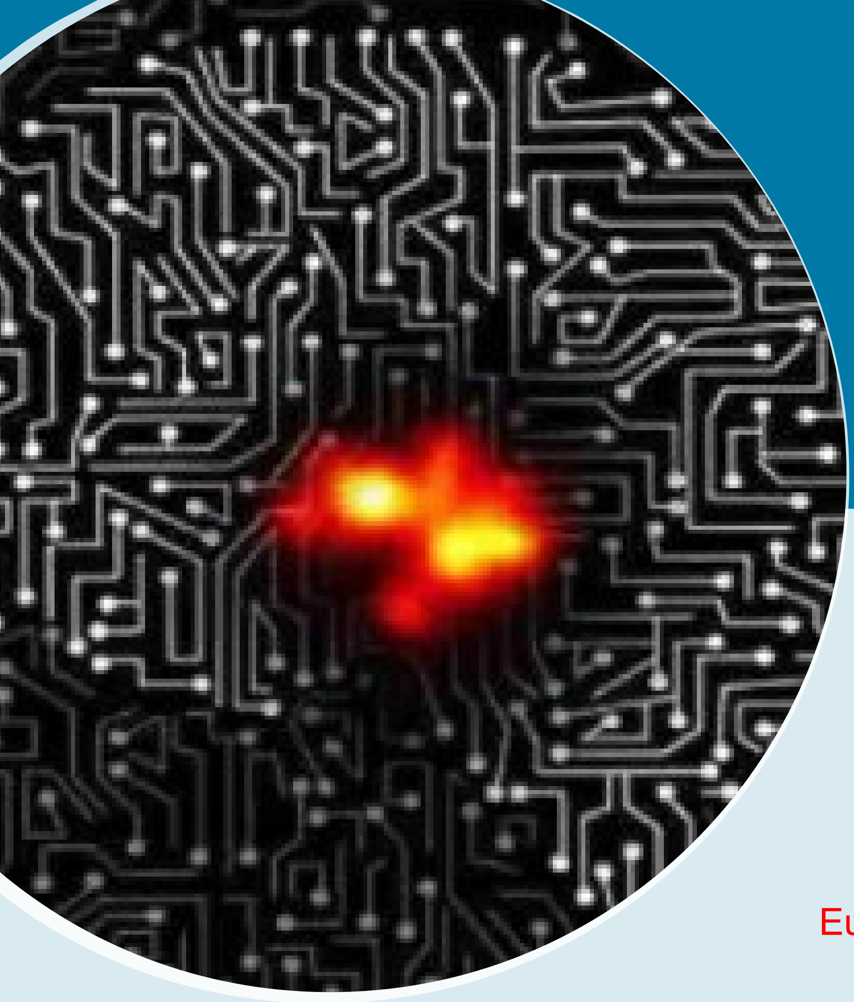


香港中文大學(深圳)
The Chinese University of Hong Kong, Shenzhen

Extreme QCD Matter Exploration meets Machine Learning

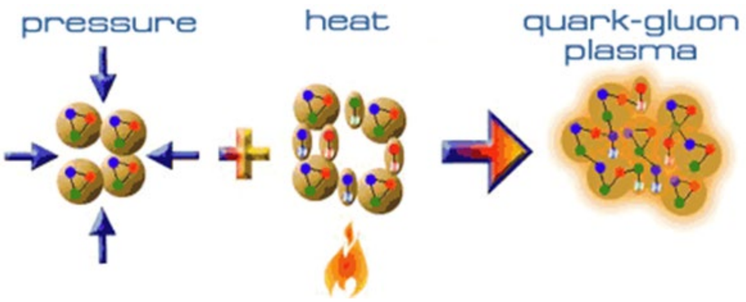
Kai Zhou (CUHK- Shenzhen)

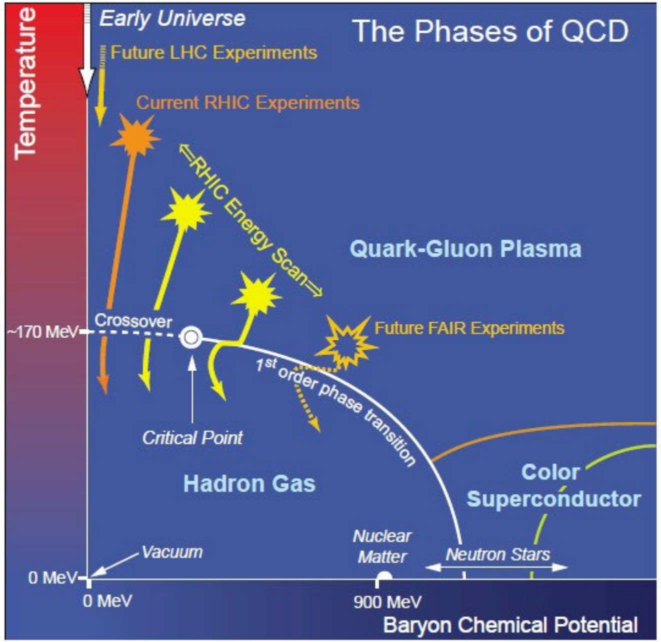
EuCAIF Conf 2025, 16-20 June, Cagliari, Italy

Overview : Golden Age of QCD matter in extreme

- **Phases** of matter : solid, liquid, gas, plasma

- Matter in extreme conditions reveals its **constituents** : <u>nuclear matter</u> → <u>quark matter</u>





<u>To study **the most elementary particle matter**</u> :

- **Nuclear Collisions** : heat & compress matter

- **Lattice Field Theory / fQCD / Effective models**

- **Neutron Star** : dense matter, astronomy constraints

Overview : Nuclear Physics meets Machine Learning

- **2012** : Discovery of Higgs boson

The New York Times

Physicists Find Elusive Particle Seen as Key to Universe

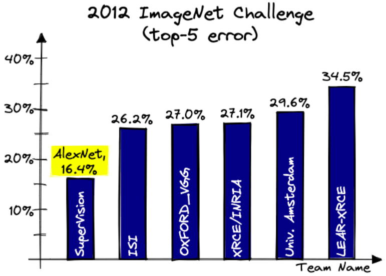
- AlexNet - Birth of Deep Learning

The New York Times

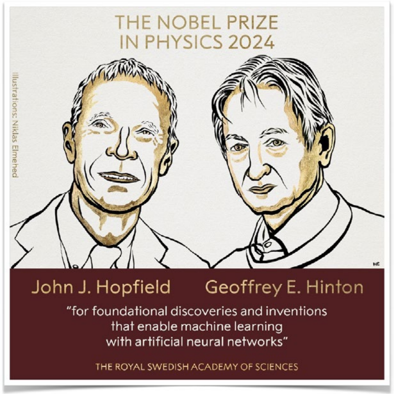
Chatbots › OpenAI Unveils GPT-4 What GPT-4 Can and Can't Do Funding Frenzy Escalates How C

Scientists See Promise in Deep-Learning Programs

Give this article

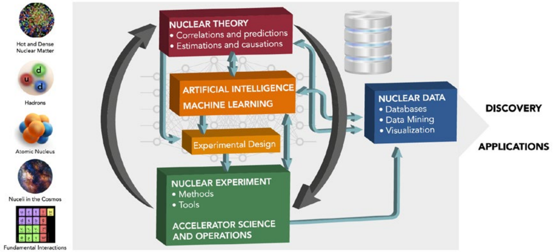


- **2024** : Nobel Prize in Physics

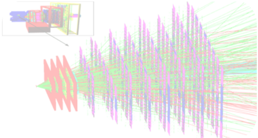


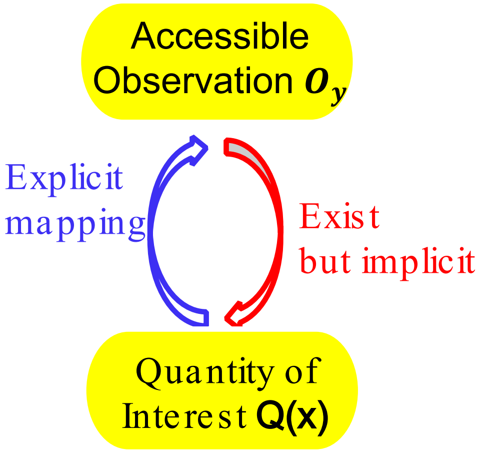
- ML4Physics, AI4Science

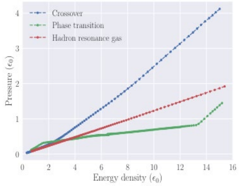
***Colloquium*: Machine learning in nuclear physics**

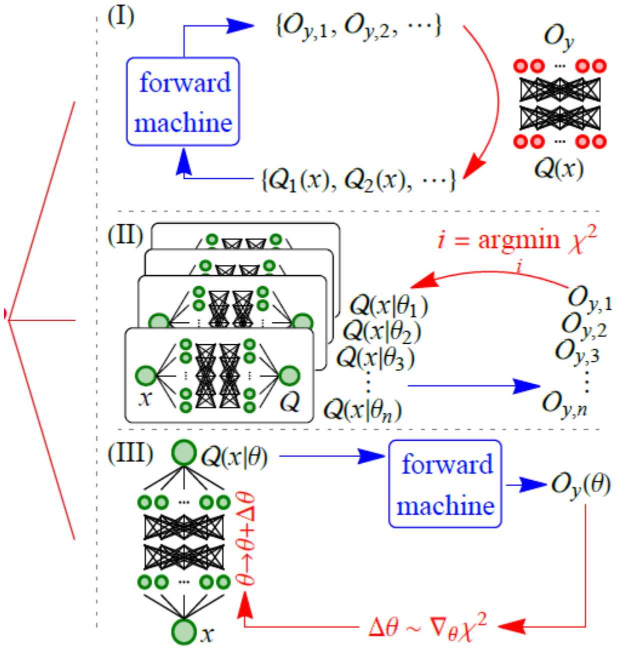


Inverse Problems Solving with ML









- **Direct inverse mapping capturing :** with Supervised Learning
- **Statistical approach to χ^2 fitting :** Bayesian Reconstruction for posterior or Heuristic (Generic) Algorithm to min.

$$\chi^2 = \sum_y \left(\frac{\mathcal{F}_y[\mathcal{Q}_{\mathrm{NN}}(x|\boldsymbol{\theta})] - \mathcal{O}_y}{\Delta \mathcal{O}_y} \right)^2$$

- **Automatic Differentiation :** fuse physical prior into reconstruction via differentiable programming strategy

$$\frac{1}{2}\nabla_{\boldsymbol{\theta}}\chi^2 = \sum_y \frac{\mathcal{F}_y[\mathcal{Q}_{\mathrm{NN}}(x|\boldsymbol{\theta})] - \mathcal{O}_y}{(\Delta \mathcal{O}_y)^2} \int \mathrm{d}x \frac{\delta \mathcal{F}_y[\mathcal{Q}(x)]}{\delta \mathcal{Q}(x)}\bigg|_{\mathcal{Q}(x)=\mathcal{Q}_{\mathrm{NN}}(x|\boldsymbol{\theta})} \nabla_{\boldsymbol{\theta}} \mathcal{Q}_{\mathrm{NN}}(x|\boldsymbol{\theta})$$

Outline: Initial state + Bulk matter + Generative model

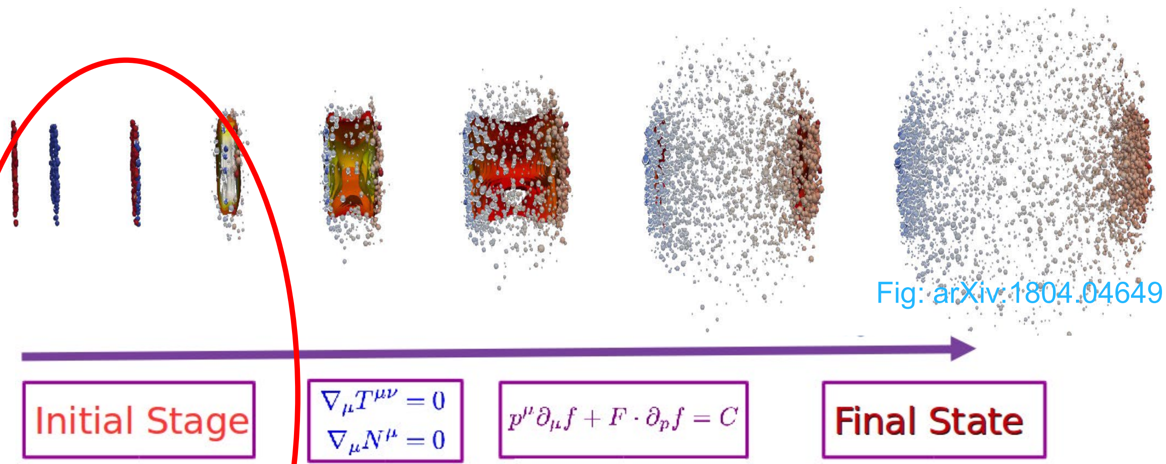


Fig: arXiv:1804.04649

Impact parameter
Nuclear structure

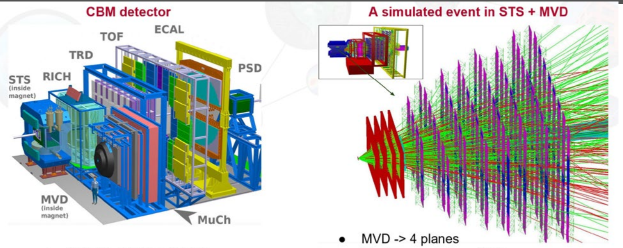
Bulk Matter properties:
Phase Transition
EOS
Shear/Bulk viscosities
Hard Probes

Event Generation
Final observables

Applications to Lattice QFT

End-to-End online impact parameter/centrality regression for CBM

- **sensor data has inherent point cloud structure**
  - Point clouds: collection of points in space
- **PointNet** based models learn directly from point clouds.
  - respects the **order invariance** of point clouds
  - Ideal real-time online analysis for HIC

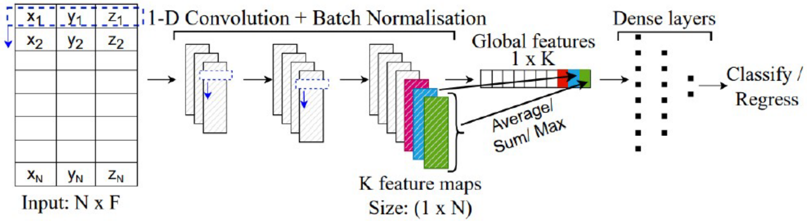


- Upto 45 AGeV collisions
- 10^7 collisions/ Second
- 1000 tracks per collision
- 1 TBytes/Second raw data

- MVD -> 4 planes
  Position resolution: 3.5-6 μm
  Secondary vertex resolution: 50 μm
- STS-> 8 planes
  Momentum resolution: 1 %

M. OK, J. S, K. Z, H. S,
PLB 811,135872 (2020)

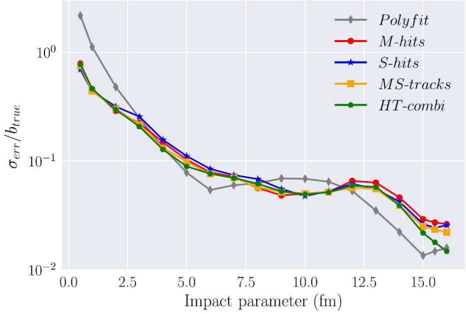
PointCloud Network
(on UrQMD + CBMRoot event)
End-to-end b estimation



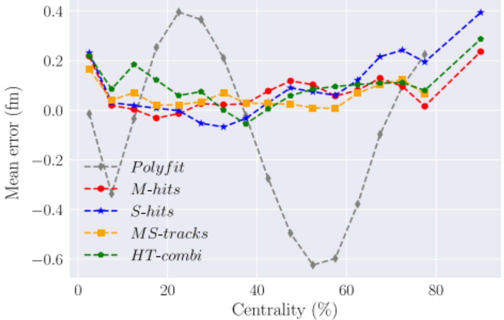
- With Hits/Tracks online b-meter: PointNet

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

- Quantifies **precision**
- Polyfit fails for central events!
- Similar precision for b>3 fm

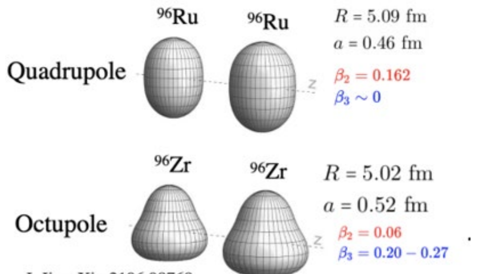


- Quantifies **accuracy**
- DL: -0.3 - 0.2 fm for b = 2-14fm
- Polyfit fluctuating



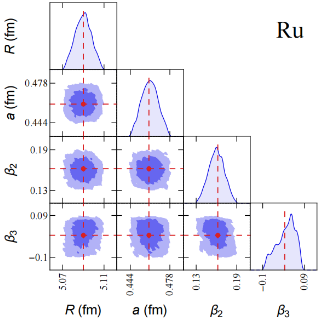
Bayesian Imaging for Nuclear Structure in Isobar Collisions

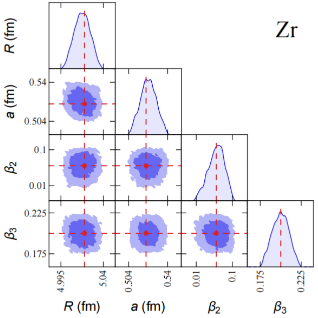
- Nuclear Structure imaging for single system ? (caveat: model dependent)
- Simultaneous inference for isobar systems with ratio?
- **Bayesian Inference:** Gaussian Process emulator + PCA dim reduction + MCMC
  Data: MC-Glauber + Matching (linear response approximation)



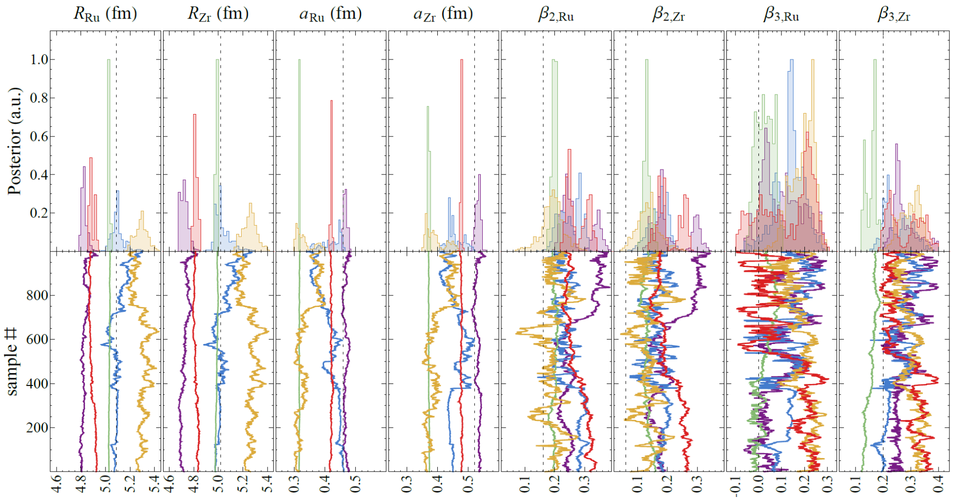
J. Jia, aXiv:2106.08768

$$\boldsymbol{y}_{\mathrm{Ru}} \equiv \{P_a^{\mathrm{Ru}}, \varepsilon_{2,a}^{\mathrm{Ru}}, \varepsilon_{3,a}^{\mathrm{Ru}}, d_{\perp,a}^{\mathrm{Ru}}\}_{a=1,\cdots,40}$$





Single system works good



With purely the Isobar-Ratios:

MCMC can not converge to a stationary inference ofthe nuclear structure

$$\boldsymbol{y}_{\mathrm{r},1} \equiv \{R_{P,a}, R_{\varepsilon_2,a}, R_{\varepsilon_3,a}, R_{d_\perp,a}\}_{a=1,\cdots,40}$$

- No unique solution : only ratios $\nRightarrow$ *nuclear structure !*

Y.Cheng, S.Shi, Y. Ma, H. S., K. Zhou,
Phys. Rev. C 107 (2023) 064909

Bayesian Imaging for Nuclear Structure in Isobar Collisions

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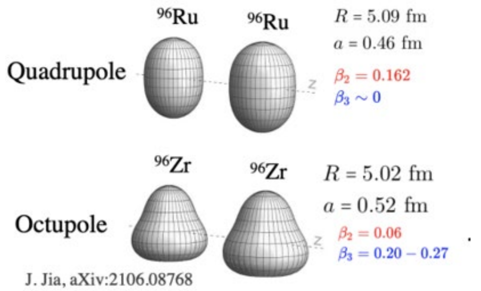
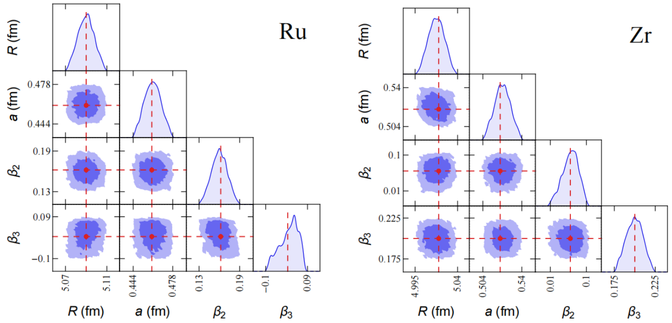
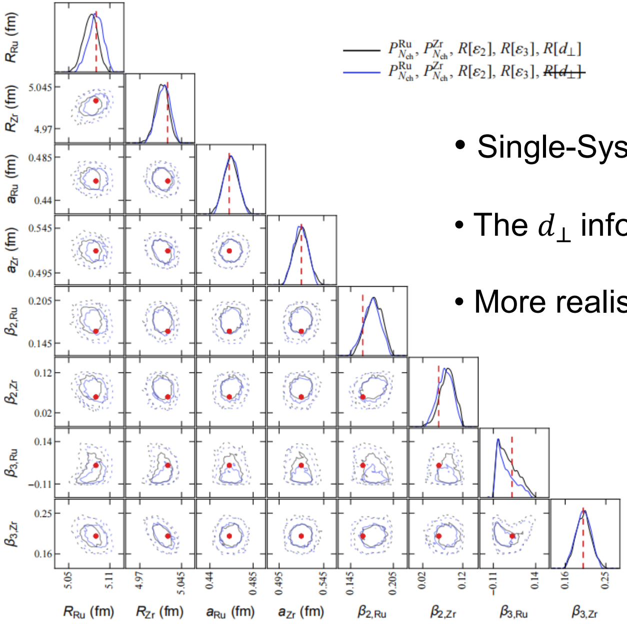


$$\boldsymbol{y}_{\mathrm{Ru}} \equiv \{P_a^{\mathrm{Ru}}, \varepsilon_{2,a}^{\mathrm{Ru}}, \varepsilon_{3,a}^{\mathrm{Ru}}, d_{\perp,a}^{\mathrm{Ru}}\}_{a=1,\cdots,40}$$



Single system works good



- Single-System Multiplicity makes it possible
- The $d_\perp$ information is redundant
- More realistic analysis with AMPT in progress

$$\boldsymbol{y}_{\mathrm{r},2} \equiv \{P_a^{\mathrm{Ru}}, P_a^{\mathrm{Zr}}, R_{\varepsilon_2,a}, R_{\varepsilon_3,a}, R_{d_\perp,a}\}_{a=1,\cdots,40}$$

Y.Cheng, S.Shi, Y. Ma, H. S., K. Zhou,
Phys. Rev. C 107 (2023) 064909

Outline: Initial state + Bulk matter + Generative model

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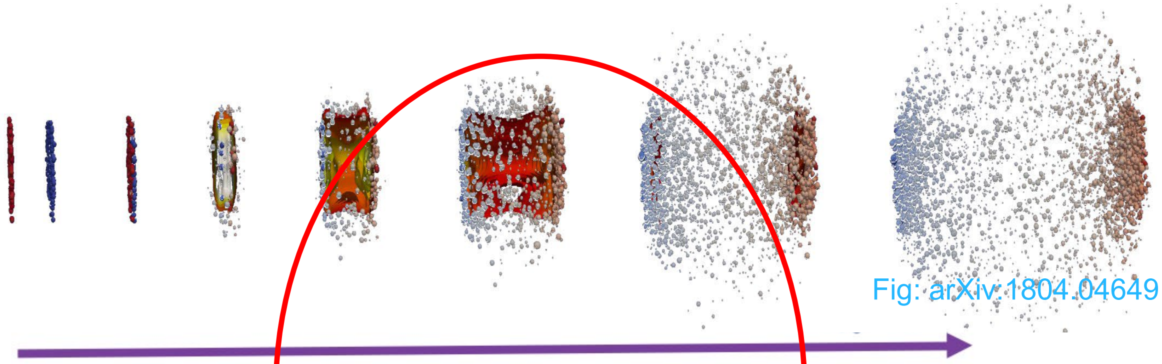


Fig: arXiv:1804.04649

Initial Stage

$$\nabla_\mu T^{\mu\nu} = 0$$
$$\nabla_\mu N^\mu = 0$$

$$p^\mu \partial_\mu f + F \cdot \partial_p f = C$$

Final State

Impact parameter
Nuclear structure

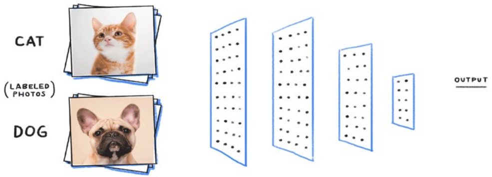
<u>Bulk Matter properties</u>:
Phase Transition
EOS

Event Generation
Final observables

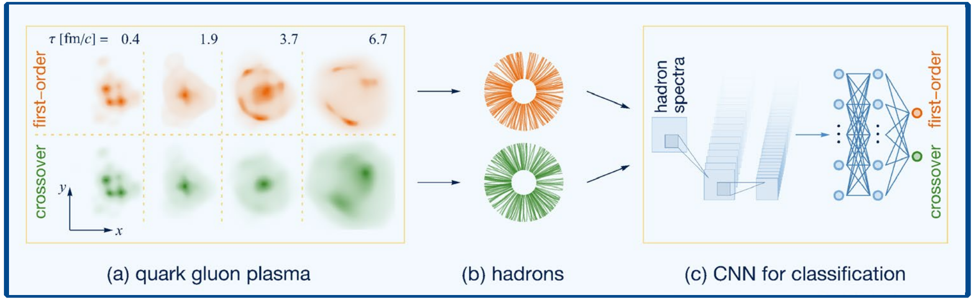
Applications to Lattice QFT

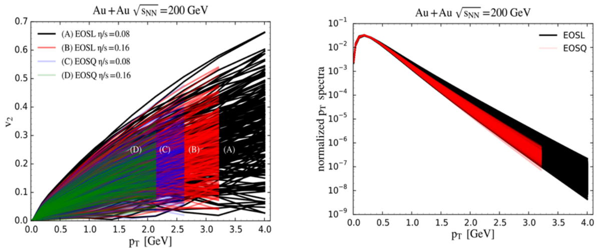
Direct inverse mapping with Data driven supervised learning

Data-driven
Inverse Mapping

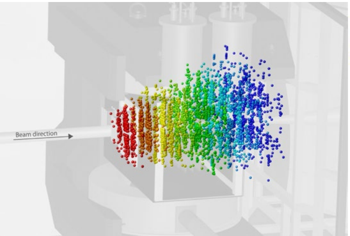


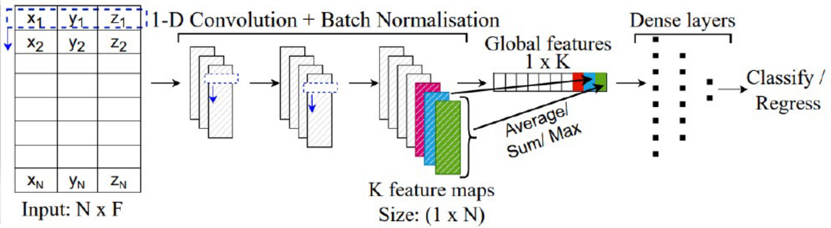
Physics Simulation
provide the Prior





Conclusion : Information of early dynamics can **survive** to the end of hydrodynamics and encoded within the final state raw spectra, immune to other uncertainties, **with deep CNN we can decode it back**. L. Pang, K. Zhou, N. Su, H. Stoecker, H. Petersen, X. Wang, **Nature Commu.**9 (2018), no.1, 210

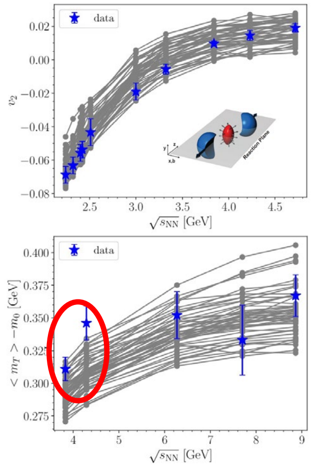


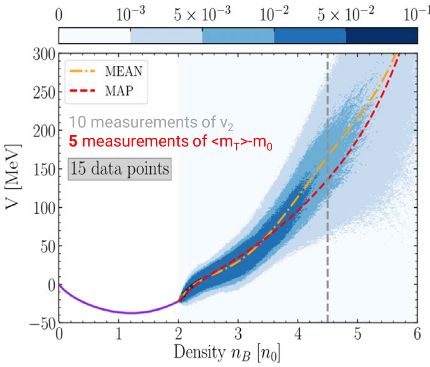


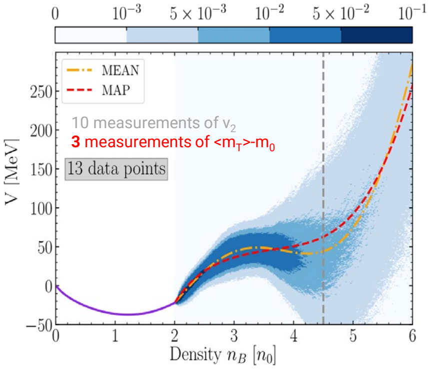
- **Collision Centrality Regression**
  M. OK, J. S, K. Zhou, H. S, **Phys.Lett.B** 811 (2020) 135872
- **EoS Classification**
  M. OK, K. Zhou, J. S, H. S, **JHEP** 10(2021) 184
- **Small/ Large-system Identification**
  S.Guo, H. Wang, K. Zhou, G. Ma, **Phy.Rev.C 110 (2024)2**

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

Bayesian Inference Dense Matter EoS from HIC and Holography





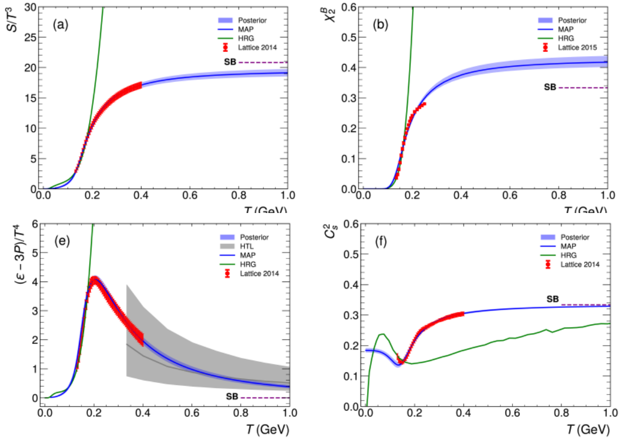


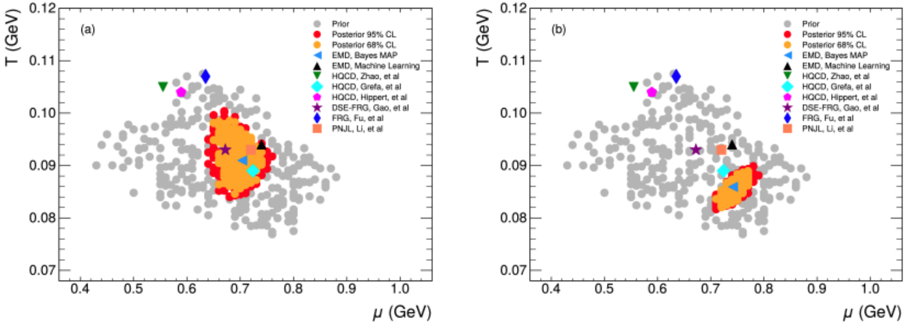
- Comprehensive Bayesian inference necessary for unambiguous solution
- Tension between data-data or model (**UrQMD**)-data
- Next-gen experiments will provide immense amount of high precision data

M.OK, J. Steinheimer, K. Zhou, H. Stoecker, **PRL131,202303(2023)**

$$S_E = \frac{1}{16\pi G_5}\int d^5x\sqrt{-g}\left[R - \frac{f(\phi)}{4}F^2 - \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)\right]$$

$$A(z) = d\ln\left(az^2+1\right) + d\ln\left(bz^4+1\right),\ f(z) = e^{cz^2 - A(z)+k}$$





- Critical endpoint from **holography (EMD)** via Bayesian Inference

L. Zhu, X. Chen, K. Zhou, H. Zhang, M, Huang, **arXiv:2501.15810**

From NS Stellar Structure (MR) to Interior EoS - AutoDiff

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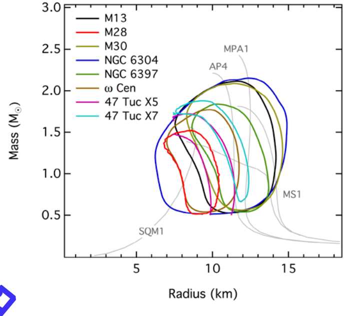
The Chinese University of Hong Kong, Shenzhen

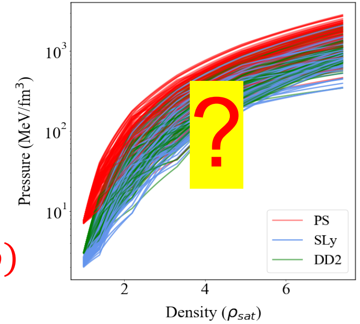
Noisy/Limited NS Observables to EoS ?



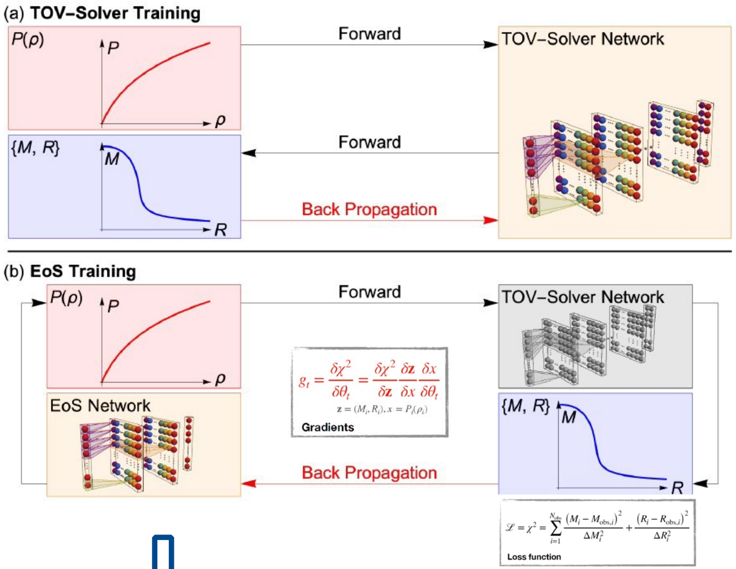
TOV eqs

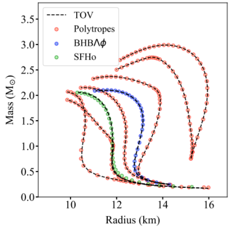
$$\frac{dP}{dr} = -\frac{G}{r^2}\left(\rho + \frac{P}{c^2}\right)\left(m + 4\pi r^3 \frac{P}{c^2}\right)\left(1 - \frac{2Gm}{c^2 r}\right)^{-1}$$

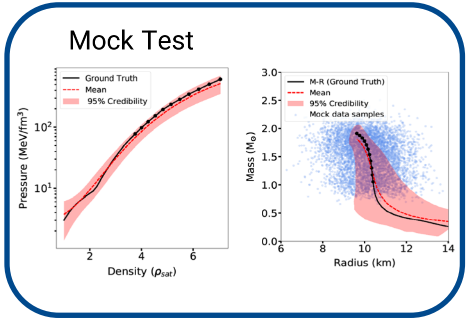
$$M = m(R) = \int_0^R 4\pi r^2 \rho \, dr$$

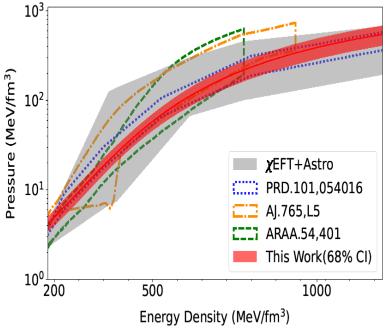


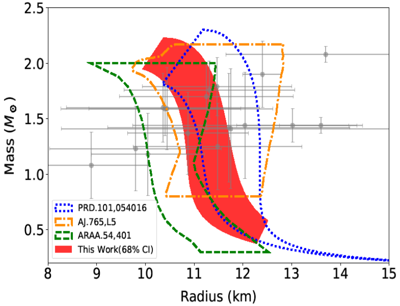
$P(\rho)$





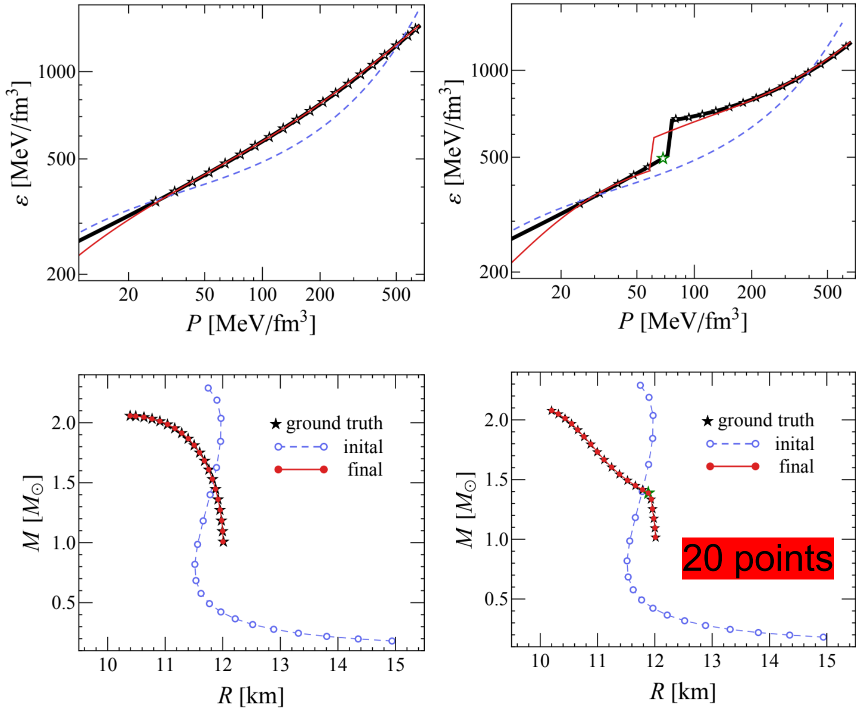






S. S, L. W, S. S, H. S, K. Z, **JCAP** 98(2022)071;**PRD**107(2023)083028

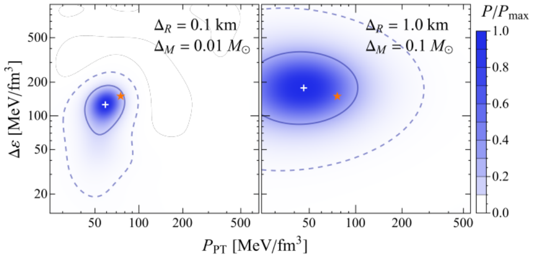
Extend to First-order phase transition reconstruction with AutoDiff

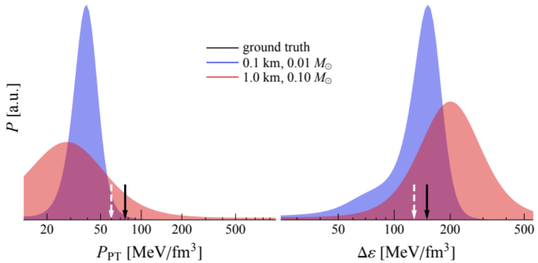


Linear response analysis get the gradients! Then use DNN :

We parameterize the inverse speed of sound squared containing both regular parts and Dirac-δ functions corresponding to possible first-order phase transitions,

We adopt SFHo as the baseline EoS and introduce a PT with latent heat $\Delta\varepsilon = 150\ \mathrm{MeV/fm^3}$ at pressure $P_{\mathrm{PT}} = 76\ \mathrm{MeV/fm^3}$. Above the PT point, we take the stiffest (causal) limit that $c_s = 1$. We employ twenty





R. Li, S. Han, Z. Lin, L. Wang, K. Zhou, S. Shi, **PRD** (2025), **arXiv:2501.15819**

Discriminative / Generative model

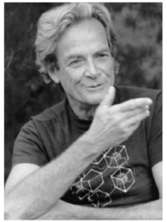
- Discriminative Learning : **prediction**

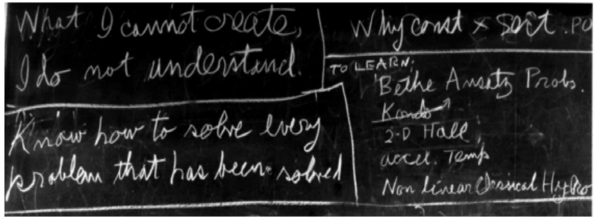
  function fitting $y = f(x)$

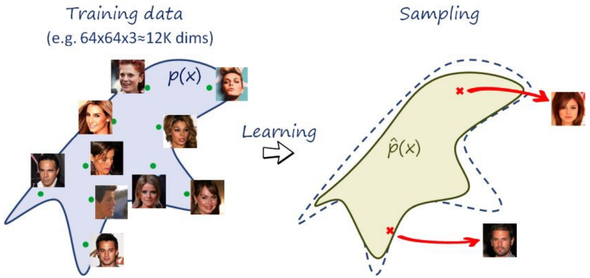
  conditional probability $p_\theta(y|x) \rightarrow p(y|x)$

- Generative Modelling : **understand**

  Joint probability distribution $p_\theta(x,y) \rightarrow p(x,y)$







“What I can not create, I do not understand”

Outline: Initial state + Bulk matter + Generative model

Fig: arXiv:1804.04649

Initial Stage

$\nabla_\mu T^{\mu\nu} = 0$

$\nabla_\mu N^\mu = 0$

$p^\mu \partial_\mu f + F \cdot \partial_p f = C$

Final State

Impact parameter
Nuclear structure

Bulk Matter properties:
Phase Transition
EOS
Shear/Bulk viscosities
Hard Probes

Event Generation
Final observables

Applications to Lattice QFT

Variational Free Energy Learning with autoregressive generative model

- Variational free energy minimization - Reverse KL divergence

$$D_{\mathrm{KL}}(q_\theta \,\|\, p) = \sum_{\mathbf{s}} q_\theta(\mathbf{s}) \ln\left(\frac{q_\theta(\mathbf{s})}{p(\mathbf{s})}\right) = \beta(F_q - F) \qquad F_q = \frac{1}{\beta}\sum_{\mathbf{s}} q_\theta(\mathbf{s})\left[\beta E(\mathbf{s}) + \ln q_\theta(\mathbf{s})\right]$$

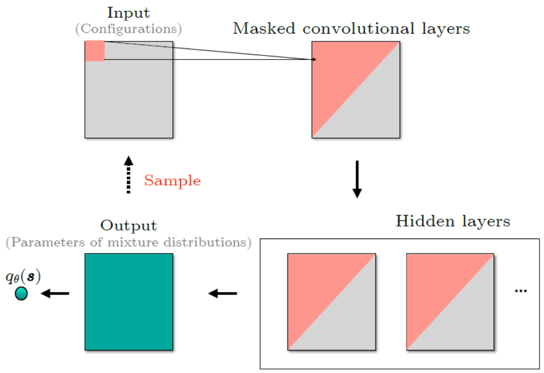
$$p(\mathbf{s}) = \frac{e^{-\beta E(\mathbf{s})}}{Z}$$

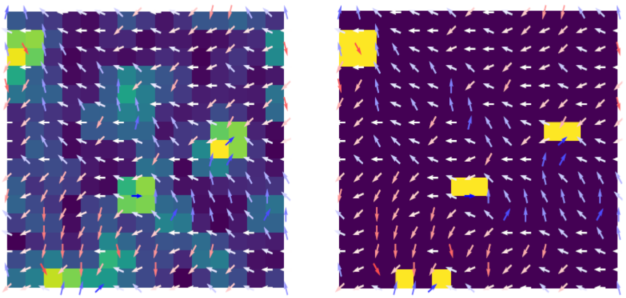
- **Autoregressive** $q_\theta(\mathbf{s}) = \prod_{i=1}^{N} q_\theta(s_i \mid s_1, \ldots, s_{i-1})$

D. Wu, Lei Wang and P. Zhang, **PRL**122,080602(2019)

- **Continuous** Autoregressive Net for XY model

L. Wang, Y. Jiang, L. He, K. Zhou, **CPL** 39, 120502 (2022)





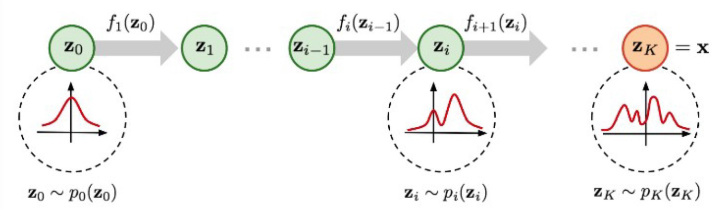
Probability distributions from CANs

Vortices

Flow based generative model to QFT

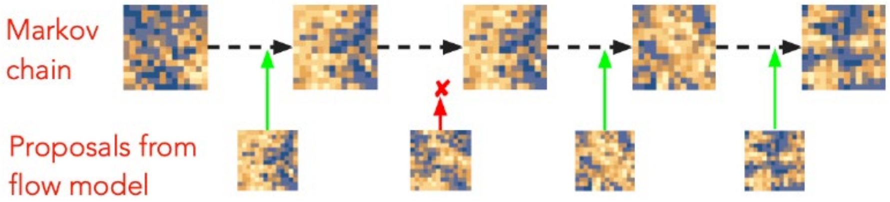
A series **(Flow)** of invertible/bijective transformations for p(z)

compose several invertible transformations to form the flow :



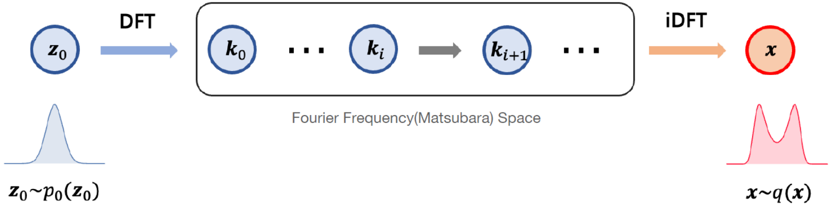
$$p_i(\mathbf{z}_i) = p_{i-1}(f_i^{-1}(\mathbf{z}_i))|\det J_{f_i^{-1}}| = p_{i-1}(\mathbf{z}_{i-1})|\det J_{f_i}|^{-1}$$

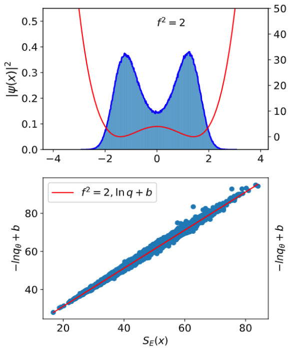
$$\rightarrow \log p(\mathbf{x}) = \log p_0(f^{-1}(\mathbf{x})) + \sum_{i=1}^{K} \log|\det J_{f_i^{-1}}| = \log p_0(\mathbf{z}_0) - \sum_{i=1}^{K} \log|\det J_{f_i}|$$

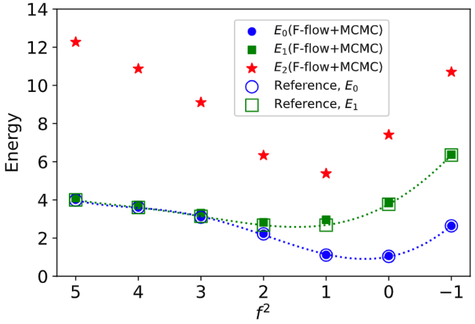


Albergo +, 1904.12072; Boyda +, 2008.05456; Favoni +, 2012.12901; Abbott +, 2208.03832; Abbott +, 2211.07541; Abbott +, 2305.02402; Bulgarelli+ 2412.00200 (SU(3)); Abbott +, arXiv:2502.00263
K.C, G. K., S. R., D. R., P. S., **Nature Reviews Physics** 5, 526-535 (2023)

Fourier Flow Model

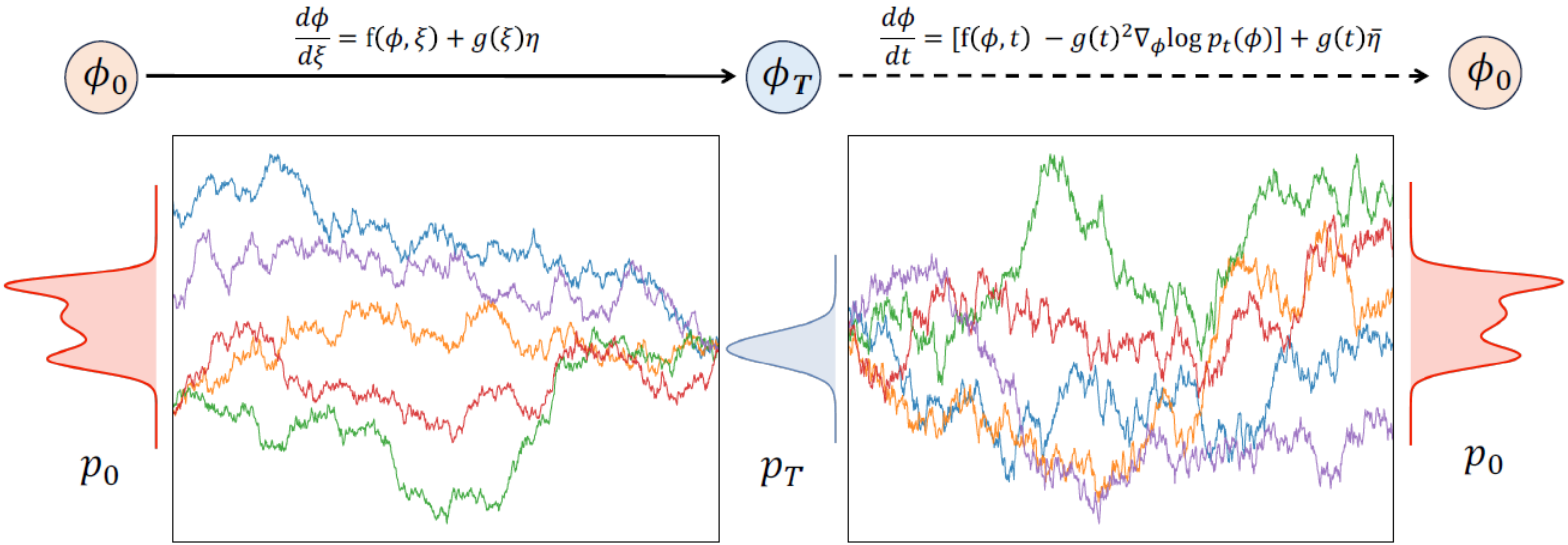






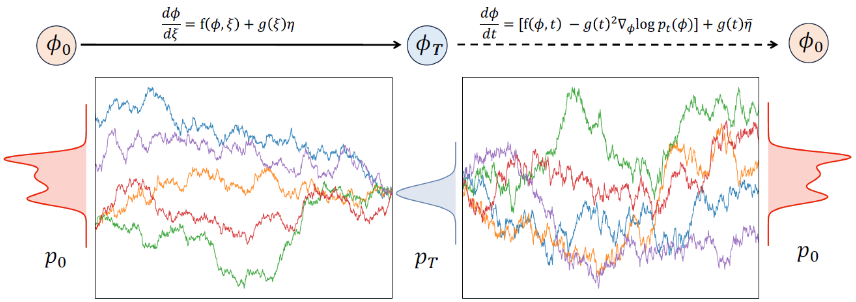
S.Chen, O. Savchuk, S. Zheng, B. Chen, H. Stoecker, L. Wang, **K. Zhou**, **PRD107, 056001(2023)**

Diffusion Model on lattice QFT configurations



L. Wang, G. Arts, K. Zhou, **JHEP** 05 (2024) 060
L. Wang, G. Arts, K. Zhou, arXiv:2311.03578 (NeurIPS 2023 workshop “ML&Physical Sciences”)
G. A, D. E. H, L. W, K. Z, arXiv:2410:21212 (NeurIPS 2024 workshop “ML&Physical Sciences)
Q. Zhu, G. Aarts, W. Wang, K. Zhou, L. Wang, arXiv:2410.19602 (NeurIPS 2024 workshop “ML&Physical Sciences)

Diffusion Model for generating field configurations



- Forward diffusion SDE

$$\frac{d\phi}{d\xi} = f(\phi,\xi) + g(\xi)\eta(\xi) \quad \langle \eta(\xi)\eta(\xi')\rangle = 2\alpha\delta(\xi-\xi')$$

- Backward diffusion SDE

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

- Score matching Training

$$\mathcal{L}_\theta = \sum_{i=1}^{N} \sigma_i^2 \mathbb{E}_{p_0(\phi_0)} \mathbb{E}_{p_i(\phi_i|\phi_0)} \left[\| s_\theta(\phi_i,\xi) - \nabla_{\phi_i} \log p_i(\phi_i|\phi_0) \|_2^2 \right] \qquad p_\xi(\phi_\xi|\phi_0) = \mathcal{N}\left(\phi_\xi; \phi_0, \frac{1}{2\log\sigma}(\sigma^{2\xi}-1)\mathbf{I}\right)$$

- **Sample generation SDE**

$$\frac{d\phi}{d\tau} = g_\tau^2 \nabla_\phi \log q_\tau(\phi) + g_\tau \bar{\eta}(\tau) \xleftarrow{\tau \,\equiv\, T - t} \frac{d\phi}{dt} = \left[f(\phi,t) - g^2(t) s_{\hat{\theta}}(\phi,t)\right] + g(t)\bar{\eta}(t).$$

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

$$\nabla_\phi S_{\mathrm{DM}} \equiv -\nabla_\phi \log q_\tau(\phi) \qquad p_{\mathrm{eq}}(\phi) \propto e^{-S_{\mathrm{DM}}/\bar{\alpha}}$$

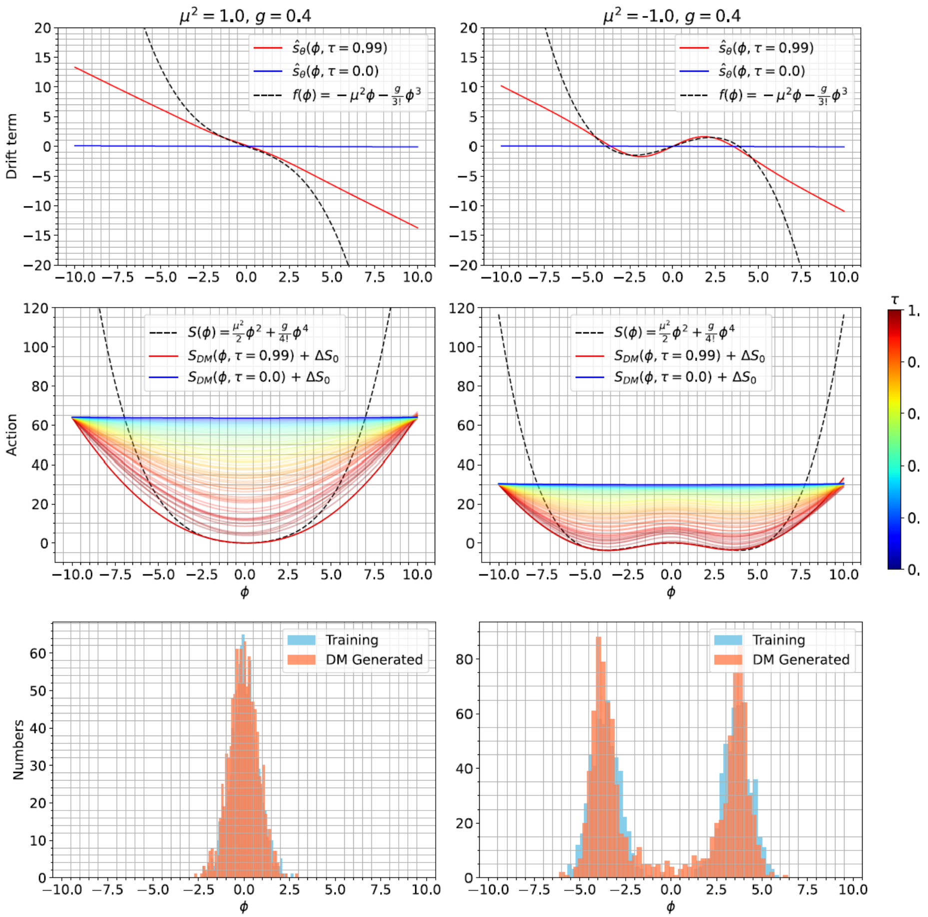
$$\boxed{\begin{gathered} p_{\tau=T}(\phi) \to P[\phi,T] \\ O(\bar{\alpha}) \sim O(\hbar) \end{gathered}}$$

- A flow of **effective action** will be learned in DMs

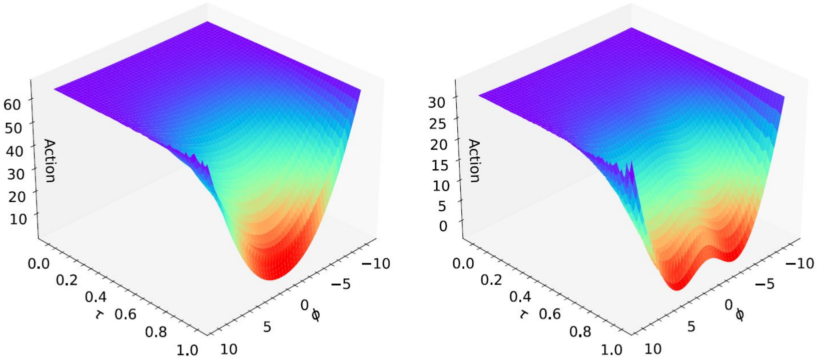
sampling from a DM is equivalent to optimizing a stochastic trajectory to approach the "equilibrium state"

L. Wang, G. Arts, K. Zhou, **JHEP** 05(2024) 060

Effective Action on toy model



- Flow of an effective action

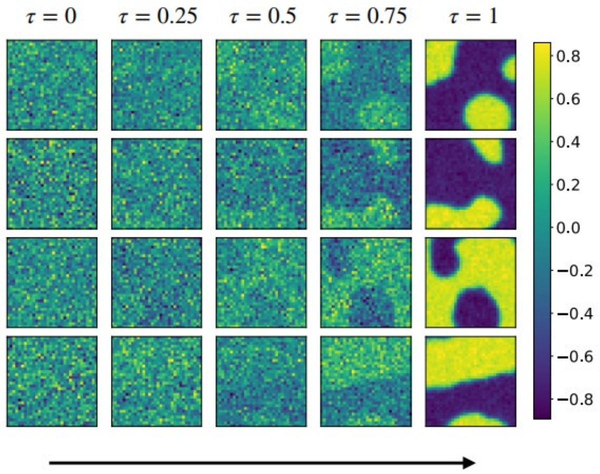


DM on 2d scalar ϕ^4 model

- 32x32 lattice, HMC generated 5120 configurations for training

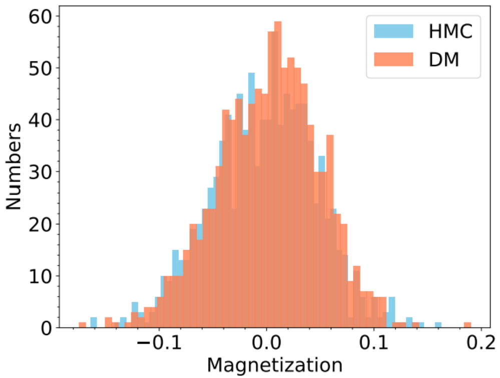
$$S_E = \sum_x [-2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4].$$

Broken phase :



"bulk" patterns emerge from DM

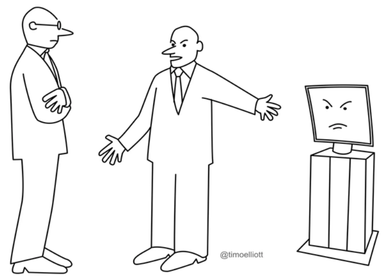
symmetric phase :



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

Further progresses on gauge fields and with more efficient generation recently

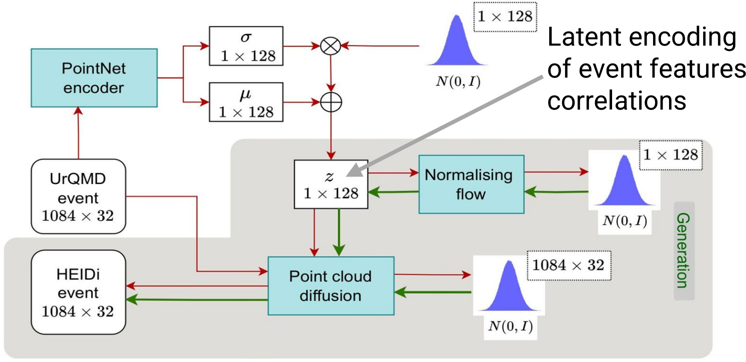
Point Cloud Diffusion Model for HICs – AI clone of simulation

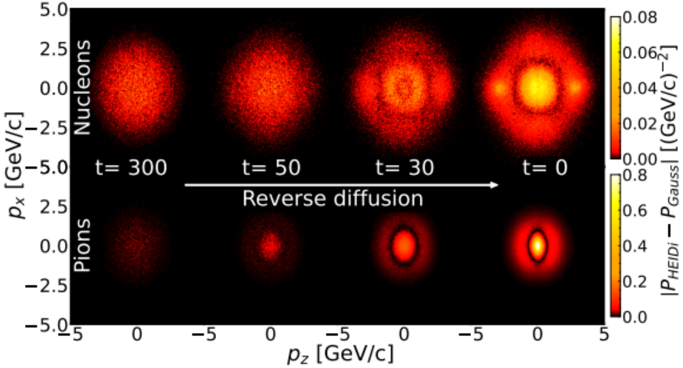


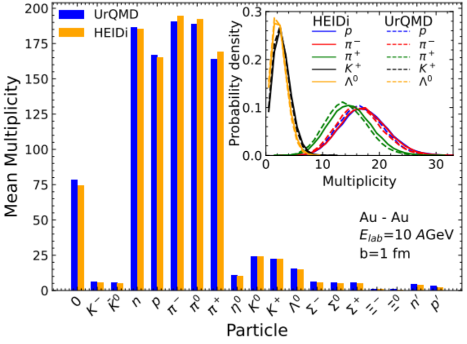
His decisions aren't any better than yours — but they're WAY faster...

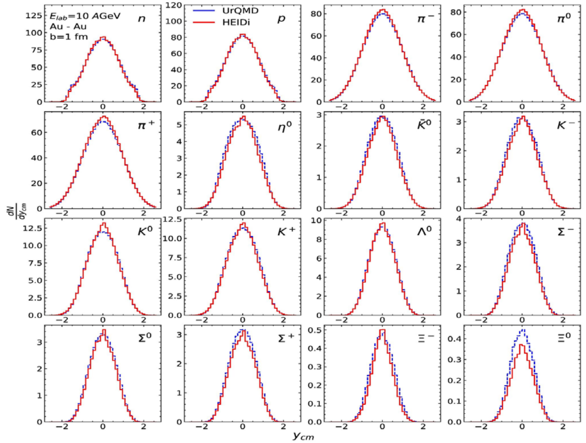
- 18k UrQMD simulation events for central Au-Au@10 AGeV collisions
- HEIDi:
  Heavy-ion Events through Intelligent Diffusion

PointNet encoder + Normalizing flow decoder + Pointcloud diffusion →









M. O.K, K. Z, J. S, H. S, arXiv:**2502.16330**, arXiv:**2412.10352**

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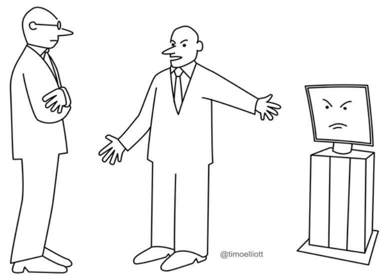

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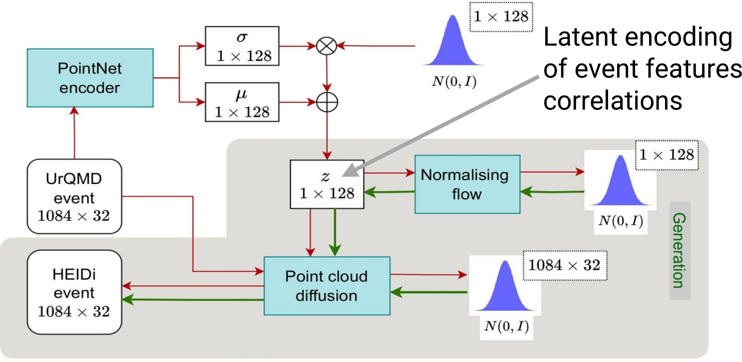

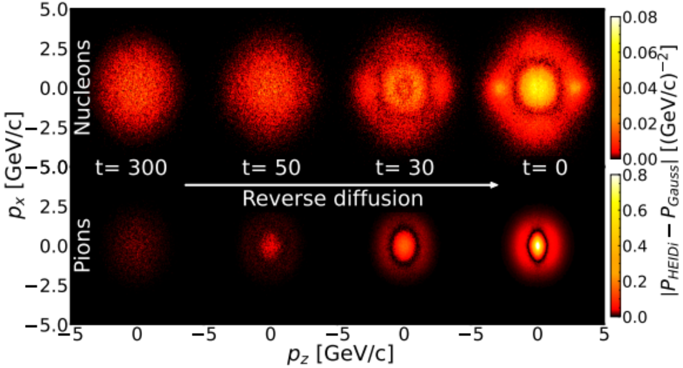

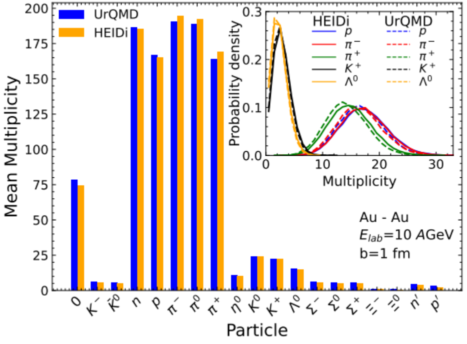

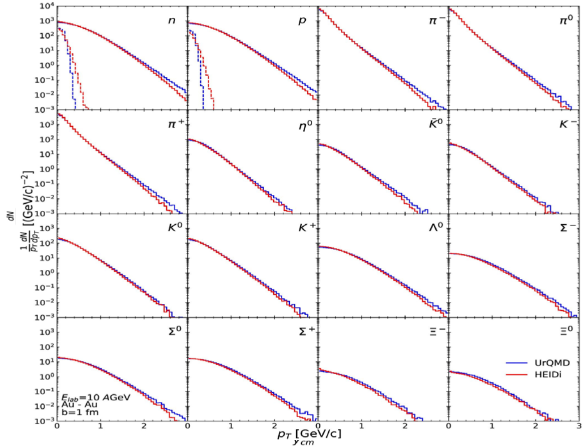

M. O.K, K. Z, J. S, H. S, arXiv:**2502.16330**, arXiv:**2412.10352**

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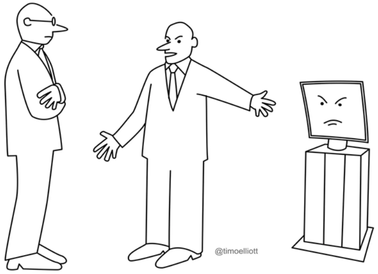

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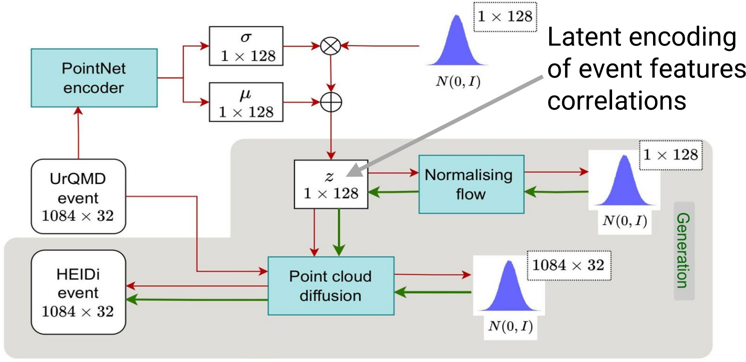

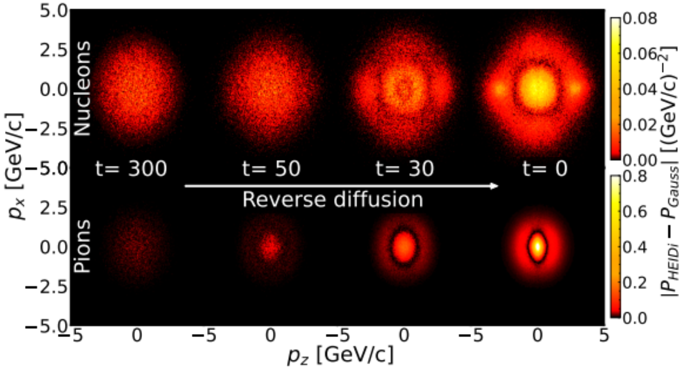

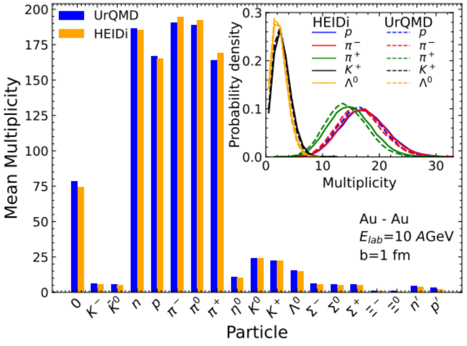

- **running time,** UrQMD
  cascade : ~ 3 sec/event;
  with potential : ~ 3 min/event;
  hybrid : ~ 1 hour/event
- HEIDI on A100: ~ 30 ms/event
- Speedup 2 ~ 5 orders of magnitude

M. O.K, K. Z, J. S, H. S, arXiv:**2502.16330**, arXiv:**2412.10352**

Summary: Machine Learning and HENP

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The Chinese University of Hong Kong, Shenzhen

nature reviews physics
https://doi.org/10.1038/s42254-024-00798-x

Perspective

Check for updates

Physics-driven learning for inverse problems in quantum chromodynamics

Gert Aarts[1], Kenji Fukushima[2], Tetsuo Hatsuda[3], Andreas Ipp[4], Shuzhe Shi[5], Lingxiao Wang[3] & Kai Zhou[6,7]

Abstract

The integration of deep learning techniques and physics-driven designs is reforming the way we address inverse problems, in which accurate physical properties are extracted from complex observations. This is particularly relevant for quantum chromodynamics (QCD) – the theory of strong interactions – with its inherent challenges in interpreting

Sections

Nature Review Physics (2025)

Thanks !

Progress in Particle and Nuclear Physics 135 (2024) 104084

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Review

Check for updates

Exploring QCD matter in extreme conditions with Machine Learning

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

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Prog. Part. Nucl. Phys. 135 (2024) 104084

A R T I C

Keywords:
Machine learn
Heavy ion coll
Lattice QCD
Neutron star
Inverse proble

Nuclear Science and Techniques (2023) 34:88
https://doi.org/10.1007/s41365-023-01233-z

REVIEW ARTICLE

Check for updates

High-energy nuclear physics meets machine learning

Wan-Bing He[1,2] · Yu-Gang Ma[1,2] · Long-Gang Pang[3] · Hui-Chao Song[4] · Kai Zhou[5]

Received: 10 March 2023 / Revised: 13 April 2023 / Accepted: 18 April 2023 / Published online: 21 June 2023

Nucl. Sci. Tech. 34 (2023) 6, 88

Abstract

Although seemingly disparate, high-energy nuclear physics (HENP) and machine learning (ML) have begun to merge in the last few years, yielding interesting results. It is worthy to raise the profile of utilizing this novel mindset from ML in HENP, to help interested readers see the breadth of activities around this intersection. The aim of this mini-review is to inform the community of the current status and present an overview of the application of ML to HENP. From different aspects and using examples, we examine how scientific questions involving HENP can be answered using ML.

Keywords Heavy-ion collisions · Machine learning · Initial state · Bulk properties · Medium effects · Hard probes · Observables