



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

Machine Learning in High Energy Nuclear Physics

Kai Zhou (CUHK-Shenzhen)

HENPIC Seminar 2025



• The discovery of the Higgs boson in 2012

The New York Times

Physicists Find Elusive Particle Seen as Key to Universe





AlexNet-ImageNet : birth of Deep Learning





• Physics Nobel Prize 2024



THE ROYAL SWEDISH ACADEMY OF SCIENCES

• ML for Nuclear Physics



Colloquium: Machine learning in nuclear physics



A Living Review of Machine Learning for Particle Physics

Modern machine learning techniques, including deep learning, is rapidly being applied, adapted, and developed for high energy physics. The goal of this document is to provide a nearly comprehensive list of citations for those developing and applying these approaches to experimental, phenomenological, or theoretical analyses. As a living document, it will be updated as often as possible to incorporate the latest developments. A list of proper (unchanging) reviews can be found within. Papers are grouped into a small set of topics to be as useful as cossible. Suggestions are most velocome.



Overview : Machine- and Deep-Learning









Find and Decode the mapping/representations into Deep Neural Network

Universal approximator (Hastad et al 86 & 91)



Differentiable programming Backward Propagation Gradient Descent Algorithm

Overview: Machine learning, Deep Neural Networks, Representation learning







Non-linear activation

Layer by layer





Discriminative / Generative

• 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"



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>





To study the most elementary particle matter :

- Nuclear Collisions : heat & compress matter
- Neutron Star : dense matter, astronomy constraints
- Lattice Field Theory / fQCD / Effective models

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.

$$\chi^{2} = \sum_{y} \left(\frac{\mathcal{F}_{y}[\mathcal{Q}_{\text{NN}}(x|\theta)] - \mathcal{O}_{y}}{\Delta \mathcal{O}_{y}} \right)^{2}$$

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

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

7

Inverse Problems Solving with ML





7

Early attempts : impact parameter determination



 $0.0 \le b \le 3.3$ $3.3 \le b \le 6.6$ $6.6 \le b \le 10$ 3 x 3 10 600 (a)stimated impact parameter (fm) $\sim \frac{1}{6}$ $\sim \frac{1}{6}$ $p_t (MeV)$ 400 200 5 x 5 600 p_t (MeV) 400 200 full input, symmetric binning 0 10 x 10 10 600 (b) imated impact parameter (fm) $p_t (MeV)$ 400 200 20 x 20 600 P_t (MeV) 400 200 filtered input, asymmetric binning 0 1000 -10000 -10001000 2 10 p_z (MeV) true impact parameter (fm)

Simple DNN Trained on QMD data Input 5X5

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

Further dev for impact parameter determination



12

10

★ NN

-- CNN

LightGBM

b (fm)

15 20 25 30

Centrality (%)

---- MLP + CNN

P. Xiang, Y. Zhao, X. Huang, **Chi. Phys. C** 53, 2358 (2022)

MLP and CNN (on AMPT event)

F. Li, Y. Wang, H. Lue, P. Li, Q. Li, F. Liu, JPG 47, 115104 (2020)

CNN and LightGBM (on UrQMD event)



PointCloud Network

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



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

Initial clustering structure identification in HICs



40



80

60

50

0

100

12C. Woods-Saxon

pion

Man Manufacture Manufacture

C-Au, N_{Event}=1000 C-Au, N_{Event}=2000

C-Au, N_{Event}=4000

O-Au, N_{Event}=1000 O-Au, N_{Event}=2000 O-Au, N_{Event}=4000

400

500

300

200

Epoch

Bayesian CNN

on AMPT events (multiple-event basis) Charged pions (phi, pT) from 12C/16O + 197Au collisions at 200 GeV

Multiple event basis





dynamical edge convolution network followed by a point cloud net is used to identify <u>self-similarity</u> and <u>critical fluctuations</u> in HIC

Repeating the **KNN** and **edge convolution** blocks twice helps to find long-range multi-particle correlations that are the key to searching for critical fluctuations.

PLB 827(2022) 137001, Y.-G. Huang, L.-G. Pang, X.F. Luo and X.-N. Wang.,





$$(\mu_{BC}, \alpha_{\text{diff}}, w, \rho) \mapsto P(T, \mu_B) \mapsto \{\text{acceptable, unstable, acause} \\ Stable : P, s, \varepsilon, n_B, \chi_2^B, \left(\frac{\partial S}{\partial T}\right)_{n_B} > 0 \\ \text{Causal : } 0 \le c_s^2 \le 1. \end{cases}$$

Classify EoS physical relevance based on <u>3D Ising model parameters</u>

D. Mroczek, M. Hjorth-Jensen, J. Noronha-Hostler, P. Parotto, C. Ratti, and R. Vilalta, PRC107, 054911





PHYSICAL REVIEW RESEARCH 2, 043202 (2020)

Nuclear liquid-gas phase transition with machine learning

Rui Wang⁰,^{1,2,*} Yu-Gang Ma,^{1,2,†} R. Wada,³ Lie-Wen Chen⁰,⁴ Wan-Bing He,¹ Huan-Ling Liu,² and Kai-Jia Sun^{3,5}



EbE charge-weighted charge multiplicity distribution of quasiprojectile as input \rightarrow

Autoencoder + confusion scheme (on NIMROD experiment)

Nuclear EoS, Nuclear matter properties from NS observables





Lsym

Jsym

Direct inverse mapping with CNN for identifying QCD transition







- Conventional obs. hard to distinguish
- Strongly influence from initial fluctuations and other uncertainties
- CNN : 95% <u>event-by-event</u> accuracy!
- <u>Robust to initial conditions, eta/s</u>

<u>Conclusion</u> : Information of early dynamics can **survive** to the end of hydrodynamics and encoded within the final state raw spectra, immune to evolution's uncertainties, **with deep CNN we can decode it back**.





Point Cloud Network for Physics online analysis for HICs



Experimental data has inherent point cloud structure

- collection of particles as 2D array :
- PointNet based models learn directly from point clouds.
 - respects the **order invariance** of point clouds
 - direct processing of experimental data from detector ⇒ ideal online analysis algorithm

X1

X2

Xn Vn

Px

1.07

0.06

6.84

40.4

Pv

4.5

0.54

Pz

6.83

40

pid

211

321

optimal for higher dimensional data



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



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 2024

Inverse Problems Solving with ML





Bayesian (Statistical) Inference of hot matter EoS from HIC data



PRL 114, 202301 (2015)

PHYSICAL REVIEW LETTERS

week ending 22 MAY 2015

Constraining the Equation of State of Superhadronic Matter from Heavy-Ion Collisions

Scott Pratt,¹ Evan Sangaline,¹ Paul Sorensen,² and Hui Wang² ¹Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory Michigan State University, East Lansing, Michigan 48824, USA ²Brookhaven National Laboratory, Upton, New York 11973, USA (Received 19 January 2015; published 19 May 2015)

$$c_s^2(\epsilon) = c_s^2(\epsilon_h) + \left(\frac{1}{3} - c_s^2(\epsilon_h)\right) \frac{X_0 x + x^2}{X_0 x + x^2 + X'^2},$$
$$X_0 = X' R c_s(\epsilon) \sqrt{12}, \quad x \equiv \ln \epsilon / \epsilon_h,$$

$$P(D|\theta) = \prod_i \exp(-(z_i(\theta) - z_{i,\exp})^2/2),$$

14 model parameters

speed of sound squared slightly softer than lattice EoS But significantly overlap



Bayesian (Statistical) global fit on HICs



Gel

18



5/8

[GeV] 0.16

0 (

0.15

100 130

norm

160 -1.0 0.0

p

1.0 0.8 1.5 2.2 0.4

 $_{k}$

0.7

w [fm]

1.0 0.0 0.15 0.3 0.0

 $\eta/s \min$

1.0 2.0 0.0

 η/s slope[†]

1.0

 ζ/s norm

2.0 0.14 0.15 0.16

 $T_{\rm sw}$ [GeV]

E 0.14

G. Nijs, W. Schee, U. Guersoy, R. Snellings, PRC103,054909; JETSCAPE, PRL126,242301; U. Heinz+, 2302.14184 (VAH) M. R. Heffernan, C. Gale, S. Jeon, J. Pauet, PRC109,065207;

Jet quenching/diffusion:

...

Y. He, L. Pang, X. Wang, PRL 122 (25) 252302 M. Xie, W. Ke, H. Zhang, X. Wang, PRC108 (2023) L011901;

Bayesian (Statistical) global fit on HICs



OPEN ACCESS

IOP Publishing

Journal of Physics G: Nuclear and Particle Physics

J. Phys. G: Nucl. Part. Phys. 51 (2024) 103001 (43pp)

https://doi.org/10.1088/1361-6471/ad6a2b

Topical Review

Applications of emulation and Bayesian methods in heavy-ion physics

	References	Pre-hydro	Hydro	Cooper-Frye	Data	Covariance
Jean-François Paquet®	Bernhard et al [28]	Trento+f.s.	DNMR	P.T.B.; σ meson production	Pb–Pb @ 2.76 TeV and 5.02 TeV	Σ_{emul} +diag. Σ_{expt}^{stat} +non-diag. Σ_{expt}^{syst} + Σ_{extra}
	Moreland et al [89]	Trento w/ subnucleonic d.o. f.+f.s.	DNMR	P.T.B.; σ meson production	p-Pb & Pb–Pb @ 5.02 TeV	Σ_{emul} +diag. Σ_{expt}^{stat} +non-diag. Σ_{expt}^{syst}
	JETSCAPE [15, 53]	Trento+f.s.	DNMR	Grad, Chapman– Enskog, P.T.B.	Au–Au @ 0.2 TeV and Pb–Pb @ 2.76 TeV	Σ_{emul} +diag. Σ_{expt}^{stat} +diag. Σ_{expt}^{syst}
	Nijs et al [111, 112]	Trento w/ subnucleonic d.o. f. + modified streaming	DNMR	P.T.B.; σ meson production	Pb–Pb @ 2.76 TeV; p-Pb and Pb– Pb @ 5.02 TeV; added differential observables	Σ_{emul} +diag. $\Sigma_{\text{expt}}^{\text{stat}}$ +non-diag. $\Sigma_{\text{expt}}^{\text{syst}}$
	Parkkila <i>et al</i> [52, 113]	Trento+f.s.	DNMR	P.T.B. σ meson production	Pb–Pb @ 2.76 TeV and 5.02 TeV; added event-plane correlations	Σ_{emul} +diag. Σ_{expt}^{stat} +non-diag. Σ_{expt}^{syst} + Σ_{extra}
	Liyanage et al [35]	Trento + anisotropic hydro parameters	Viscous aniso- tropic hydro	P.T.M.A.	Pb–Pb @ 2.76 TeV	Σ_{emul} +diag. Σ_{expt}^{stat} +diag. Σ_{expt}^{syst}
	Heffernan <i>et al</i> [24, 26]	IP-Glasma	DNMR	Grad, Chapman– Enskog	Pb–Pb @ 2.76 TeV; added event- plane correlations	Σ_{emul} +diag. Σ_{expt}^{stat} +diag. Σ_{expt}^{syst}

Bayesian Reconstruction for dense matter EoS from HICs



- Hadronic cascade dominant
- UrQMD model adapted to any density dependent EoS \rightarrow

via density dependent potential





Evidence : p's v2 and transverse kinetic energy



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

Closure Test:



Test the extracted EoS on different observables (not used in Bayesian analysis)

Use real exp. Data:













FIG. 7. Considering the MDI: the posterior PDFs of K. Left: observable only $-v_2(y_0)$, right: observables $-v_2(y_0)$ and $-v_2(u_{t_0})$.

Bayesian inference of nuclear incompressibility from proton elliptic flow in central Au+Au collisions at 400 MeV/nucleon

J. M. Wang (汪金梅),^{1,2} X. G. Deng (邓先概) ⁽³⁾,^{1,2,*} W. J. Xie (谢 文杰),³ B. A. Li (李宝安) ⁽⁵⁾,^{4,†} and Y. G. Ma (马余刚) ⁽⁵⁾,^{1,2,‡} *arXiv:2406.07051*

> IQMD simulation of proton v2 Au+Au at E=400 MeV/Nucleon

MDI: momentum dependent Interaction

$$E/A = \frac{\alpha}{2} \frac{\rho}{\rho_0} + \frac{\beta}{\gamma + 1} \left(\frac{\rho}{\rho_0}\right)^{\gamma} + \frac{3}{10m} \left(\frac{3\pi^2 \hbar^3 \rho}{2}\right)^{2/3} + \frac{1}{2} t_4 \frac{\rho}{\rho_0} \int f\left(\vec{p}\right) \ln^2 \left[1 + t_5 \left(\vec{p} - \langle \vec{p}' \rangle\right)^2\right] d^3p,$$
(1)

$$P = \rho^{2} \frac{\partial E/A}{\partial \rho} = \frac{\alpha}{2} \frac{\rho^{2}}{\rho_{0}} + \frac{\beta \gamma \rho}{\gamma + 1} \left(\frac{\rho}{\rho_{0}}\right)^{\gamma} + \frac{1}{5m} \left(\frac{3}{2} \pi^{2} \hbar^{3}\right)^{\frac{2}{3}} \rho^{\frac{5}{3}} + \frac{t_{4}}{2} \frac{\rho^{2}}{\rho_{0}} \ln^{2} \left(1 + t_{5} P_{F}^{2}\right),$$
(2)

$$K = 9\rho^{2} \frac{\partial^{2} E/A}{\partial \rho^{2}} |_{\rho_{0}} = -\frac{3}{5m} \left(\frac{3\pi^{2}\hbar^{3}\rho_{0}}{2}\right)^{2/3} + \frac{9\beta\gamma\left(\gamma-1\right)}{\gamma+1} + \ln\left(1+t_{5}P_{F}^{2}\right)\frac{6t_{4}t_{5}P_{F}^{2}}{1+t_{5}P_{F}^{2}},$$
(3)

20

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)





Critical Endpoint from Holographic QCD via Bayesian Inference



22



Bayesian inference of the critical endpoint from holographic QCD



22



Bayesian reconstruction for h-h interaction from <u>femtoscopy</u> – mock test





$$C(k) = \int S(\mathbf{r}) \mid \boldsymbol{\psi}_k(\mathbf{r}) \mid^2 \mathrm{d}^3 r,$$

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi + V \psi = E \psi,$$

$$S(r) = \frac{1}{(4\pi r_0^2)^{3/2}} \exp\left(-\frac{r^2}{4r_0^2}\right),$$

$$r_0 = 1.0 \text{ fm}$$

DNN emulator + PCA for correlation + PyMC With O. L, J. Z, X. C, etc., <u>in preparation</u>

$$V(r) = \sum_{i=1,2} a_i e^{-(r/b_i)^2} + a_3 m_{\pi}^4 f(r, b_3) \frac{e^{-2m_{\pi}r}}{r^2}$$

$$f(r, b_3) = \left(1 - e^{-(r/b_3)^2}\right)^2$$

There are six parameters are a_i, b_i (i = 1,2,3) for this potential !





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.

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

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

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

Deep Learning composes differentiable components to a program, e.g. DNN, then optimizes it with gradients



From EoS to NS Stellar Structure (MR)





 $P(\rho)$

• Gravity $\leftarrow \rightarrow$ Pressure

$$egin{aligned} rac{dP}{dr} &= -rac{G}{r^2}\left(
ho+rac{P}{c^2}
ight)\left(m+4\pi r^3rac{P}{c^2}
ight)\left(1-rac{2Gm}{c^2r}
ight)^{-1} \ M &= m(R) = \int_0^R 4\pi r^2
ho\,dr \end{aligned}$$

Dense matter Equation of State

• Noisy/Limited NS Observables to EoS?



From EoS to NS Stellar Structure (MR) -- Inverse ?

 $P(\rho)$





• Gravity $\leftarrow \rightarrow$ Pressure

$$egin{aligned} rac{dP}{dr} &= -rac{G}{r^2}\left(
ho+rac{P}{c^2}
ight)\left(m+4\pi r^3rac{P}{c^2}
ight)\left(1-rac{2Gm}{c^2r}
ight)^{-1} \ M &= m(R) = \int_0^R 4\pi r^2
ho\,dr \end{aligned}$$

Dense matter Equation of State

• Noisy/Limited NS Observables to EoS ?



Auto-diff framework and Results





S. Soma, L. Wang, S. Shi, H. Stoecker, K. Zhou, Phys. Rev. D 107 (2023)083028





R. Li, S. Han, Z. Lin, L. Wang, K. Zhou, S. Shi, arXiv:2501.15819

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 $\Delta \varepsilon = 150 \text{ MeV/fm}^3$ at pressure $P_{\rm PT} = 76 \text{ MeV/fm}^3$. Above the PT point, we take the stiffest (causal) limit that $c_s = 1$. We employ twenty



Quasi-particle analysis of IQCD thermodynamics





HQ Potential Model, Inverse Shroedinger Eq.





Proof of Concept



limited spectrum { En } to continuous interaction V(r) ?

-- Yes! But to some range decided by the used states.

Learn V(r) from 5 eigenvalues :

{ En } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV



Deviation @ given states' wavefunction vanishes

 $\delta E_n = \langle \psi_n \, | \, \delta V(r) \, | \, \psi_n \rangle$







S.S, K. Z, J.Z, S.M., P. Z, Phys. Rev. D 105 (2022) 1, 1



31 $K(\omega, \tau, T) = \frac{\cosh \omega(\tau - \frac{1}{2T})}{\sinh \frac{\omega}{2T}}$

0.5



Spectral function reconstruction from Euclidean correlator

0.75

0.50

0.25

0.00



Offler+ 1912.12900; [Kades+ PRD102 (2020) 096001; Chen+ 2110.13521; Zhou+ PRD104(2021)076011 Horak+ PRD105 (2022) 036014



Hadron emission source reconstruction via femtoscopy



31

100 125 150 175 200

k[MeV/c]

50 75



50 75

100 125 150 175 200

k[MeV/c]

ML Holography (EMD model) with lattice QCD reference





0.00

0.5

1.0

μ

1.5

X. Chen, M. Huang, Phys.Rev.D 109 (2024) L051902; JHEP02 (2025)123



Want to **model** the observed data's underlying but unknown **distribution**, to further :

- Understand/Inference the data (inherent structure, properties, features...)
- Sample according to the distribution

Suppose observation dataset :

$$\mathbf{X} = \{x^{(1)}, x^{(2)}, ..., x^{(N)}\} \stackrel{i.i.d}{\sim} p_{data}(x)$$

We use parametric model to approach the data distribution :

$$p_{\theta}(x) \to p_{data}(x)$$

• Maximize Likelihood Estimation :

$$\theta^* = \underset{\theta}{\arg\max} \log p_{\theta}(\mathbf{X}) = \underset{\theta}{\arg\max} \frac{1}{N} \sum_{i=1}^{N} \log p_{\theta}(x^{(i)})$$



GAN to generate complex scalar field configurations





Autoregressive network for variational many-body physics calculation







$$D_{\mathrm{KL}}(q_{\theta} \| p) = \sum_{\mathbf{s}} q_{\theta}(\mathbf{s}) \ln\left(\frac{q_{\theta}(\mathbf{s})}{p(\mathbf{s})}\right) = \beta(F_q - F_q)$$

$$F_q = \frac{1}{\beta} \sum_{\mathbf{s}} q_{\theta}(\mathbf{s}) \left[\beta E(\mathbf{s}) + \ln q_{\theta}(\mathbf{s})\right]$$



Probability distributions from CANs

Vortices





T. Xu, L. Wang, L. He, K. Zhou, Y. Jiang, Chi. Phys. C 2024



Flow based generative model (given unnormalized distribution)



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

compose several invertible transformations to form the flow :



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





"A heavy quark move inside quark-gluon plasma"



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) → **Best Physics for Al Paper Award !** Q. Zhu, G. Aarts, W. Wang, K. Zhou, L. Wang, arXiv:2410.19602 (NeurIPS 2024 workshop "ML&Physical Sciences)

Diffusion Model for field configurations



 p_0

Forward diffusion SDE

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

1 /

Backward diffusion SDE

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

• Score matching Training $\mathcal{L}_{\theta} = \sum_{i=1}^{n} \sigma_i^2 \mathbb{E}_{p_0(\phi_0)} \mathbb{E}_{p_i(\phi_i|\phi_0)} \left[\|s_{\theta}(\phi_i, \xi) - \nabla_{\phi_i} \log p_i(\phi_i|\phi_0)\|_2^2 \right]$

• Sample generation SD

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

 $\frac{\partial p_{\tau}(\phi)}{\partial \tau} = \int d^n x \left\{ g_{\tau}^2 \frac{\delta}{\delta \phi} \left(\bar{\alpha} \frac{\delta}{\delta \phi} + \nabla_{\phi} S_{\rm DM} \right) \right\} p_{\tau}(\phi), \qquad \nabla_{\phi} S_{\rm DM} \equiv -\nabla_{\phi} \log q_{\tau}(\phi) \qquad p_{\rm eq}(\phi) \propto e^{-S_{\rm DM}/\bar{\alpha}} \qquad p_{\tau=T}(\phi) \to P[\phi, T]$

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

 $p_{\xi}(\phi_{\xi}|\phi_0) = \mathcal{N}\left(\phi_{\xi}; \phi_0, \frac{1}{2\log\sigma}(\sigma^{2\xi} - 1)\mathbf{I}\right)$

 $\frac{a\phi}{dt} = [f(\phi, t) - g(t)^2 \nabla_{\phi} \log p_t(\phi)] + g(t) dt$

 p_T

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

 ϕ_0

 p_0

A flow of <u>effective action</u> will be learned in DMs L. Wang, G. Arts, K. Zhou, JHEP 05(2024) 060 sampling from a DM is equivalent to optimizing a stochastic trajectory to approach the "equilibrium state"

Effective Action on toy model

φ





DM on 2d scalar ϕ^4 model



• **32x32 lattice, HMC generated** <u>5120 configurations</u> 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 :



numerous "bulk" patterns emerge

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)	$0.0017 {\pm}~0.0015$	2.4227 ± 0.1035	0.0484 ± 0.0959

Relation to (inverse) RG



39

• Forward diffusion kernel: **gaussian smoothing**

$$p_{\xi}(\phi_{\xi}|\phi_0) = \mathcal{N}\left(\phi_{\xi}; \phi_0, \frac{1}{2\log\sigma}(\sigma^{2\xi} - 1)\mathbf{I}\right)$$

$$\phi_{\tau}(\mathbf{x}) = \phi_0(\mathbf{x}) + \sqrt{\frac{\sigma^{2\tau} - 1}{2 \log \sigma}} \epsilon(\mathbf{x}) \text{ with } \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

• In Fourier space:

$$\phi_{\tau}(p) = \phi_0(p) + \sqrt{\frac{\sigma^{2\tau} - 1}{2\log\sigma}} \epsilon(p).$$

 ! the above evolution will perturb (smear) higher momentum modes faster because of the gradually increasing noise level

In FRG, the high frequency (short-distance) degrees of freedom is progressively integrated out ! See Semon's and Mathis's talk!



U-net Emulator for relativistic hydrodynamics



PHYSICAL REVIEW RESEARCH 3, 023256 (2021)

Applications of deep learning to relativistic hydrodynamics

Hengfeng Huang,^{1,2} Bowen Xiao,³ Ziming Liu,¹ Zeming Wu,^{1,2} Yadong Mu,^{3,4} and Huichao Song ^{[],2,5}

tic heavy-ion collisions. Using 10 000 initial and final profiles generated from (2+1)-dimensional relativistic hydrodynamics VISH2+1 with Monte Carlo Glauber (MC-Glauber) initial conditions, we train a deep neural network based on the stacked U-net, and use it to predict the final profiles associated with various initial conditions, including MC-Glauber, MC Kharzeev-Levin-Nardi (MC-KLN), a multiphase transport (AMPT) ^{0.50} model, and the reduced thickness event-by-event nuclear topology (TRENTO) model. A comparison with the VISH2+1 results shows that the network predictions can nicely capture the magnitude and inhomogeneous $_{0.25}$. structures of the final profiles, and creditably describe the related eccentricity distributions $P(\varepsilon_n)$ (n = 2, 3, 4).







CNN Emulator to hydrodynamic results of heavy-ion collisions



PHYSICAL REVIEW C 108, 034905 (2023)

Deep learning for flow observables in ultrarelativistic heavy-ion collisions



As an input, the DenseNet model uses discretized initial energy density in the transverse-coordinate (x, y)plane calculated from the EKRT model with a grid size 269×269 and a resolution of 0.07 fm. The DenseNet model is trained to reproduce a set of final state p_T integrated observables v_n , average transverse momentum $[p_T]$, and charged particle multiplicity $dN_{ch}/d\eta$ for each event. The input energy density is normalized in such a



Similar study for intermediate energies with IBUU +DNN emulation see: **B. Li+, arXiv:2406.18421**

Generative diffusion model to heavy-ion collisions



An end-to-end generative diffusion model for heavy-ion collisions

Jing-An Sun,^{1,2} Li Yan,^{1,3} Charles Gale,² and Sangyong Jeon²



tor. We carried out (2+1)D minimum bias simulations of Pb-Pb collisions at 5.02 TeV, choosing the shear viscosity η/s to be one of three distinct values: 0.0, 0.1, and 0.2. For each value of η/s , we generate 12,000 pairs of initial entropy density profiles and final particle spectra, corresponding to 12,000 simulated events, as the training dataset. 70% of the total events are used for training and the rest are used for validation.

Considering that the spectra \mathbf{S}_0 depend on the initial entropy density profiles \mathbf{I} and the shear viscosity η/s , we train a conditional reverse diffusion process $p(\mathbf{S}_0|\mathbf{I},\eta/s)$ without modifying the forward process.

one single central collision event in just 10^{-1} seconds on a GeForce GTX 4090 GPU.

ble precision, as the traditional numerical simulation of hydrodynamics for one central event typically takes approximately 120 minutes (10^4 seconds) on a single CPU.

arXiv:2410.13069

Point Cloud Diffusion Model for HICs



UrQMD

30

20

HEIDI

10

.9

Probability 0

0.0

- 18k UrQMD simulation events for Au-Au@10 AGeV
- HEIDi: Heavy-ion Events through Intelligent Diffusion
- Point-cloud representation: momentum + ID



200

175

Multiplicity 100 100 UrQMD

HEIDi

What's the future? – Generative AI and LLM maybe the future



Should artificial intelligence be interpretable to humans?

Matthew D. Schwartz ☑



Machine vs. Biological intelligence

- Biological intelligence grows by a factor of 2 in one million years
- Machine intelligence grows by a factor of 10 in 1 year



Summary: Machine Learning and HENP



nature reviews physics

https://doi.org/10.1038/s42254-024-00798-

Perspective

Check for updates

arning

outlook

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 ©⁶⁷

Abstract	Sections
The integration of deep learning techniques and physics-driven designs	Introduction
is reforming the way we address inverse problems, in which accurate	Physics-driven le
physical properties are extracted from complex observations. This is	QCD physics
of strong interactions – with its inherent challenges in interpreting	Conclusions and

Nature Review Physics (2025)

Thanks!



Review

Exploring QCD matter in extreme conditions with Machine Learning

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

REVIEW ARTICLE



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

High-energy nuclear physics meets machine learning

Wan-Bing He^{1,2} · Yu-Gang Ma^{1,2} · Long-Gang Pang³ · Hui-Chao Song⁴ · Kai Zhou⁵

Received: 10 March 2023 / Revised: 13 April 2023 / Accepted: 18 April 2023 / Published online: 21 June 2023 © The Author(s) 2023

Abstract

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



Experimental data has inherent point cloud structure

- Point clouds: collection of points in space
- Point clouds are represented as 2D array.
 - each row= a point in the point cloud
 - each column =a dimension of the point cloud
- PointNet based models learn directly from point clouds.
 - respects the order invariance of point clouds
 - direct processing of experimental data
- Advantages:
 - Iess processing time ⇒ideal online algorithm
 - optimal for higher dimensional data
- We consider the CBM experiment as a use case
 - Au-Au collisions
 - 10 AGeV
 - CBM Challenges 🚽





Upto 45 AGeV collisions

1000 tracks per collision

TBytes/Second raw data

107 collisions/ Second



- STS-> 8 planes
 - Momentum resolution: 1 %

models





05

b ~ (0-16)fm

12

Third order polynomial fit to

multiplicity vs. impact parameter

•

curve

Polyfit (non-ML baseline)

Regressive and Generative AI for High Energy Nuclear Physics

- Nuclear properties prediction
 - Dripline locations, atomic masses, separation energies, superheavy nuclei location...
 - ➢ ANN application since 1992, later to beta-decay etc., → BNN
 - Different ML methods, SVM, Gradient boost, BDT,...
- Interpo-/extrapolation of nuclear data, augment nuclear model
 - Nuclear masses, nuclear charge radii, alpha-decay rate,
 - Fission yield constrain, fusion cross-section estimation, isotopic cross-section prediction
 - Within nuclear DFT, Energy density functional (EDF) need to be adjusted to exp data – with ML (1)
- Nuclear matter equation of state and Neutron Star properties
 - Inverse problems in heavy ion collisions and EoS extraction
 - Experimental global analysis, for QGP properties and PDF
 - Neutron Star analysis with Bayesian, DNN, Auto-diff...
 - Fast Simulation (Emulator) for HICs
- In lattice QCD
 - Inverse problem: spectral function or interaction or PDF reconstruction
 - Bayesian inference and DNN, and also auto-diff
 - Configurations Generation via Generative models



(particle phy) Supervised Learning – Regressive Tasks



• Jet Tagging, PID, - <u>BDT, CNN, GNN, PCN (CMS-DeepJet, ATLAS)</u>

- B-tagging (identifying jets originating from b-quarks)
- Tau-jet : Lepton/photon vs. hadron separation
- Heavy-flavor jets (specific particle decays)
- Pion, kaon, proton identification, medium-like/vacuum-like jets

Reconstruction – <u>GNN, CNN, Self-Supervised</u> (ML4ParticleFlow)

- Convert raw detector signals to physical variables (4 mom, vertex)
- > Calibrating reconstructed energies in calorimeter
- Correcting measured momenta from tracking detectors

• Real-Time Trigger / Filtering system - CNN, RL, Q-learning

- Ultra-low latency classification of collision event / signals
- Implementing ML inference on specialized hardware (FPGAs)
- Online distillation reducing raw data flow from Terabytes/second to manageable levels

Inference – <u>cINN</u>, flows

- Learn param of theory from high-d exp data simulation based inference
- Inverse problem solving





(particle phy) Unsupervised Learning – Generative or Detection tasks



• Simulation – GAN, VAE, flow, Diffusion (CaloGAN)

- Fast simulation of collision events and detector responses.
- Use classical simulation or collider data as input, train surrogate
- > 3D voxel image or Point Cloud
- Replace time-consuming full GEANT4 simulations to accelerate experimental analyses.
- **Unfolding** <u>GNN, CNN, Self-Supervised</u> (ML4ParticleFlow)
 - Recover theoretical-level physical distributions (e.g., transverse momentum) from detector-level data.
 - Calibrating reconstructed energies in calorimeter
 - Correct for detector effects such as resolution and efficiency.
 - NN based direct unfolding, or Generative based probabilistic unfolding
- Anomaly Detection Classifier, PCA, AutoEncoder,
 - Detect physics phenomena beyond standard models.
 - Search for rare events, such as dark matter signals or new resonances.



Fast Calorimeter Simulation Challenge 2022

new on GitHub

Welcome to the home of the first-ever Fast Calorimeter Simulation Challenge!

The purpose of this challenge is to spur the development and benchmarking of fast and high-fidelity calorimeter shower generation using deep learning methods. Currently, generating calorimeter showers of interacting particles (electrons, pitons, u) sugge GENT4 is a major computational bottleneck at the LHC, and it is forecast to overwhelm the computing budget of the LHC experiments in the near future. Therefore there is an urgent need to develop GEAN14 emulators that are both fast (computationally lightweight) and accurate. The LHC collaborations have been developing fast simulation methods for some time, and the hope of this challenge is to directly compare new deep learning approaches on common benchmarks. It is expected that participants will make use of cutting edge techniques in generative modeling with deep learning, e.g. GANs, VAEs and normalizing flows.

This challenge is modeled after two previous, highly successful data challenges in HEP – the top tagging community challenge and the LHC Olympics 2020 anomaly detection challenge.

Test results







validation R2 ~0.96



CNN to detect CME, and regress stochastic dynamics in HICs





Y. Zhao, L. Wang, K. Zhou, X. Huang, PRC 106, L051901(Letter)



L. Jiang, L. Wang, K. Zhou, PRD 103, 116023

Critical Endpoint from Holographic QCD via Bayesian Inference



