the most expensive parts is solving the Dirac equation
- ▶ Preconditioners can accelerate this

Preconditioners

- ▶ State of the art: algebraic multigrid (AMG)
- ▶ But AMG needs costly setup
- ▶ Can this setup be avoided?
- ▶ **Goal:** Preconditioner competitive with AMG, but with very little (or even no) setup



Status quo

Previous work

- ▶ Exploratory studies with different kinds of Machine Learning models [1,2]
- ▶ Multigrid coarse grid solver and smoother were reformulated in a learnable way [3]
- ▶ Prolongation and restriction operators were translated into ML language [4]

Shortcomings

- ▶ Focus on preconditioning the high modes
- ▶ expensive AMG setup is still needed
- ▶ no generalization to unseen configurations

[1] S. Calì et al., PRD **107**, 034508 (2023)

[2] Y. Sun et al., arXiv:2509.10378 [hep-lat] (2025)

[3] C. Lehner and T. Wettig, PRD **108**, 034503 (2023)

[4] C. Lehner and T. Wettig, PRD **110**, 034517 (2024)

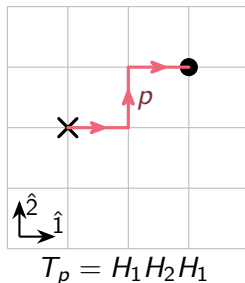


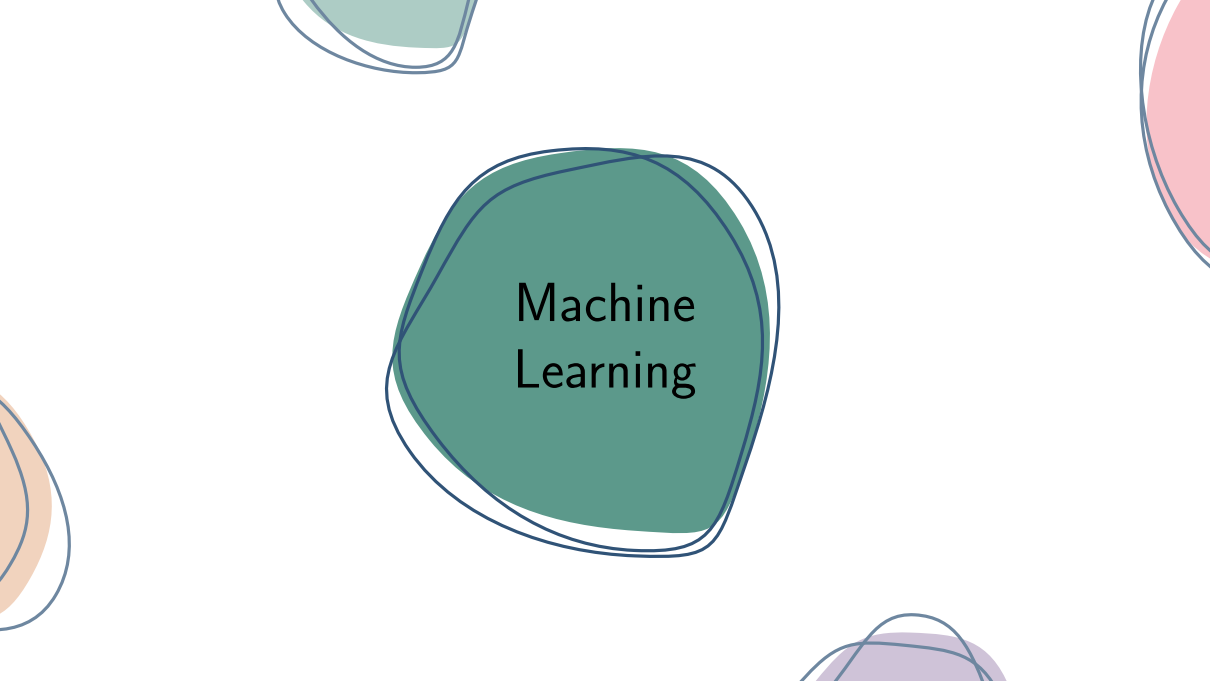
Gauge equivariance

- ▶ Gauge-equivariant transport of information between adjacent lattice sites:
hop operator

$$H_{p_i}\varphi(x) = U_{p_i}^\dagger(x - \hat{p}_i)\varphi(x - \hat{p}_i)$$

- ▶ Combining multiple hops leads to **parallel transports** T_p along a path p
- ▶ weighted linear combinations of parallel transports are gauge-equivariant



The background features several abstract, hand-drawn shapes in various colors: a teal shape at the top center, a pink shape at the top right, an orange shape at the bottom left, and a purple shape at the bottom right. These shapes are outlined with thin, dark blue lines.

Machine Learning

Network Architecture

Dense linear (L) layer

- ▶ n spin-color fields
 $\varphi \in \mathbb{C}^{L_x \times L_y \times L_z \times L_t \times N_c \times N_s}$
- ▶ build m linear combinations of the input fields, with spin matrices $W_{ij} \in \mathbb{C}^{N_s \times N_s}$ as weights:

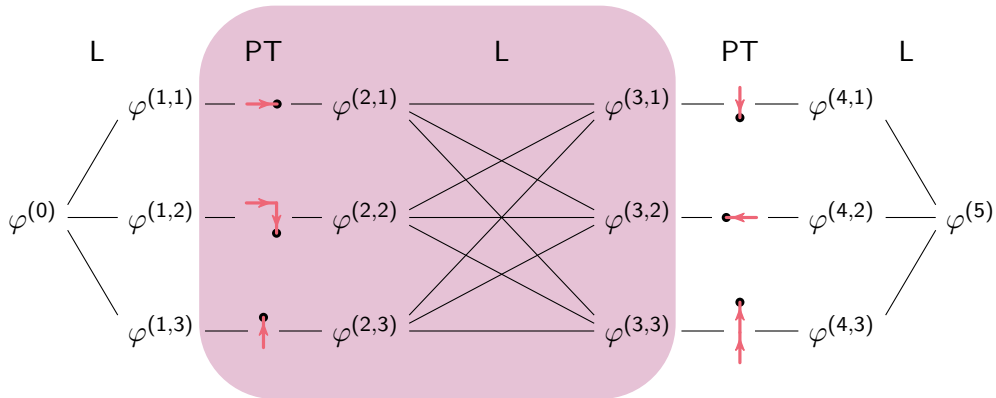
$$\psi_i(x) \stackrel{\text{L}}{=} \sum_{j=1}^n W_{ij} \varphi_j(x)$$

Parallel Transport (PT) layer

- ▶ n spin-color fields
 $\varphi \in \mathbb{C}^{L_x \times L_y \times L_z \times L_t \times N_c \times N_s}$
- ▶ apply a different parallel transport $p^{(i)}$ to every input field:

$$\psi_i(x) \stackrel{\text{PT}}{=} T_{p^{(i)}} \varphi_i(x)$$

Network Architecture



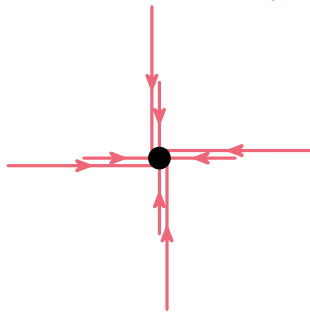
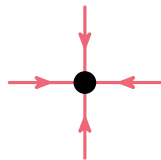
Choice of PT paths

► 1-hop paths:

$$P = \{H_p | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}\}$$

► long straight paths:

$$P = \{H_p^n | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}, \\ n \in \{2^0, 2^1, \dots, 2^{L_p/2}\}\}$$



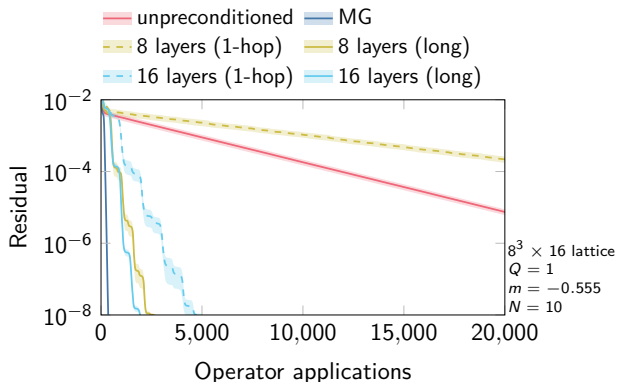
Choice of PT paths

► 1-hop paths:

$$P = \{H_p | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}\}$$

► long straight paths:

$$P = \{H_p^n | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}, \\ n \in \{2^0, 2^1, \dots, 2^{L_p/2}\}\}$$



Score function

► Standard choice:

$$C = \|MD\varphi - \varphi\|^2$$

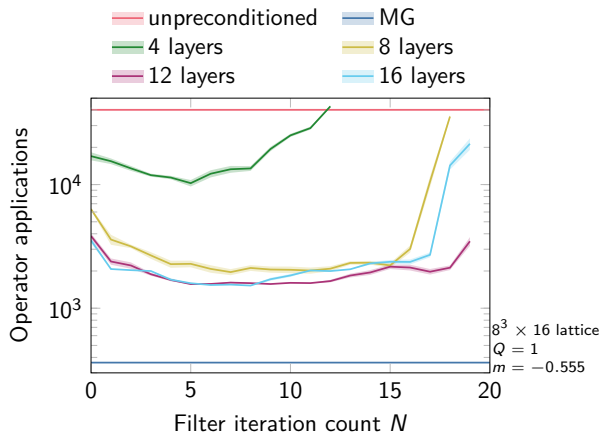
with random field φ

► Filtered cost function:

$$C = \|MD\tilde{\varphi} - \tilde{\varphi}\|^2$$

where $\tilde{\varphi}$ is obtained through N iterations of GMRES for $D\varphi = 0$ with random initial guess

⇒ Stronger emphasis on the low modes!





Results

Gauge configurations

$8^3 \times 16$ ensemble¹:

- ▶ Wilson action
- ▶ quenched, heat bath
- ▶ Wilson-clover Dirac operator
- ▶ configurations with $|Q| \in \{0, 1, 2\}$

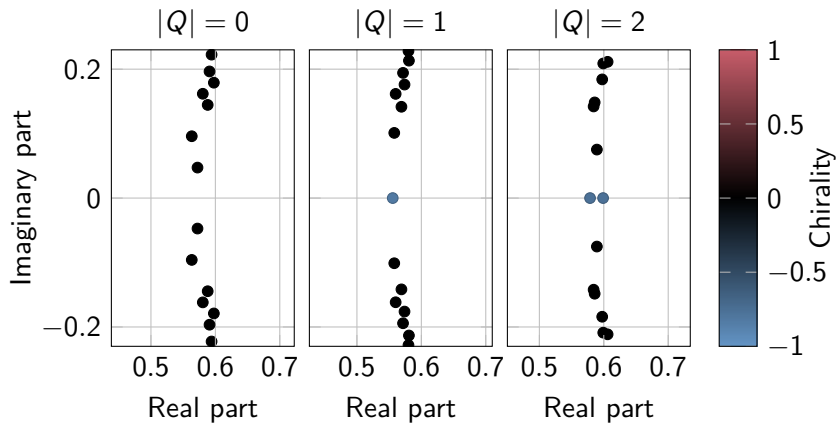
$16^3 \times 32$ ensemble:

- ▶ Wilson action
- ▶ quenched, HMC
- ▶ Wilson-clover Dirac operator
- ▶ configurations with $|Q| \in \{0, 4\}$

¹ <https://doi.org/10.5281/zenodo.15018324>

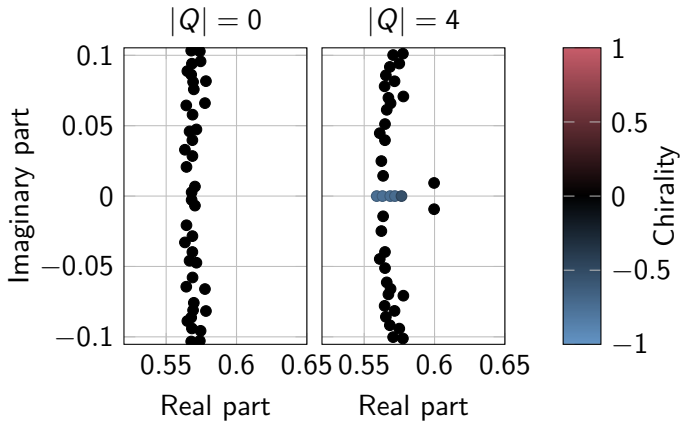
Gauge configurations

$8^3 \times 16$ lattice

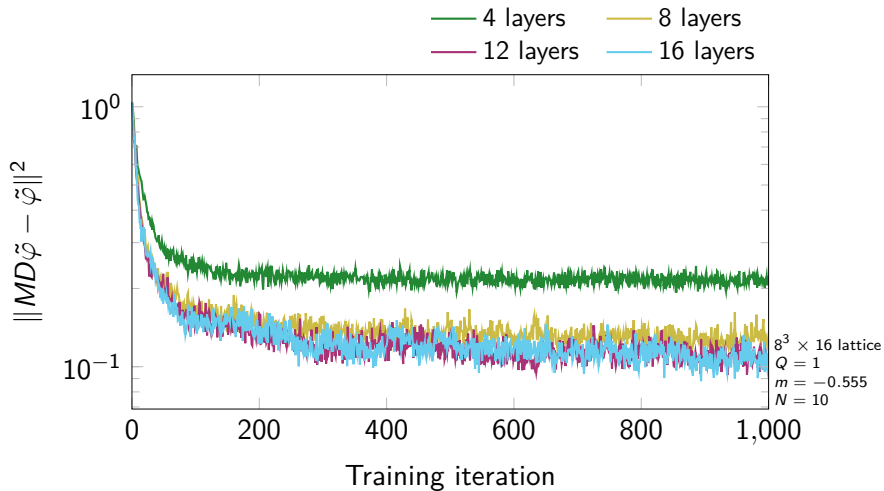


Gauge configurations

$16^3 \times 32$ lattice

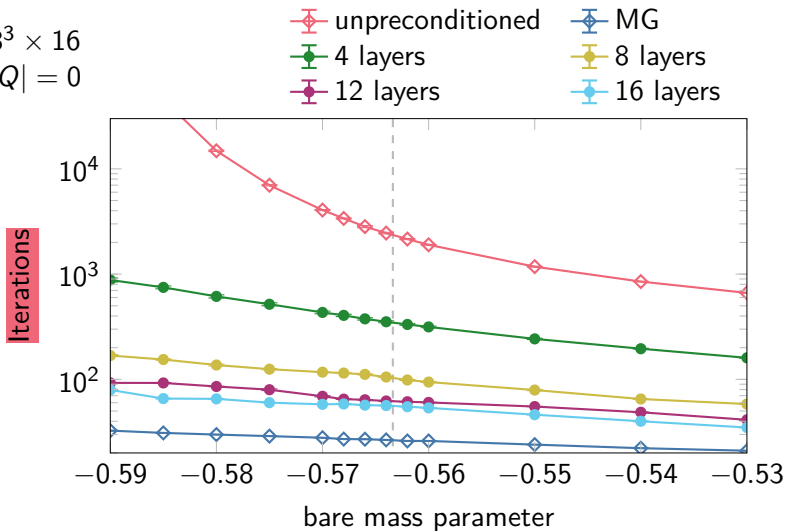


Training cost



Iteration count gain?

$$8^3 \times 16$$
$$|Q| = 0$$

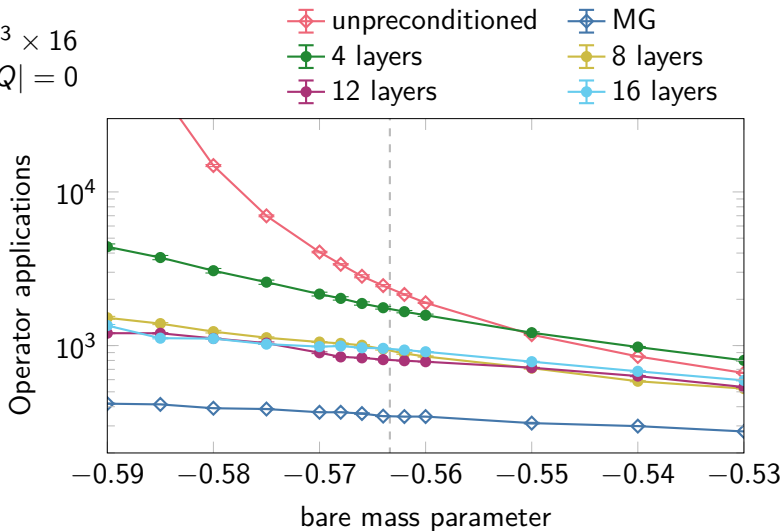


Critical slowing down

$$8^3 \times 16$$
$$|Q| = 0$$

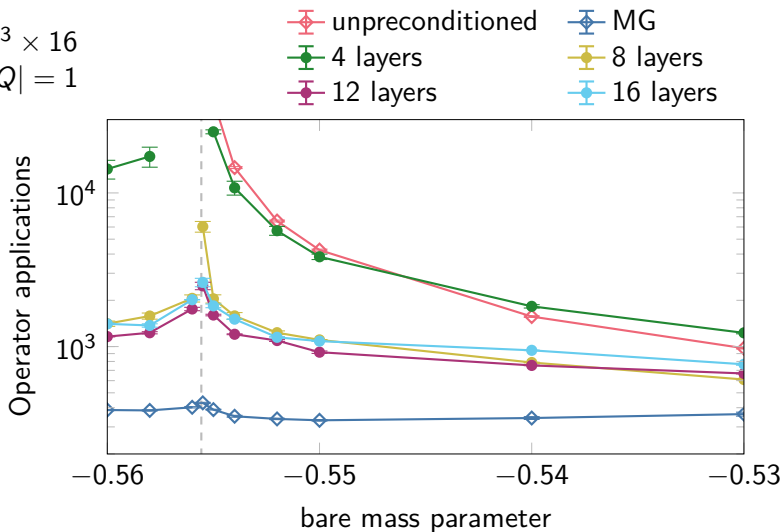
applications of:

- D_{fine}
- PT layer



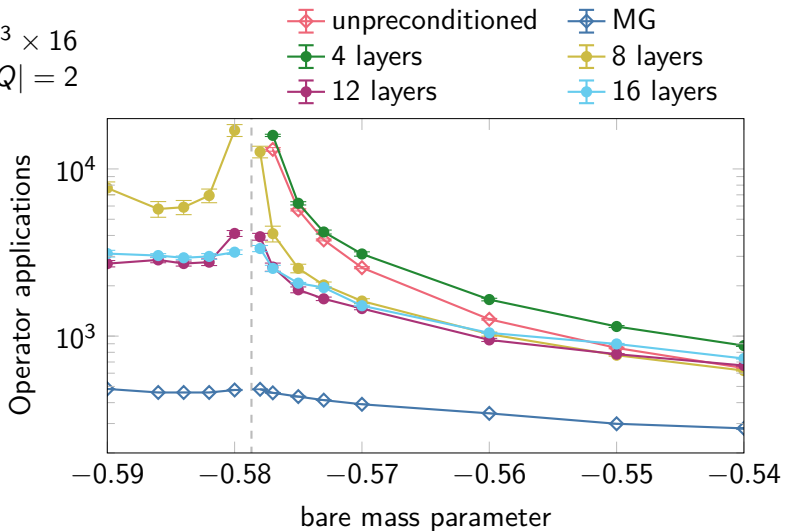
Critical slowing down

$$8^3 \times 16$$
$$|Q| = 1$$



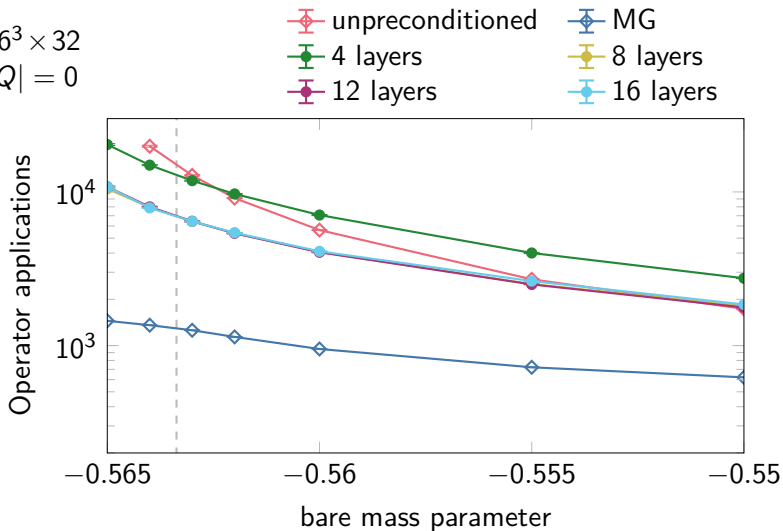
Critical slowing down

$$8^3 \times 16$$
$$|Q| = 2$$



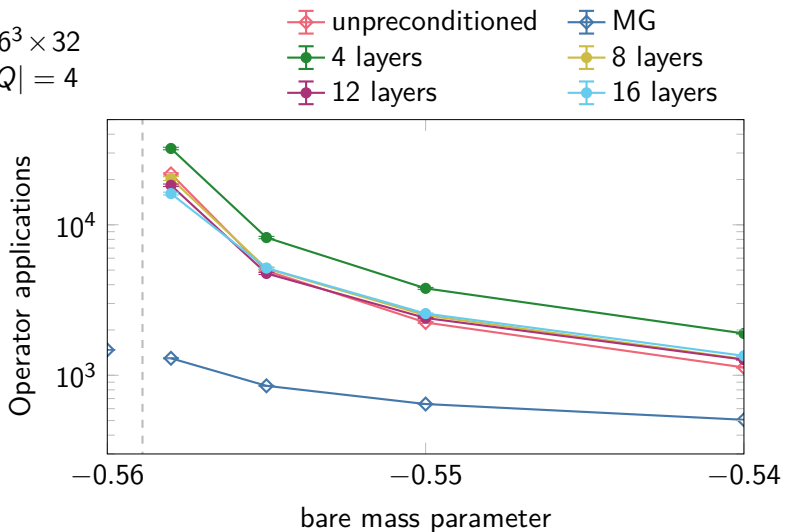
Critical slowing down

$16^3 \times 32$
 $|Q| = 0$



Critical slowing down

$16^3 \times 32$
 $|Q| = 4$



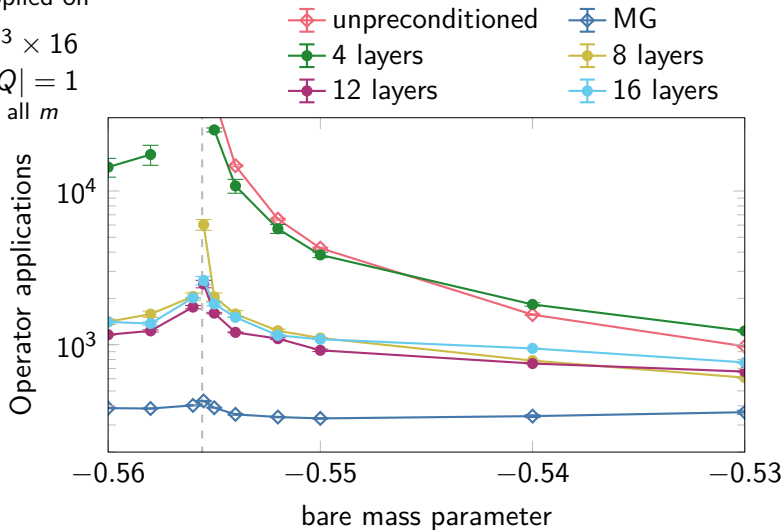
Transfer

trained and
applied on

$$8^3 \times 16$$

$$|Q| = 1$$

all m



Transfer

trained on

$$8^3 \times 16$$

$$|Q| = 0$$

$$m = -0.56$$

applied on

$$8^3 \times 16$$

$$|Q| = 1$$

$$\text{all } m$$

\rightarrow

unpreconditioned

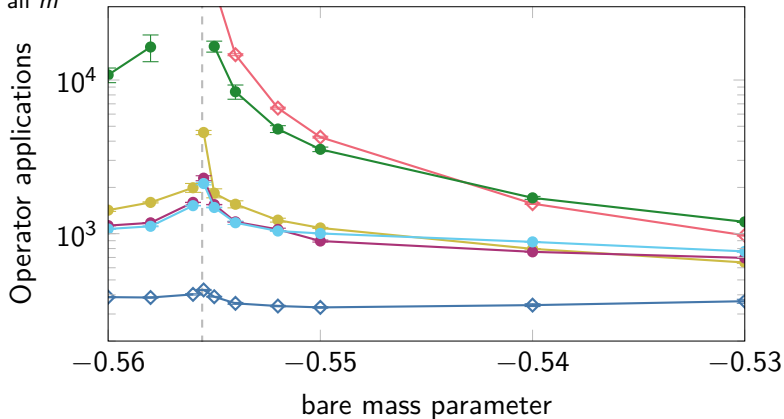
4 layers

12 layers

MG

8 layers

16 layers

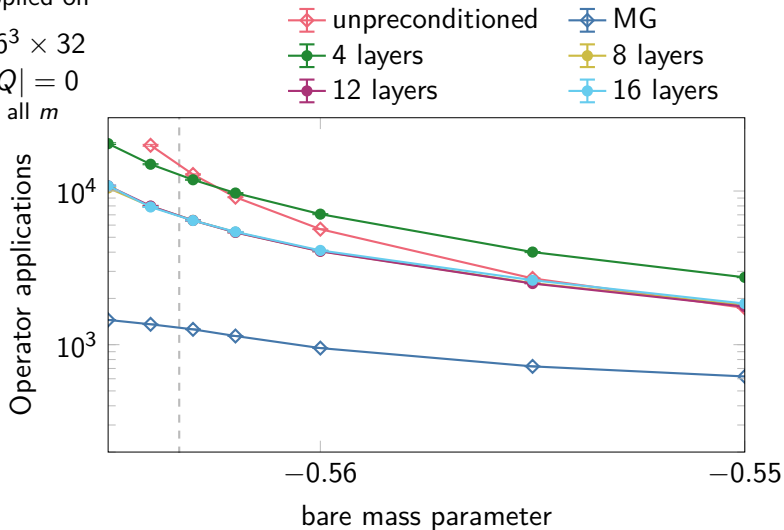


Transfer

trained and
applied on

$16^3 \times 32$

$|Q| = 0$
all m



Transfer

trained on

$$8^3 \times 16$$

$$|Q| = 0$$

$$m = -0.56$$

applied on

$$16^3 \times 32$$

$$|Q| = 0$$

$$\text{all } m$$

→

unpreconditioned

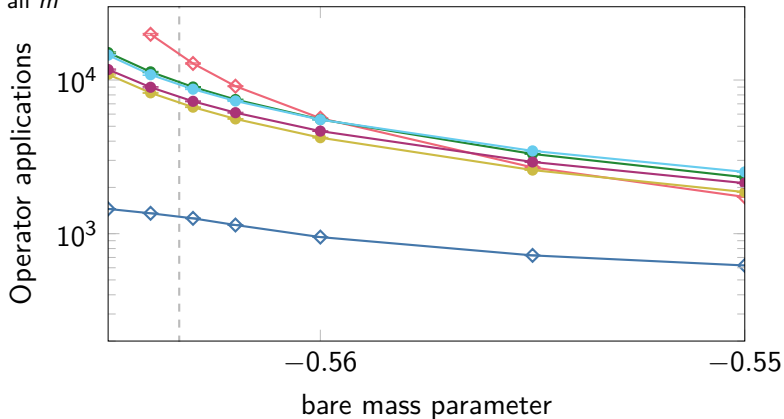
4 layers

12 layers

MG

8 layers

16 layers



The background features several abstract, hand-drawn shapes in muted colors: a teal shape at the top left, a pink shape at the top right, an orange shape at the bottom left, and a purple shape at the bottom right. The central focus is a large, irregular pink shape with a dark blue outline, which contains the word "Conclusion".

Conclusion

Conclusion

Goals

- ✓ Build a preconditioner using ML that mitigates critical slowing down
- ✓ Transfer to unseen configurations without retraining
→ No costly setup
- ✗ Handle topological modes nicely

Next steps

- ▶ Understand why the architecture fails for topological modes
 - ▶ First study easier systems like Laplace operator or Schwinger model
 - ▶ Identify what is problematic about topological modes
- ▶ Explore models to generate representative near-null space vectors economically



Slides and code:
simon-pfahler.github.io