

Physics-informed neural networks for solving FRG

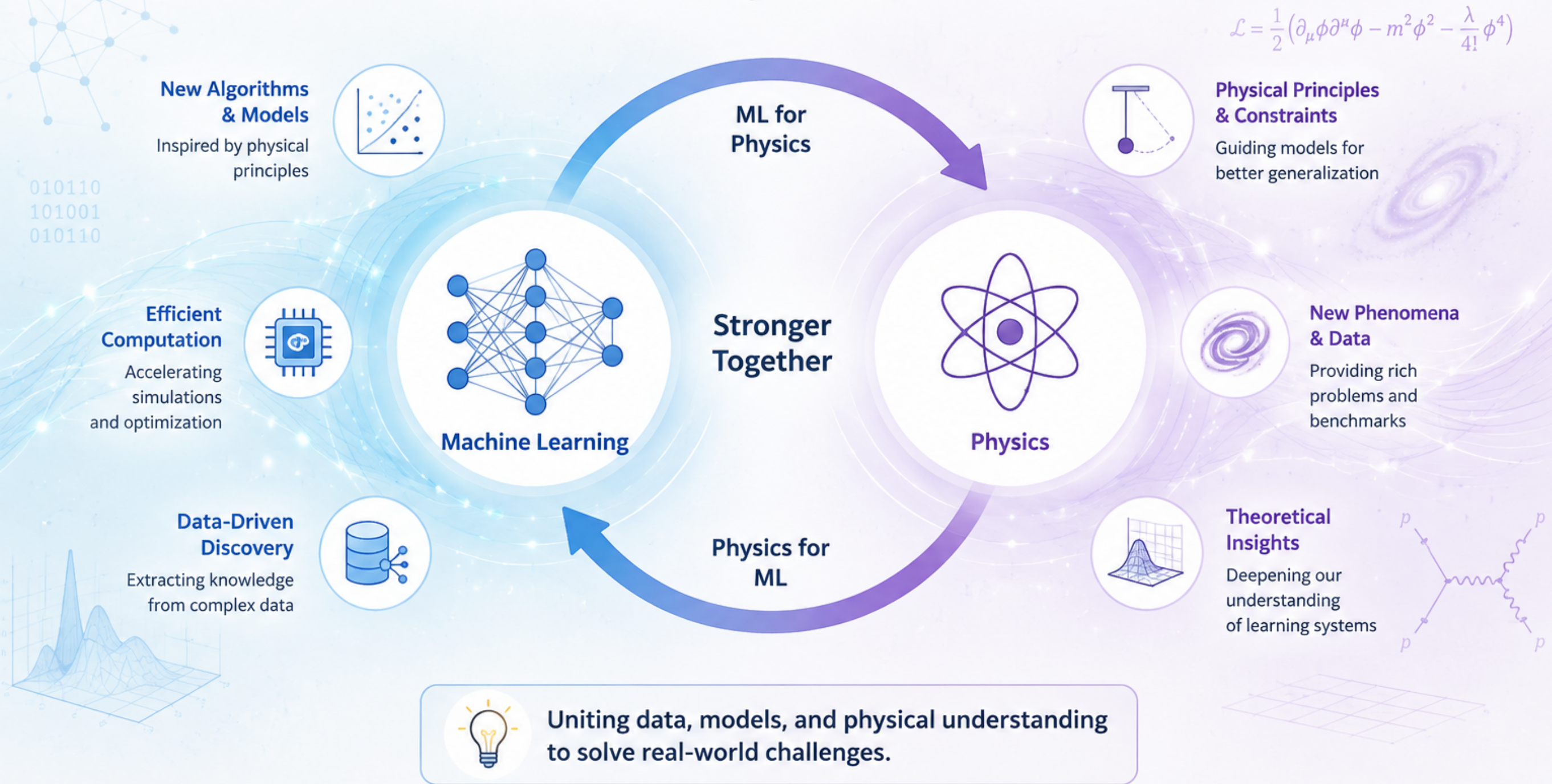
Takeru Yokota (Osaka Institute of Technology, RIKEN iTHEMS)

Refs. [1] TY, Phys. Rev. B 109, 214205 (2024)
[2] Miyagawa, TY, NeurIPS2024 (2024)
[3] TY, in prep

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University of Sussex, Brighton, UK, 4th September 2026

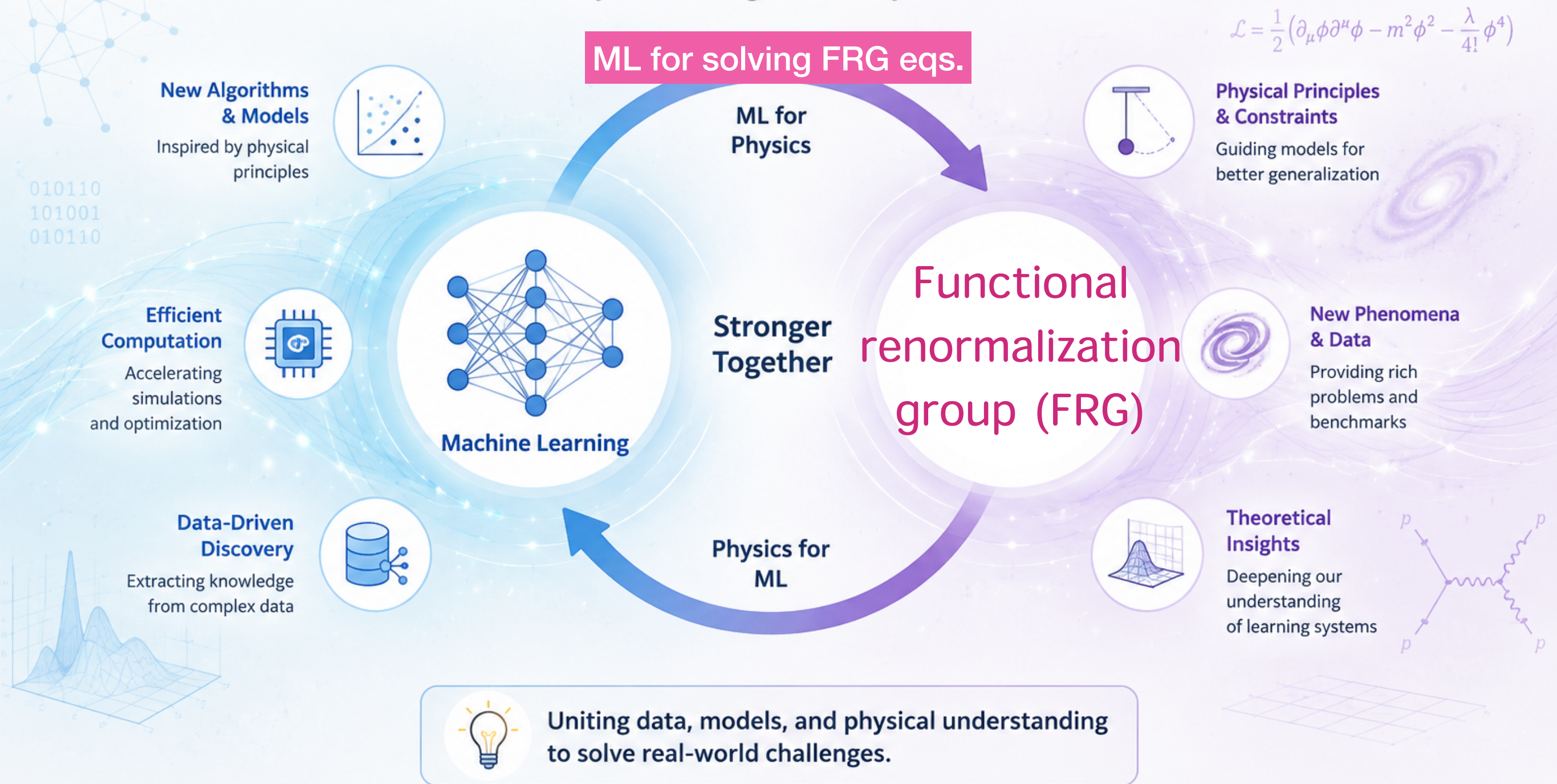
Machine Learning ↔ Physics

A virtuous cycle driving discovery and innovation



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Contents

1. Physics-informed neural networks (PINNs) for FRG

- Motivation & method
- Network architecture

2. Demonstration in a toy model

- Calculation w/ multi-layer perceptron
- Calculation w/ input-convex neural network

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Why is solving FRG eqs. difficult?

Wetterich eq. $\partial_k \Gamma_k[\varphi] = \frac{1}{2} \text{Tr} \left[\partial_k R_k \cdot \left(\frac{\delta^2 \Gamma_k[\varphi]}{\delta \varphi \delta \varphi} + R_k \right)^{-1} \right]$

► Functional diff. eq. (FDE) = Infinite-dim. PDE

- A function ($\varphi(x)$) = An infinite-dim. vector

c.f.) Basis function expansion $\varphi(x) = \varphi_1 e_1(x) + \varphi_2 e_2(x) + \dots$

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► Reduction to finite DOF ($\varphi(x) \rightarrow \boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_M)$)

- Basis function expansion: $\varphi(x) \approx \varphi_1 e_1(x) + \dots + \varphi_M e_M(x)$
- Finite-volume lattice: $\varphi(x) \rightarrow \{\varphi_n\}_{n=1}^M$

$\Rightarrow$ FDE $\approx$ High-dim. PDE (HDPDE)

$$\partial_k \Gamma_k(\boldsymbol{\varphi}) = \frac{1}{2} \text{tr} \left[\partial_k R_k \cdot \left(\text{Hess}_{\boldsymbol{\varphi}} \left(\Gamma_k(\boldsymbol{\varphi}) + \Delta S_k^{\text{reg}}(\boldsymbol{\varphi}) \right) \right)^{-1} \right]$$

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Solving FRG $\approx$ Solving HDPDE

Why is solving FRG eqs. difficult?

Numerically tough!

- ▶ Direct discretization of the input φ suffers from **the curse of dimensionality** (#grid points $\sim \exp(cM)$)
- ▶ Conventional methods: Reduction of PDE by vertex expansion, derivative expansion...
 - Truncation of form of Γ_k based on Taylor expansion

Other possible approaches that retain richer form of $\Gamma_k(\varphi)$?

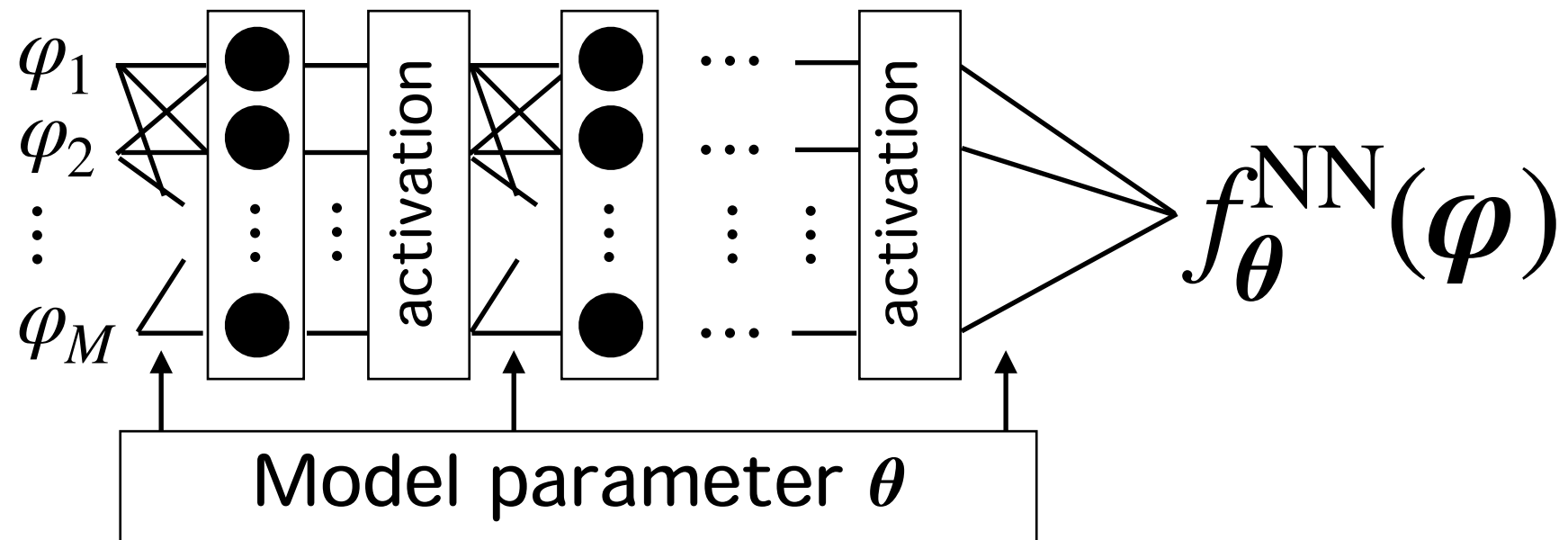
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Solving FRG $\approx$ Solving HDPDE

Neural networks (NNs)

Ansatz for a multivariable function



- ▶ The derivatives $(\frac{\partial}{\partial \varphi} f_{\theta}(\varphi), \frac{\partial^2}{\partial \varphi \partial \varphi} f_{\theta}(\varphi) \dots)$ are efficiently evaluated even for **high-dim. input**.
 - Efficient evaluation via the chain rule (**automatic differentiation**).
 - No explicit grid in the φ -space is required!

Machine-learning-based method for HDPDE & FRG

HDPDE

► Physics-informed NNs (PINNs)

*Psichogios, Ungar, AIChE (1992), Lagaris, Likas, Fotiadis (1998)
Raissi, Perdikaris, Karniadakis (2017); JCP (2019)*

- e.g.) **1M-dim.** PDEs

Z. Shi, Z. Hu, M. Lin, K. Kawaguchi, NeurIPS (2024) Best paper

- Poisson eq., Sine-Gordon eq., Allen-Cahn eq.
- Few minutes on a single NVIDIA A100 GPU
- Typical error $\lesssim 1\%$ compared to exact solutions

- **FRG** *TY, PRB (2024); TY, in prep*

- Demonstration: Up to 101-dim. PDE

► Rayleigh-Ritz variational method

E, Yu, Comm. Math. Stat. (2018), Khoo, Lu, Ying, Res. Math. Sci. (2018),...

► Backward stochastic differential equation...

*E, Han, Jentzen, Comm. Math. Stat. (2017), Han, Jentzen, E (2018), Raissi (2018),
Beck, E, Jentzen, J. Nonlinear Science (2019),...*

Other ML-based studies for solving FRG eqs.

► Gaussian process

Yang, Darcy, Hudes, Alexander, Eyink, Owhadi, J. Comp. Phys. (2026)

- 2-dim. PDE demonstration

► PINN-based method for LPA flow eq.

Tan, Fu, He, Wang, PRD (2026)

Yang-yang's talk

Machine-learning-based method for HDPDE & FRG

HDPDE

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Today's talk!

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Yang-yang's talk

PINNs for FRG (PINN-FRG)

TY, PRB (2024)

► NN ansatz for the solution: $\Gamma_k(\varphi) \approx f_{\theta}^{\text{NN}}(k, \varphi)$

► Loss for optimization of $f_{\theta}^{\text{NN}}(k, \varphi)$

$$L(\theta) = \frac{1}{N_{\text{col}}} \sum_{i=1}^{N_{\text{col}}} r_{\theta} \left(k^{(i)}, \varphi^{(i)} \right)^2$$

- Residual (LHS – RHS of the Wetterich eq.)

$$r_{\theta}(k, \varphi) = \partial_k f_{\theta}^{\text{NN}}(k, \varphi) - \frac{1}{2} \text{tr} \left[\partial_k R_k \cdot \left(\text{Hess}_{\varphi} \left(f_{\theta}^{\text{NN}}(k, \varphi) + \Delta S_k^{\text{reg}}(\varphi) \right) \right)^{-1} \right]$$

- $(k^{(i)}, \varphi^{(i)})$ ($i = 1, \dots, N_{\text{col}}$): Collocation points
 - Sampled from $k_{\text{IR}} \leq k \leq k_{\text{UV}}$ & the domain of φ

► The initial condition $\Gamma_{k_{\text{UV}}}(\varphi) = S(\varphi)$ (bare action) is implemented in the ansatz $f_{\theta}^{\text{NN}}(k, \varphi)$.

NN architecture for stable training

- ▶ Multi-layer perceptron (MLP) based model for $f_{\theta}^{\text{NN}}(k, \varphi)$ TY, PRB (2024)

- But, the convexity of $f_{\theta}^{\text{NN}}(k, \varphi) + \Delta S_k^{\text{reg}}(\varphi)$ is not guaranteed

$$r_{\theta}(k, \varphi) = \partial_k f_{\theta}^{\text{NN}}(k, \varphi) - \frac{1}{2} \text{tr} \left[\partial_k R_k \cdot \left(\text{Hess}_{\varphi} \left(f_{\theta}^{\text{NN}}(k, \varphi) + \Delta S_k^{\text{reg}}(\varphi) \right) \right)^{-1} \right]$$

- Loss of convexity → Loss of Hessian regularity
→ Breakdown of matrix inv. calc. → Breakdown of training

NN architecture for stable training

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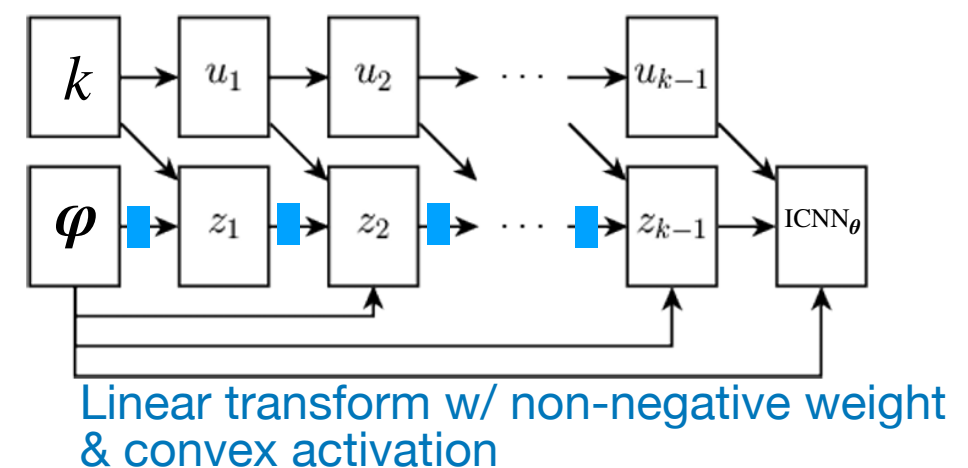
- ▶ Input convex NN (ICNN) for $f_{\theta}^{\text{NN}}(k, \varphi)$

- ICNN guarantees the convexity

Amos, Xu, Kolter, ICML (2017)

- Ansatz for $f_{\theta}^{\text{NN}}(k, \varphi)$

TY, in prep



$$f_{\theta}^{\text{NN}}(k, \varphi) = \lambda_{\theta_1}(k) \left(S(\varphi) + \Delta S_{k_{\text{UV}}}^{\text{reg}}(\varphi) \right) + \left(1 - \lambda_{\theta_1}(k) \right) \text{ICNN}_{\theta_2}(k, \varphi) - \Delta S_k^{\text{reg}}(\varphi)$$

- $\lambda_{\theta_1}(k)$: Gate function ($\lambda_{\theta_1}(k_{\text{UV}}) = 1, 0 \leq \lambda_{\theta_1}(k) \leq 1$)
- The convexity & initial condition are satisfied.

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Toy-model demonstration: 0-dim classical $O(N)$ model

Model

$$S(\boldsymbol{\varphi}) = \frac{1}{2}m^2\boldsymbol{\varphi}^2 + \frac{g}{4!}(\boldsymbol{\varphi}^2)^2$$

- Exactly solvable E.g., Keitel, Bartosch, JPA (2012)
- Non-perturbative region: $\tilde{g} = Ng/m^4 \gtrsim 1$

- ▶ Wetterich eq.: $(N+1)$ -dim. PDE (We do **not** use the reduction of variable $\boldsymbol{\varphi} \rightarrow \rho = \boldsymbol{\varphi}^2$)
- ▶ We calculate $\Gamma_k(\boldsymbol{\varphi})$ for $1 \leq N \leq 100$ and both $m^2 > 0$ and $m^2 < 0$ cases
 - The convexity problem becomes severe for $m^2 < 0$.

PINN-FRG setup

- ▶ Regulator: $R_k = k^2 \mathbf{1}_{N \times N}$
- ▶ NN: (1) MLP based model TY, PRB (2024)

$$f_{\theta}^{\text{NN}}(k, \boldsymbol{\varphi}) = S(\boldsymbol{\varphi}) + \text{MLP}_{\theta}(k, \boldsymbol{\varphi}) - \text{MLP}_{\theta}(k_{\text{UV}}, \boldsymbol{\varphi})$$

MLP structure: 3 hidden layers, 256 units/layer, Softplus activation functions

(2) ICNN based model TY, in prep

$$f_{\theta}^{\text{NN}}(k, \boldsymbol{\varphi}) = \lambda_{\theta_1}(k) \left(S(\boldsymbol{\varphi}) + \Delta S_{k_{\text{UV}}}^{\text{reg}}(\boldsymbol{\varphi}) \right) + \left(1 - \lambda_{\theta_1}(k) \right) \text{ICNN}_{\theta_2}(k, \boldsymbol{\varphi}) - \Delta S_k^{\text{reg}}(\boldsymbol{\varphi})$$

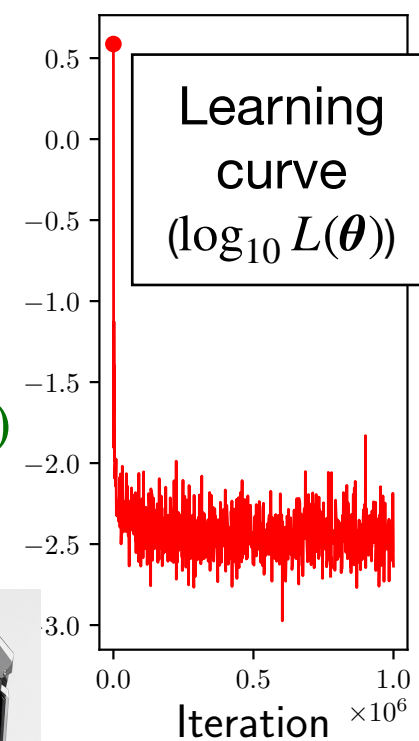
ICNN structure: 4 hidden layers, 64 units/layer, Softplus & tanh activation functions

- ▶ Time for optimization: few minutes ~ few hours

- Resource: NVIDIA A100 & RTX5080 GPU

- Code implementation: PyTorch

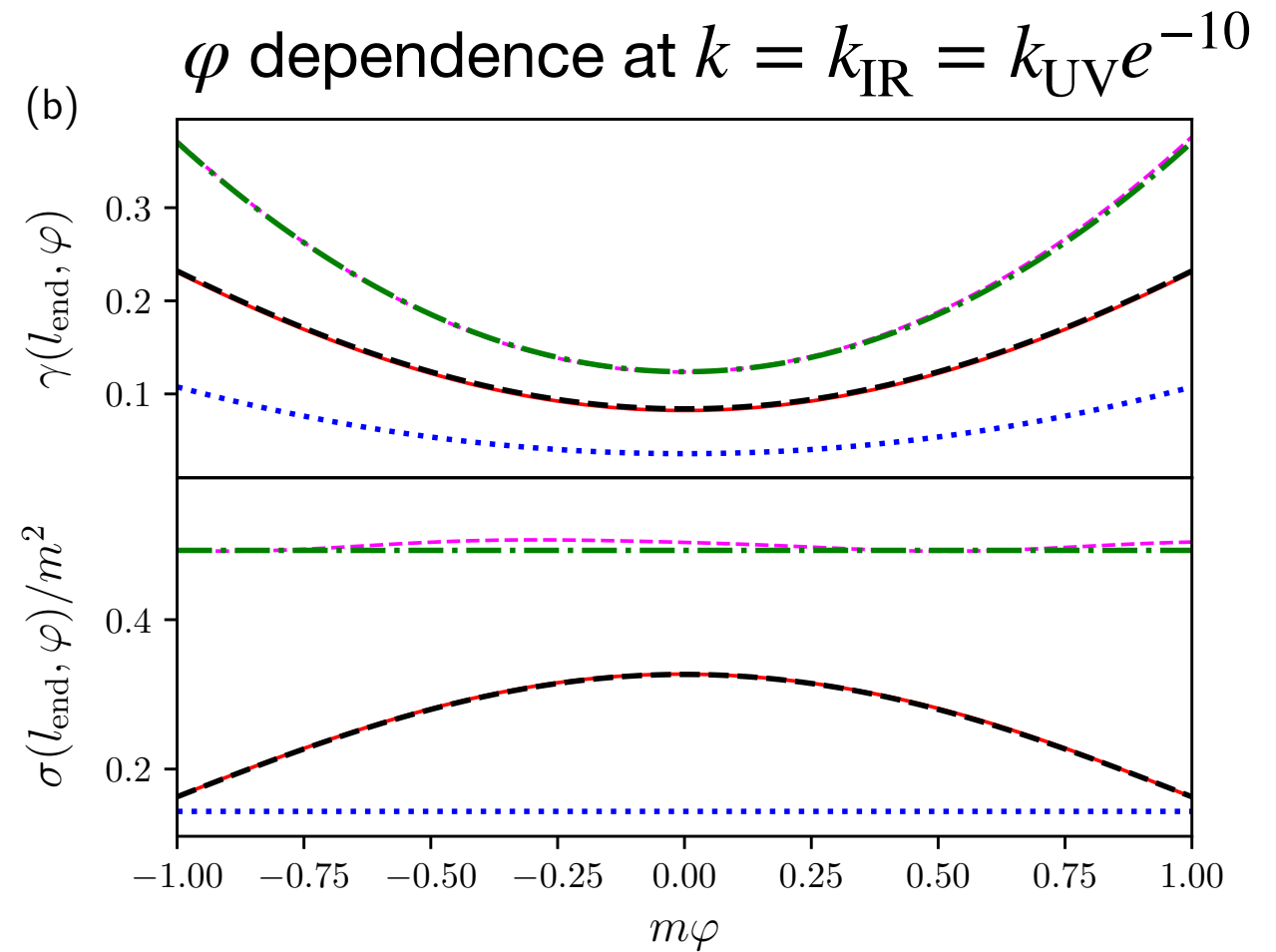
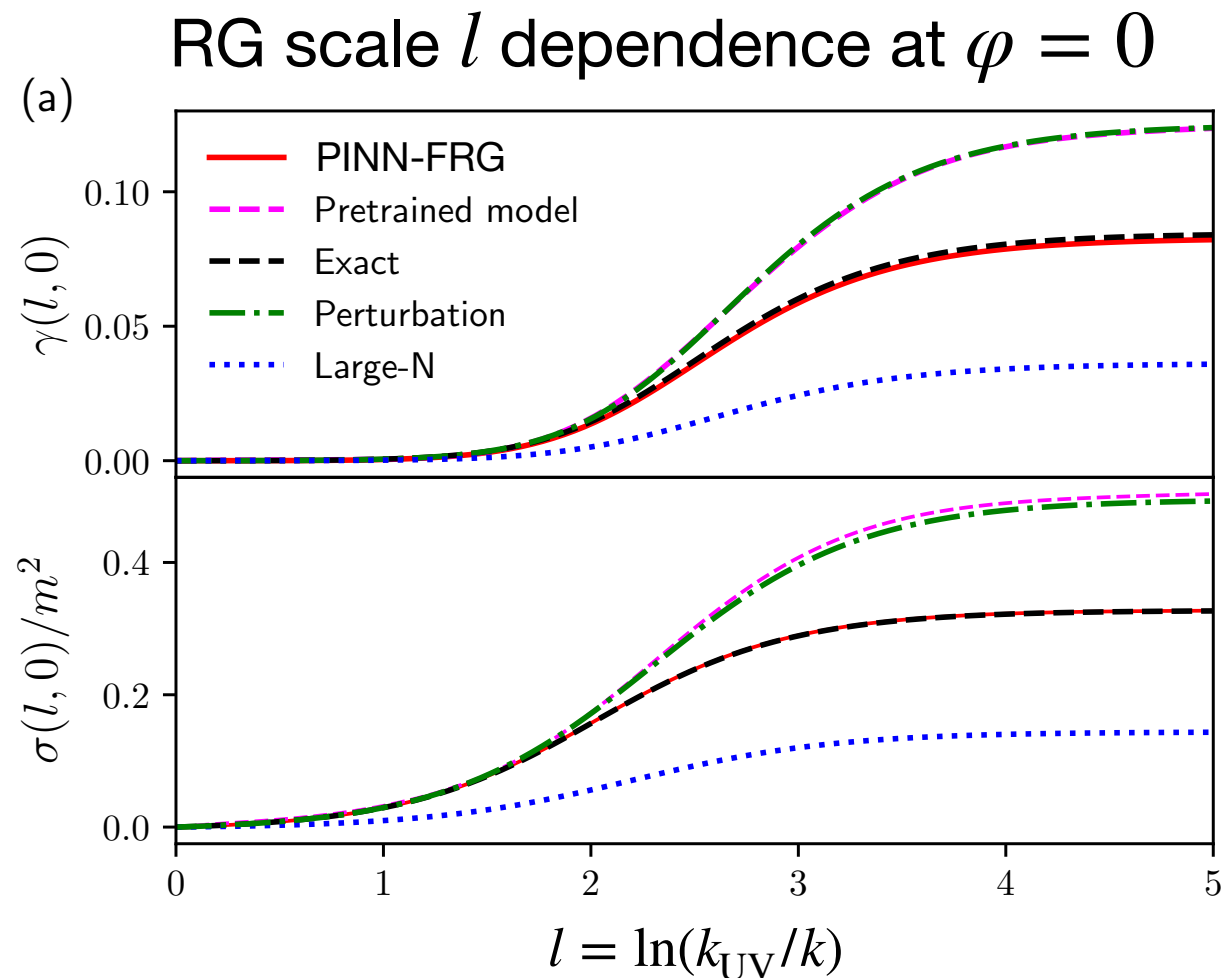
- <https://github.com/TakeruYokota/PINNLFRG.git>



$N = 1, \tilde{g} = 1, m^2/k_{UV}^2 = 0.01$ case (MLP based model)

TY, PRB (2024)

- Reduced effective action: $\gamma(l, \varphi) = \Gamma_k(\varphi) - S(\varphi) - \Delta\Gamma_k^{\text{free}}$ ($l = \ln(k_{UV}/k)$)
- Reduced self-energy $\sigma_\alpha(l, \varphi) = \frac{\partial^2}{\partial \varphi_\alpha^2} \gamma(l, \varphi)$



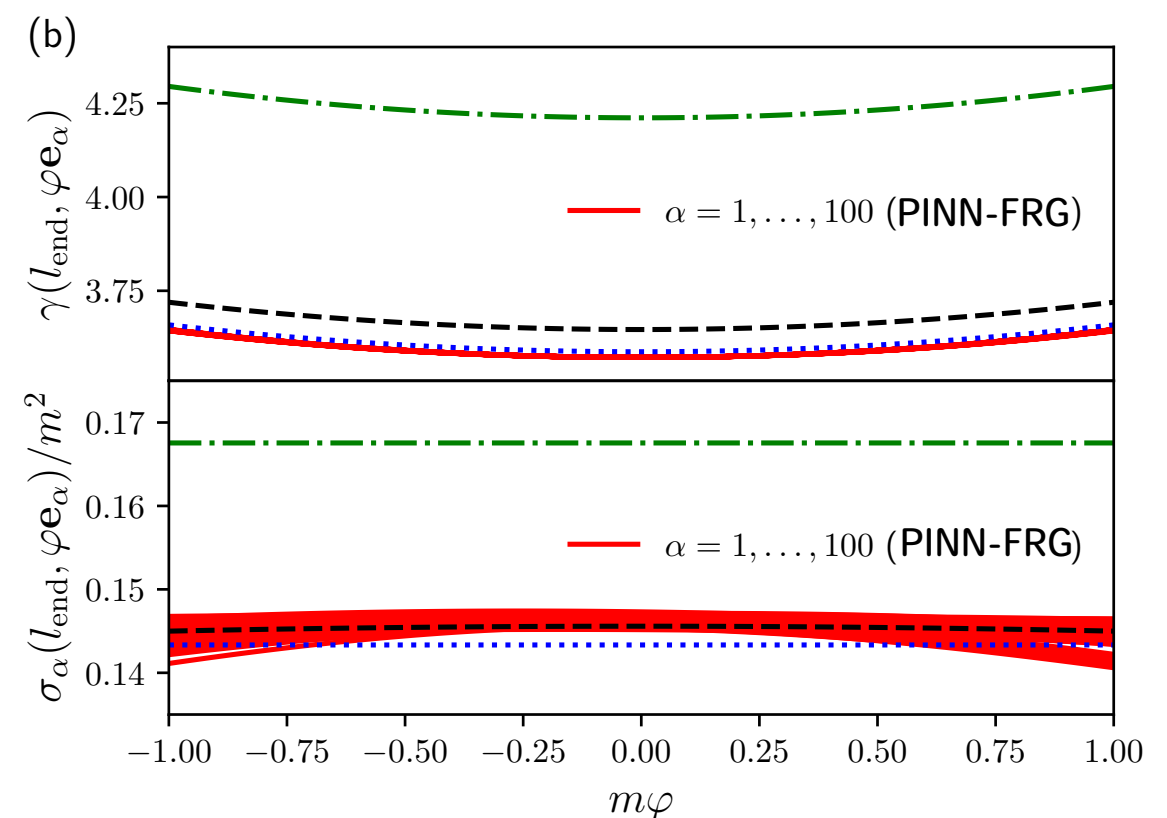
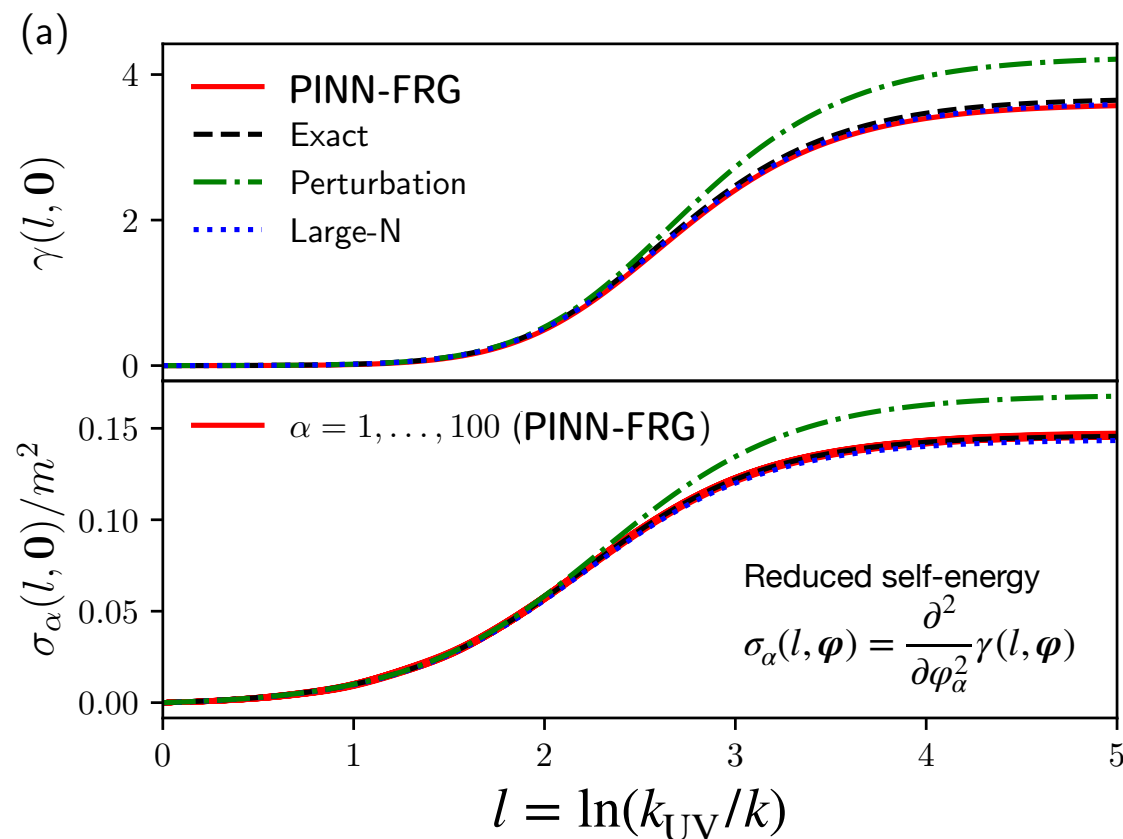
- $\gamma(l, \varphi)$ is simultaneously obtained for a domain of φ in our method (PINN-FRG).
- PINN-FRG shows accurate results compared to 1st-order perturbation & leading-order large-N expansion

$N = 100, \tilde{g} = 1, m^2/k_{\text{UV}}^2 = 0.01$ case (MLP based model)

TY, PRB (2024)

RG scale l dependence at $\varphi = 0$

φ dependence at $k = k_{\text{IR}} = k_{\text{UV}}e^{-10}$

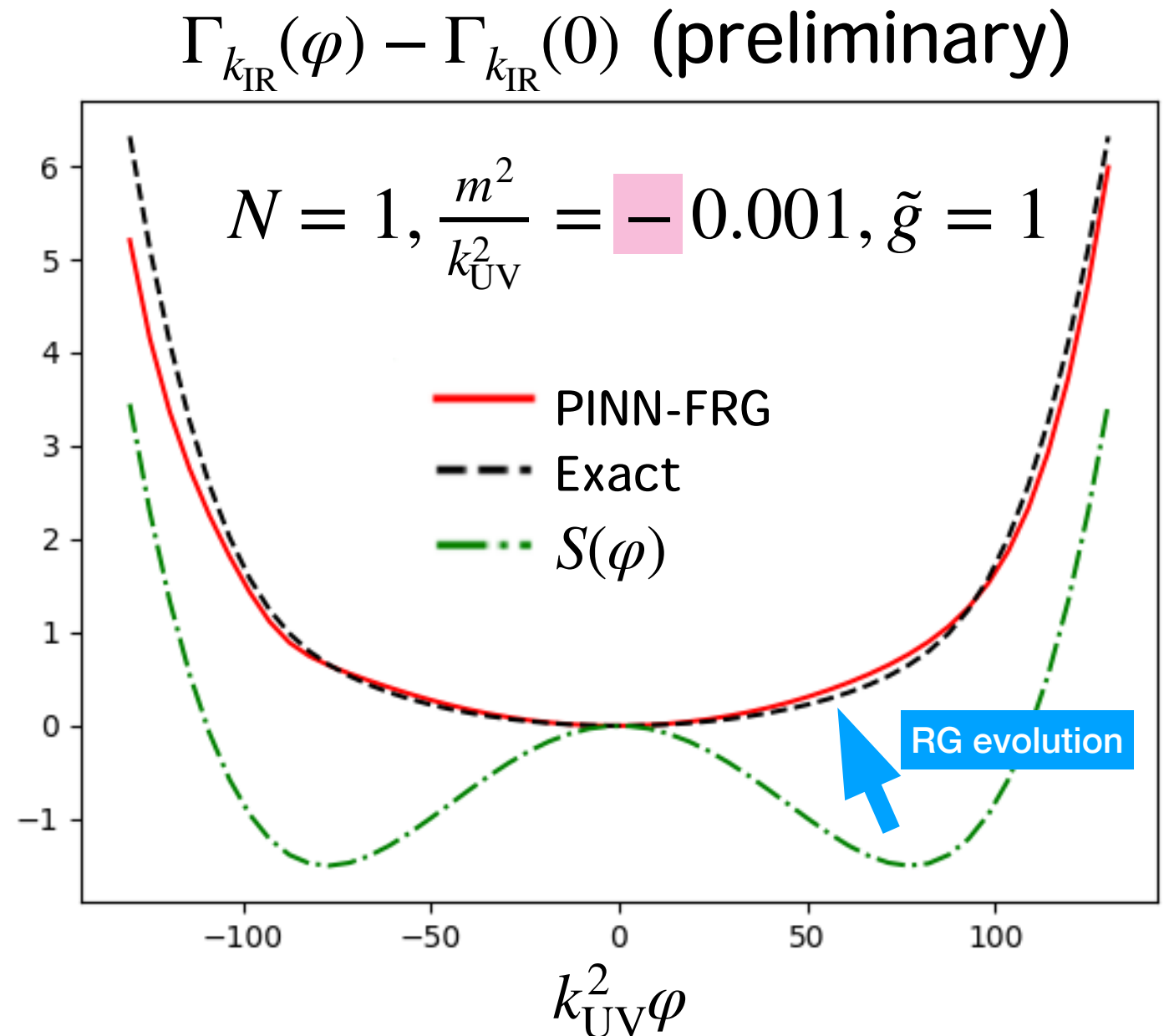


- ▶ Except for $\gamma(l, \mathbf{0})$, PINN-FRG results are given by $N = 100$ lines corresponding to the N -direction in φ space.
- ▶ PINN-FRG shows comparable results with large-N expansion, which should be accurate for $N = 100$.
- ▶ $O(N)$ symmetry is reproduced in PINN-FRG.

$m^2 < 0$ case (ICNN based model)

TY, in prep

- ▶ In the case of MLP-based models, the loss of convexity becomes severe, causing the training to fail.
- ▶ In models based on ICNN, there is no loss of convexity, and the calculations can be performed.



Next step: Localization phase transition in the Caldeira-Leggett model

- Double-well potential + external noise
- 0-dim. quantum model

Summary

TY, PRB (2024)
TY, in prep

- ▶ **Physics-informed neural networks (PINNs)** may offer a new approach to solving FRG eqs.
- ▶ The use of **input convex neural networks (ICNNs)** is key to the success of PINN-FRG.
- ▶ We have demonstrated the performance of PINN-FRG using 0-dim. classical $O(N)$ model.
 - Numerical demonstration up to **101-dim.** PDE

Outlook

- ▶ Application to the localization phase transition in the Caldeira-Leggett model
- ▶ Application to other functional diff. eqs. *Miyagawa, TY, NeurIPS2024 (2024)*
 - Fokker-Planck, Hopf...

Backup

Hessian's invertibility & pretraining (MLP)

$$L_{\theta} = \mathbb{E}_{\substack{\varphi \sim \mathcal{P}_{\varphi} \\ l \sim \mathcal{P}_l}} \left[\left(\partial_l \Gamma_l^{\theta}(\varphi) - \frac{1}{2} \text{tr} \left[\partial_l R_l \left(\frac{\partial^2 \Gamma_l^{\theta}(\varphi)}{\partial \varphi \partial \varphi} + R_l \right)^{-1} \right] \right)^2 \right]$$


The matrix must be invertibility during the training.

In our experience, this is frequently broken with randomly chosen θ .

Pretraining with some approximate analytic results remedies this problem

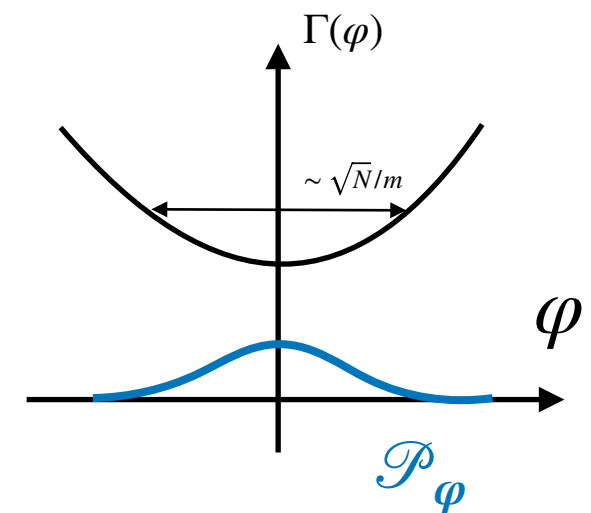
We use 1st-order perturbative result:

$$L_{\theta}^{\text{pre}} = \mathbb{E}_{\substack{\varphi \sim \mathcal{P}_{\varphi} \\ l \sim \mathcal{P}_l}} \left[\left(\gamma(l, \varphi; \theta) - \gamma^{\text{1pt}}(l, \varphi) \right)^2 \right]$$

Other details of numerical procedure

$$L_{\theta} = \mathbb{E}_{\substack{\boldsymbol{\varphi} \sim \mathcal{P}_{\boldsymbol{\varphi}} \\ l \sim \mathcal{P}_l}} \left[\left(\partial_l \Gamma_l^{\theta}(\boldsymbol{\varphi}) - \frac{1}{2} \text{tr} \left[\partial_l R_l \left(\frac{\partial^2 \Gamma_l^{\theta}(\boldsymbol{\varphi})}{\partial \boldsymbol{\varphi} \partial \boldsymbol{\varphi}} + R_l \right)^{-1} \right] \right)^2 \right]$$

- ▶ $\mathcal{P}_l$: uniform distribution in $[0, l_{\text{end}}]$ with $l_{\text{end}} = 5$
- ▶ $\mathcal{P}_{\boldsymbol{\varphi}}$: $\|\boldsymbol{\varphi}\|$ is sampled following $N(0, N/m^2)$ (w/o sign)
 $\hat{\boldsymbol{n}} = \boldsymbol{\varphi}/\|\boldsymbol{\varphi}\|$ is uniformly sampled
 - * The variance N/m^2 is needed to learn the shape of Γ .
 - * Other choices such as $N(\mathbf{0}, m^{-2}\mathbf{1})$ fail to sample the neighborhoods of $\boldsymbol{\varphi} = \mathbf{0}$ due to curse of dimensionality
- ▶ 500 collocation points are used to evaluate the expectation.
- ▶ Adam optimizer
- ▶ Pytorch
- ▶ The matrix inverse is evaluated by direct method
 - ▶ This may not be efficient but is easy to implement (`torch.linalg.inv`)



Computational time & convergence (MLP)

We conduct computations for all the combinations of

$$N = 1, 10, 100 \text{ and } \tilde{g} = 0.1, 1, 10 \quad \tilde{g} = Ng/m^4$$

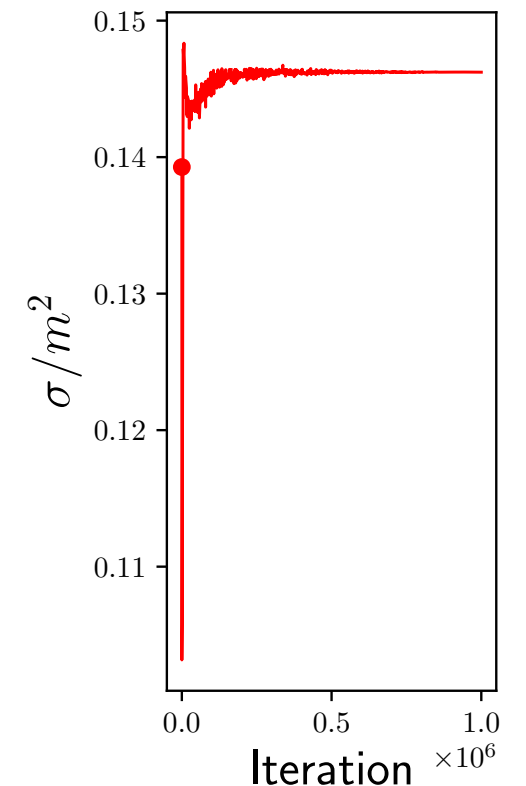
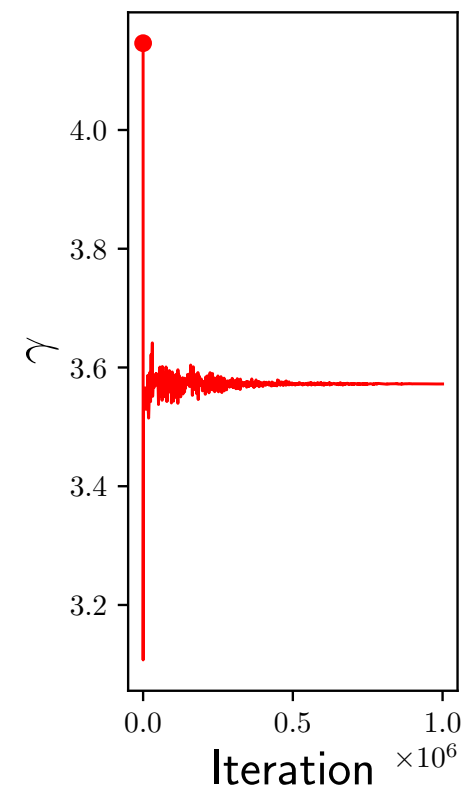
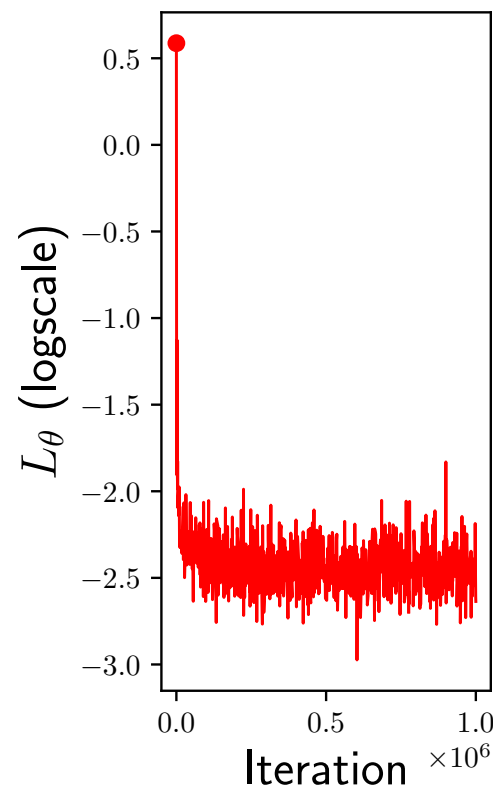
- ▶ Learning rate (Wetterich): 10^{-4} with exponential decay factor 0.99999
- ▶ Learning rate (pretraining): 10^{-3}

Learning curve & histories of physical quantities
($N = 100$ & $\tilde{g} = 1$ case)

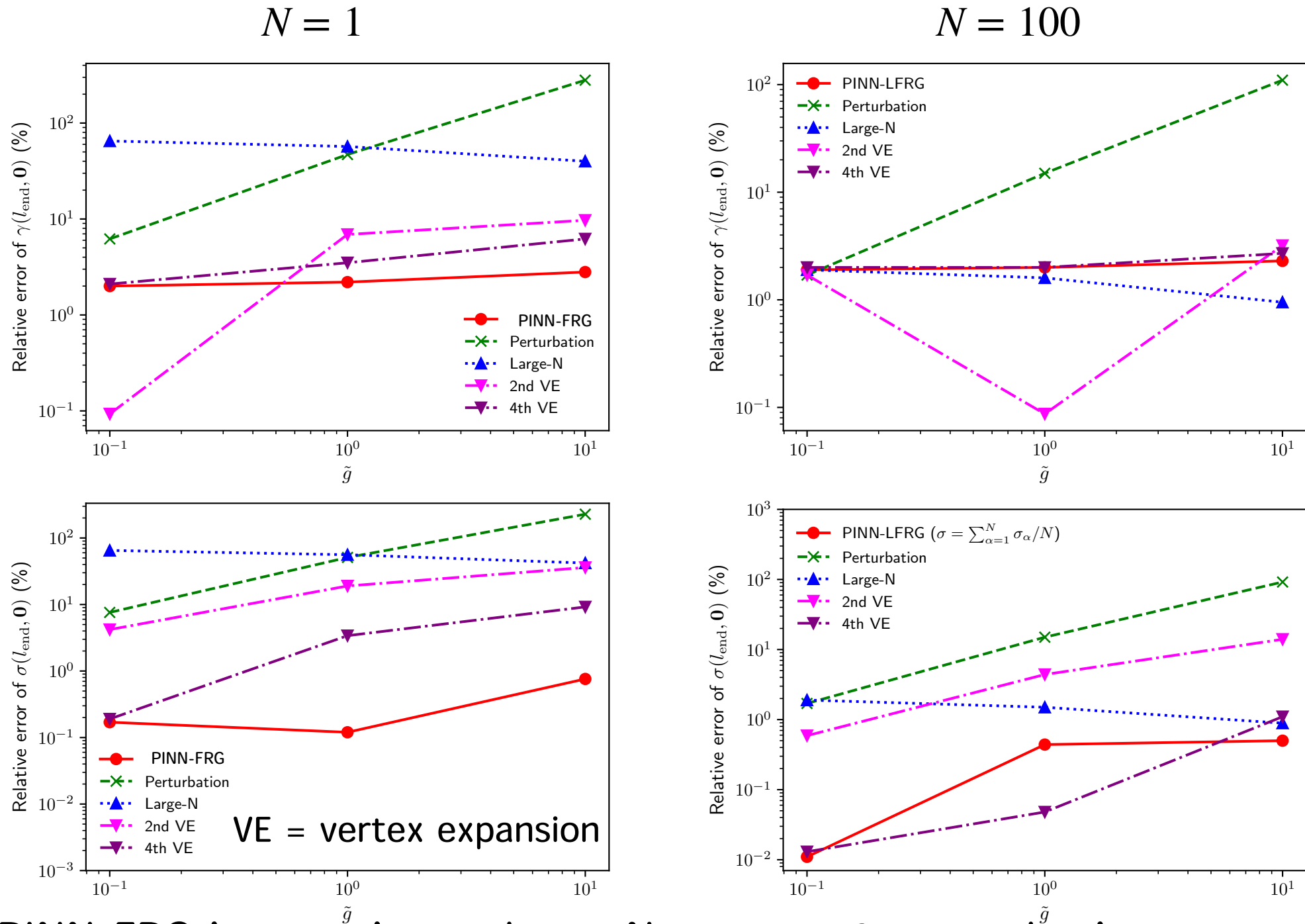
Comp. time on NVIDIA A100 GPU

N	1	10	100
Pretraining	4m	4m	6m
Wetterich	6h	7h	11h

* At larger N ($\gtrsim 1000$),
we ran out of memory.



Relative errors at $\varphi = 0$ for different N and $\tilde{g}$ (MLP)



- ▶ PINN-FRG is superior to large-N at $N=1$ & perturbation
- ▶ PINN-FRG shows better accuracy at non-perturbative region ($\tilde{g} = 10$) compared to 2nd & 4th VE.