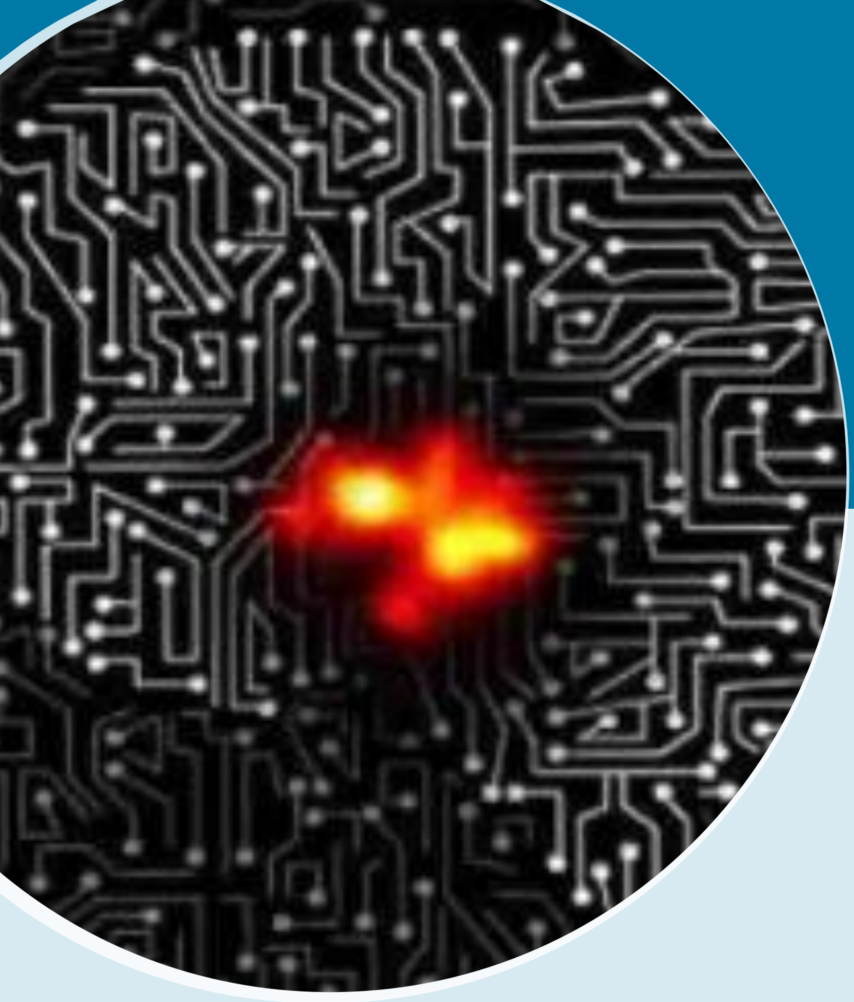

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The Chinese University of Hong Kong, Shenzhen

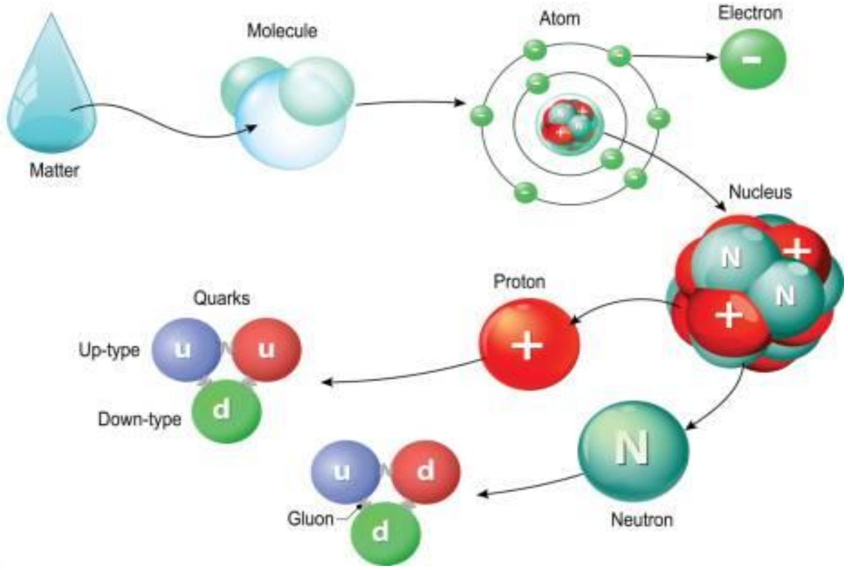
Extreme QCD Matter Exploration meets Machine Learning

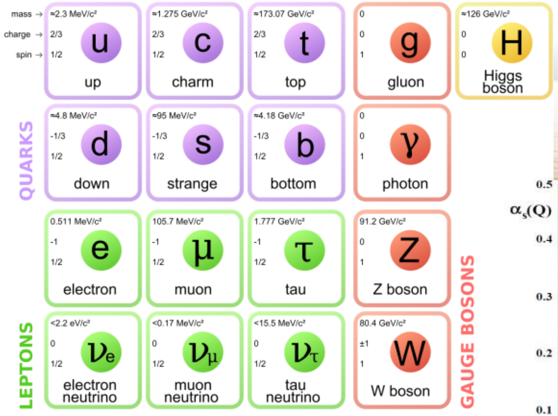
Kai Zhou (CUHK-Shenzhen)

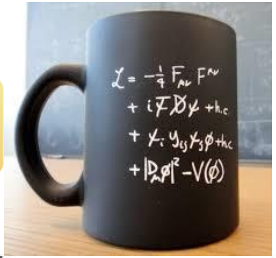
AI for Theoretical Sciences Workshop
(**IOP, Beijing,** 12-15.Nov.2024)

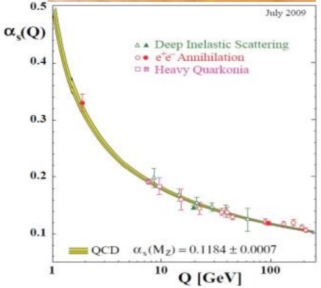
- **Reductionism** perspective for exploring matter
  Hierarchy of structures of Matter →
- Most Basic **Elements** : Quarks and Gluons
- Elementary **Interactions** :
  Quantum Chromodynamics QCD

MATTER
from molecule to quark









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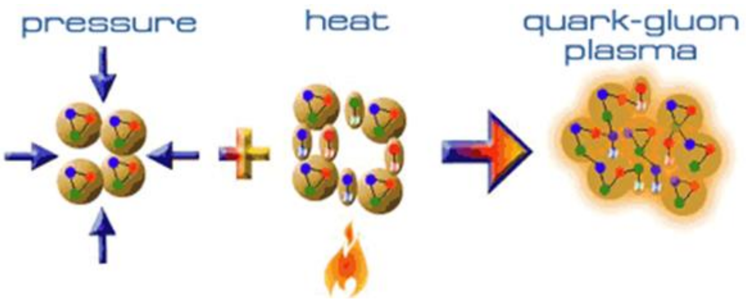
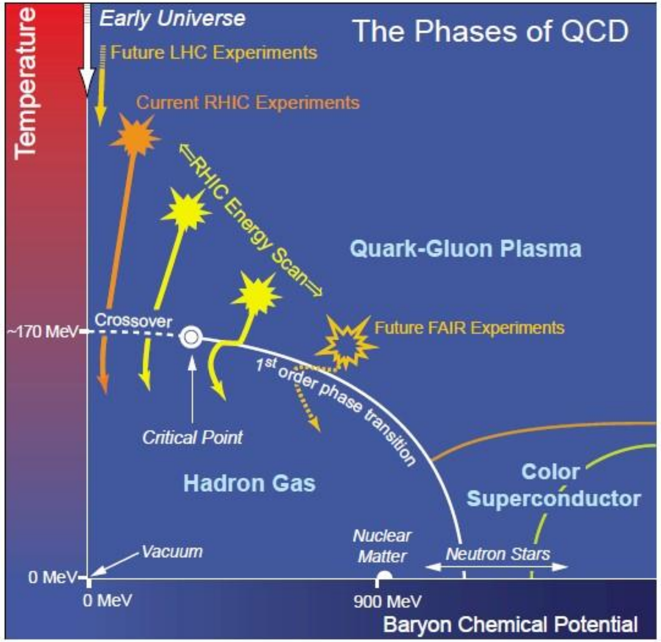
- **Phases** of matter : solid, liquid, gas, plasma
- Matter in extreme conditions reveals its **constituents** : nuclear matter → quark matter





``It would be intriguing to explore new phenomena by distributing high energy or high nuclear matter density over a relatively large volume."

- - **T.D. Lee** (1974)

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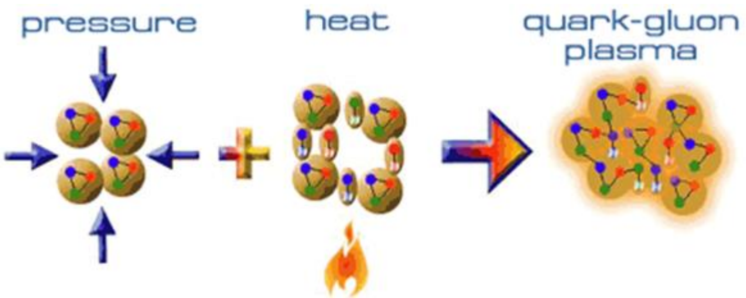
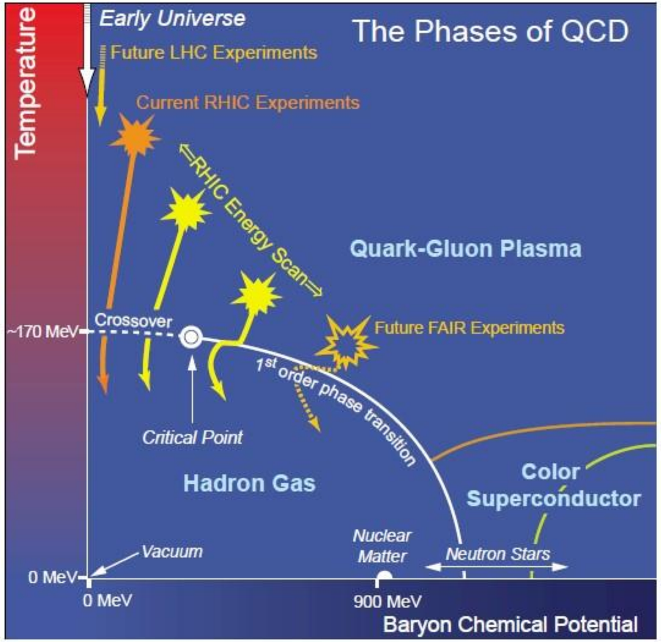
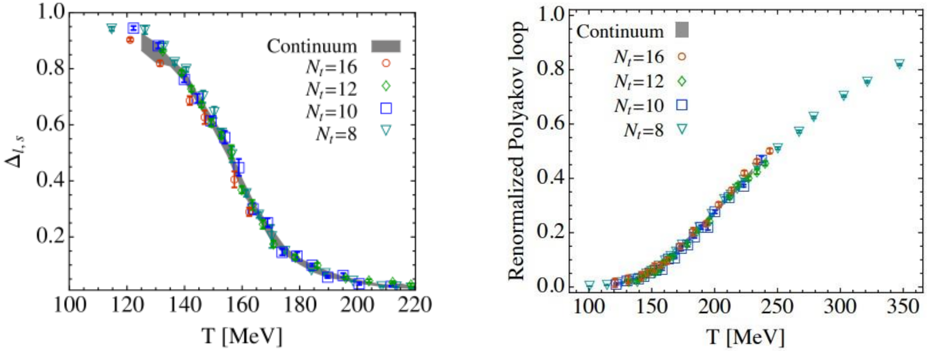




- Quark condensate and Polyakov loop
- Chiral symmetry breaking restoration and Deconfinement



Borsaenyi, et.al., JHEP(2010)73

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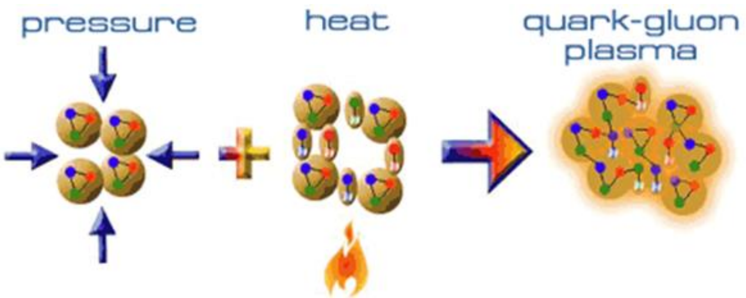
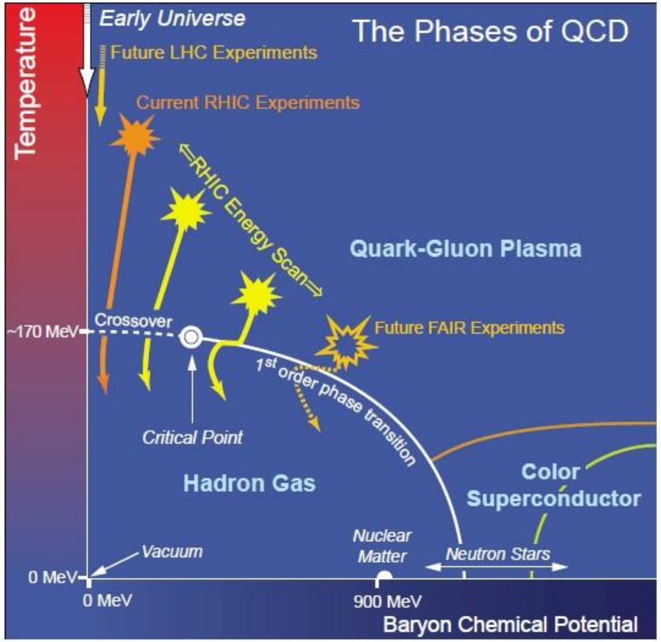
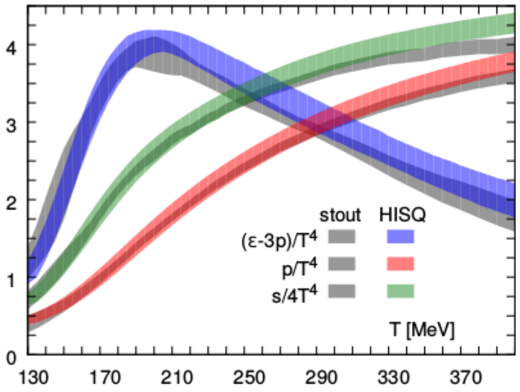
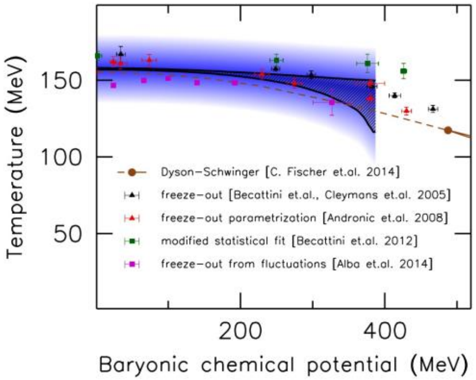




Bazavov, et.al., Nucl.Phys.A (2014) 867-871

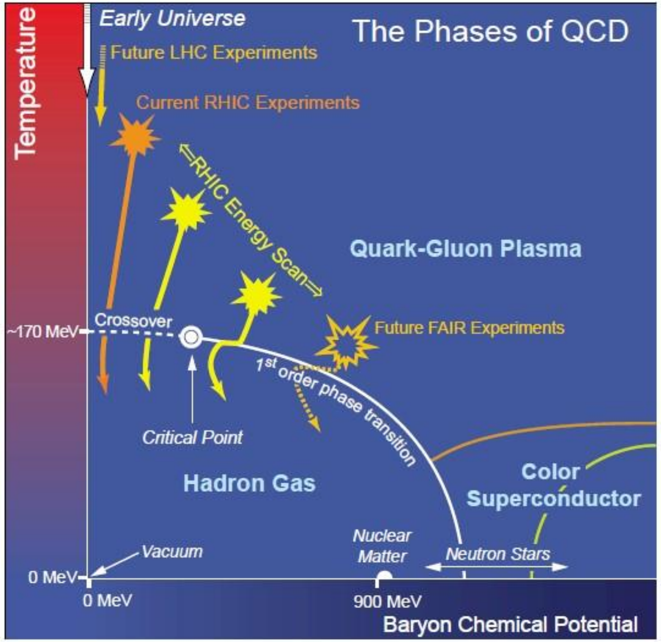


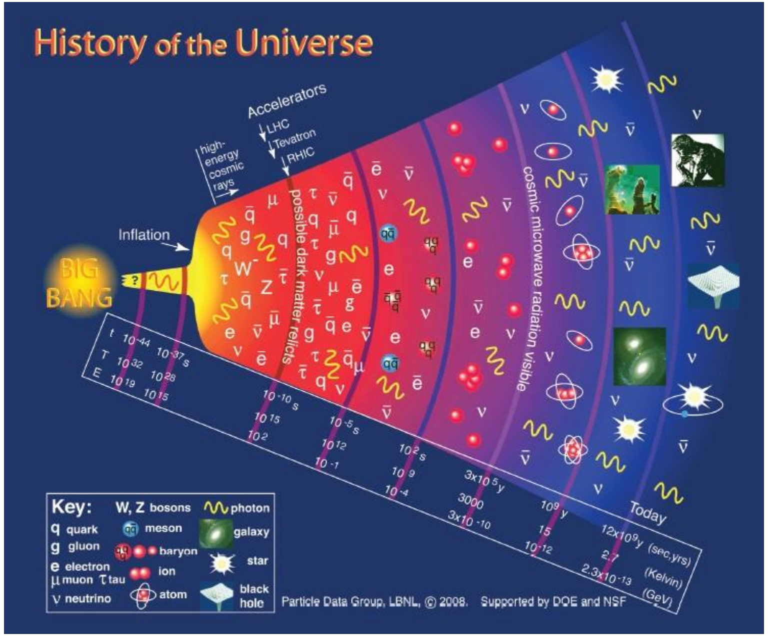


J. Guenther et al., Nucl.Phys.A 967(2017)720

Overview : Old phase of matter in Early Universe

- **Phases** of matter : solid, liquid, gas, plasma
- Matter in extreme conditions reveals its **constituents** :
  nuclear matter → quark matter





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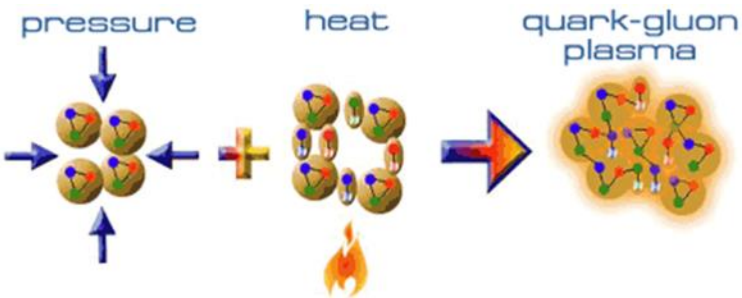

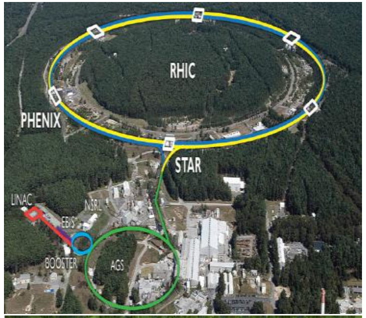

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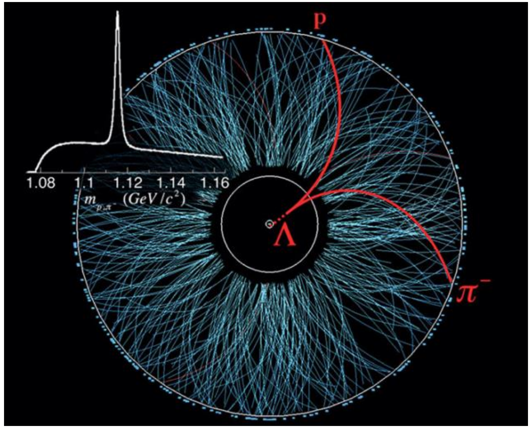

Overview : Little Bang

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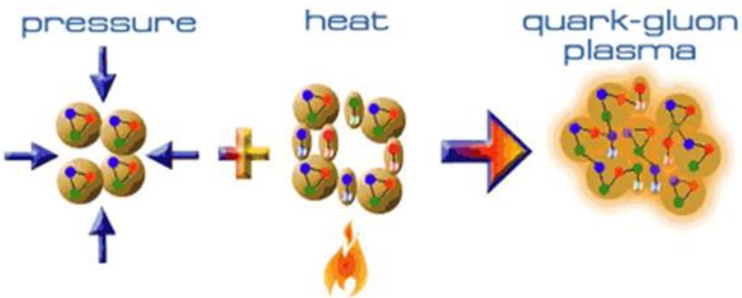
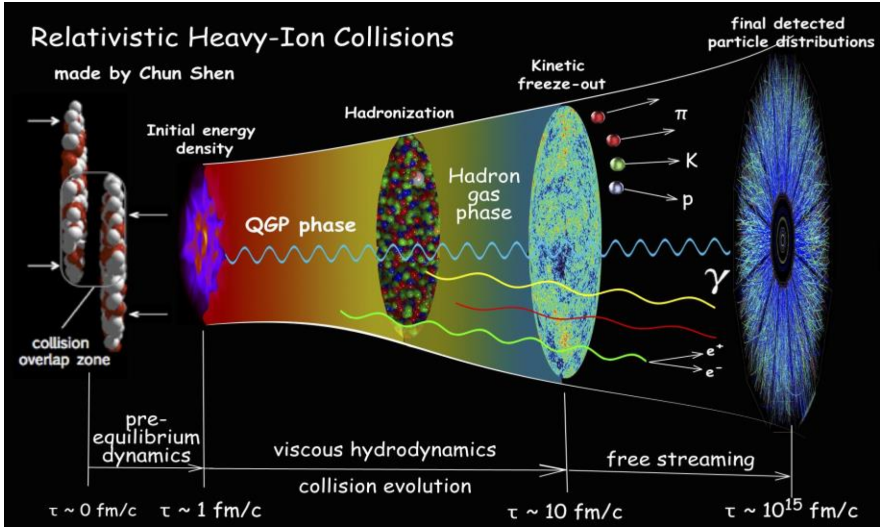


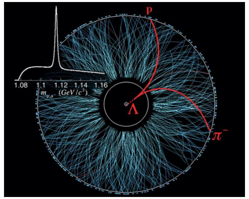
- Terrestrial Lab of ‘heat /compress’ machine

- The <u>Little Bang</u> from the collider :



- **Experiment** : measures final hadrons and leptons

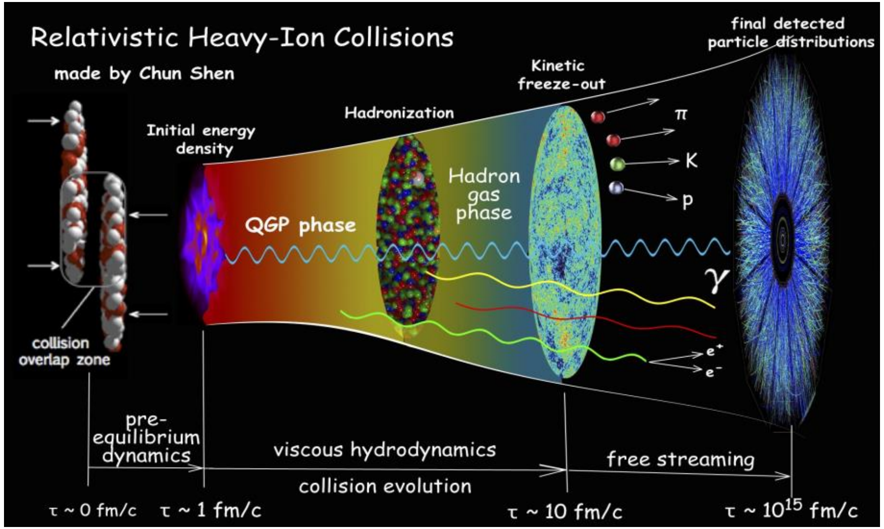
How to learn about physics from Experiment ?

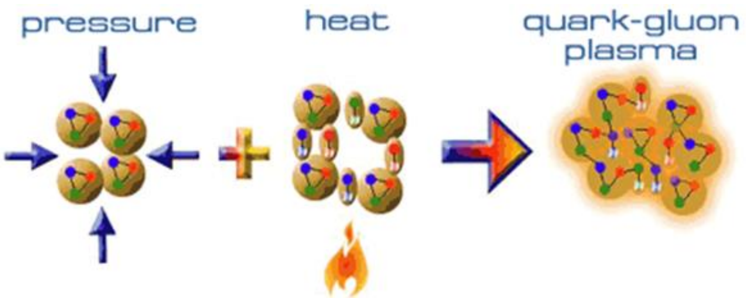


- **<u>Confront Theory/Model with Data</u>**

Overview : Little Bang

- Terrestrial Lab of ‘heat /compress’ machine
- The <u>Little Bang</u> from the collider :





- **Transport models** based on Boltzmann Equations

$$p^{\mu}\partial_{\mu}f + F\cdot\partial_{p}f = \sum_{i} C[f]$$

- **Relativistic Hydrodynamics** : macroscopic d.o.f

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

$$\partial_{\mu}N^{\mu} = 0$$

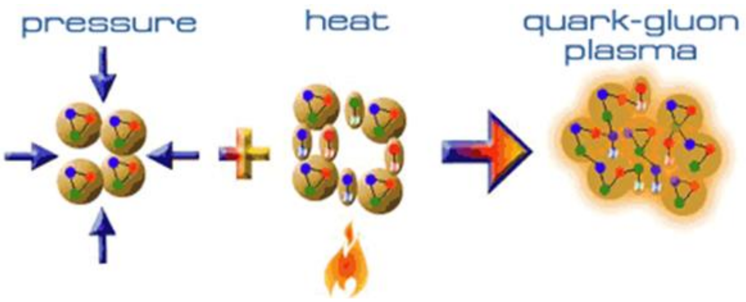
+ equation of state (EoS)

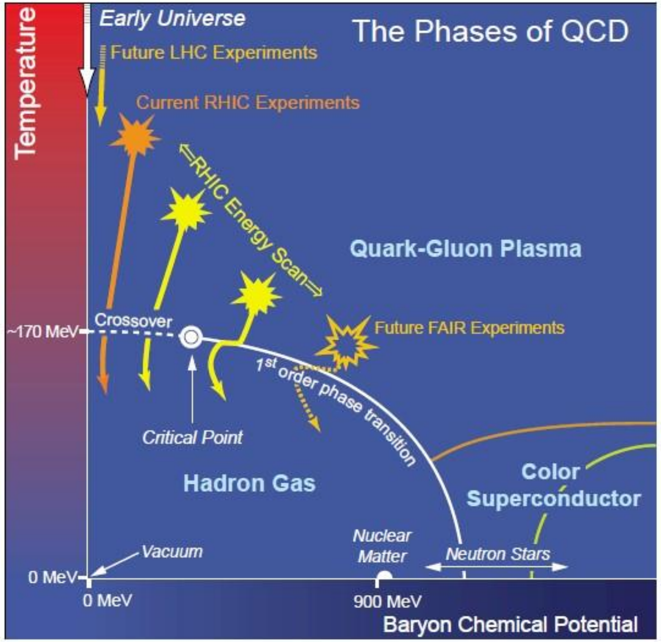
- State of the Art : **Hybrid Transport**

<u>Combine microscopic and macroscopic d.o.f</u>

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

- Matter in extreme conditions reveals its **constituents** : nuclear matter → quark matter

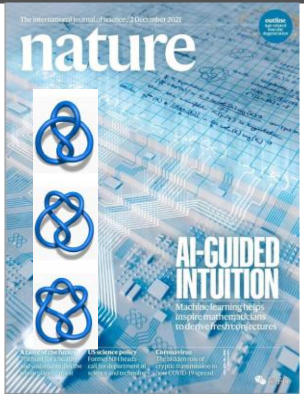


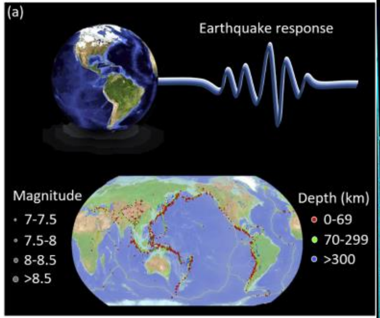


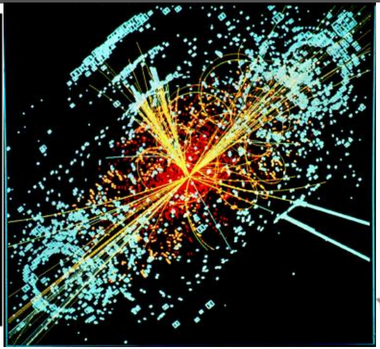
To study QCD matter under extreme conditions :

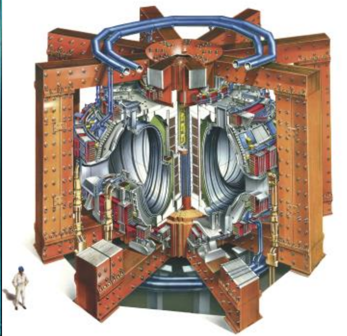
- **Nuclear Collisions** : heat & compress matter
- **Neutron Star** : dense matter, astronomy constraints
- **Lattice Field Theory** / fQCD / effective models

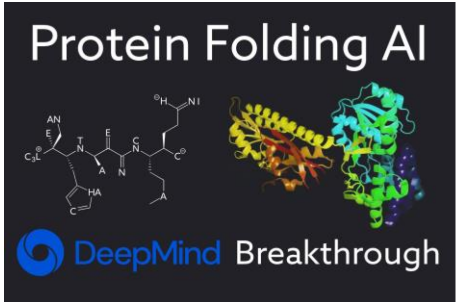
Overview : Machine- and Deep-Learning







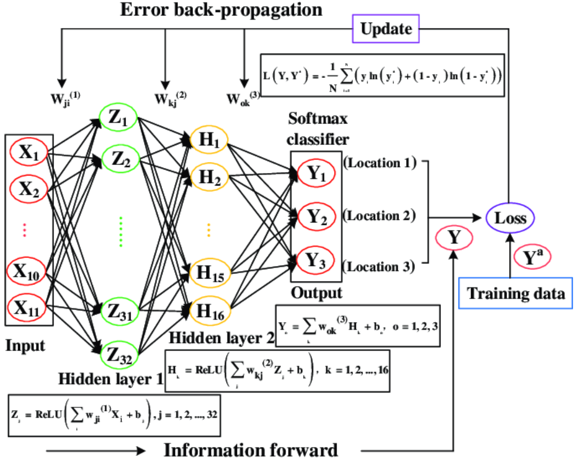




Find and Decode the mapping/representations into Deep Neural Network

➡ **Function approximator**

Universal approximator (Hastad et al 86 & 91)

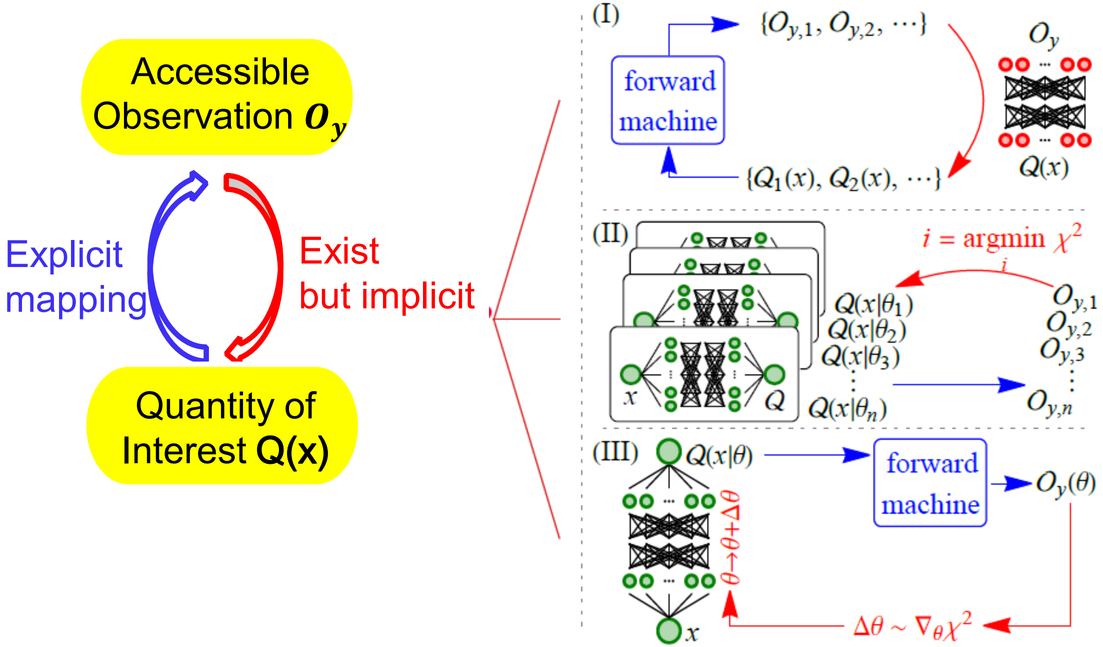


Differentiable programming

Backward Propagation

Gradient Descent Algorithm

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.

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

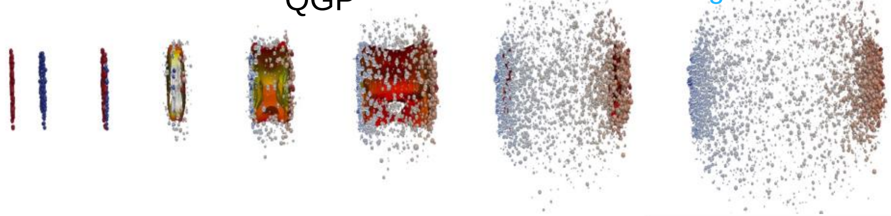
- **Automatic Differentiation :** fuse physical prior into reconstruction via differentiable programming strategy

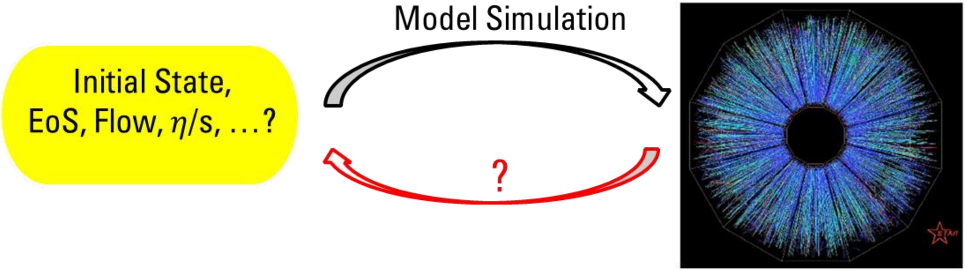
$$\frac{1}{2} \nabla_{\boldsymbol{\theta}} \chi^2 = \sum_y \frac{\mathcal{F}_y[\mathcal{Q}_{\text{NN}}(x|\boldsymbol{\theta})] - \mathcal{O}_y}{(\Delta \mathcal{O}_y)^2} \int \mathrm{d}x \frac{\delta \mathcal{F}_y[\mathcal{Q}(x)]}{\delta \mathcal{Q}(x)} \bigg|_{\mathcal{Q}(x) = \mathcal{Q}_{\text{NN}}(x|\boldsymbol{\theta})}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

Challenge in HIC and modern computational strategies

QGP

Fig: arXiv:1804.04649



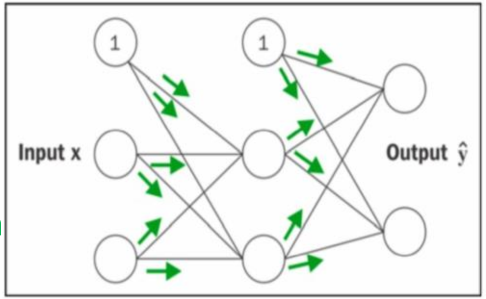


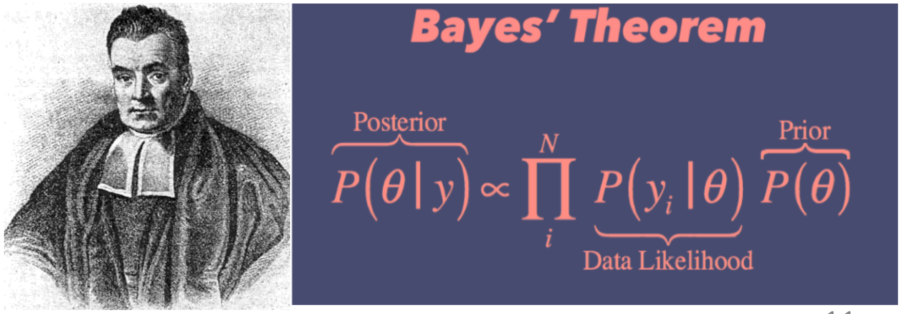
- **<u>Uncertainties</u>** in HIC modeling
- Multiple parameters **<u>entangle</u>** with multiple observables
- How to **<u>disentangle</u> different factors** to reveal fundamental physics from the dynamical environment final state?

Universal approximator

Differentiable programming

Gradient based optimization

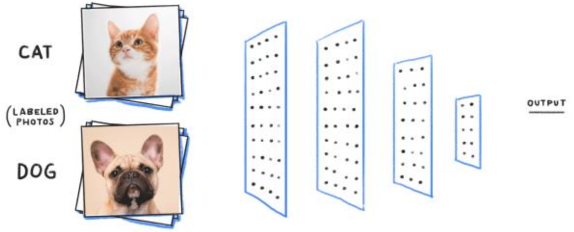


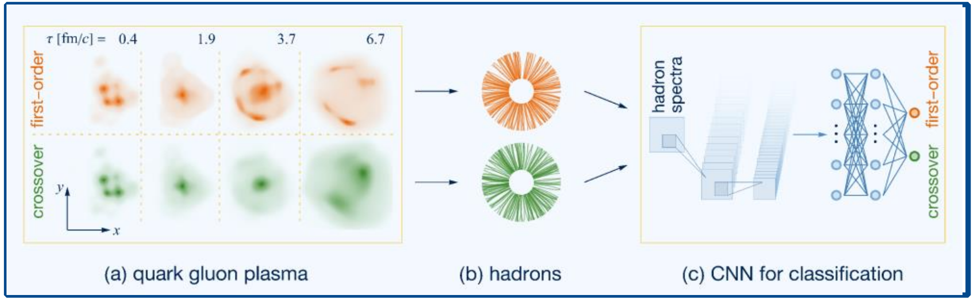


Direct inverse mapping with CNN for identifying QCD transition

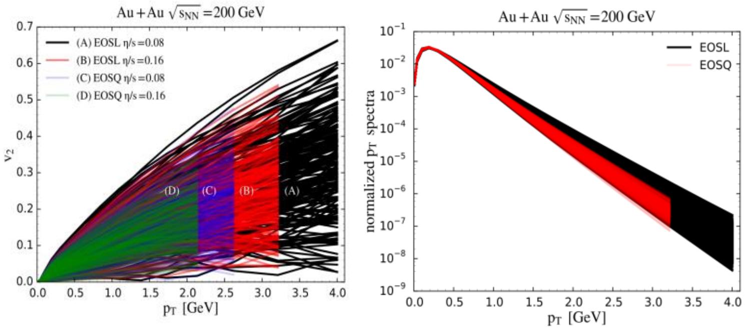
Data-driven
Inverse Mapping

Physics Simulation
provide the Prior





(a) quark gluon plasma (b) hadrons (c) CNN for classification

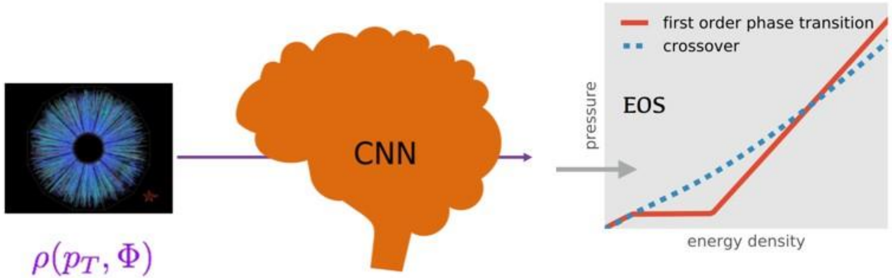


- Conventional obs. hard to distinguish
- Strongly influence from initial fluctuations and other uncertainties
- CNN : 95% event-by-event accuracy!
- Robust to initial conditions, eta/s

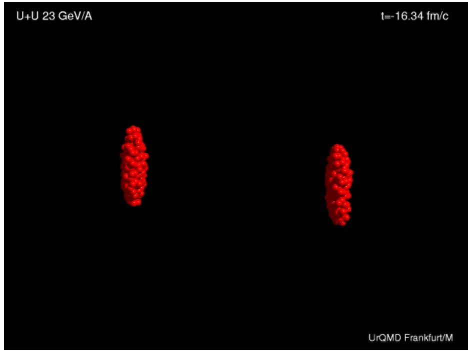
Conclusion : Information of early dynamics can **survive** to the end of hydrodynamics and encoded within the final state raw spectra, immune to evolution's uncertainties, **with deep CNN we can decode it back**.

L. Pang, K. Zhou, N. Su, H. Stoecker, H. Petersen, X. Wang, **Nature Commu.**9 (2018), no.1, 210

Into more realistic situations

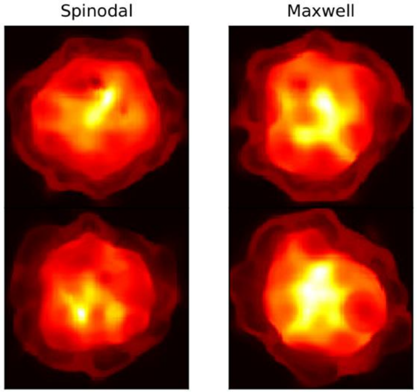


Hadronic cascade
(UrQMD considered)



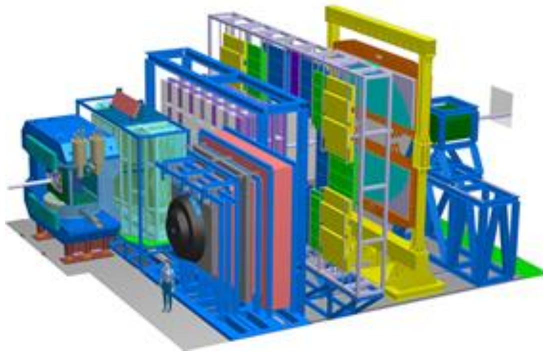
Eur. Phys. J. C 80 (2020) no.6,516

Non-equilibrium transition
(Baryon Clumping, spinodal)



JHEP 12,122(2019)
Phys. Rev. D 103,116023 (2021)

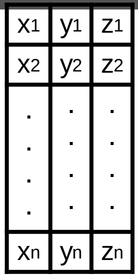
Detector effects
(Hits/Tracks, Point-Net)



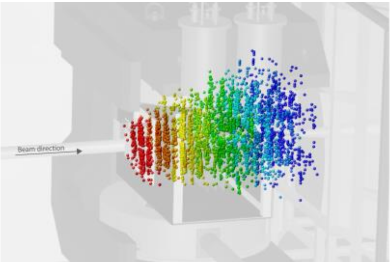
Phys. Lett. B 811, 135872
JHEP 21 (2021) 184

Point Cloud Network for Physics online analysis for HICs

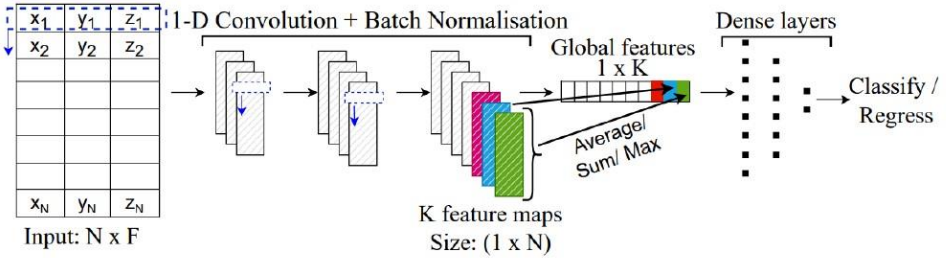
- Experimental data has inherent **point cloud structure**
  - **collection of particles** as *2D array* :



E	Px	Py	Pz	pid
6.84	1.07	4.5	6.83	211
40.4	0.06	0.54	40	321
…	…	…	…	…

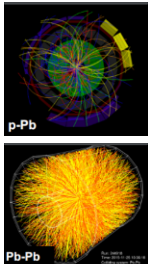


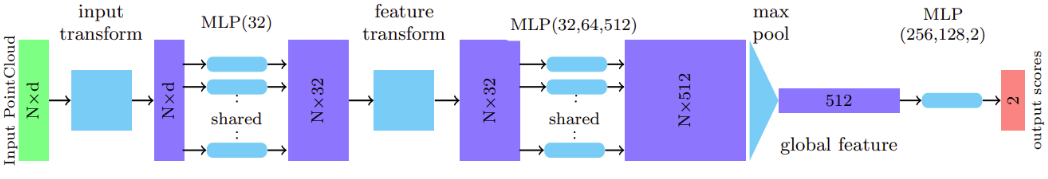
- PointNet based models learn directly from point clouds.
  - respects the **order invariance** of point clouds
  - direct processing of experimental data from detector ⇒ **ideal online analysis algorithm**
  - optimal for higher dimensional data

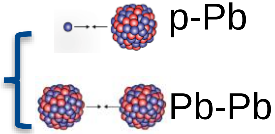


- **Collision Centrality Regression**
- **EoS Classification**
- **Small/ Large-system Identification**

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







S.Guo, H. Wang, K. Zhou, G. Ma, **Phy.Rev.C** 2024

Bayesian Reconstruction for dense matter EoS from HICs

- Hadronic cascade dominant

$$\dot{\mathbf{r}}_i = \frac{\partial \mathbf{H}}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i = -\frac{\partial \mathbf{H}}{\partial \mathbf{r}_i}$$

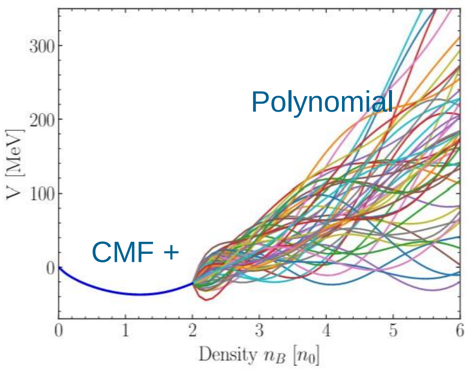
- **UrQMD model** adapted to any density dependent EoS →

$$\dot{\mathbf{p}}_i = -\frac{\partial \mathbf{H}}{\partial \mathbf{r}_i} = -\frac{\partial \mathbf{V}}{\partial \mathbf{r}_i}$$

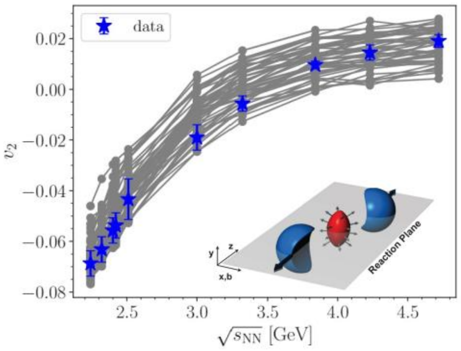
$$= -\left(\frac{\partial V_i}{\partial n_i} \cdot \frac{\partial n_i}{\partial \mathbf{r}_i}\right) - \left(\sum_{j \neq i} \frac{\partial V_j}{\partial n_j} \cdot \frac{\partial n_j}{\partial \mathbf{r}_i}\right)$$

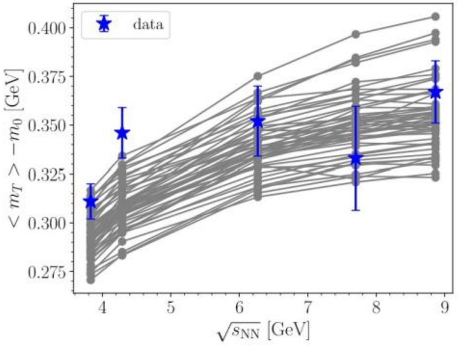
via density dependent potential

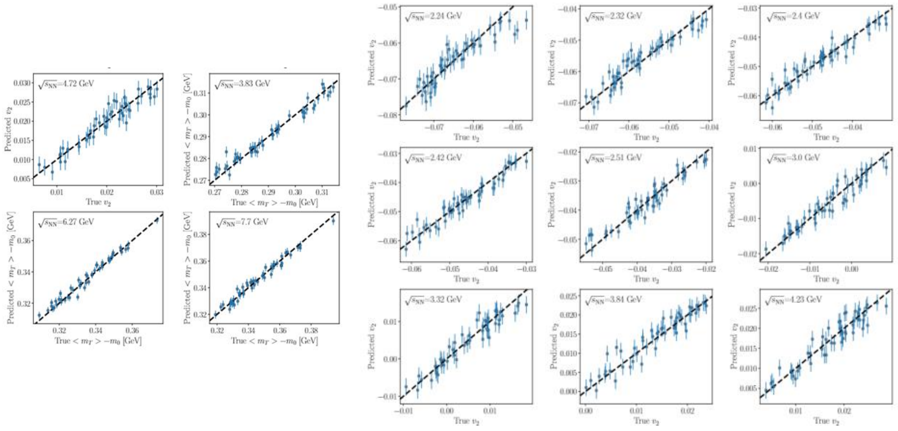
Eur.Phys.J.C82(2022)5,417



Evidence : proton's v2 and transverse kinetic energy





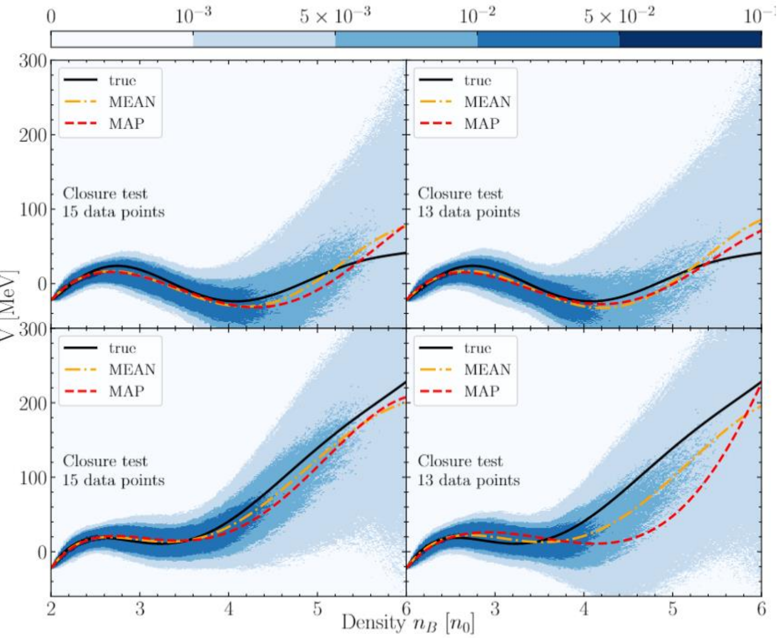


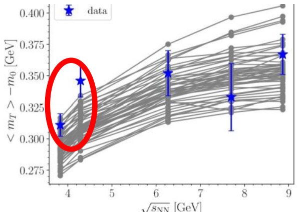
- Gaussian Process **Emulator** : $Obs_i(\boldsymbol{\theta}) \sim GP(\mu(\boldsymbol{\theta}), \kappa(\boldsymbol{\theta}, \boldsymbol{\theta}'))$
- The trained emulator predict observables well: $\boldsymbol{R^2} \sim \mathbf{0.9}$

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

Bayesian Reconstruction of dense matter EoS from HICs

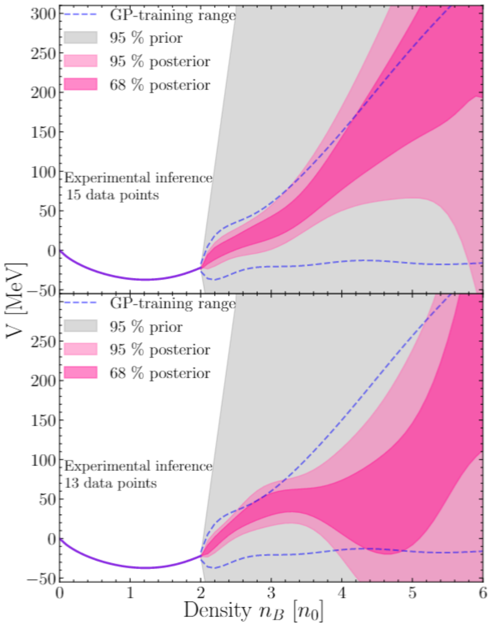
- **Posterior** ~ Likelihood * Prior

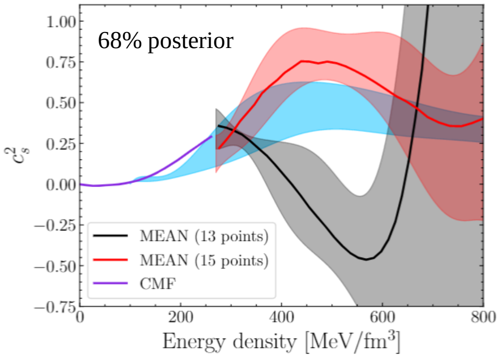


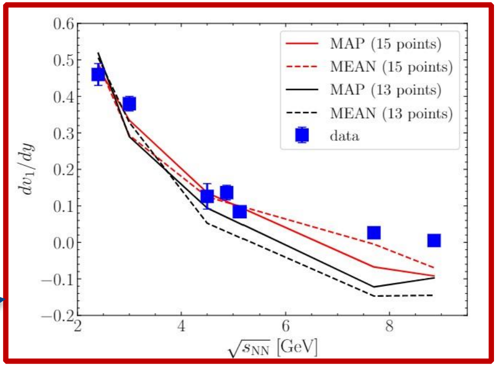


Phys. Rev. Lett.
131 (2023) 202303

- With real experimental data







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

HQ Potential Model, Inverse Shroedinger Eq.

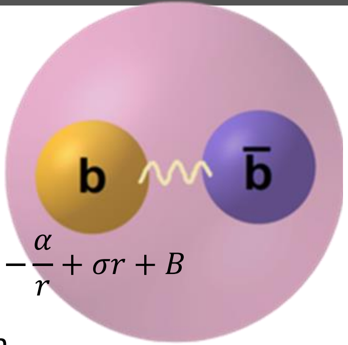
Large mass scale : $m_Q >> \Lambda_{QCD}, T, p$

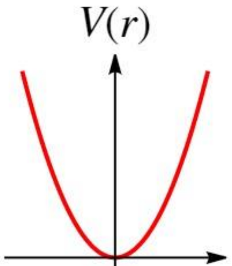
- Hard Process production in early stage
- 'Calibrated' QCD Force – HQ interaction

Vacuum: NRQCD, Cornell-like $V(r) = -\frac{\alpha}{r} + \sigma r + B$

Medium: Color Screening, Thermal width

Laine, et.al, JHEP(2



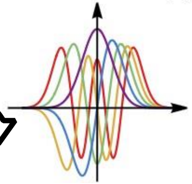


$$V(T,r) = V_R(T,r) + i \cdot V_I(T,r)$$

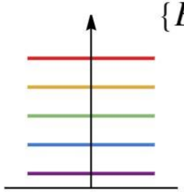
Inverse Power method

H.W.Crater, JCP(1994)

$\{\psi_n(r)\}$



$\{E_n\}$



$$\begin{cases} \mathrm{Re}[E_n] = m - 2m_b \\ \mathrm{Im}[E_n] = -\Gamma \end{cases}$$

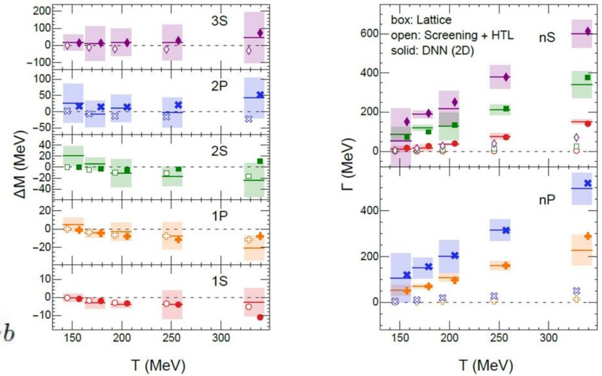
?

Large mass scale :

$$\hat{H}\psi_n = -\frac{\nabla^2}{2m_\mu}\psi_n + V(r)\psi_n = E_n\psi_n$$

M. Strickland, et.at., PRC(2015) PRD(2018), PLB(2020)

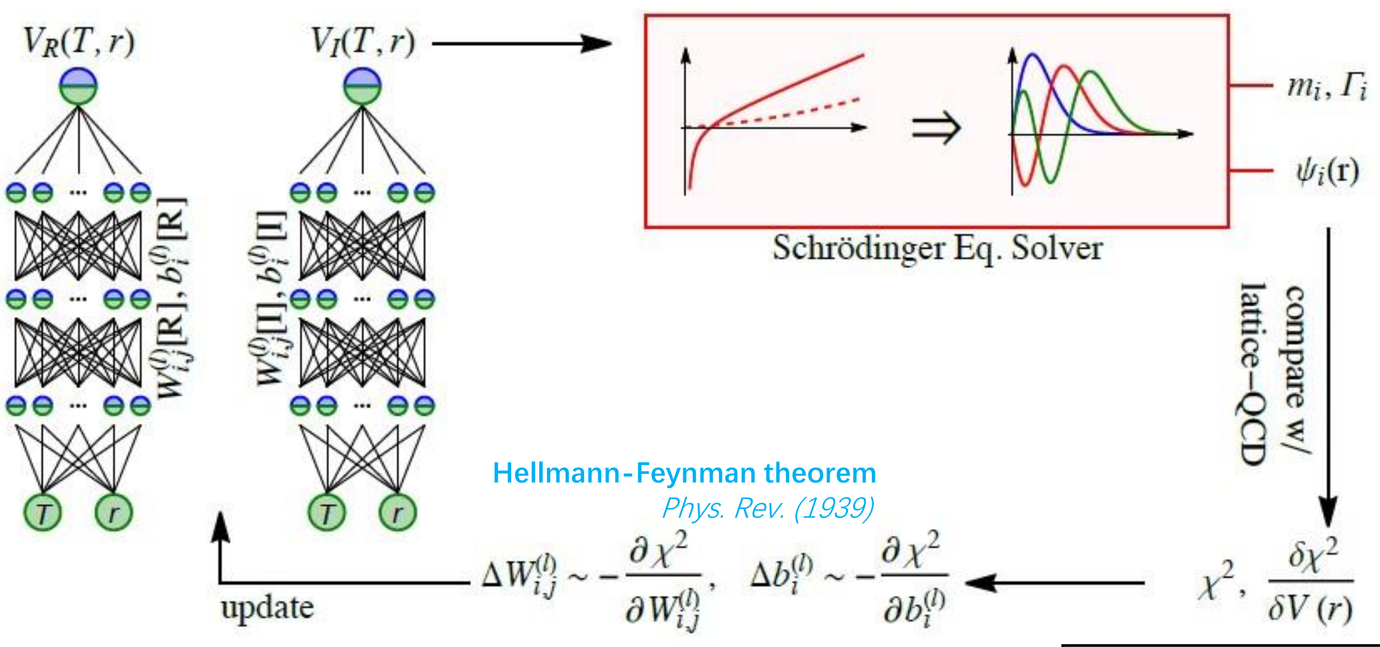
New lQCD results cannot be explained by Perturbative HTL-inspired potentials !



R. Larsen, et.al, PRD(2019), PLB(2020), PRD(2020)

How to extract effective potential given limited spectroscopy ?

Flow chart for “DNN + Schrödinger Eq.”



Hellmann-Feynman theorem
Phys. Rev. (1939)

$$\chi^2 = \sum_{T,i} \frac{(m_{T,i} - m_{T,i}^{\text{lattice}})^2}{(\delta m_{T,i}^{\text{lattice}})^2} + \frac{(\Gamma_{T,i} - \Gamma_{T,i}^{\text{lattice}})^2}{(\delta \Gamma_{T,i}^{\text{lattice}})^2}$$

$$T \in \{0, 151, 173, 199, 251, 334\} \text{ MeV}$$

$$i \in \{1S, 2S, 3S, 1P, 2P\}$$

$$J(\boldsymbol{\theta}) = \frac{1}{2}\chi^2(\boldsymbol{\theta}) + \frac{\lambda}{2}\boldsymbol{\theta} \cdot \boldsymbol{\theta},$$

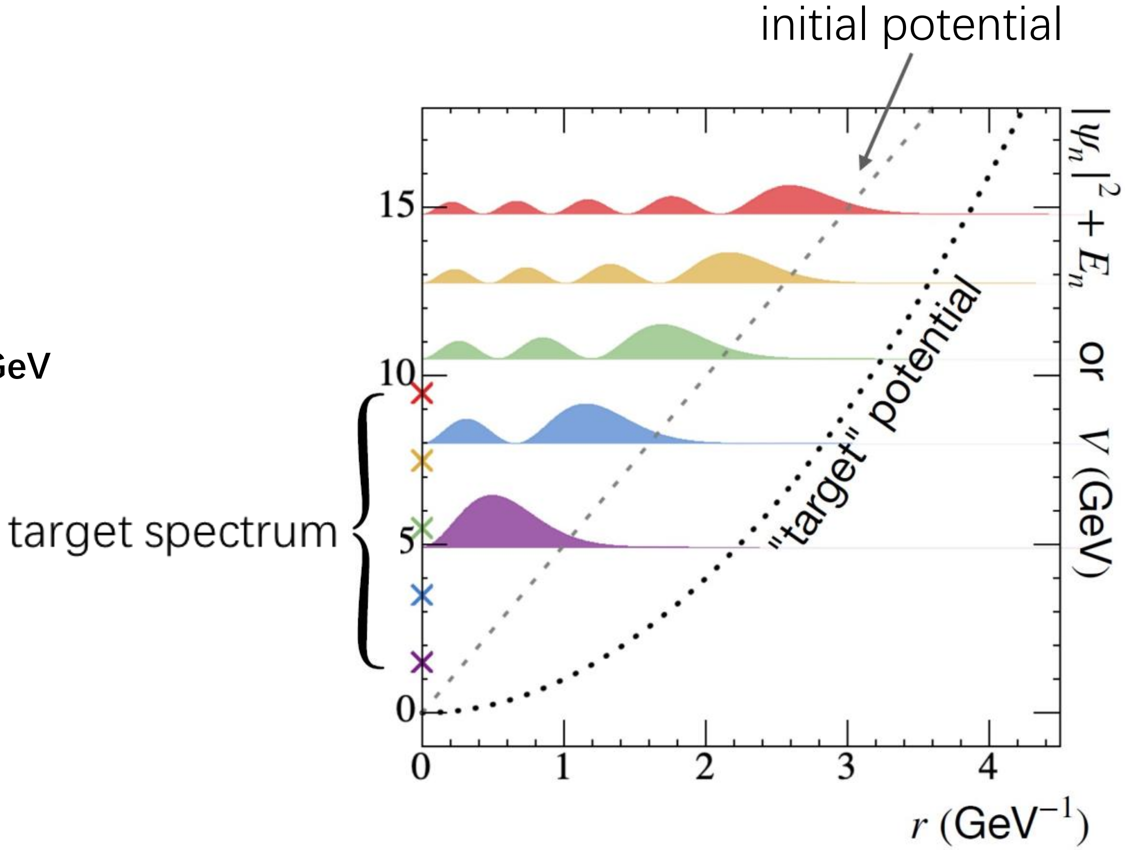
S.Shi, K. Zhou, et al., *Phys. Rev. D* 105 (2022) 1, 1

Proof of Concept

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

Learn V(r) from 5 eigenvalues :

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



<u>limited spectrum { En }</u> to <u>continuous interaction V(r)</u> ?

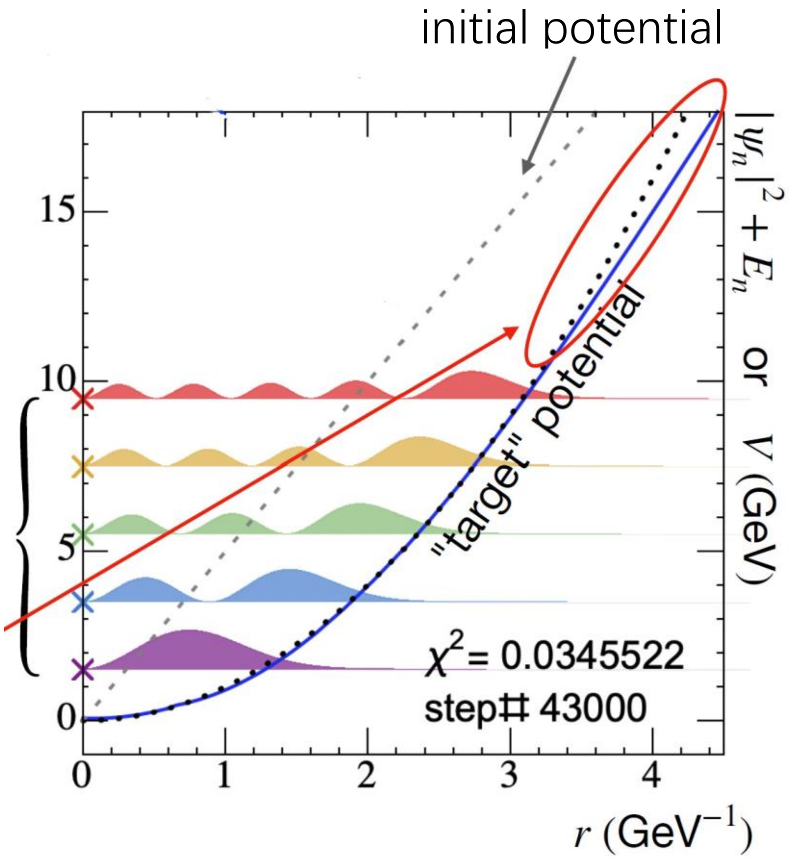
-- Yes! But to some range decided by the used states.

Learn V(r) from 5 eigenvalues :

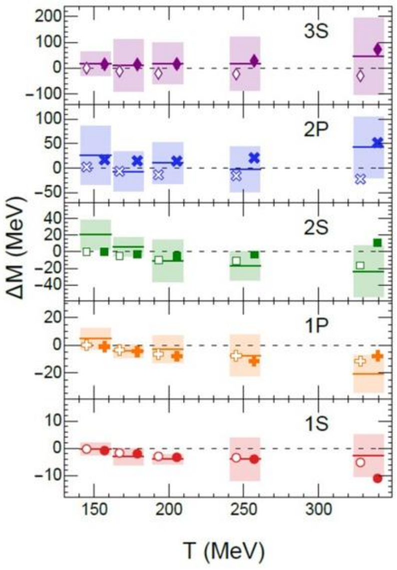
{ En } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV

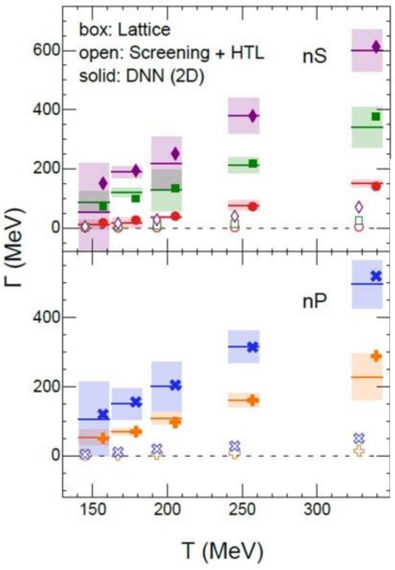
Deviation @ given states' wavefunction vanishes

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



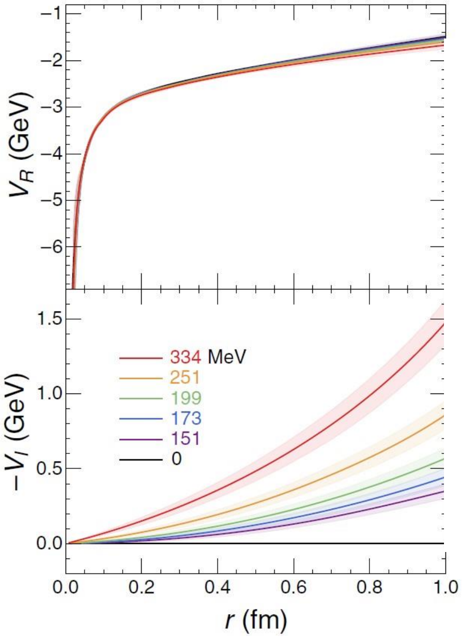
Results with lattice data for mass/width and the reconstructed HQ Potential

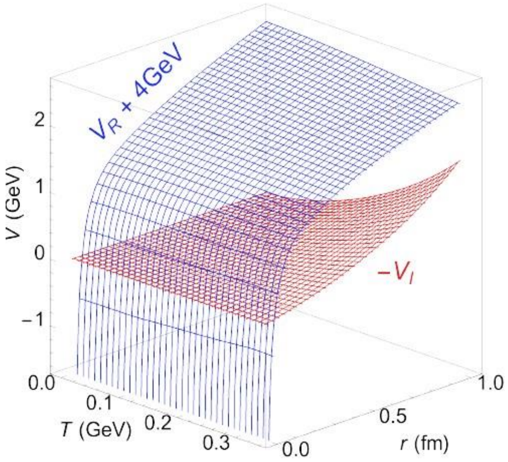




Chi2-per-data=16.5/30

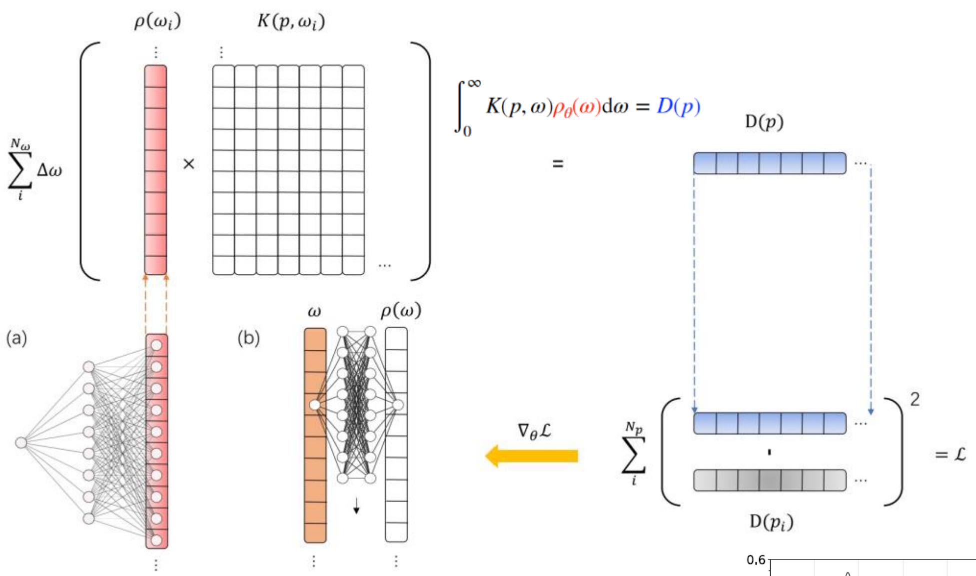
The reconstructed T, r dependent potential

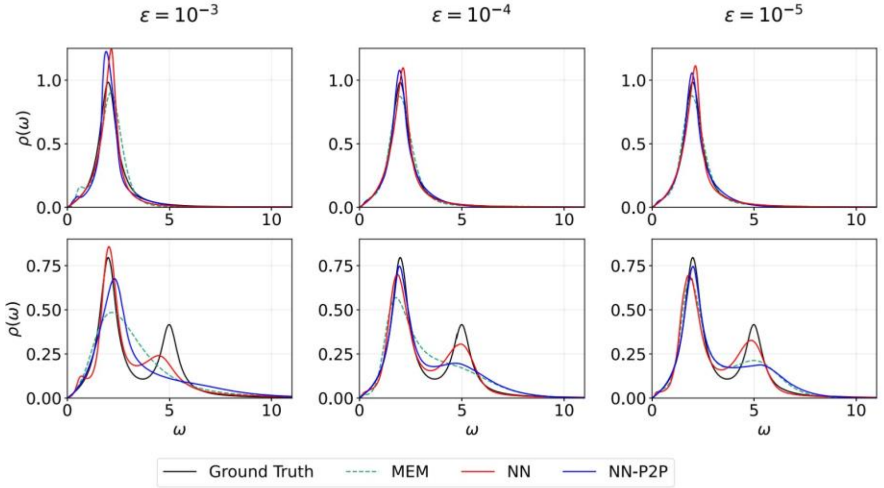


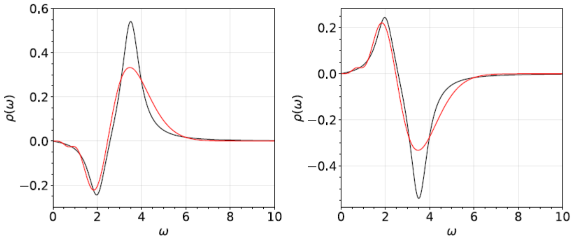


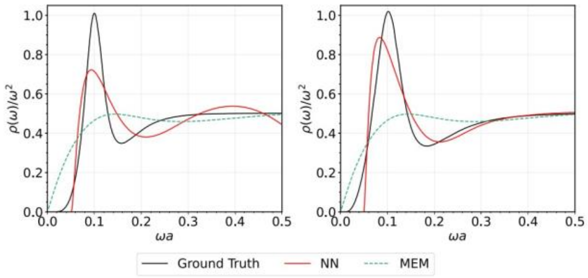
S. Shi, K. Zhou, et al., *Phys. Rev. D* 105 (2022) 1, 1

Spectral function reconstruction from Euclidean correlator









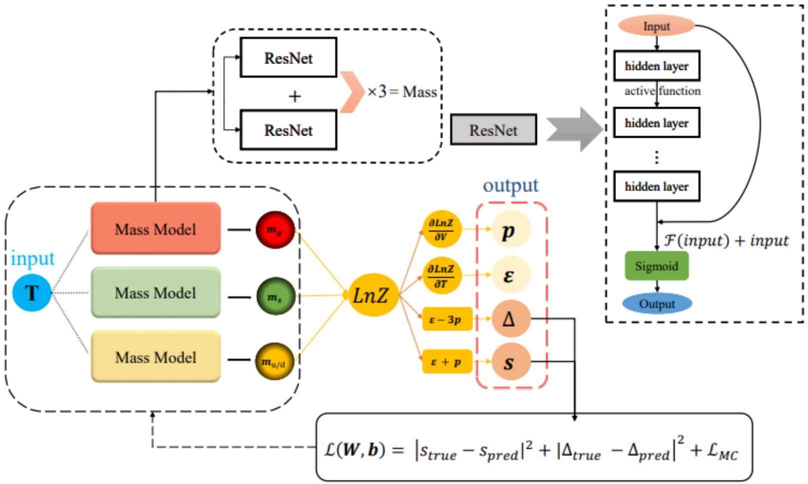
$$G(\tau, T) = \int_0^\infty \frac{d\omega}{2\pi} K(\omega, \tau, T)\rho(\omega, T)$$

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

L. Wang, S. Shi and K. Zhou

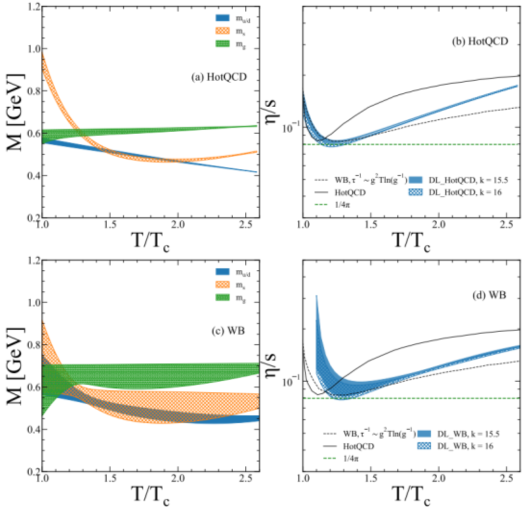
NeurIPS2021 ‘Machine learning and the Physical Science’,
Phys. Rev. D 106, L051502 (Letter),
Computer Physics Communications (2022) 108547,

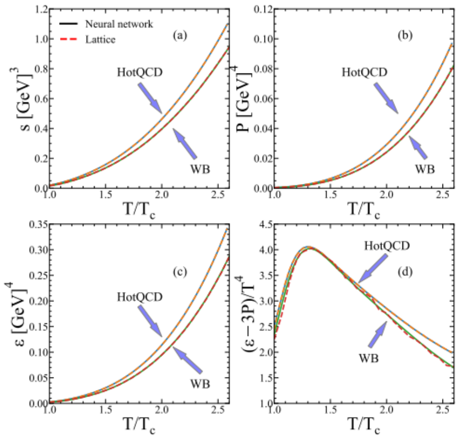
Quasi-particle analysis of lQCD thermodynamics



$$\ln Z_g(T) = -\frac{16V}{2\pi^2}\int_0^\infty p^2 dp \ln\left[1-\exp\left(-\frac{1}{T}\sqrt{p^2+m_g^2(T)}\right)\right], \quad (2)$$

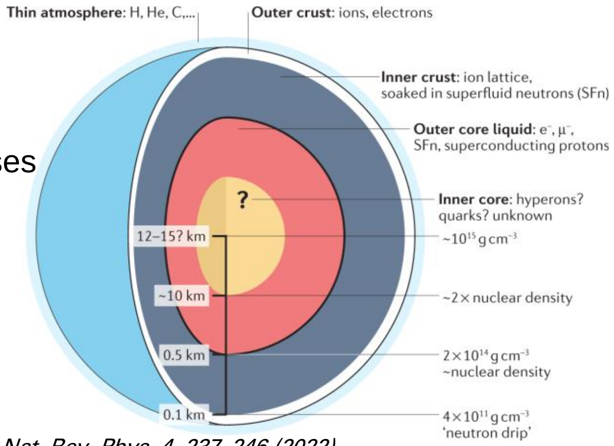
$$\ln Z_{q_i}(T) = +\frac{12V}{2\pi^2}\int_0^\infty p^2 dp \ln\left[1+\exp\left(-\frac{1}{T}\sqrt{p^2+m_{q_i}^2(T)}\right)\right], \quad (3)$$





F. Li, H. Lue, L. Pang and G. Qin, Phys. Lett. B 844 (2023) 138088

From EoS to NS Stellar Structure (MR)



Nat. Rev. Phys. 4, 237–246 (2022)

- Mass ~ 2 solar masses
- Radii ~ 10 km
- Densities 5-8 ρ_0

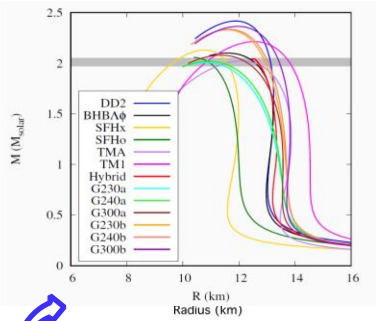
- Gravity ← → Pressure

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

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

- Dense matter Equation of State $P(\rho)$

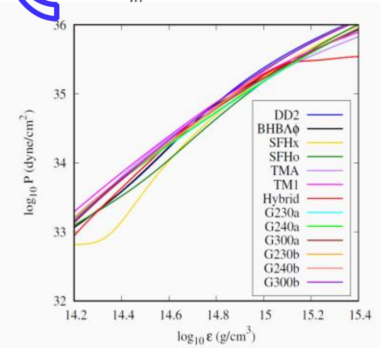
- <u>Noisy/Limited NS Observables</u> to <u>EoS</u> ?



TOV equations

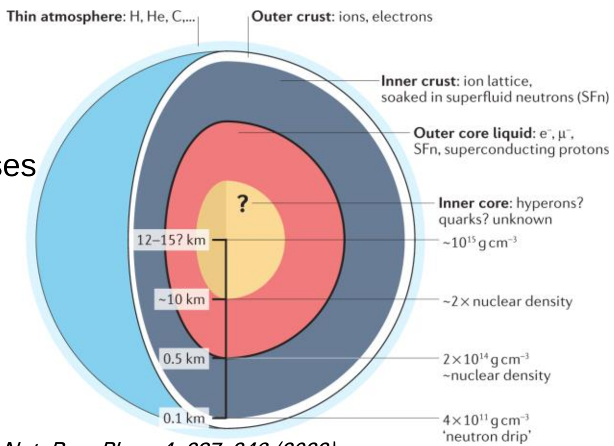
$$-\frac{dP}{dr} = \frac{[\epsilon(r) + P(r)][M(r) + 4\pi r^3 P(r)]}{r[r - 2M(r)]}$$

$$\frac{dM(r)}{dr} = 4\pi r^2 \epsilon(r),$$



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

- Mass ~ 2 solar masses
- Radii ~ 10 km
- Densities 5-8 ρ_0



Nat. Rev. Phys. 4, 237–246 (2022)

- Gravity ← → Pressure

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

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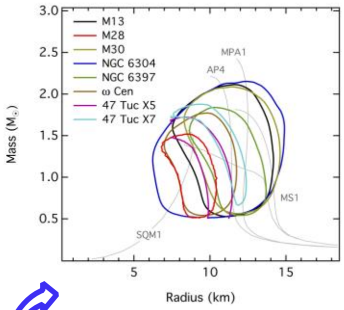
- Noisy/Limited NS Observables to EoS ?



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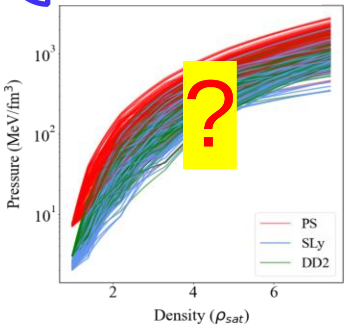
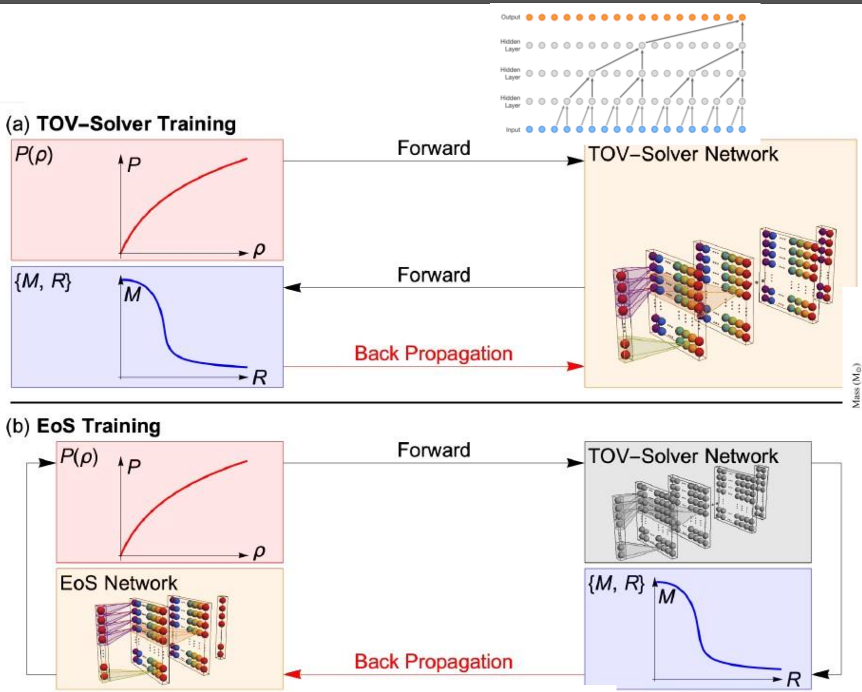


Auto-diff framework and Results



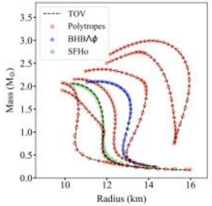
$$\mathscr{L} = \chi^2 = \sum_{i=1}^{N_{\rm obs}} \frac{(M_i - M_{{\rm obs},i})^2}{\Delta M_i^2} + \frac{(R_i - R_{{\rm obs},i})^2}{\Delta R_i^2}$$

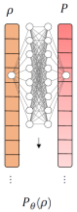
Loss function

$$g_t = \frac{\delta \chi^2}{\delta \theta_t} = \frac{\delta \chi^2}{\delta \mathbf{z}} \frac{\delta \mathbf{z}}{\delta x} \frac{\delta x}{\delta \theta_t}$$

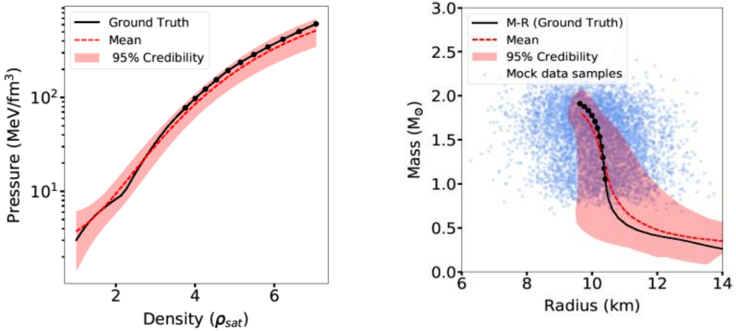
$\mathbf{z} = (M_i, R_i), x = P_i(\rho_i)$

Gradients

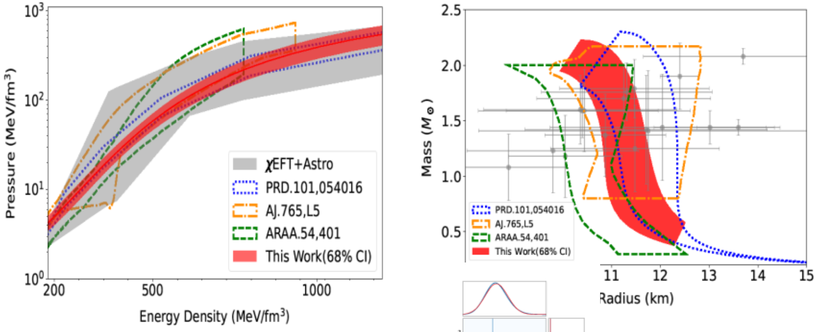


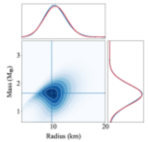


- Well validated through **Mock Tests**



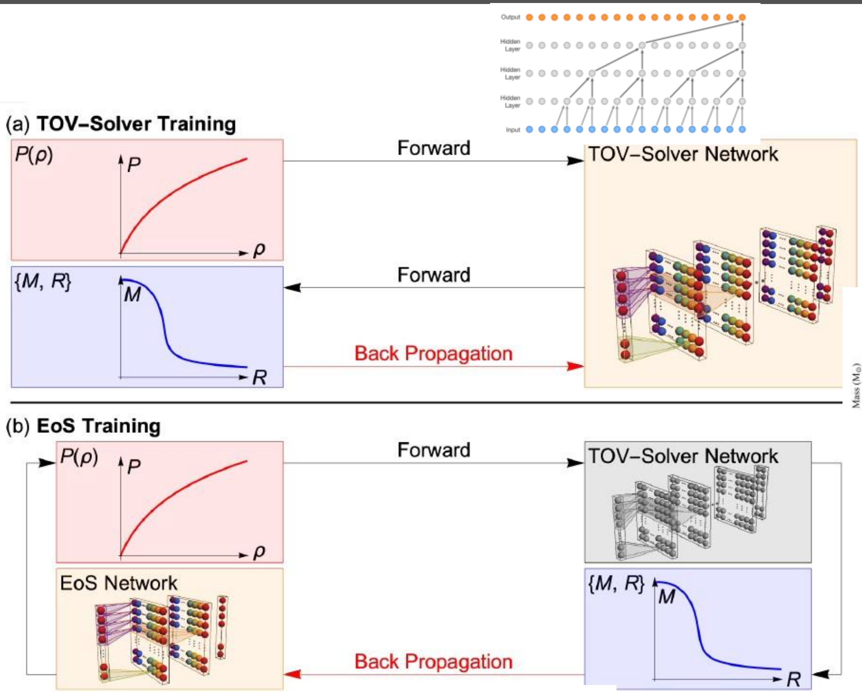
- With **real observable** we reconstruct the NS EoS also





S. Soma, L. Wang, S. Shi, H. Stoecker, K. Zhou, **JCAP** 98 (2022) 071
S. Soma, L. Wang, S. Shi, H. Stoecker, K. Zhou, **Phys. Rev. D** 107 (2023)083028

Auto-diff framework and Results



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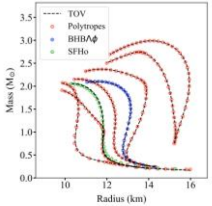
Loss function

$$g_t = \frac{\delta\chi^2}{\delta\theta_t} = \frac{\delta\chi^2}{\delta \mathbf{z}}\frac{\delta \mathbf{z}}{\delta x}\frac{\delta x}{\delta\theta_t}$$

$\mathbf{z} = (M_i, R_i), x = P_i(\rho_i)$

Gradients



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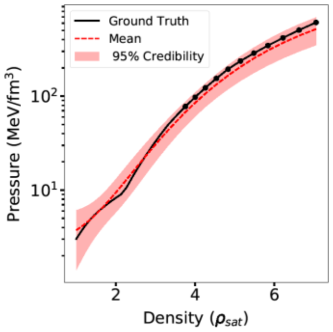

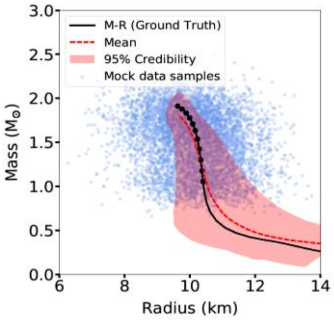

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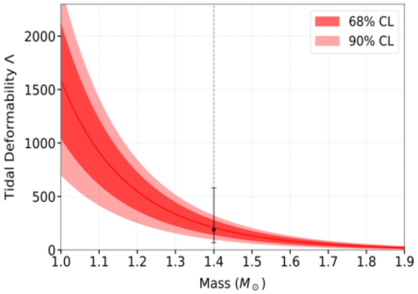
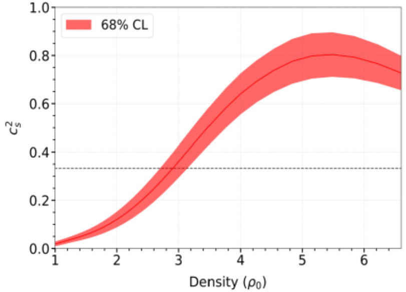
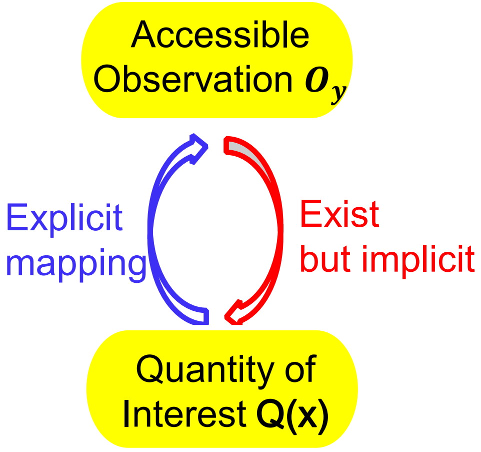
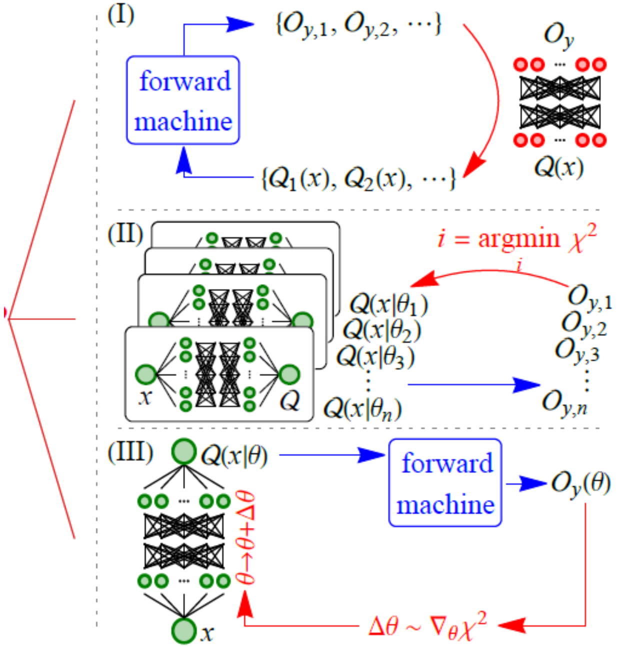




S. Soma, L. Wang, S. Shi, H. Stoecker, K. Zhou, **JCAP** 98 (2022) 071
S. Soma, L. Wang, S. Shi, H. Stoecker, K. Zhou, **Phys. Rev. D** 107 (2023)083028

Summary : 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

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

Summary

- **Deep Learning** can help bridging HIC experiment with theory/model for physics exploration caveat: model dependency
- **Bayesian Inference** for EoS from different beam energy experiment data (v2 and mT) perform well - consistent with dv1/dy measurements and BNSM constraint
  sensitivity check reveals tension: measurement uncertainty or model limitation
- **Auto-diff** can help physics extraction for lattice measurements
- **Flexible DNN represented** EoS of Neutron Star can be inferred from astro-obs. (M-R) via **auto-diff based inference** with uncertainty well estimated

→ Combined global fit of EoS from HIC and NS obs. ? (need to take care of isospin dependence)

Thanks！

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

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

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

Progress in Particle and Nuclear Physics 135 (2024) 104084

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

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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*

ARTICLE INFO

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

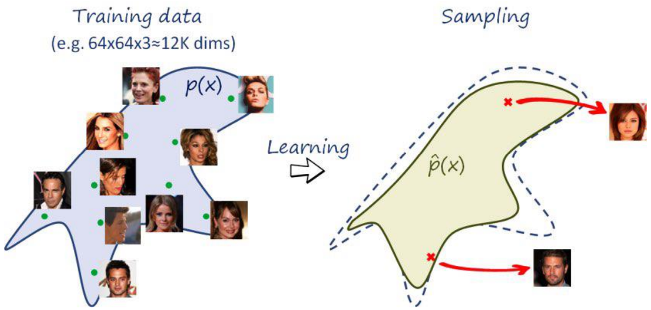
ABSTRACT

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.

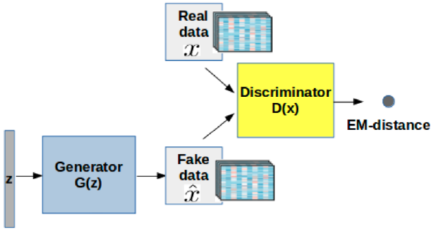
Prog. Part. Nucl. Phys. 135 (2024) 104084

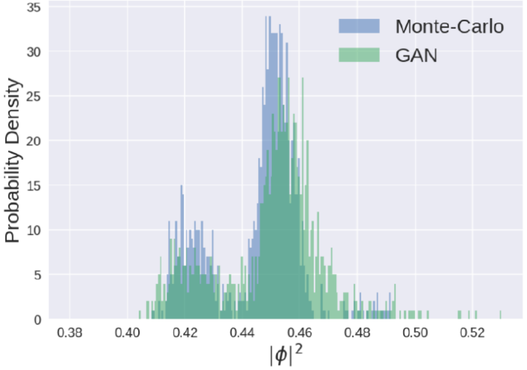
Thanks!

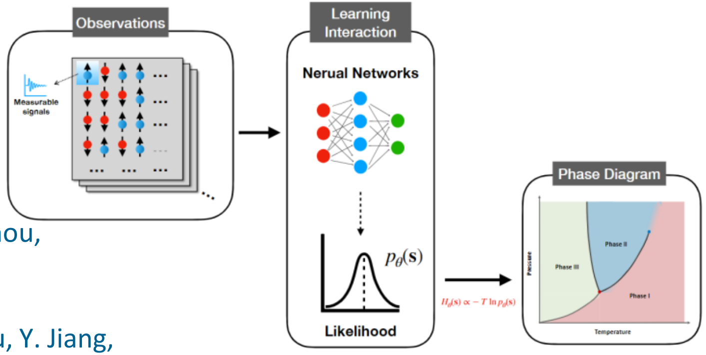
Generative AI: Given an ensemble of data from the target distribution

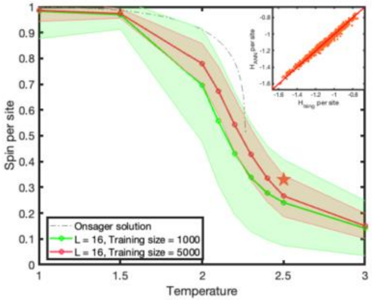


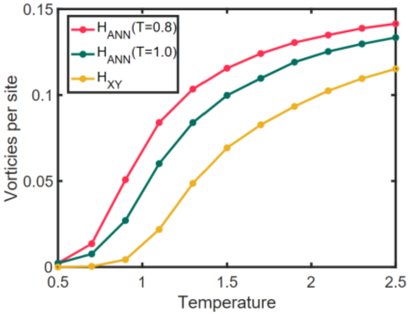
K. Zhou, G. Endrődi, L.-G. Pang, and H. Stöcker,
PRD 100, 011501 (2019)











L. Wang, L. He, Y. Jiang, K. Zhou,
arXiv:2007.01037

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

Suppose knowing unnormalized probability distribution

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

- Reverse KL divergence

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

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

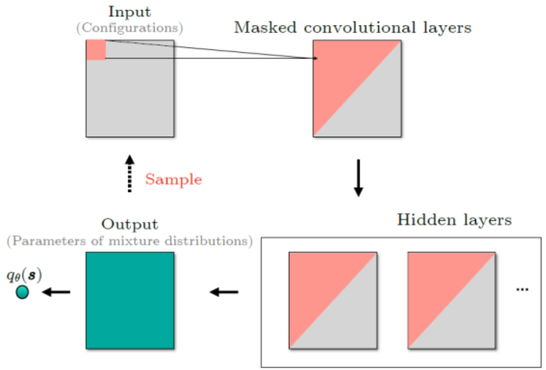
- Autoregressive

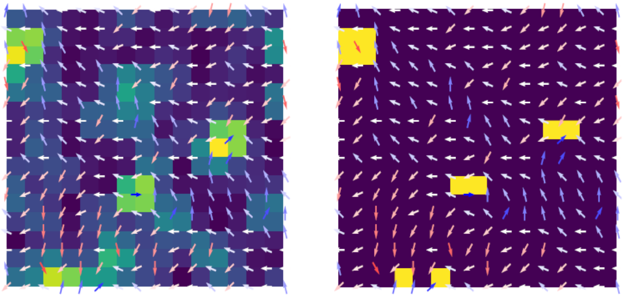
$$q_\theta(\mathbf{s}) = \prod_{i=1}^{N} q_\theta(s_i \mid s_1, \ldots, s_{i-1})$$

D. Wu, Lei Wang and P. Zhang, **PRL122,080602(2019)**

- Continuous Autoregressive for XY model

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





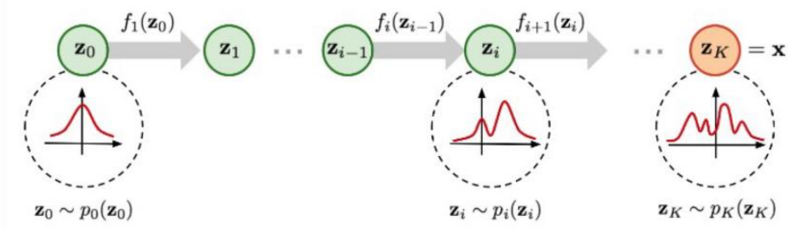
Probability distributions from CANs

Vortices

Flow based generative model given unnormalized distribution

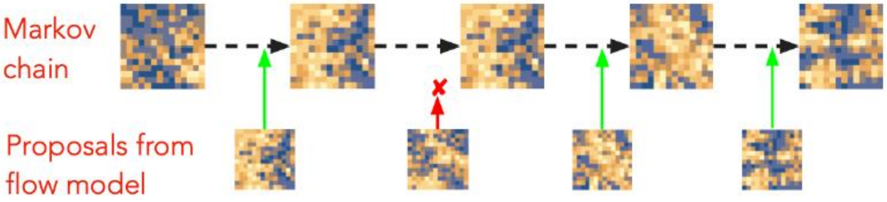
A series **(Flow)** of invertible/bijective transformations for p(z)

<u>compose several invertible transformations to form the flow :</u>



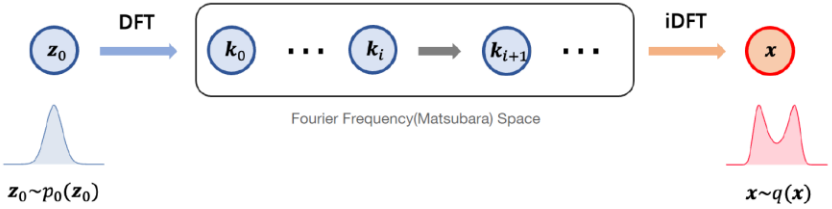
$$p_i(\mathbf{z}_i) = p_{i-1}(f_i^{-1}(\mathbf{z}_i))|\det J_{f_i^{-1}}| = p_{i-1}(\mathbf{z}_{i-1})|\det J_{f_i}|^{-1}$$

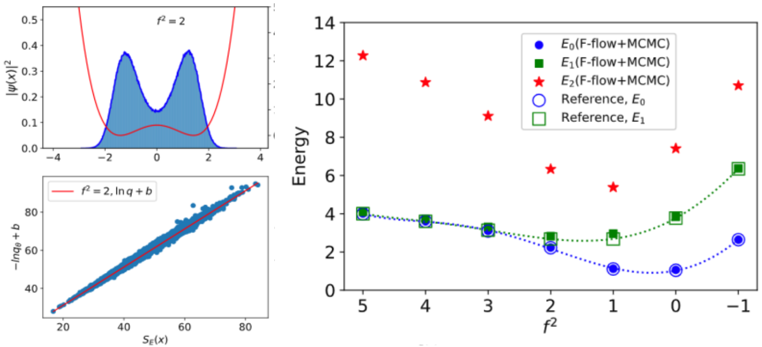
$$\rightarrow \log p(\mathbf{x}) = \log p_0(f^{-1}(\mathbf{x})) + \sum_{i=1}^{K} \log|\det J_{f_i^{-1}}| = \log p_0(\mathbf{z}_0) - \sum_{i=1}^{K} \log|\det J_{f_i}|$$



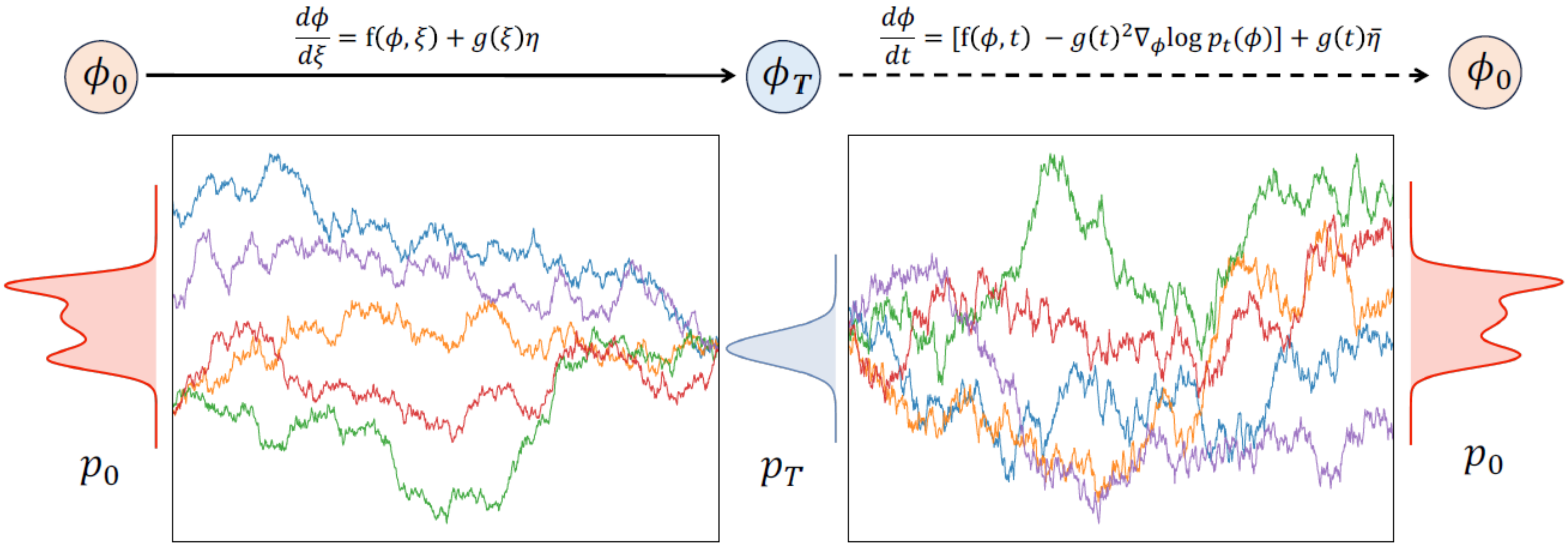
Fourier Flow Model

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





Diffusion Model on lattice QFT configurations



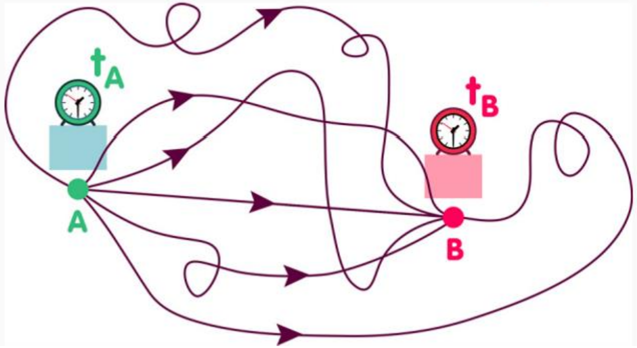
L. Wang, G. Arts, K. Zhou, JHEP 05 (2024) 060
L. Wang, G. Arts, K. Zhou, arXiv:2311.03578 (NeurIPS 2023 workshop “ML&Physical Sciences”)
G. Aarts, D. E. Habibi, L. Wang, K. Zhou, arXiv:2410:21212 (NeurIPS 2024 workshop “ML&Physical Sciences)
Q. Zhu, G. Aarts, W. Wang, K. Zhou, L. Wang, arXiv:2410.19602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

- **Stochastic vibration**

$$i\hbar\frac{\partial}{\partial t}\Psi=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

$$\frac{\partial\phi(x,t)}{\partial t}=D\frac{\partial^2\phi(x,t)}{\partial x^2}$$

In Feynman's formulation of quantum mechanics in Euclidean space:



$$\mathcal{Z}=\int \mathcal{D}x\, e^{-S_E[x]/\hbar}$$

$$\langle 0|\hat{x}^N|0\rangle=\frac{1}{\mathcal{Z}}\int \mathcal{D}x\, x^N e^{-S_E[x]/\hbar}$$

One can construct stochastic process to reproduce the quantum path Integral with its equilibrium:

$$e^{-S_E[x]/\hbar}\rightarrow\frac{\partial x}{\partial\tau}=-\frac{\delta S_E[x]}{\delta x}+\eta\begin{cases}\langle\,\eta(t,\tau)\,\rangle_\eta=0\\ \langle\,\eta(t,\tau)\eta(t',\tau')\,\rangle_\eta=2\hbar\delta(t-t')\delta(\tau-\tau')\end{cases}$$

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

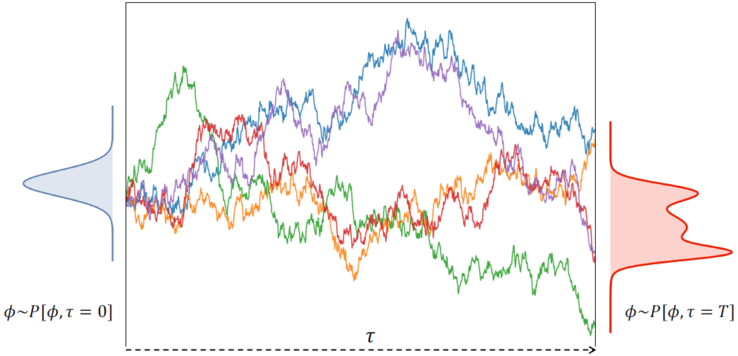
Stochastic Quantization

- **Stochastic quantization** $Z = \int D\phi\, e^{-S_E}$ $\qquad p(\phi) = \dfrac{e^{-S_E(\phi)}}{Z}$

$$\frac{\partial \phi(x,\tau)}{\partial \tau} = -\frac{\delta S_E[\phi]}{\delta \phi(x,\tau)} + \eta(x,\tau) \qquad \langle \eta(x,\tau)\rangle = 0, \qquad \langle \eta(x,\tau)\eta(x',\tau')\rangle = 2\alpha\delta(x-x')\delta(\tau-\tau')$$

- **Fokker-Planck equation** $\dfrac{\partial P[\phi,\tau]}{\partial \tau} = \int d^n x \left\{ \dfrac{\delta}{\delta\phi}\left(\alpha \dfrac{\delta}{\delta\phi} + \dfrac{\delta S_E}{\delta \phi}\right)\right\} P[\phi,\tau]$

long time equilibrium limit → $P_{\text{eq}}[\phi] \propto e^{-\frac{1}{\alpha}S_E[\phi]}$

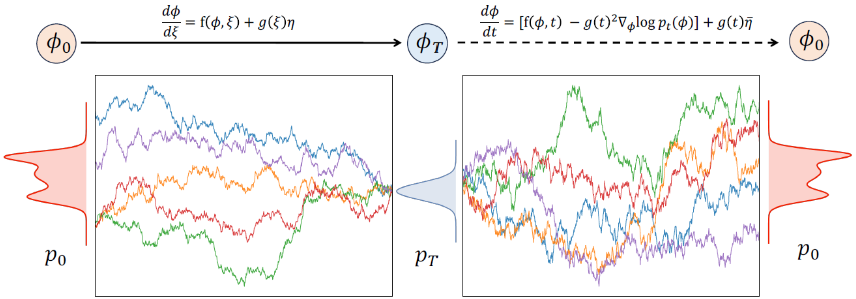


- **Observables** $\langle \mathcal{O}[\phi]\rangle_\tau = \int D\phi\, \mathcal{O}[\phi] P[\phi,\tau]$

$$\langle \mathcal{O}[\phi]\rangle_{\tau\to\infty} = \frac{\int D\phi\, \mathcal{O}(\phi) e^{-\frac{1}{\hbar}S_E(\phi)}}{\int D\phi\, e^{-\frac{1}{\hbar}S_E(\phi)}} = \langle \mathcal{O}[\phi]\rangle_{\text{quantum}}$$

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

Diffusion Model for field configurations



- Forward diffusion SDE

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

- 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**

$$\frac{d\phi}{dt} = \left[f(\phi,t) - g^2(t)s_{\hat{\theta}}(\phi,t)\right] + g(t)\bar{\eta}(t).$$

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

Denoising within DM as Stochastic Quantization

- Backward diffusion SDE in **variance expanding** scheme (i.e., vanishing drift in Forward)

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

- Redefine time $\tau \equiv T - t$ and denoting $g_\tau = g(T-\tau),\ q_\tau(\phi) = p_{T-\tau}(\phi)$

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

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

- The corresponding Fokker-Planck equation and equilibrium

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

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

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

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

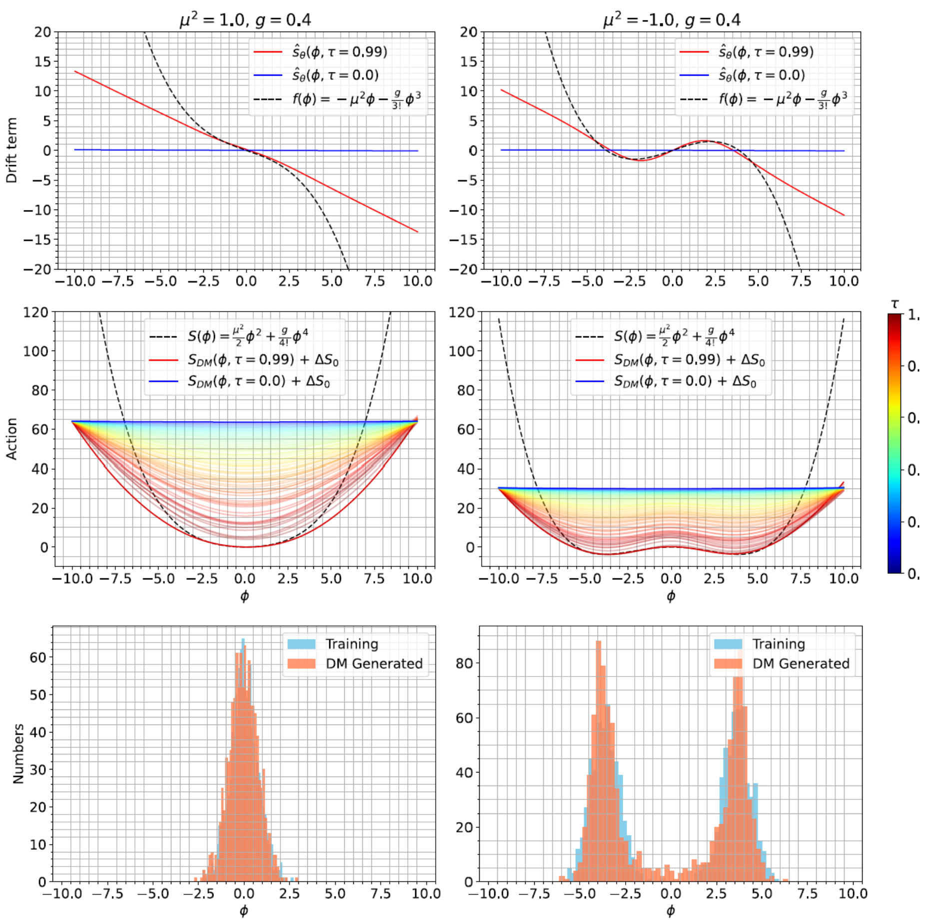
$$p_{\tau=T}(\phi) \to P[\phi, T]$$

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

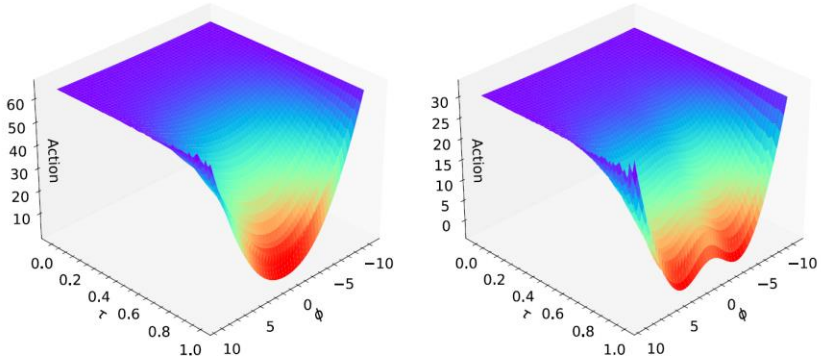
sampling from a DM is equivalent to optimizing a stochastic trajectory to approach the "equilibrium state"

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

Effective Action on toy model



- Flow of an effective action



DM on scalar phi4 model

- Consider a real scalar field with action:

$$S = \int \mathrm{d}^d x \mathrm{d}t \mathcal{L} = \int \mathrm{d}^d x \mathrm{d}t (\frac{1}{2}(\partial^2 \phi_0^2 - m^2 \phi_0^2) - \frac{\lambda_0}{4!}\phi_0^4),$$

- In Euclidean space, the discretized action with dimension less form:

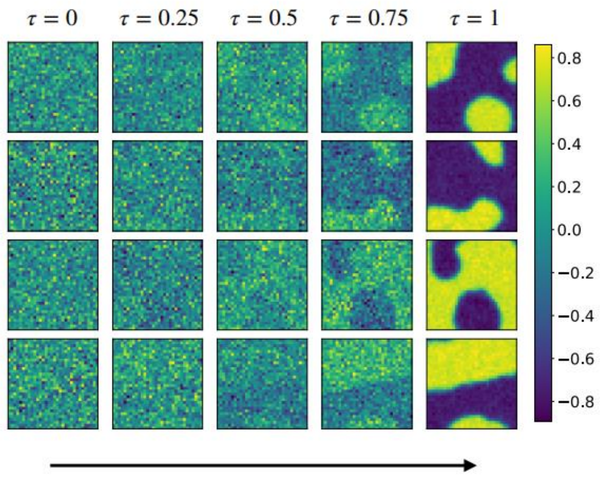
$$S_E = \sum_x [-2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4].$$

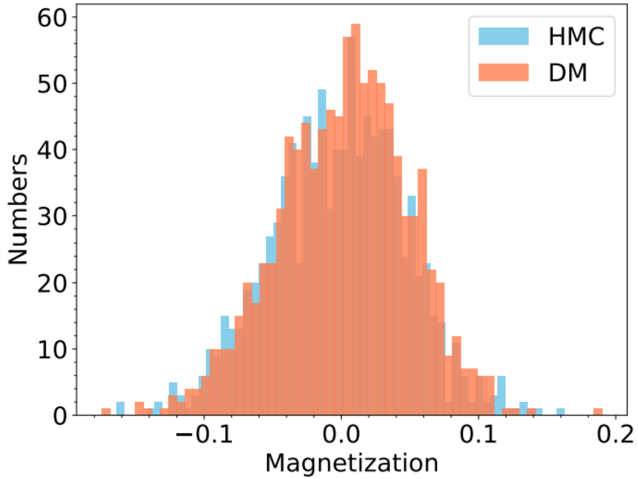
$$a^{\frac{d-2}{2}}\phi_0 = (2\kappa)^{1/2}\phi, (am_0)^2 = \frac{1-2\lambda}{\kappa} - 2d, a^{-d+4}\lambda_0 = \frac{6\lambda}{\kappa^2},$$

- Broken phase and symmetric phase

$$\kappa_c(\lambda) = \frac{1-2\lambda}{2d}.$$

- **2d 32x32 lattice size, HMC generated <u>5120 configurations</u> for training**
- **Broken phase :** **symmetric phase :**

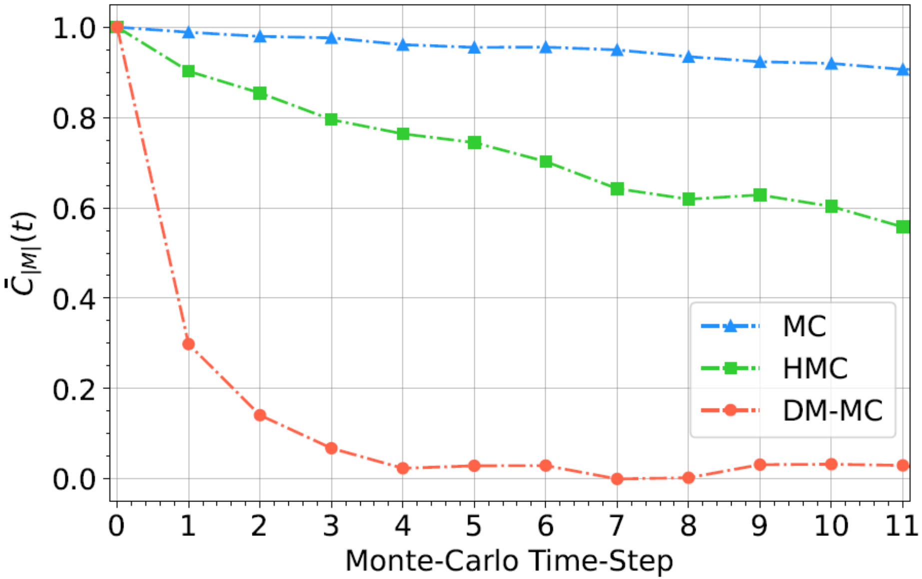




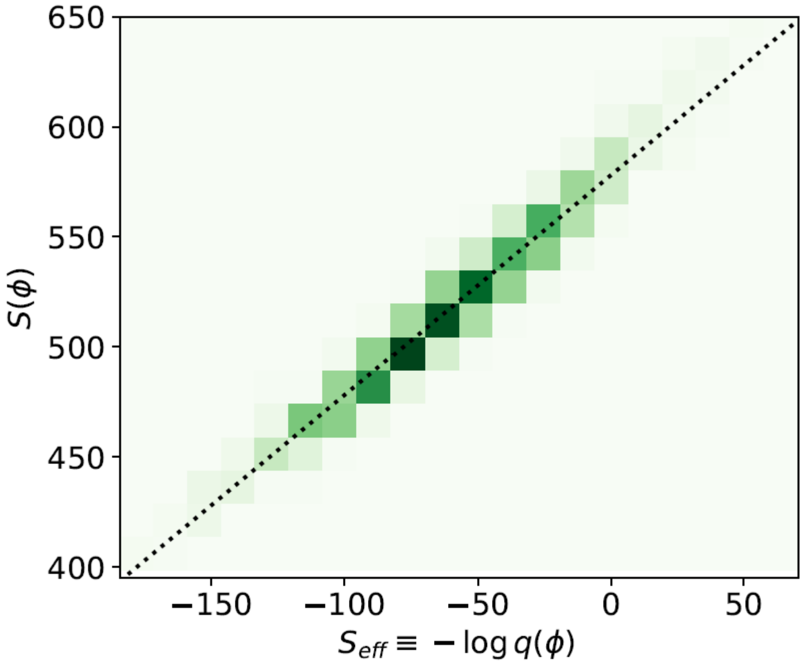
numerous "bulk" patterns emerge

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

Results: Autocorrelation time and final captured eff action



validation R2 ~0.96

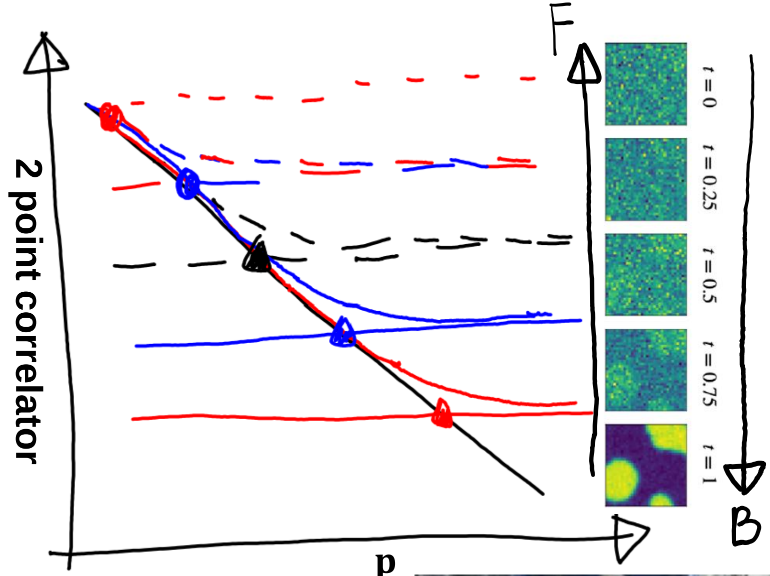


Relation to (inverse) RG

- Forward diffusion kernel: <u>**gaussian smoothing**</u>

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

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



- 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!

Closure Test – HTL potential case

$$V_R(T,r) = \frac{\sigma}{\mu_D}\left(2-(2+\mu_D r)e^{-\mu_D r}\right) - \alpha\left(\mu_D + \frac{e^{-\mu_D r}}{r}\right) + B\,,$$

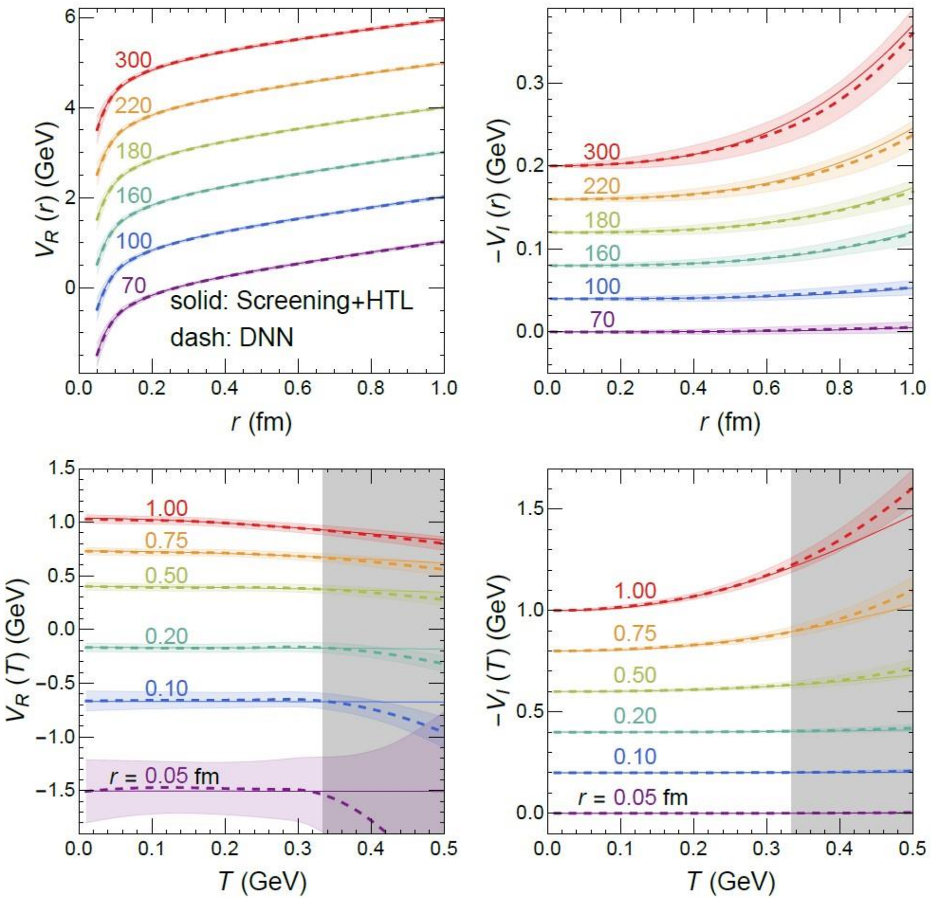
$$V_I(T,r) = -\frac{\sqrt{\pi}}{4}\mu_D T \sigma r^3 G^{2,2}_{2,4}\left(\begin{matrix}-\frac{1}{2},-\frac{1}{2} \\ \frac{1}{2},\frac{1}{2},-\frac{3}{2},-1\end{matrix}\middle| \frac{\mu_D^2 r^2}{4}\right) - \alpha T\,\phi(\mu_D r)\,,$$

$m_b = 4.676$ GeV, $\alpha = 0.39$,
$\sigma = 0.223\ \mathrm{GeV}^2$, $B = 0$ GeV,
assume that $\mu_D(T) = T/2$.

Provide mass and width of

1S, 2S, 3S, 1P, and 2P states.

@$(0, 151, 173, 199, 251, 334)$ MeV



Back up