Challenges in Theoretical Physics

Koji Hashimoto (Kyoto U.)
Director of MLPhys, Director of ARiSE AI4MP



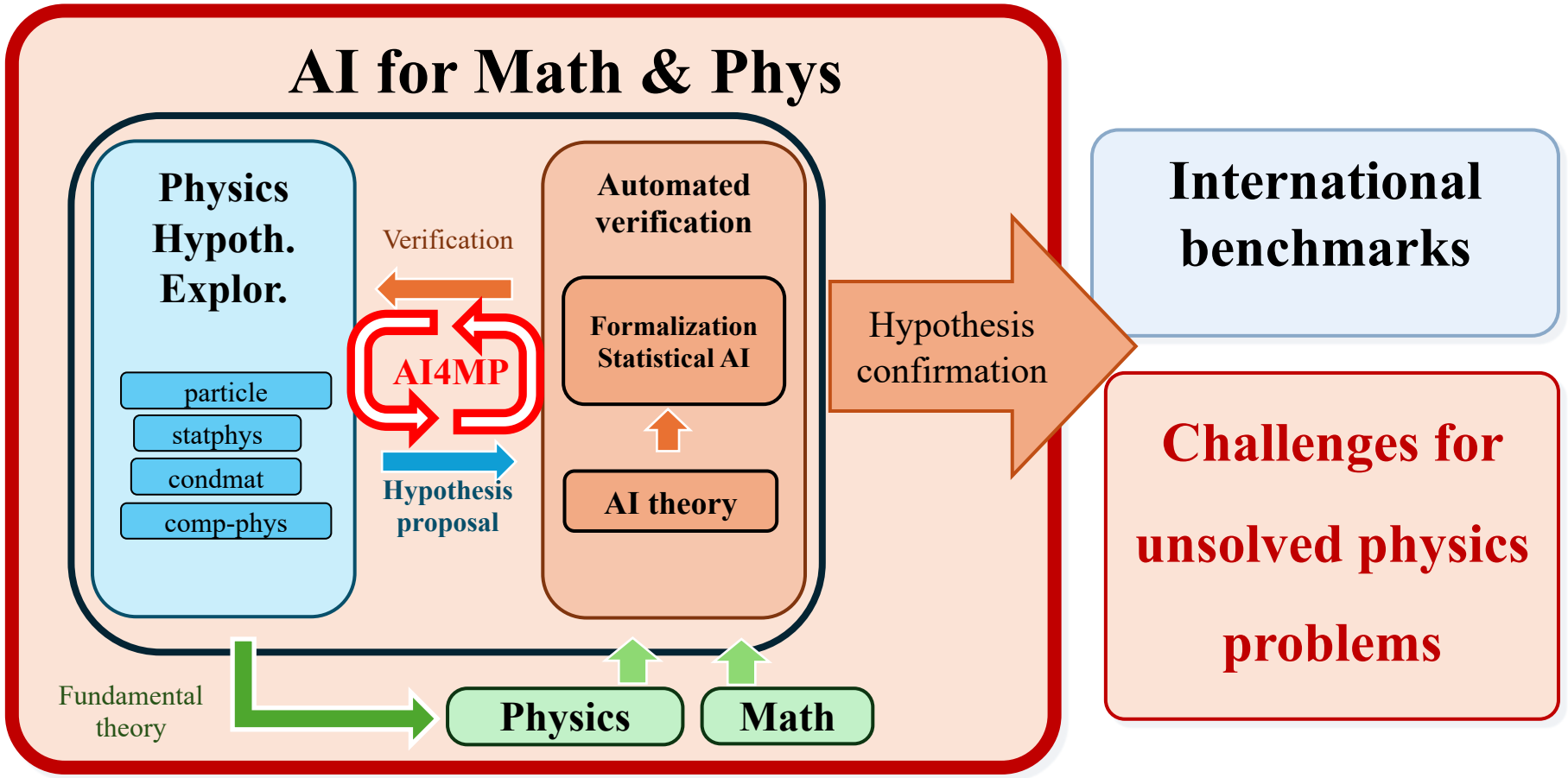
The challenge is:

to keep
our sustainable community of theorists,
to cope and develop with AI agents

ARiSE AI4MP (2026-2029, 4M USD)

Director: Koji Hashimoto, Co-director: Masataka Imaizumi
+ A.Tomiya + T.Otsuki + M.Nojiri + Y.Kabashima + M.Sugiyama + S.Iso

AI agents with math and physics verification for unsolved physics problems





MLPhYs

Foundation of "Machine Learning Physics"





Deep learning and physics 2018

研究会「深層学習と物理2018」

> 大阪大学　南部陽一郎ホール
>
> 2018年6月1日～2日
>
> 招待講演者（敬称略）：
> 青木健一（金沢大），安藤康伸（産総研），大関真之(東北大)，
> 大槻東巳（上智大），柏浩司（福岡工業大），久良尚任（東大），
> 斎藤弘樹（電通大），柴正太郎（KEK），福嶋健二（東大），
> 藤田浩之（東大物性研），田中章詞（理研），富谷昭夫（CCNU），
> 永井佑紀（原子力機構），橋本幸士（阪大）



> 組織委員：
> 田中章詞（理研）
> 富谷昭夫（CCNU）
> 永井佑紀（原子力機構）
> 橋本幸士（阪大）



Deep Learning And Physics

DLAP2019

> Yukawa Institute for Theoretical Physics
> Kyoto, Japan
> 31 Oct - 2 Nov 2019

Target scope of Conference

Deep learning plays a central role in recent developments in research in artificial intelligence (AI). Various ideas based on physics are found in the research of deep learning, and consequently, deep learning and physics are related intimately. This international conference is dedicated to (1) applications of deep learning to physics, (2) discovering similarities among deep learning and physics, and (3) leading to new paradigm in physics motivated by deep learning. Researchers in related fields are welcome to attending discussions at the conference.

Organizers

Koji Hashimoto (Osaka U), Masatoshi Imada (Toyota RIKEN / Waseda U), Kouji Kashiwa (Fukuoka Institute of Technology), Yuki Nagai (JAEA), Masayuki Ohzeki (Tohoku U), Enrico Rinaldi (Riken & Arithmer Inc.), Akinori Tanaka (RIKEN AIP), Akio Tomiya (Riken BNL)



2020: DLAP seminar series started (now 82th)

Deep learning and Physics

Project maintained by cometscome　　Hosted on GitHub Pages — Theme by mattgraham

「ディープラーニングと物理学　オンライン」とはオンラインWeb会議システムを利用したセミナーです。2023年10月より、学習物理領域セミナーと合同で開催されています。

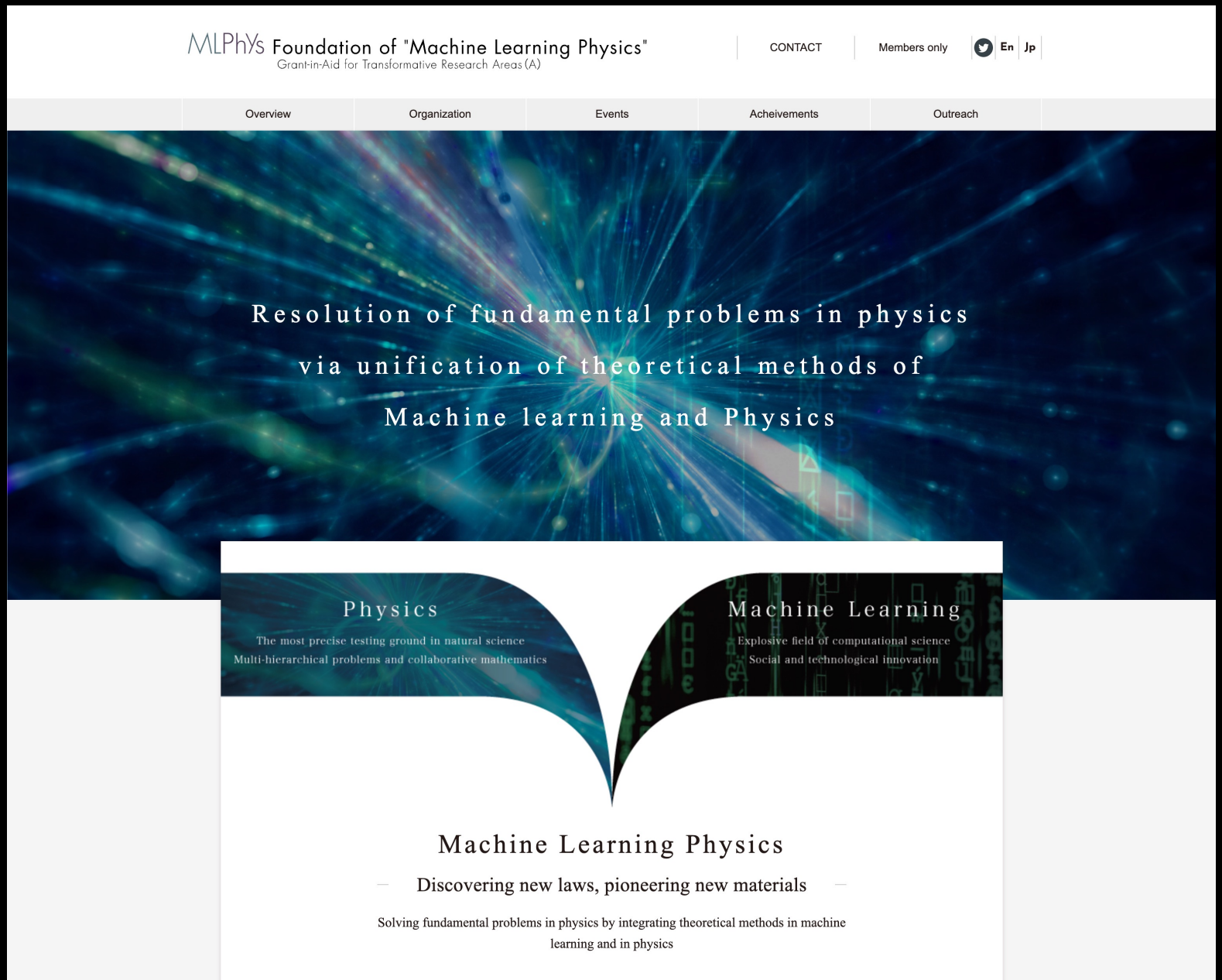
DLAP世話人:　橋本幸士（京都大)、富谷昭夫（東京女子大)、永井佑紀（東京大)、田中章詞（理研AIP/iTHEMS）(順不同)

領域セミナー世話人：橋本幸士（京都大)、広野雄士（大阪大)、三内顕義（京都大)、金子隆威（上智大）(順不同)

本セミナーシリーズは、科学研究費補助金学術変革領域研究(A)「学習物理学の創成」の補助を受けております。

- 第30回領域セミナ・第82回DLAP：　松原 崇 氏 「データの幾何学と深層学習　～画像やテキストの構造を見つける～」 7/23
- 第29回領域セミナ・第81回DLAP：　野村 悠祐 氏 「機械学習手法を用いた量子多体問題の解析」 7/9
- 第28回領域セミナ・第80回DLAP：　野尻 美保子 氏 「科学計算コード生成におけるLLMエージェントのタスク分解と監査」 6/25
- 第27回領域セミナ・第79回DLAP：　Ling Xiao Wang 氏 「Diffusion Models as Stochastic Quantization on the Lattice」 6/11
- 第26回領域セミナ・第78回DLAP：　宮戸 岳 氏 「物理に着想を得たモデルによる、長期的かつコ

2022: MLPhys initiative started



2023: MLPhys conference (Kyoto)

MLPhYs 学術変革領域研究(A) 学習物理学の創成
Foundation of "Machine Learning Physics"





2023

11/13-15

International lectures

Sebastian Goldt (SISSA), *"Analytical approaches to the learning dynamics of two-layer neural networks"*

Sven Krippendorf (LMU Munich), *"Machine learning as a method in mathematical physics"* *lecture 1* *lecture 2* *lecture 3*

Lei Wang (Chinese Academy of Sciences), *"Generative models for physicists"*

2023: lectures4mlphys started (now 22th)

View on GitHub

lectures4mlphys

物理屋のための機械学習講義

Youtube チャンネル

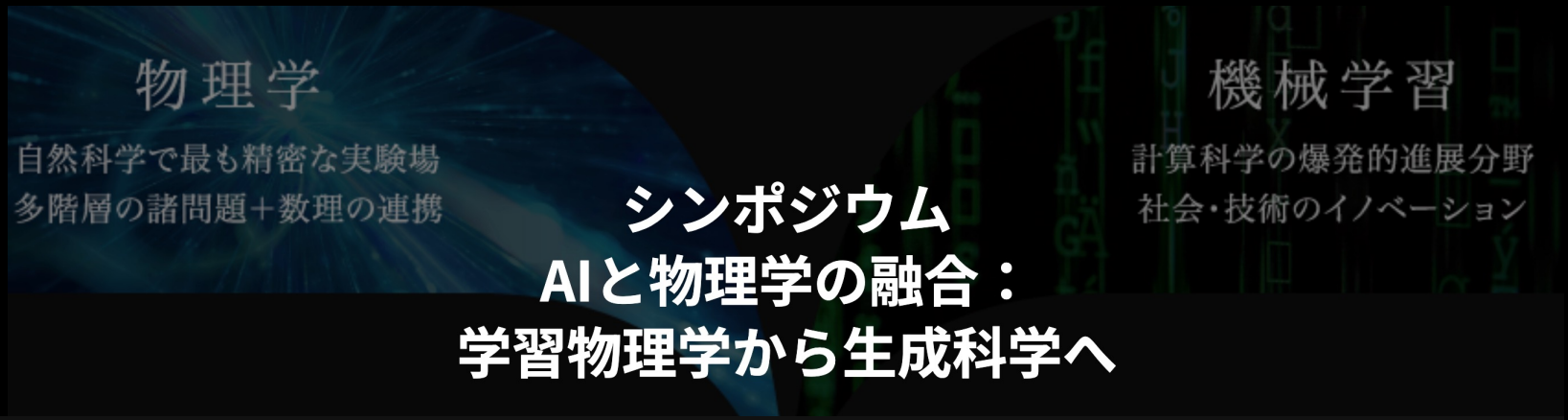
開催趣旨

機械学習は物理学の幅広い分野で、 一部既存手法を超える性能を見せるなど、 有効に活用され始めています。 一方で、物理学研究者および学習者にとって、 機械学習で用いられる個々の手法は理解できたとしても、 その幅広い分野全体を概観することは簡単ではありません。 そこで、物理学研究者および学習者が機械学習の様々な 基礎知識に触れられるよう、 本講義シリーズを企画しました。 幅広い参加者をお待ちしています。

- 世話人: 大野 浩史 (筑波大)、柏 浩司 (福岡工業大)、富谷 昭夫 (東京女子大)、二村 保徳 (筑波大)（順不同)

本講義シリーズは、科学研究費補助金学術変革領域研究(A)「学習物理学の創成」の補助を受けております。

June 2025: Symposium
“From MLPhys to Generative Sciences”



シンポジウム
AIと物理学の融合：
学習物理学から生成科学へ

概要

日時：2025年6月22日（日）13:30〜18:30　その後自由形式議論会 ~20:30
場所：京都大学理学部セミナーハウス（吉田キャンパスマップ#10）

研究会趣旨

物理学と機械学習を融合する研究領域として誕生した学習物理学領域は、発足から3年が経ち、様々な融合研究の成果が生まれています。一方で、生成AIの推論能力の向上により、物理学の現場においても、生成AIを共同研究者としても利用するような状況が生まれつつあります。 本研究会は、学習物理学領域における多様な物理学の生成の成果を紹介し、一方で、それらの学術的意義や将来の物理学にどのようにつながっていくかを多様な観点から議論するものです。第一部では、学習物理学領域の多様な研究成果を概観し、次に第二部では、情報学、数学、英文学、といった周辺の分野で生成AIもしくはそこから生まれる統合された「生成科学」の方向性を紹介していただきます。パネルでは、物理学とAIのさらなる学際融合研究領域の進展に向けて、現状と未来を議論します。

プログラム

挨拶
　北川進 京都大学 理事・副学長
挨拶

第二部 生成科学に向けて

16:20

第三部 パネルディスカッション

MLPhys 2026 conference

MLPhys 学術変革領域研究(A) 学習物理学の創成
Foundation of "Machine Learning Physics"



Schedule

2026

07/13-15

International conference

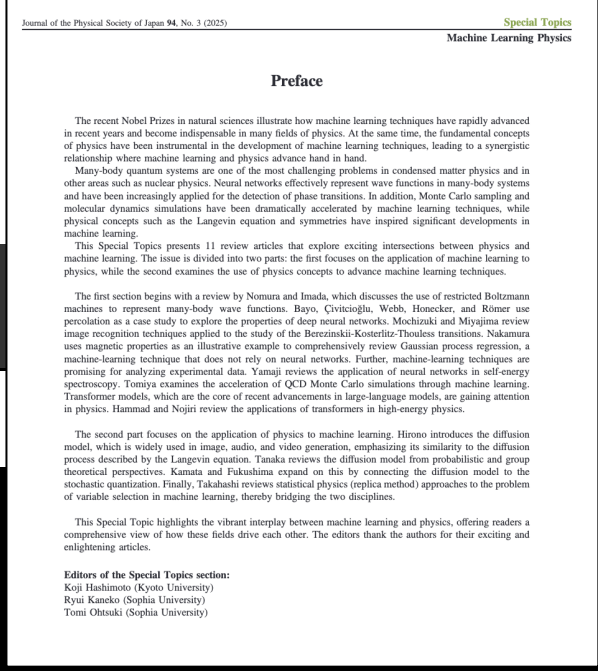
Journal of the Physical Society of Japan

SPECIAL TOPICS: Machine Learning Physics

J. Phys. Soc. Jpn. 94 (2025) No. 3 (11 articles)

Editors: Koji Hashimoto, Ryui Kaneko,
Tomi Ohtsuki

- Quantum many-body solvers using artificial neural networks
  Yusuke Nomura, Masatoshi Imada
- The percolating cluster is invisible to image recognition with deep learning
  D. Bayo, A. Honecker, R.A. Römer
- Machine learning detections of the Berezinskii-Kosterlitz-Thouless transitions in classical spin models
  Masahito Mochizuki, Yusuke Miyajima
- Machine learning as an improved estimator for magnetization curve and spin gap
  Tota Nakamura
- Self-energy spectroscopy by artificial neural network
  Youhei Yamaji
- Machine learning assisted lattice QCD
  Akio Tomiya
- Transformer faces high energy physics
  Ahmed Hammad, Mihoko Nojiri
- Physics-motivated Approaches in Machine Learning
  Yuji Hirono
- Diffusion model and stochastic quantizatio
  Syo Kamata, Kenji Fukushima
- Diffusion models in physics context
  Akinori Tanaka
- Mean-field analysis of stability selection
  Takashi Takahashi



Preface

The recent Nobel Prizes in natural sciences illustrate how machine learning techniques have rapidly advanced in recent years and become indispensable in many fields of physics. At the same time, the fundamental concepts of physics have been instrumental in the development of machine learning techniques, leading to a synergistic relationship where machine learning and physics advance hand in hand.

Many-body quantum systems are one of the most challenging problems in condensed matter physics and in other areas such as nuclear physics. Neural networks effectively represent wave functions in many-body systems and have been increasingly applied for the detection of phase transitions. In addition, Monte Carlo sampling and molecular dynamics simulations have been dramatically accelerated by machine learning techniques, while physical concepts such as the Langevin equation and symmetries have inspired significant developments in machine learning.

This Special Topics presents 11 review articles that explore exciting intersections between physics and machine learning. The issue is divided into two parts: the first focuses on the application of machine learning to physics, while the second examines the use of physics concepts to advance machine learning techniques.

The first section begins with a review by Nomura and Imada, which discusses the use of restricted Boltzmann machines to represent many-body wave functions. Bayo, Çivitcioğlu, Webb, Honecker, and Römer use percolation as a case study to explore the properties of deep neural networks. Mochizuki and Miyajima review image recognition techniques applied to the study of the Berezinskii-Kosterlitz-Thouless transitions. Nakamura uses magnetic properties as an illustrative example to comprehensively review Gaussian process regression, a machine-learning technique that does not rely on neural networks. Further, machine-learning techniques are promising for analyzing experimental data. Yamaji reviews the application of neural networks in self-energy spectroscopy. Tomiya examines the acceleration of QCD Monte Carlo simulations through machine learning. Transformer models, which are the core of recent advancements in large-language models, are gaining attention in physics. Hammad and Nojiri review the applications of transformers in high-energy physics.

The second part focuses on the application of physics to machine learning. Hirono introduces the diffusion model, which is widely used in image, audio, and video generation, emphasizing its similarity to the diffusion process described by the Langevin equation. Tanaka reviews the diffusion model from probabilistic and group theoretical perspectives. Kamata and Fukushima expand on this by connecting the diffusion model to the stochastic quantization. Finally, Takahashi reviews statistical physics (replica method) approaches to the problem of variable selection in machine learning, thereby bridging the two disciplines.

This Special Topic highlights the vibrant interplay between machine learning and physics, offering readers a comprehensive view of how these fields drive each other. The editors thank the authors for their exciting and enlightening articles.

Editors of the Special Topics section:
Koji Hashimoto (Kyoto University)
Ryui Kaneko (Sophia University)
Tomi Ohtsuki (Sophia University)

Format of MLPhys (2022-)

Steering committee

B01: ML models for physics

B02: Numerical sampling efficiency

B03: Topology and ML

A01: AI computational physics

A02: AI particle physics

A03: AI condensed matter physics

A04: AI quantum + gravity

MLPhys

Giving-up Interpretability, while bridging

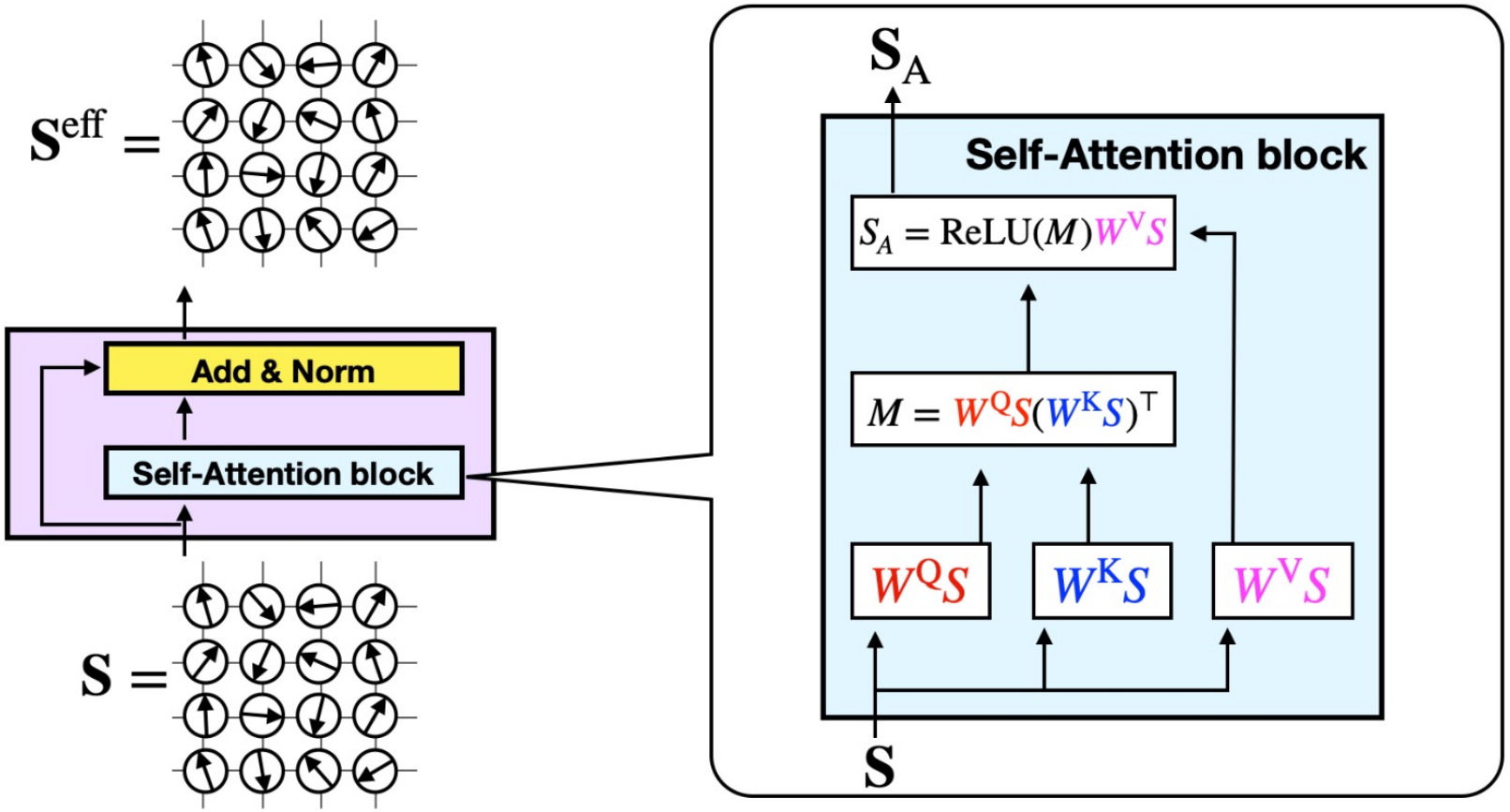
AI comp. phys. : Spin MC by transformer	A01 Tomiya
AI particle phys. : Jet tag by transformer	A02 Nojiri
AI cond-mat phys. : Identifying fractal phases	A03 Ohtsuki
AI superconductor : Material dependence	A03 Imada
AI molecular dynamics : quasicrystals	A03 Nagai
Stat-mech AI : Faster diffusion model	B02 Kabashima
AI emergent spacetime : AdS/CFT inverted	A04 Hashimoto
Path-integral AI : Diffusion is QM	B01 Tanaka
Gravity AI : Symmetry in neurons	A04 Hashimoto

AI comp. phys. : spin MC by transformer

A01

Attention mechanism describes nonlocality

[Tomiya, Nagai, *PoS* LATTICE2023 (2024) 001]

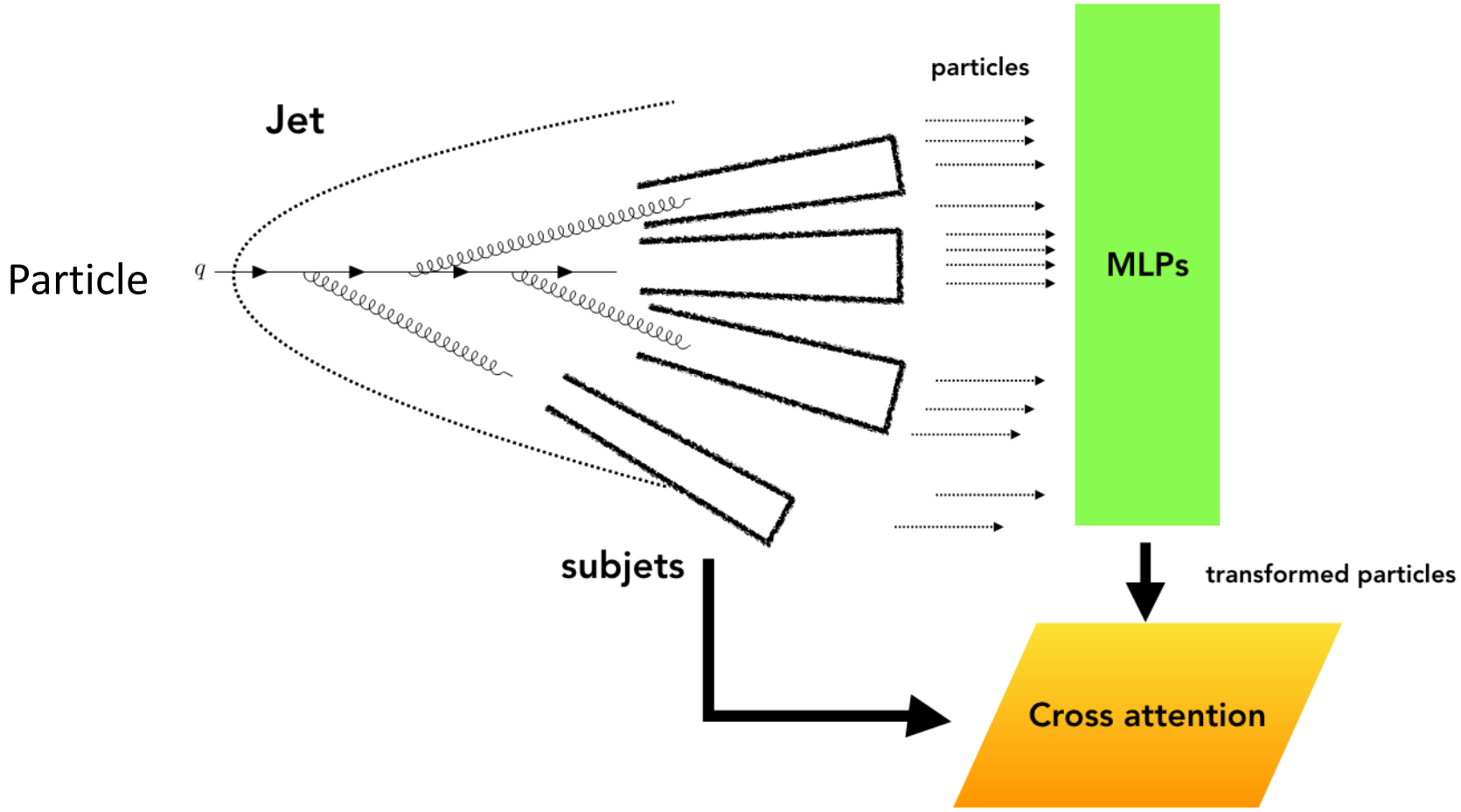


AI particle phys. : jet tag by transformer

A02

Cross-attention learns
Physical energy scales

[Hammad, Nojiri, JHEP 06(2024)176,
JHEP 03 (2024) 114]

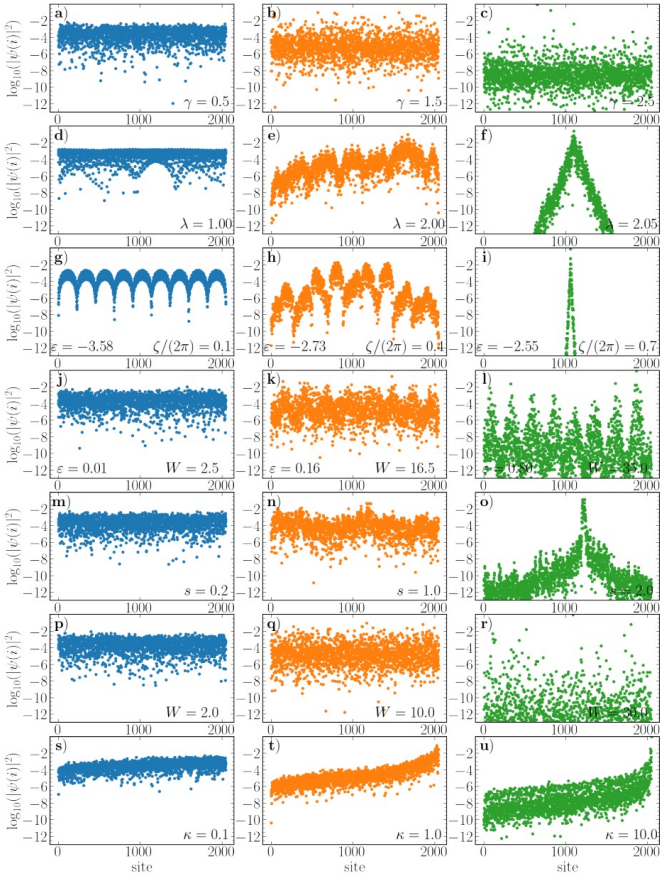


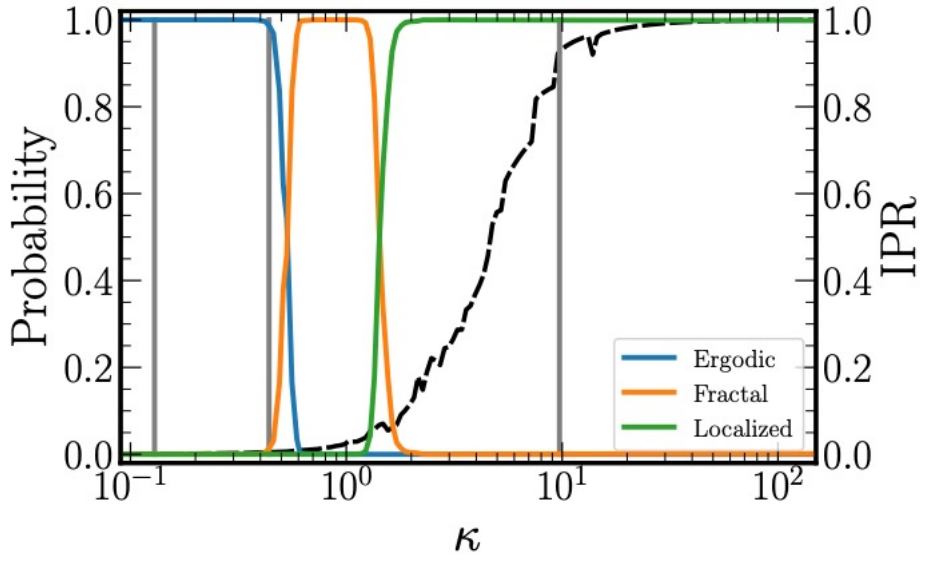
AI cond-mat phys. : finding fractal phases

A03

Learning fractal quantum phases that generalize across different quantum systems

[Cadez, Dietz, Rosa, Andreanov, Slevin, Ohtsuki, Phys. Rev. B 108, 184202 (2023)]



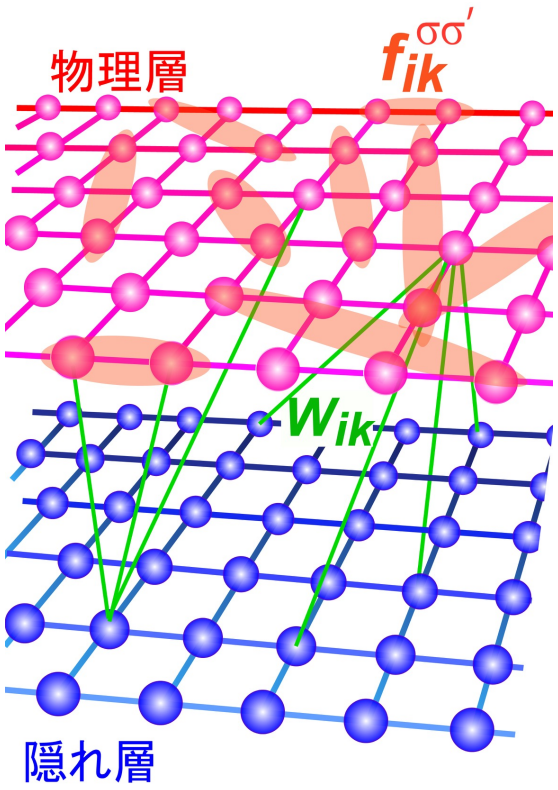


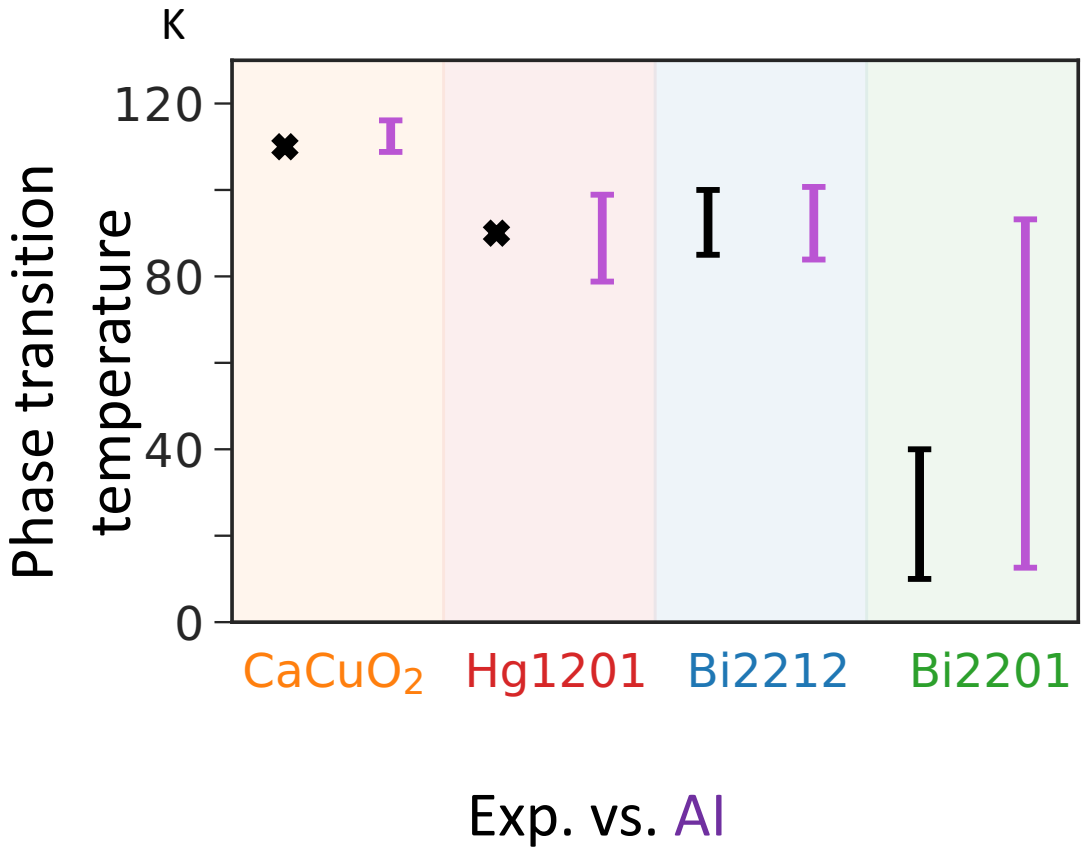
AI superconductor : material dependence

A03

Quantum many-body wave functions by Boltzmann machine

[Schmid, Morée, Kaneko, Yamaji, Imada, Phys. Rev. X 13, 041036 (2023)]





AI molcular dynamics : quasicrystals

A03

Higher-dim. structure learned by Machine

[Nagai et al., Phys.Rev. Lett. 102, 041124 (2024)]

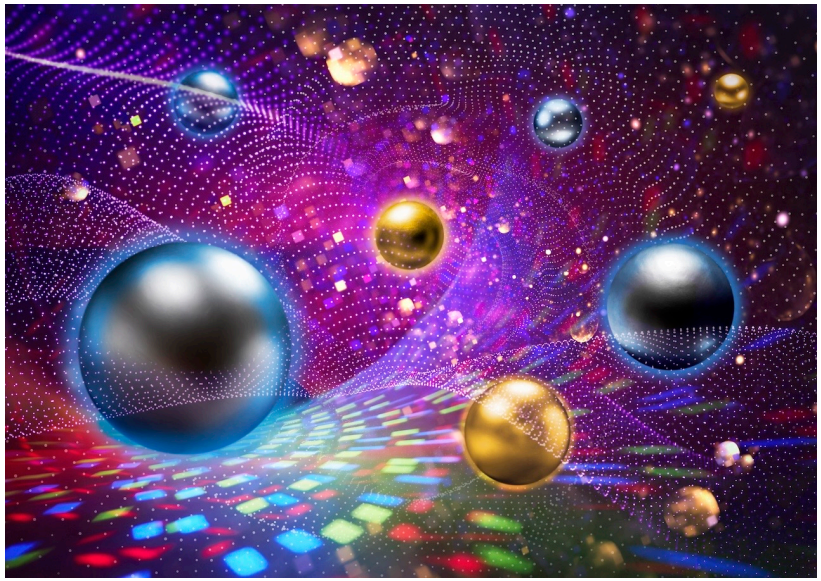
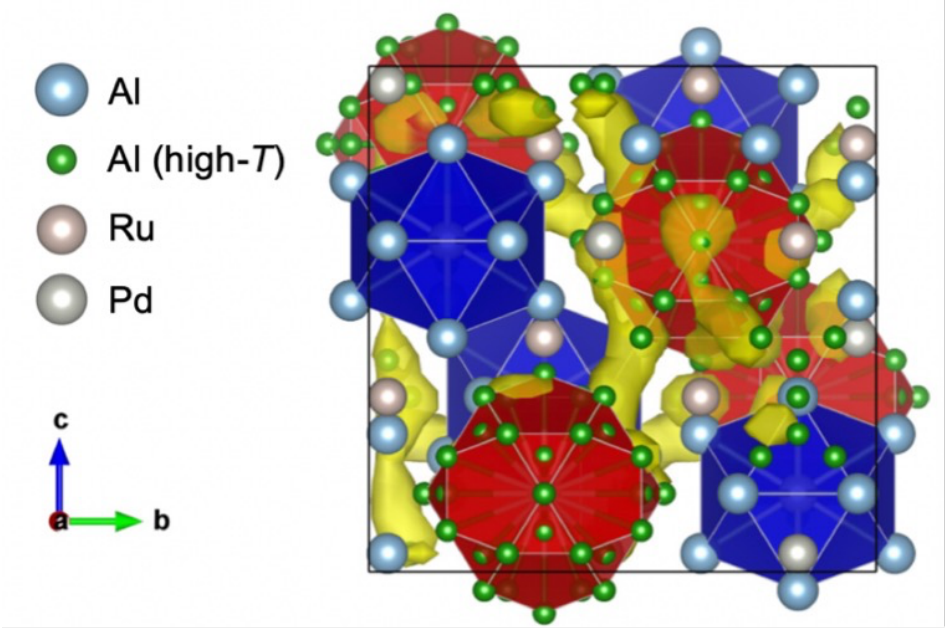


Image of higher-dimensional atoms affecting the 3-dim. world
Credit: UTokyo ITC/Shinichiro Kinoshita



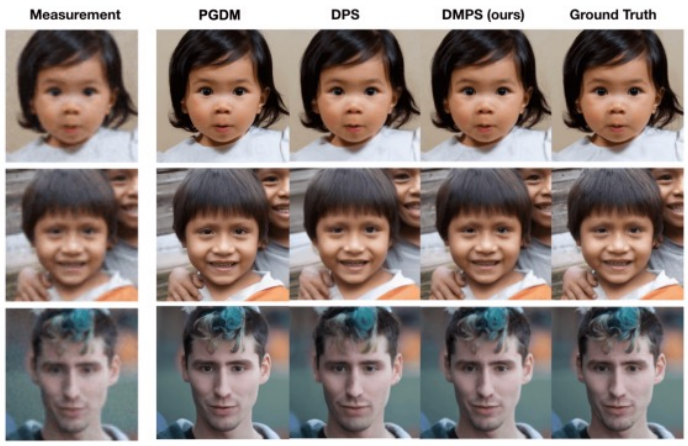
Alminium atoms floating through high-dim. paths

Stat-mech AI：Faster diffusion model

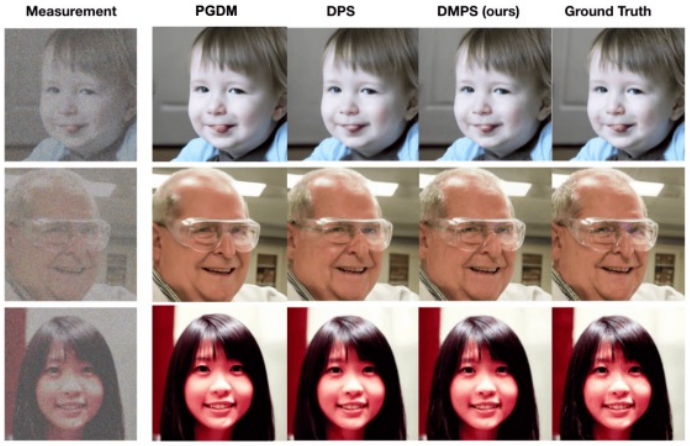
B02

Leveraging stochastic process theory for efficient gen AI

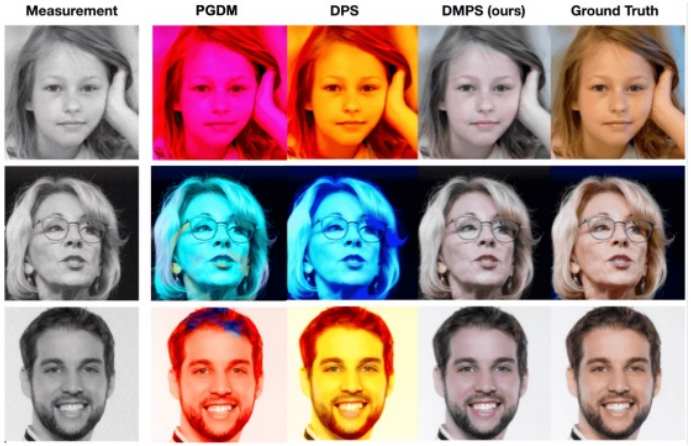
[Meng, Kabashima, ArXiv:2211.12343, ACML2024]



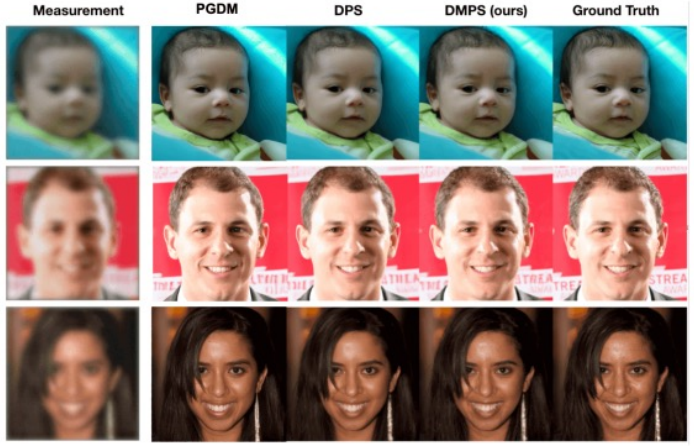
(*a*) Super-resolution (SR) (×4)



(*b*) Denoising ($\sigma = 0.5$)



(*c*) colorization



(*d*) Deblurring (uniform)

Giving-up Interpretability, while bridging

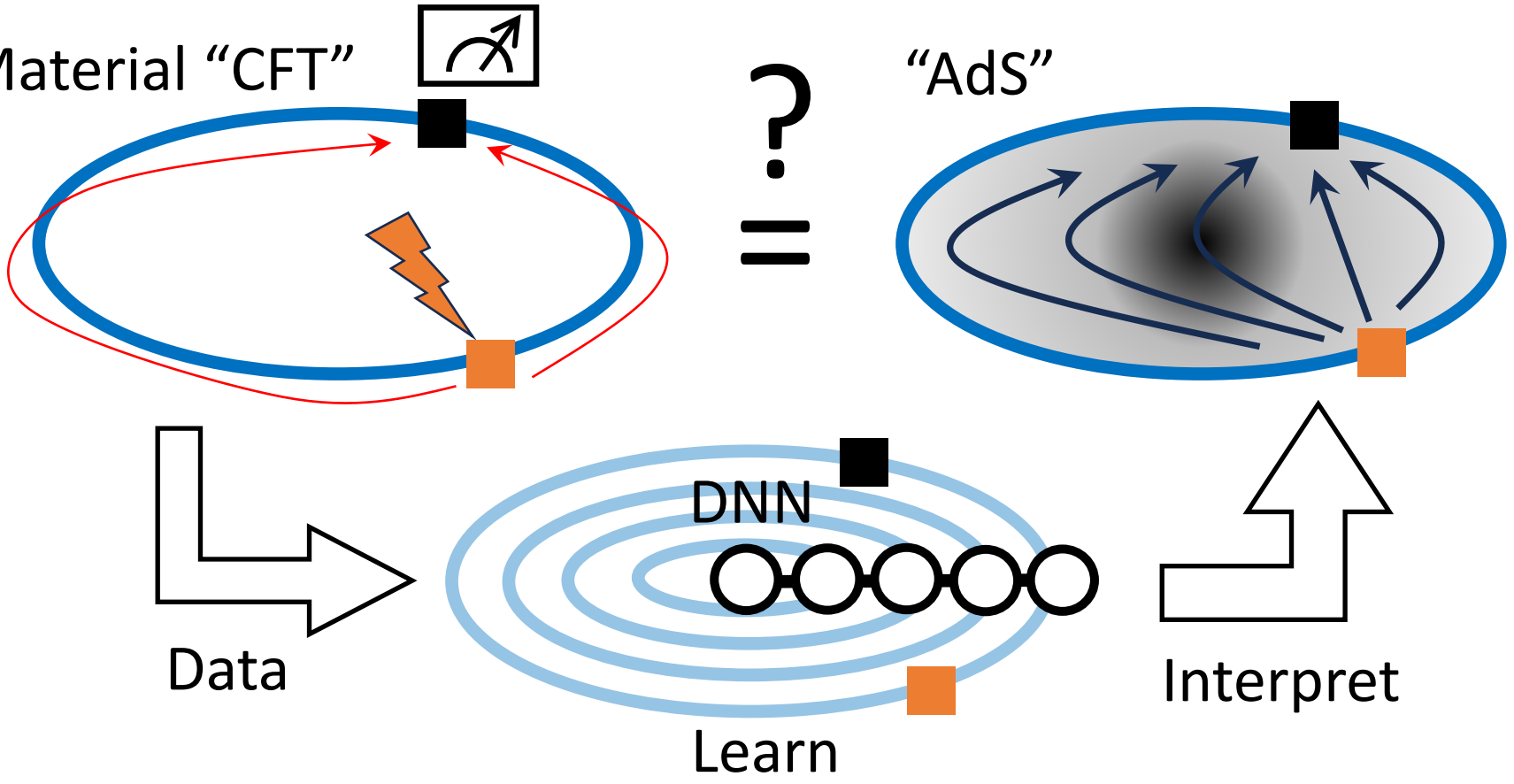
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Gravity AI : Symmetry in neurons	A04 Hashimoto

AI emergent spacetime : AdS/CFT inverted

A04

NN derives emergent bulk spacetime from data on material

[Hashimoto, Matsuo, Murata, Ogiwara, Takeda, ICML 2024 workshop poster]

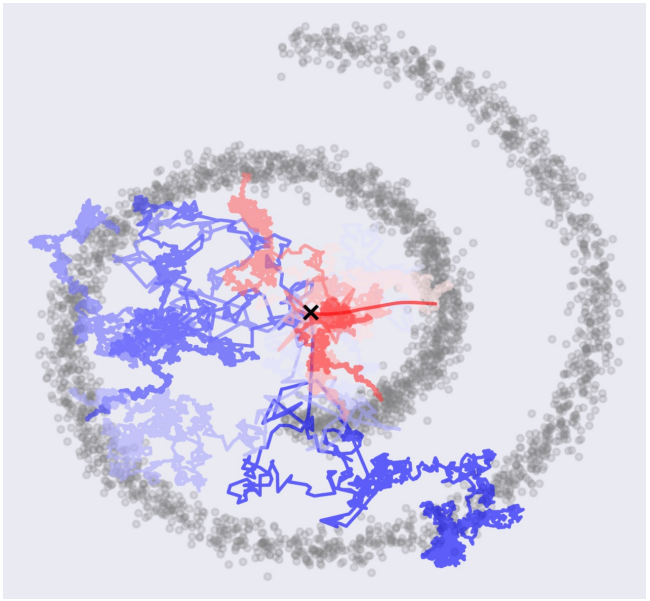


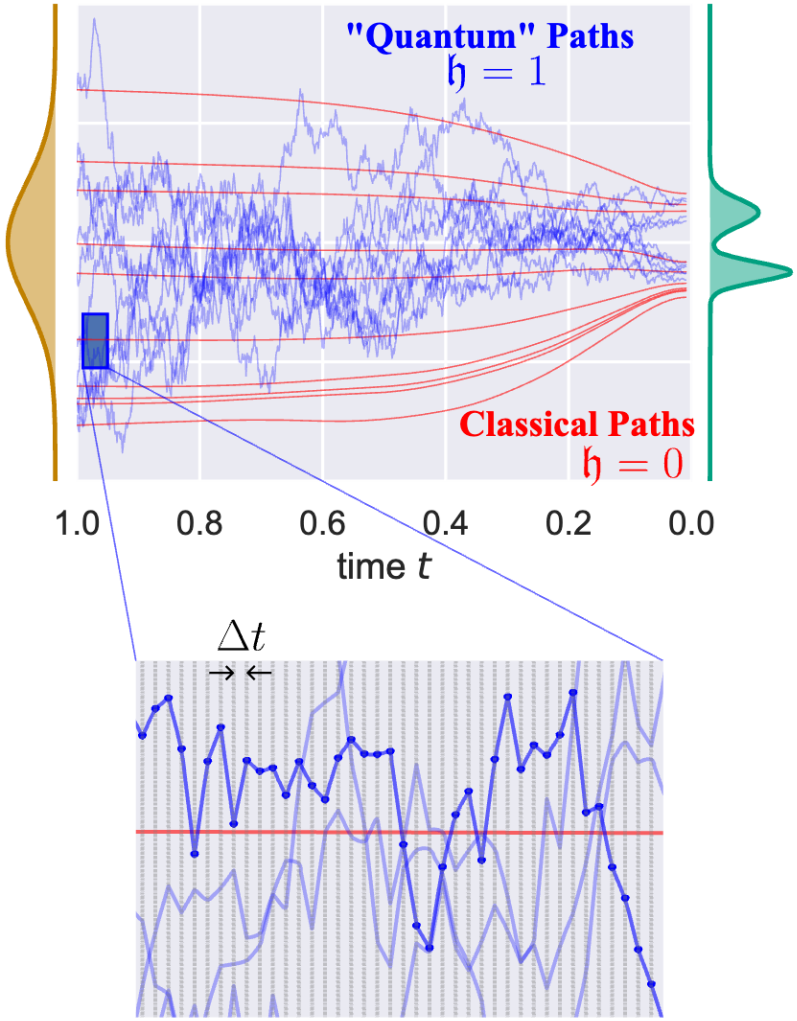
Path-integral AI：Diffusion is QM

B01+B03

[Hirono, Tanaka, Fukushima, ICML 2024, arXiv:2403.11262]

Diffusion model for generative AI is rewritten by path-integral



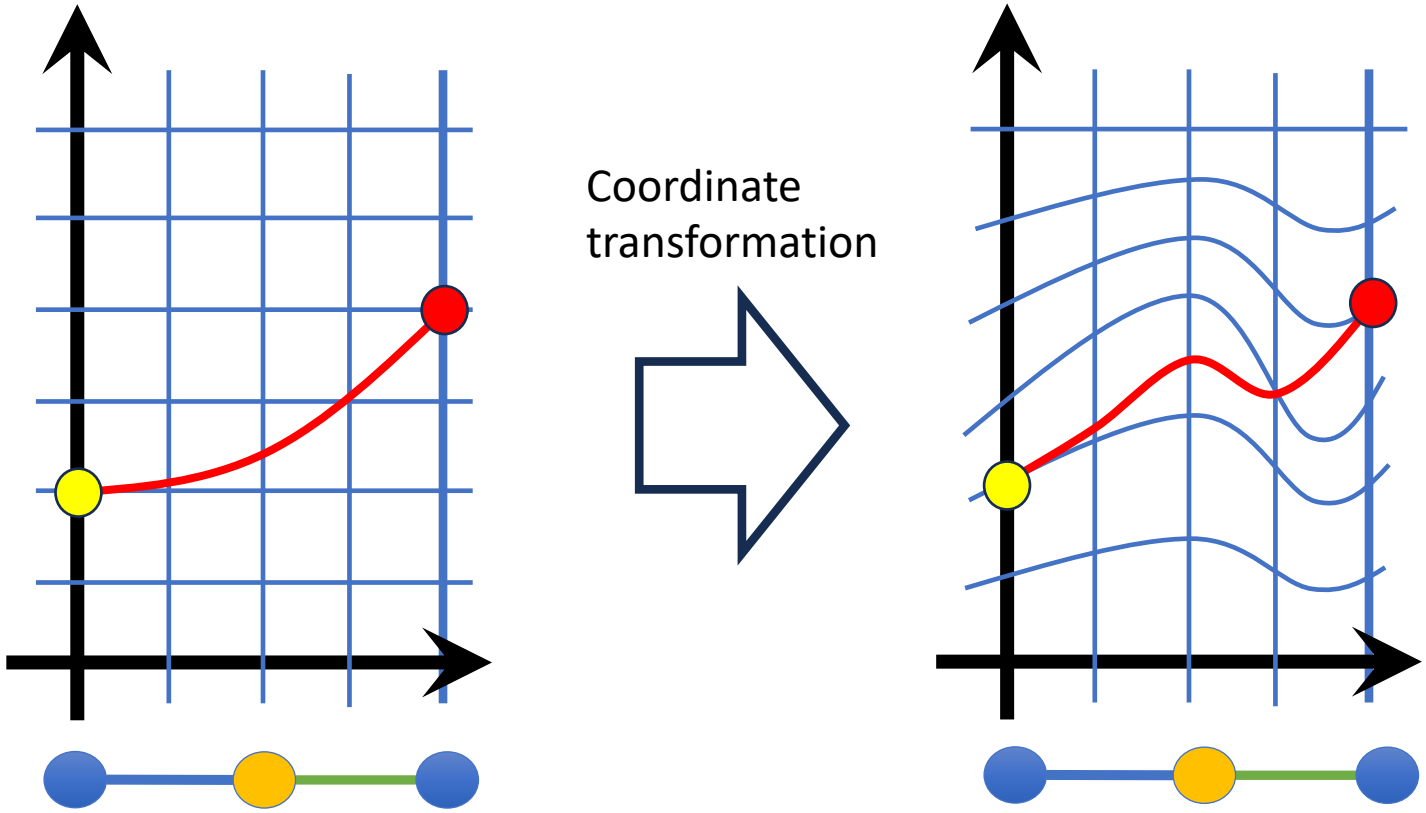


Gravity AI：Symmetry in neurons

A04+B03

Gravitational symmetry in transformers and neural ODEs

[Hashimoto, Hirono, Sannai, **Mach. Learn.: Sci. Technol. 5 025079 (2024)]**



Giving-up Interpretability, while bridging

AI comp. phys. : Spin MC by transformer	A01 Tomiya
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Giving-up Interpretability, while bridging

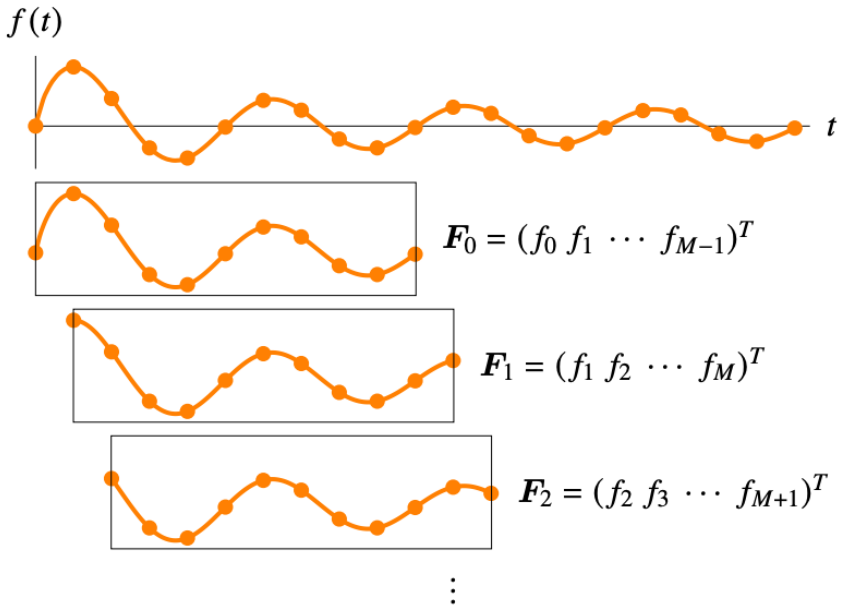
Data-driven quantum forecast	Steer. Kaneko
AI finds a physical law from exp data	Steer. Hirono
ML as a differential equation solver	Steer. Tanahashi
AI prover agent for auto-math	Steer. Sannai

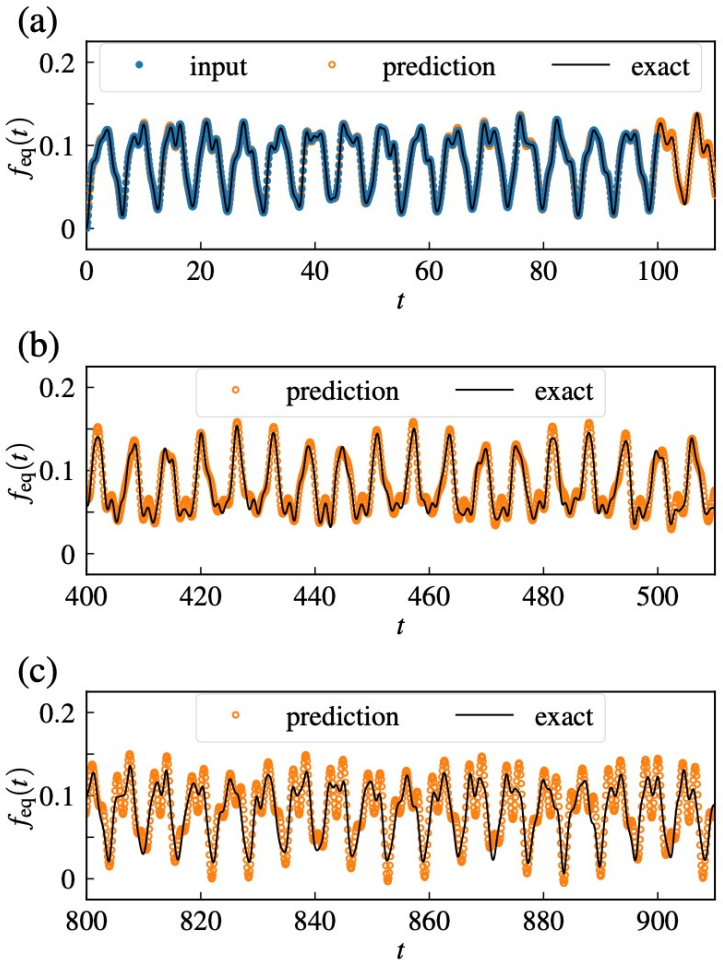
AI emergent spacetime：AdS/CFT inverted	A04 Hashimoto
Path-integral AI：Diffusion is QM	B01 Tanaka
Gravity AI：Symmetry in neurons	A04 Hashimoto

Data-driven quantum forecast

[Kaneko, Imada, Kabashima, Ohtsuki,
Phys. Rev. Research 7, 013085 (2025)

Learning quantum dynamics
from short-time data

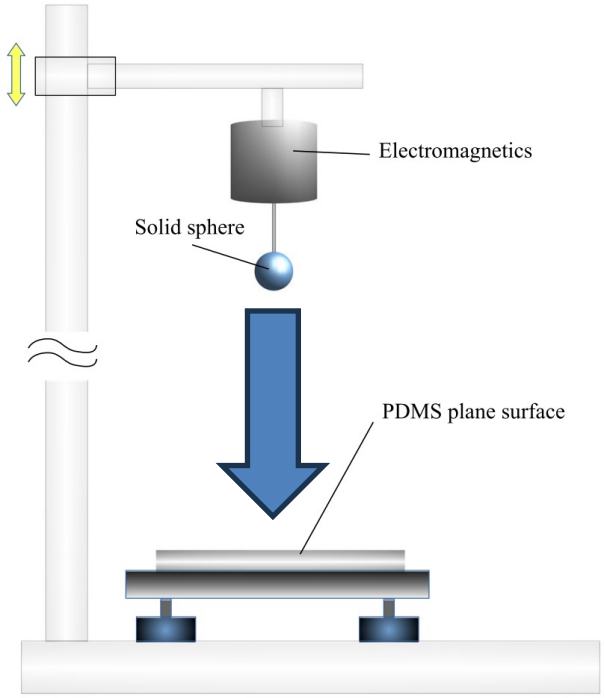




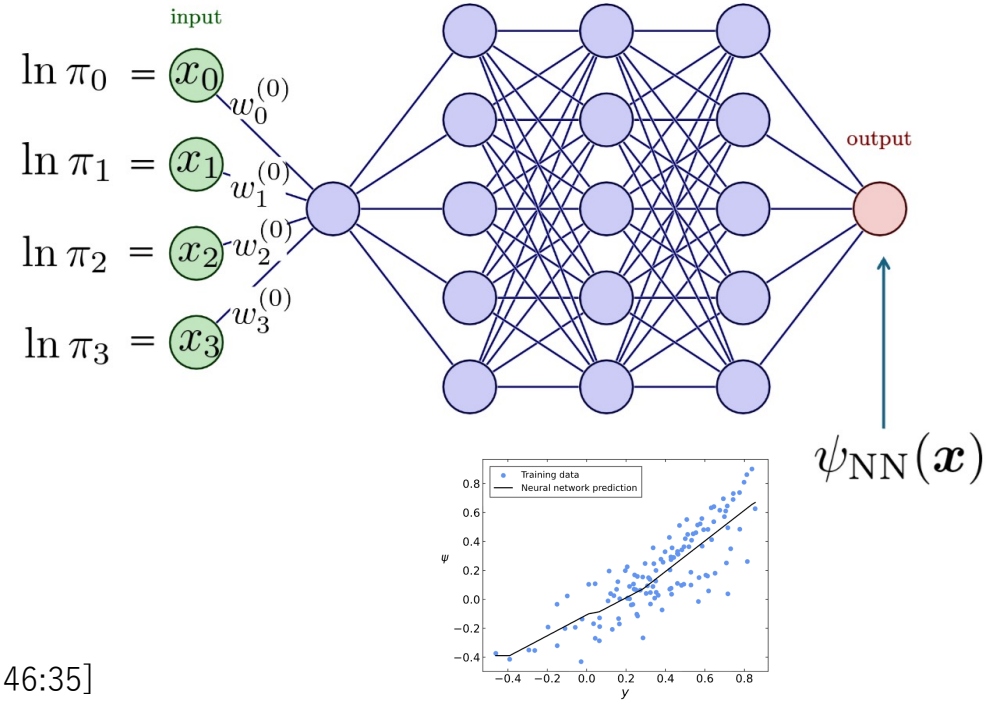
AI finds a physical law from exp data

[Watanabe, Ishii, Hirono, Maruoka, Phys. Rev. E 111, 024301 (2025)] (Editors' Suggestion)

NN extracts a new scaling law from raw exp. data



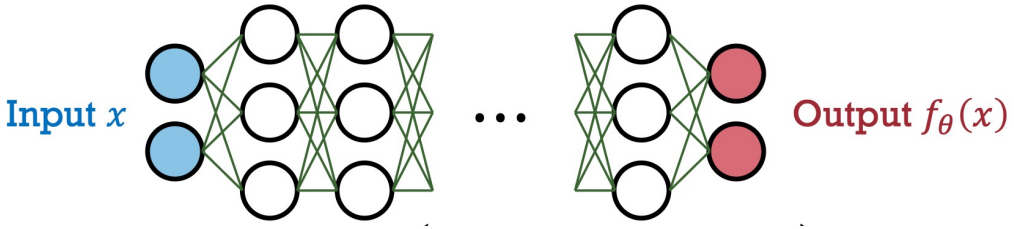
Modified from [Maruoka、Eur.Phys.J.E (2023) 46:35]



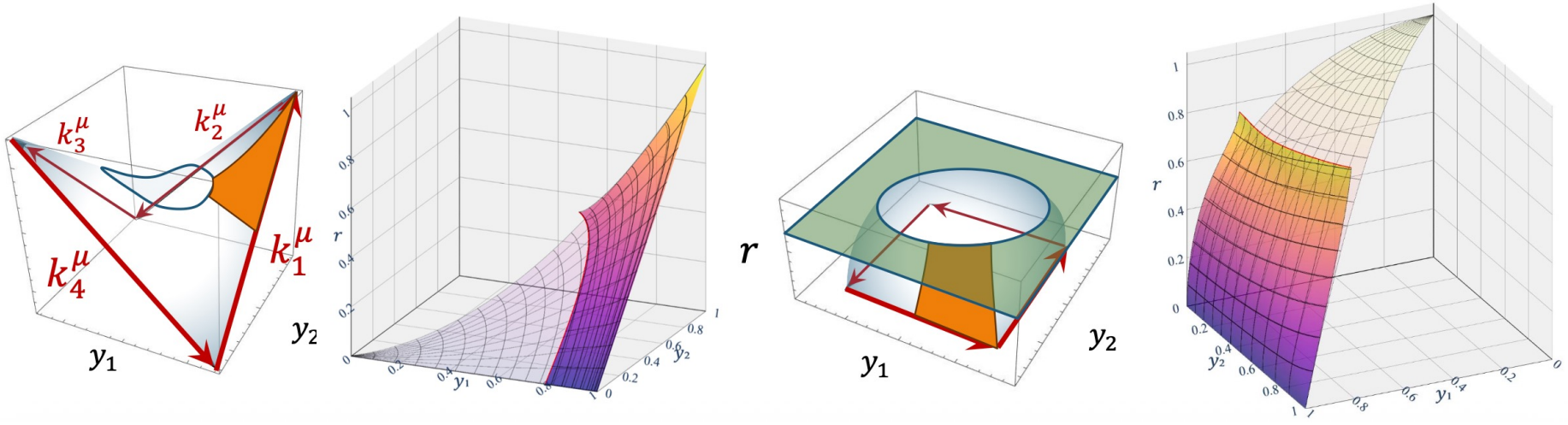
ML as a differential equation solver

[Hashimoto, Kyo, Murata, Ogiwara, Tanahashi, Mach. Learn.: Sci. Technol. 7 (2026) 015013]

Physics-Informed NN solves minimal surfaces



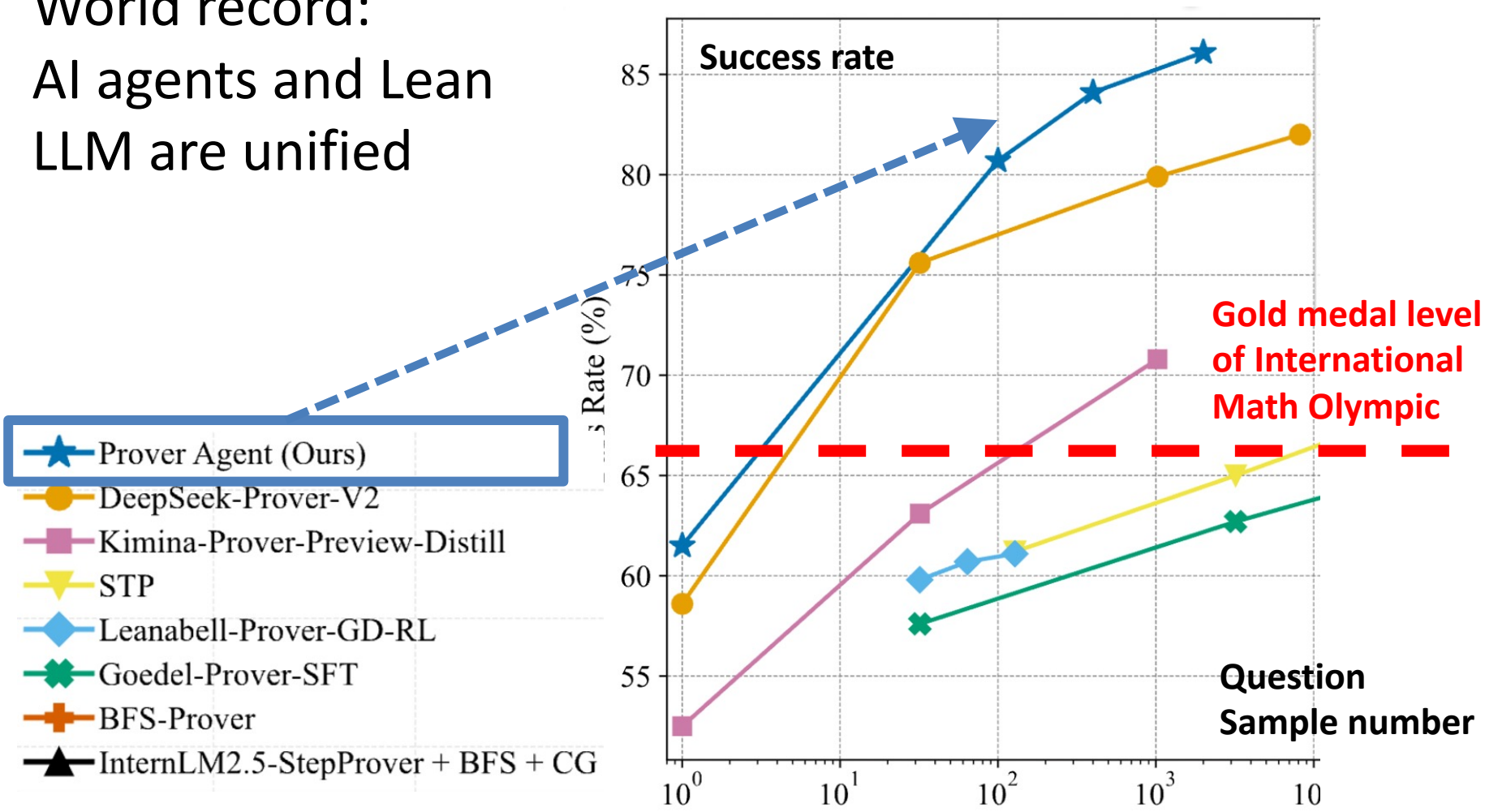
$$(\text{Loss}) = \sum(\text{EoM})^2 + \sum(\text{initial condition})^2 + \sum(\text{boundary condition})^2$$



AI prover agent for auto-math

[Baba, Liu, Kurita, Sannai, ArXiv:2506.19923]

World record:
AI agents and Lean
LLM are unified



Giving-up Interpretability, while bridging

AI comp. phys. : Spin MC by transformer

AI particle phys. : Jet tag by transformer

AI cond-mat phys. : Identifying fractal phases

AI superconductor : Material dependence

AI molecular dynamics : quasicrystals

Stat-mech AI : Faster diffusion model

AI emergent spacetime : AdS/CFT inverted

Path-integral AI : Diffusion is QM

Gravity AI : Symmetry in neurons

Future: Toward Abduction

2017	2022	2027	203X+
Entanglement Reproducibility. Validate by reproducing previous research.	**Predictive Power** Obtain predictive empirical rules w/ ML. Prepare ML math for physics.	**Abduction** Discover new laws in MLPhys. Develop new laws and materials.	

Foundation of Machine Learning Physics

We are heading for …
Generative Sciences!!

What Does Giving Up on Interpretability Bring to Machine Learning Physics?

Lessons from International Conference on Machine Learning Physics 2026: Research Design Connecting Performance, Meaning, and Internal Understanding

Koji Hashimoto

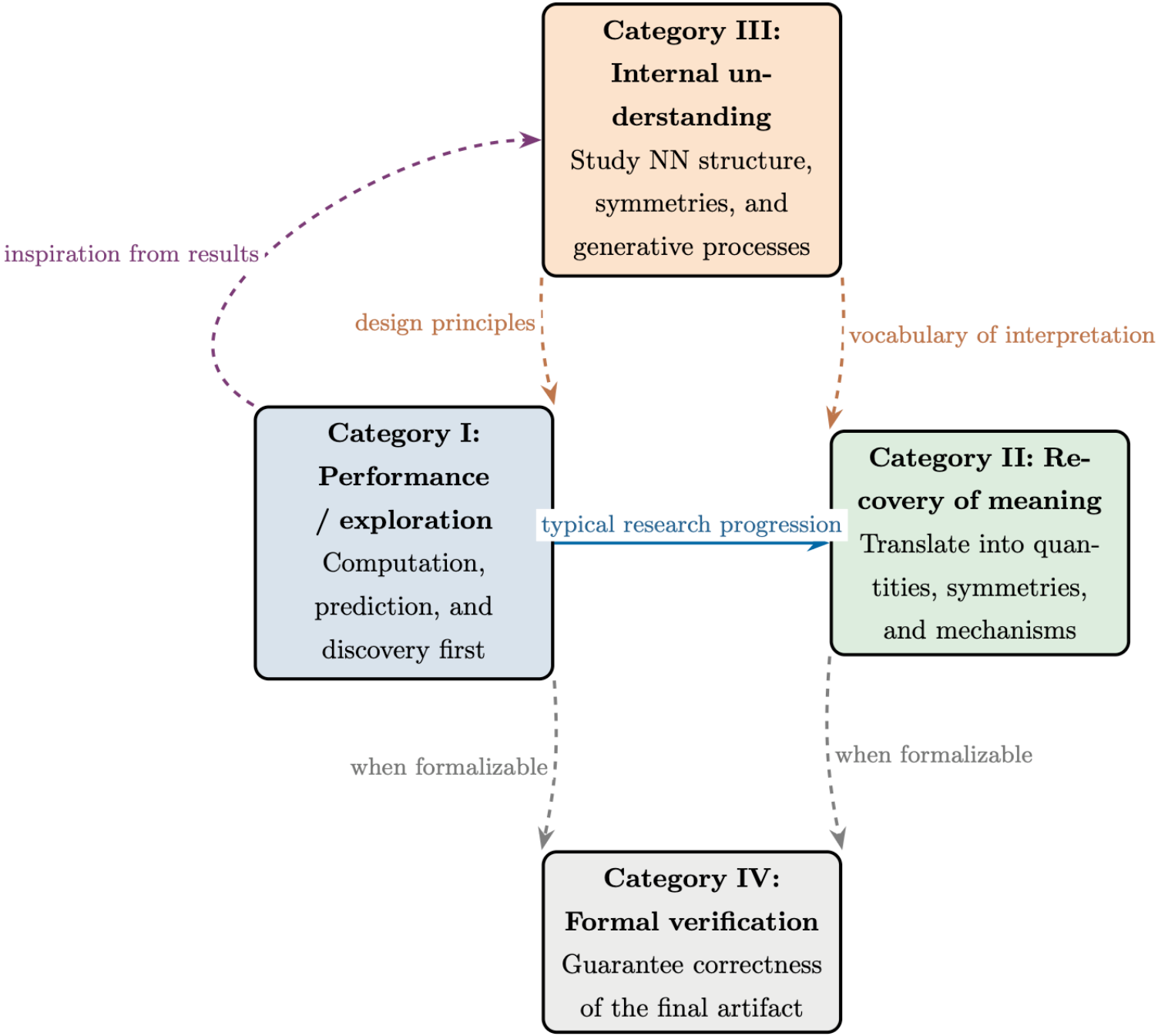
Representative, Foundation of Machine Learning Physics

Kyoto University

July 2026

Abstract

When neural networks (NNs) are used in physics, at what point should human interpretability of their internal representations be a condition of success? This article takes


Category III: Internal understanding
Study NN structure, symmetries, and generative processes
inspiration from results
design principles
vocabulary of interpretation
Category I: Performance / exploration
Computation, prediction, and discovery first
typical research progression
Category II: Recovery of meaning
Translate into quantities, symmetries, and mechanisms
when formalizable
when formalizable
Category IV: Formal verification
Guarantee correctness of the final artifact

ARiSE AI4MP (2026-2029)

Koji Hashimoto + Masataka Imaizumi
+ Tomiya + Otsuki + Nojiri + Kabashima + Sugiyama + Iso

AI agents with math and physics verification for unsolved physics problems

