

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)

Precision Frontier of QCD Matter:
Inference and Uncertainty Quantification

01-13 Sep, CCNU, Wuhan

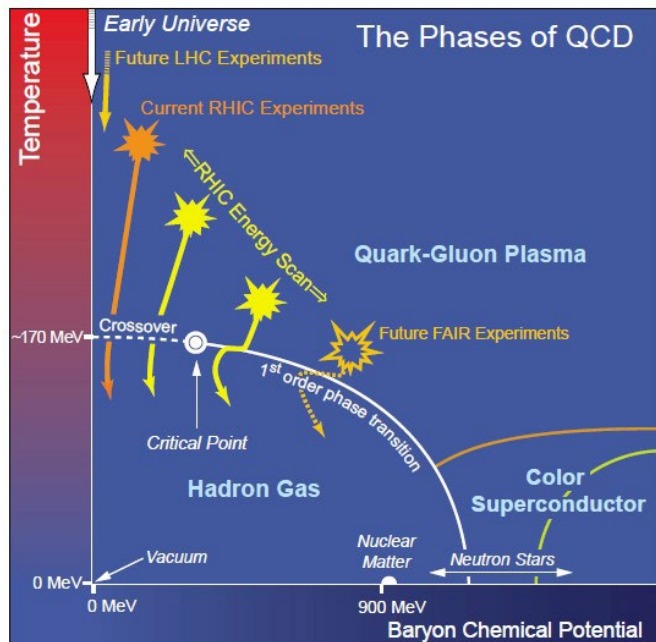
Overview : **Golden Age** of QCD matter in extreme

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



To study the most elementary particle matter :

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



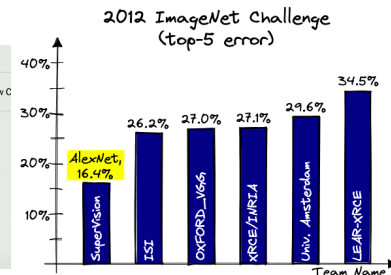
Overview : Nuclear Physics meets Machine Learning

- **2012** : Discovery of Higgs boson

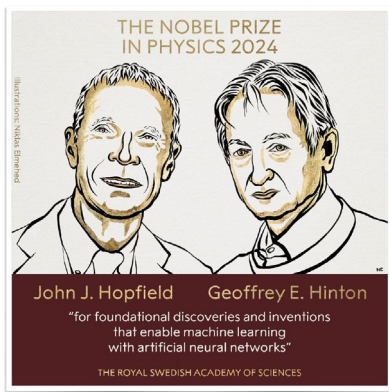


The New York Times
Physicists Find Elusive Particle Seen as Key to Universe

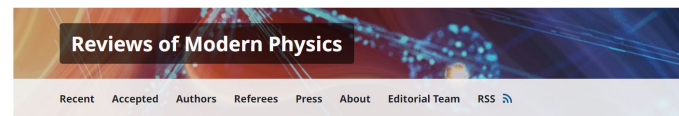
- AlexNet - Birth of Deep Learning



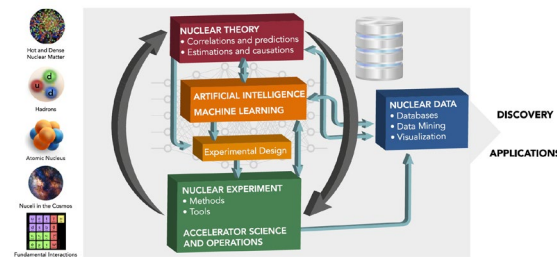
- **2024** : Nobel Prize in Physics

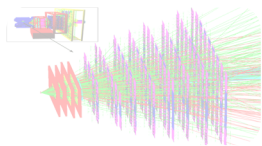


- ML4Physics, AI4Science



Colloquium: Machine learning in nuclear physics



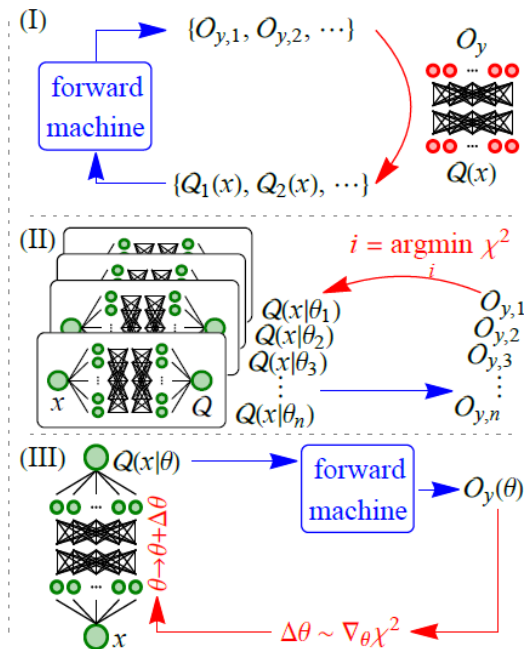
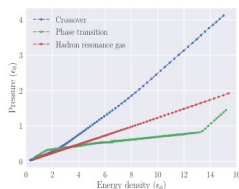


Accessible
Observation \mathcal{O}_y

Explicit
mapping

Exist
but implicit

Quantity of
Interest $\mathcal{Q}(x)$



- **Direct inverse mapping capturing :**
with Supervised Learning

- **Statistical approach to χ^2 fitting :**
Bayesian Reconstruction for posterior
or Heuristic (Generic) Algorithm to min.

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

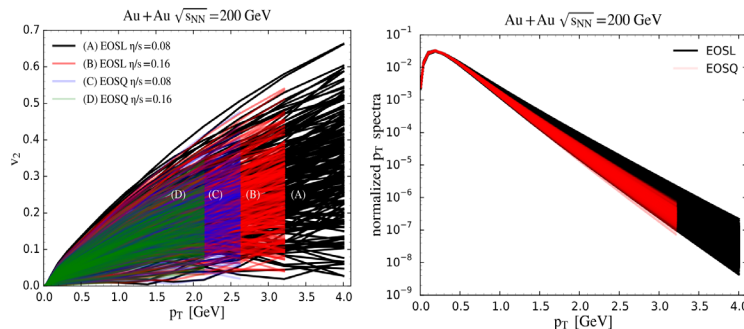
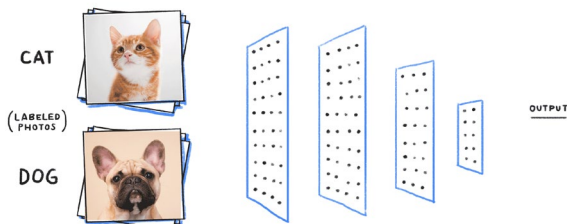
- **Automatic Differentiation :**
fuse physical prior into reconstruction
via differentiable programming strategy

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

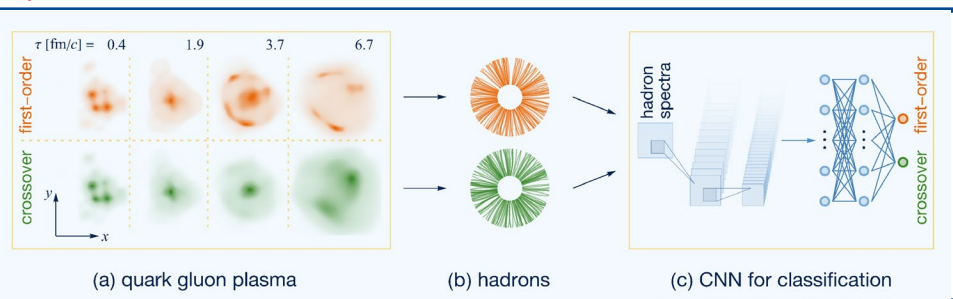
Direct inverse mapping with CNN for identifying QCD transition

Data-driven
Inverse Mapping

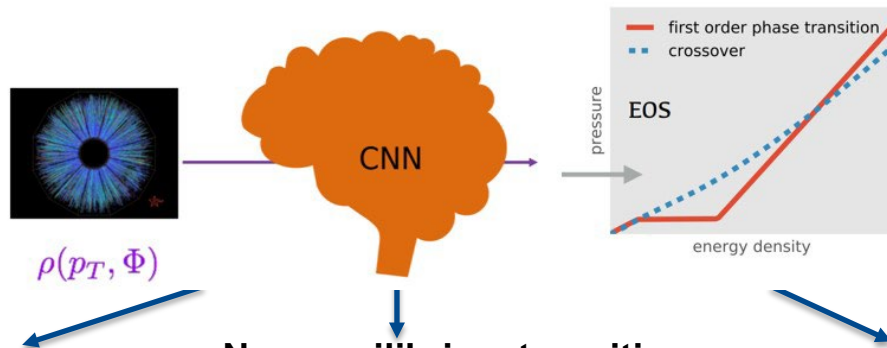
Physics Simulation
provide the Prior



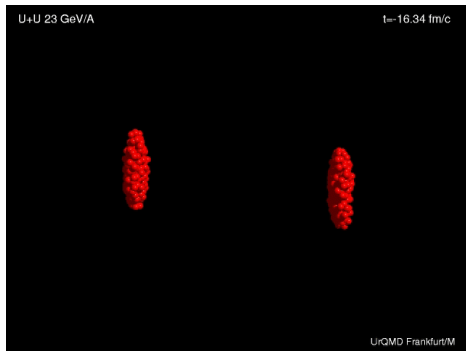
- Conventional obs. hard to distinguish
- Strongly influence from initial fluctuations and other uncertainties
- CNN : 95% event-by-event accuracy!
- Robust to initial conditions, eta/s



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.**

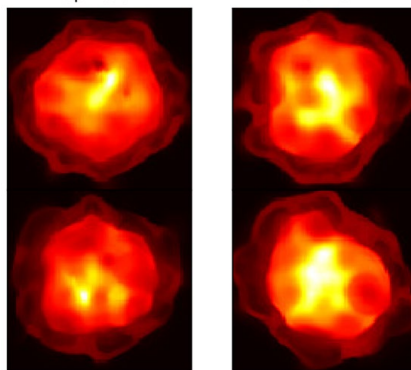


Hadronic cascade (UrQMD considered)



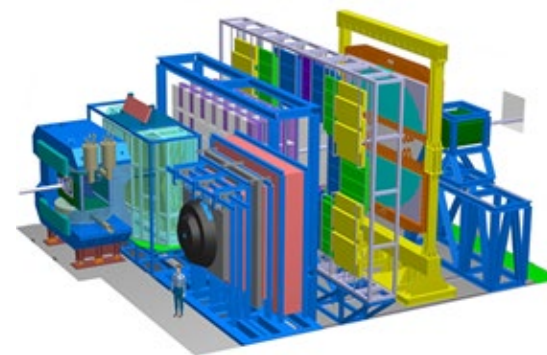
Eur. Phys. J. C 80 (2020) no.6,516

Non-equilibrium transition (Baryon Clumping, spinodal)



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

Detector effects (Hits/Tracks, Point-Net)



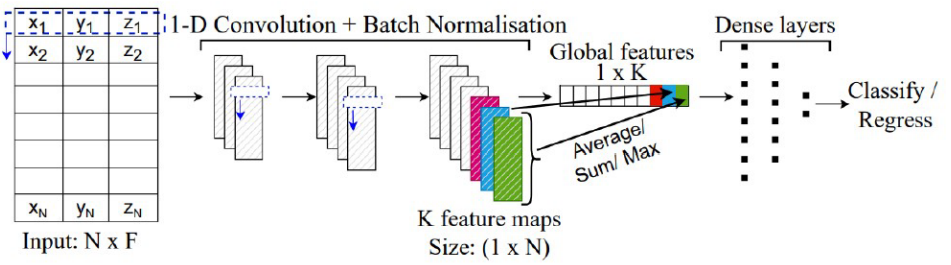
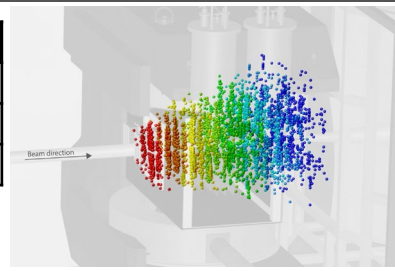
Phys. Lett. B 811, 135872
JHEP 21 (2021) 184

Point Cloud Network for Physics online analysis for HICs

- Sensor 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 process \Rightarrow **ideal online analysis algorithm**

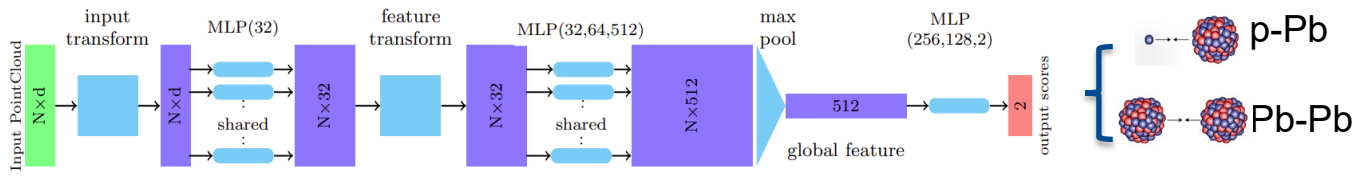
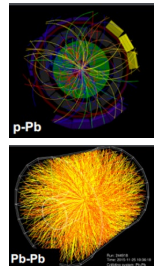
X1	y1	Z1
X2	y2	Z2
.	.	.
.	.	.
.	.	.
.	.	.
Xn	yn	Zn

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

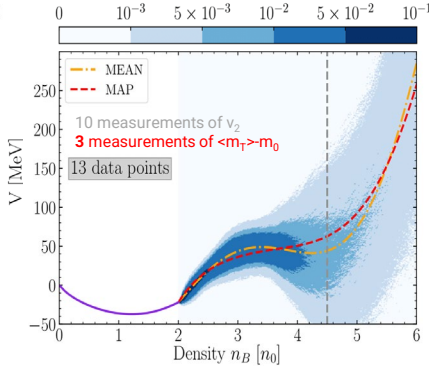
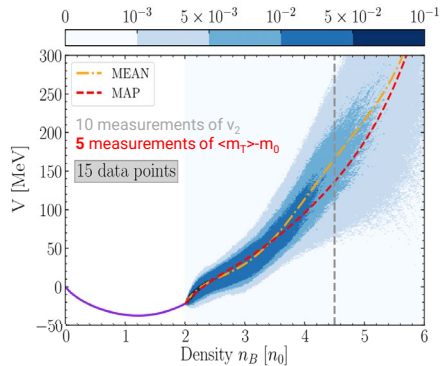
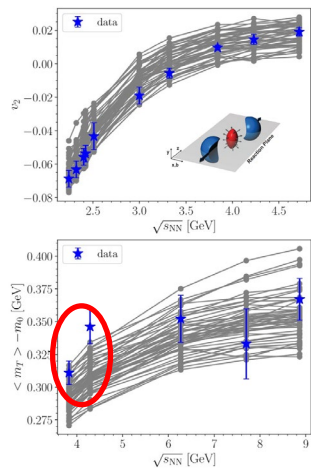


- Collision Centrality Regression**
M. OK, J. S, K. Zhou, H. S, *Phys.Lett.B* 811 (2020) 135872
- EoS Classification**
M. OK, K. Zhou, J. S, H. S, *JHEP* 10(2021) 184
- Small/ Large-system Identification**
S.Guo, H. Wang, K. Zhou, G. Ma, *Phys.Rev.C* 110 (2024)2

Manjunath O.K. and Kai Zhou, etc. *Phys.Lett.B* 811 (2020) 135872; *JHEP*10(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

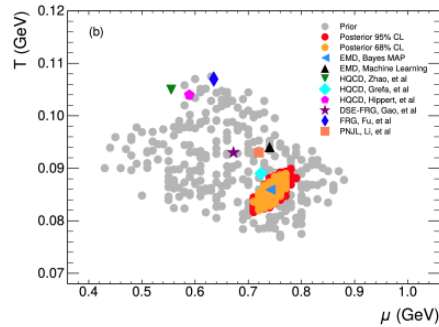
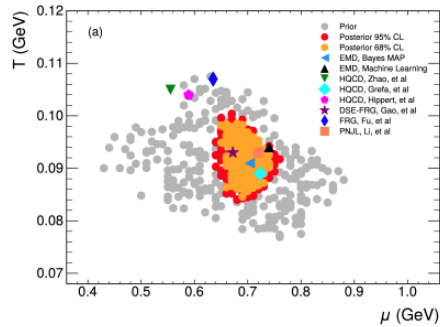
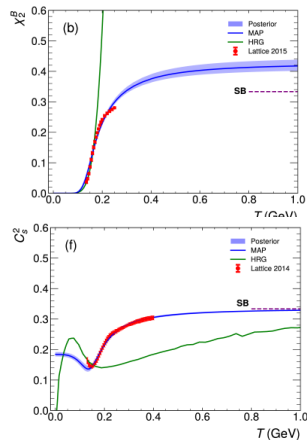
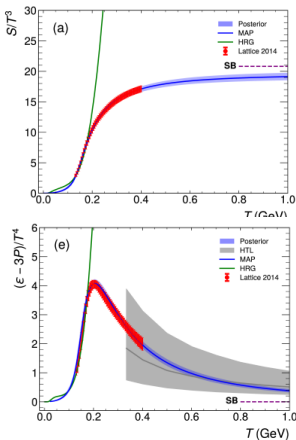
- Next-gen experiments will provide immense amount of high precision data

M.OK, J. Steinheimer, K. Zhou,
H. Stoecker, [PRL 131, 202303 \(2023\)](#)

See talk by Manjunath. O.K (this afternoon)

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

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



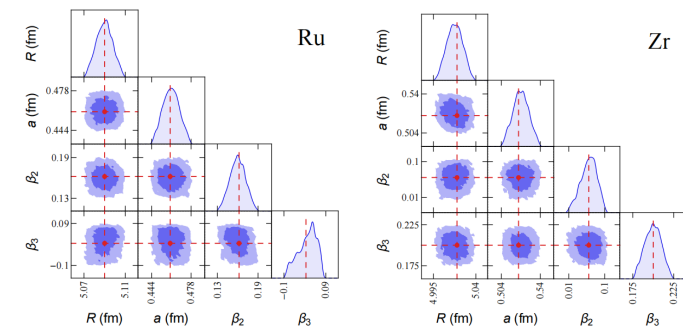
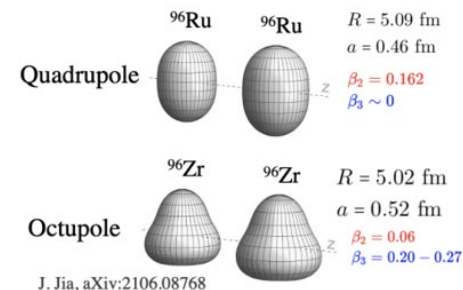
- Critical endpoint from **holography (EMD)** via Bayesian Inference

L. Zhu, X. Chen, K. Zhou,
H. Zhang, M. Huang,
[arXiv:2501.17763](#)

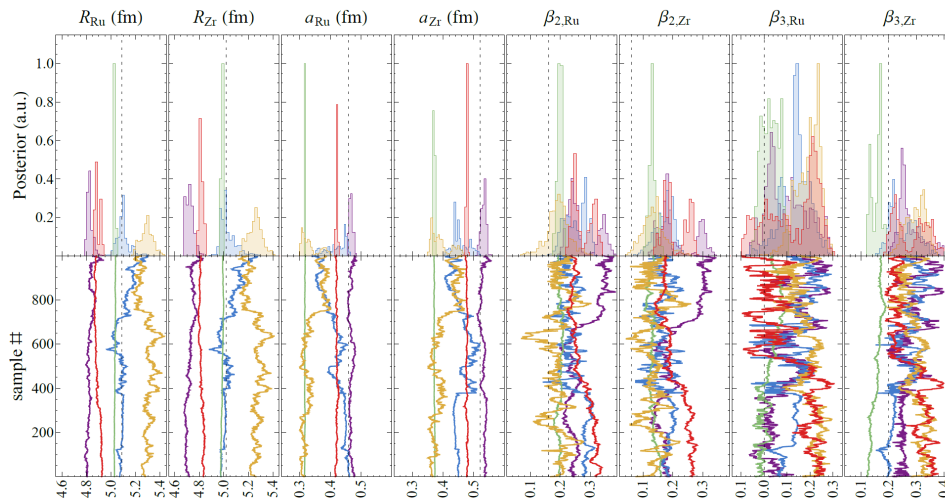
Bayesian Imaging for Nuclear Structure in Isobar Collisions

- 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)

$$\mathbf{y}_{\text{Ru}} \equiv \{P_a^{\text{Ru}}, \varepsilon_{2,a}^{\text{Ru}}, \varepsilon_{3,a}^{\text{Ru}}, d_{\perp,a}^{\text{Ru}}\}_{a=1,\dots,40}$$



Single system works good



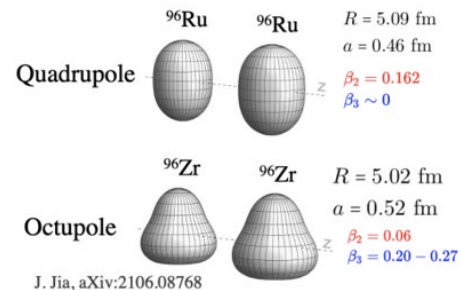
With purely the Isobar-Ratios:

MCMC can not converge to a stationary inference of the nuclear structure

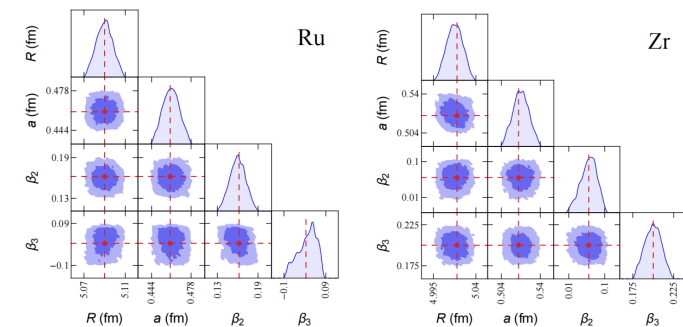
$$\mathbf{y}_{\text{r},1} \equiv \{R_{P,a}, R_{\varepsilon_{2,a}}, R_{\varepsilon_{3,a}}, R_{d_{\perp,a}}\}_{a=1,\dots,40}$$

Bayesian Imaging for Nuclear Structure in Isobar Collisions

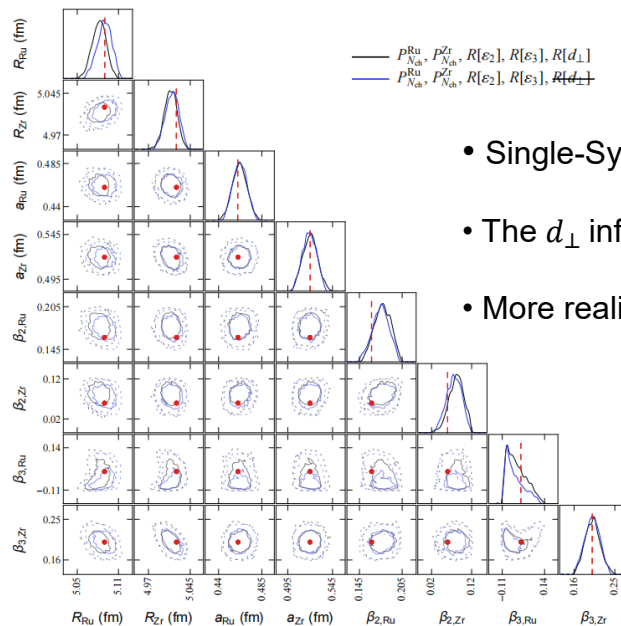
- Nuclear Structure imaging for single system ? (caveat: model dependent)
- Simultaneous inference for isobar systems with ratio?
- Bayesian Inference:** Gaussian Process emulator + PCA dim reduction + MCMC
Data: MC-Glauber + Matching (linear response approximation)



$$\mathbf{y}^{\text{Ru}} \equiv \{P_a^{\text{Ru}}, \varepsilon_{2,a}^{\text{Ru}}, \varepsilon_{3,a}^{\text{Ru}}, d_{\perp,a}^{\text{Ru}}\}_{a=1, \dots, 40}$$



Single system works good

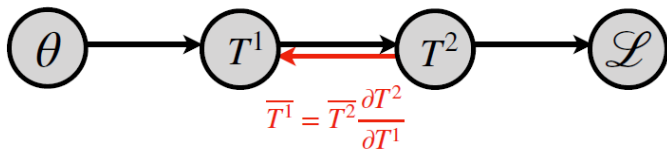


- Single-System Multiplicity makes it possible
- The d_{\perp} information is redundant
- More realistic analysis with AMPT in progress

$$\mathbf{y}_{r,2} \equiv \{P_a^{\text{Ru}}, P_a^{\text{Zr}}, R_{\varepsilon_{2,a}}, R_{\varepsilon_{3,a}}, R_{d_{\perp,a}}\}_{a=1, \dots, 40}$$

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

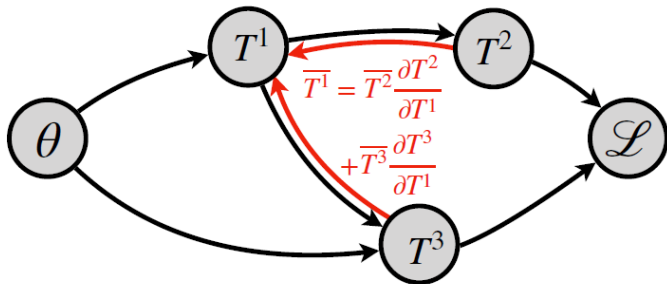
(a)



Chain rule for gradients : $\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\partial \mathcal{L}}{\partial T^n} \frac{\partial T^n}{\partial T^{n-1}} \cdots \frac{\partial T^2}{\partial T^1} \frac{\partial T^1}{\partial \theta}$

Defining adjoint variables : $\bar{T} = \partial \mathcal{L} / \partial T$

(b)

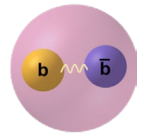


$$\bar{T}^i = \bar{T}^{i+1} \frac{\partial T^{i+1}}{\partial T^i}$$

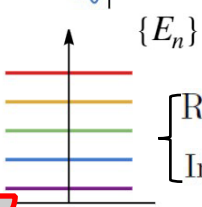
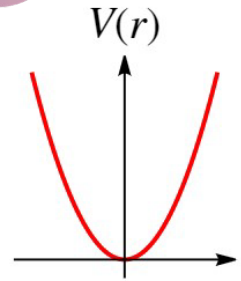
$$\bar{\theta} = \bar{T}^1 \frac{\partial T^1}{\partial \theta}$$

$$\bar{T}^i = \sum_{j: \text{child of } i} \bar{T}^j \frac{\partial T^j}{\partial T^i}$$

HQ Potential Model, Inverse Shroedinger Eq.



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



$\{E_n\}$ *R. Larsen, et.al, PRD(2019), PLB(2020), PRD(2020)*

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

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

?

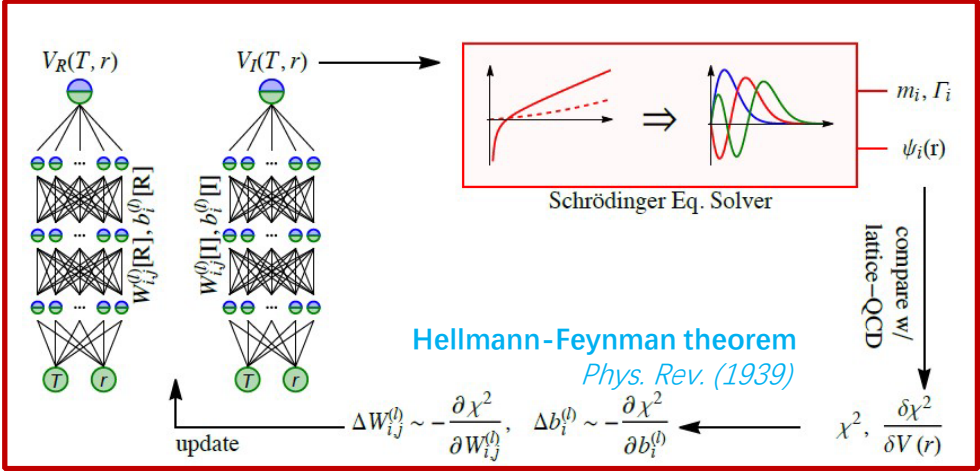
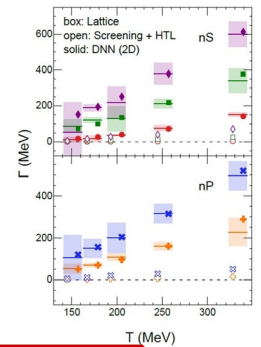
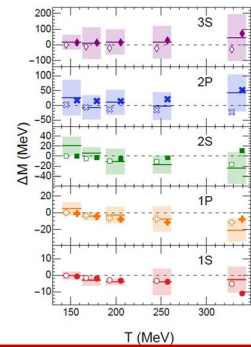
How to extract **effective potential** given **limited spectroscopy**? →

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

$T \in \{0, 151, 173, 199, 251, 334\}$ MeV
 $i \in \{1S, 2S, 3S, 1P, 2P\}$

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

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

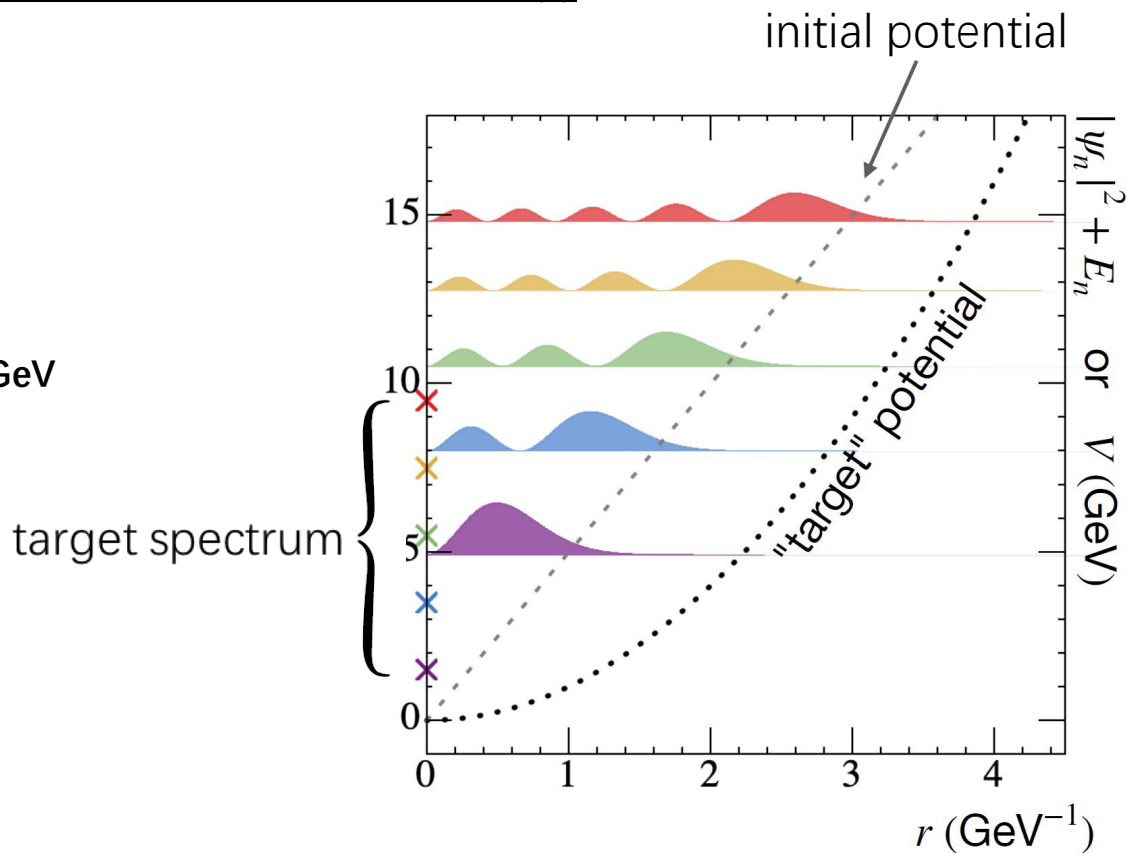


Proof of Concept

limited spectrum $\{ E_n \}$ to continuous interaction $V(r)$?

Learn $V(r)$ from 5 eigenvalues :

$\{ E_n \} = \{ 3/2, 7/2, 11/2, 15/2, 19/2 \}$ GeV



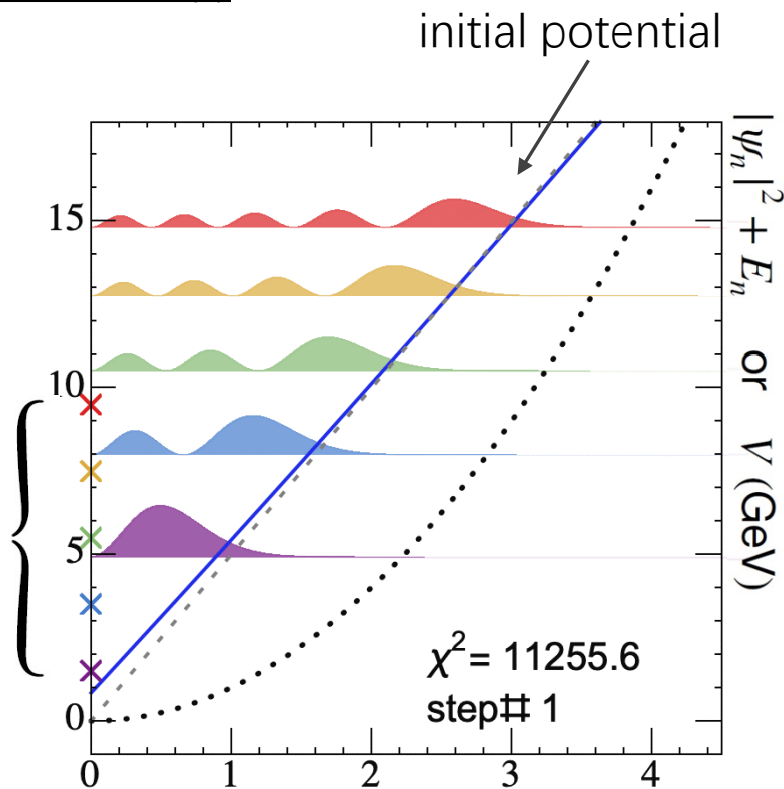
Proof of Concept

limited spectrum $\{ E_n \}$ to continuous interaction $V(r)$?

Learn $V(r)$ from 5 eigenvalues :

$\{ E_n \} = \{ 3/2, 7/2, 11/2, 15/2, 19/2 \}$ GeV

target spectrum



Proof of Concept

limited spectrum $\{E_n\}$ to continuous interaction $V(r)$?

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

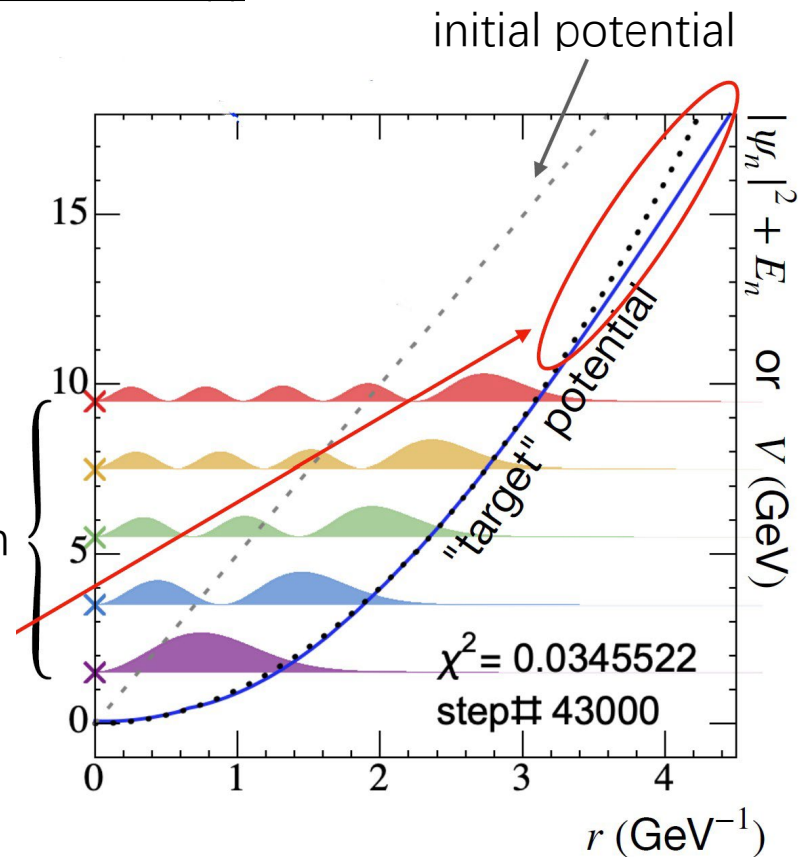
Learn $V(r)$ from 5 eigenvalues :

$\{E_n\} = \{3/2, 7/2, 11/2, 15/12, 19/2\}$ GeV

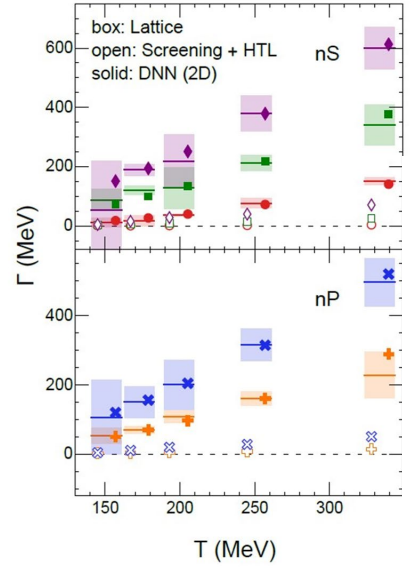
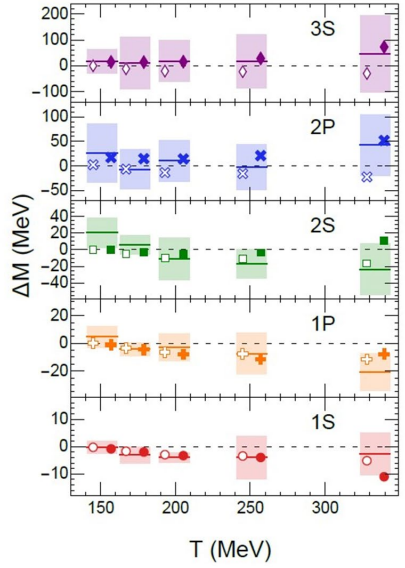
target spectrum

Deviation @ given states' wavefunction vanishes

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

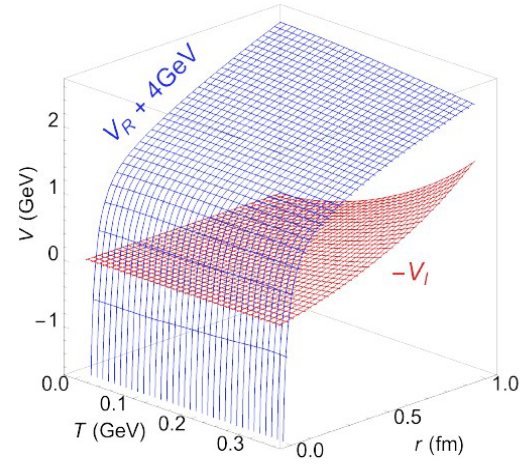
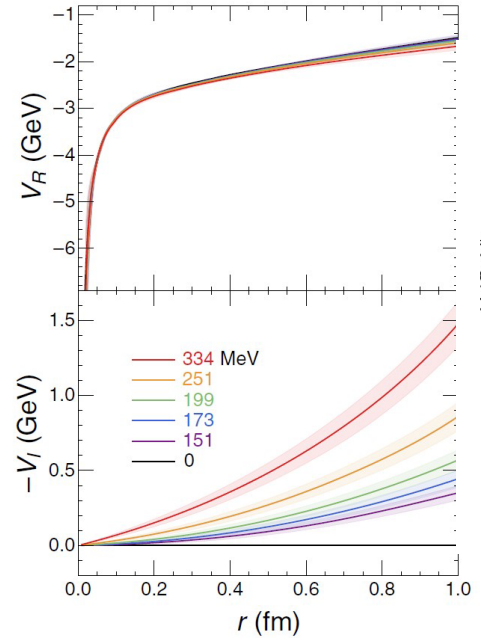


Results with lattice data for mass/width and the reconstructed HQ Potential



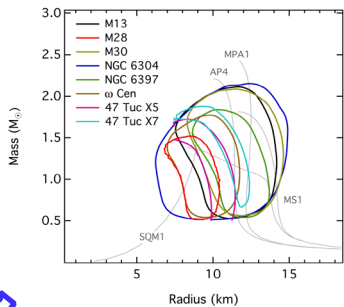
Chi2-per-data=16.5/30

The reconstructed T, r dependent potential



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

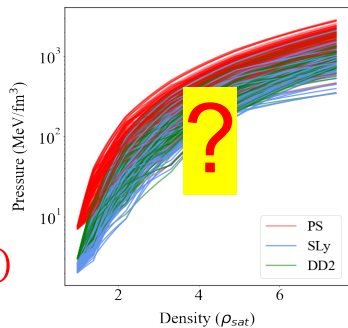
Noisy/Limited NS Observables to EoS ?



TOV
eqs

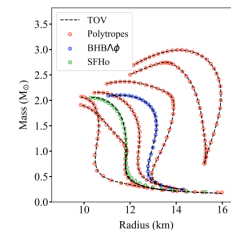
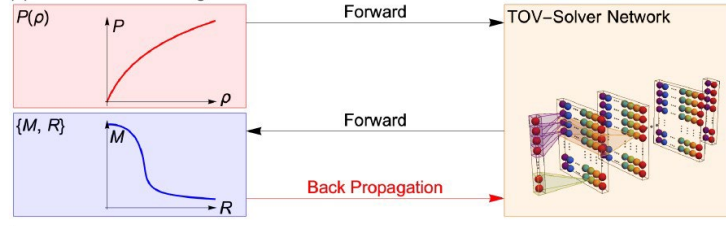
$$\frac{dP}{dr} = -\frac{G}{r^2} \left(\rho + \frac{P}{c^2} \right) \left(m + 4\pi r^3 \frac{P}{c^2} \right) \left(1 - \frac{2Gm}{c^2 r} \right)^{-1}$$

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

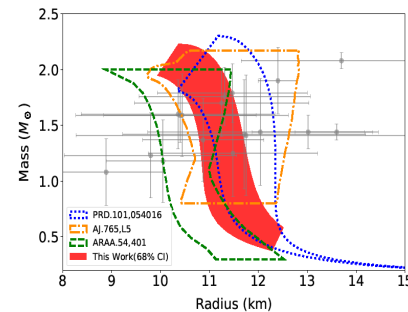
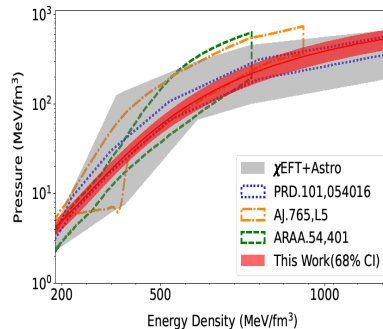
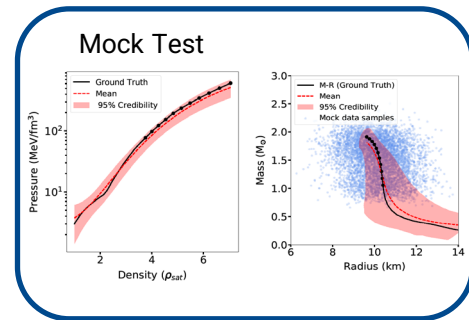
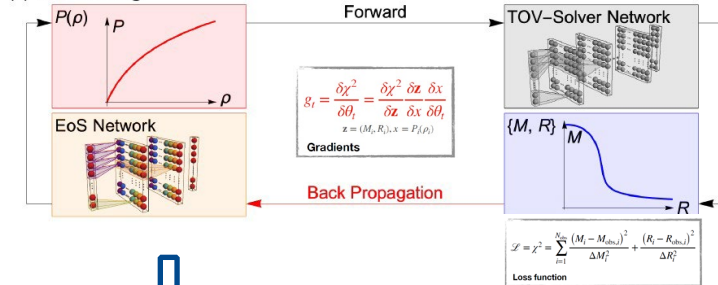


$P(\rho)$

(a) TOV-Solver Training

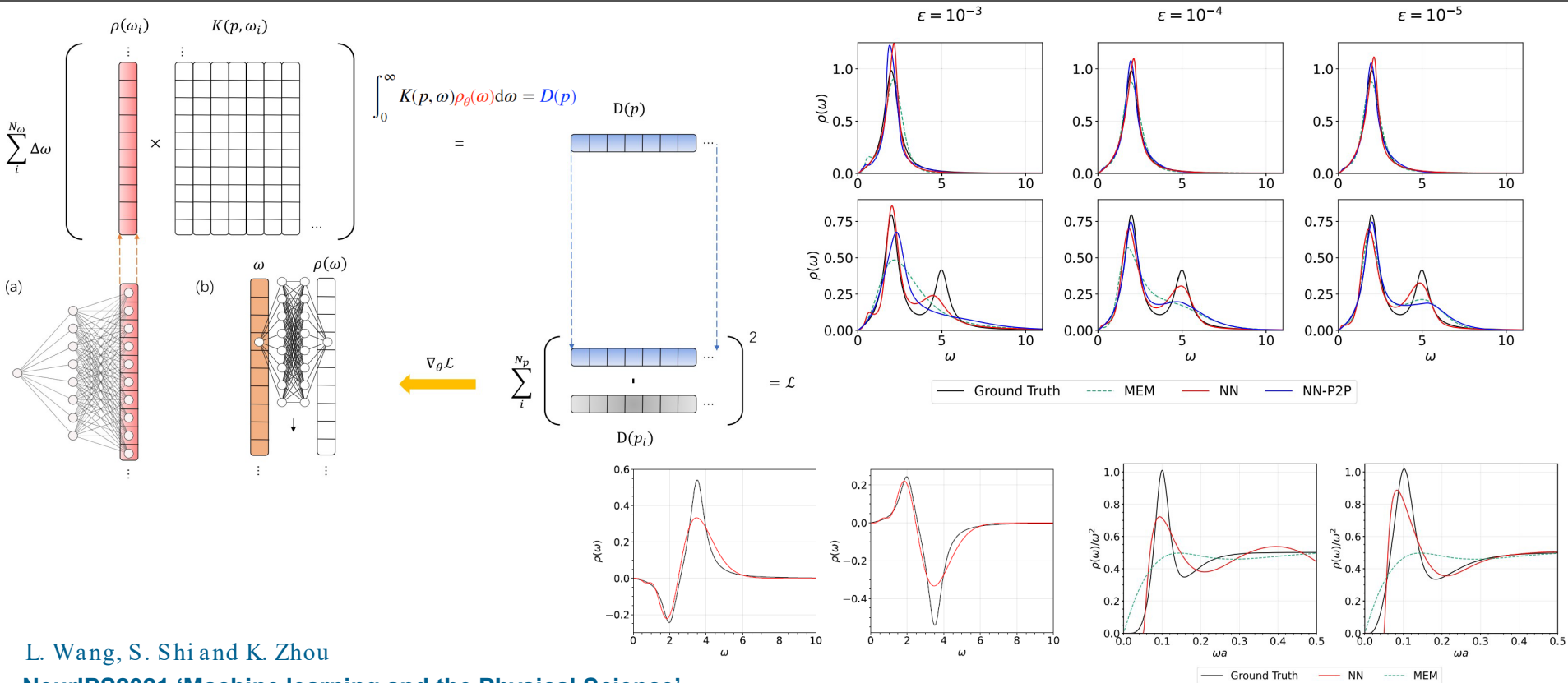


(b) EoS Training



S. S, L. W, S. S, H. S, K. Z, JCAP
98(2022)071;PRD107(2023)083028

Spectral function reconstruction from Euclidean correlator via AD



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,

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

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

- Discriminative Learning : **prediction**

function fitting

$$y = f(x)$$

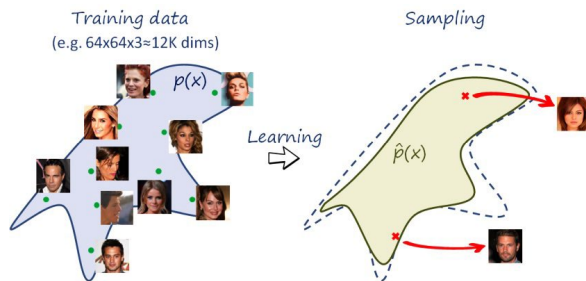
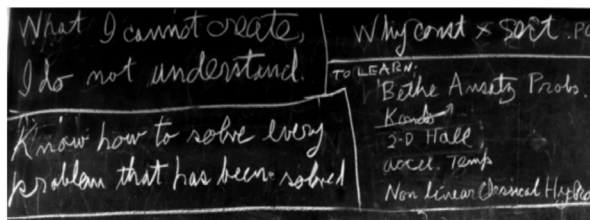
conditional probability

$$p_{\theta}(y|x) \rightarrow p(y|x)$$



- Generative Modelling : **understand**

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



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

- Variational free energy minimization - Reverse KL divergence

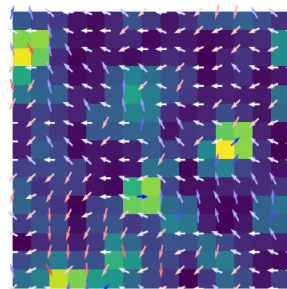
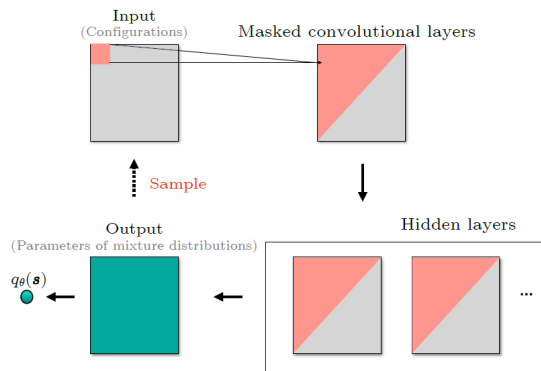
$$D_{\text{KL}}(q_{\theta} \parallel p) = \sum_{\mathbf{s}} q_{\theta}(\mathbf{s}) \ln \left(\frac{q_{\theta}(\mathbf{s})}{p(\mathbf{s})} \right) = \beta(F_q - F) \quad F_q = \frac{1}{\beta} \sum_{\mathbf{s}} q_{\theta}(\mathbf{s}) [\beta E(\mathbf{s}) + \ln q_{\theta}(\mathbf{s})]$$

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

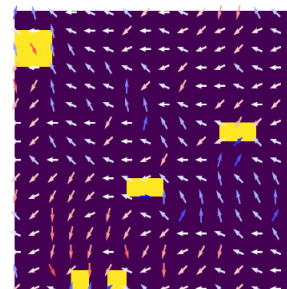
- **Autoregressive** $q_{\theta}(\mathbf{s}) = \prod_{i=1}^N q_{\theta}(s_i \mid s_1, \dots, s_{i-1})$
- **Continuous Autoregressive Net for XY model**

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

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



Probability distributions from CANs

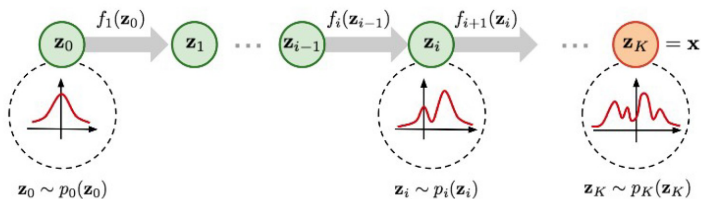


Vortices

Flow based generative model to QFT

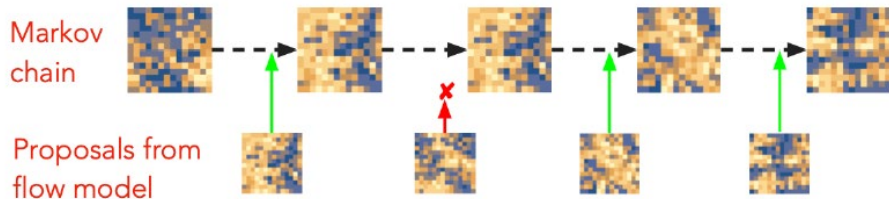
A series (Flow) of invertible/bijective transformations for $p(\mathbf{z})$

compose several invertible transformations to form the flow :



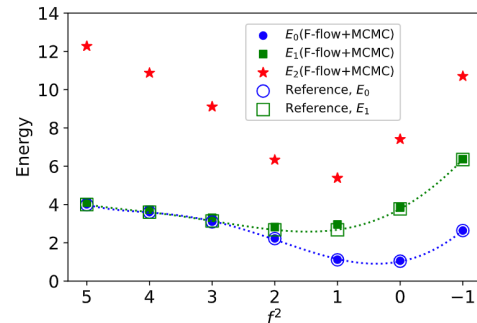
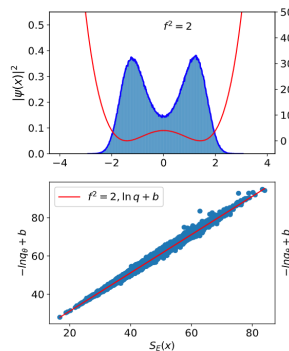
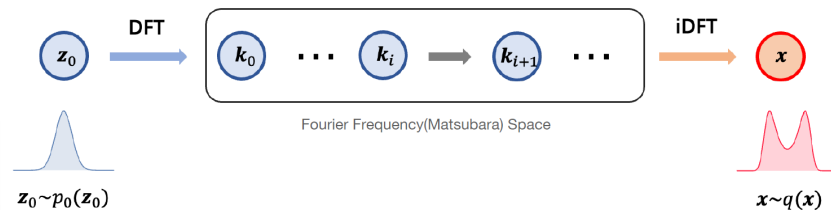
$$p_i(z_i) = p_{i-1}(f_i^{-1}(z_i)) |\det J_{f_i^{-1}}| = p_{i-1}(z_{i-1}) |\det J_{f_i}|^{-1}$$

$$\rightarrow \log p(\mathbf{x}) = \log p_0(f^{-1}(\mathbf{x})) + \sum_{i=1}^K \log |\det J_{f_i^{-1}}| = \log p_0(z_0) - \sum_{i=1}^K \log |\det J_{f_i}|$$



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

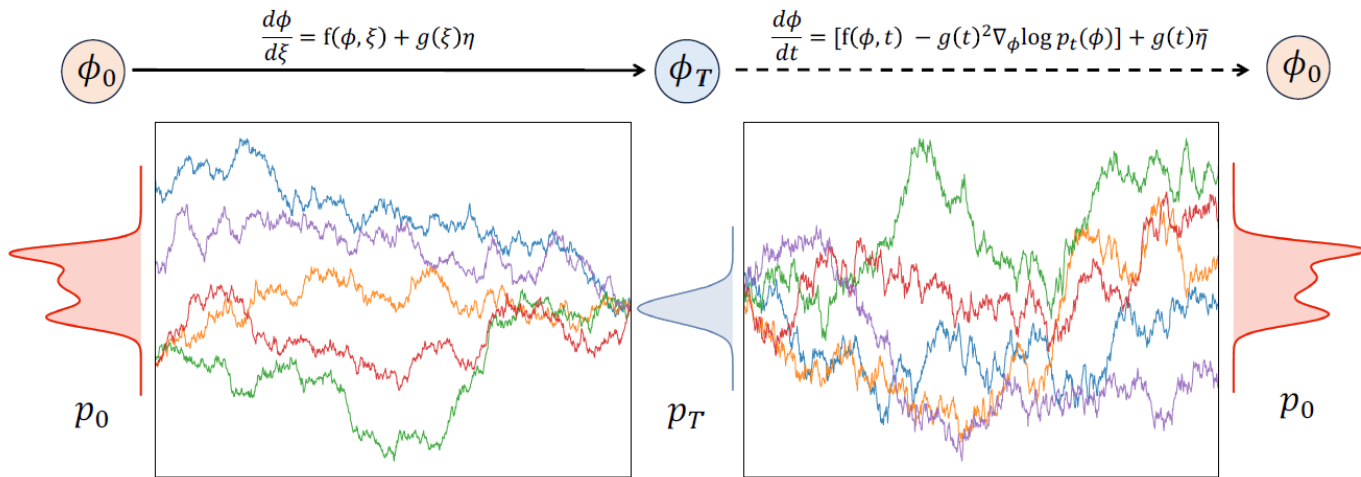
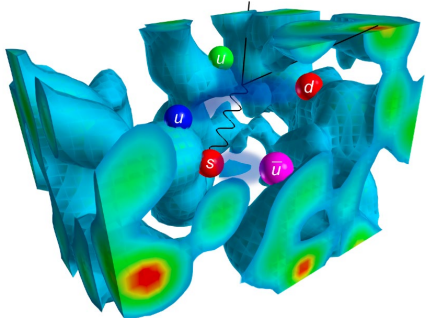


S.Chen, O. Savchuk, S. Zheng, B. Chen, H. Stoecker, L. Wang, K. Zhou, **PRD107, 056001(2023)**

Diffusion Model on lattice QFT configurations

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

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



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 AI Paper” Award**

Q. Zhu, G. Aarts, W. Wang, K. Zhou, L. Wang, arXiv:2410.19602 (NeurIPS 2024 workshop “ML&Physical Sciences”)

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

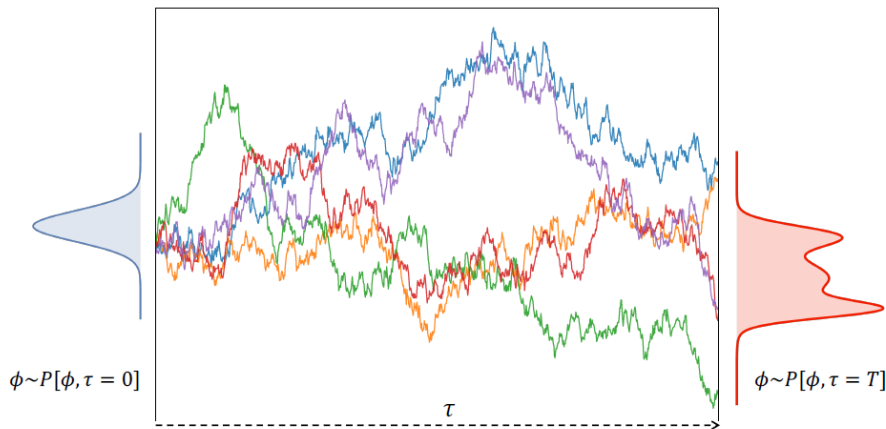
$\langle \eta(x, \tau) \rangle = 0$, $\langle \eta(x, \tau) \eta(x', \tau') \rangle = 2\alpha \delta(x - x') \delta(\tau - \tau')$
 τ : fictitious time, α : diffusion constant

- Fokker-Planck equation

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

Equilibrium solution (long-time limit),

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



Thermal equilibrium limit \rightarrow Quantum distribution

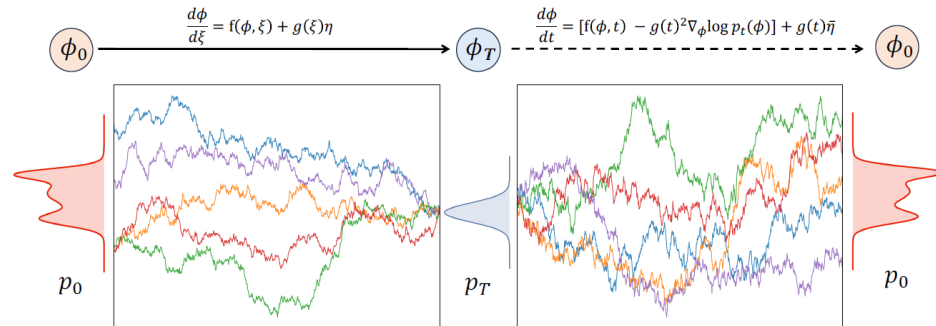
- Set the diffusion constant as $\alpha = \hbar$

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

DM generation SDE and Stochastic Quantization

$$\frac{\partial \phi(x, \tau)}{\partial \tau} = g^2(\tau) \nabla_{\phi} \log P(\phi; \tau) + g(\tau) \eta(x, \tau)$$

$$\frac{\partial \phi(x, \tau)}{\partial \tau} = -\nabla_{\phi} S(\phi) + \sqrt{2} \eta(x, \tau)$$



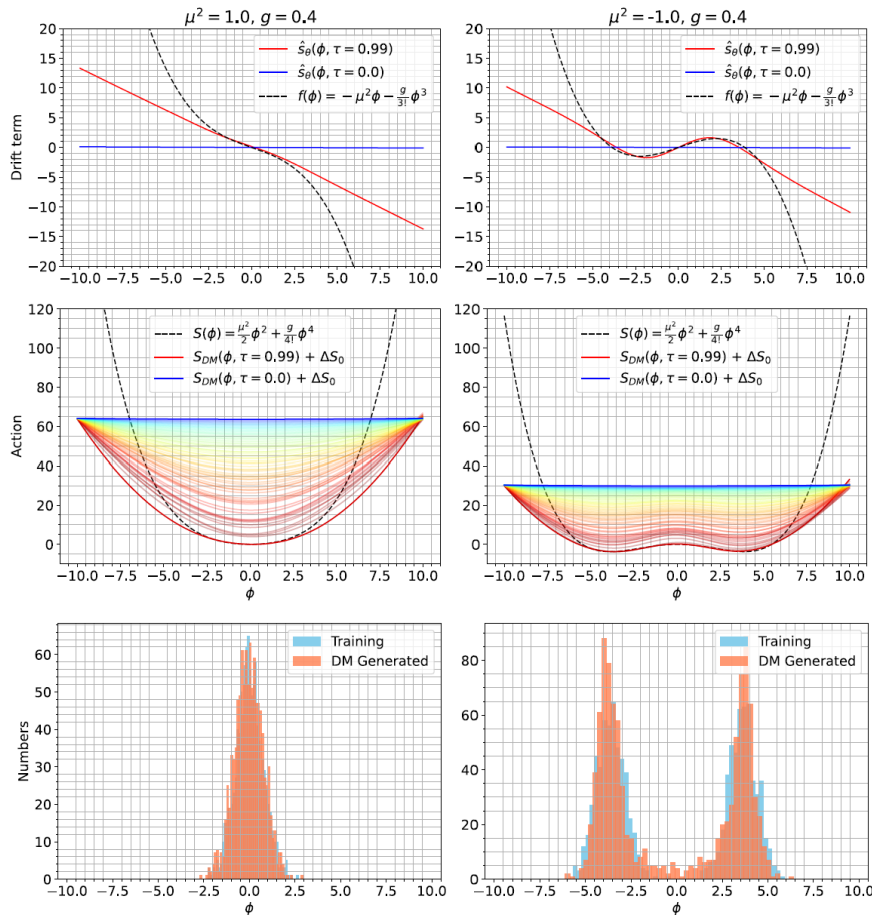
Similarities and differences:

- ✓ SQ: fixed drift, determined from known action
constant noise variance (but can be generalised using kernels)
thermalisation followed by long-term evolution in equilibrium
- ✓ DM: drift and noise variance time-dependent, learn from data
evolution between $0 \leq \tau \leq T = 1$, many short runs

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

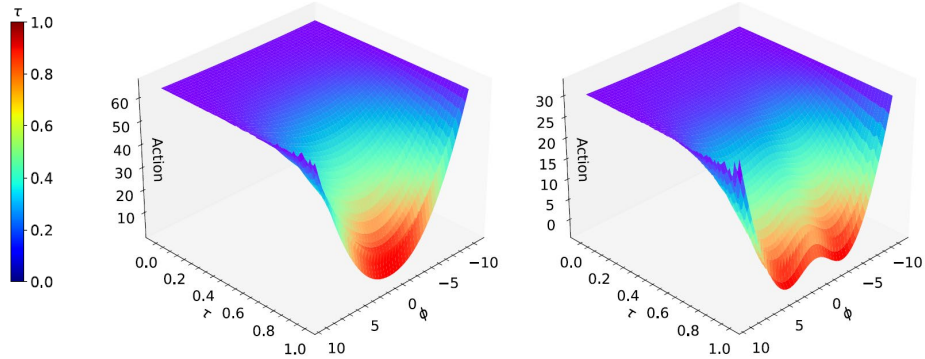
$$O(\bar{\alpha}) \sim O(\hbar)$$

Effective Action on A Toy model



- Flow of the effective action

$$S(\phi) = \frac{\mu^2}{2}\phi^2 + \frac{g}{4!}\phi^4, \quad f(\phi) = -\frac{\partial S(\phi)}{\partial \phi} = -\mu^2\phi - \frac{g}{3!}\phi^3$$



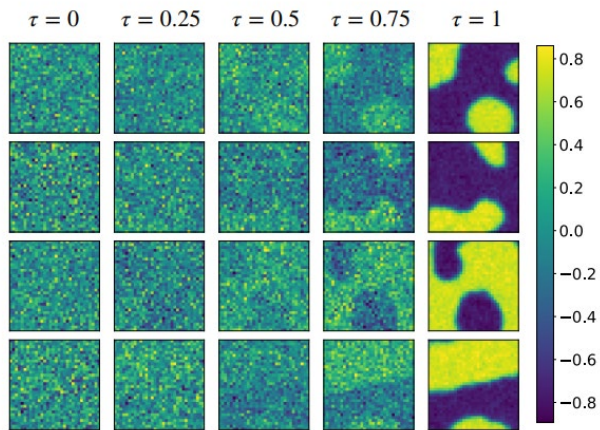
$$S_{DM}(\phi, \tau) = \int \hat{s}_\theta(\tilde{\phi}, \tau) d\tilde{\phi}$$

DM on 2d scalar ϕ^4 model

- 32x32 lattice, HMC generated 5120 configurations for training

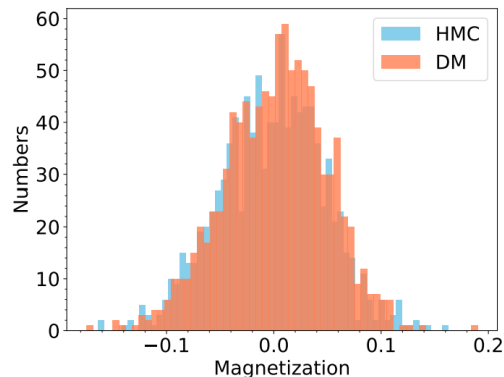
$$S_E = \sum_x [-2\kappa \sum_{\mu=1}^d \phi(x)\phi(x + \hat{\mu}) + (1 - 2\lambda)\phi(x)^2 + \lambda\phi(x)^4].$$

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

- Forward diffusion kernel: **gaussian smoothing**

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

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

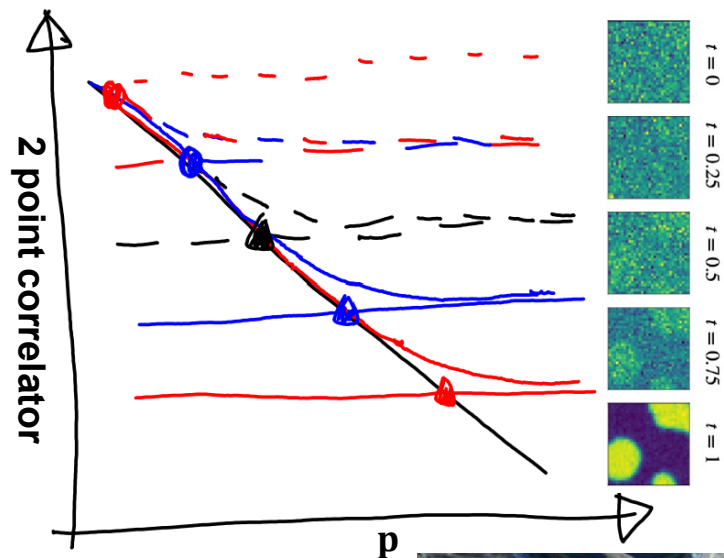
- In Fourier space:

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

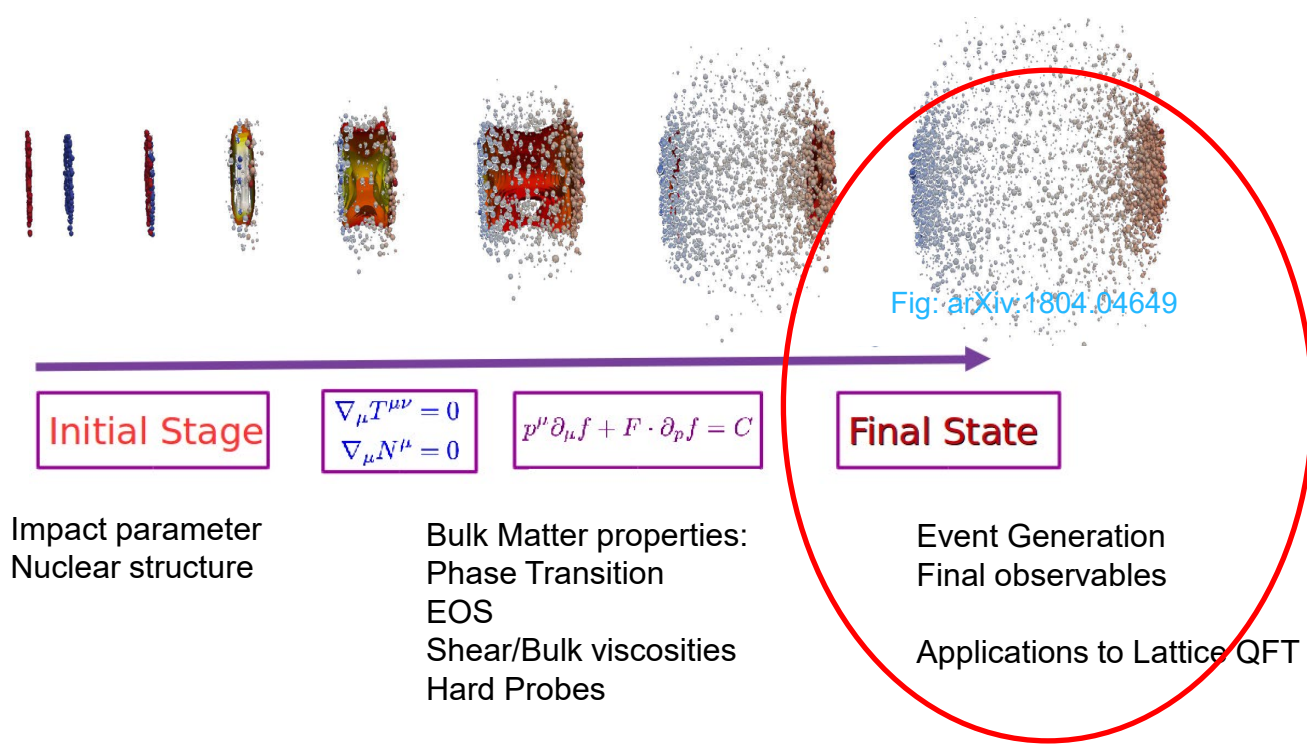
- ! the above evolution will perturb (smear) higher momentum modes first,
With decreasing cut scale because of the gradually increasing noise level !



In **FRG**, the high frequency (short-distance) degrees of freedom is progressively integrated out !



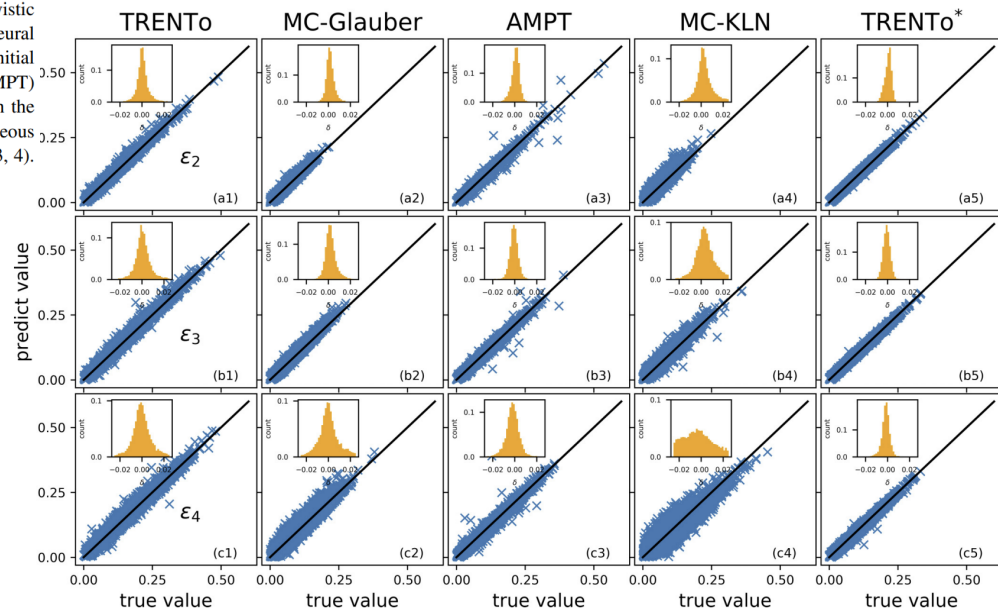
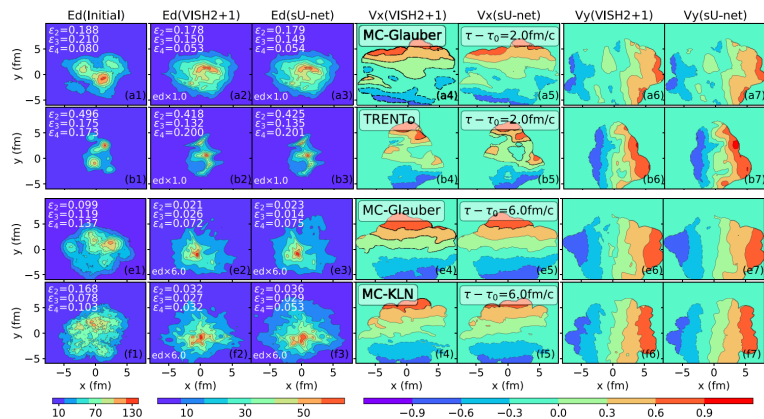
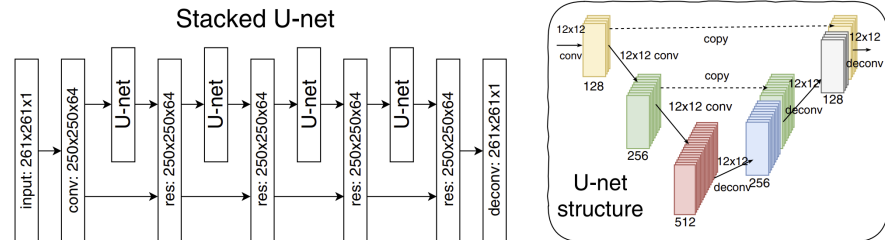
Initial state + Bulk matter + Generative model



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^{1,2,5}

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) 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 structures of the final profiles, and creditably describe the related eccentricity distributions $P(\epsilon_n)$ ($n = 2, 3, 4$).



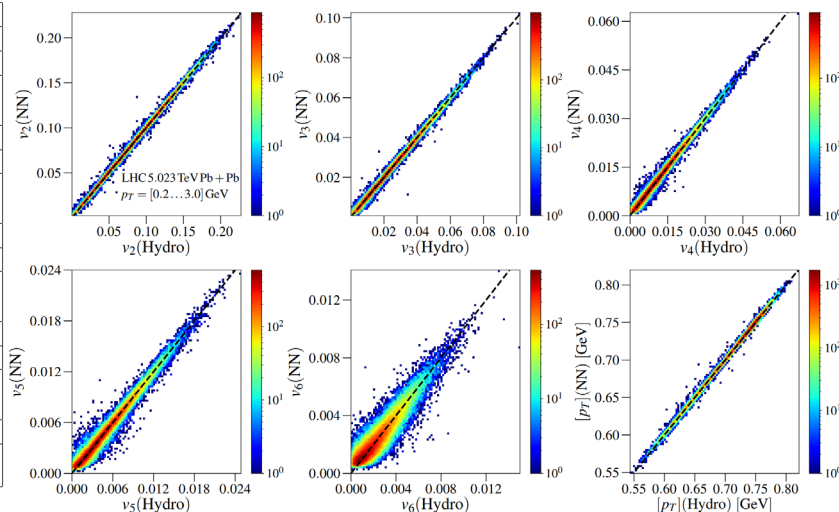
PHYSICAL REVIEW C **108**, 034905 (2023)

Deep learning for flow observables in ultrarelativistic heavy-ion collisions

H. Hirvonen , K. J. Eskola , and H. Niemi 

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

Block	Output size	Layers
Convolution	134x134x64	7x7 conv, stride 2
Pooling	67x67x64	3x3 max pool, stride 2
Dense Block	67x67x256	1x1 conv 3x3 conv x 6
Transition Layer	67x67x128	1x1 conv
	33x33x128	2x2 average pooling, stride 2
Dense Block	33x33x512	1x1 conv 3x3 conv x 12
Transition Layer	33x33x256	1x1 conv
	16x16x256	2x2 average pooling, stride 2
Dense Block	16x16x896	1x1 conv 3x3 conv x 20
Transition Layer	16x16x448	1x1 conv
	8x8x448	2x2 average pooling, stride 2
Dense Block	8x8x1216	1x1 conv 3x3 conv x 24
Output Layer	1x1x1216	8x8 global average pooling
	N_{out}	Fully connected layer with ReLU activation

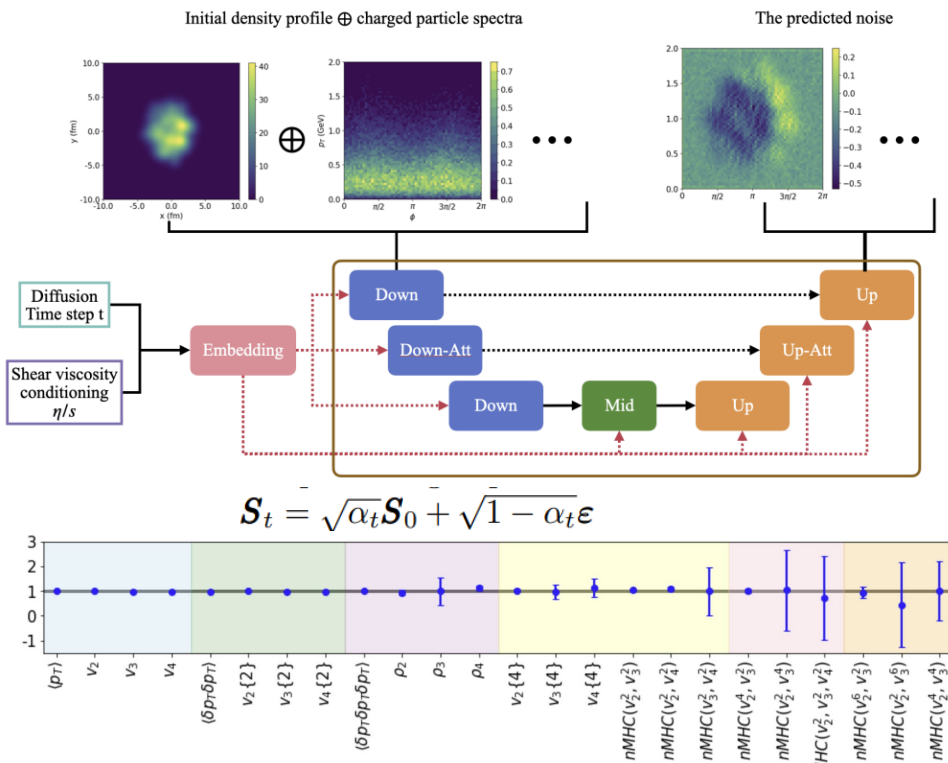


10^7 events using the neural network, which takes around 20 h with the GPU. This is a very substantial difference compared to doing full hydrodynamic simulations using CPU, which would take about 5×10^6 CPU hours.

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

arXiv:2410.13069

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



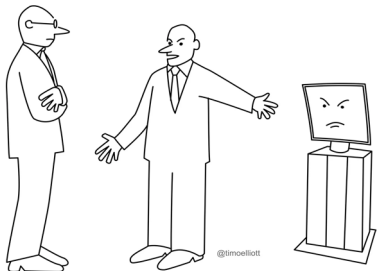
We carried out (2+1)D minimum bias simulations of Pb-Pb collisions at 5.02 TeV, choosing the shear viscosity η/s to be one of three distinct values: 0.0, 0.1, and 0.2. For each value of η/s , we generate 12,000 pairs of initial entropy density profiles and final particle spectra, corresponding to 12,000 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 S_0 depend on the initial entropy density profiles I and the shear viscosity η/s , we train a conditional reverse diffusion process $p(S_0|I, \eta/s)$ 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.

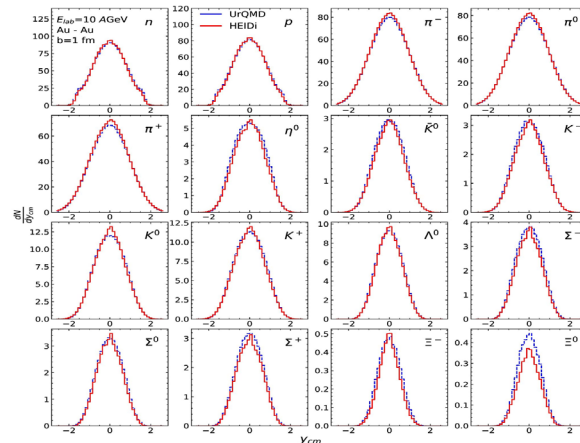
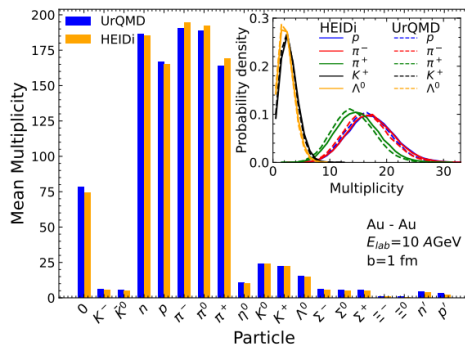
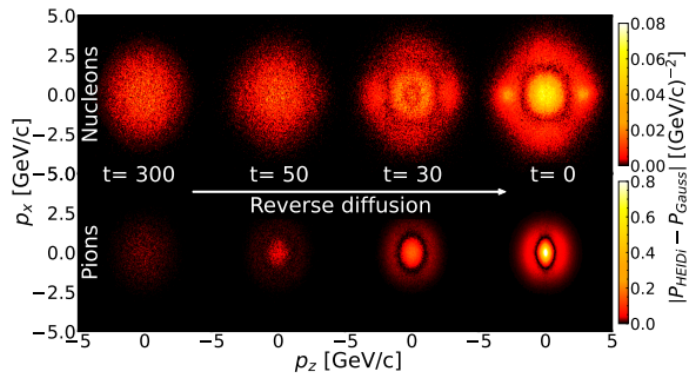
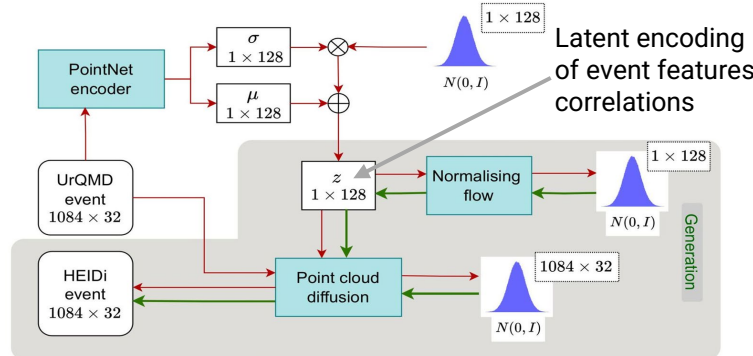
Point Cloud Diffusion Model for HICs – AI clone of simulation



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

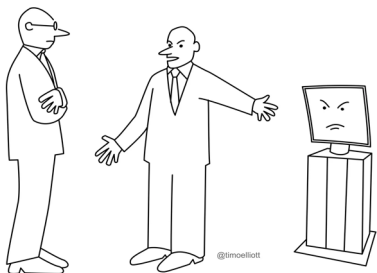
- 18k UrQMD simulation events for central Au-Au@10 AGeV collisions
- **HEIDI:**
Heavy-ion Events through Intelligent Diffusion

PointNet encoder + Normalizing flow decoder + Pointcloud diffusion →



See talk by Manjunath. O.K (this afternoon)

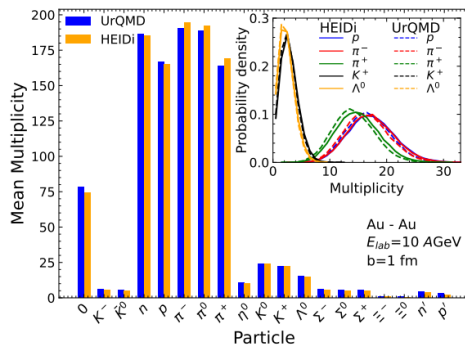
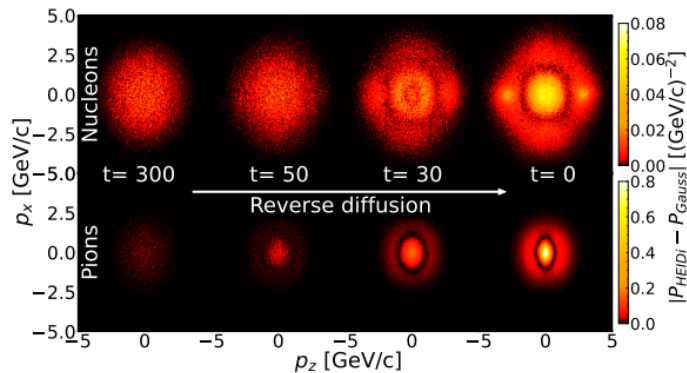
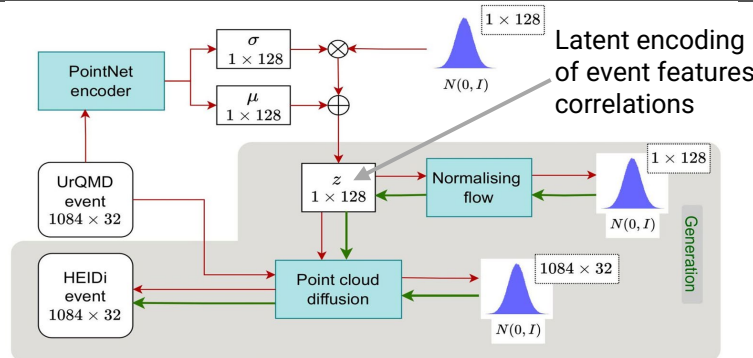
Point Cloud Diffusion Model for HICs – AI clone of simulation



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

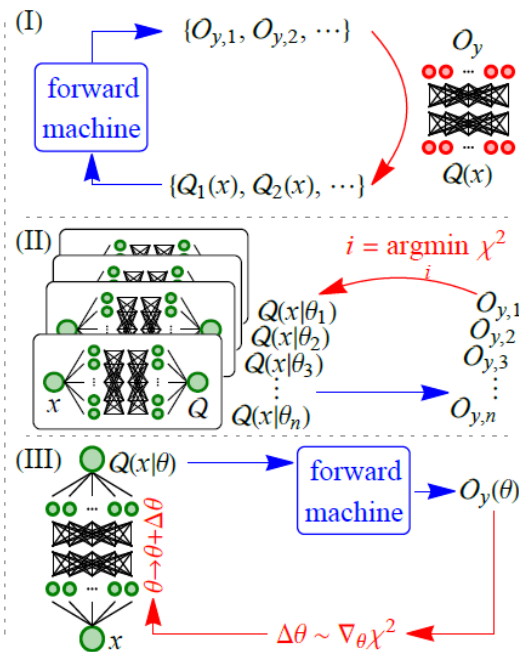
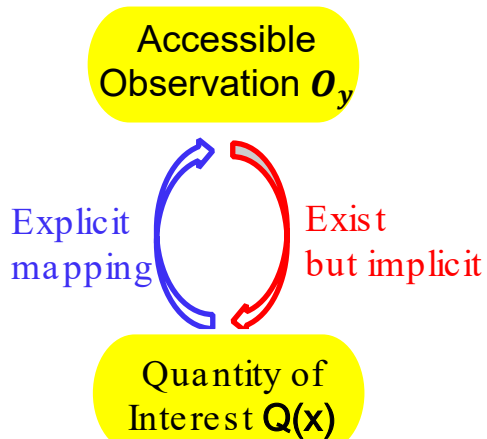
- 18k UrQMD simulation events for central Au-Au@10 AGeV collisions
- **HEIDI:**
Heavy-ion Events through Intelligent Diffusion

PointNet encoder + Normalizing flow decoder + Pointcloud diffusion →



- **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

- **Deep Learning** help bridging HIC experiment with theory/model for physics exploration/inversion *caveat: model dependency*
 - **Bayesian Inference** for EoS from different beam energy experiment data (v_2 and m_T) perform well - consistent with dv_1/dy measurements and BNSM constraint
sensitivity check reveals tension: measurement uncertainty or model limitation
 - **Auto-diff** help physics extraction taking advantage of GPU and DNN
 - **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*)



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

$$\chi^2 = \sum_y \left(\frac{\mathcal{F}_y[Q_{NN}(x|\theta)] - O_y}{\Delta O_y} \right)^2$$
- **Automatic Differentiation :** fuse physical prior into reconstruction via differentiable programming strategy

Thanks !

Nature Review Physics (2025)

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

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

$$\frac{1}{2} \nabla_{\theta} \chi^2 = \sum_y \frac{\mathcal{F}_y[Q_{NN}(x|\theta)] - O_y}{(\Delta O_y)^2} \int dx \frac{\delta \mathcal{F}_y[Q(x)]}{\delta Q(x)} \Big|_{Q(x)=Q_{NN}(x|\theta)} \nabla_{\theta} Q_{NN}(x|\theta)$$