Machine Learning for QCD matter: from Inverse Problem to Generative models

Lingxiao Wang(王凌霄) (FIAS)

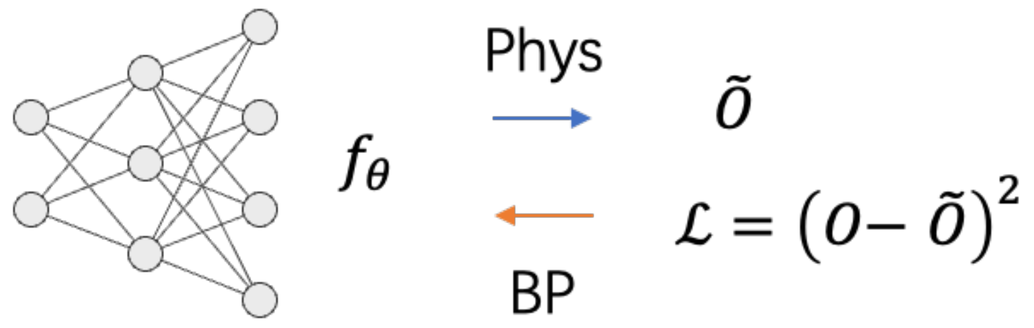
Dec 18, 2023, QPT 2023

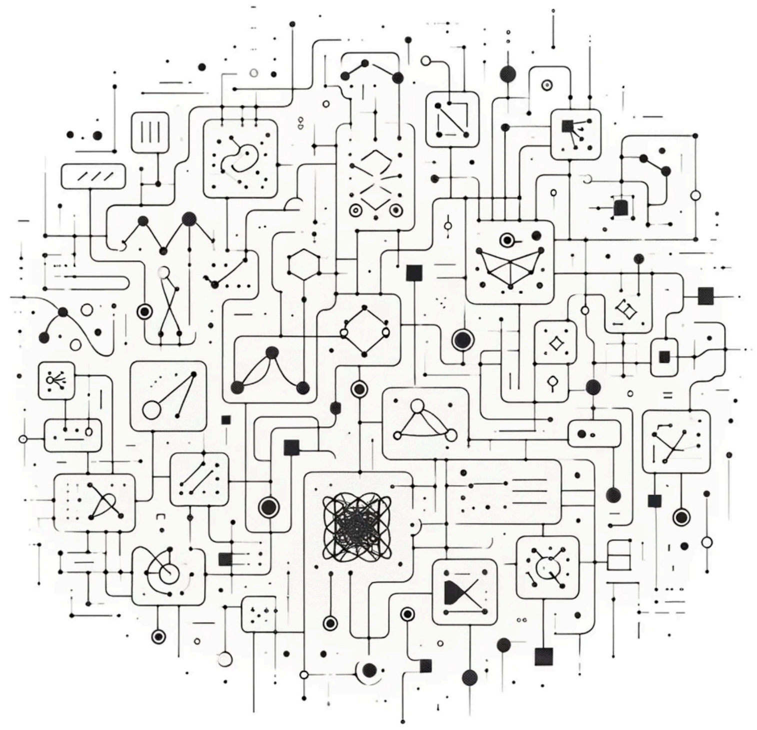
Prog.Part.Nucl.Phys. 104084(2023);
Phys. Rev. D 103, 116023, Phys. Rev. C 106, L051901, Phys. Rev. D 107, 083028, Phys. Rev. D 106, L051502;
Chin. Phys. Lett. 39, 120502, Phys. Rev. D 107, 056001, arXiv: 2309.17082.

Collaborators: Kai Zhou(FIAS), Shuzhe Shi(THU), Tetsuo Hatsuda(RIKEN), Gert Aarts(Swansea Uni.), ...

Outline

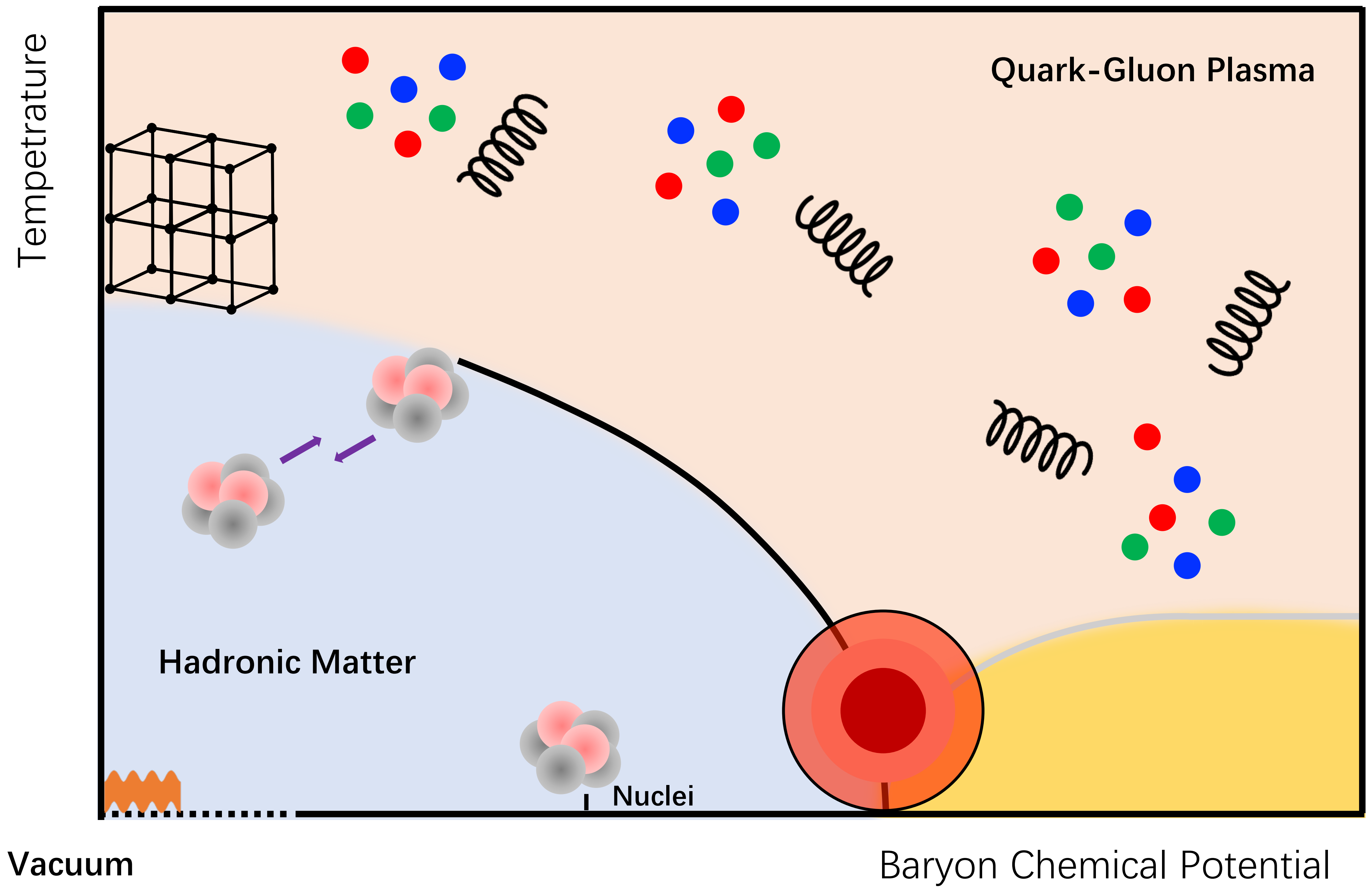
- **Machie Learning for QCD Matter**
- **Inverse Problems**
  - Data-Driven Learning
  - Physics-Driven Learning
- **Generative Models**
  - Generating Samples
  - Diffusion Models
- **Outlooks**

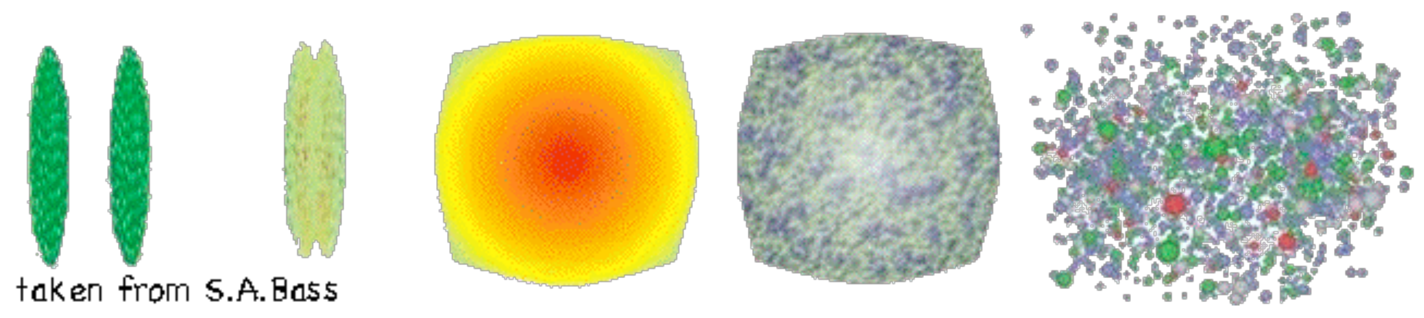




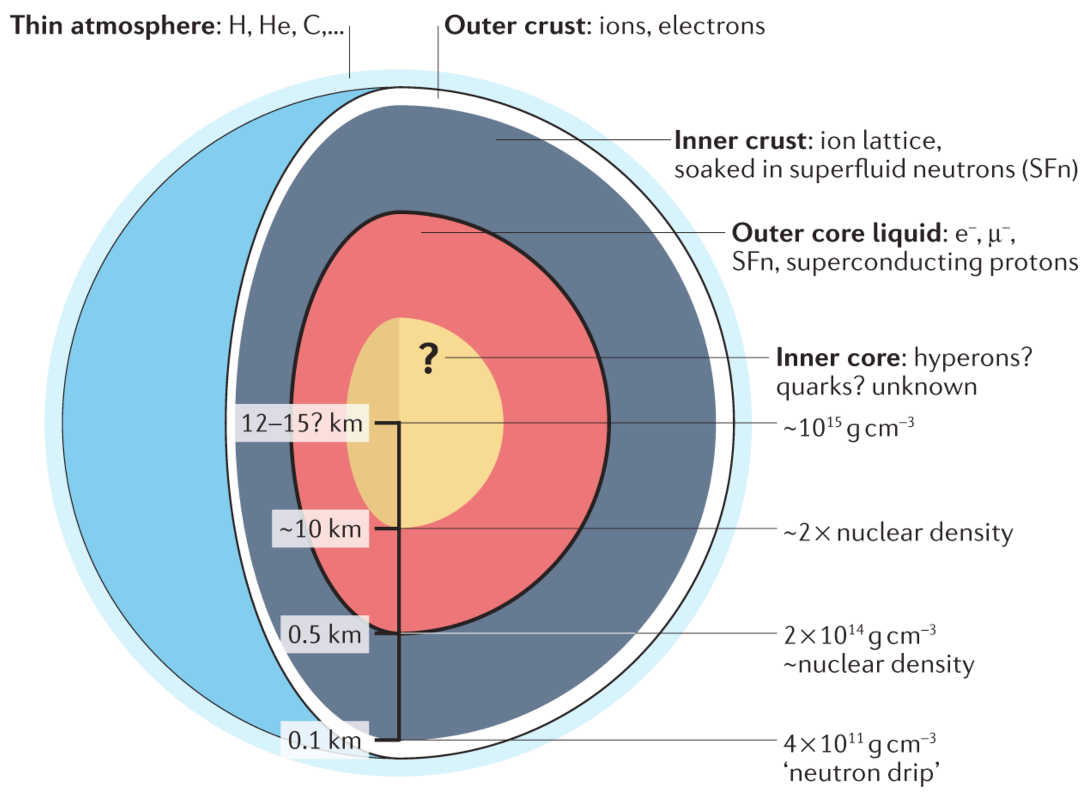
Generated by ChatGPT-4 + DALL·E

QCD Matter





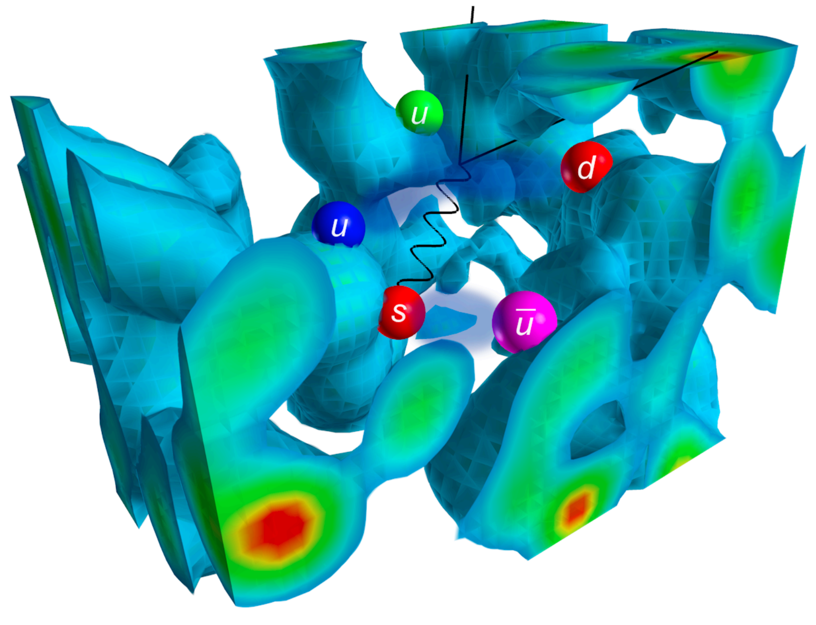
Heavy-Ion Collisions



Nat. Rev. Phys. 4, 237–246 (2022)

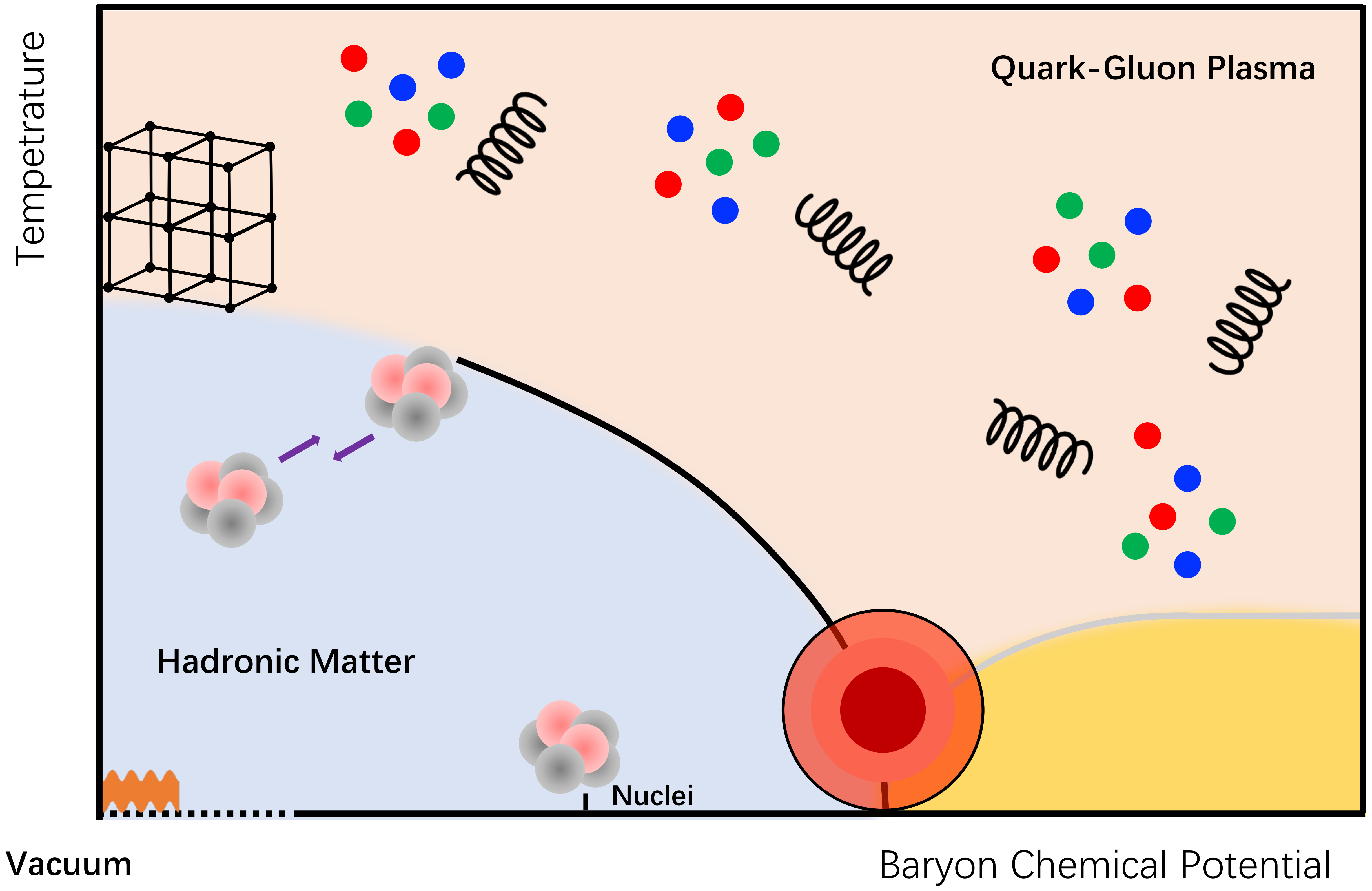
Exploring QCD matter in three "**labs**",

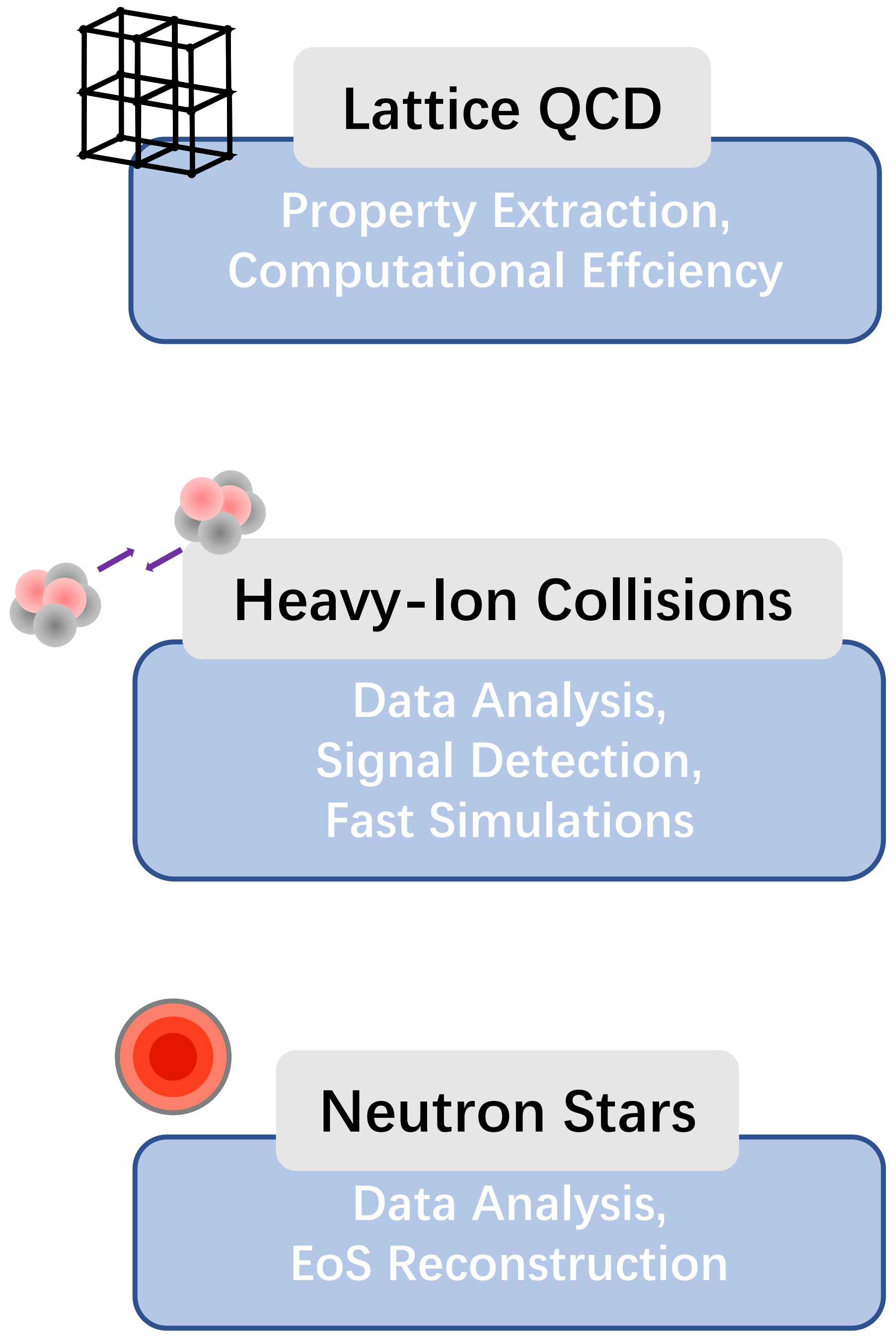
- **Heavy-Ion Collisions** : compress matter to **high-T** and **high-μ_B**
- **Neutron Star** : dense matter, merger events at **low-T** and **high-μ_B**
- **Lattice QCD** : numerically solve QCD Lagrangian at **finite-T** and $\mu_B \sim 0$



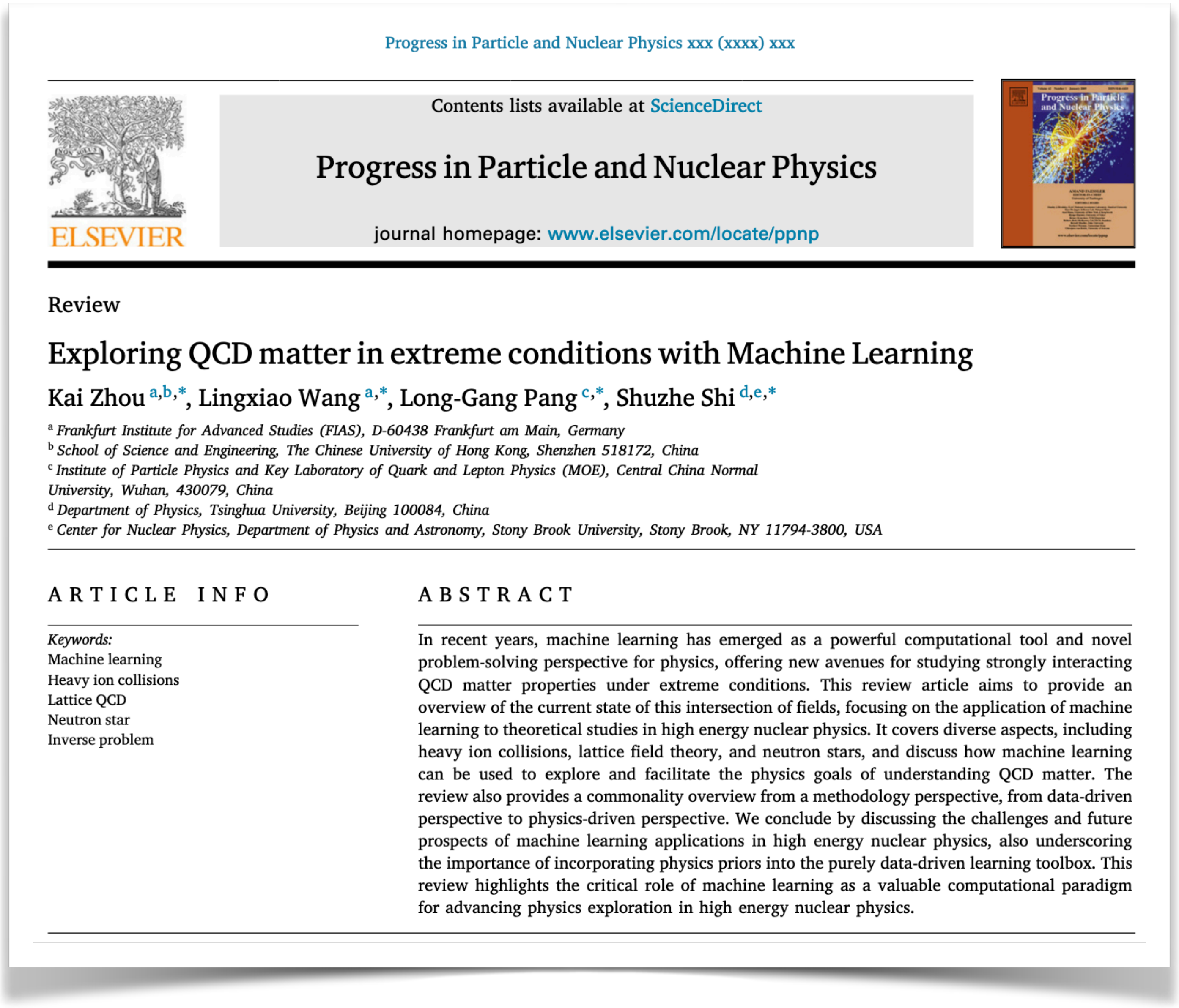
Lattice QCD © Derek Leinweber/CSSM/University of Adelaide

Why Machine Learning?





Prog.Part.Nucl.Phys. 104084(2023) **(Invited Review)**



Progress in Particle and Nuclear Physics xxx (xxxx) xxx

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

ELSEVIER

Review

Exploring QCD matter in extreme conditions with Machine Learning

Kai Zhou [a,b,*], Lingxiao Wang [a,*], Long-Gang Pang [c,*], Shuzhe Shi [d,e,*]

[a] Frankfurt Institute for Advanced Studies (FIAS), D-60438 Frankfurt am Main, Germany
[b] School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen 518172, China
[c] Institute of Particle Physics and Key Laboratory of Quark and Lepton Physics (MOE), Central China Normal University, Wuhan, 430079, China
[d] Department of Physics, Tsinghua University, Beijing 100084, China
[e] Center for Nuclear Physics, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794-3800, USA

A R T I C L E I N F O

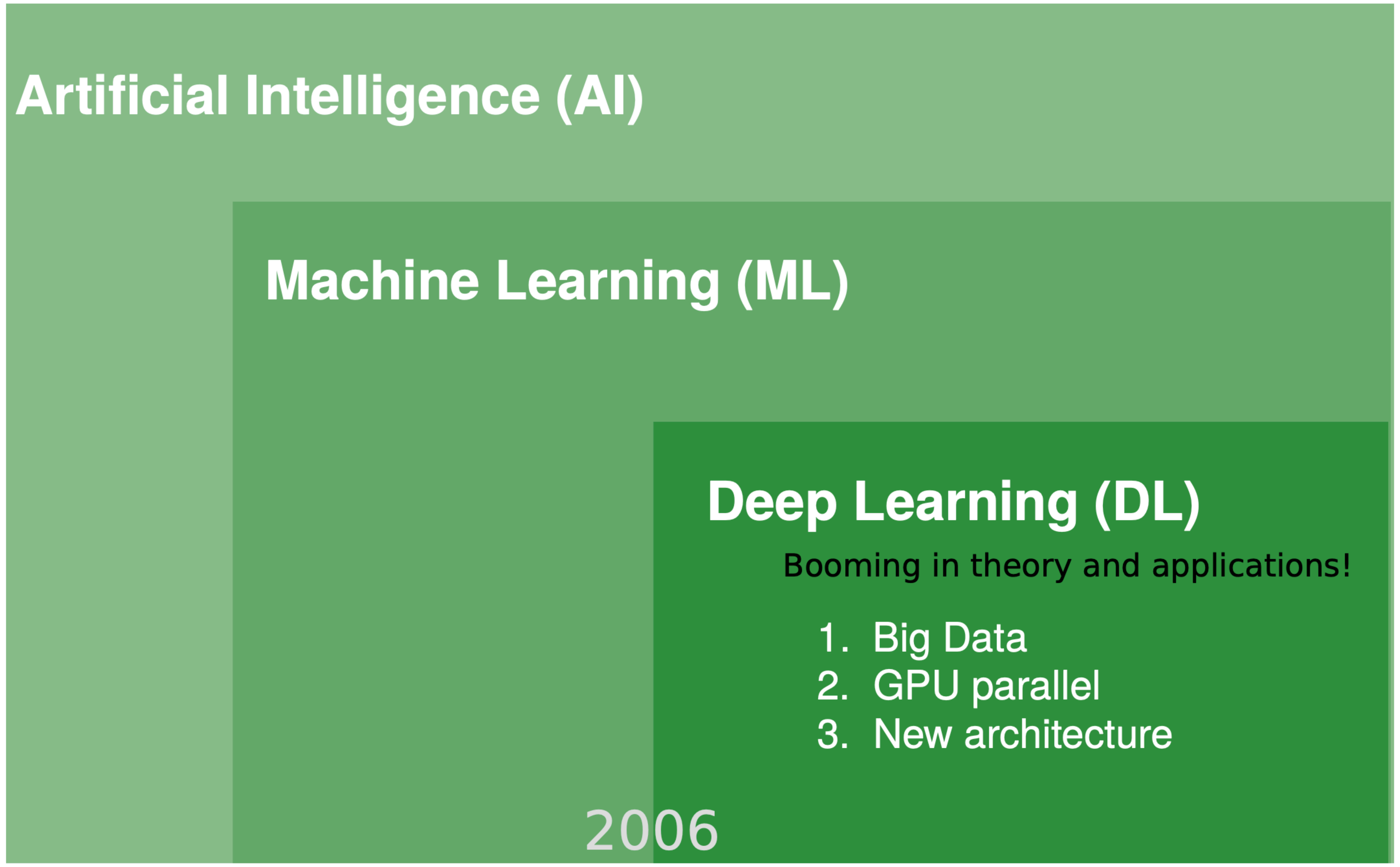
Keywords:
Machine learning
Heavy ion collisions
Lattice QCD
Neutron star
Inverse problem

A B S T R A C T

In recent years, machine learning has emerged as a powerful computational tool and novel problem-solving perspective for physics, offering new avenues for studying strongly interacting QCD matter properties under extreme conditions. This review article aims to provide an overview of the current state of this intersection of fields, focusing on the application of machine learning to theoretical studies in high energy nuclear physics. It covers diverse aspects, including heavy ion collisions, lattice field theory, and neutron stars, and discuss how machine learning can be used to explore and facilitate the physics goals of understanding QCD matter. The review also provides a commonality overview from a methodology perspective, from data-driven perspective to physics-driven perspective. We conclude by discussing the challenges and future prospects of machine learning applications in high energy nuclear physics, also underscoring the importance of incorporating physics priors into the purely data-driven learning toolbox. This review highlights the critical role of machine learning as a valuable computational paradigm for advancing physics exploration in high energy nuclear physics.

- **Heavy-Ion Collisions** : **Large number of data!** Complicated simulations!
- **Neutron Star** : **Accumulating observations!** Poor signal-noise ratio!
- **Lattice QCD** : **Computationally consuming!** Physics extraction!

What is ML?



Geoffrey Hinton

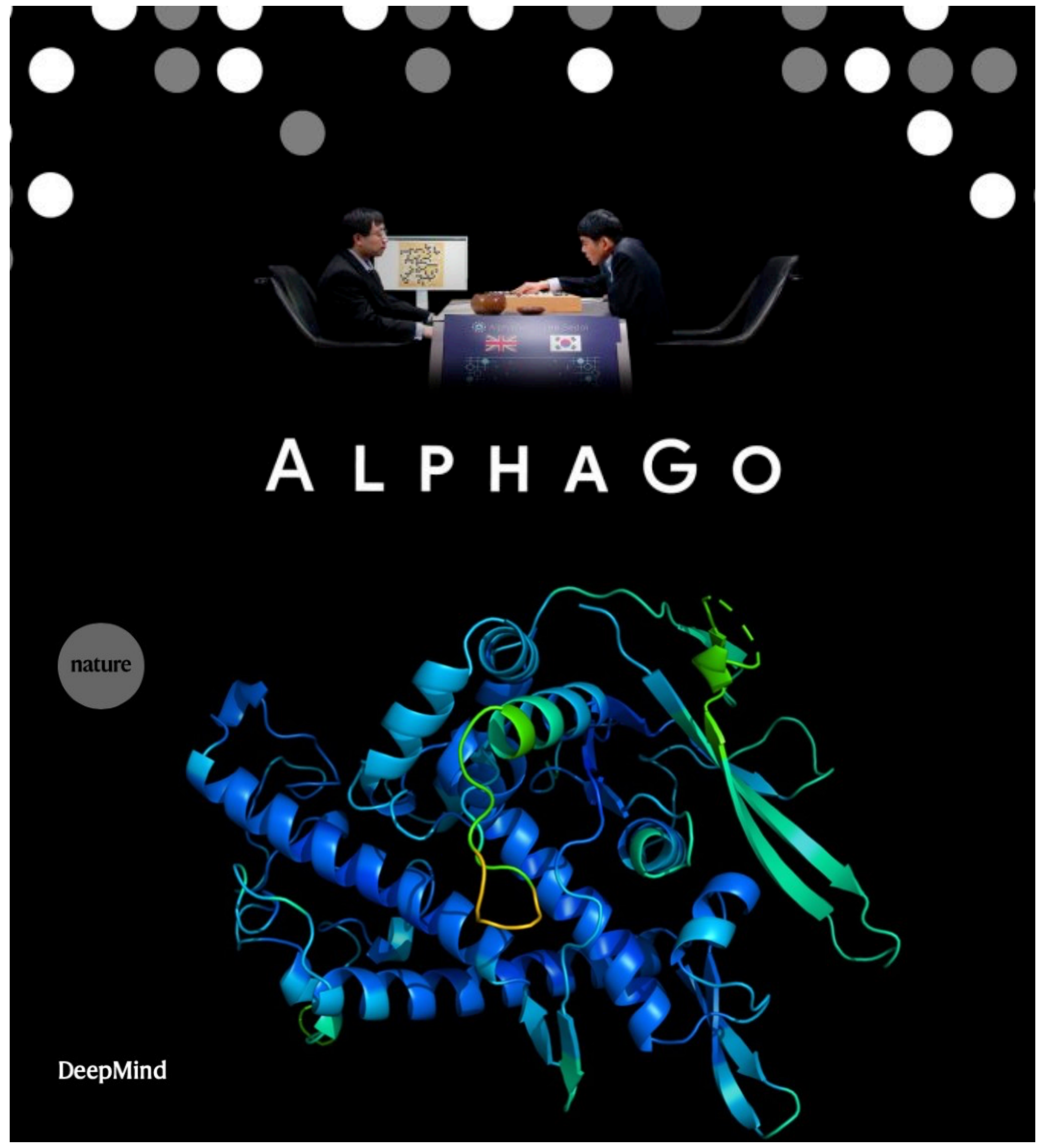
Machine Learning (ML) is a subset of artificial intelligence that involves the creation of algorithms that allow computers to learn from and make decisions or predictions based on data. It's essentially a way for computers to "learn" from data without being explicitly programmed to do so.

— **ChatGPT-4**

Big Data + Deep Models

↓ GPU

Successful Deep Learning!



Machine Learning and Inference

Maximum Likelihood Estimation(MLE)

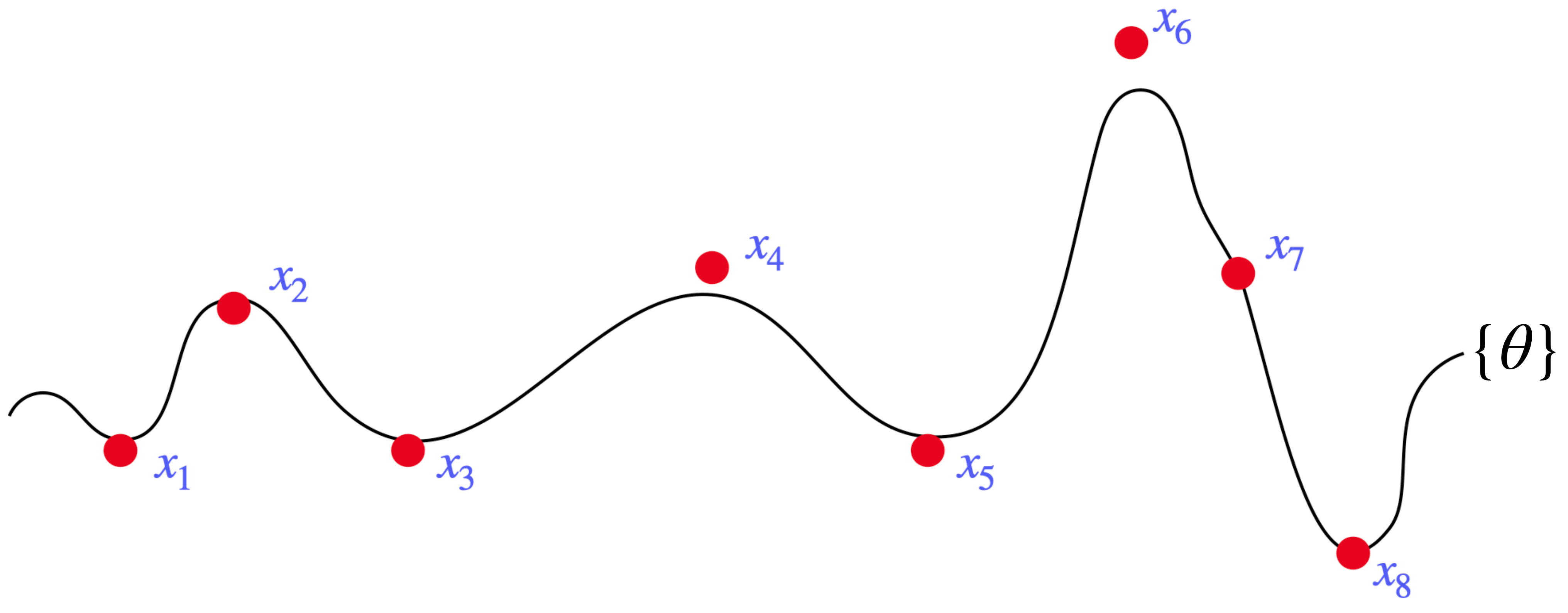
$$\max_{\theta} \prod_{i=1}^{N} p(\mathbf{x}_i \mid \theta)$$

Bayesian Inference

Maximum A Posterior(MAP)

$$p(\theta \mid X) = \frac{p(X \mid \theta)\pi(\theta)}{p(X)}$$

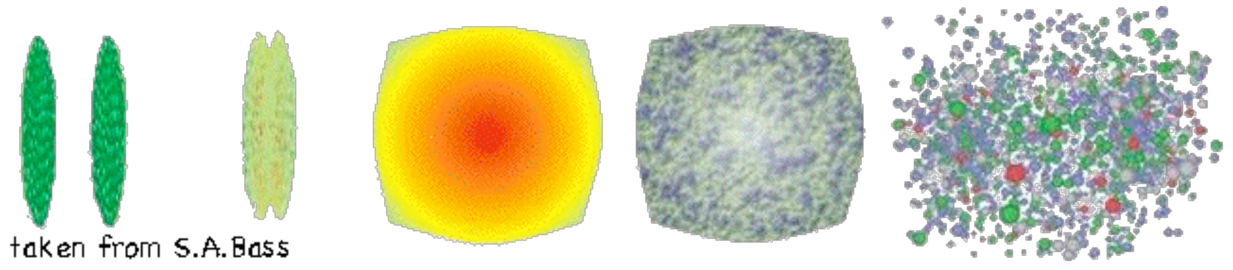
Posterior $p(\theta \mid X)$, **Prior** $\pi(\theta)$, **Evidence** $p(X)$



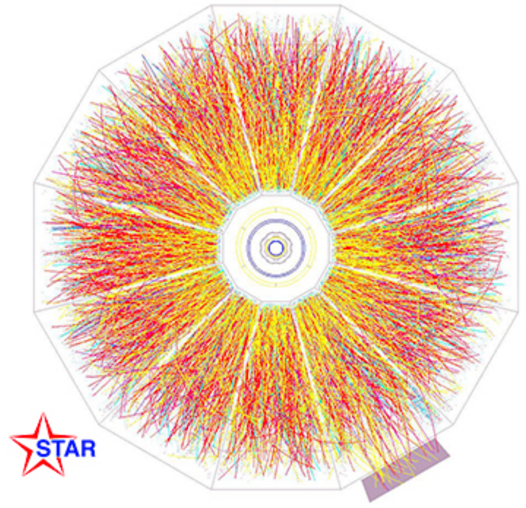
Inverse Problems

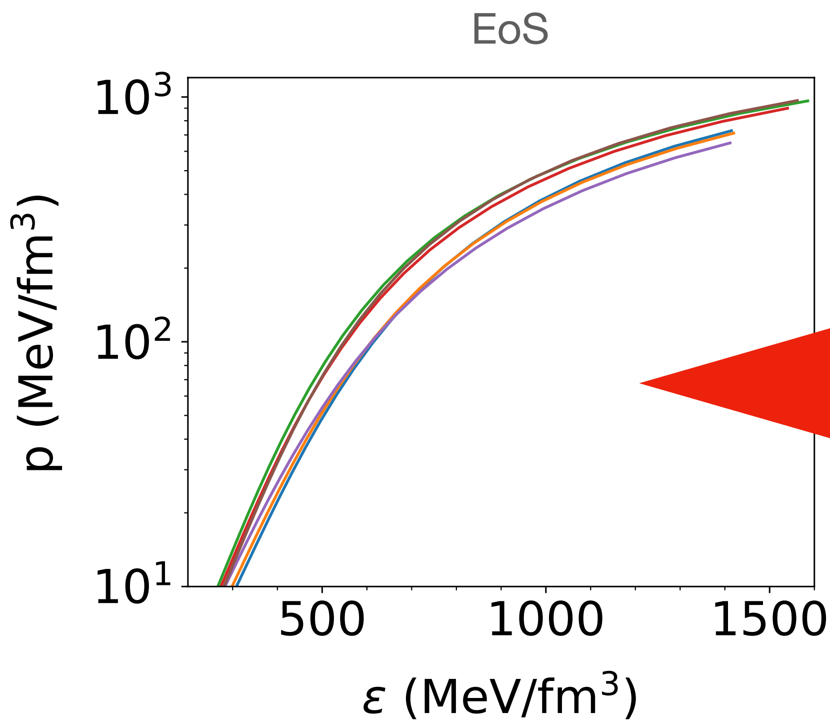
Physics

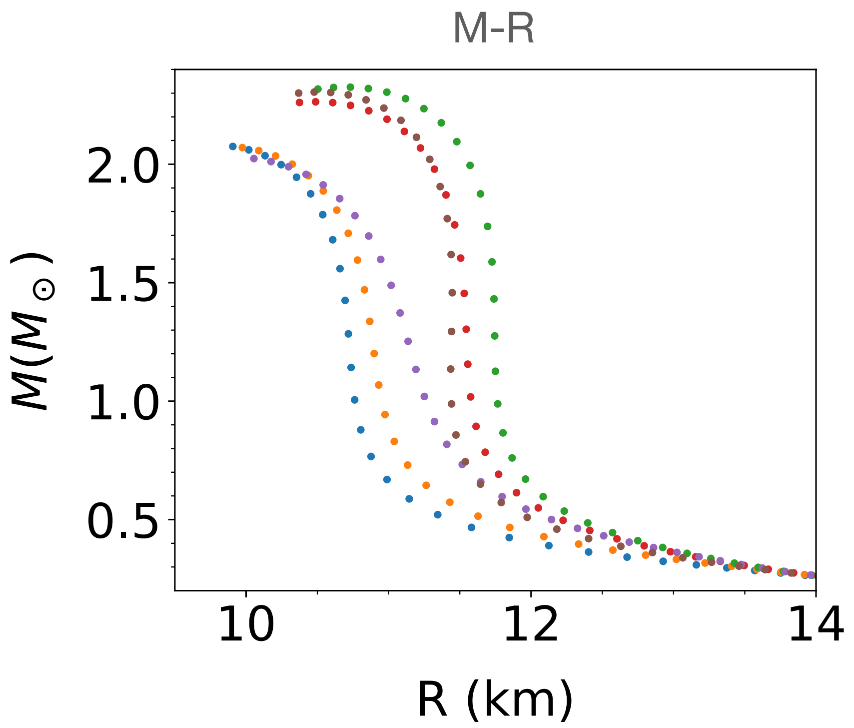
Data

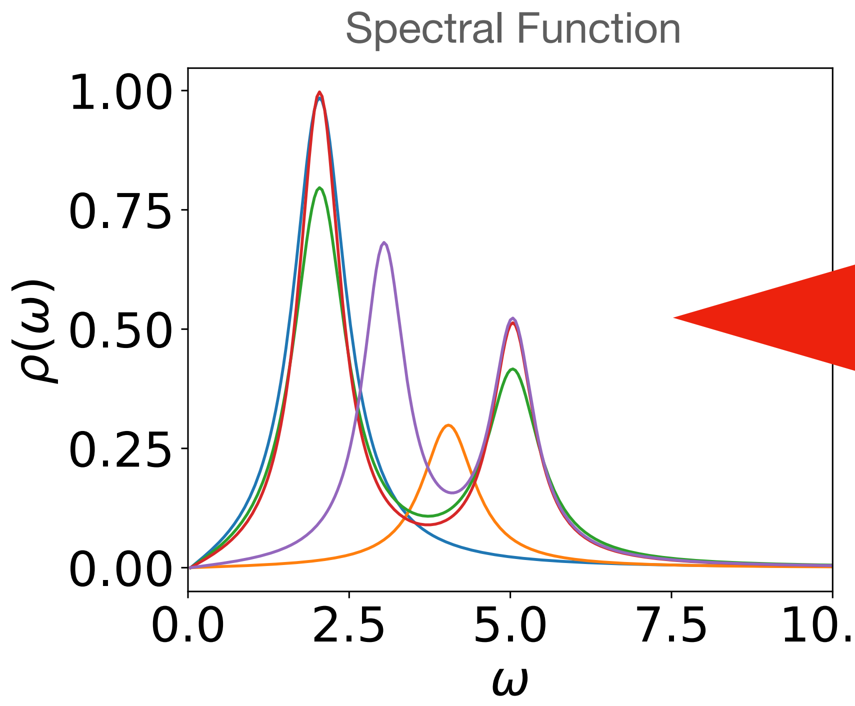


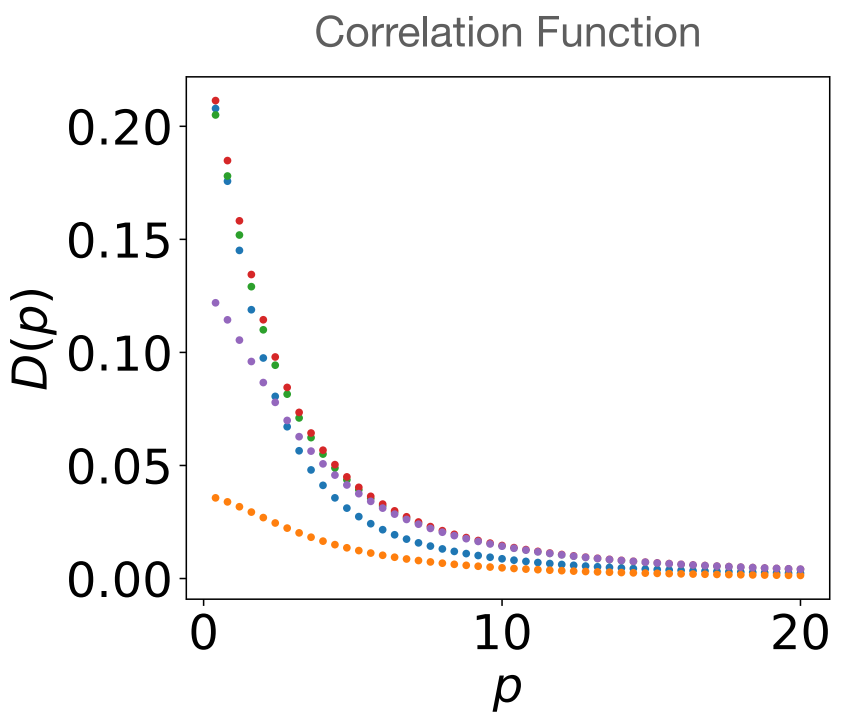
QCD matter properties





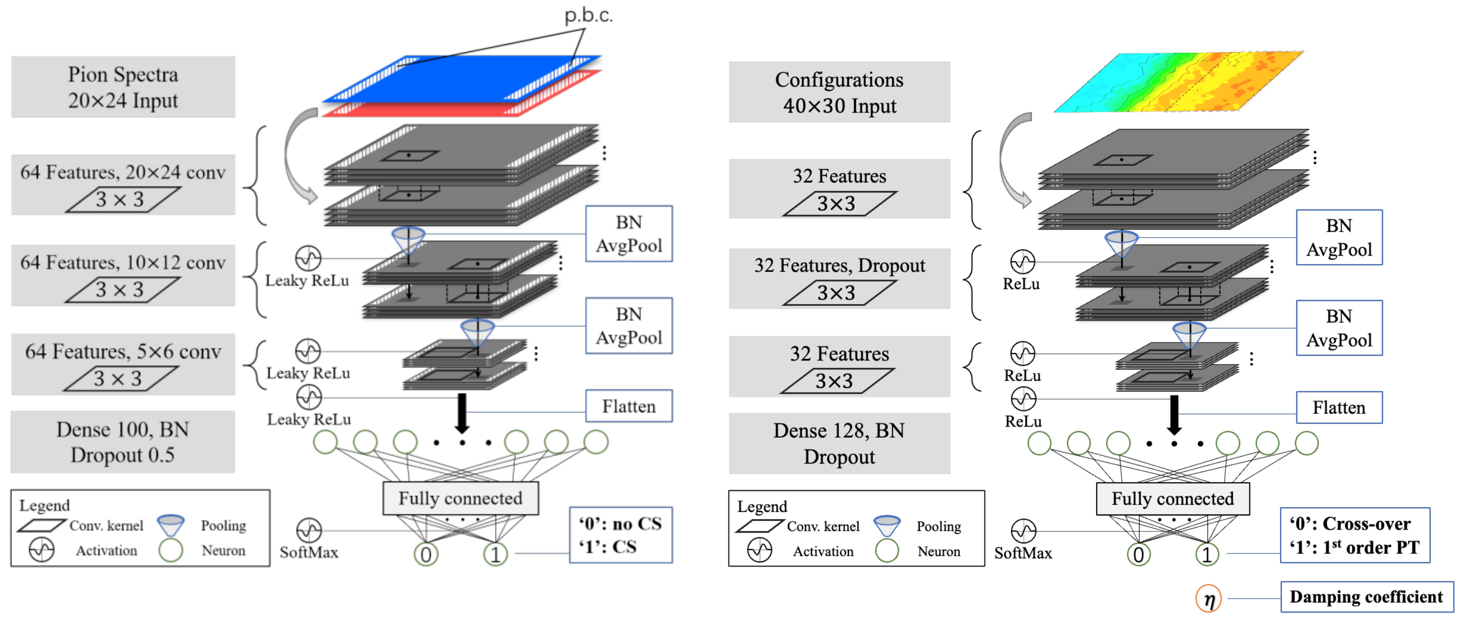






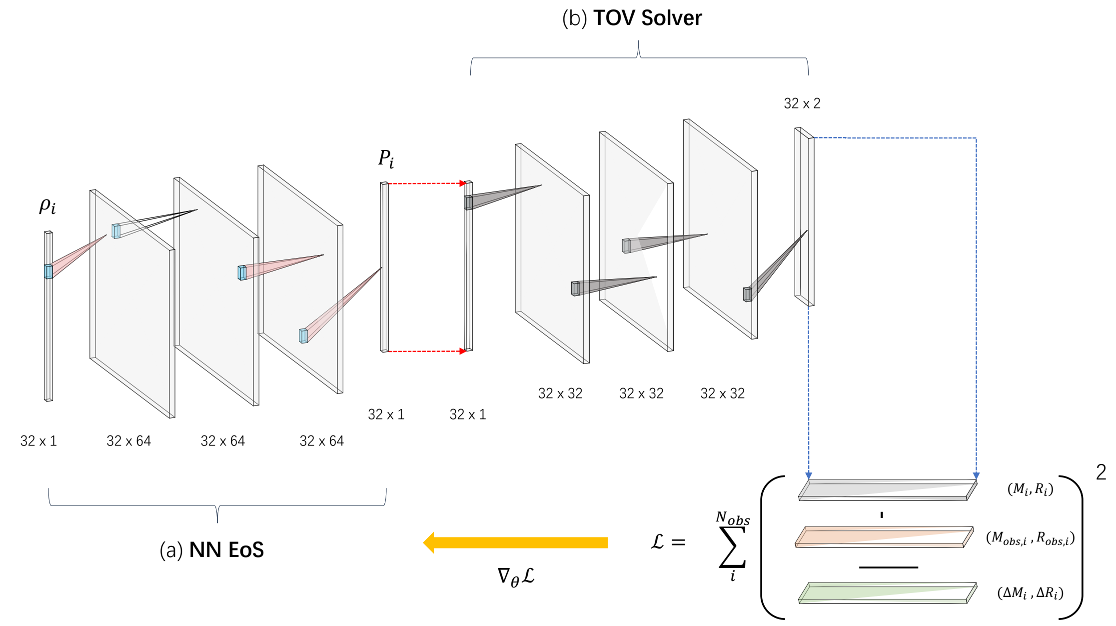
Heavy-Ion Collisions

Phys. Rev. C 106, L051901; Phys. Rev. D 103, 116023



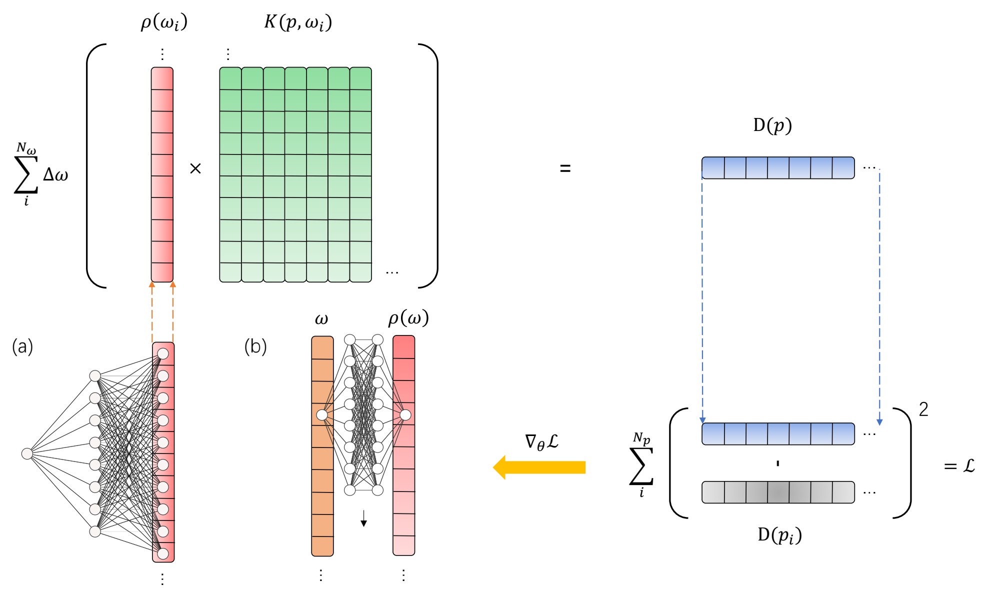
Neutron Star

Phys. Rev. D 107, 083028; JCAP08 (2022) 071



Lattice QCD

Phys. Rev. D 106, L051502; Comput. Phys. Commun. 282, 108547 (2023);



Data-Driven Learning

$$f_\theta : X \to Y$$

Forward process

Physics

Model Parameters/ Properties/States

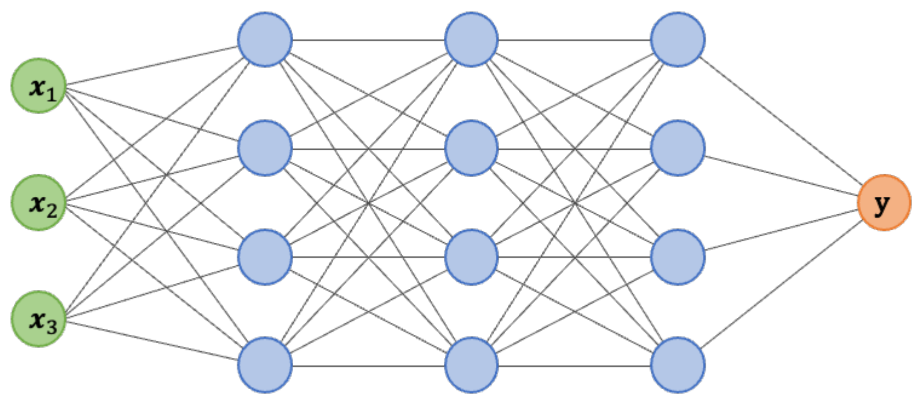
Data

Observations

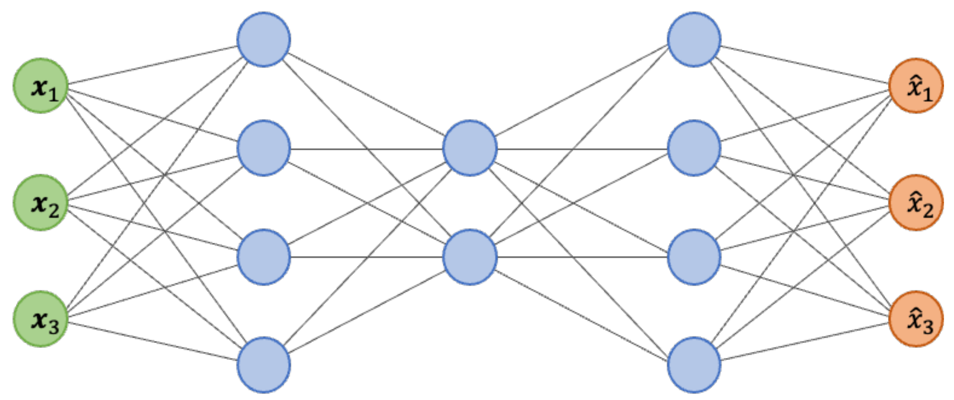
Inverse Mapping, f_θ

Data-Driven Learning

$$f_\theta : X \to Y$$



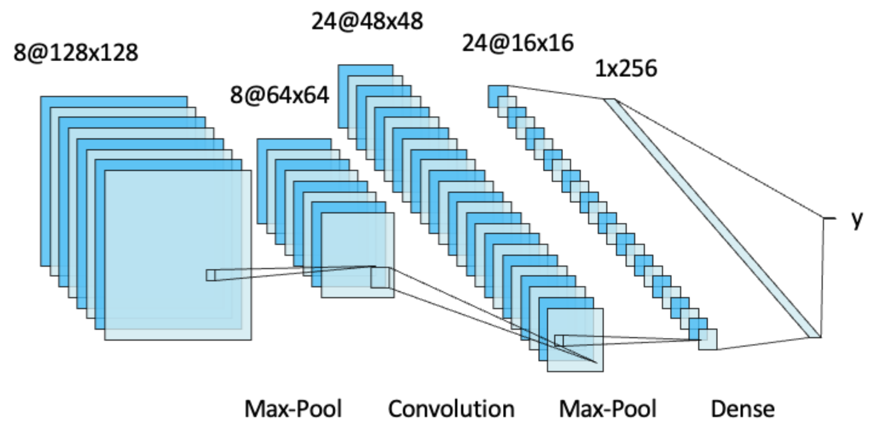
Deep Neural Network



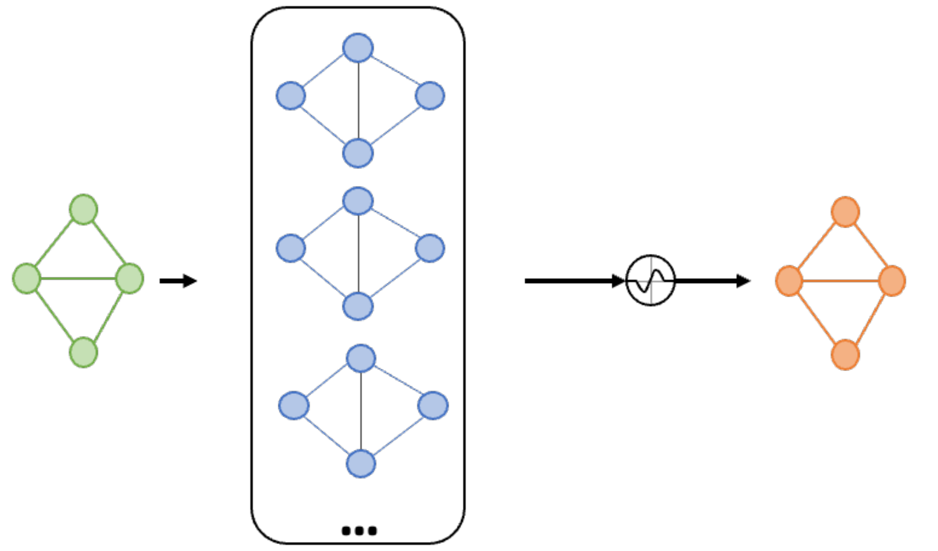
AutoEncoder

Universal Approximation Theorem (1989,1991)

A feed-forward network with *a single hidden layer* containing *a finite number of neurons* can approximate arbitrary continuous functions.



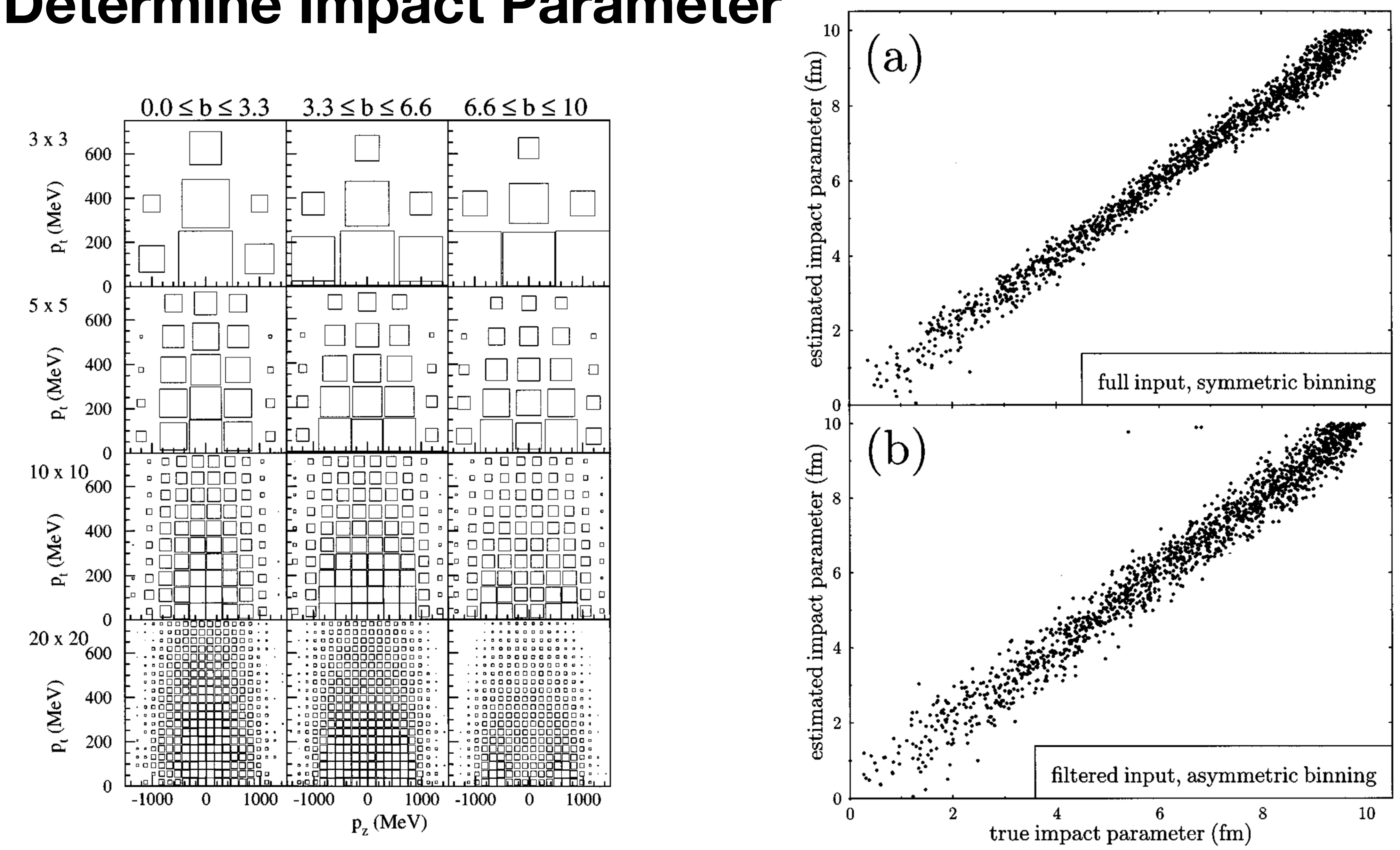
Convolutional Neural Network



Graph Neural Network

Data-Driven Learning

Determine Impact Parameter



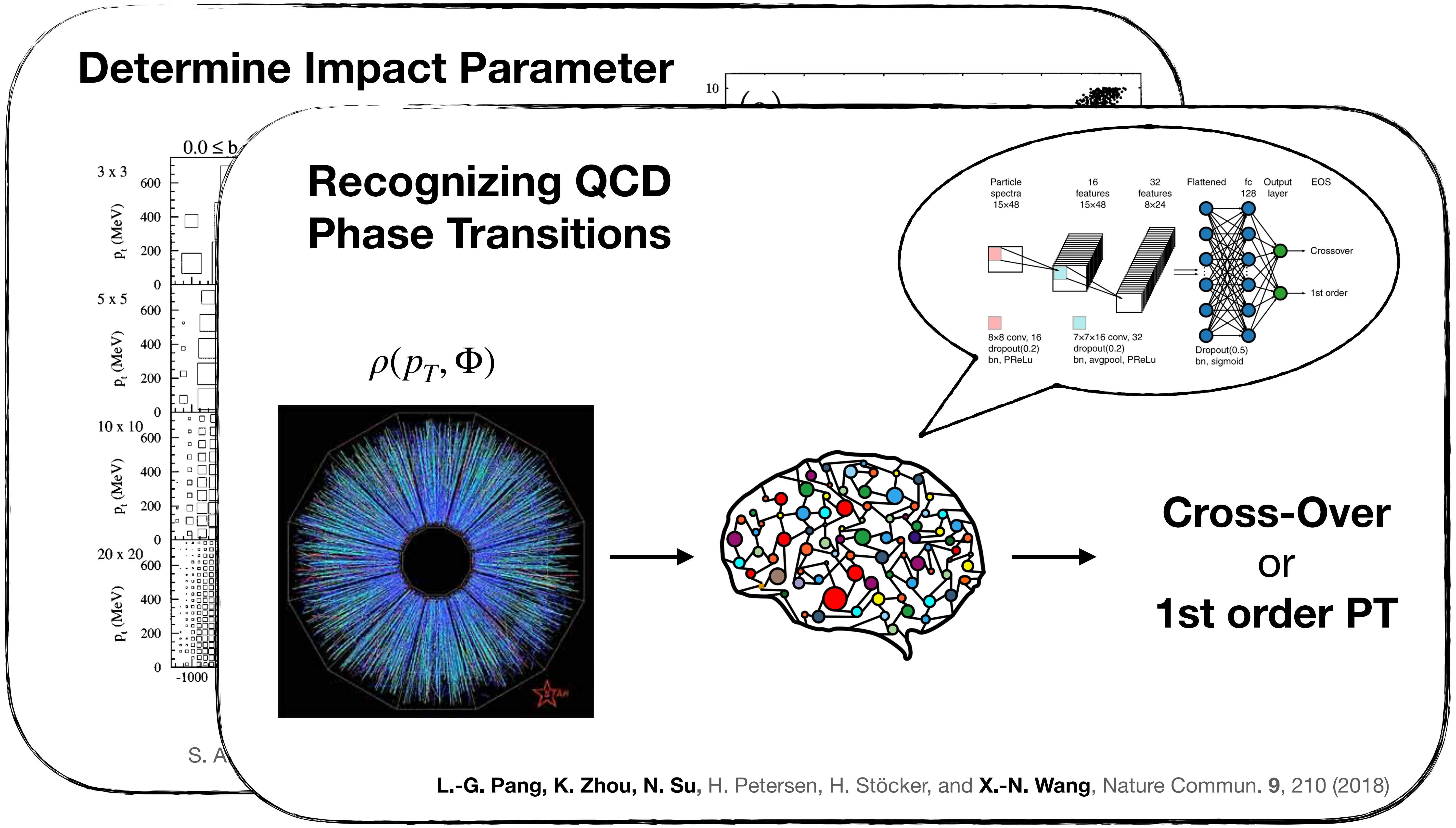
S. A. Bass, A. Bischoff, J. A. Maruhn, H. Stöcker, and W. Greiner, Phys. Rev. C **53**, 2358 (1996)

QMC data

1 hidden layer with 20 neurons

Input 5X5

Data-Driven Learning



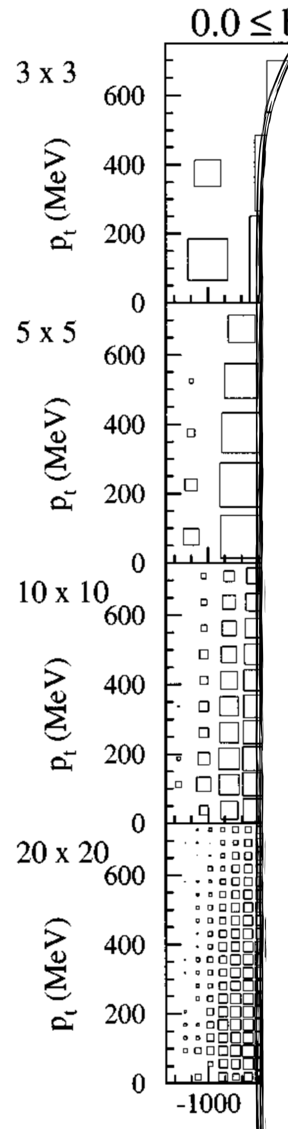
Hydro data

CNNs+DNNs

Input 15X48

Data-Driven Learning

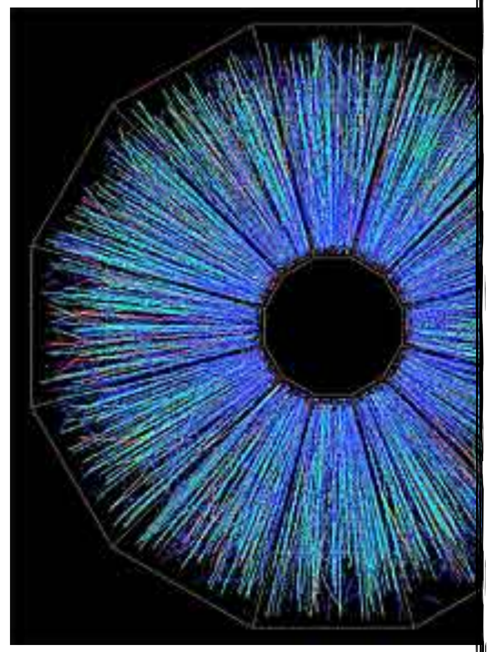
Determine Impact Parameter



S. A

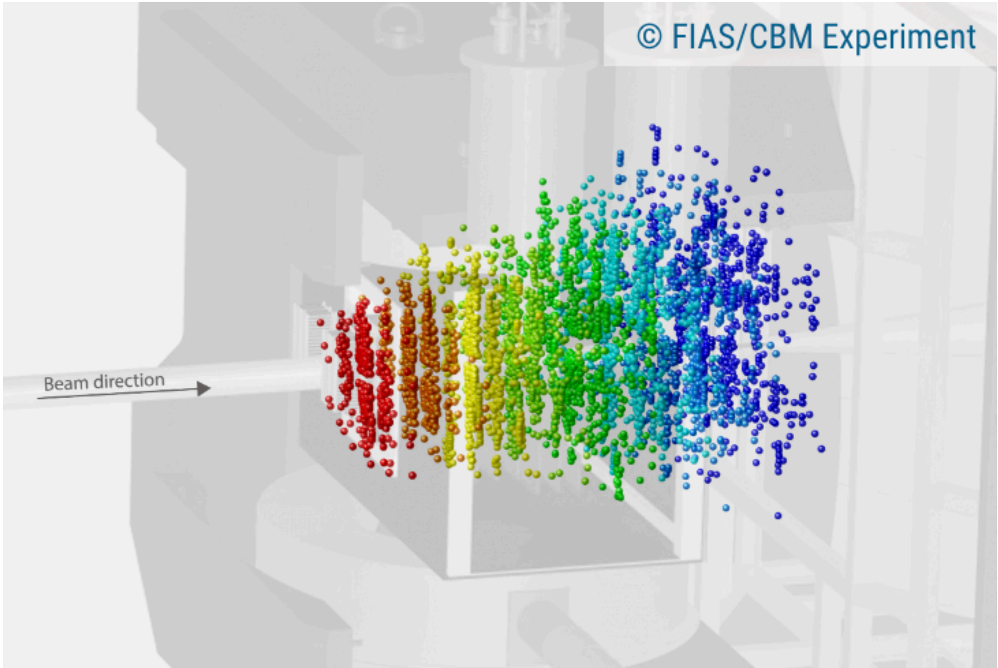
Recognizing QCD Phase Tran

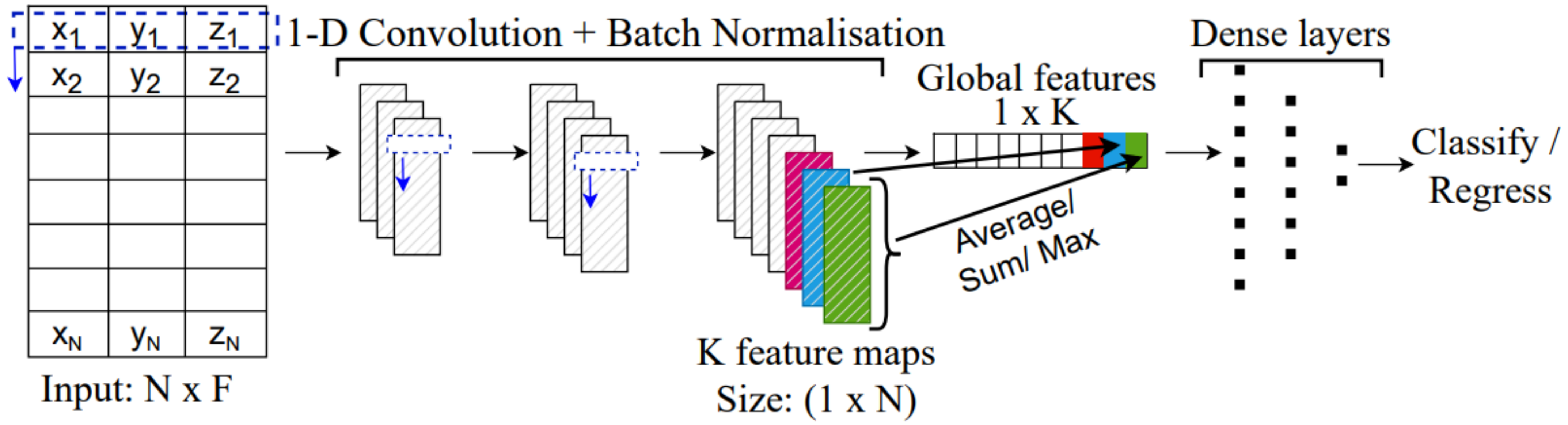
$\rho(p_T, \Phi)$



L.-G. Pa

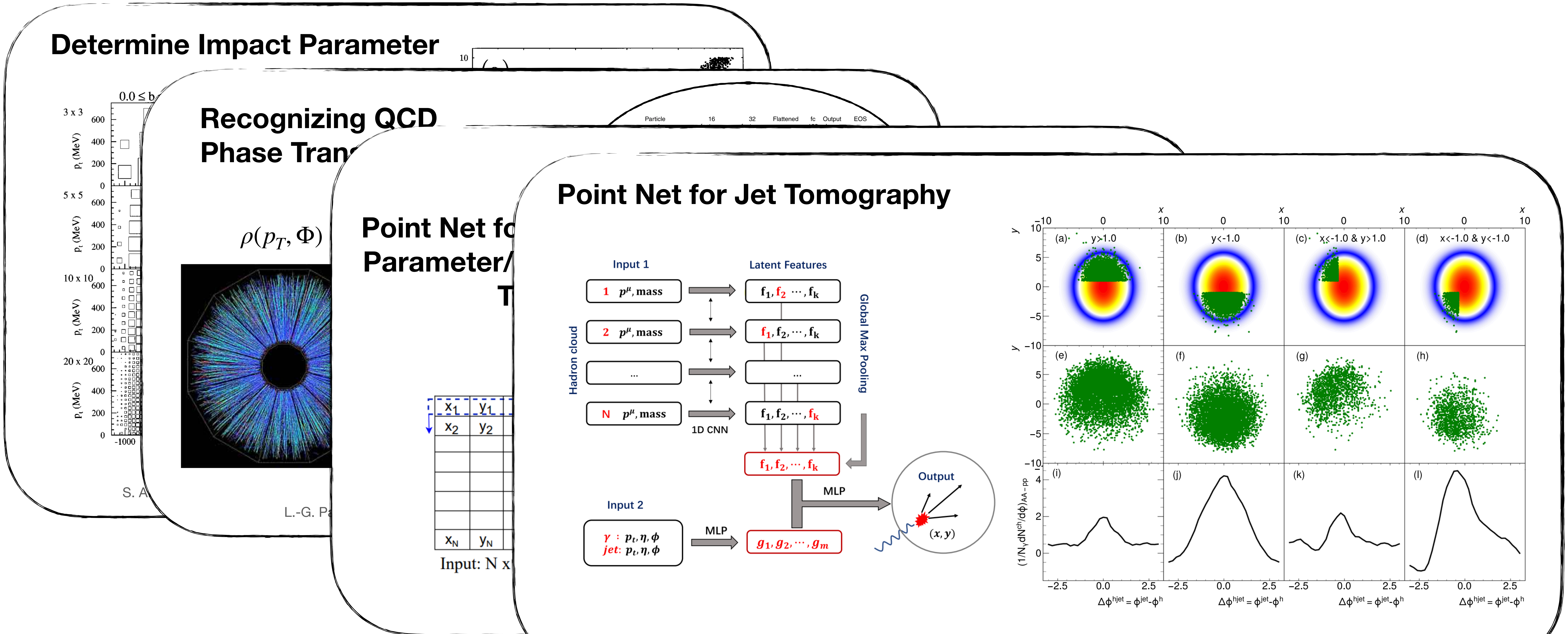
Point Net for Determing Impact Parameter/ Recognizing Phase Transitions





Manjunath O.K. and Kai Zhou, etc. *Phys.Lett.B* 811 (2020) 135872; JHEP10(2021)184.

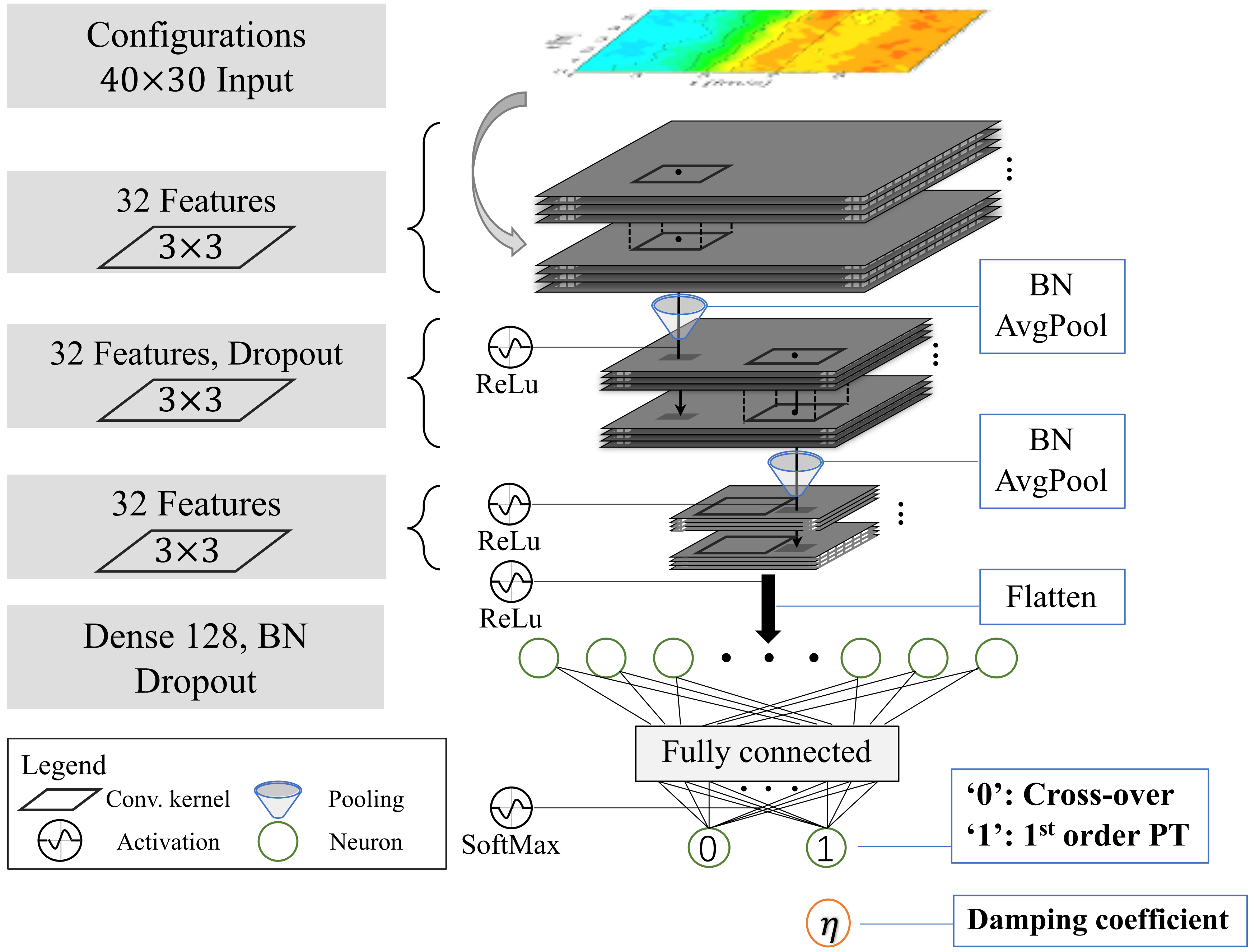
Data-Driven Learning



Z. Yang, Y. He, W. Chen, W.-Y. Ke, **L.-G. Pang**, and **X.-N. Wang**, Eur. Phys. J. C **83**, 652 (2023).

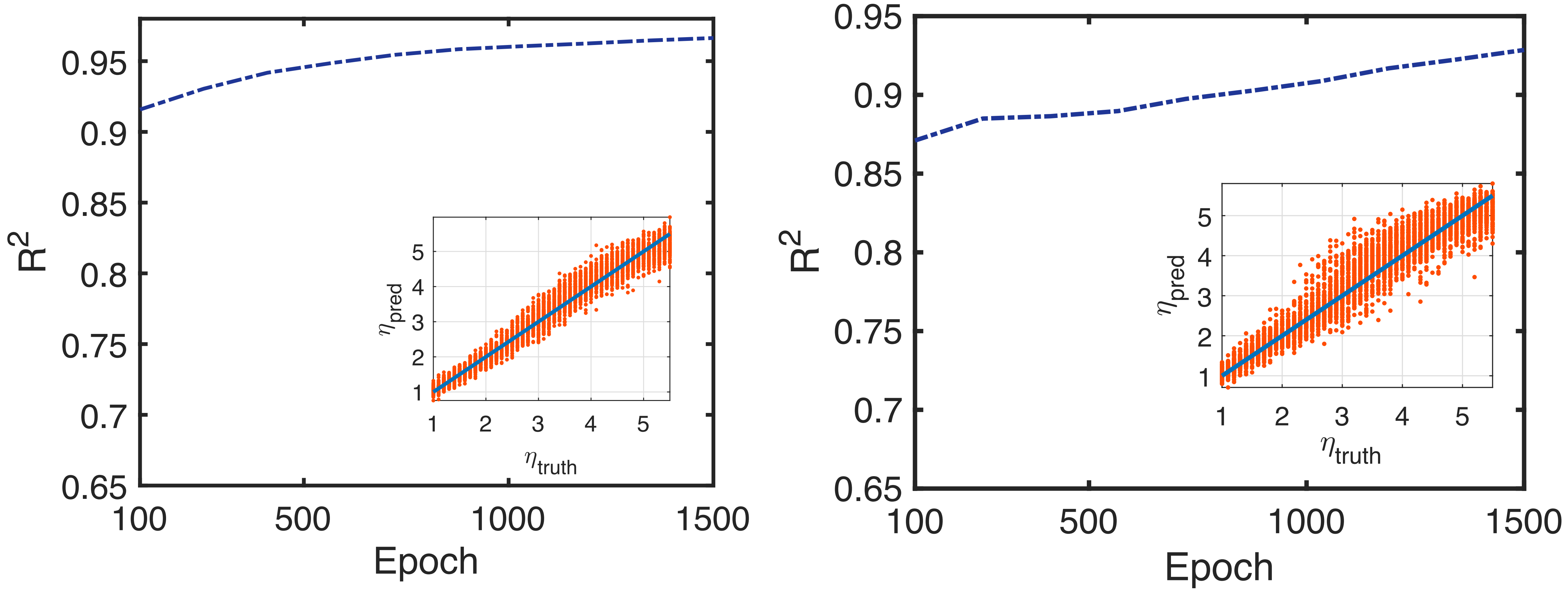
...

Our Current Works



Phys. Rev. D 103, 116023

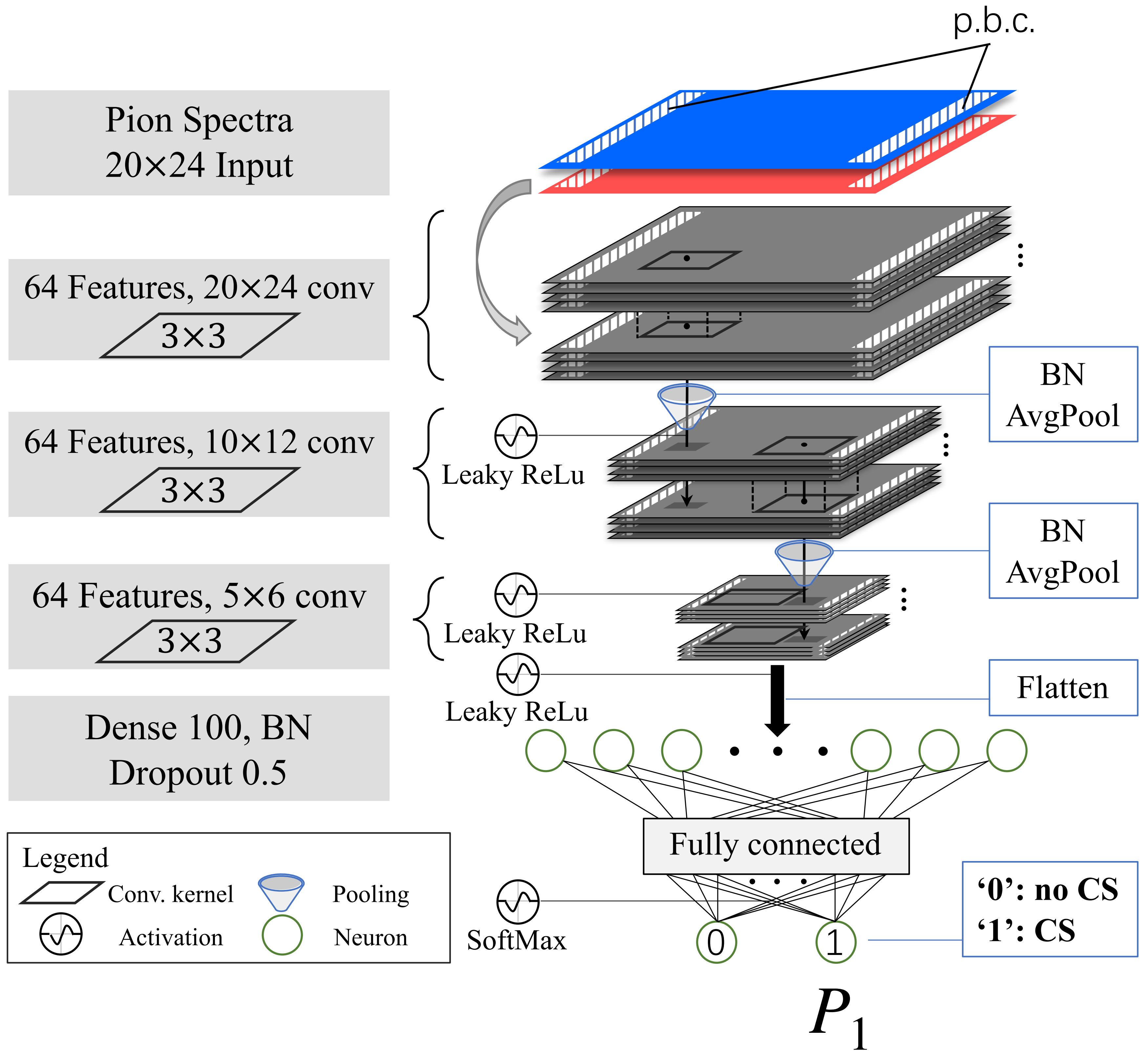
with Lijia and Kai

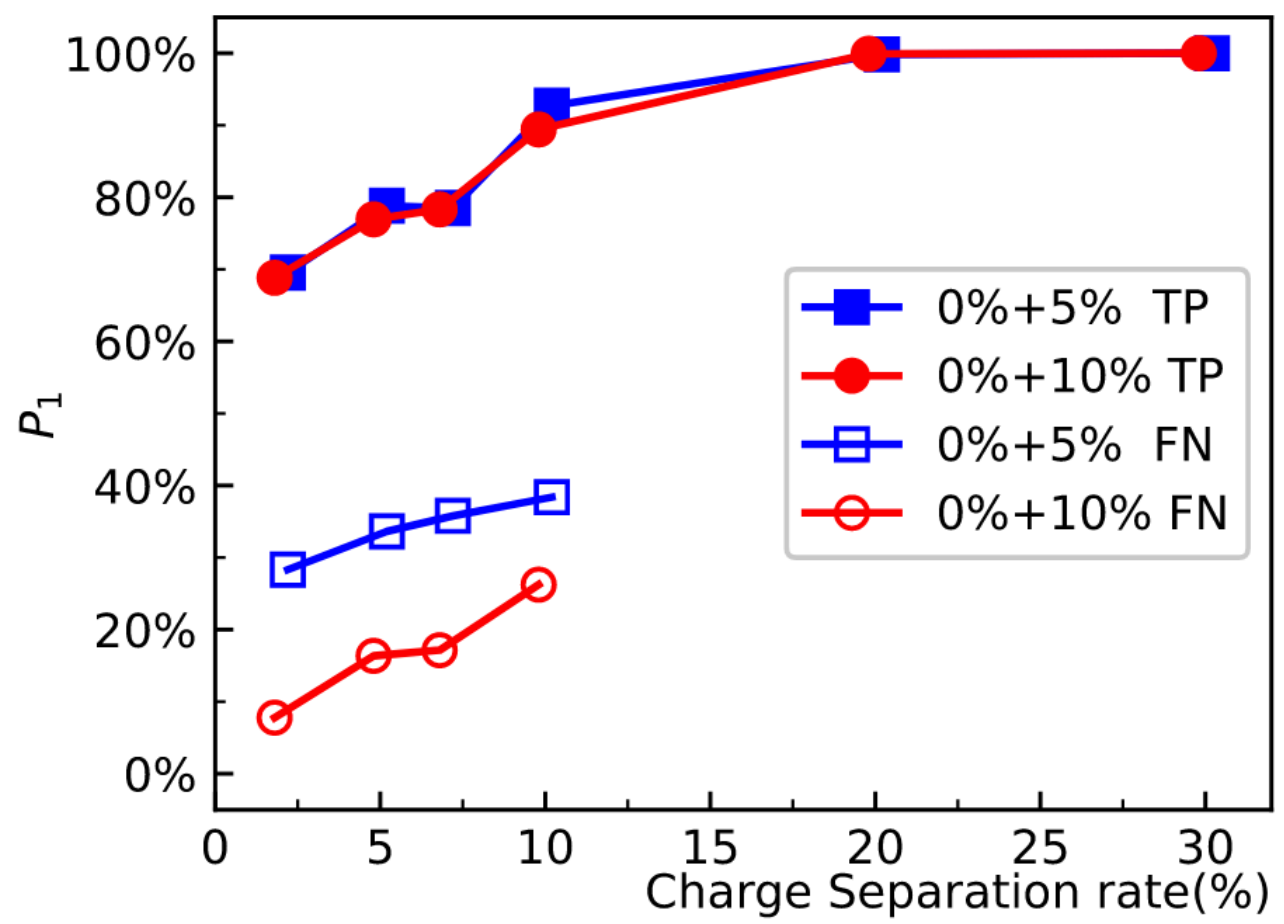


Learning dynamics of stochastic processes from configurations

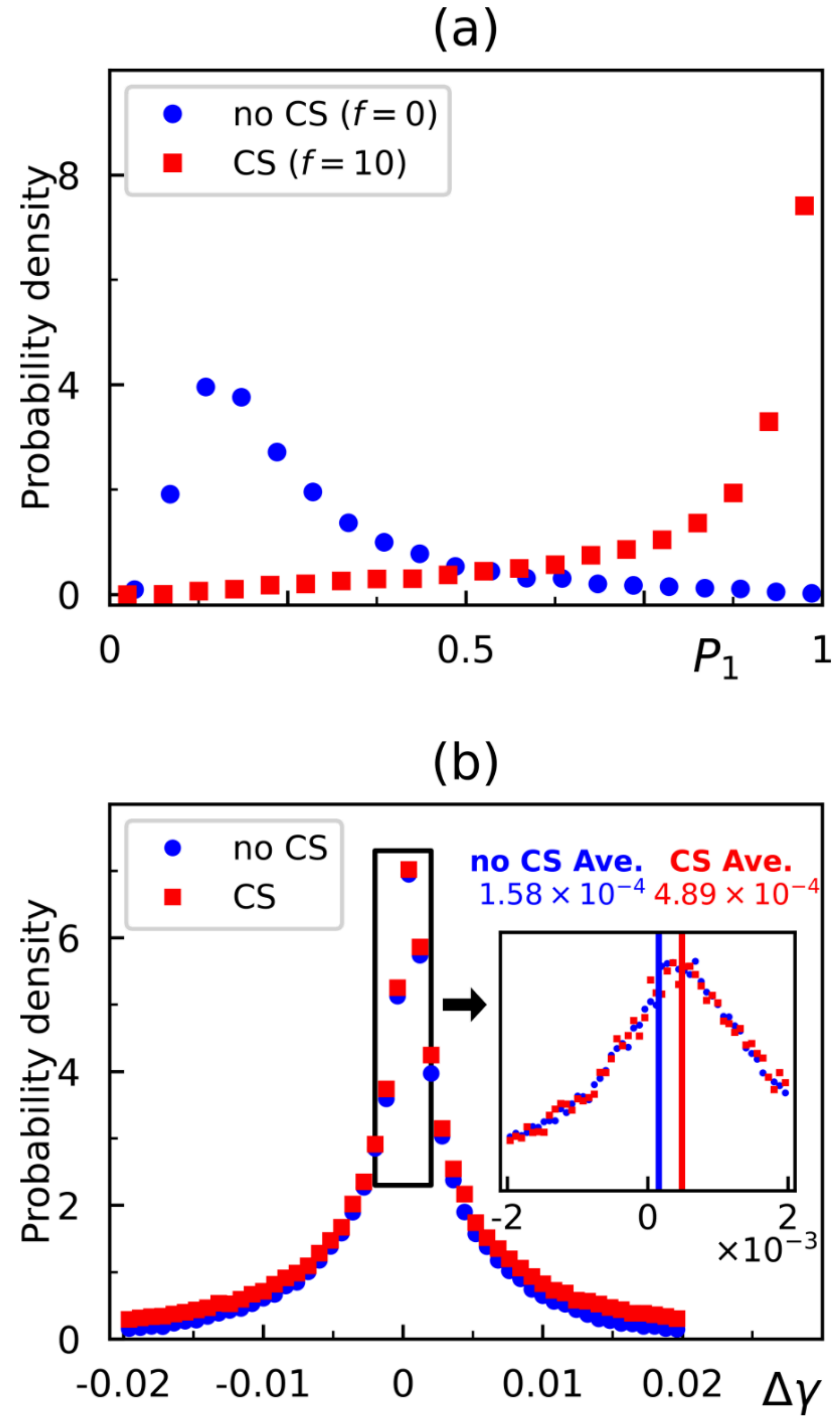
Our Current Works

Phys. Rev. C 106, L051901(Letter) **with Yuan-Sheng, Xu-Guang and Kai**





0%+5%(10%) Model
traned on differnt data-set with
charge seperation fraction, f = 5%(10%)



Au + Au $\sqrt{s_{NN}}$= 200 GeV, centrality 40–50%

Neural networks for detecting CME

Physics-Driven Learning

$$\hat{\theta} = \mathbf{arg\,max}_{\theta}\{p(X \mid \theta)\}$$

Forward process

Physics

Model Parameters/ Properties/States

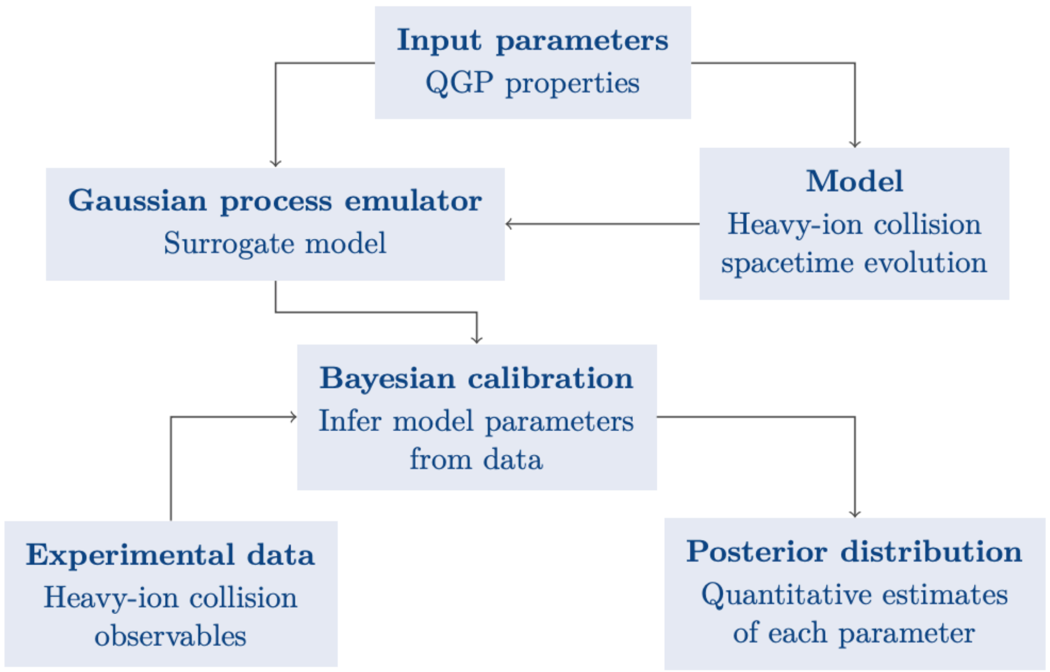
Data

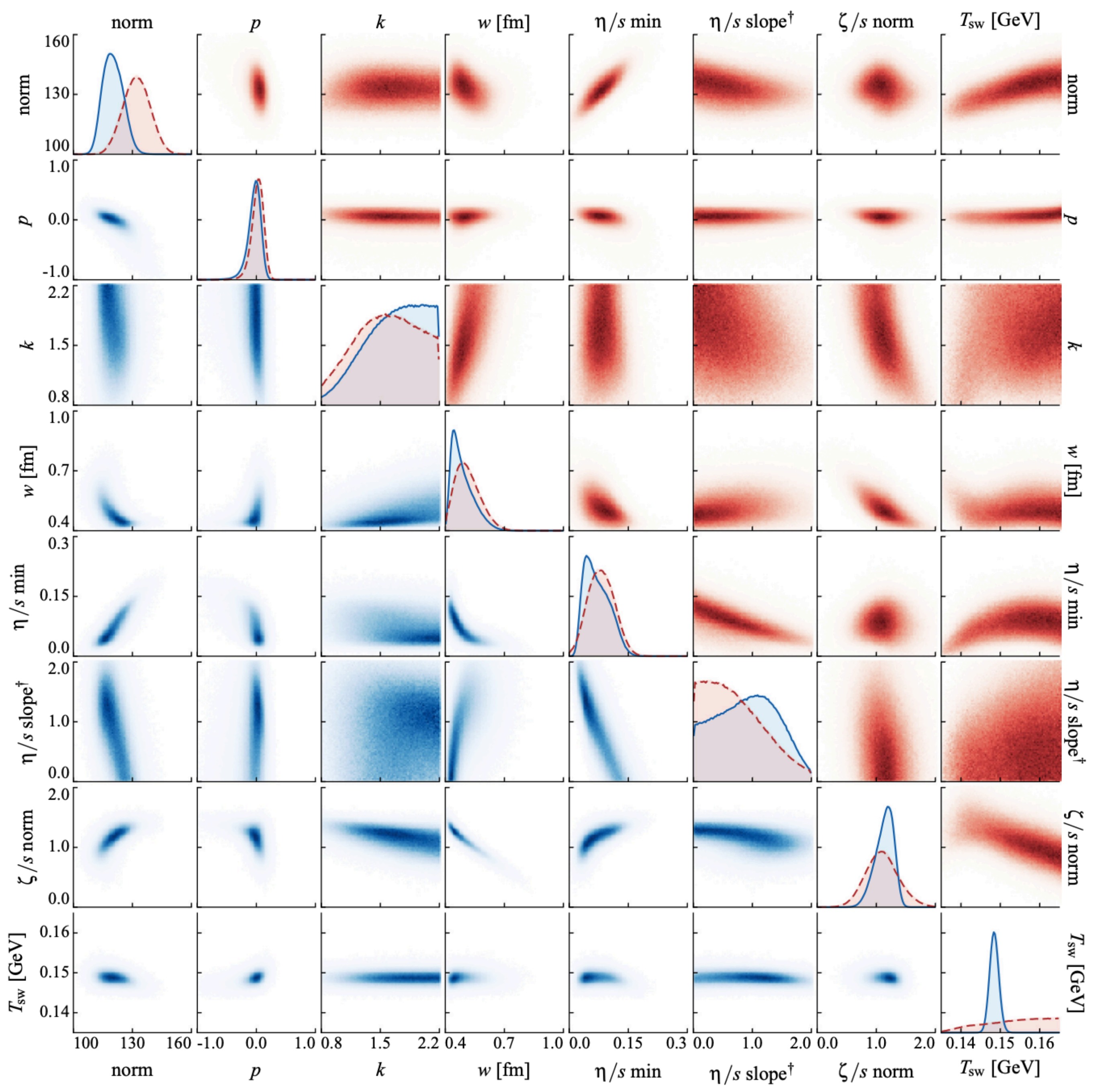
Observations

Inference

Physics-Driven Learning

Inferring Dynamical Information

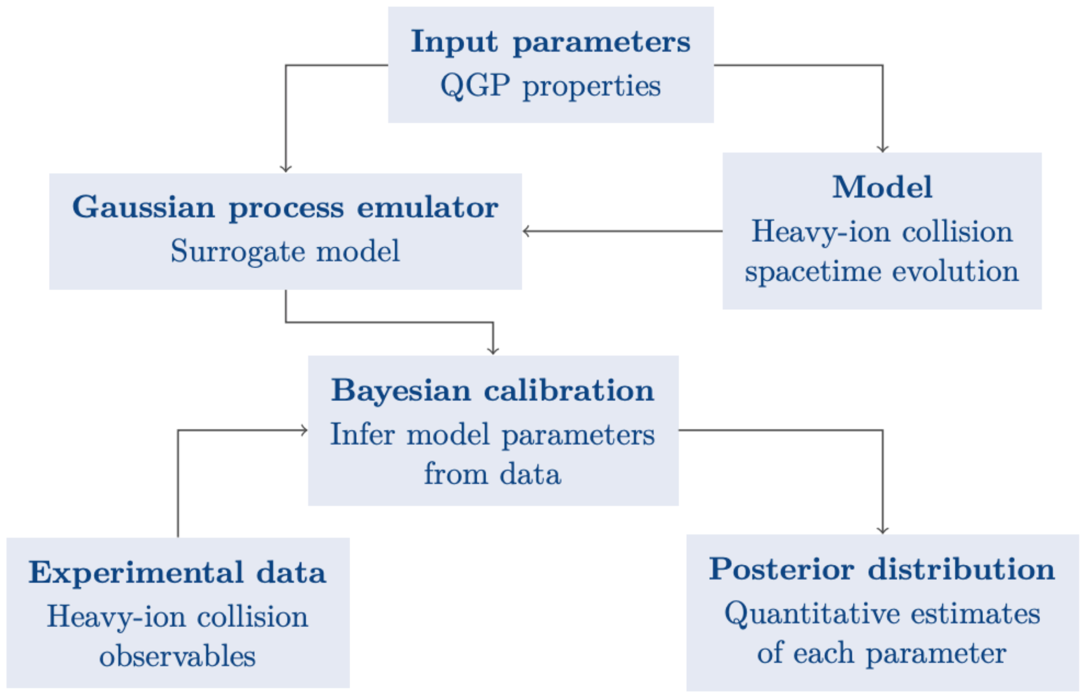




J. E. Bernhard, etc.(Duke Group), arXiv:1804.06469 and Nat Phy **15**, 1113 (2019).

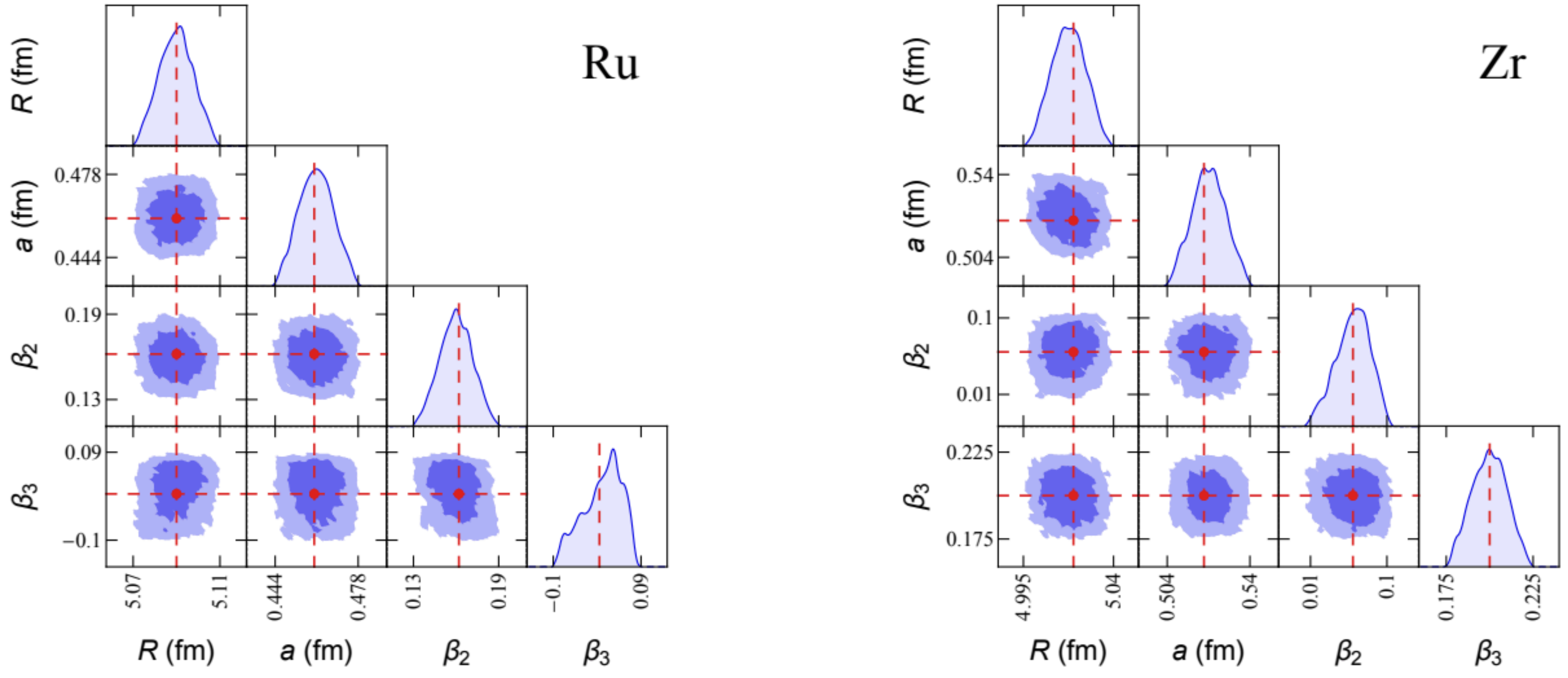
Physics-Driven Learning

Inferring Dynamical Information



J. E. Bernhard, etc.(Duke Group), arXiv:1804.06469

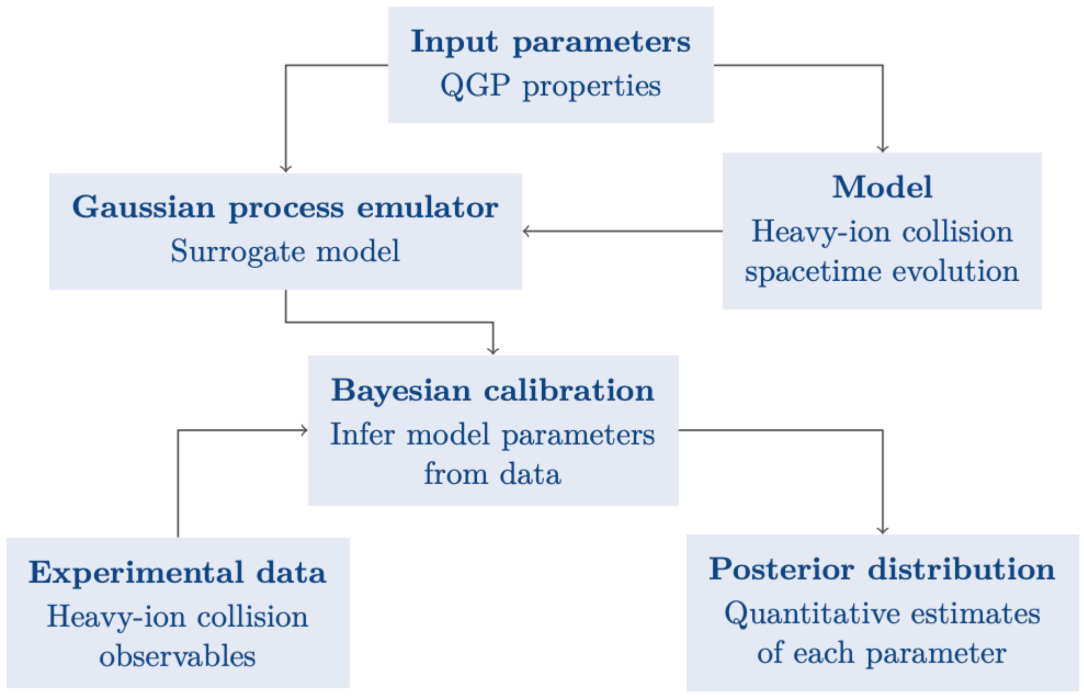
Determing Nulcear Struture



Y.-L. Cheng, **S. Shi, Y.-G. Ma**, H. Stöcker, and **K. Zhou**, Phys. Rev. C **107**, 064909 (2023)

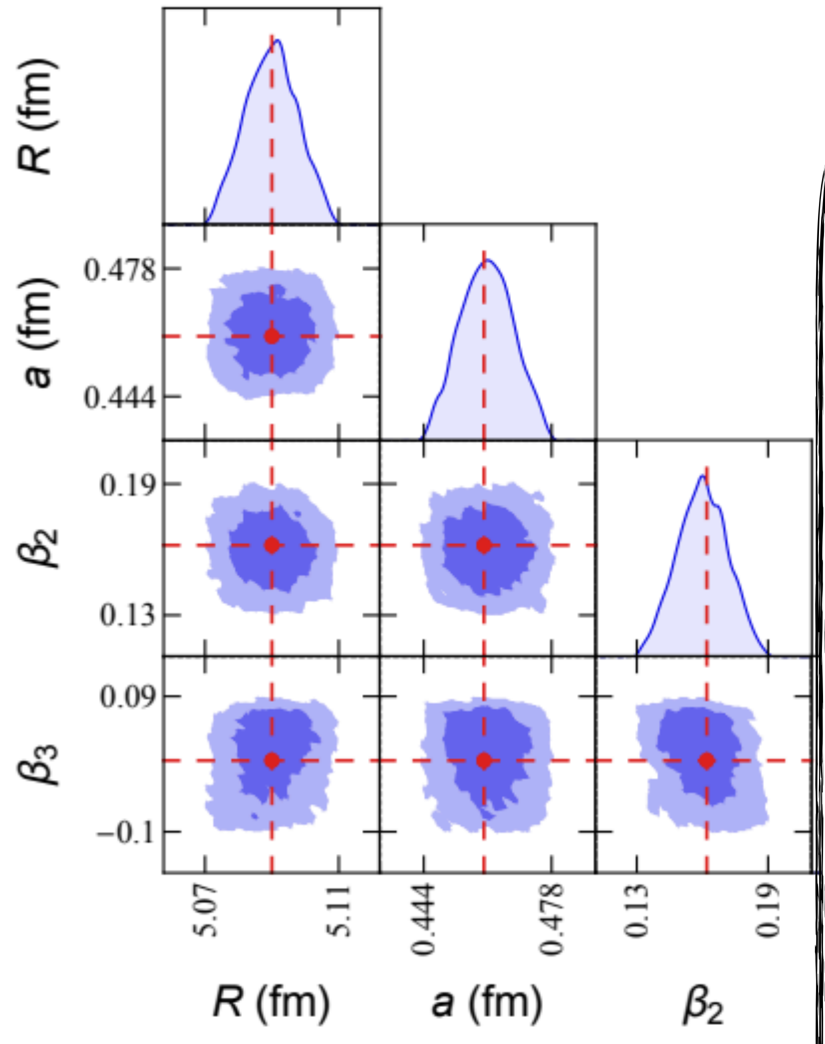
Physics-Driven Learning

Inferring Dynamical Information



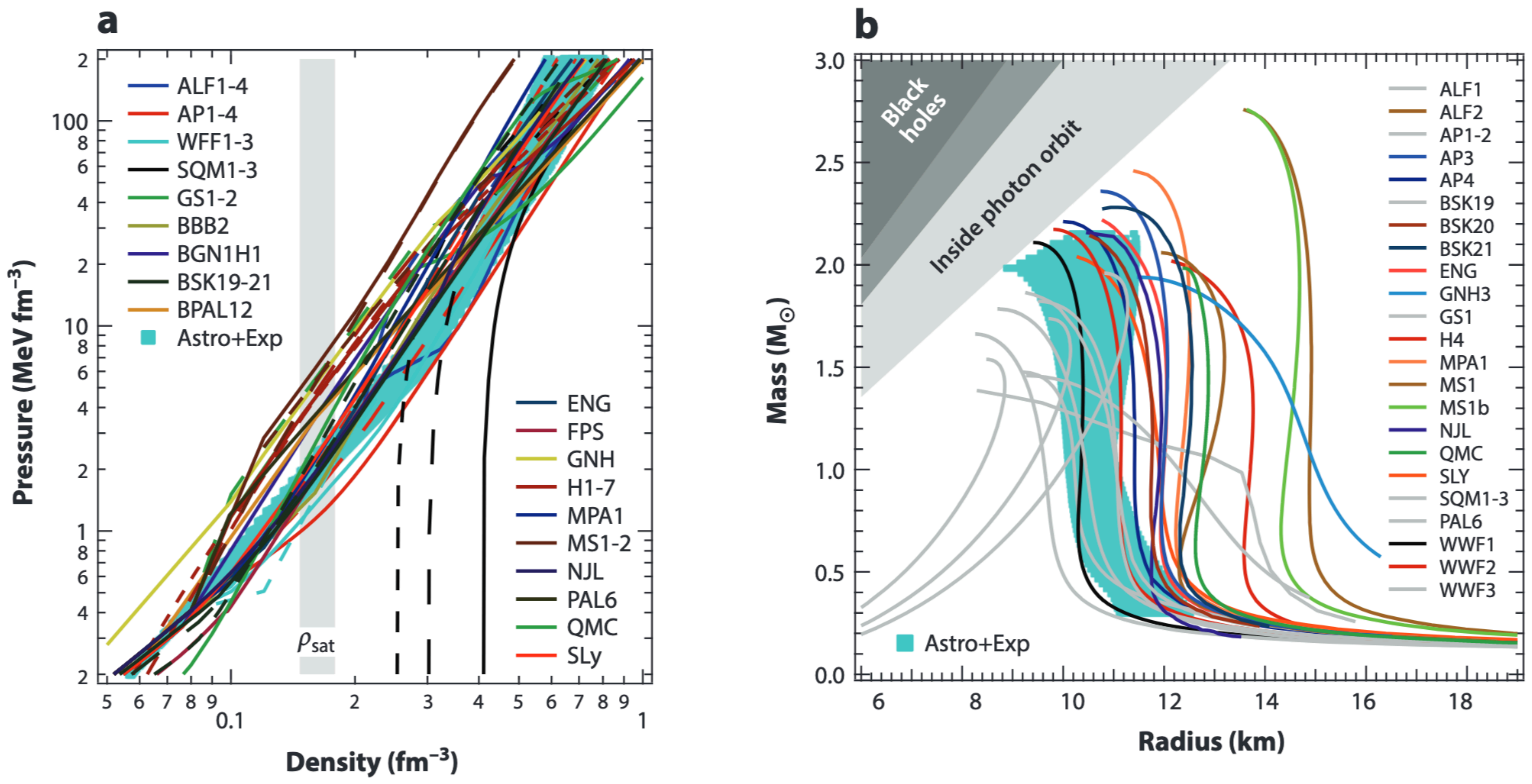
J. E. Bernhard, etc.(Duke Group), arXiv:1804.06469

Determing Nulcear Struture



Y.-L. Cheng, S. Shi, Y.

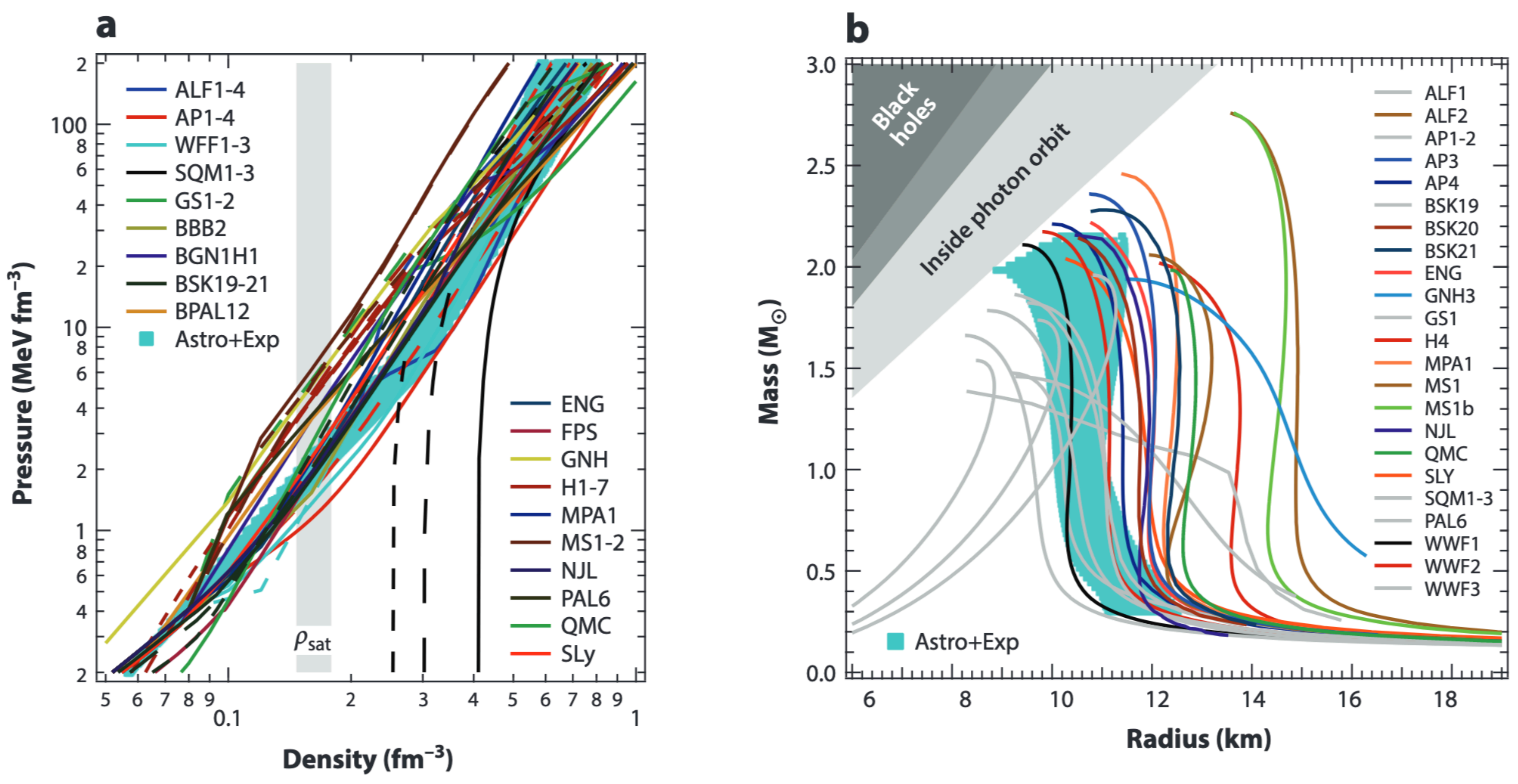
Building Nuclear Matter EoS



F. Özel and P. Freire, Annu. Rev. Astron. Astrophys. **54**, 401 (2016)

Physics-Driven Learning

Building Nuclear Matter EoS



F. Özel and P. Freire, Annu. Rev. Astron. Astrophys. **54**, 401 (2016)

Physics Parameters are Finite

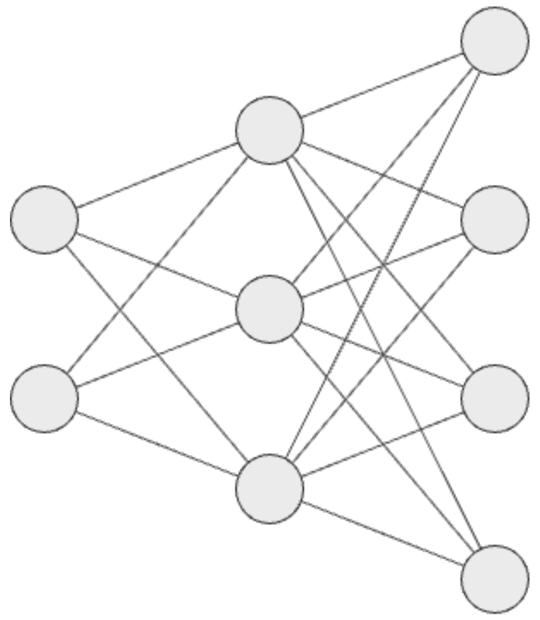
EoS, Wave-Function, Potential, …

Inference is Easy-To-Compute

ODEs, PDEs, Simulations, …

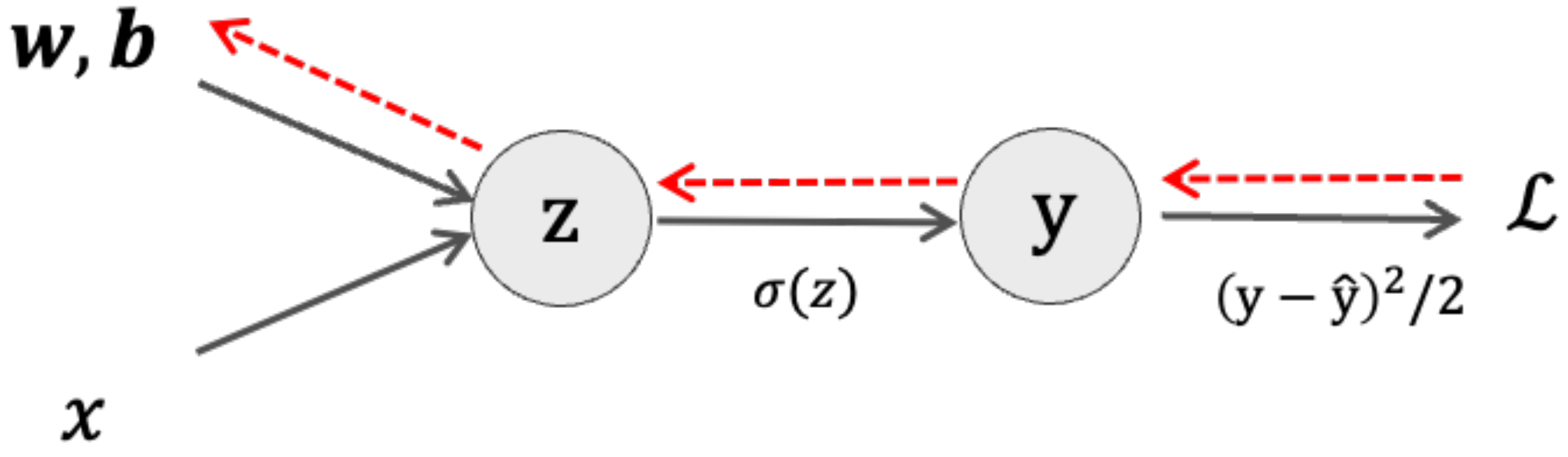
Physics-Driven Deep Learning

$$\hat{\theta} = \textbf{arg max}_{\theta}\{p(X \mid \theta)\}$$



$$f_\theta \underset{\text{BP}}{\overset{\text{Phys}}{\rightleftarrows}} \tilde{O}$$

$$\mathcal{L} = (O - \tilde{O})^2$$



Deep Neural Network represented Physics, f_θ

Flexible Representation

Back-Propagation

Easy-To-Compute on GPUs

Physics-Driven Deep Learning

1. Building Neutron Star EoS

Tolman–Oppenheimer–Volkoff equations

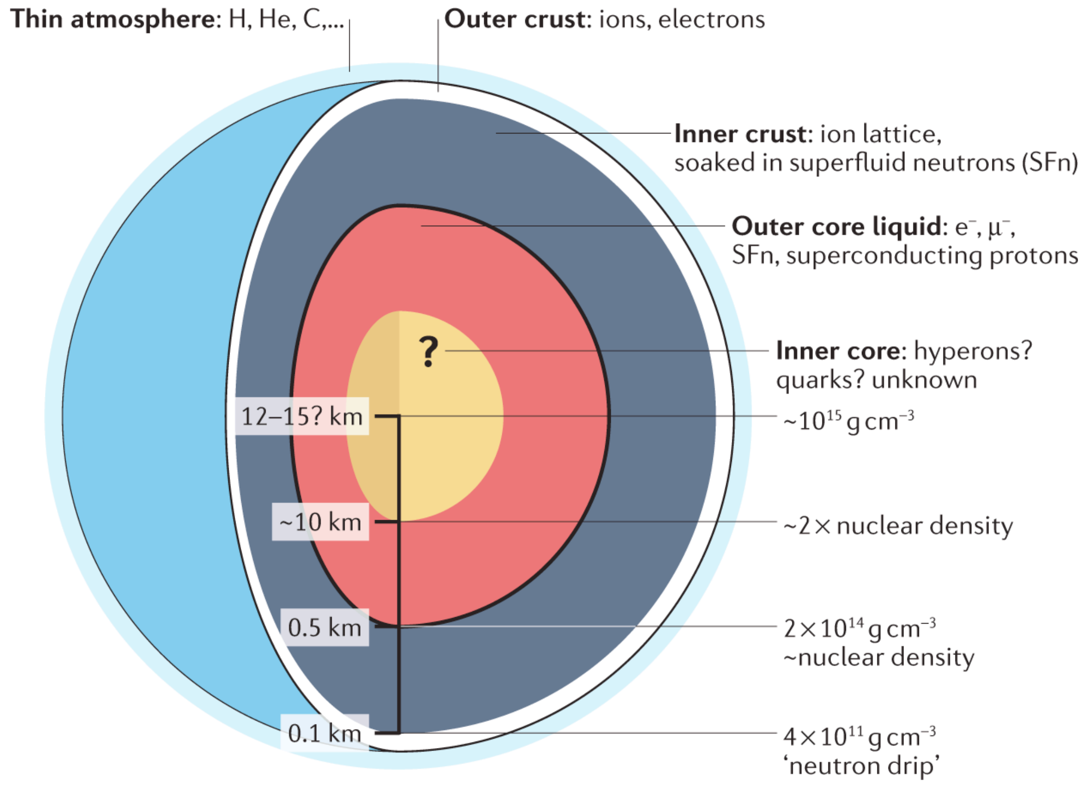
$$\begin{cases} \dfrac{dP}{dr} = -G\dfrac{m(r)\varepsilon(r)}{r^2}\left(1+\dfrac{P(r)}{\varepsilon(r)}\right)\left(1+\dfrac{4\pi r^3 P(r)}{m(r)}\right)\left(1-\dfrac{2Gm(r)}{r}\right)^{-1} \\ \dfrac{dm(r)}{dr} = 4\pi r^2 \varepsilon(r) \end{cases}$$

EoS $P(\varepsilon) = 0$

Core $r = 0, \varepsilon(r=0) = \varepsilon_c, P(r=0) = P(\varepsilon_c)$

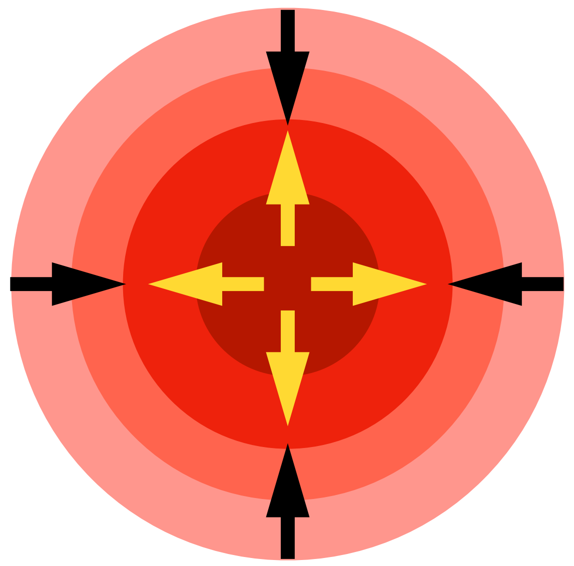
Surface $r = R, \varepsilon(r=R) \simeq 0, M = \int 4\pi r^2 \varepsilon(r) dr$

M, R

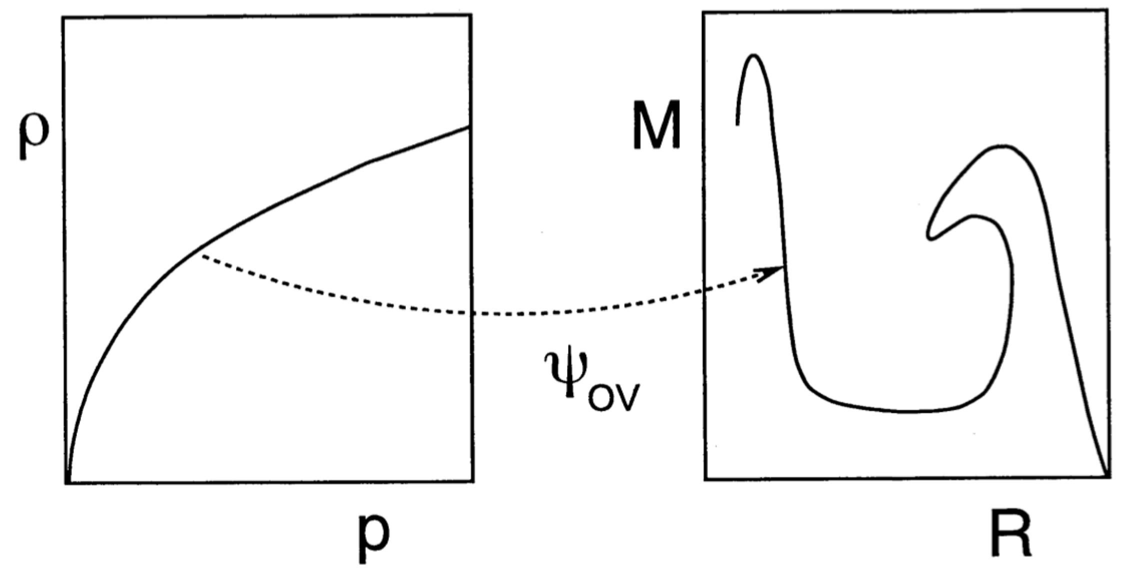


Nat. Rev. Phys. 4, 237–246 (2022)

Hydrostatic condition in each shell (dr)



Pressure Gravity

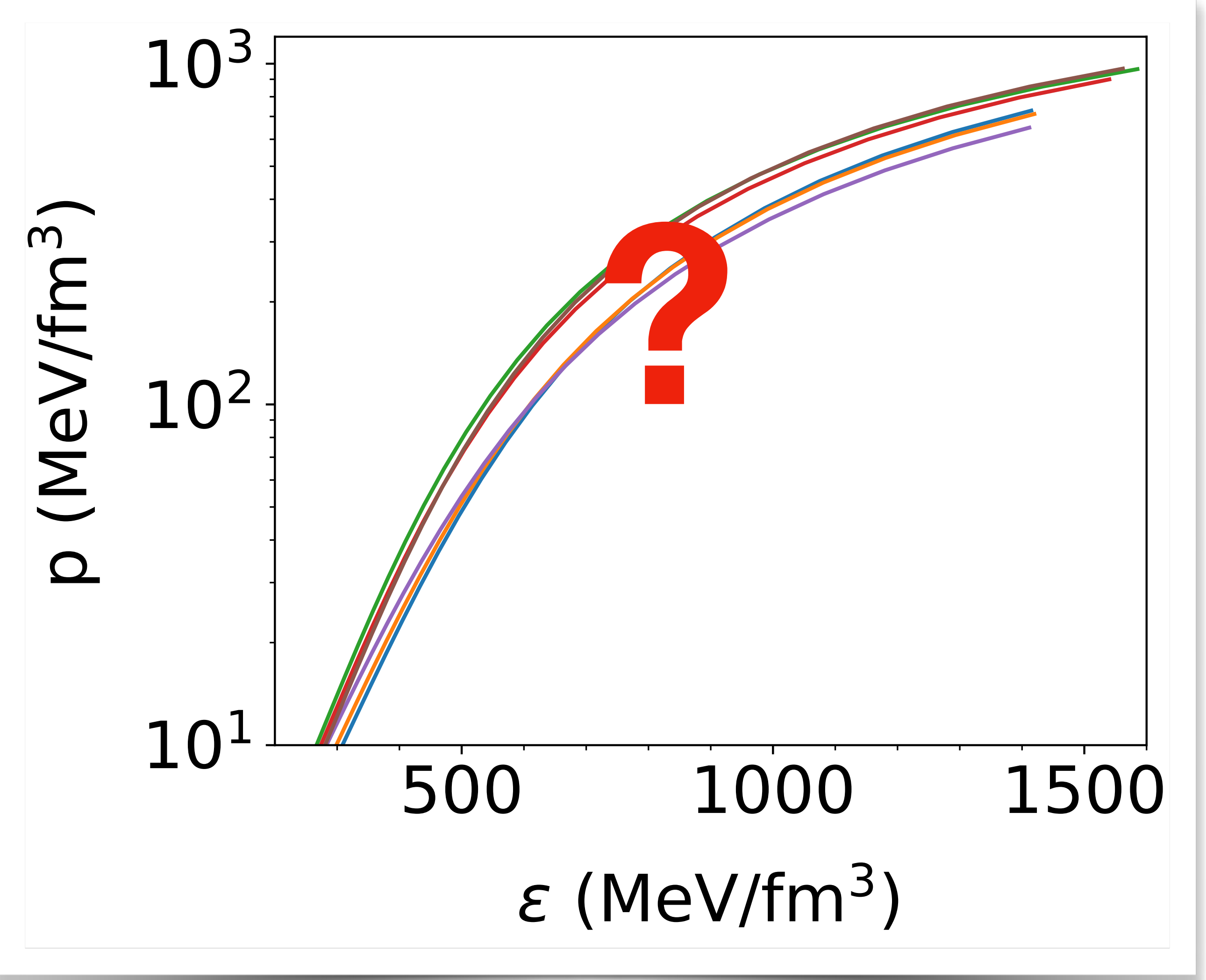


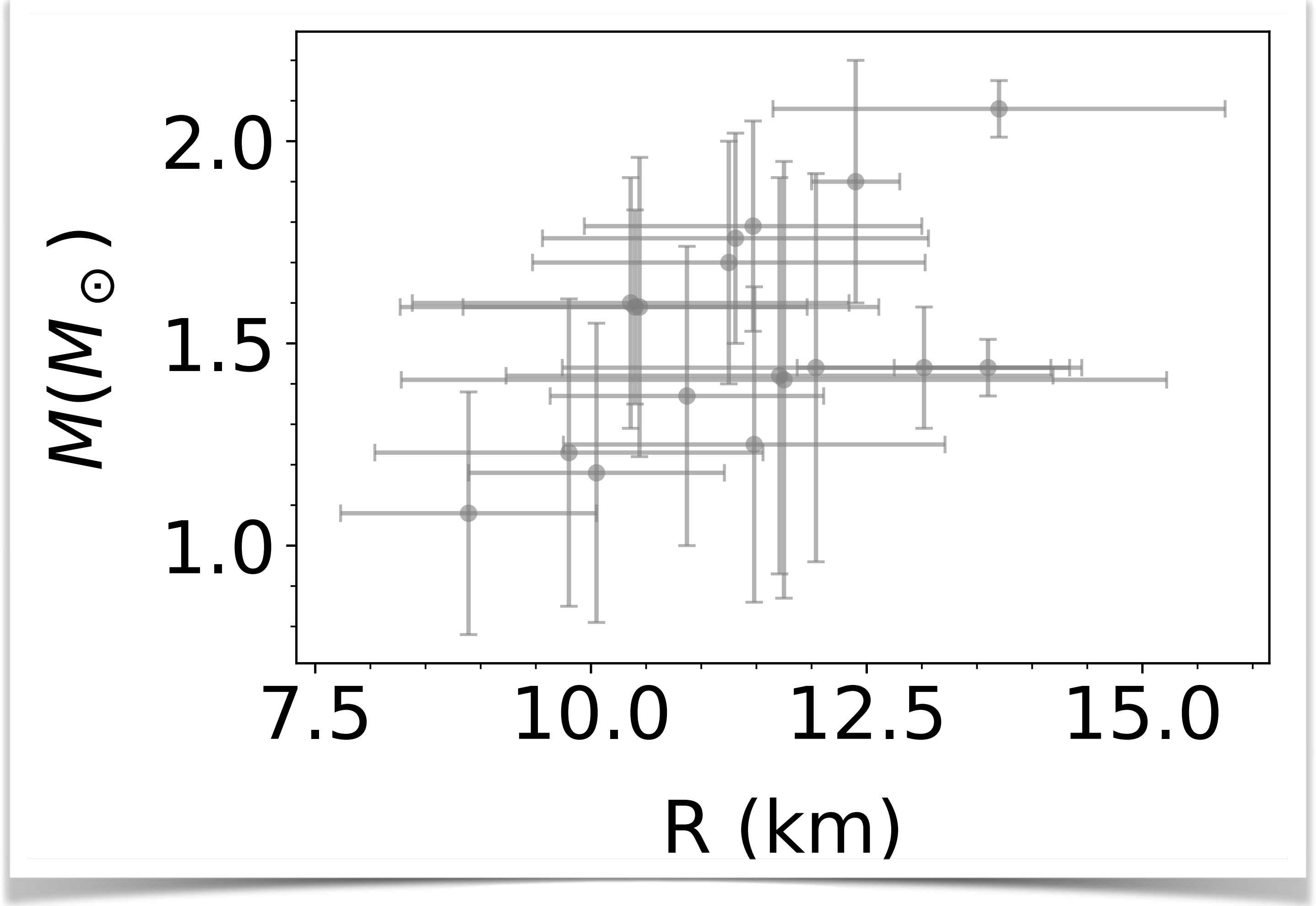
L. Lindblom, *A.J., 398, 569 (1992).*
If the **whole M(R)** is known,it's well-defined problem.

Physics-Driven Deep Learning

1. Building Neutron Star EoS

Tolman–Oppenheimer–Volkoff equations

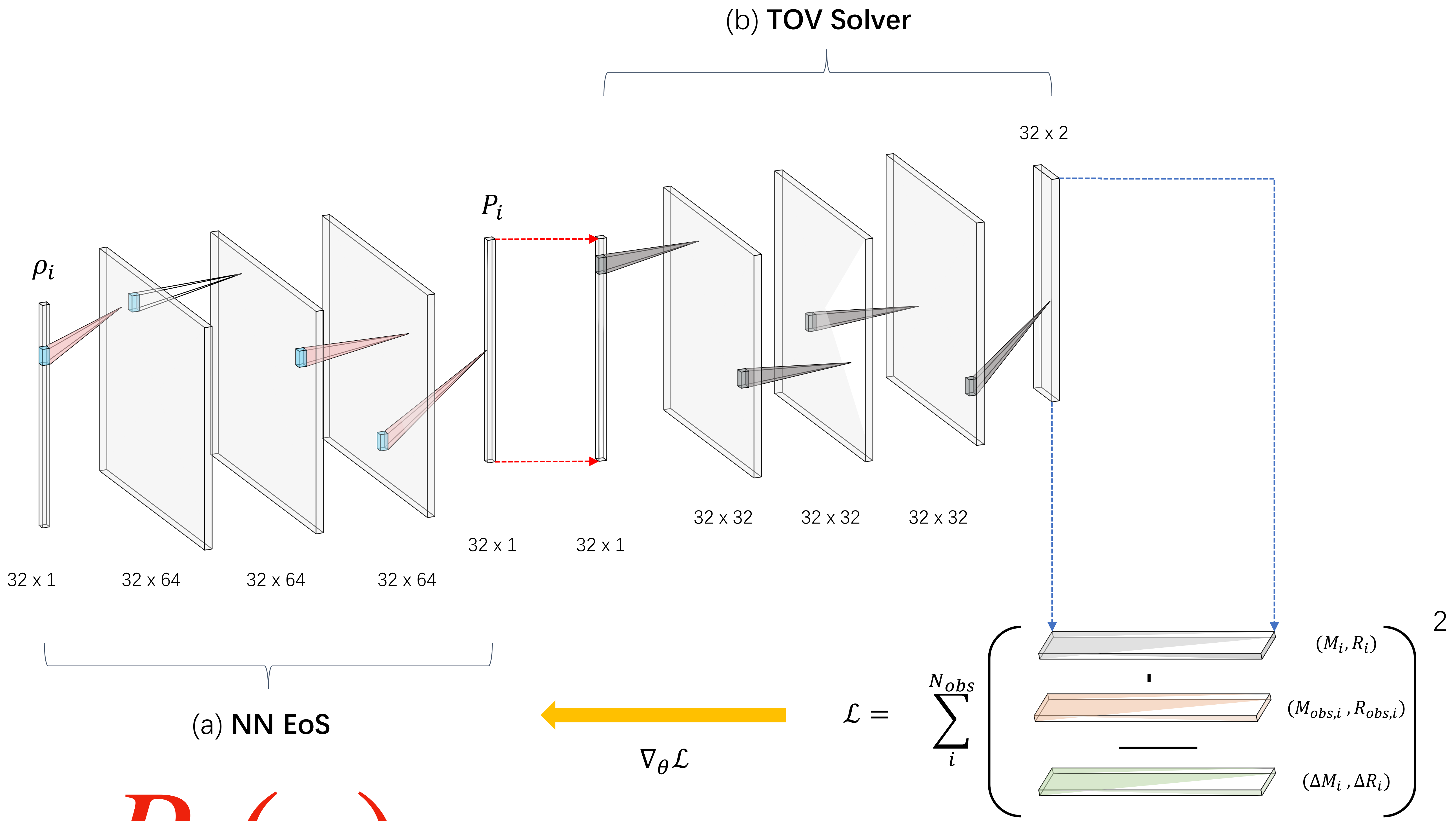




Physics-Driven Deep Learning

1. Building Neutron Star EoS

Phys. Rev. D 107, 083028; JCAP08 (2022) 071



$$P_\theta(\rho)$$

$$\mathscr{L} = \chi^2 = \sum_{i=1}^{N_{\rm obs}} \frac{\left(M_i - M_{{\rm obs},i}\right)^2}{\Delta M_i^2} + \frac{\left(R_i - R_{{\rm obs},i}\right)^2}{\Delta R_i^2}$$

Loss function

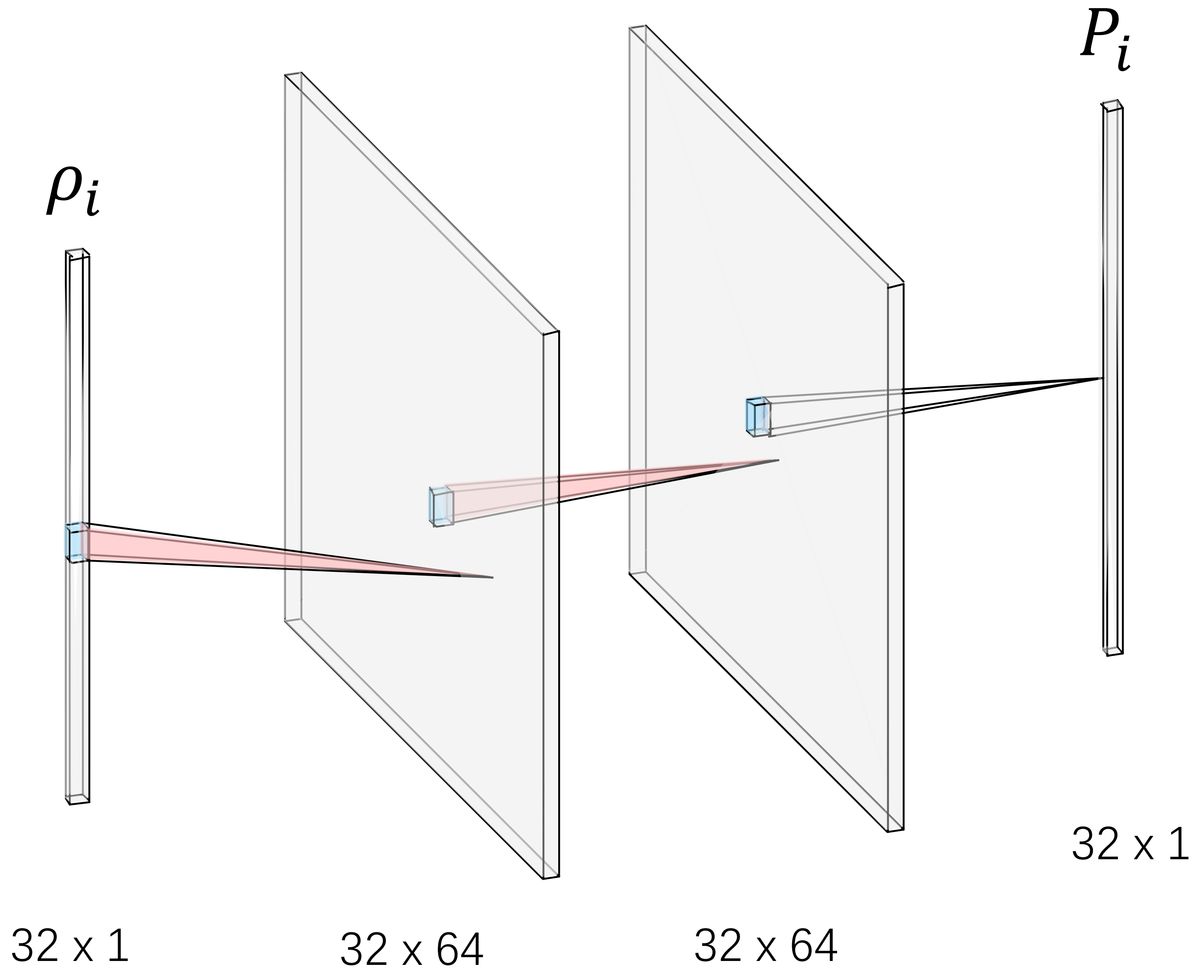
- (M_i, R_i) : predicted Mass-Radius
- $(M_{obs,i}, R_{obs,i})$: observed Mass-Radius
- $(\Delta M_i, \Delta R_i)$: uncertainties

Physics-Driven Deep Learning

1. Building Neutron Star EoS

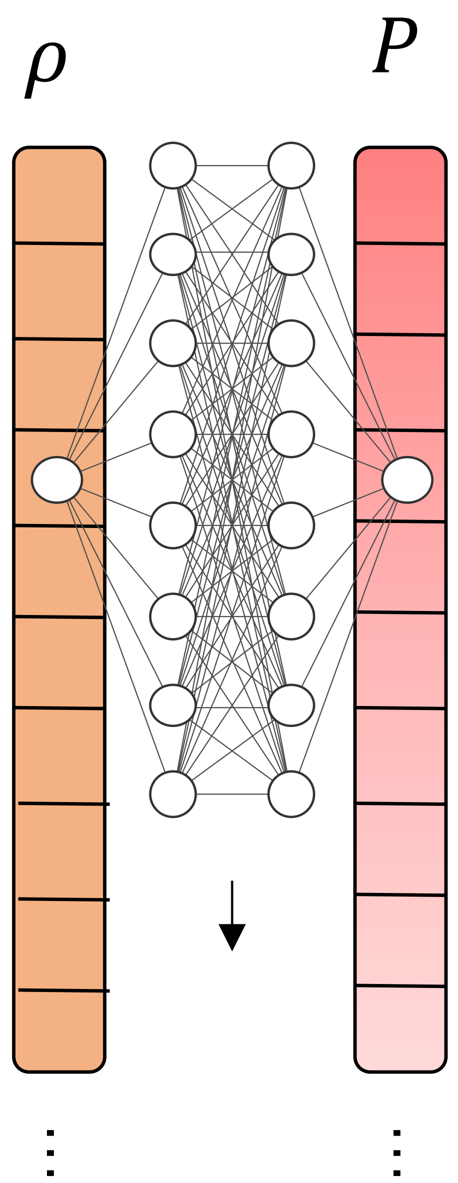
Phys. Rev. D 107, 083028; JCAP08 (2022) 071

Module A. NN EoS



A Trainable Neural Network

$\simeq$



$P_\theta(\rho)$

$\{\theta\}$: weights and bias of the neural network
Size of $\{\theta\}$ = 4353

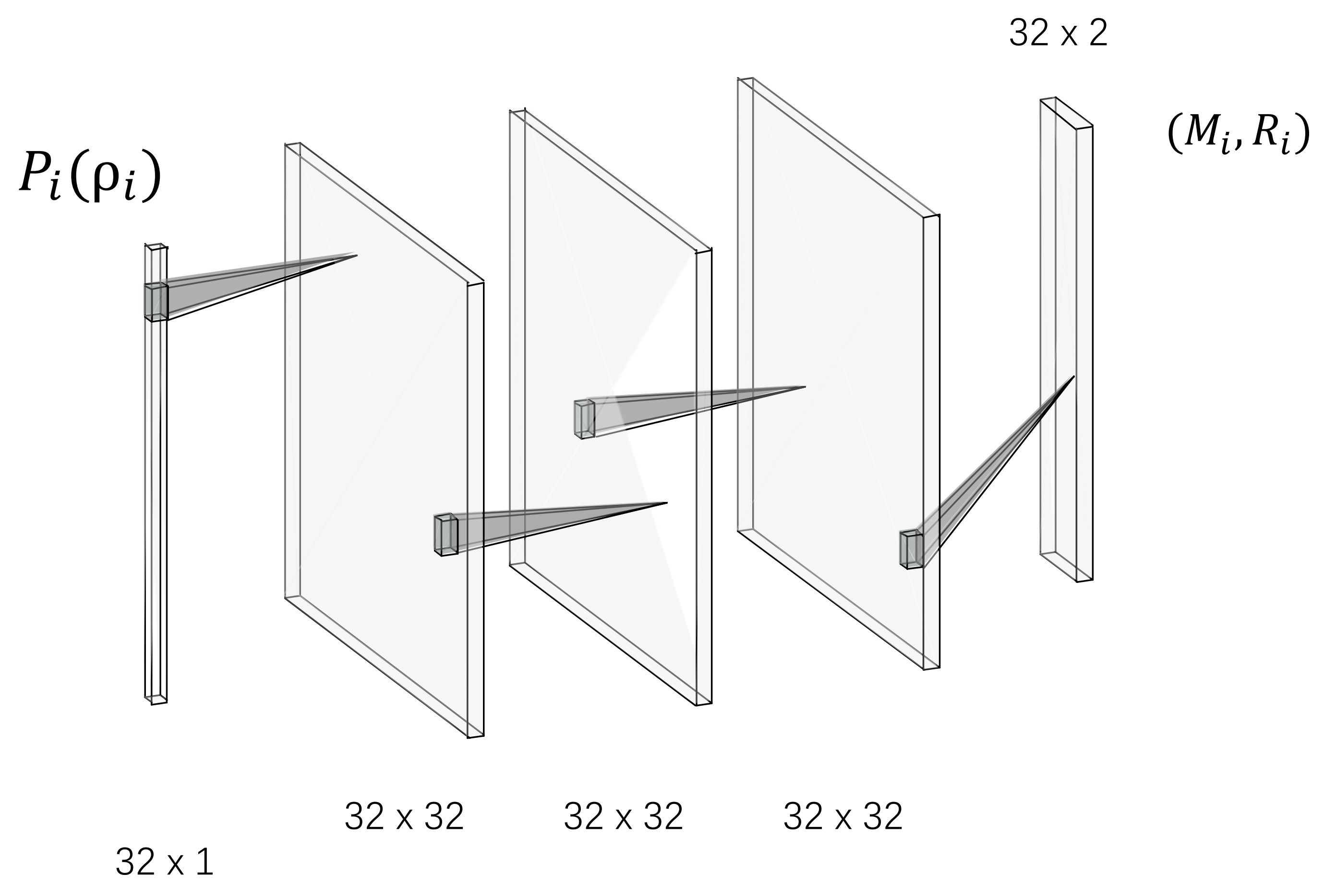
NS crust: **DD2**, inner: $P_\theta(1.1\rho_{\text{sat}} \leq \rho)$

Physics-Driven Deep Learning

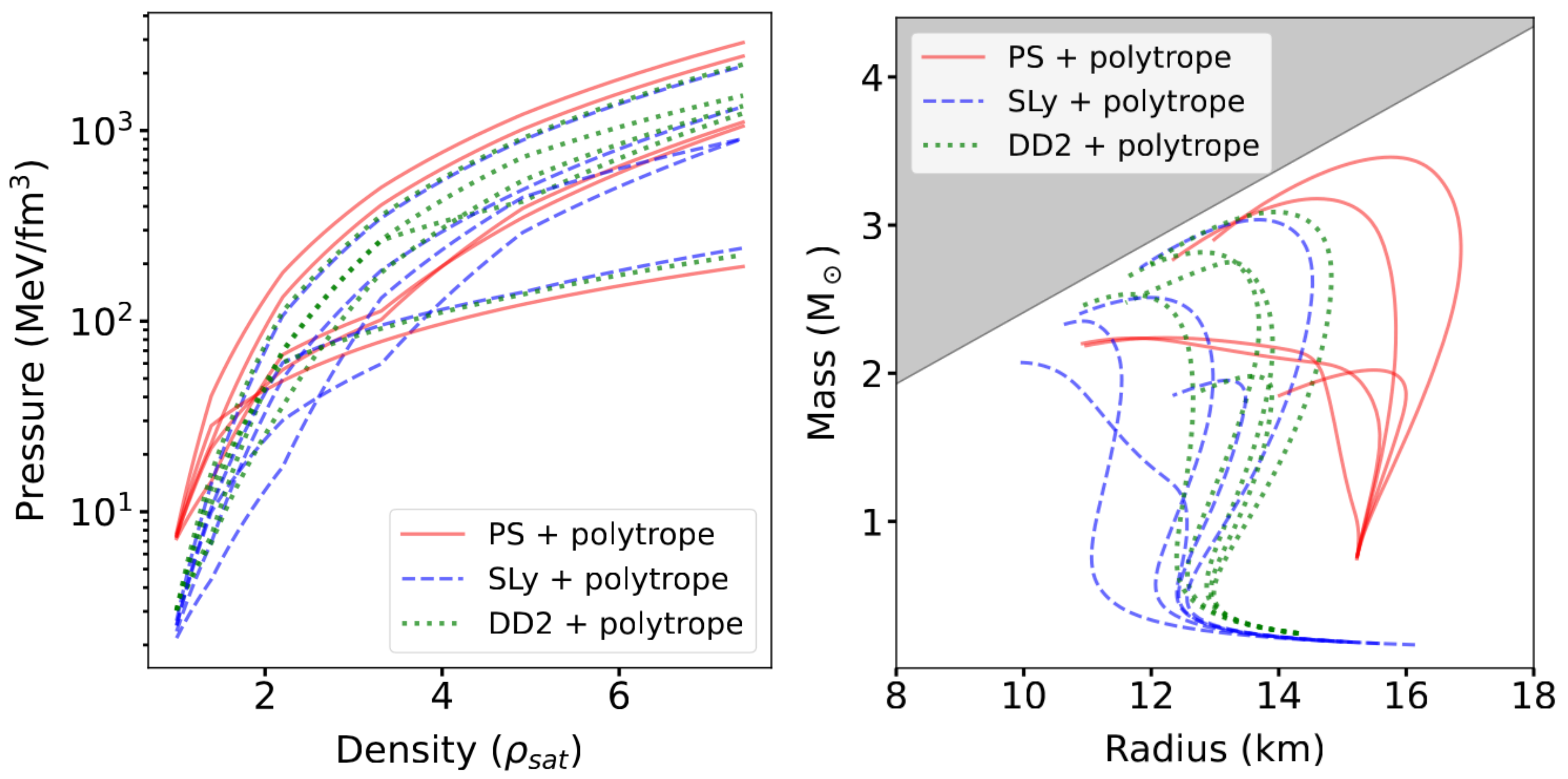
1. Building Neutron Star EoS

Phys. Rev. D 107, 083028; JCAP08 (2022) 071

Module B. TOV eq. Solver

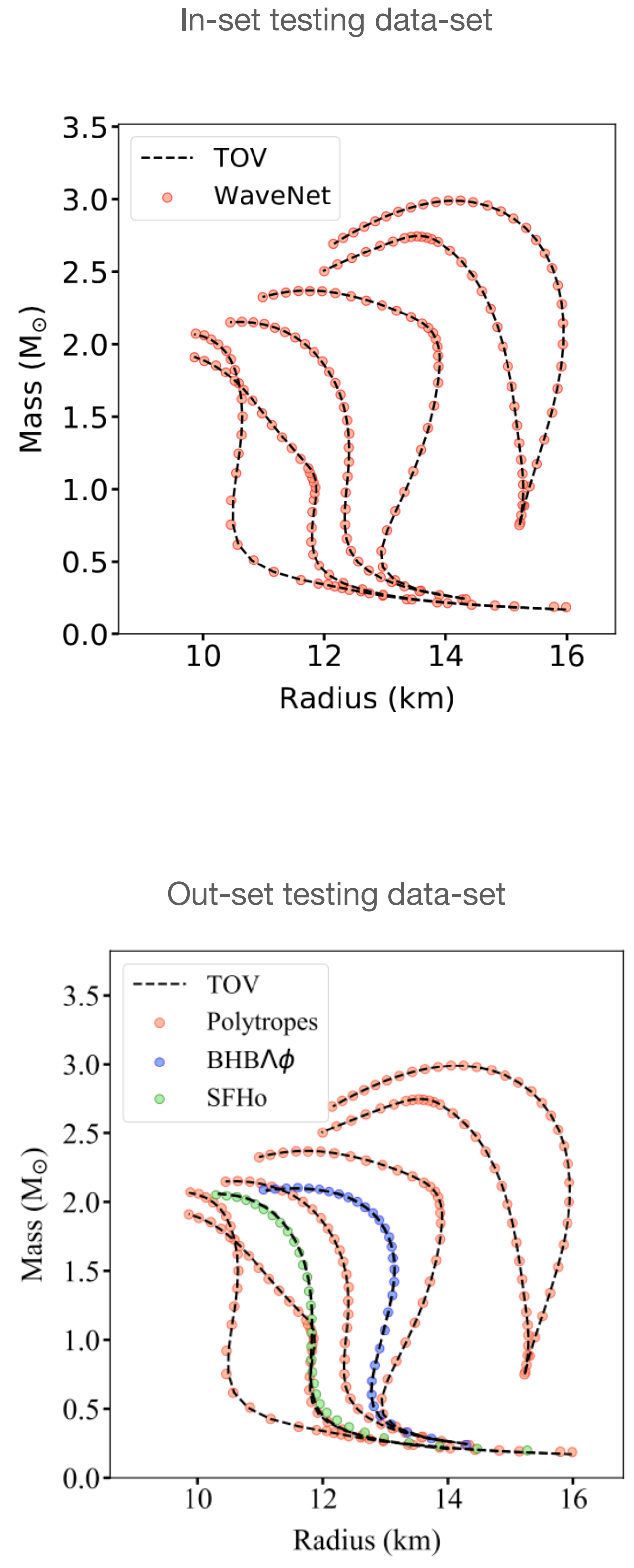


A **Pre-Trained** Neural Network



Training data-set
300,000 polytropic EoS functions with 3 low density models

$$P = K_i \rho^{\Gamma_i}, \quad i = [1,5], \quad 1.1\rho_{sat} \le \rho \le 7.4\rho_{sat}$$

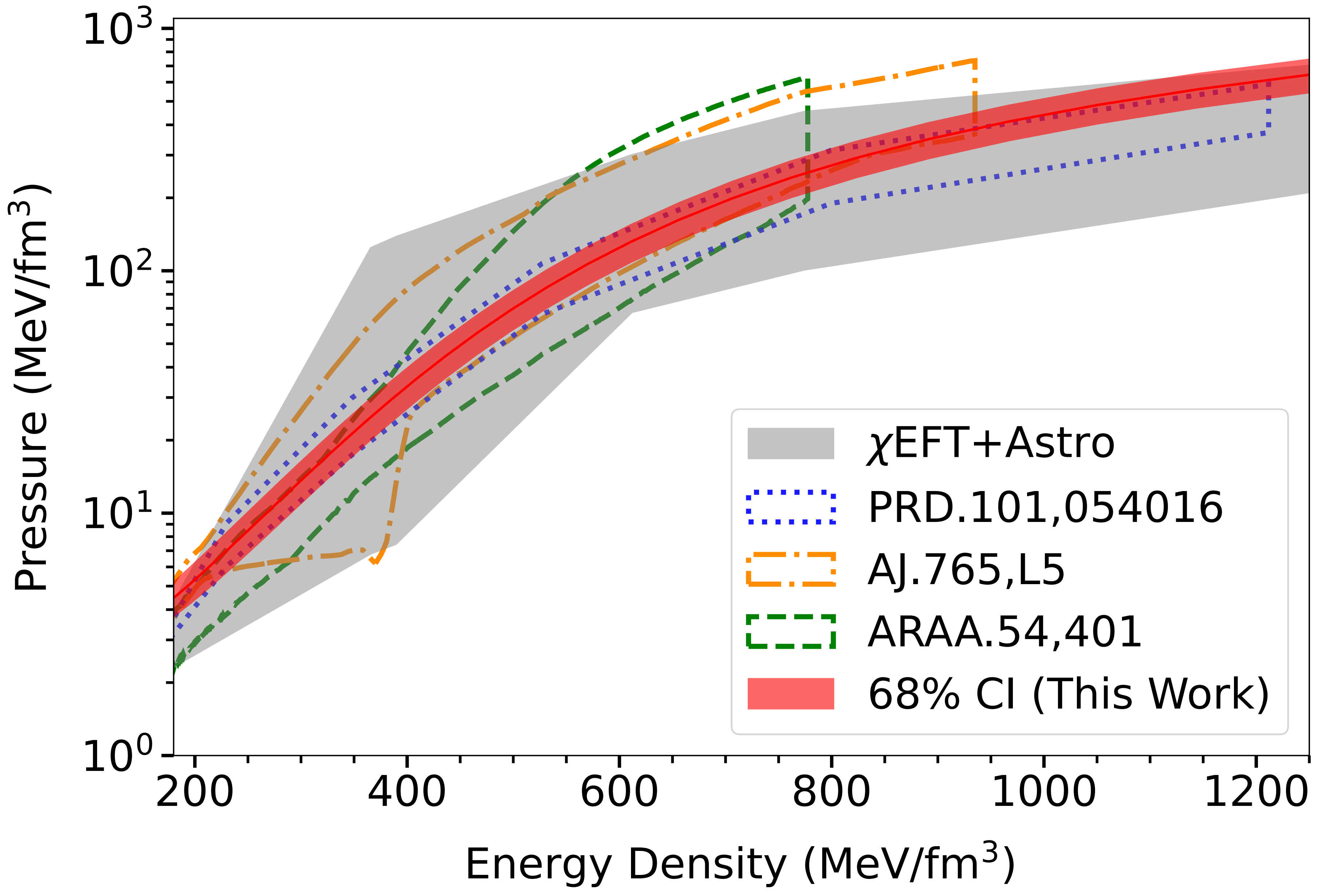


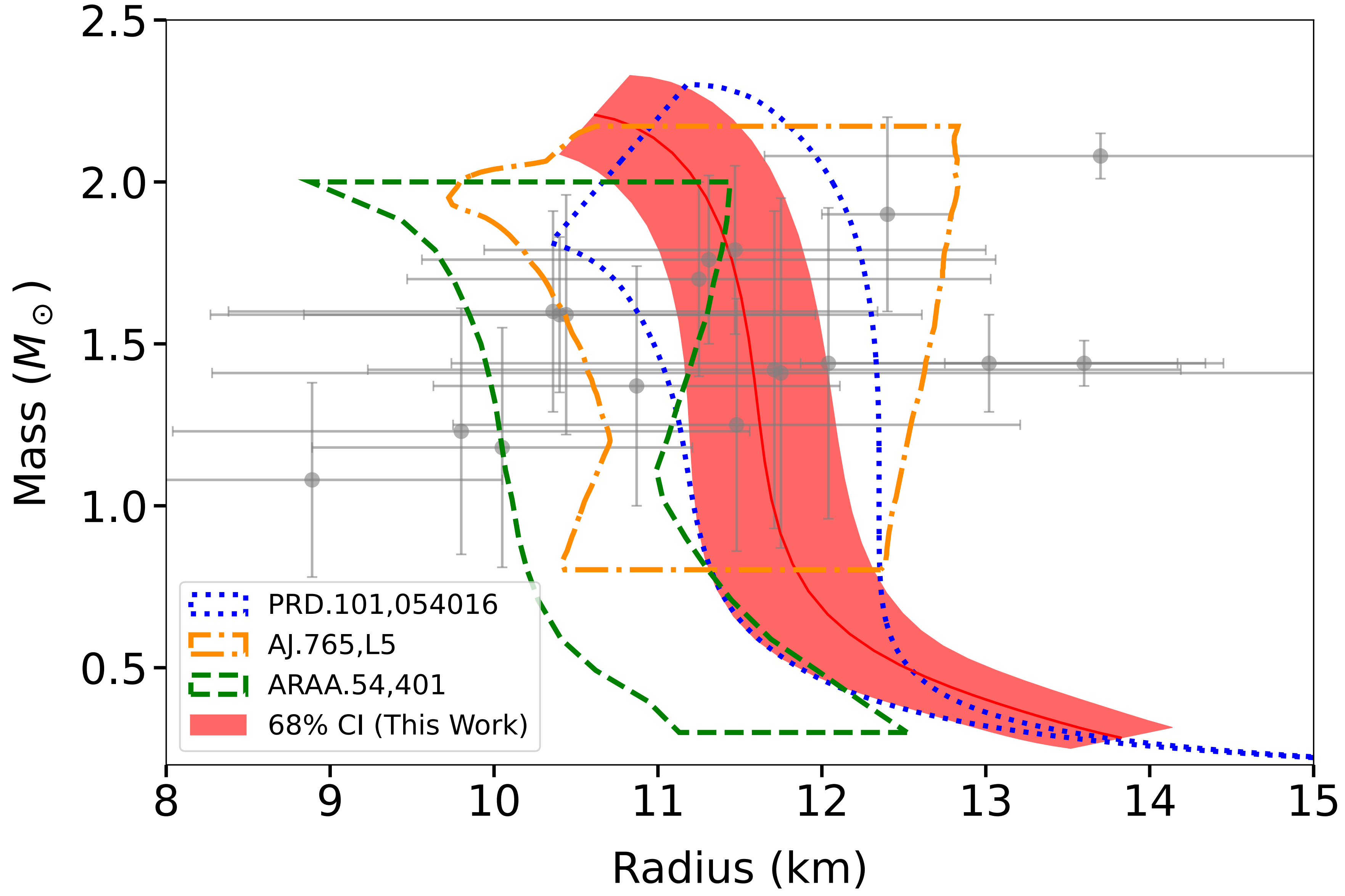
Physics-Driven Deep Learning

1. Building Neutron Star EoS

Phys. Rev. D 107, 083028

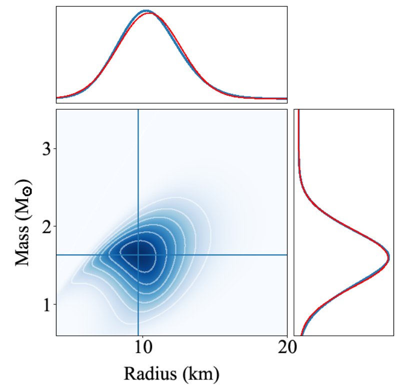
Blue dots: NN results, Fujimoto-Fukushima-Murase
Yellow and Green dashed lines: Bayesian Approaches





Our results: $R_{1.4} = 11.6 \pm 0.43$ **km (68% CI)**

18 (M_i, R_i) , sample size = **10k**
causality ($d\epsilon/dp < 1$)
Maximum mass $\geq 1.9\,M_\odot$



Observable	Mass($M_\odot$)	Radius(km)
M13	1.42±0.49	11.71±2.48
M28	1.08±0.30	8.89±1.16
M30	1.44±0.48	12.04±2.30
NGC 6304	1.41±0.54	11.75±3.47
NGC 6397	1.25±0.39	11.48±1.73
ωCen	1.23±0.38	9.80±1.76
4U 1608-52	1.60±0.31	10.36±1.98
4U 1724-207	1.79±0.26	11.47±1.53
4U 1820-30	1.76±0.26	11.31±1.75
EXO 1745-248	1.59±0.24	10.40±1.56
KS 1731-260	1.59±0.37	10.44±2.17
SAX J1748.9-2021	1.70±0.30	11.25±1.78
X5	1.18±0.37	10.05±1.16
X7	1.37±0.37	10.87±1.24
4U 1702-429	1.90±0.30	12.40±0.40
PSR J0437–4715	1.44±0.07	13.60±0.85
PSR J0030+0451	1.44±0.15	13.02±1.15
PSR J0740+6620	2.08±0.07	13.70±2.05

Physics-Driven Deep Learning

2. Reconstructing Spectral Function

Correlation Function

$$\bar{D}_{\eta\eta'} = \mathrm{Tr}(\mathrm{T}_\tau[J_\eta(\tau,\mathrm{x})J^\dagger_{\eta'}(0,0)]e^{-H/T})/Z$$

$$\equiv T\sum_n \int \frac{d^3k}{(2\pi)^3} D_{\eta\eta'}(i\omega_n,\mathrm{k})e^{-i(\omega_n\tau-\mathrm{k}\cdot\mathrm{x})}$$

M. Asakawa, Y. Nakahara, and T. Hatsuda, Prog. Part. Nucl. Phys. 46, 459 (2001)

$\mathbf{k}=0, \eta=\eta'$

$\mathbf{k}=0, \eta=\eta', T\to 0$

Spectrum representation

$$G(\tau,T) = \int_0^\infty K(\omega,\tau,T)\rho(\omega,T)d\omega$$

$$K(\omega,\tau,T) = \frac{\cosh\omega(\tau-\frac{1}{2T})}{\sinh\frac{\omega}{2T}}$$

Thermal Kernel

$T \to 0$

Energy eigenspace

$$C(\tau) = \sum_{n=0} e^{-E_n\tau} \mid <\Omega_0 \mid J(0) \mid \Omega_n> \mid^2$$

$$\equiv \sum_{n=0} c_n{}^2 e^{-E_n\tau}$$

Discretization

$$G(\tau) = \int_0^\infty e^{-\tau\omega}\rho(\omega)d\omega$$

Laplace Kernel

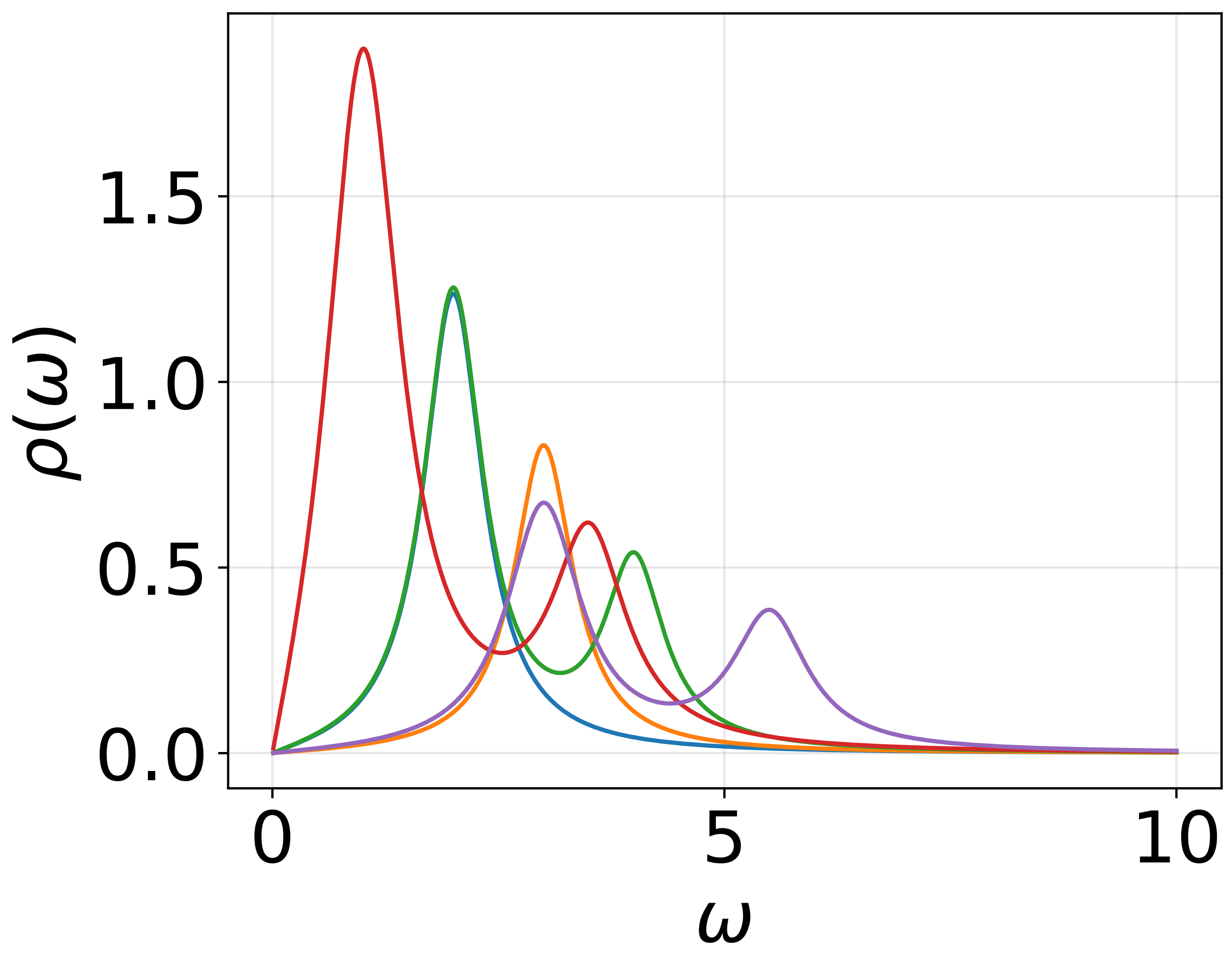
Spectral Function $\rho(\omega), \quad E_n$

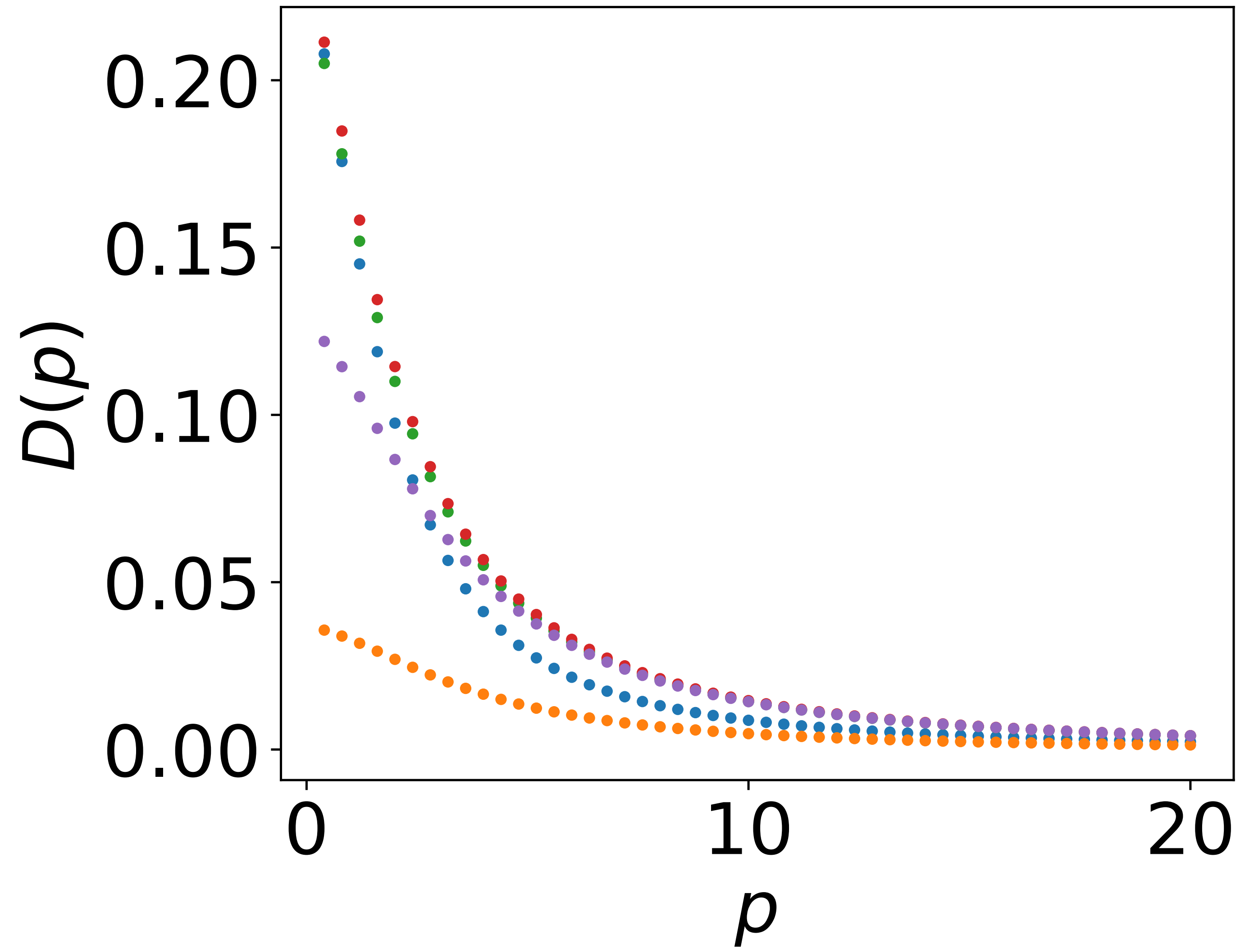
Physics-Driven Deep Learning

2. Reconstructing Spectral Function

***Kallen—Lehmann(KL)* representation**

$$D(p) \equiv \int_0^\infty K(p,\omega)\rho(\omega)\mathrm{d}\omega \quad K(p,\omega) = \frac{\omega}{\pi(\omega^2+p^2)}$$



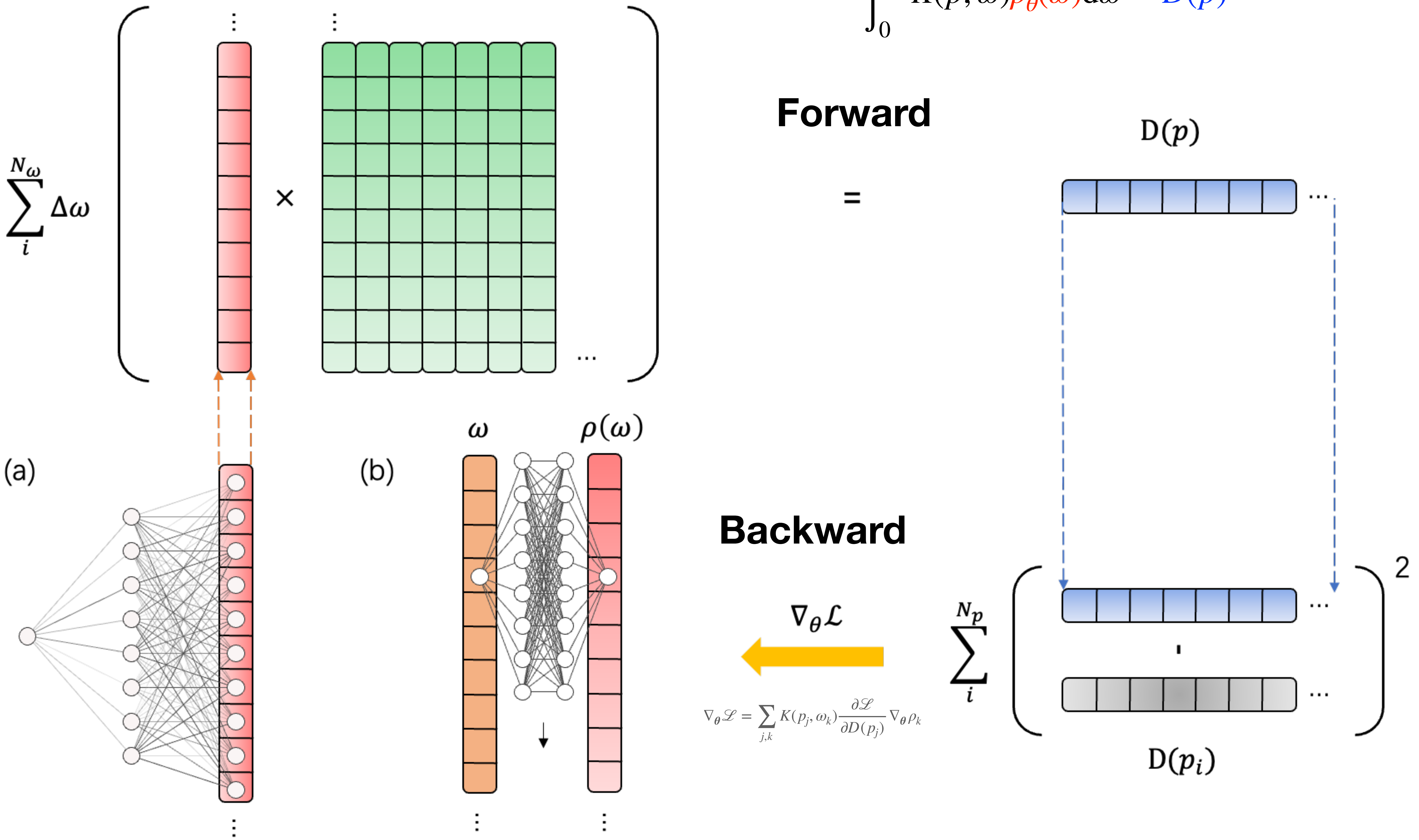


Physics-Driven Deep Learning

2. Reconstructing Spectral Function

Phys. Rev. D 106, L051502

$$\int_0^\infty K(p,\omega)\rho_\theta(\omega)\mathrm{d}\omega = D(p)$$



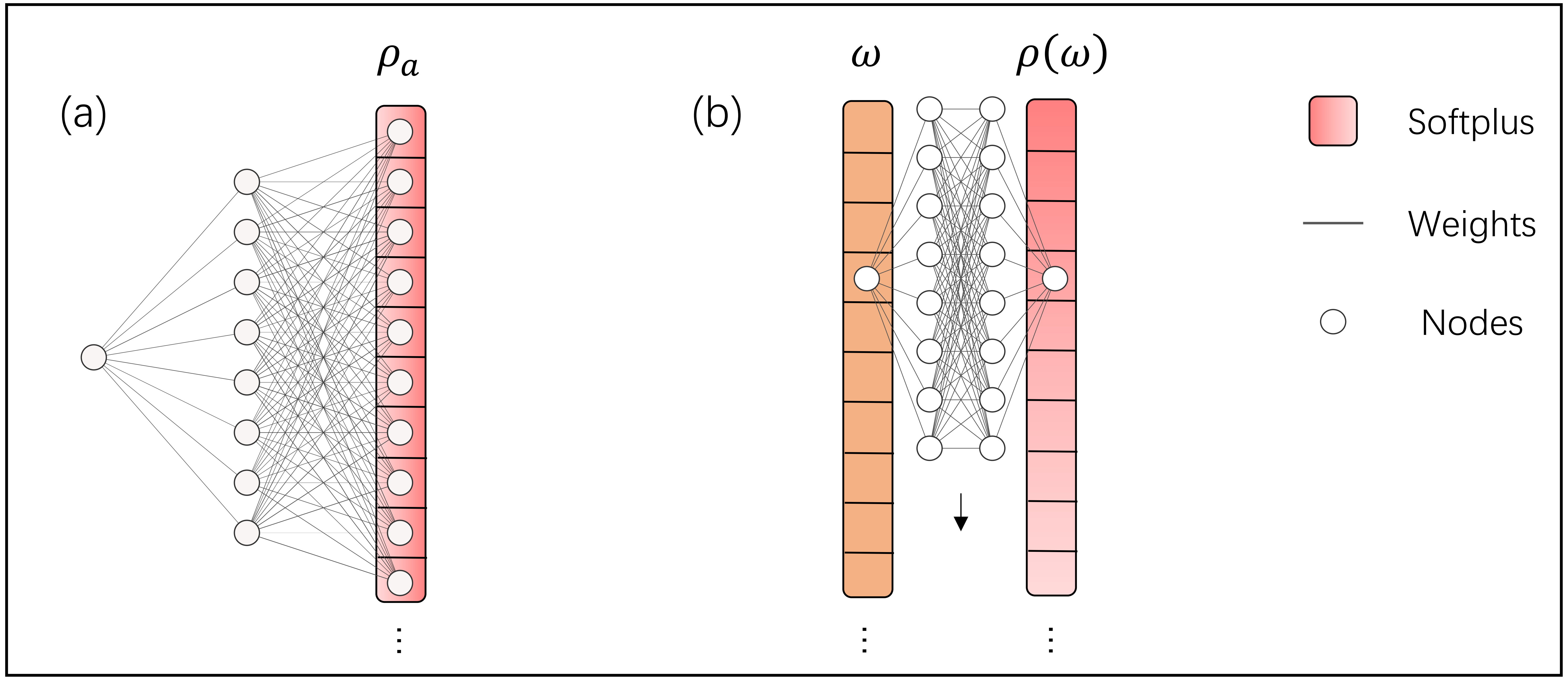
χ^2 Loss function

$$\mathscr{L} = \sum_i^{N_p} w_i(\mathrm{D}_i - D(p_i))^2$$

Physics-Driven Deep Learning

2. Reconstructing Spectral Function

Phys. Rev. D 106, L051502



NN : $(\rho_1, \rho_2, \cdots, \rho_{N_\omega})$

Differentiable variables : Network weights $\{\theta\}$

Adam, L2 ($\lambda = 10^{-3} \rightarrow 10^{-8}$), Smoothness ($\lambda_s = 10^{-4} \rightarrow 0$)

width = 64 and depth = 3 with bias

NN-P2P : $\rho(\omega)$

Differentiable variables : Network weights $\{\theta\}$

Adam, L2 ($\lambda = 10^{-6} \rightarrow 0$)

width = 64 and depth = 3 with bias

Regularization

L2 : $\lambda \mid \theta \mid_2^2$

Smoothness: $\lambda_s \sum_i^{N_\omega} (\rho_i - \rho_{i-1})^2$

Gradient-based Optimization

Adam : $\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$

Physical Prior

Positive-defined condition(for hadrons):
Softplus $log(1 + e^x)$

Physics-Driven Deep Learning

2. Reconstructing Spectral Function

Phys. Rev. D 106, L051502

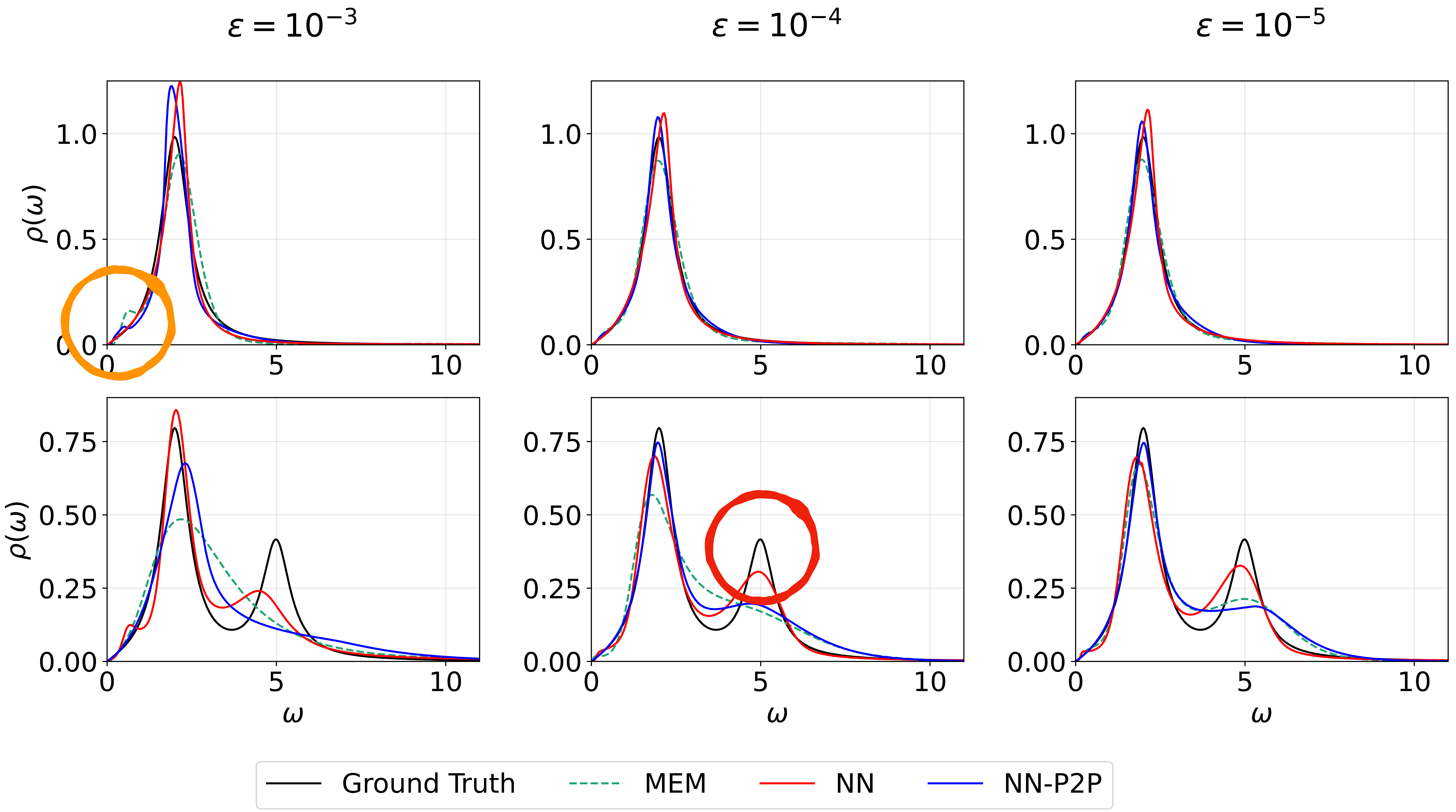
Mock Test I.

$$\rho^{(\mathrm{BW})}(\omega) = \frac{4A\Gamma\omega}{\left(M^2+\Gamma^2-\omega^2\right)^2+4\Gamma^2\omega^2}$$

$A = 1.0, \Gamma = 0.5, M = 2.0$

$A_1 = 0.8, A_2 = 1.0, \Gamma_1 = \Gamma_2 = 0.5$
$M_1 = 2.0, M_2 = 5.0$

noise level ϵ
$N_p = 25$ points



Physics-Driven Deep Learning

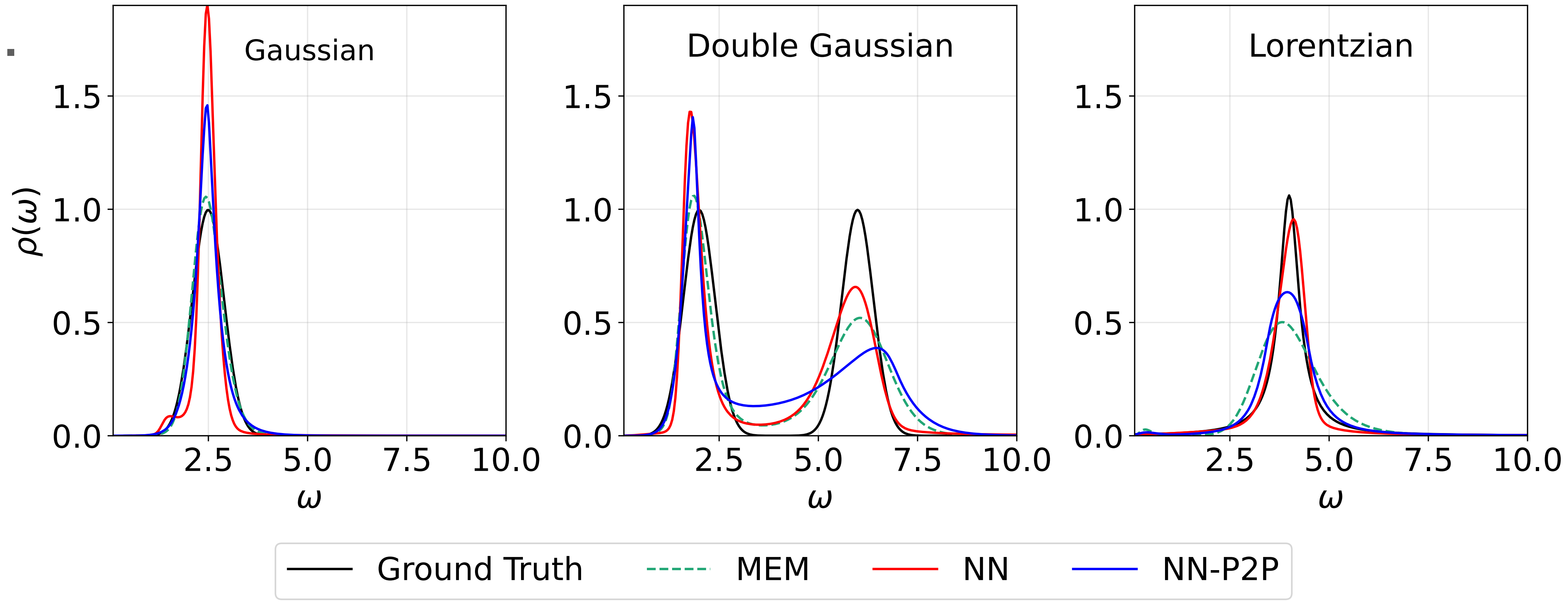
2. Reconstructing Spectral Function

Phys. Rev. D 106, L051502

Mock Test II.

noise level $\epsilon = 10^{-4}$ with $N_p = 25$ points

1.



1. Single-peak functions

2. Non-positive-definited SPs

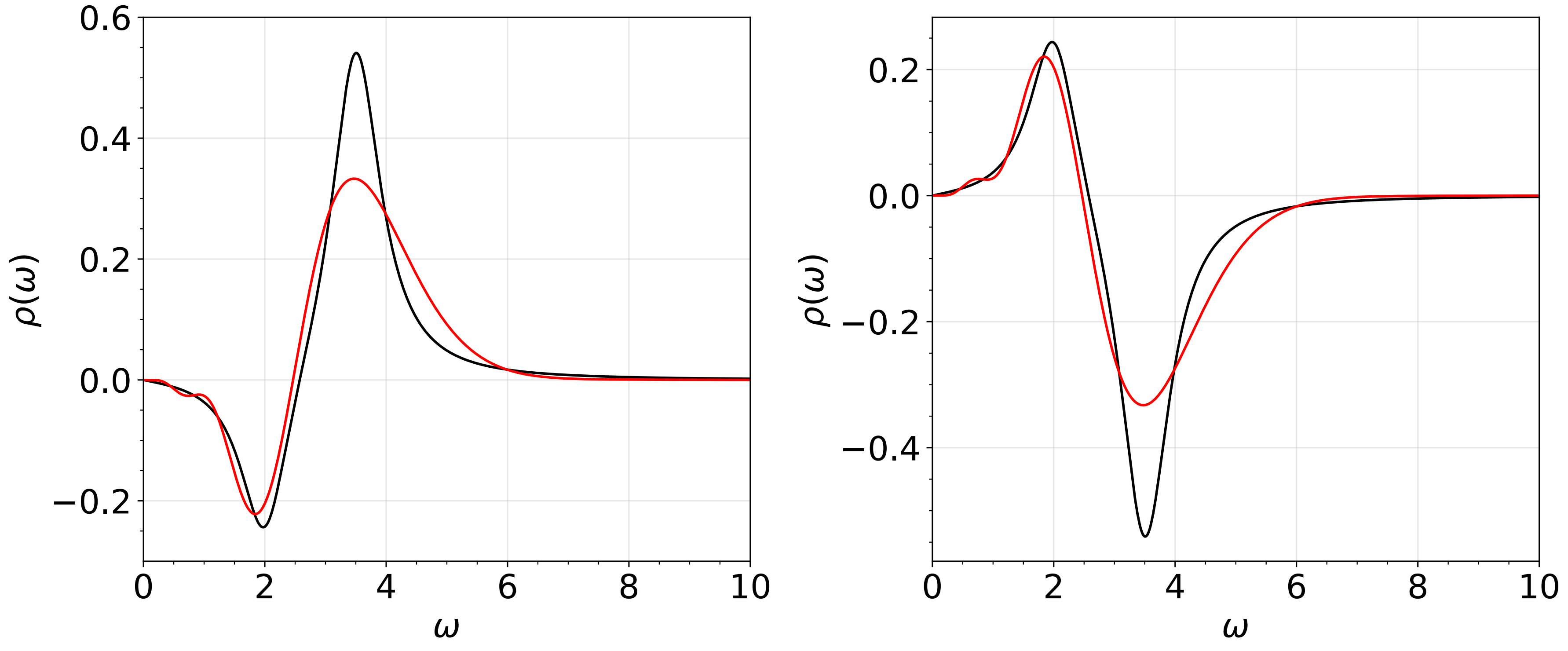
3. Lattice QCD mock data

Thermal (details see arXiv:2110.13521)

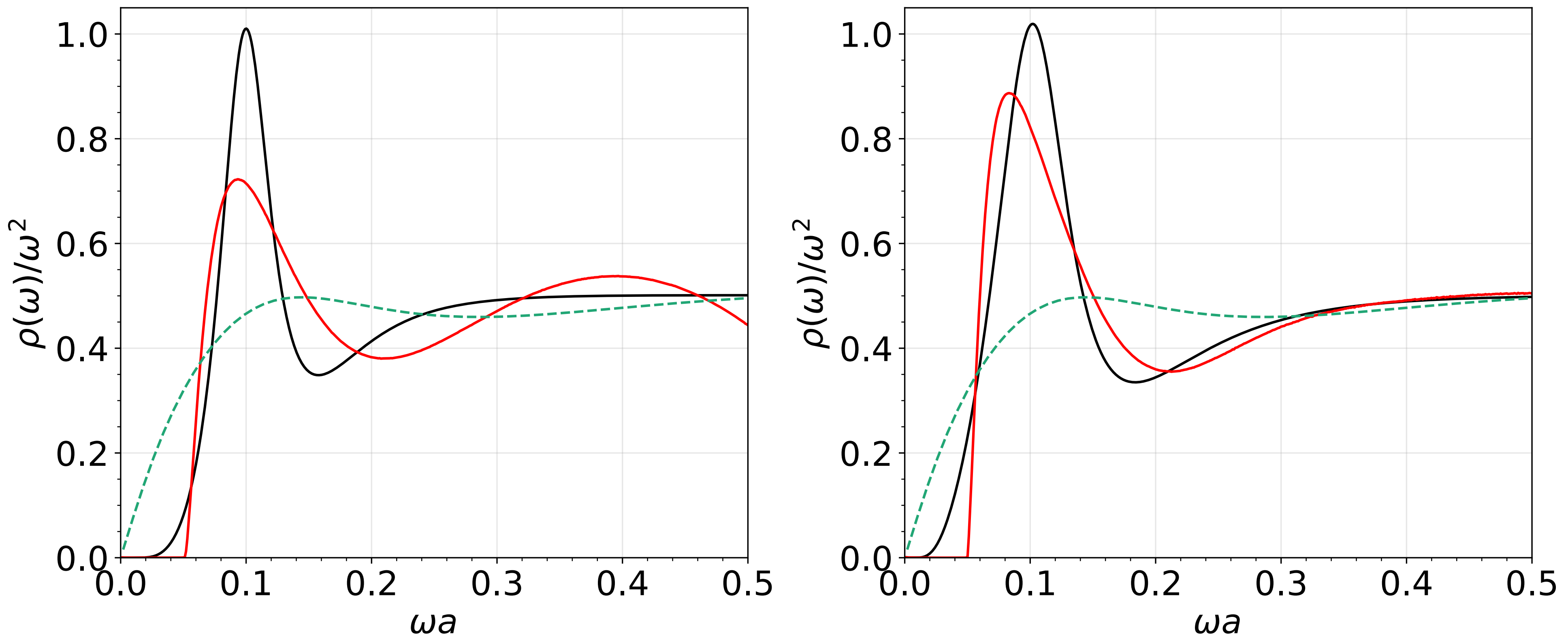
$$G(\tau, T) = \int_0^\infty \frac{d\omega}{2\pi} K(\omega, \tau, T)\rho(\omega, T)$$

$$K(\omega, \tau, T) = \frac{\cosh \omega(\tau - \frac{1}{2T})}{\sinh \frac{\omega}{2T}}$$

2.



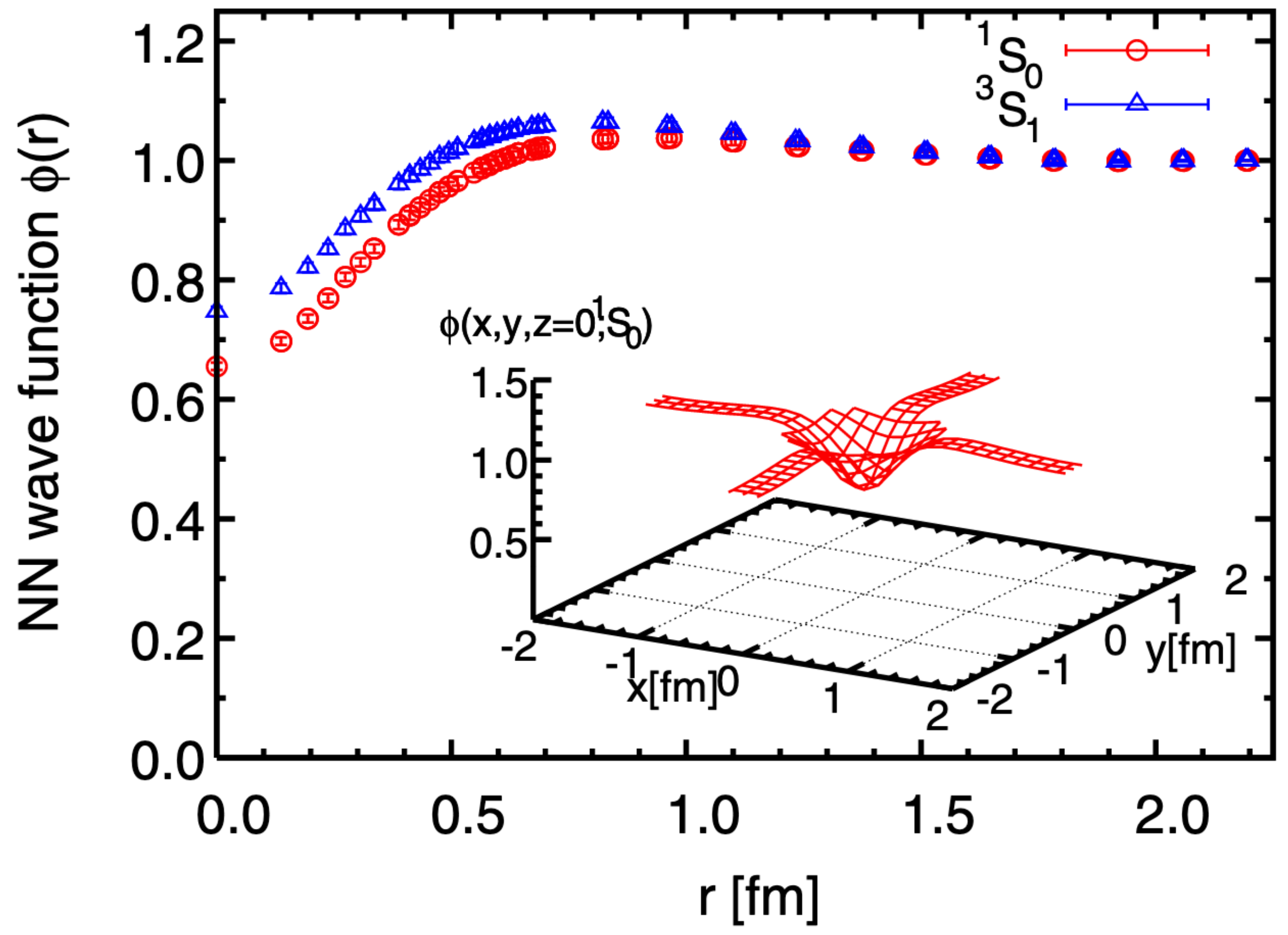
3.

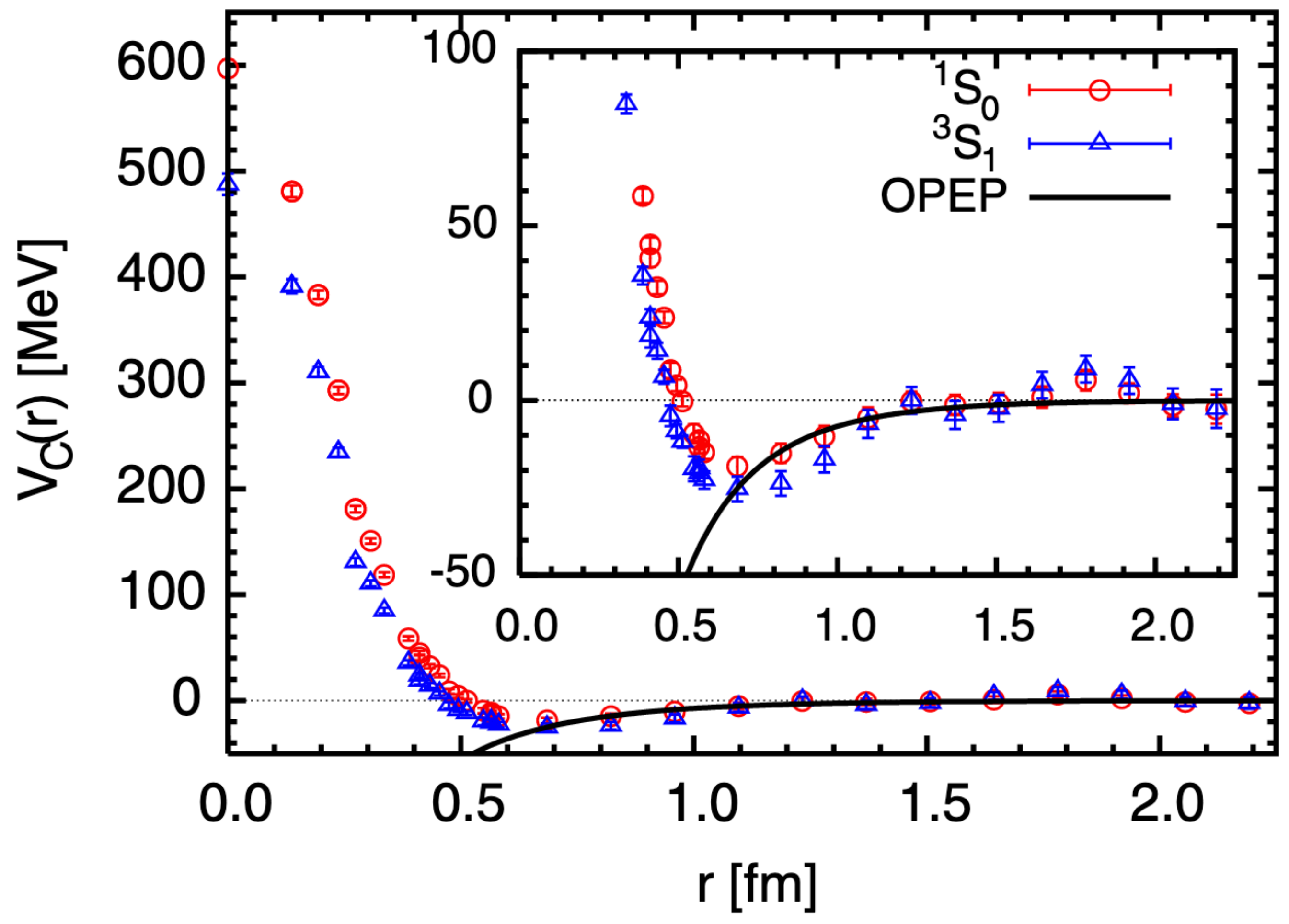


Physics-Driven Deep Learning

3. Extracting Nuclear Force

N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. **99**, 022001 (2007)





Local Approx.
Gradient Expansion

Nambu-Bethe-Salpeter (NBS) wave function

$$\psi_{NBS}(\vec{r}) = \langle 0|N(\vec{r})N(\vec{0})|N(\vec{k})N(-\vec{k}), in\rangle$$
$$\simeq e^{i\delta_l(k)} \sin(kr - l\pi/2 + \delta_l(k))/(kr)$$

(at asymptotic region)

HAL QCD method

Nulcear Force

$$(k^2/m_N - H_0)\,\psi_{NBS}(\vec{r}) = \int d\vec{r}'\, U(\vec{r},\vec{r}')\psi_{NBS}(\vec{r}')$$

(Schrodinger eq.)

Physics-Driven Deep Learning

3. Extracting Nuclear Force

in preparation (with HAL QCD)

Separable Potential

$$U(\mathbf{r},\mathbf{r}') \equiv \omega\nu(\mathbf{r})\nu(\mathbf{r}'), \qquad \nu(\mathbf{r}) \equiv e^{-\mu r}$$

$$\phi_k^0(r) = \frac{e^{i\delta_0(k)}}{kr}\left[\sin\{kr+\delta_0(k)\} - \sin\delta_0(k)e^{-\mu r}\left(1+\frac{r(\mu^2+k^2)}{2\mu}\right)\right]$$

$$k\cot\delta_0(k) = -\frac{1}{4\mu^2}\left[2\mu(\mu^2-k^2) - \frac{3\mu^2+k^2}{4\mu^3}(\mu^2+k^2)^2 + \frac{(\mu^2+k^2)^4}{8\pi m\omega}\right]$$

Nambu-Bethe-Salpeter (NBS) wave function

$$\phi_{\mathbf{k}}(\mathbf{r})e^{-W_{\mathbf{k}}t} \equiv \langle 0 \;\; N(\mathbf{x}+\mathbf{r},t)N(\mathbf{x},t) \;\; NN, W_k\rangle$$

$$(E_k - H_0)\phi_{\mathbf{k}}(\mathbf{r}) = \int d^3 r' U(\mathbf{r},\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}')$$

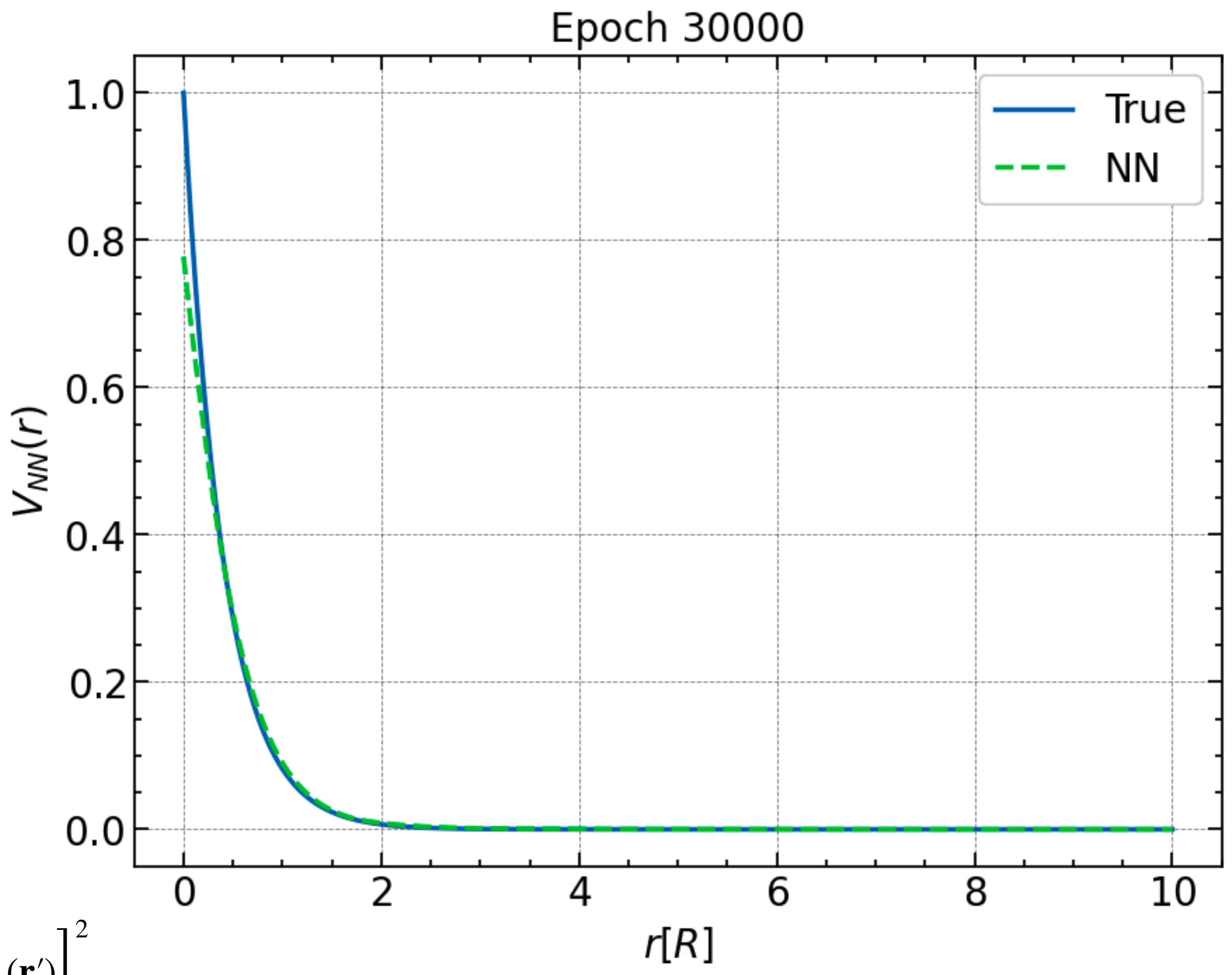
$$E_k = \frac{k^2}{2m}, \quad H_0 = -\frac{\nabla^2}{2m}, \quad m = \frac{m_N}{2}$$

No Approx.

$$\mathscr{L} = \sum_k \int d^3 r \left[\left(E_k - H_0\right)\phi_{\mathbf{k}}(\mathbf{r}) - \int d^3 r' U_\theta(\mathbf{r},\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}')\right]^2$$

Neural Network Hadron Force

$$U_\theta(\mathbf{r},\mathbf{r}') = \omega\exp(-\mu r)f_\theta(r'), \quad f_\theta(r) \equiv V_{NN}(r)$$

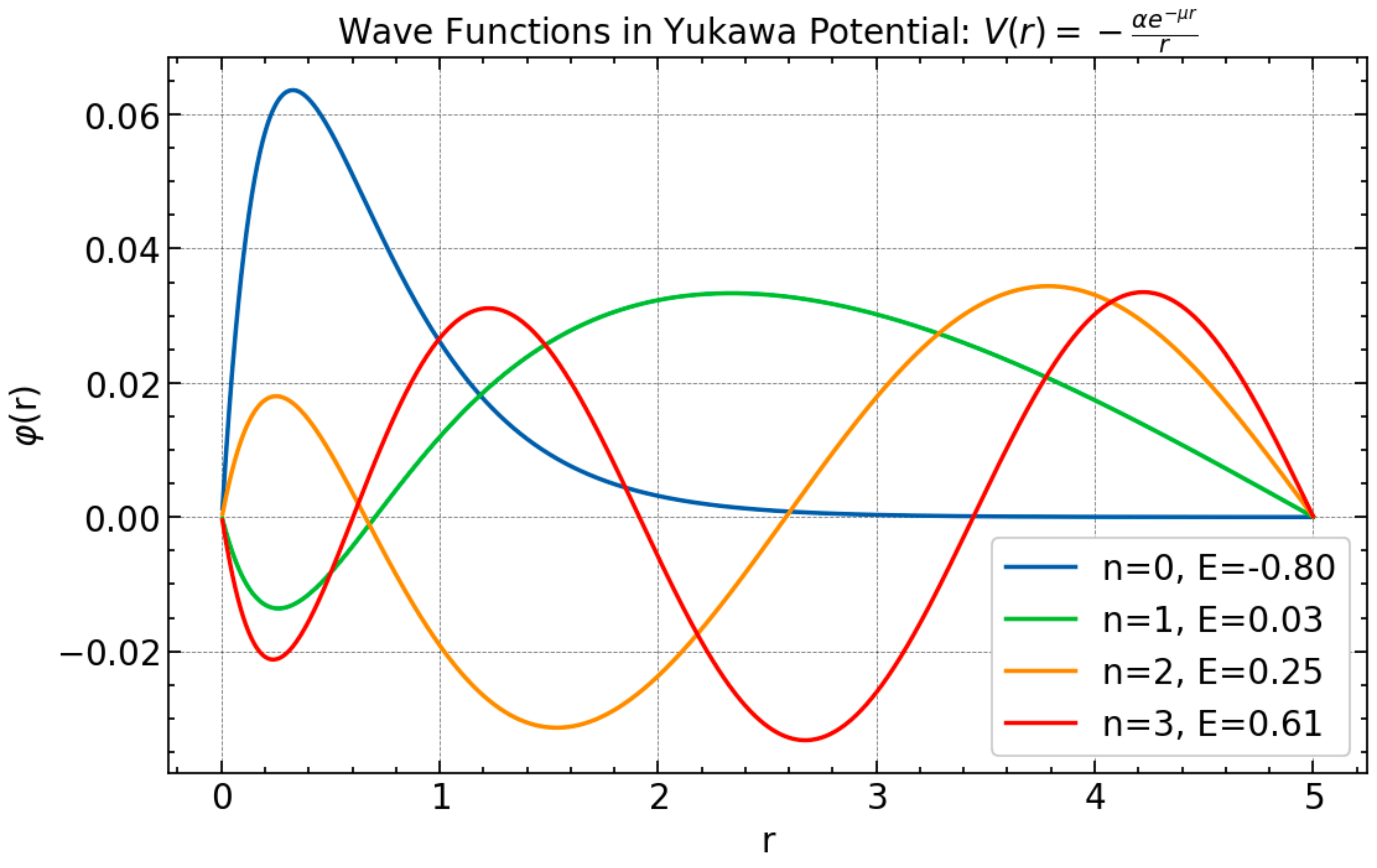


3. Extracting Nuclear Force

in preparation (with HAL QCD)

Yokawa Potential

$$\left(-\frac{\nabla^2}{2m} + V(r)\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \qquad V(r) = -\alpha\frac{e^{-\mu r}}{r}$$



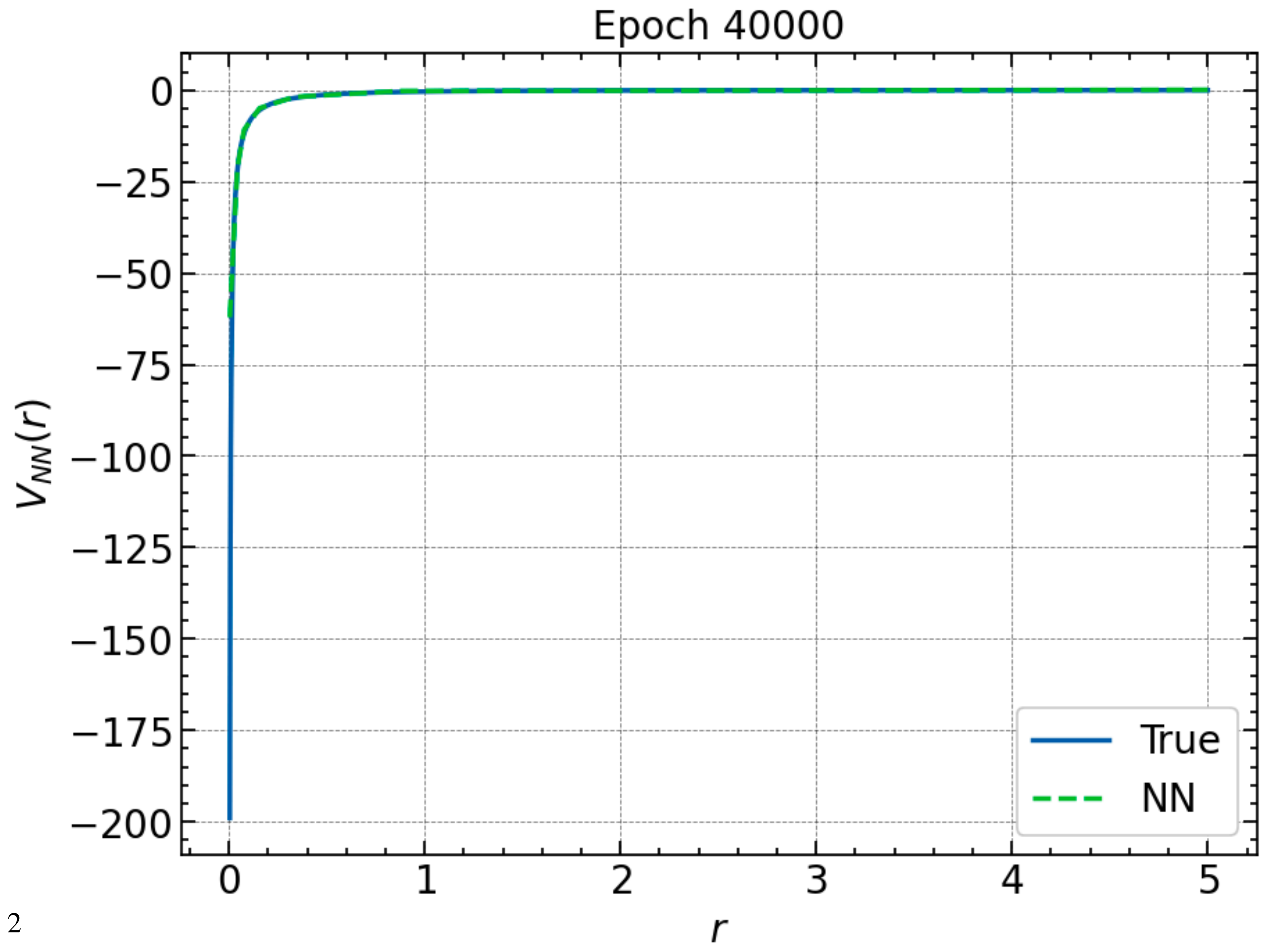
$\mu = 1, \alpha = 2, m = 3.3\mu$

No Approx.

$$\mathscr{L} = \sum_r \sum_n \left[\left(E_n - H_0\right)\phi_{\mathbf{n}}(r) - V_{NN}(r)\phi_{\mathbf{n}}(r)\right]^2$$

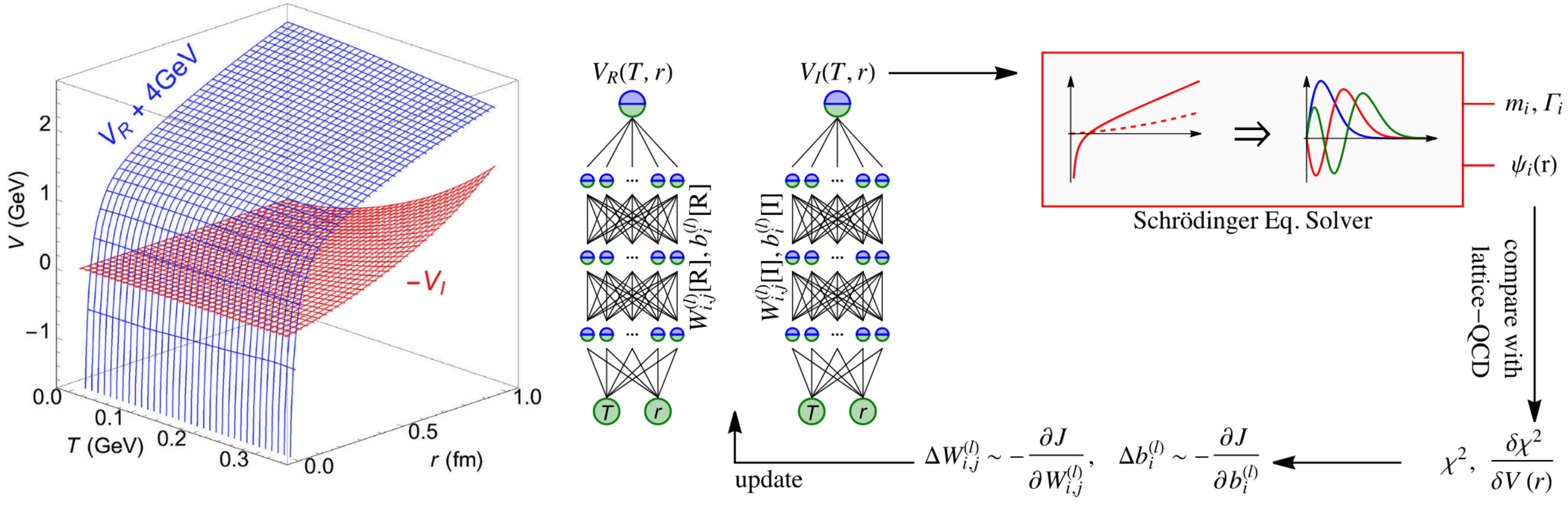
Neural Network Hadron Force

$$V_{NN}(r) \equiv f_\theta(r)$$



Other Works

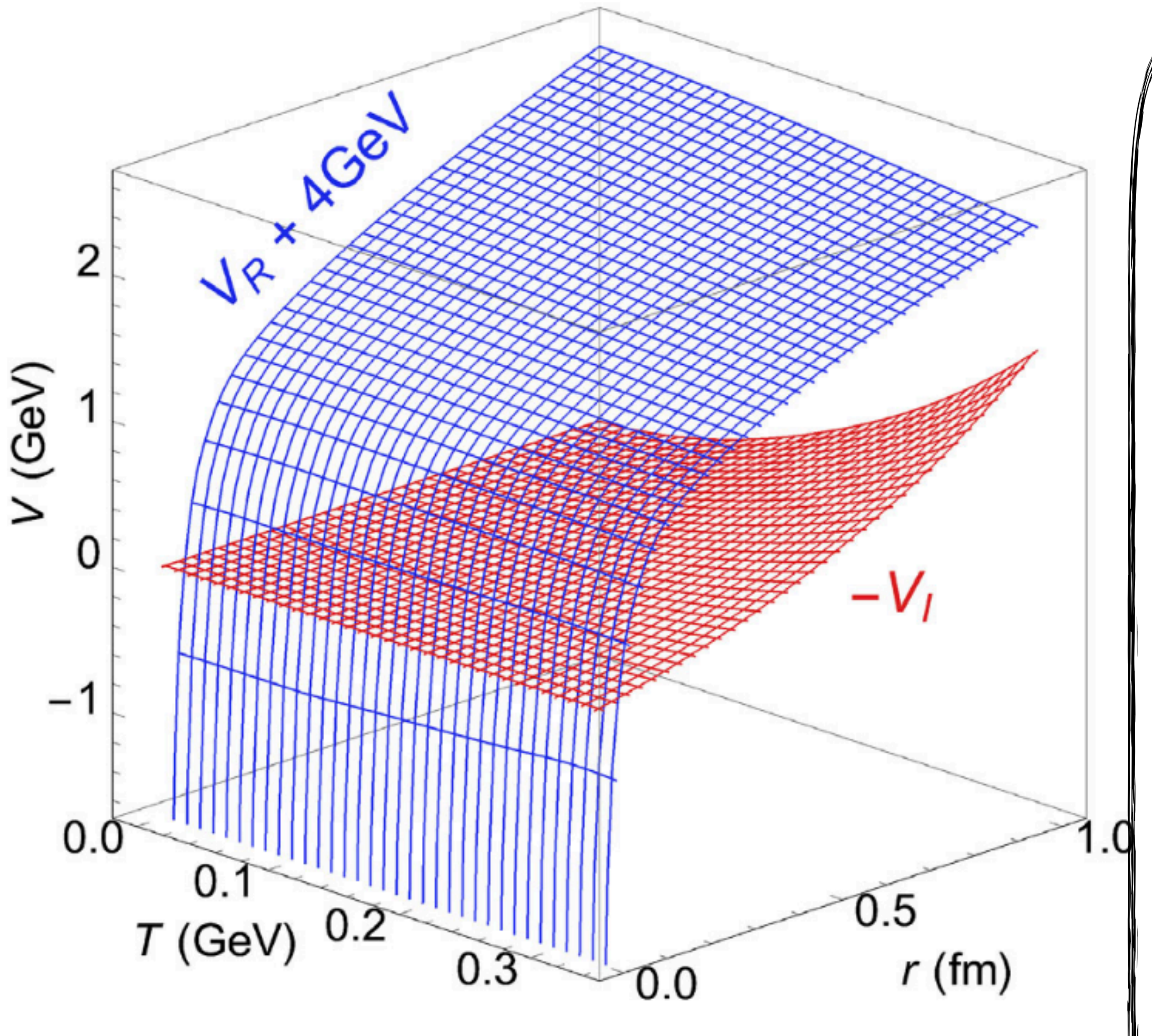
Extracting heavy quark potential



S. Shi, K. Zhou, J. Zhao, S. Mukherjee, and **P. Zhuang**, Phys. Rev. D **105**, 014017 (2022).

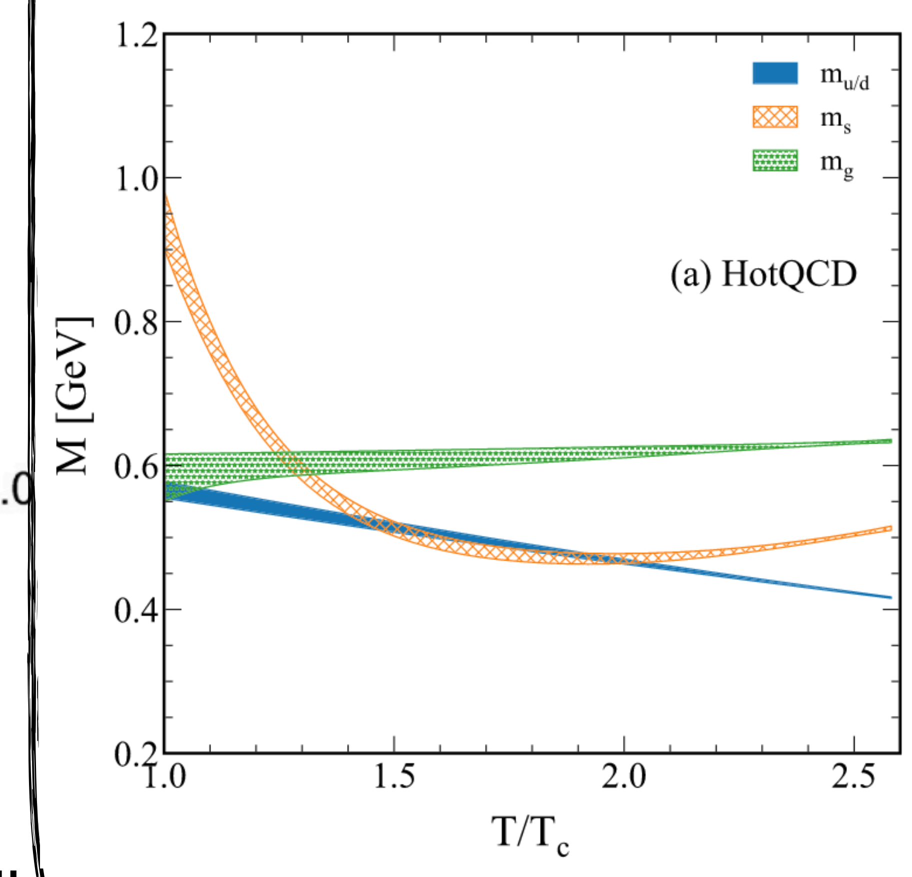
Other Works

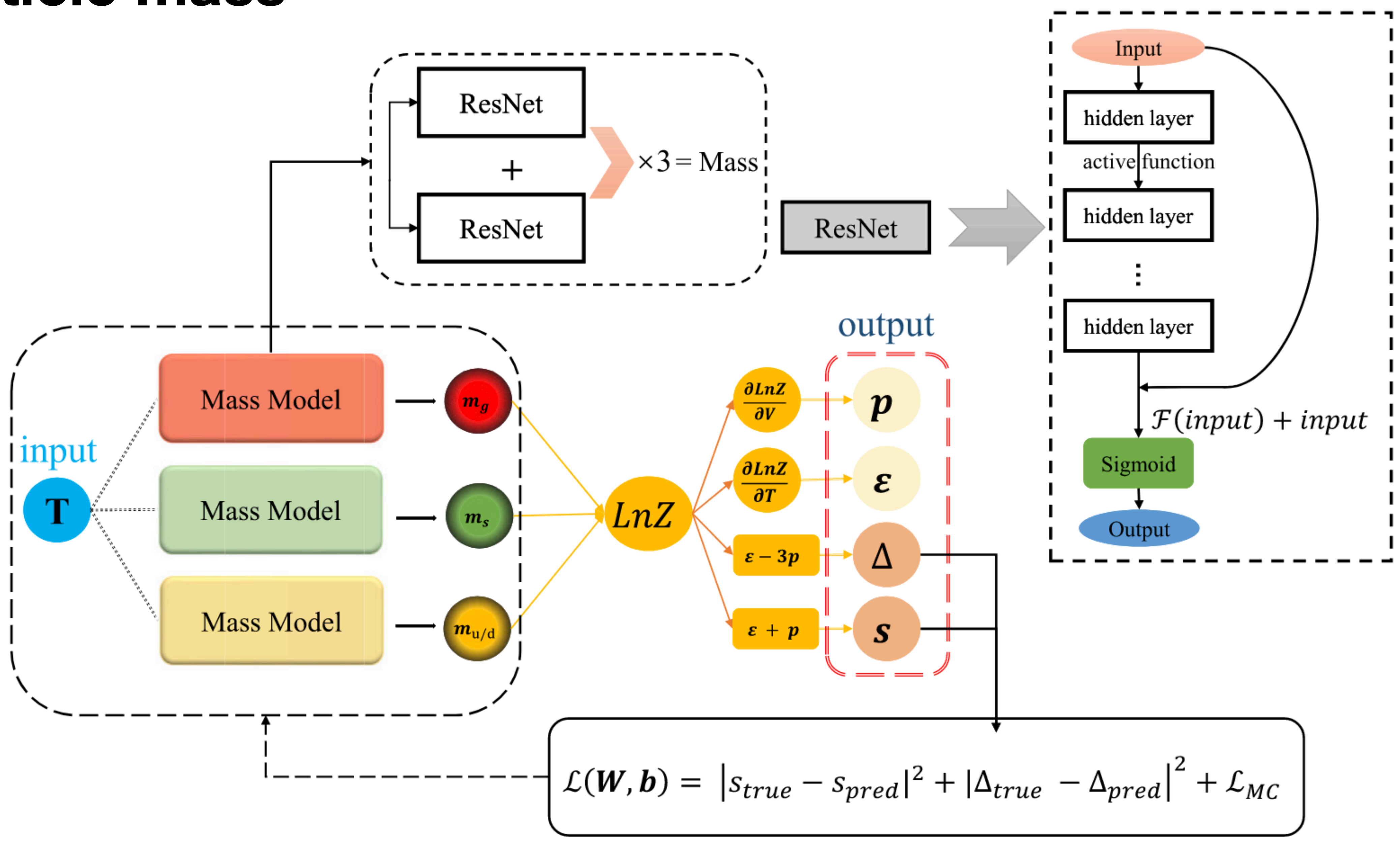
Extracting heavy quark potential



S. Shi, K. Zhou,

Learning quasi-particle mass



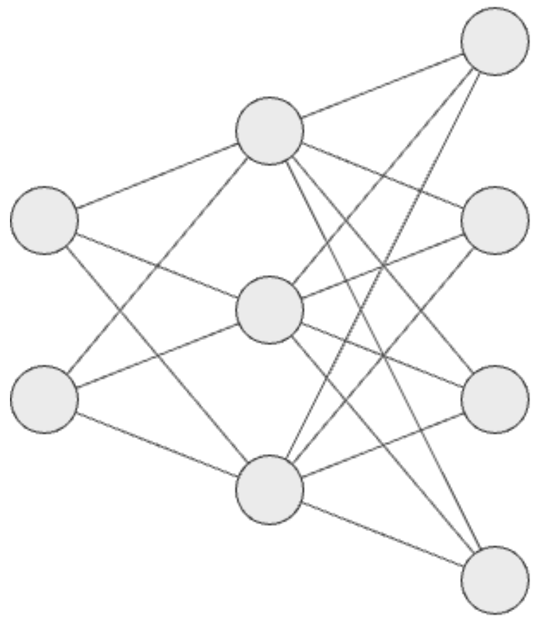


F.-P. Li, H.-L. Lü, **L.-G. Pang**, and **G.-Y. Qin**, Deep-Learning Quasi-Particle Masses from QCD Equation of State, Phys. Lett. B 138088 (2023).

...

Summary I

- **Inverse Problems**
  - Data-driven learning
  - Physics-driven learning
  - Physics-driven **deep** learning
    - Neural network representations
    - Gradient-based optimization
- **Future works**
  - Nuclear Matter EoS
  - Spectroscopy [github1, github2]
  - NN-Nulcear Force



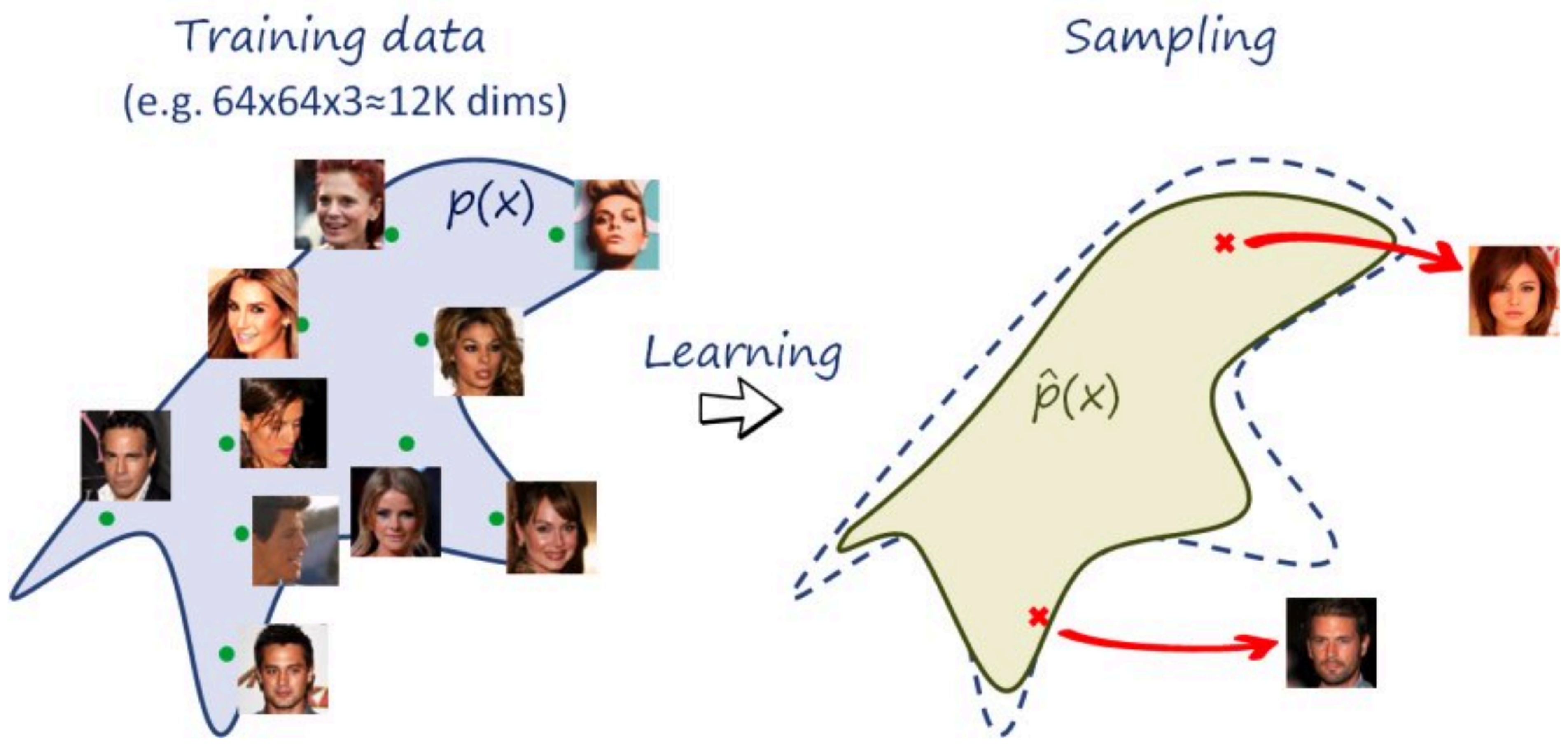
$f_\theta \xrightarrow{\text{Phys}} \tilde{O}$

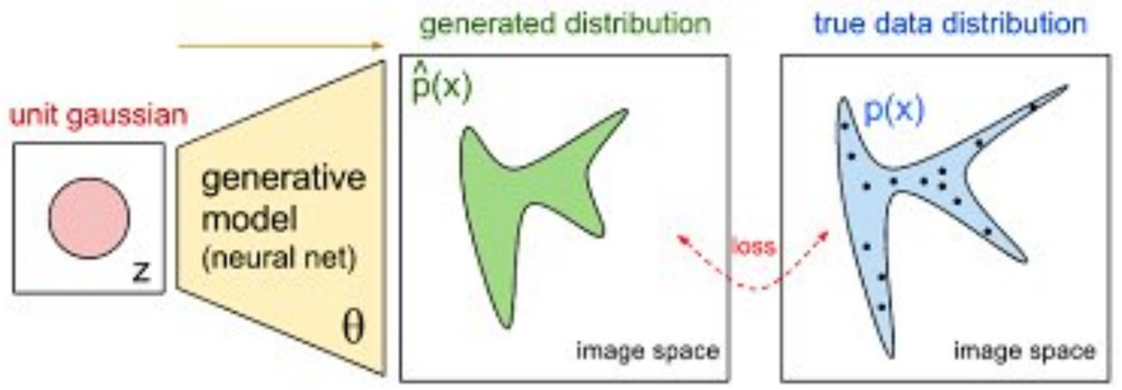
$\mathcal{L} = (O - \tilde{O})^2 \xrightarrow{\text{BP}} f_\theta$

$$\hat{\theta} = \mathbf{arg\,max}_\theta \{p(X \mid \theta)\}$$

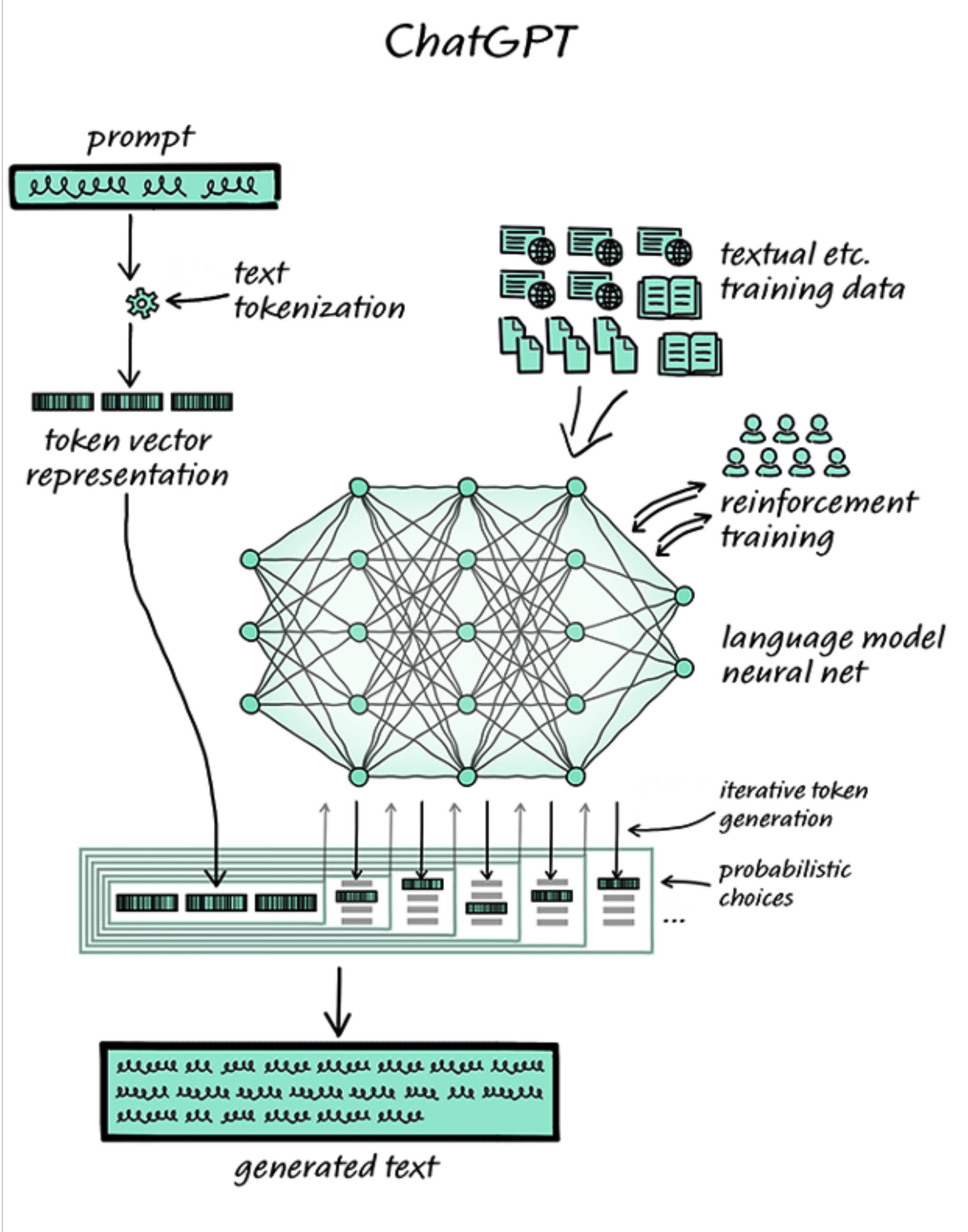
Generative Models

Generative Models





@blogs of OpenAI



Generative models

→ **Underlying Distributions in Data**

$$\max_{\theta} \prod_{i=1}^{N} p_\theta(\mathbf{x}_i)$$

Generating Samples

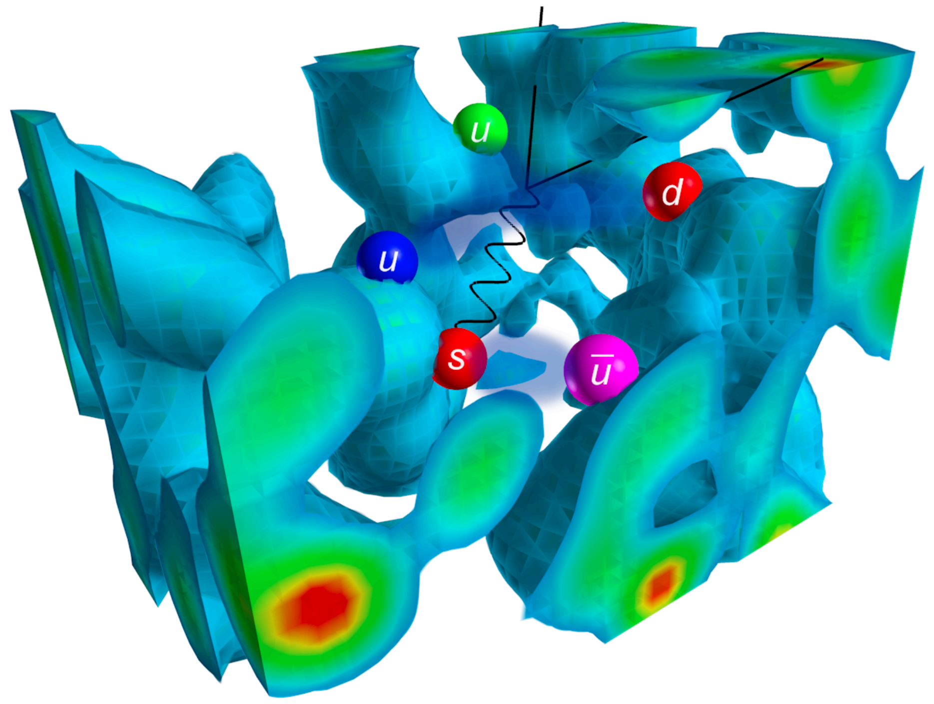
$$p(\phi) = e^{-S(\phi)}/Z$$

$$\langle O \rangle \approx \frac{1}{N} \sum_i O_i$$

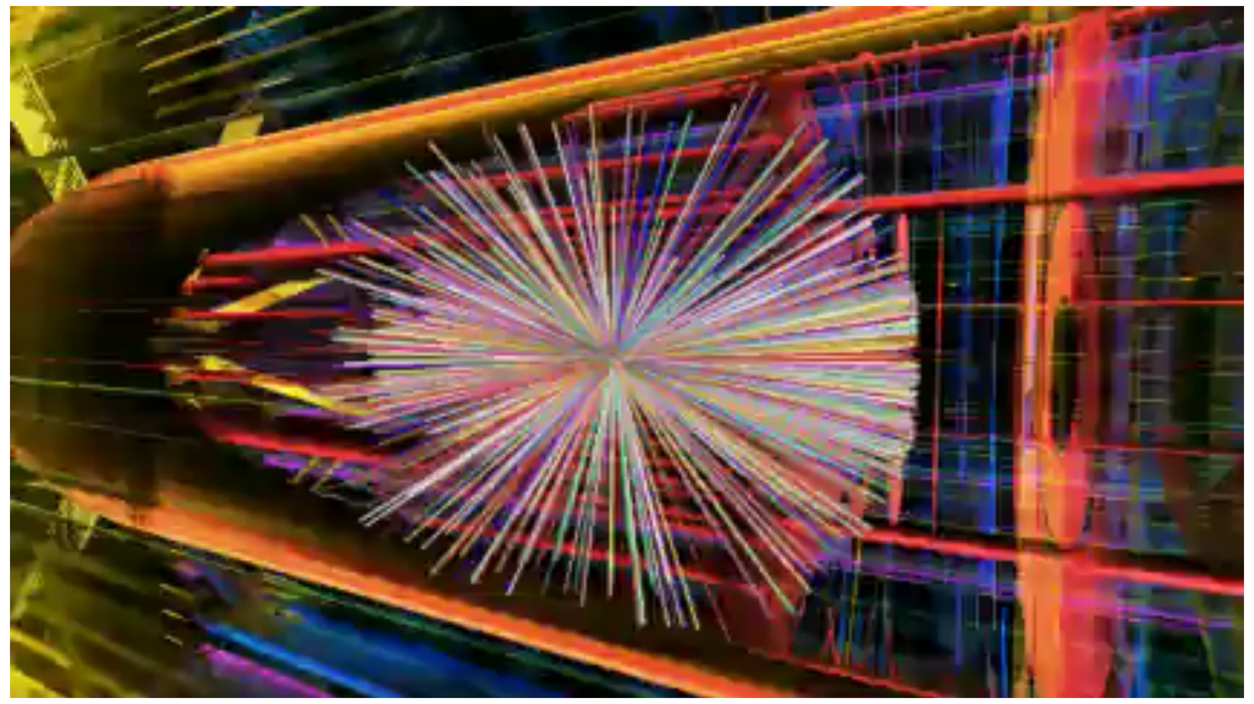
→ **Physical Distribution, Sampling** via Generative Models

Global Sampling

Fast and Independent Sampler



Lattice QCD © Derek Leinweber/CSSM/University of Adelaide



Heavy-Ion Collisions © 2010 CERN

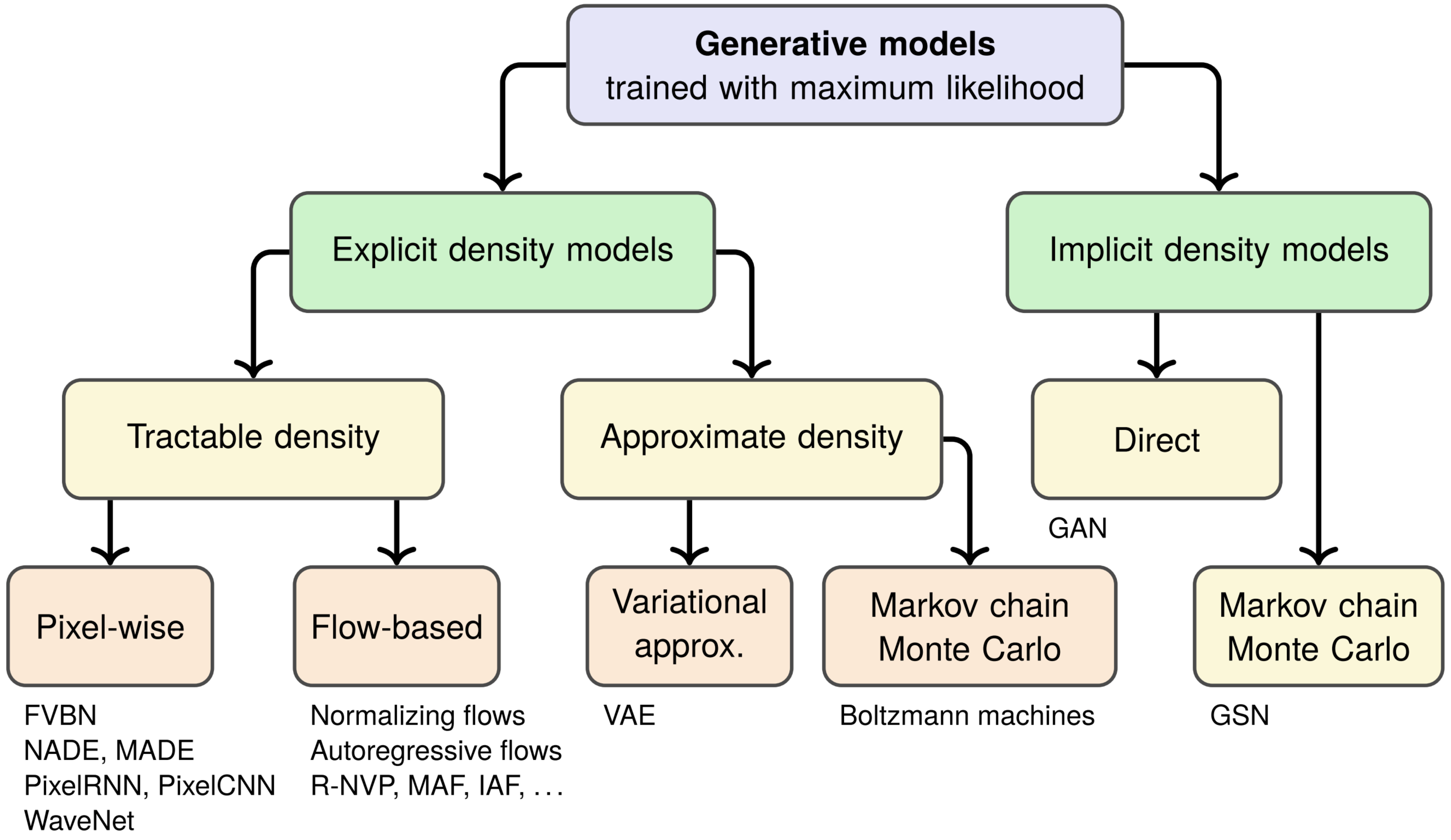
Generating Samples

Maximum Likelihood Estimation(MLE)

$$\max_{\theta} \prod_{i=1}^{N} p(\mathbf{x}_i \mid \theta)$$

$$p_\theta(\mathbf{x}) = \frac{e^{-f_\theta(\mathbf{x})}}{Z_\theta}$$

from a **statistical phsyics** perspective



I. Goodfellow, arXiv:1701.00160 (2017)

Generating Samples

Event Generation and Detector Simulation

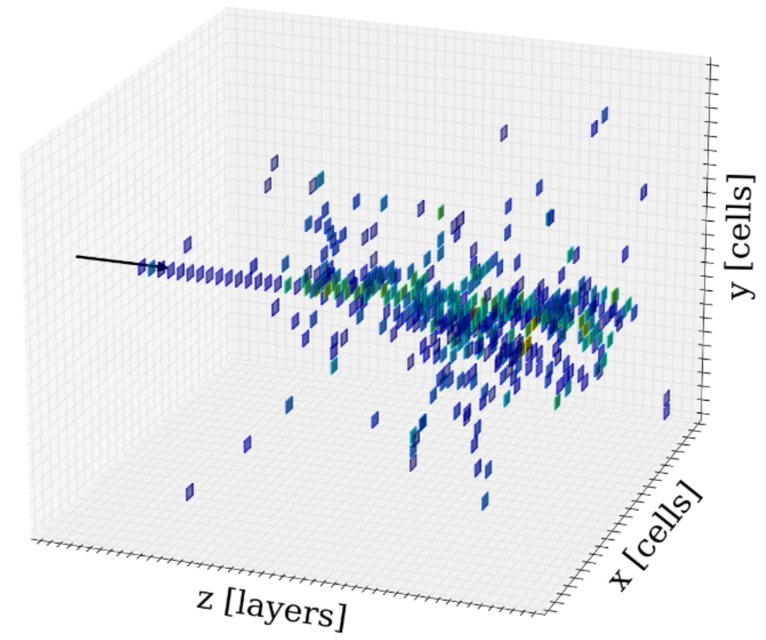
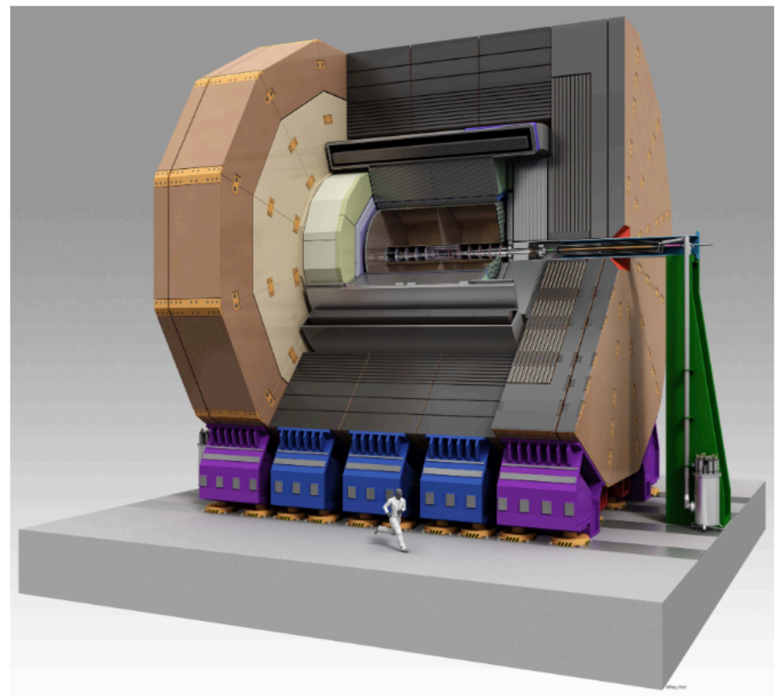
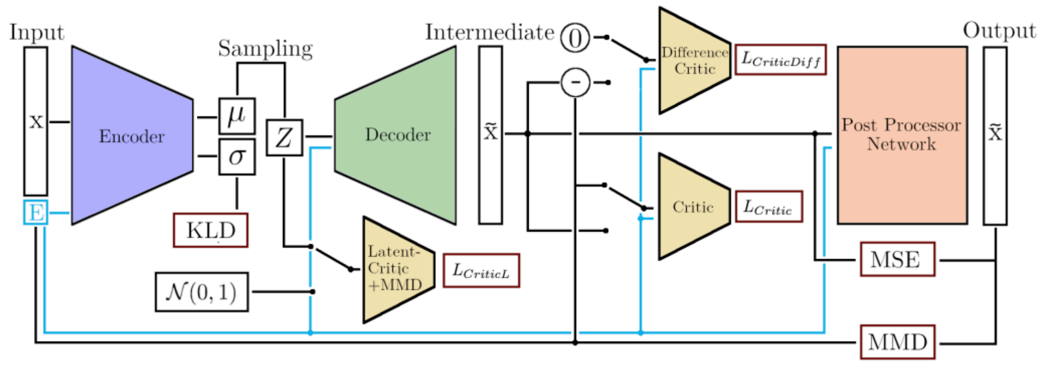


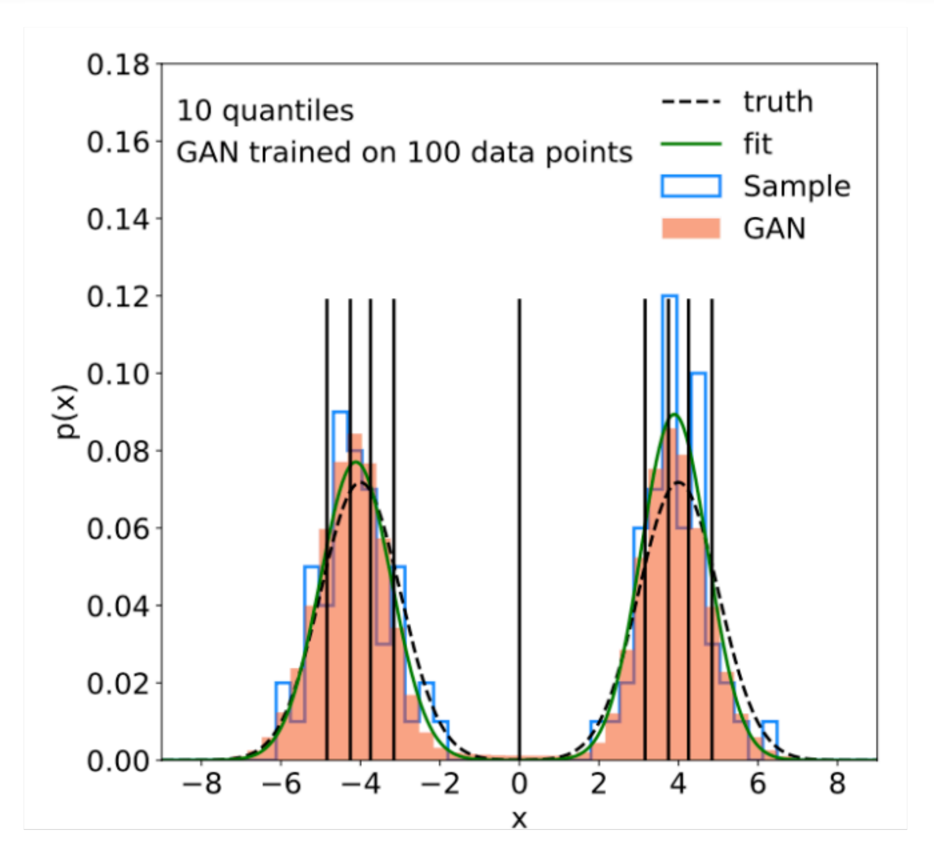
Image: S. Diefenbacher/UHH



"View of the ILD detector concept.", International Large Detector (ILD) collaboration. From: ILC technical design report, Volume 4: Detectors



Gregor Kasieczka ,etc. (Hamburg Group)



Generating Samples

Event Generation and Detector Simulation

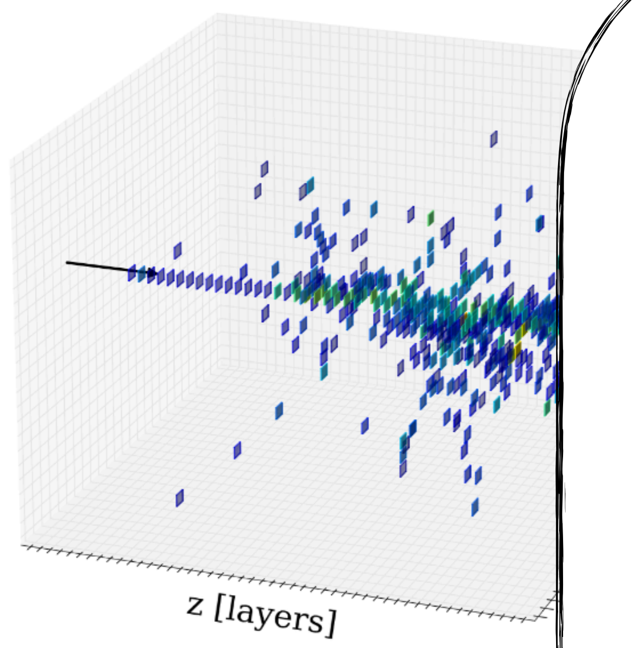
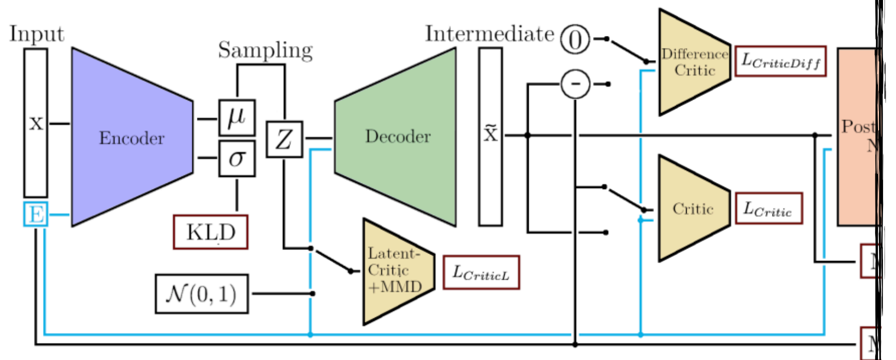
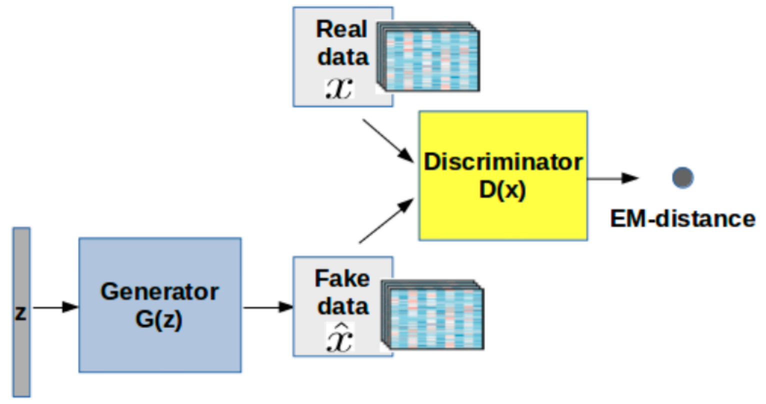
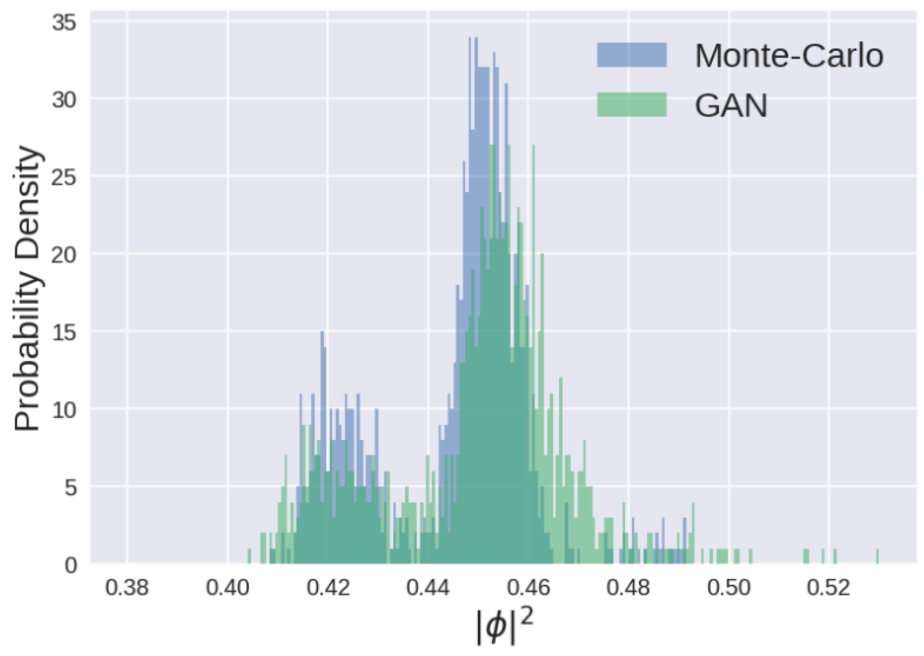


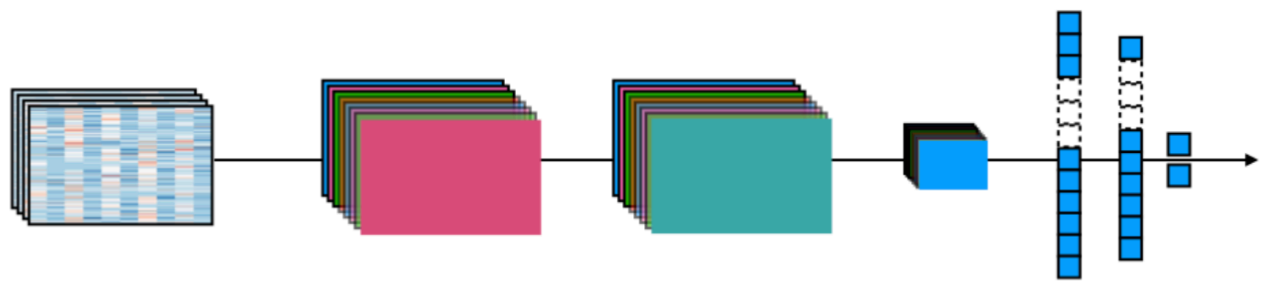
Image: S. Diefenbacher/UHH



Generating Field Configurations







K. Zhou, G. Endrődi, **L.-G. Pang**, and H. Stöcker, Phys. Rev. D **100**, 011501 (2019)

Generating Samples

Event Generation and Detector Simulation

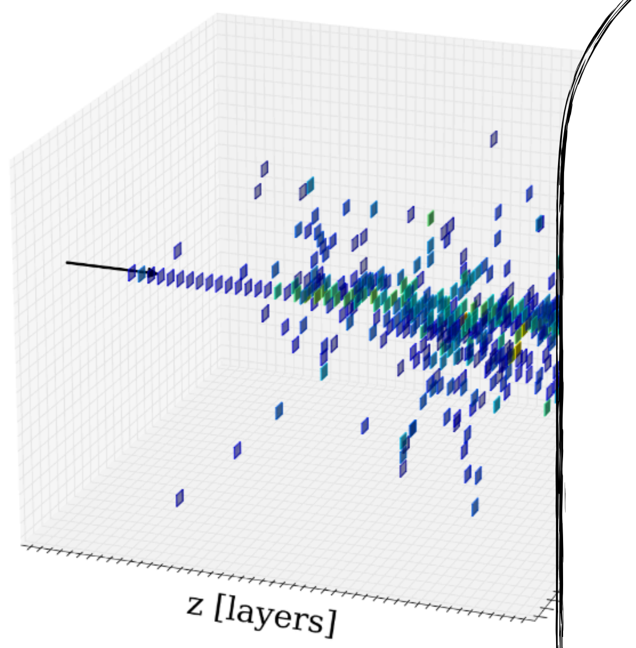
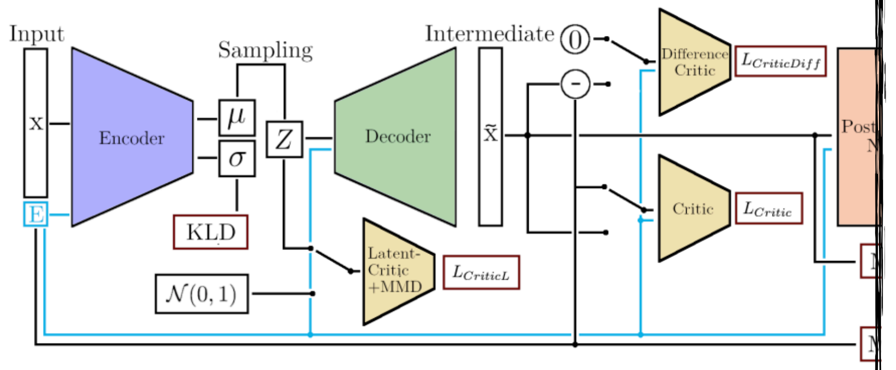
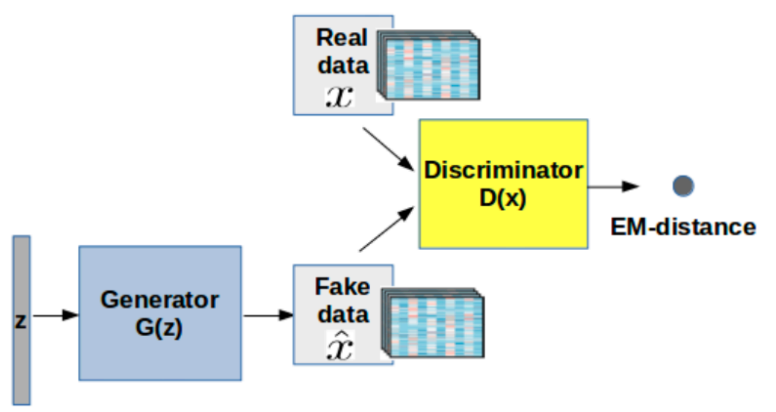
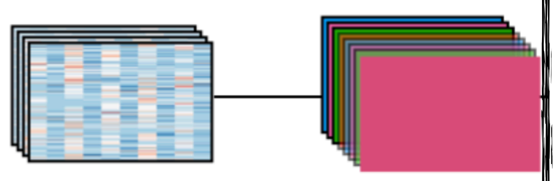


Image: S. Diefenbacher/UHH



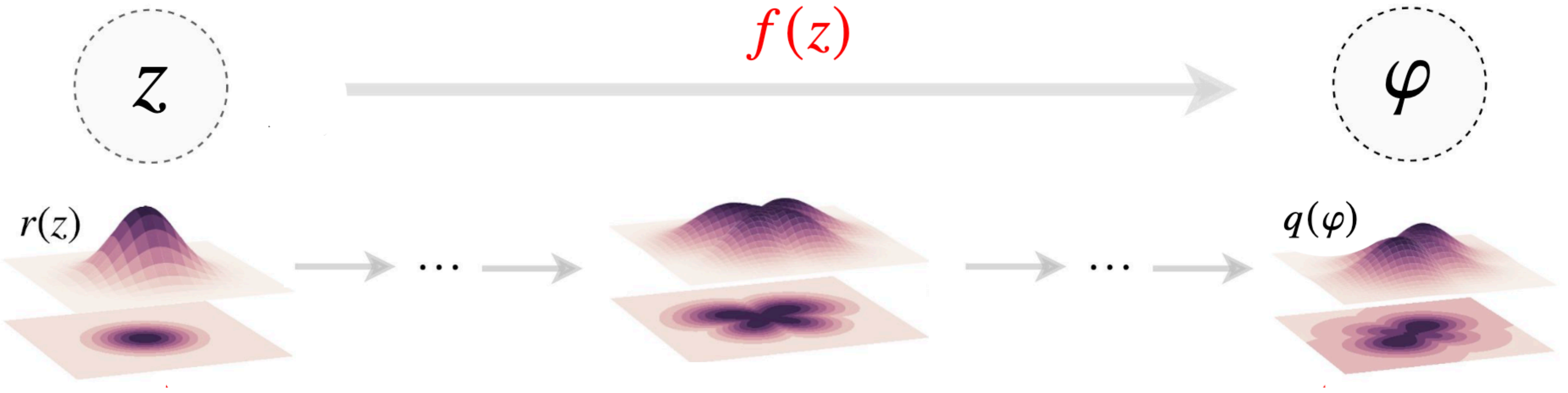
Generating Field Configurations

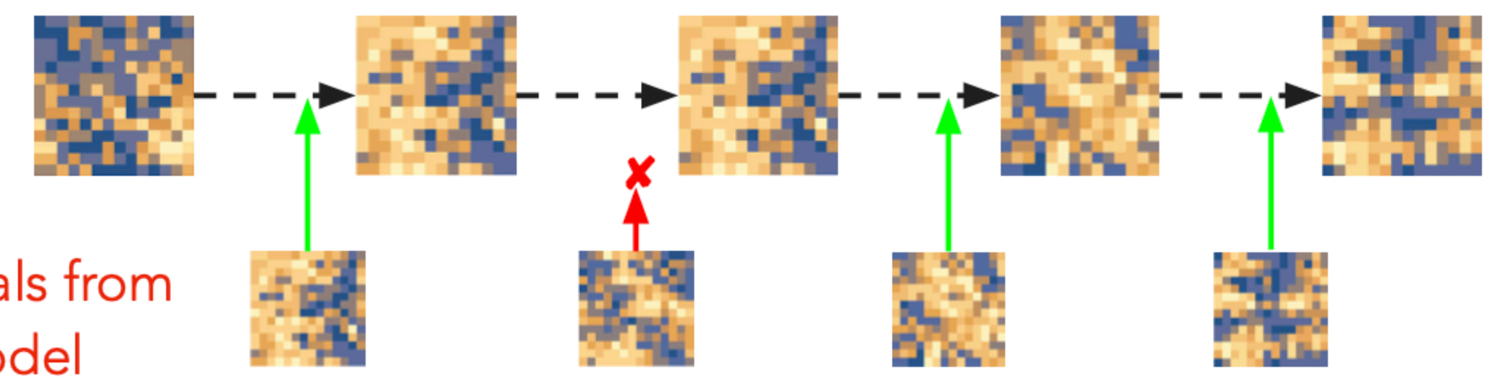




K. Zhou, G. Endrődi, L.-G. Pang, an

Flow-based Monte-Carlo





Phiala Shanahan,etc. (MIT Group)

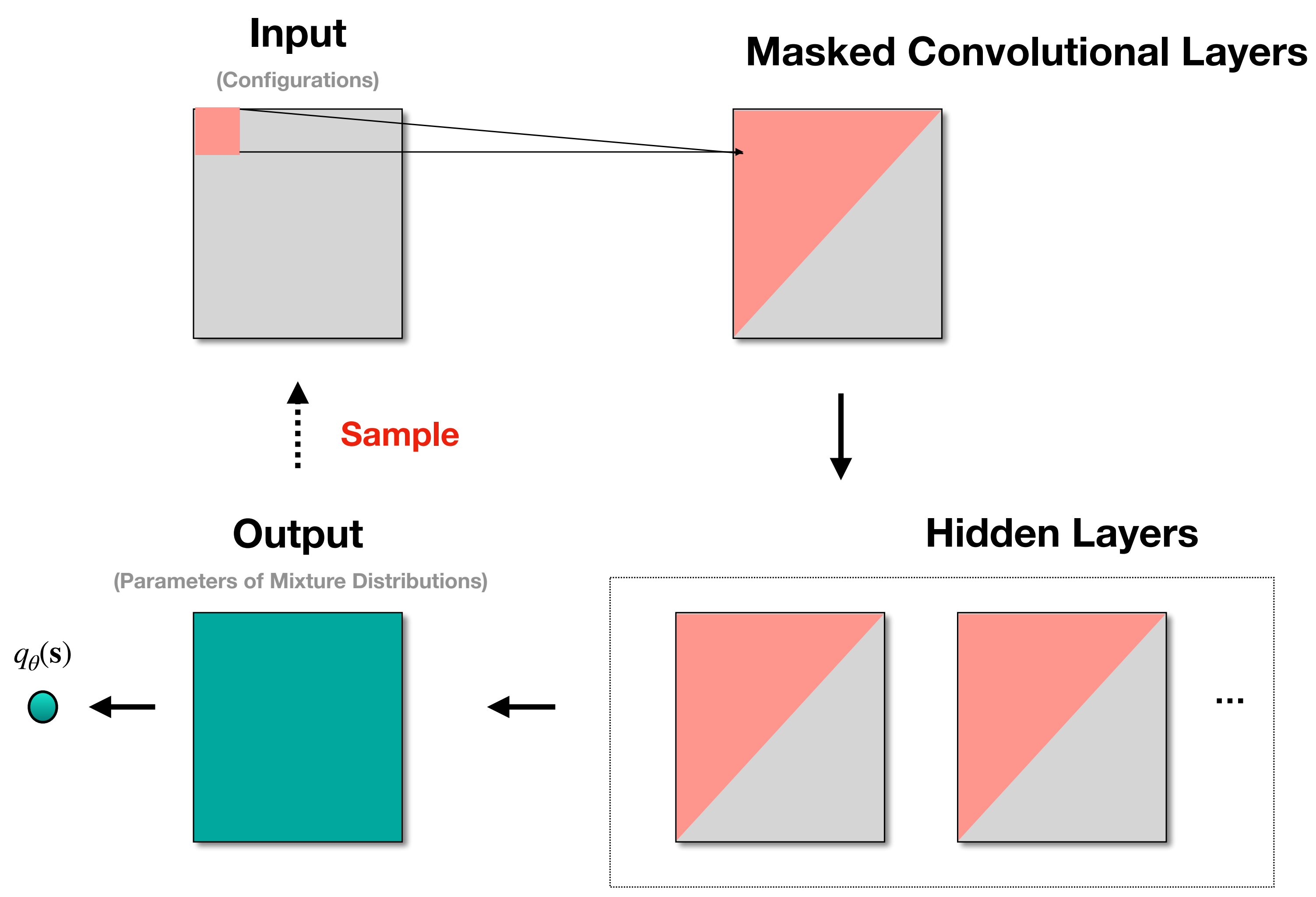
Generating Samples

1. Spin Configurations

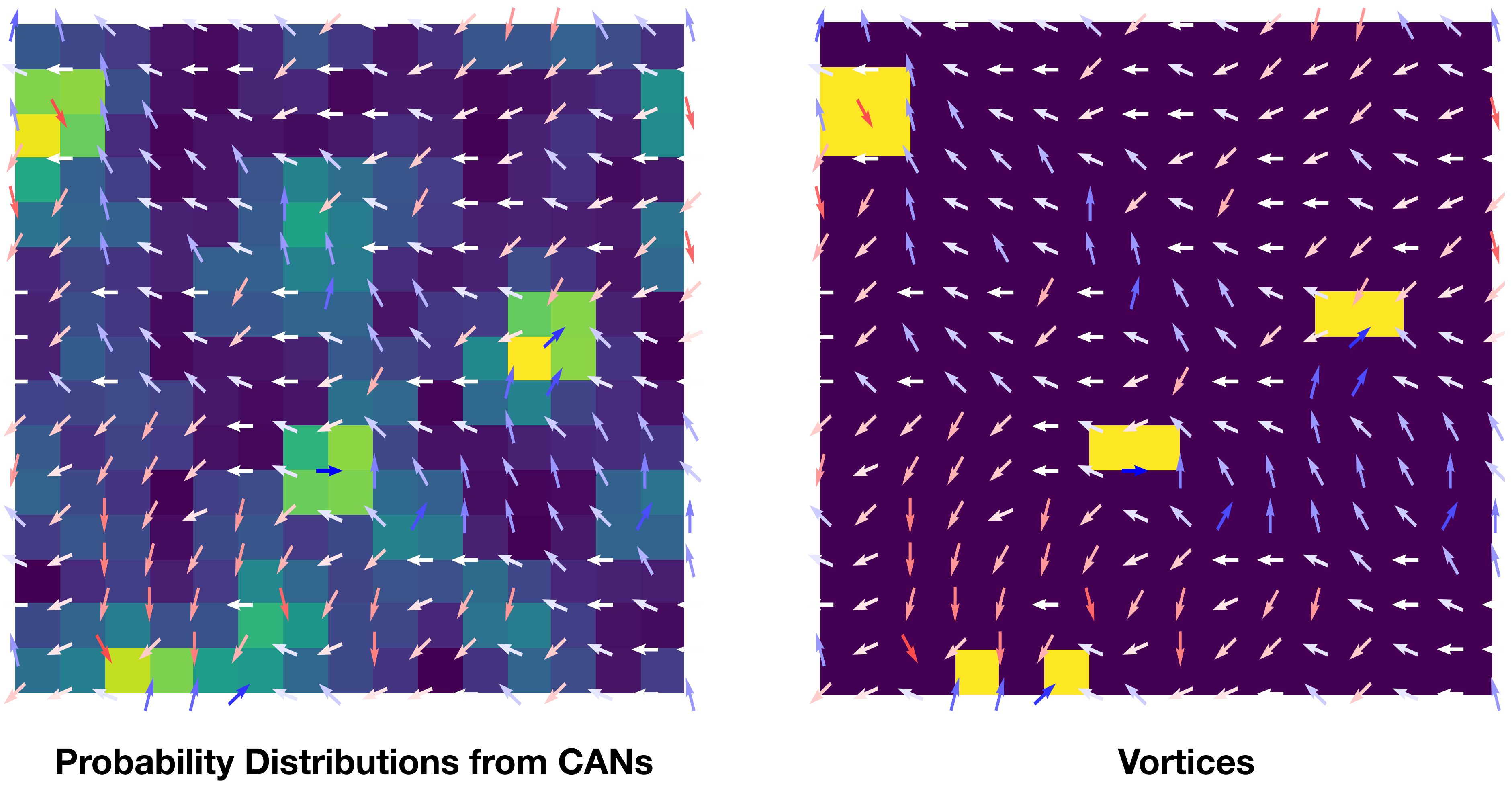
Chinese Phys. Lett. 39, 120502 (2022)

Autoregressive Networks model Likelihood $q_\theta(s)$ explicitly

$$q_\theta(s) \to p(s) = \frac{e^{-E(s)}}{Z}$$



Kosterlitz-Thouless(KT) transition, with (Vortices)

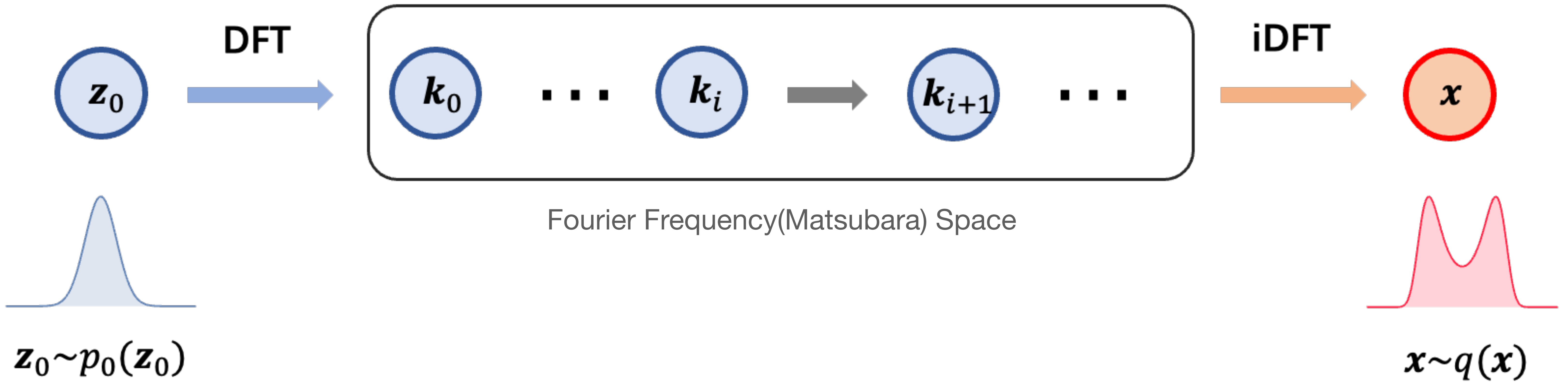


Generating Samples

2. Field Configurations

Phys. Rev. D 107, 056001

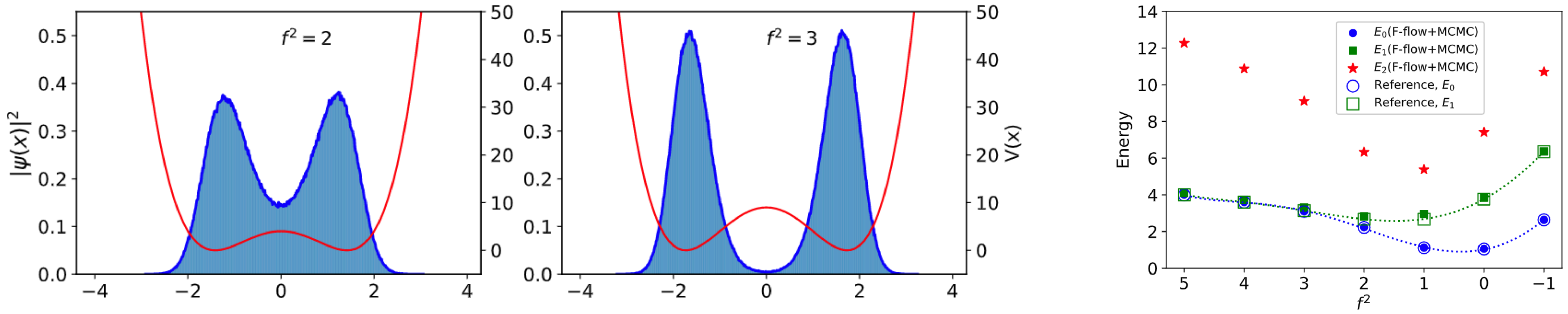
Fourier Flow Model



More priors. More stable!
for training neural networks

$$X_k = \sum_{n=0}^{N-1} e^{-i\frac{2\pi}{N}kn} x_n$$

Discrete Fourier transformation (DFT)



Space Opera, Jason Allen via Midjourney

Diffusion Models

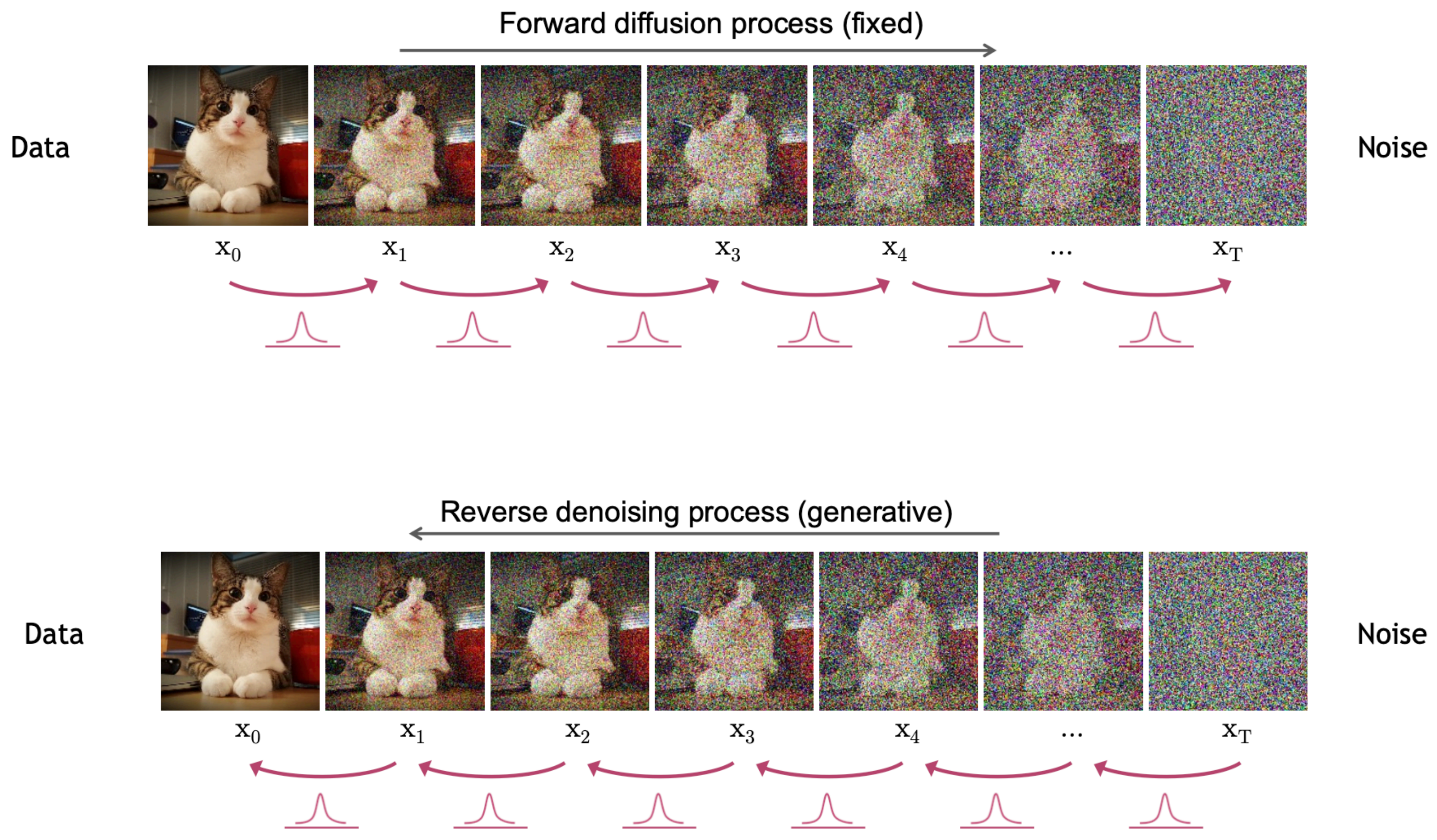
Lingxiao Wang via Dreamstudio

Quark-gluon plasma under electromagnetic fields

Quark-gluon plasma under strongly rotating

Diffusion Models

- Forward diffusion process **gradually adds noise** to input
- Reverse denoising process learns to **generate data by denoising**
- Train **Probabilistic Models** to learn how to **convert a simple distribution to a target distribution**



Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020

Diffusion Models

- **Forward Diffusion SDE**
  - **Drift term**: pulls towards mode
  - **Diffusion term**: injects noise

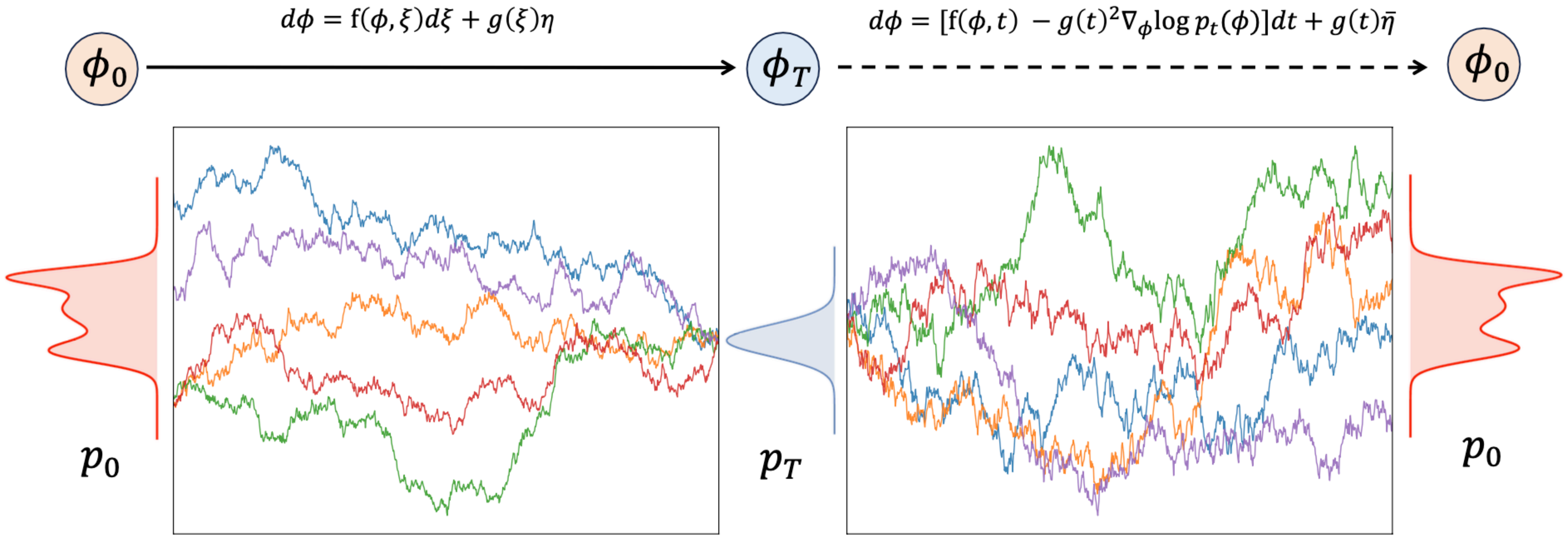
Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021

Anderson, in Stochastic Processes and their Applications, 1982

$$\frac{d\phi}{d\xi} = \boxed{f(\phi, \xi)} + \boxed{g(\xi)\eta(\xi)}$$

- **Reverse Generative Diffusion SDE**
  - Drift term is adjusted with a "**Score Function**"
  - Represent the score function with **neural networks**

$$\frac{d\phi}{dt} = \boxed{\left[f(\phi, t) - g^2(t)\, \nabla_\phi \log p_t(\phi)\right]} + \boxed{g(t)\bar{\eta}(t)}$$



Diffusion Models

Stochastic Quantization

$$\frac{\partial \phi(x,\tau)}{\partial \tau} = -\frac{\delta S_E[\phi]}{\delta \phi(x,\tau)} + \eta(x,\tau)$$

$$\langle \eta(x,\tau)\rangle = 0, \quad \langle \eta(x,\tau)\eta(x',\tau')\rangle = 2\alpha\delta(x-x')\delta(\tau-\tau')$$

τ: fictitious time, α: diffusion constant

- **Fokker-Planck equation**

$$\frac{\partial P[\phi,\tau]}{\partial \tau} = \alpha \int d^n x \left\{ \frac{\delta}{\delta \phi}\left(\frac{\delta}{\delta \phi} + \frac{\delta S_E}{\delta \phi}\right)\right\} P[\phi,\tau]$$

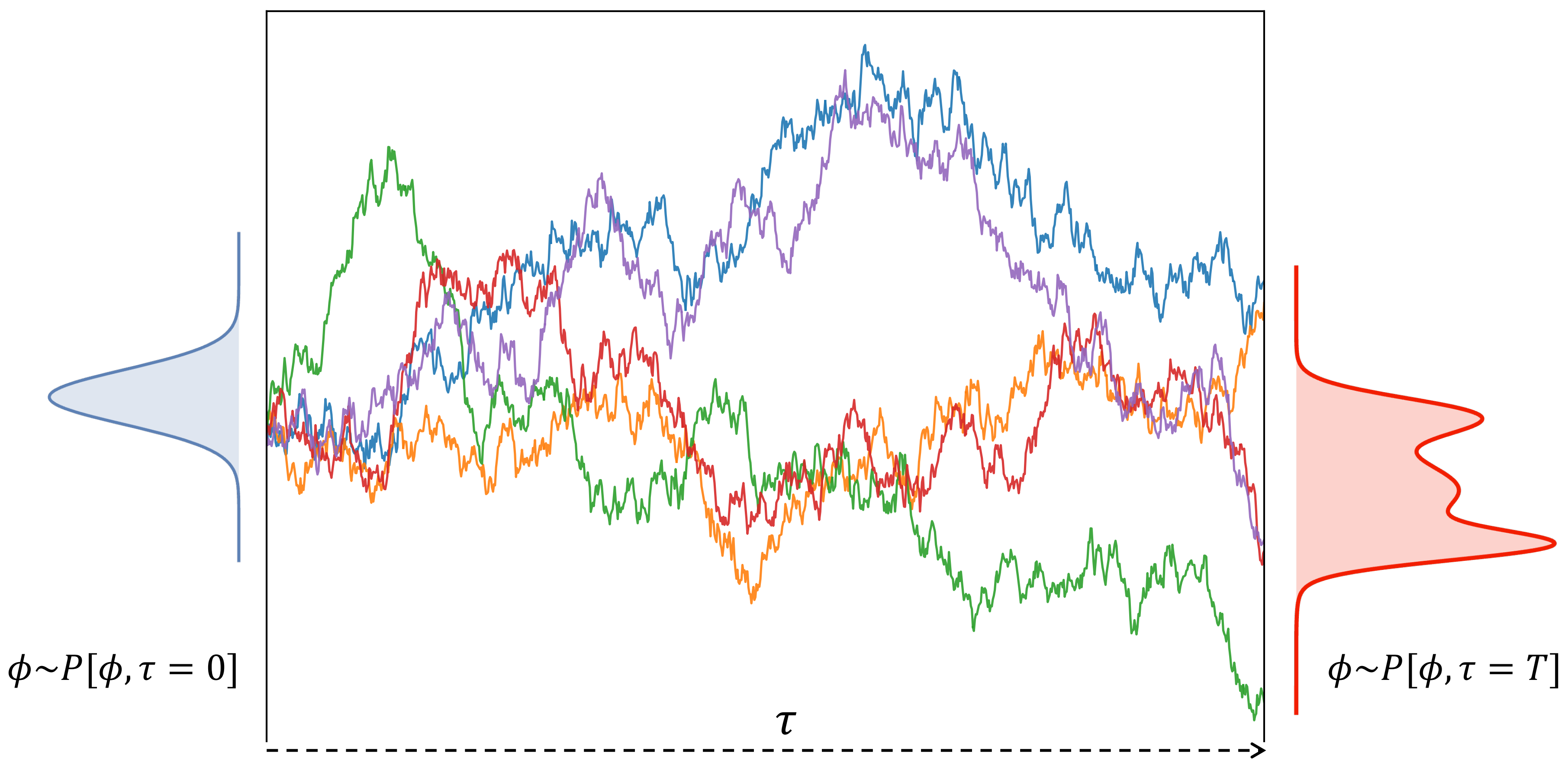
Equilibrium solution (long-time limit),

$$P_{\text{eq}}[\phi] \propto e^{-\frac{1}{\alpha}S_E[\phi]}$$

- Set the diffusion constant as $\alpha = \hbar$

$$P_{\text{eq}}[\phi] \sim e^{-\frac{1}{\hbar}S_E[\phi]} = P_{\text{quantum}}[\phi]$$

Parisi G. and Wu Y. S., Sci. China, A **24**, ASITP-80-004 (1980).



Thermal equilibrium limit → Quantum distribution

1. No need gauge-fixing!
2. Can handle fermionic fields naturally
→(Complex Langevin method)
....

P. H. Damgaard and H. Hüffel, Stochastic Quantization, Phys. Rept. 152, 227 (1987).
M. Namiki, Basic Ideas of Stochastic Quantization, PTPS 111, 1 (1993).
G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty, and I.-O. Stamatescu, Eur. Phys. J. A **49**, 89 (2013).

Diffusion Models

DMs as SQ

- **Diffusion models(Reverse SDE):**

$$\frac{d\phi}{dt} = -g(t)^2 \nabla_\phi \log p_t(\phi) + g(t)\bar{\eta}$$

  - **Define:** $\tau \equiv T - t(d\tau \equiv -dt)$

$$\frac{d\phi}{d\tau} = g_\tau^2 \nabla_\phi \log q_\tau(\phi) + g_\tau \bar{\eta}$$

$$\phi(\tau_{n+1}) = \phi(\tau_n) + g_\tau^2 \nabla_\phi \log q_{\tau_n}[\phi(\tau_n)]\Delta\tau + g_\tau \sqrt{\Delta\tau}\bar{\eta}(\tau_n)$$

introducing **Noise scale:** $\langle \bar{\eta}^2 \rangle \equiv 2\bar{\alpha}$, **time scale:** $g_\tau^2 \Delta\tau$

- **FP equation**

$$\frac{\partial p_\tau(\phi)}{\partial \tau} = \int d^n x \left\{ g_\tau^2 \bar{\alpha} \frac{\delta}{\delta\phi} \left(\frac{\delta}{\delta\phi} + \frac{1}{\bar{\alpha}} \nabla_\phi S_{\mathbf{DM}} \right) \right\} p_\tau(\phi)$$

$\nabla_\phi S_{\mathbf{DM}} \equiv -\nabla_\phi \log q_\tau(\phi)$

$$p_{eq}(\phi) \propto e^{-\frac{S_{DM}}{\bar{\alpha}}}$$

$$p_{\tau=T}(\phi) \to P[\phi, T]$$

$$O(\bar{\alpha}) \sim O(\hbar)$$

The reverse mode of
a well-trained diffusion model at $\tau \to T$ serves as
the stochastic quantization for the input

Diffusion Models

DM for Scalar Field

arXiv: 2309.17082

- **Euclidean action** on lattice

$$S_E = \sum_x a^d [\sum_{\mu=1}^{d} \frac{(\phi_0(x+a\hat{\mu}) - \phi_0(x))^2}{a^2} + \frac{m_0^2}{2}\phi_0^2 + \frac{\lambda_0}{4!}\phi_0^4]$$

- Dimensionless form

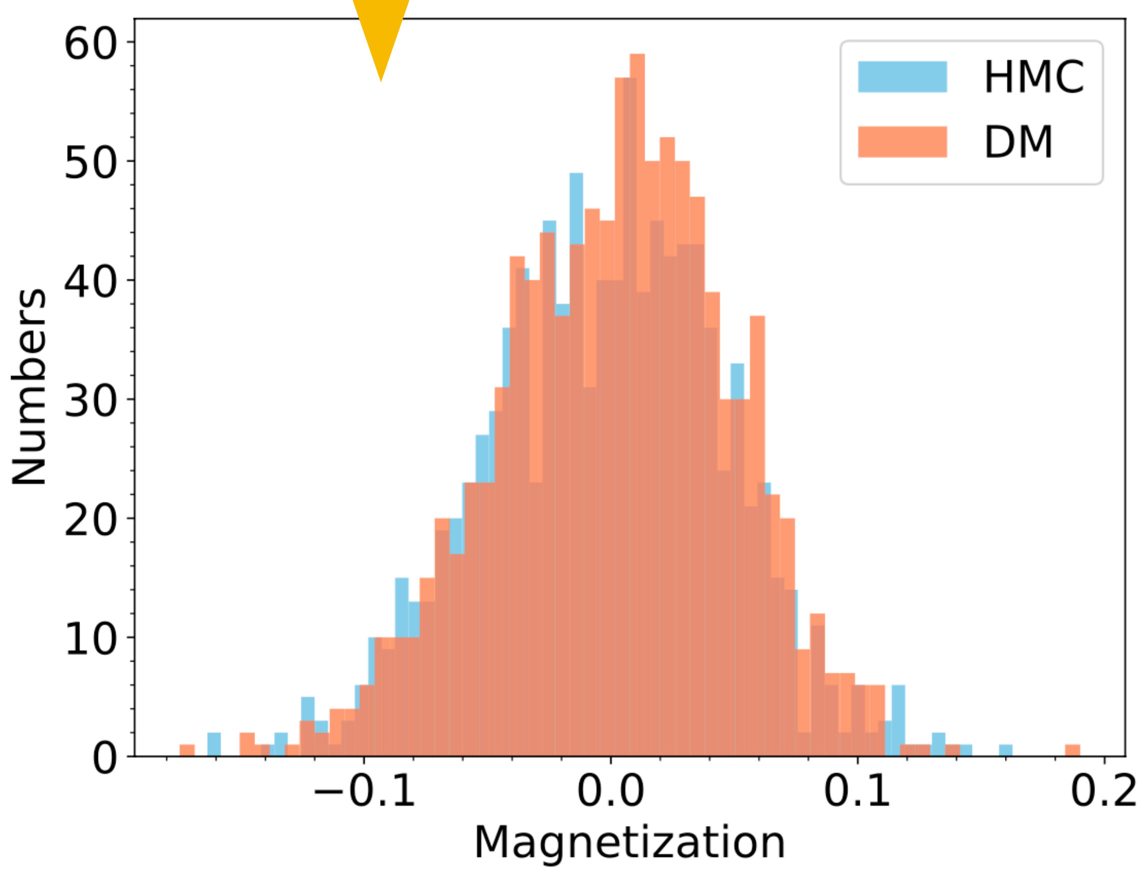
$$S_E = \sum_x [-2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4]$$

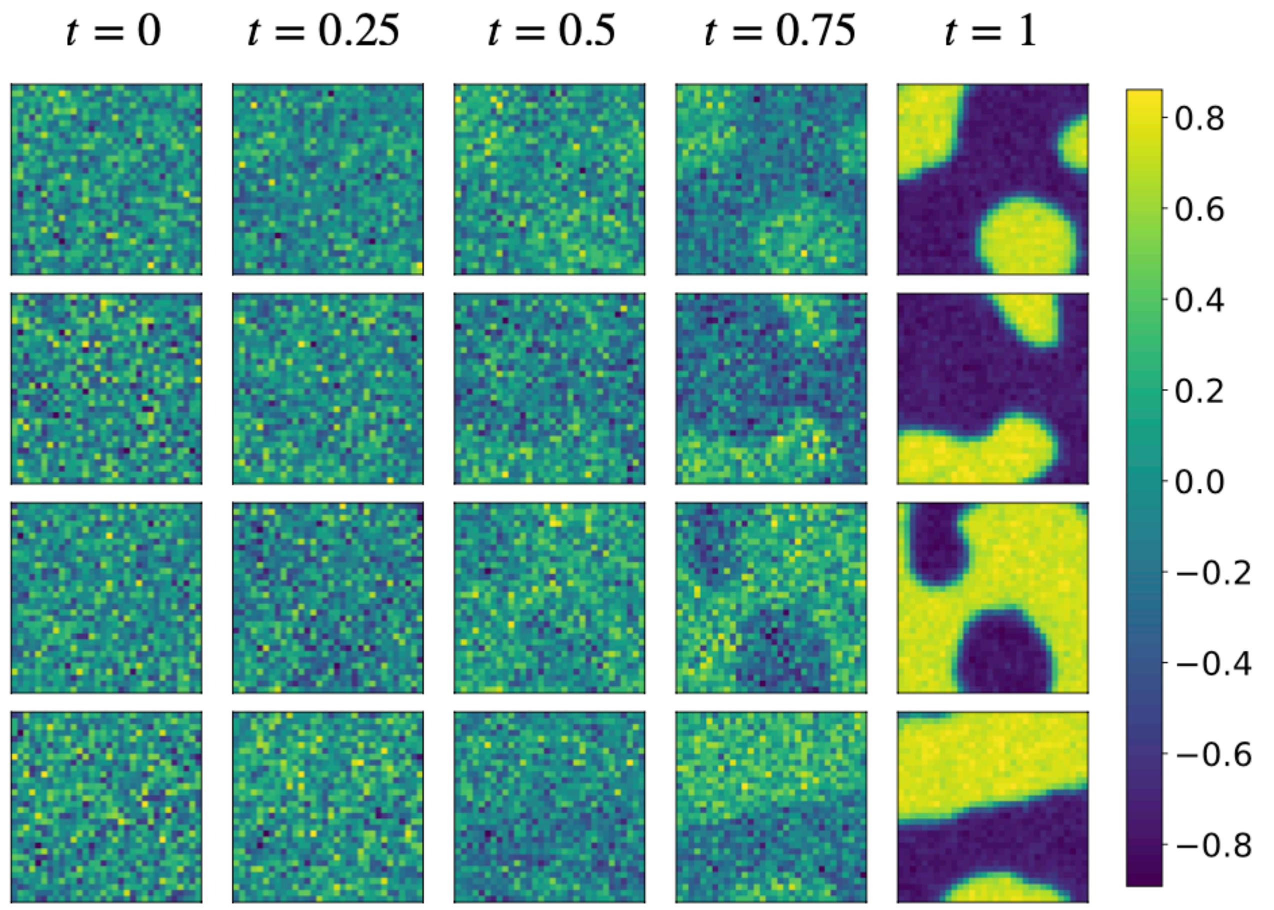
$$a^{\frac{d-2}{2}}\phi_0 = (2\kappa)^{1/2}\phi$$

$$(am_0)^2 = \frac{1-2\lambda}{\kappa} - 2d, \quad a^{-d+4}\lambda_0 = \frac{6\lambda}{\kappa^2}$$

- Hopping parameter κ, Coupling constant λ

- **Diffusion models**
  - $T = 1.0, \sigma = 25$
- **Data generation**
  - 2-d 32×32 lattice; Hamiltonian Monte Carlo(HMC); 5120 configurations for training.
  - Broken phase: $\kappa = 1.0, \lambda = 0.022$
  - Symmetric phase: $\kappa = 0.21, \lambda = 0.022$

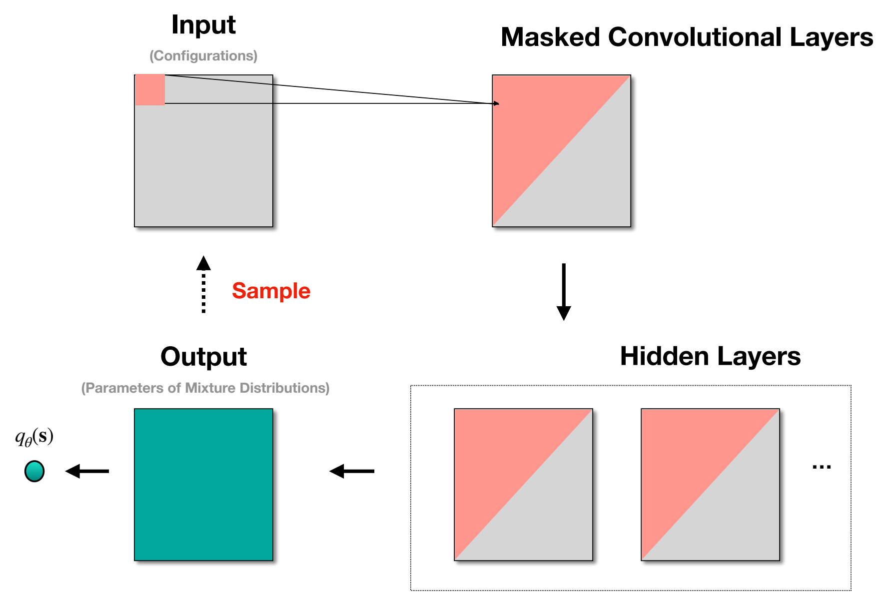


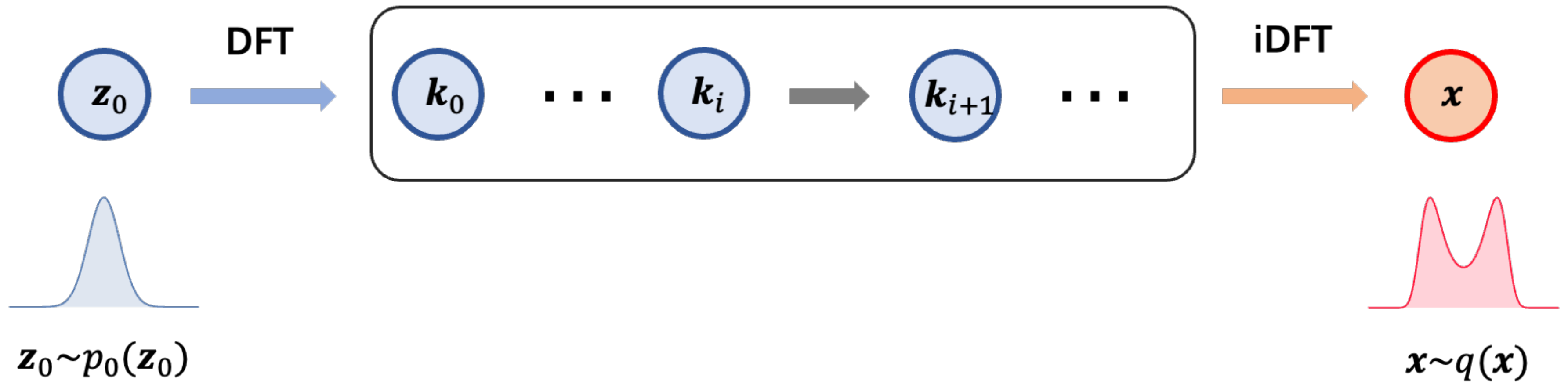


data-set	$\langle M \rangle$	χ_2	U_L
Training(HMC)	0.0012± 0.0007	2.5160 ± 0.0457	0.1042 ± 0.0367
Testing(HMC)	0.0018 ± 0.0015	2.4463 ± 0.1099	-0.0198 ± 0.1035
Generated(DM)	0.0017± 0.0015	2.4227 ± 0.1035	0.0484 ± 0.0959

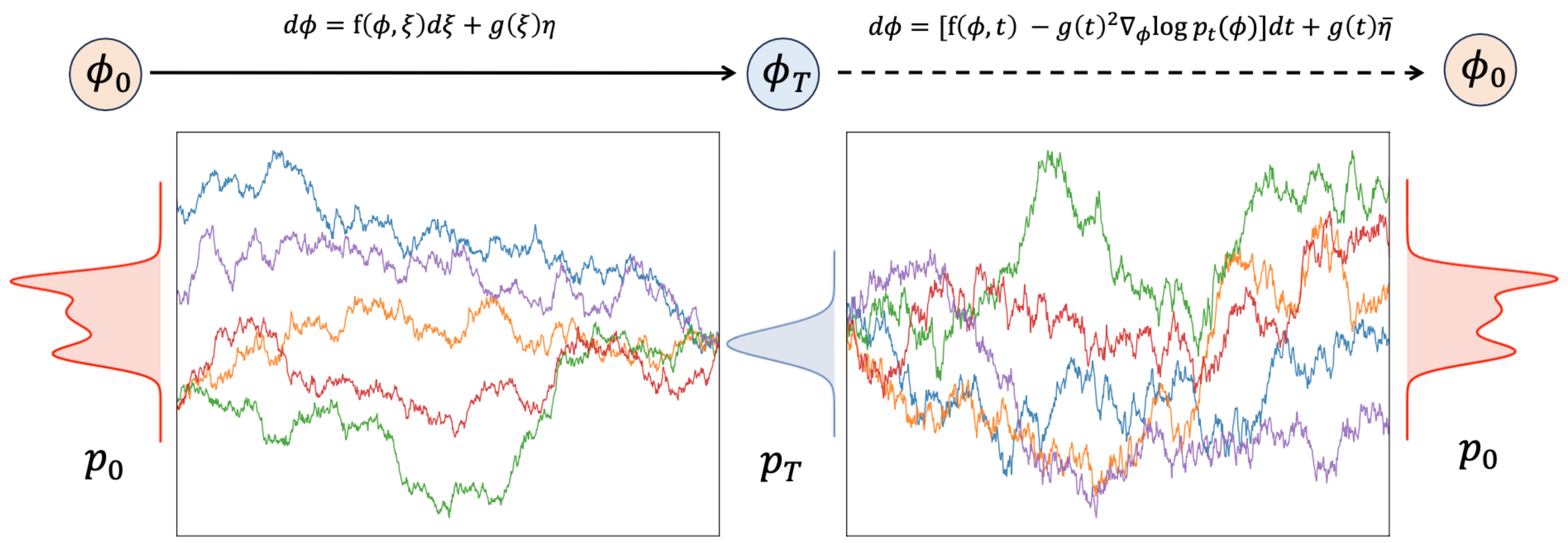
Summary II

- **Generative Models**
  - Generating Samples
    - **Spin system**: Continuous autoregressive networks
    - **Field**: Fourier-Flow model
  - Diffusion Models
    - **Stochastic Quantization** scheme





- **Future works**
  - **Diffusion models as SQ**
  - 2+1D **Gauge Field**
  - Complex Langevin Method(CLM) for **Fermions**



Representation Learning

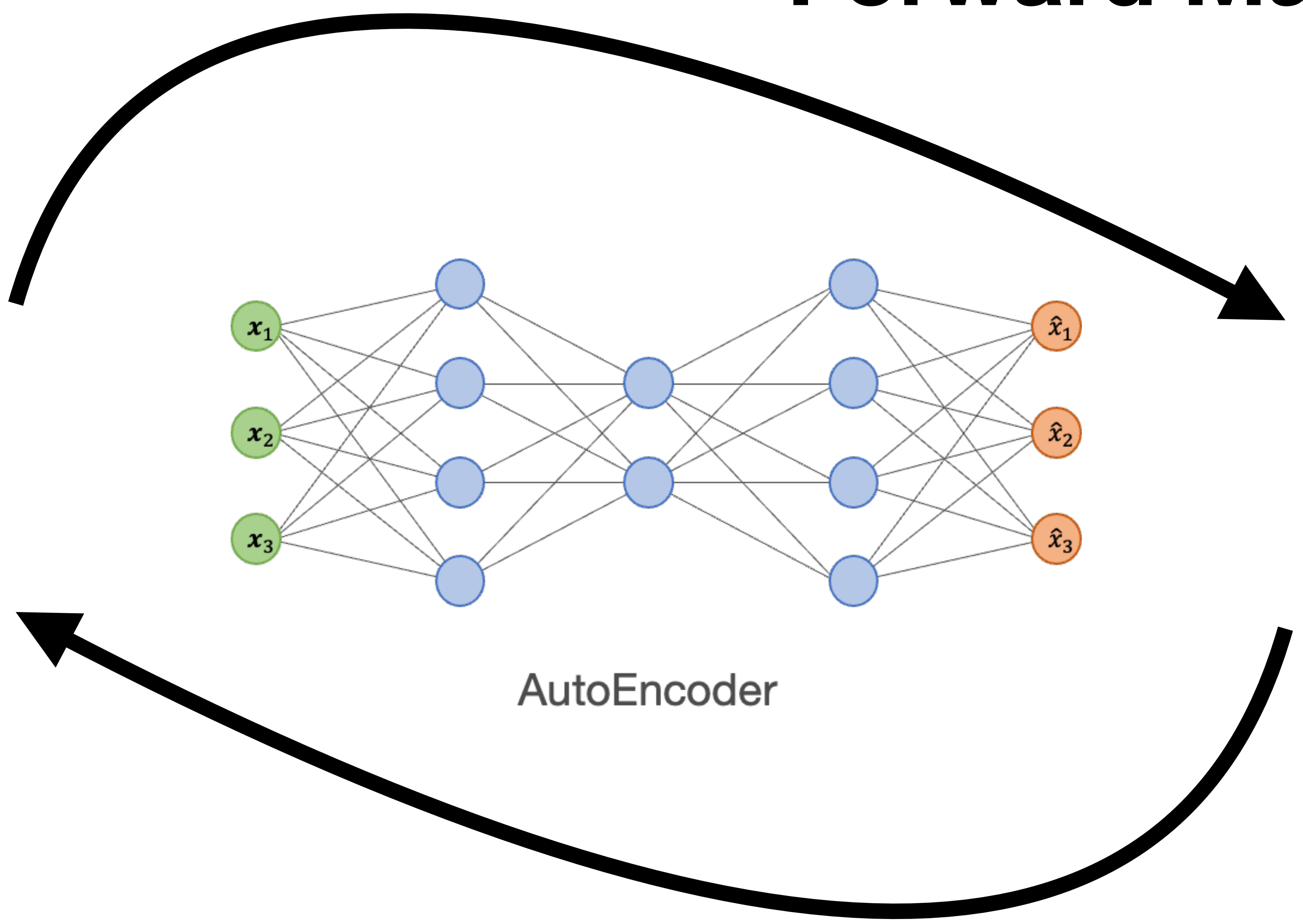
$$g_\theta : X \to Y$$

$$f_\theta : Y \to X$$

Forward Mapping, f_θ

Physics

Model Parameters/ Properties/States



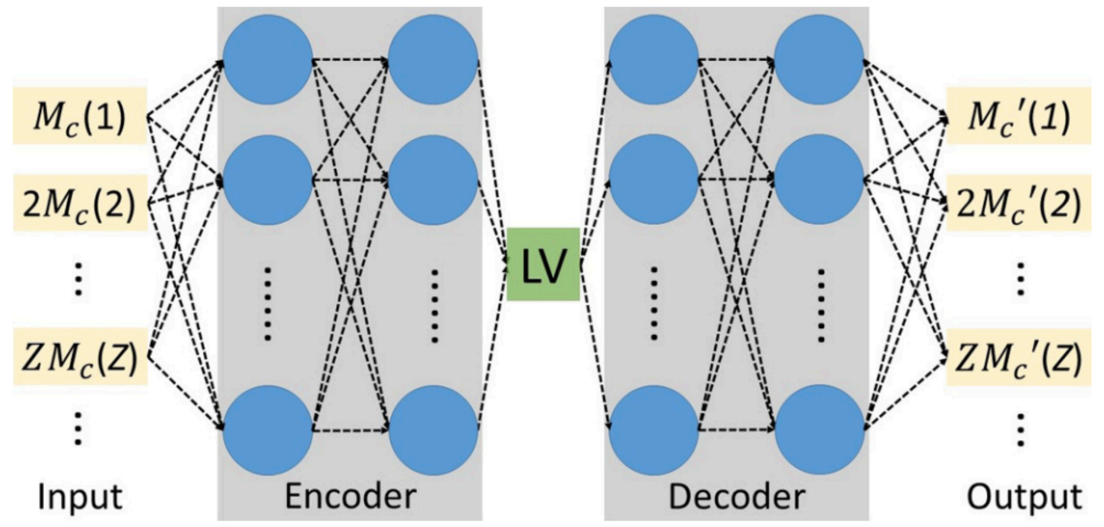
Data

Observations

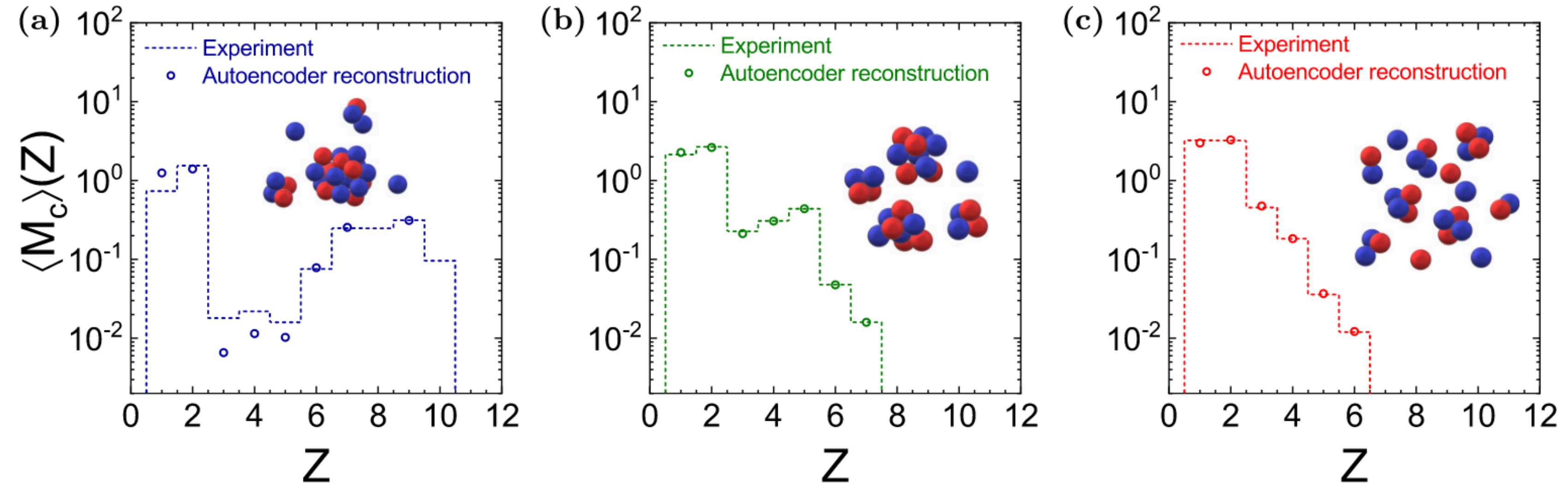
Inverse Mapping, g_θ

Representation Learning

Recognizing nuclear liquid-gas phase transition



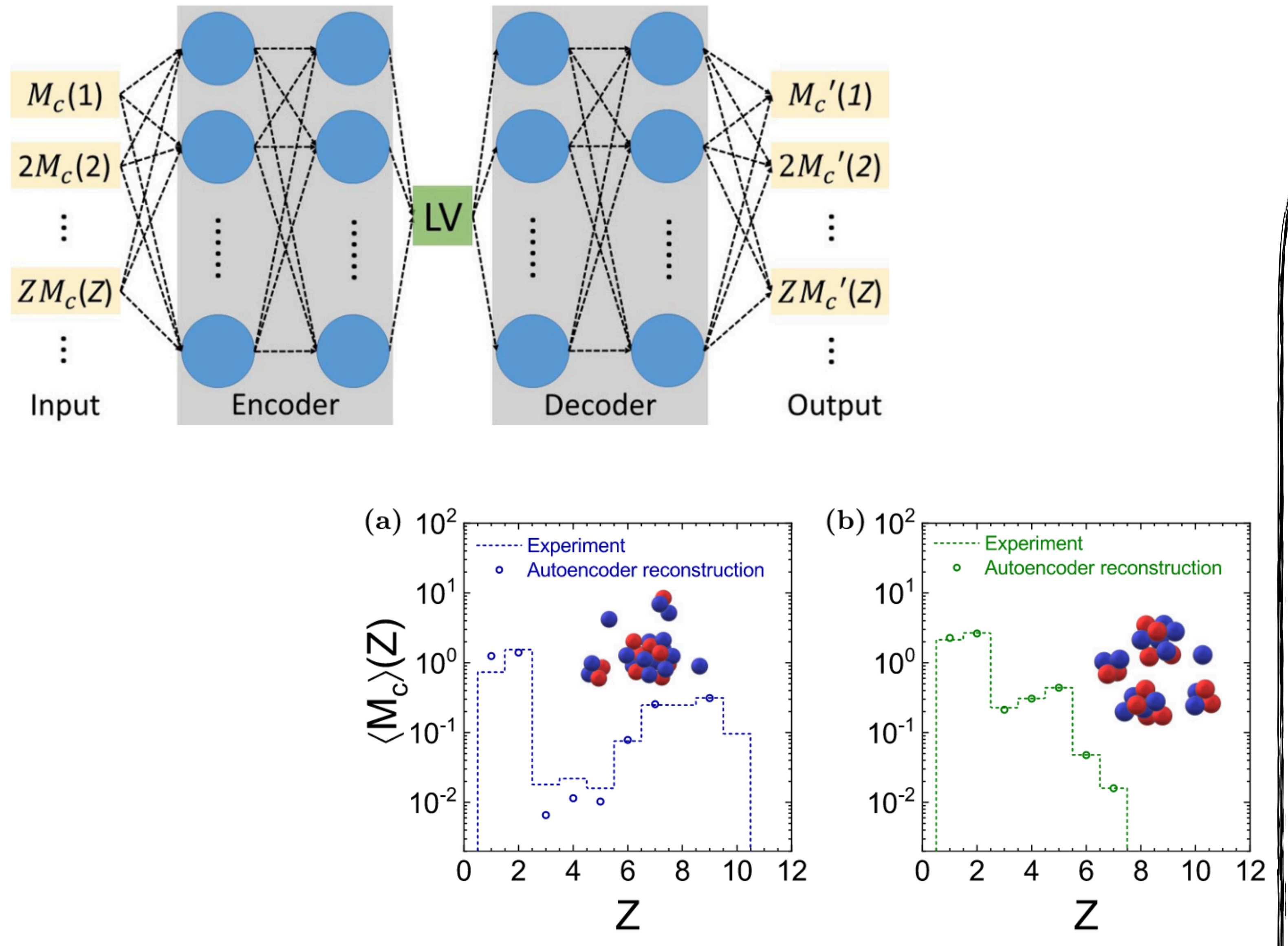
Anomaly Detection
Latent Variable Extraction



R. Wang, **Y.-G. Ma**, R. Wada, L.-W. Chen, W.-B. He, H.-L. Liu, and K.-J. Sun, Phys. Rev. Res. **2**, 043202 (2020)

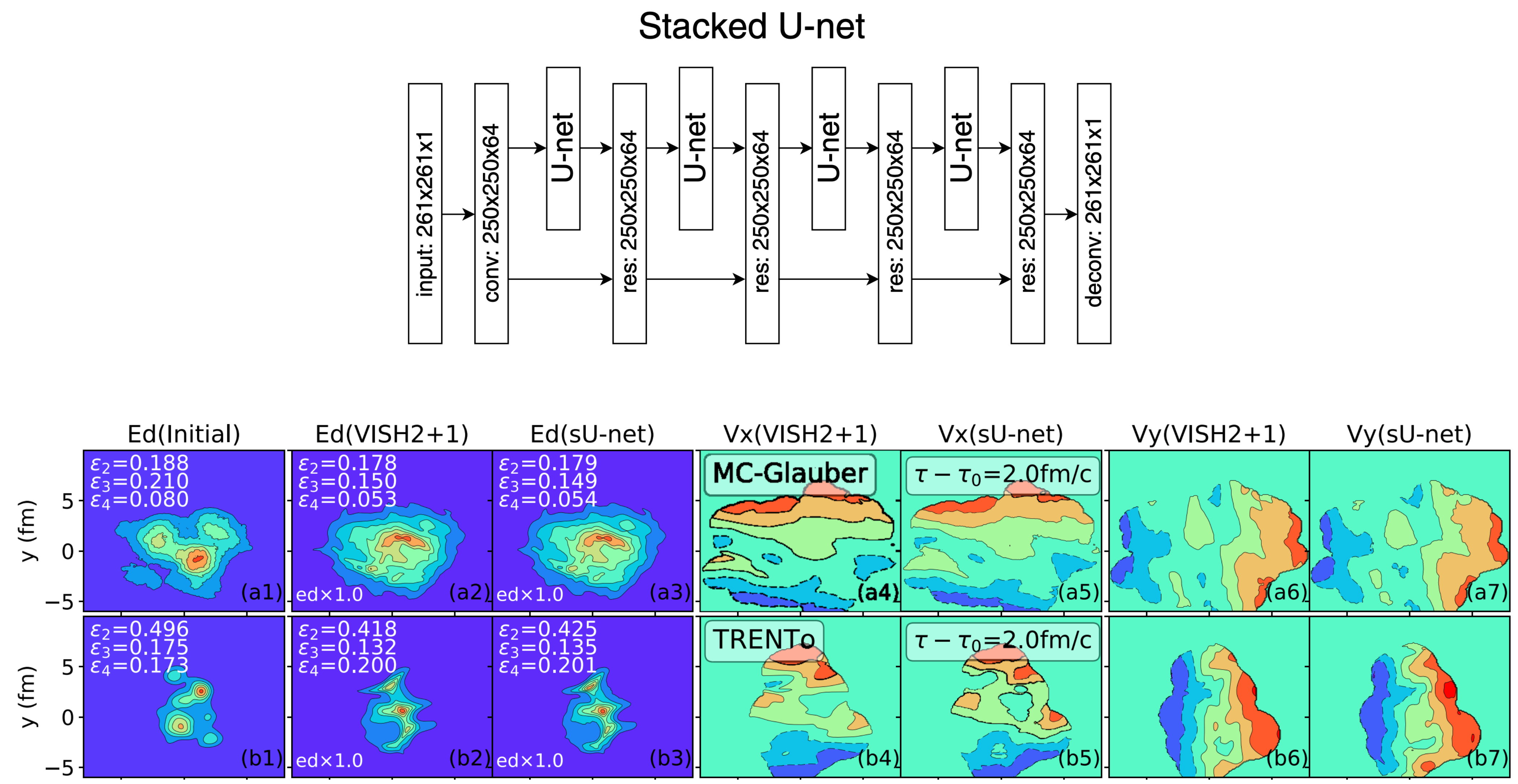
Representation Learning

Recognizing nuclear liquid-gas phase transition



R. Wang, **Y.-G. Ma**, R. Wada, L.-W. Chen, W.-B. He, H.-L. Liu, and K.-J. Sun,

Predict relativistic hydrodynamics

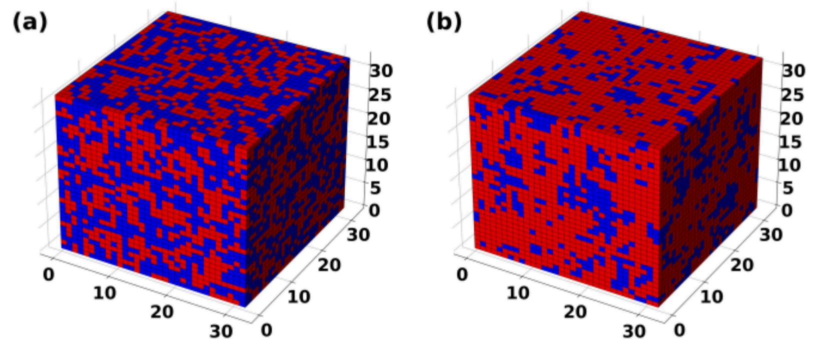


H. Huang, B. Xiao, Z. Liu, Z. Wu, Y. Mu, and **H. Song**, Phys. Rev. Res. **3**, 023256 (2021)

Rapidly Developing

12.15 Poster Session

Exploring percolation phase transition in the Ising model with machine learning	冉冉 郭



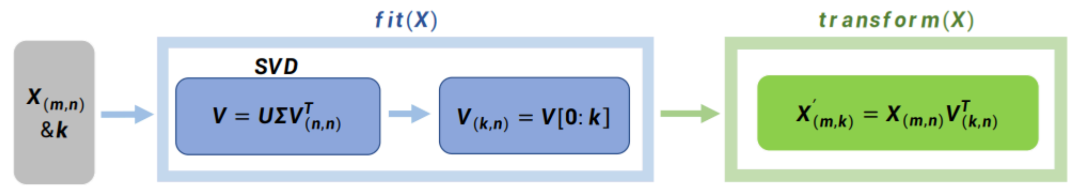
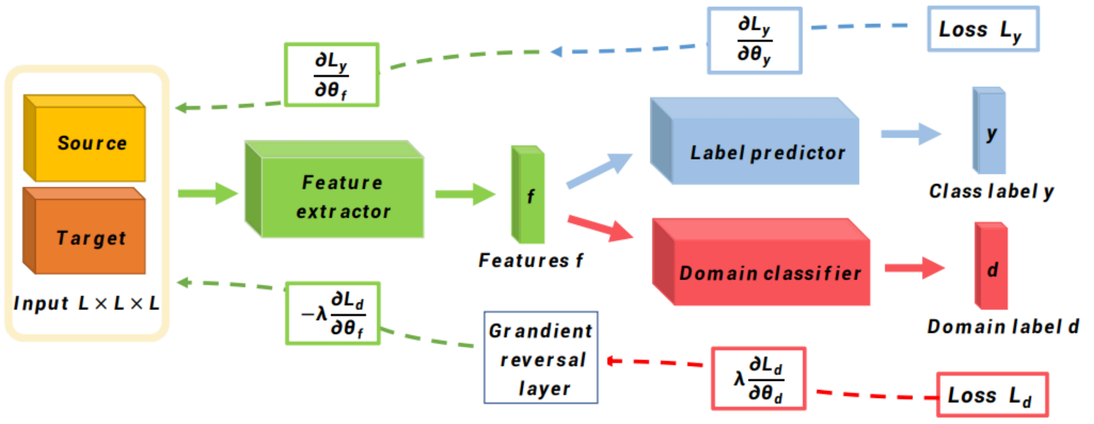
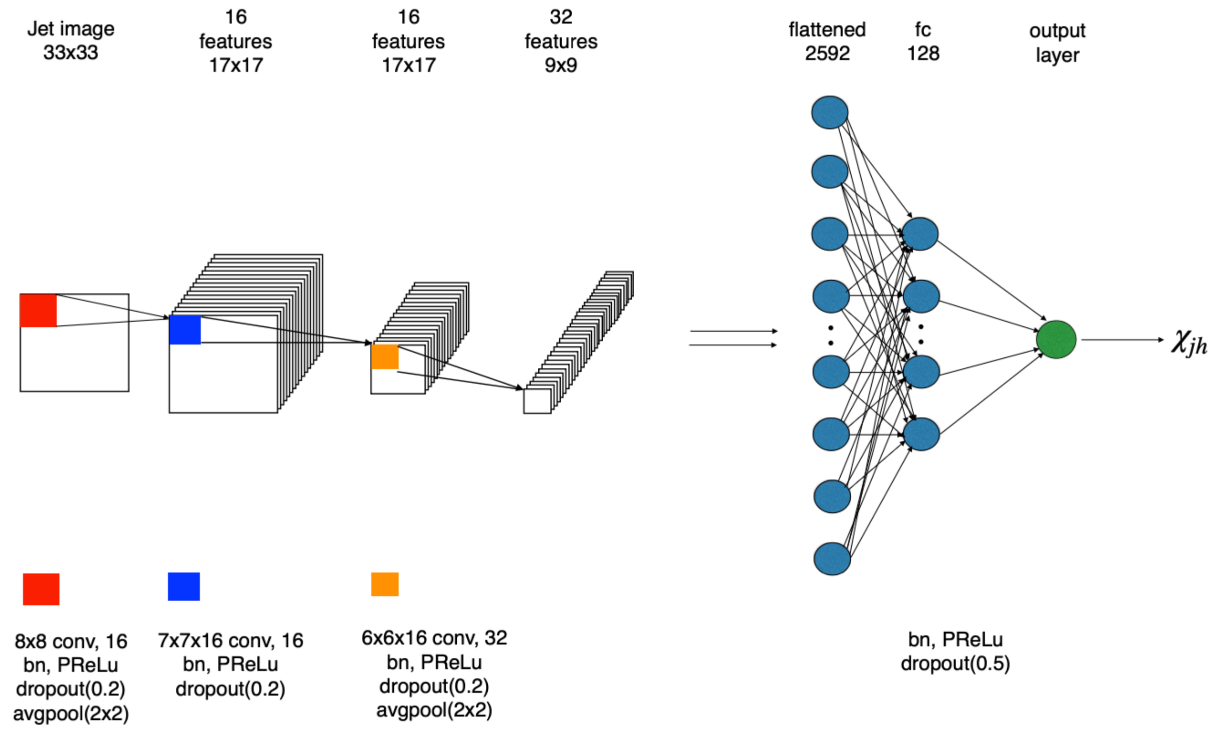


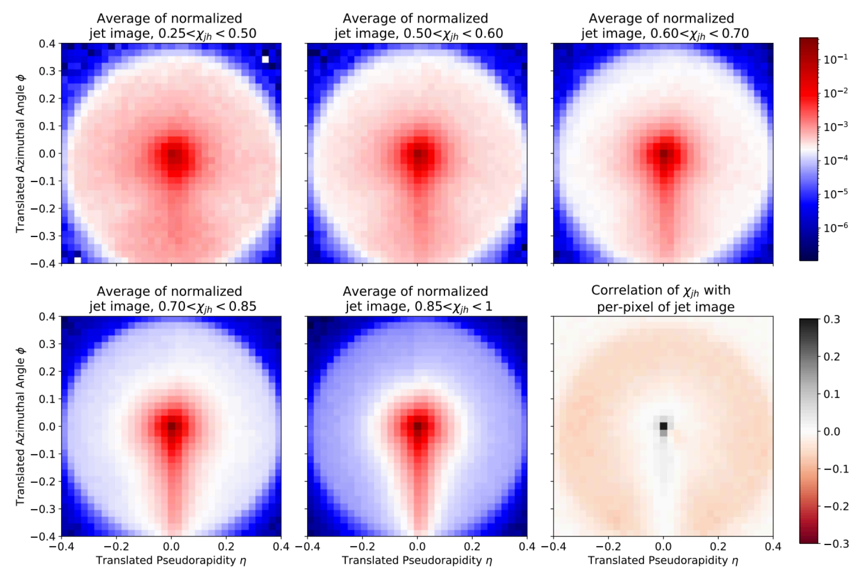
FIG. 2: (color online) The PCA architecture used in our analysis.



12.17 morning

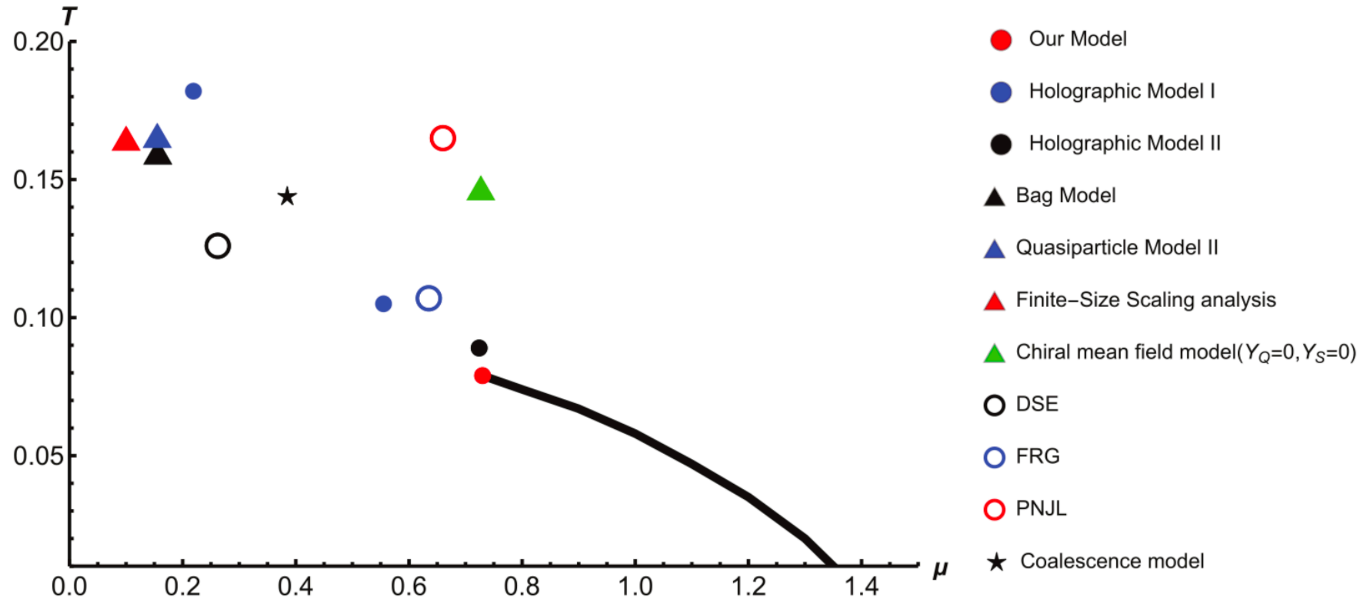
9:20-9:40	Deep learning jet modifications in heavy-ion collisions	Yilun Du





12.18 morning

9:00-9:20	Searching CEP in a holographic model with machine learning	Xun Chen



Thank You !

ML meets Physics, Opportunities and Challenges

Kouzou Sakai @Quanta Magazine