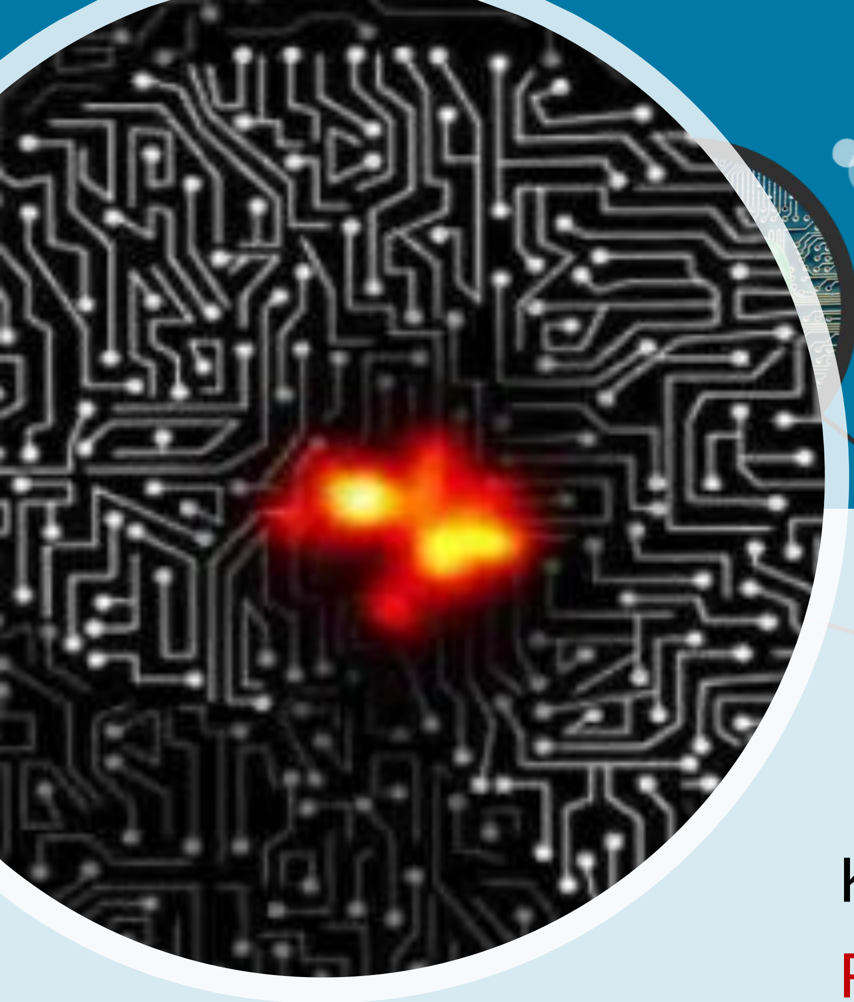


FIAS Frankfurt Institute for Advanced Studies

Exploration of Matter in Extreme conditions with Machine Learning

Kai Zhou (FIAS)

RHIC-BES Seminar

Outline

- **Overview** : 1, QCD matter in extreme;
  2, AI/ML/DL techs

- **Heavy Ion Collisions** with ML
  1.1 Hot matter EOS identification from HIC with DL
  1.2 Online event impact parameter determination with Point-Net for CBM
  1.3 Bayesian Inference of dense matter EOS from HIC data

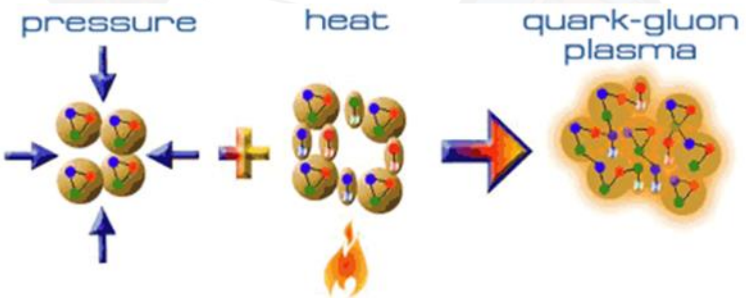
- **Lattice QCD data** analysis with ML
  2.1 In-medium heavy quark potential reconstruction with DNN
  2.2 Unsupervised Spectral function reconstruction with DNN

- **Neutron Star** EOS inference with ML

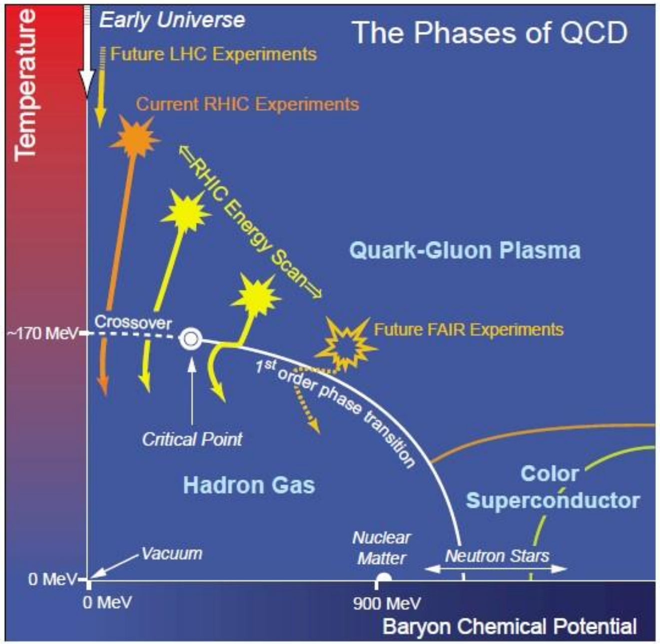
- **Summary**

Overview : 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>



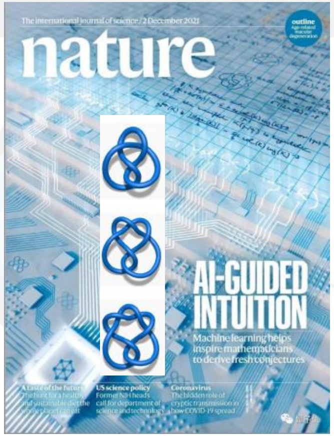
``It would be intriguing to explore new phenomena by distributing high energy or high nuclear matter density over a relatively large volume.'' - - **T.D. Lee** (1974)

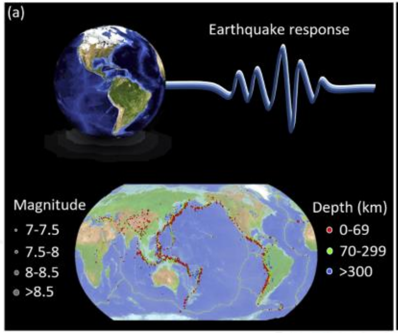


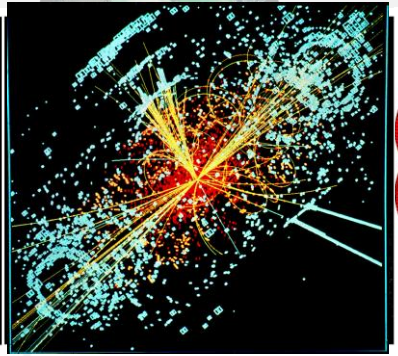
<u>To study QCD matter under extreme conditions :</u>

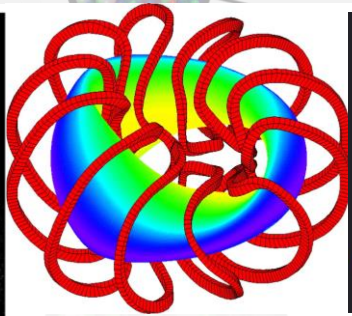
- Nuclear Collisions : heat & compress matter
- Lattice Field Theory : numerically solve partition function
- Neutron Star : dense matter, astronomy constraints

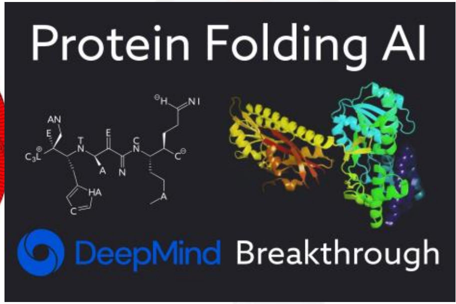
Overview: Deep Learning

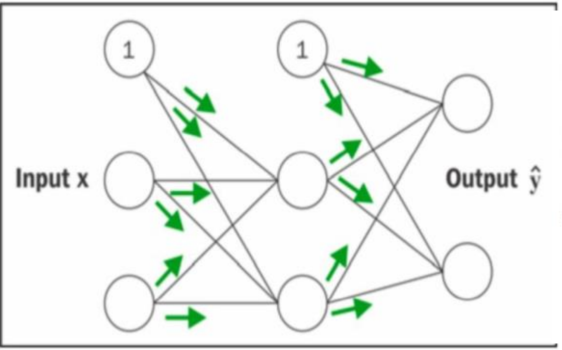








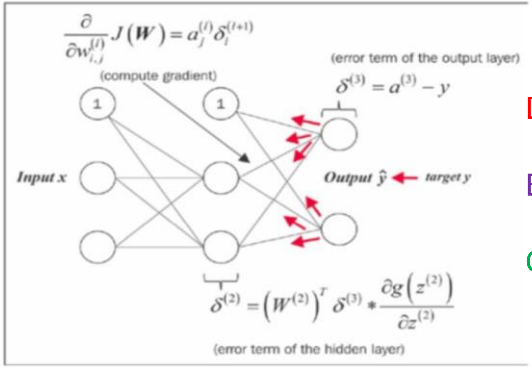




Find and **Decode** the mapping/representations into
Deep **N**eural **N**etwork

➡ **Function approximator**

Universal approximator (Hastad et al 86 & 91)

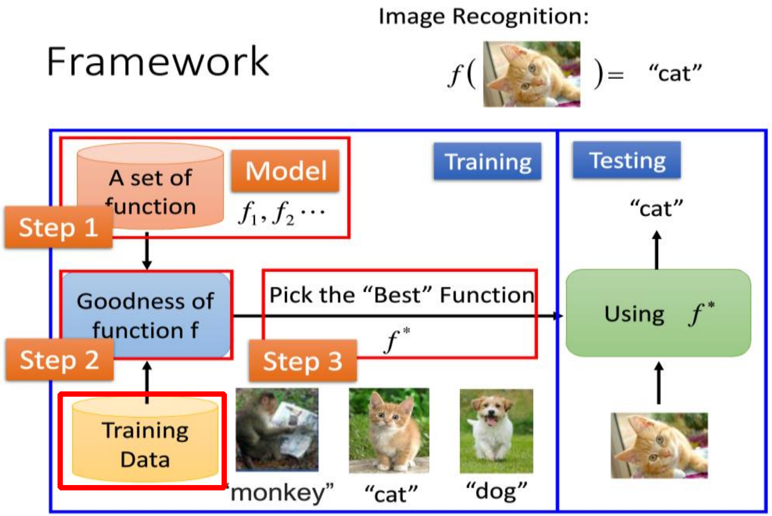


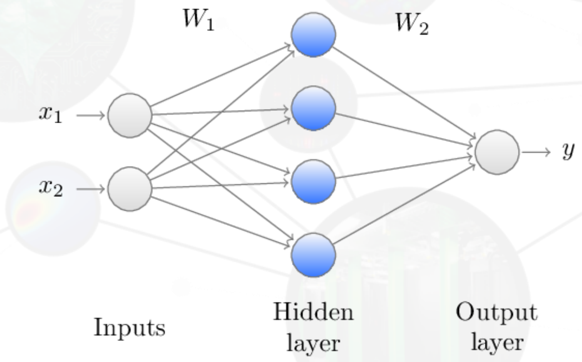
Differentiable programming

Backward Propagation

Gradient Descent Algorithm

Overview: Machine learning, Deep Neural Networks, Representation learning



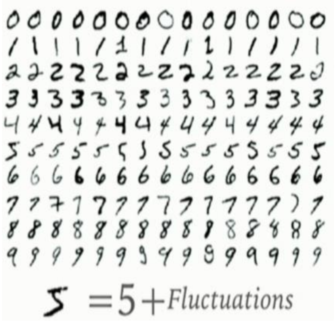


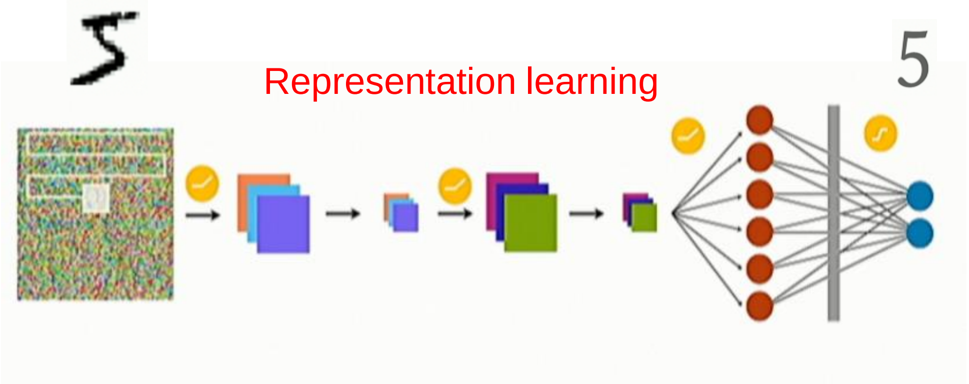
Composing :

Linear affine transformation
+
Non-linear activation

Layer by layer

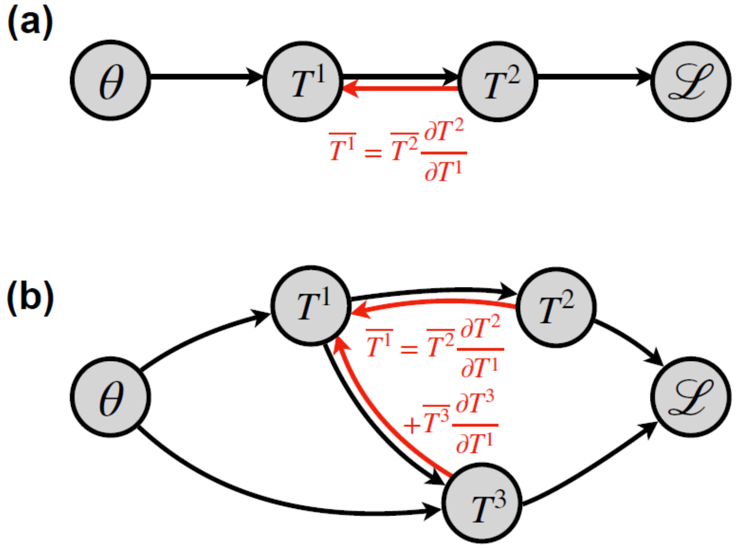
$$f_{NN}(x;\theta) = h_2(w_2 h_1(w_1 x + b_1) + b_2)$$





Overview: Deep Learning, Differentiable Programming and Automatic differentiation

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



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 : $\overline{T} = \partial \mathcal{L} / \partial T$

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

$$\boxed{\overline{\theta} = \overline{T^1}\frac{\partial T^1}{\partial \theta}}$$

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

Overview: Discriminative and Generative learning

- Discriminative learning : **prediction** (classification / regression)

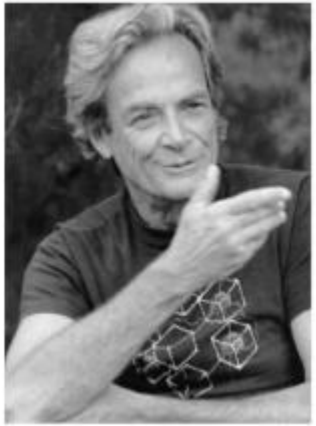
  Function Fitting $y = f(x)$

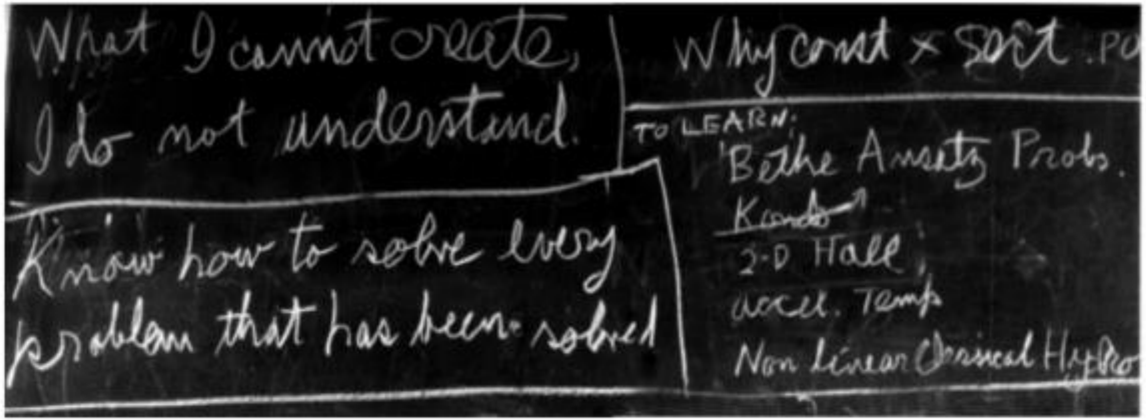
  Conditional Probability $p_\theta(y|x) \rightarrow p(y|x)$

- Generative learning : **understand** (generation / clustering)

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

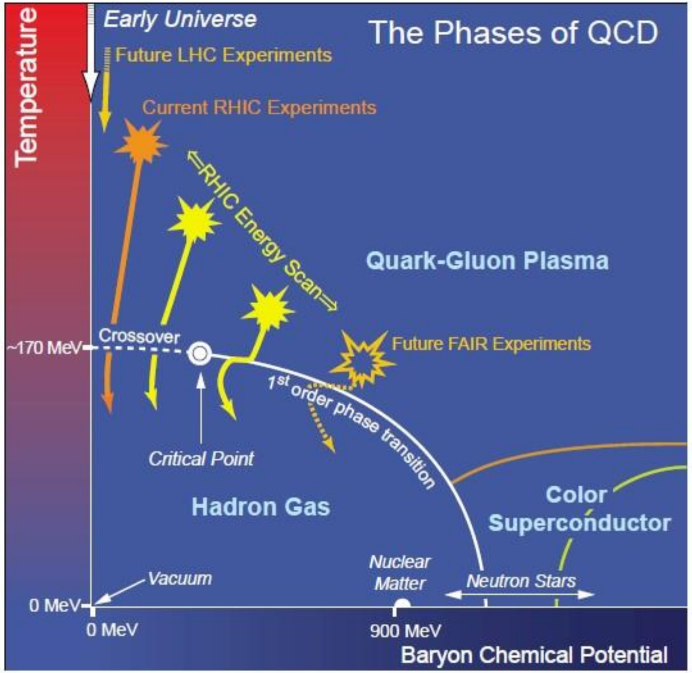
"What I can not create I do not understand"





Overview : Our focus of Matter Exploration in extreme with Machine Learning

Questions we will discuss →



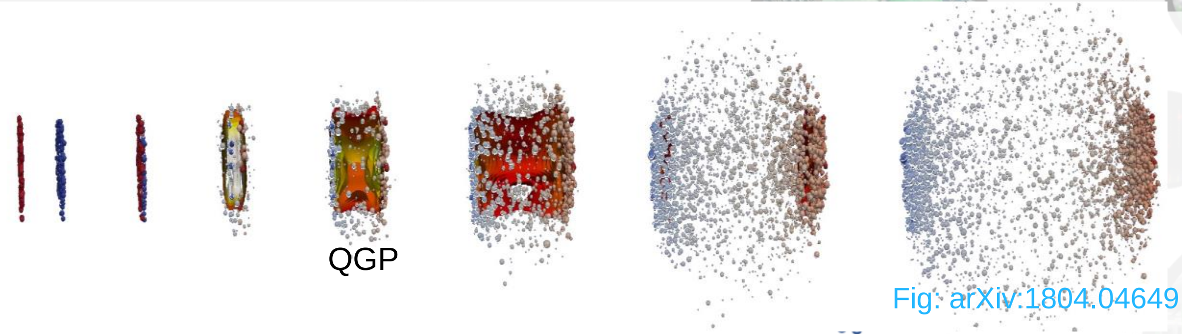
- Nuclear Collisions :
  - ✓ Will early dynamic-info survive the evolution? How to decode?
  - ✓ How to more effectively connect experiment to theory/model?
  - ✓ Dense matter EoS underlies current low energy HIC observable
- Lattice QCD data:
  - ✓ Could physical observable evaluation from configs and also partition function be captured by Machine Learning?
  - ✓ Inverse problem solving: convert measurement to physics?
- Neutron Star :
  - ✓ How to maximumly exploit the astronomy observation?

1.1, Hot matter EoS identification from Heavy Ion Collisions with Deep Learning

With **Longgang Pang**, Nan Su, Yilun Du, Jan Steinheimer, Lijia Jiang, Lingxiao Wang, Hanna Peterson, Horst Stoecker, Xinnian Wang, etc.,

Nature Communications 9 (2018), no.1, 210
JHEP 12 (2019) 122
Eur.Phys.J.C 80 (2020) 6, 516
Phys. Lett. B 811 (2020)
JHEP 21 (2021) 184
Phys. Rev. D 103 (2021) 11, 116023

Challenges in heavy ion collisions



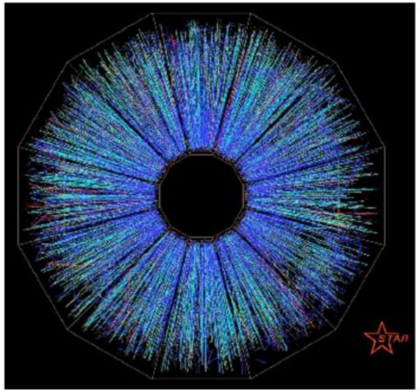
Initial Stage | $\nabla_\mu T^{\mu\nu} = 0$, $\nabla_\mu N^\mu = 0$ | $p^\mu \partial_\mu f + F \cdot \partial_p f = C$ | Final State

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

EoS, η/s,
initial state, … ?
…

Model simulation

?



L.G.Pang, **K. Zhou**, N.Su et al., **Nature Commu.9 (2018), no.1, 210**

Direct inverse mapping?

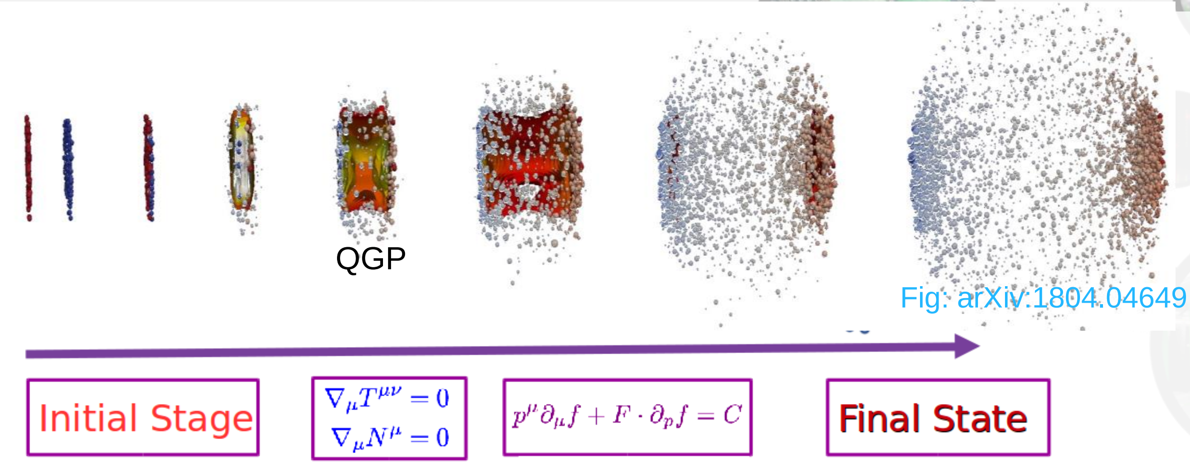
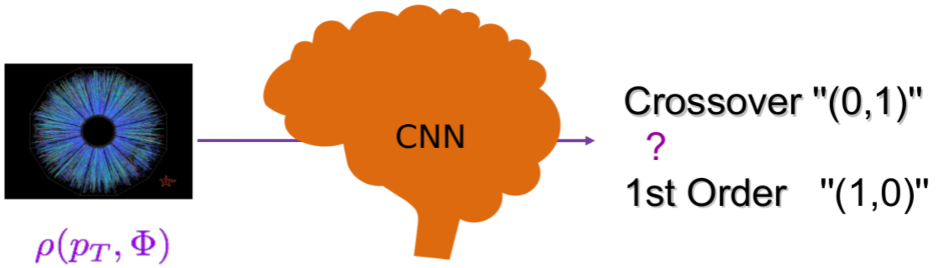
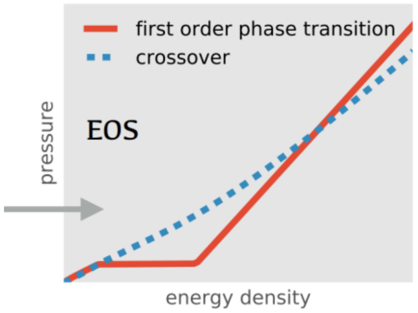


Fig: arXiv:1804.04649

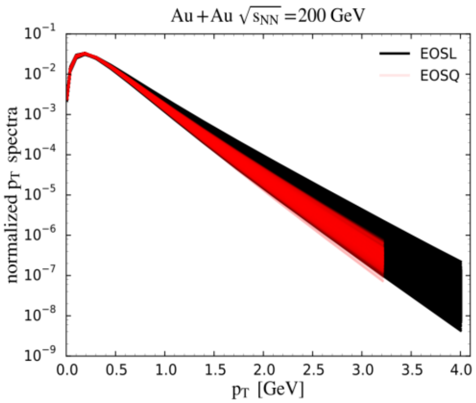
- Uncertainties in HIC modeling
- Multiple parameters <u>entangle</u> with multiple observables
- How to disentangle different factors to reveal fundamental physics from the dynamical environment?
- **DNN make the road!**

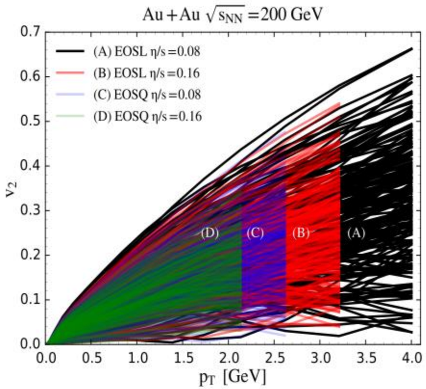


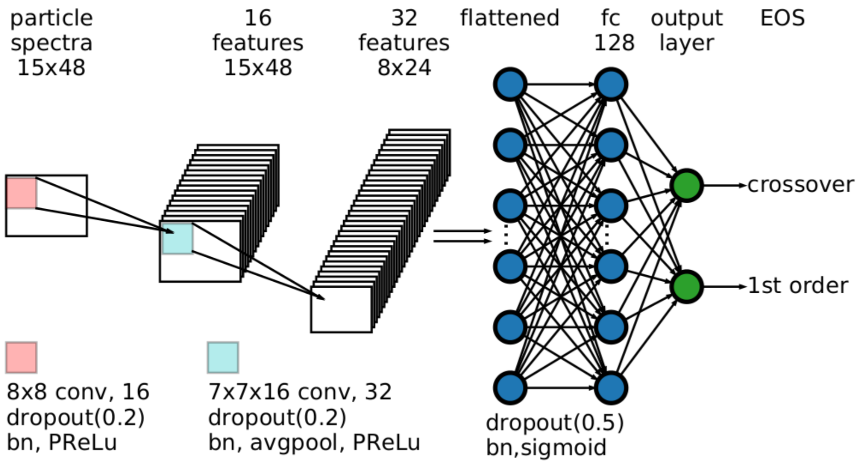


L.G.Pang, **K. Zhou**, N.Su et al., **Nature Commu.9 (2018), no.1, 210**

Prototype study of deploy AI to decode dynamical physics in Heavy Ion Collisions





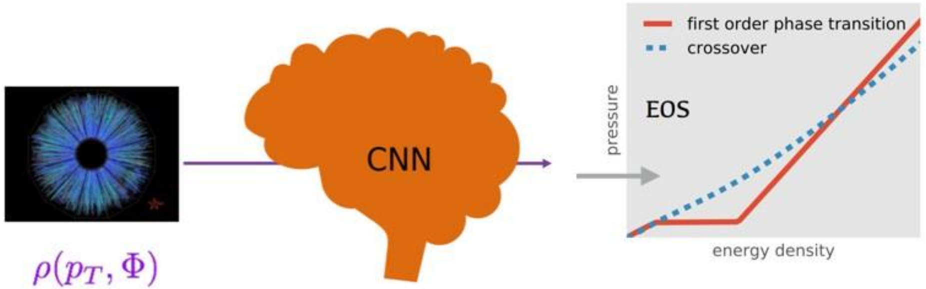


- Conventional observable fail !
- Strongly depends on the initial fluctuations and other uncertainties

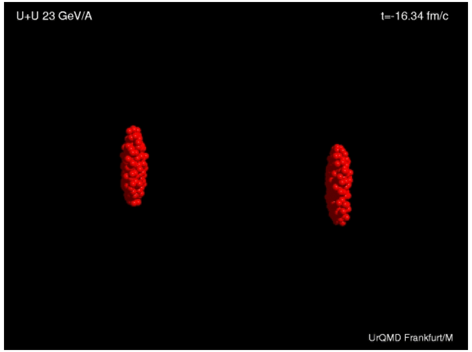
- ~ 95% EbE classification accuracy!
- Robust against initial condition, eta/s

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

Into more realistic cases

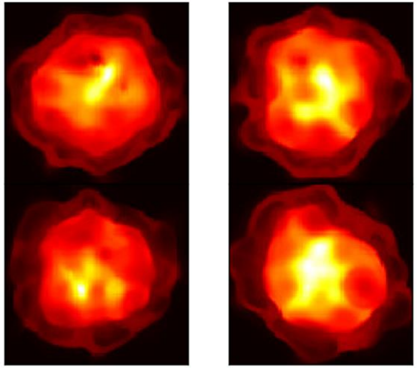


Hadronic cascade
(UrQMD considered)



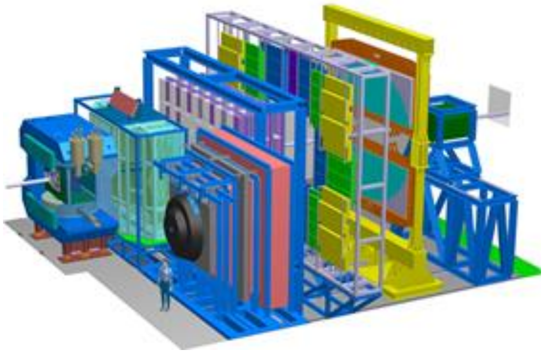
Y.L. Du, **K. Zhou**, et at.,
Eur.Phys.J.C 80 (2020) no.6,516

Non-equilibrium transition
(Baryon Clumping, spinodal)



J.S, L.G. Pang, **K. Zhou**, et at.,
JHEP 12,122(2019)

Detector effects
(Hits/Tracks, Point-Net)



M.O.K, J.S, **K. Zhou**, et at.,
Phys. Lett. B 811, 135872
JHEP 21 (2021) 184

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1.2, End-to-End Online Event Characteristics for CBM with PointNet

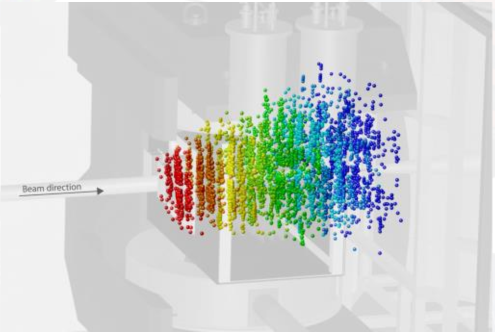
With **Manjunath O.K**, Jan Steinheimer, Andreas Redelbach, Horst Stoecker

Phys.Lett.B 811 (2020) 135872
Particles 2021, 4(1), 47-52

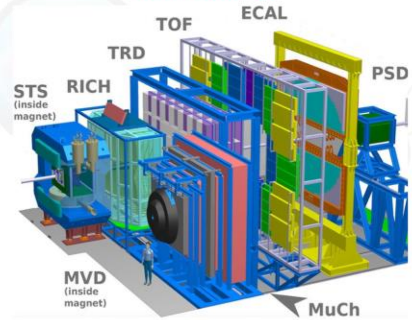
Motivation : point cloud data structure, and CBM challenge

- **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:
  - less 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** →

x_1	y_1	z_1
x_2	y_2	z_2
.	.	.
.	.	.
.	.	.
.	.	.
x_n	y_n	z_n

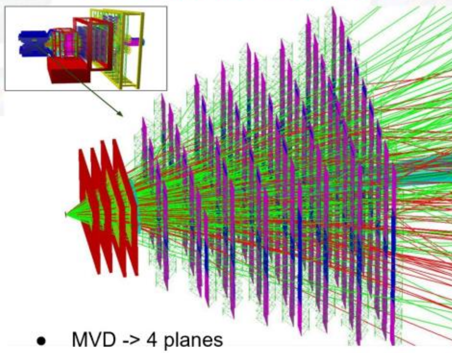


CBM detector



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

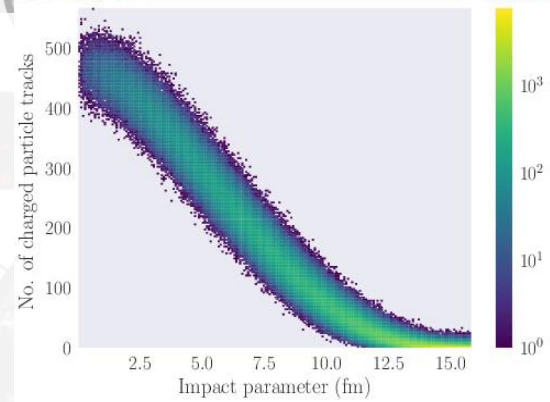
A simulated event in STS + MVD



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

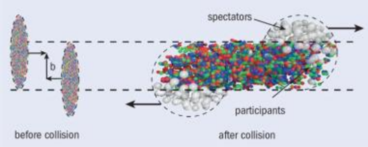
Take impact parameter for example

- ‘b’ is not directly measurable in exp
- Final state observables carry the information
  - MC Glauber
  - Percentiles of Nch, Espec are mapped to centrality
  - Only a likely distribution for b in a centrality bin is known

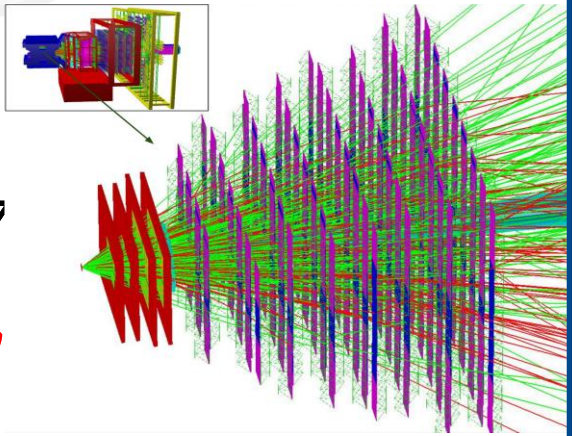


- UrQMD + cbmROOT generate data
- With **hits/tracks** from detector,

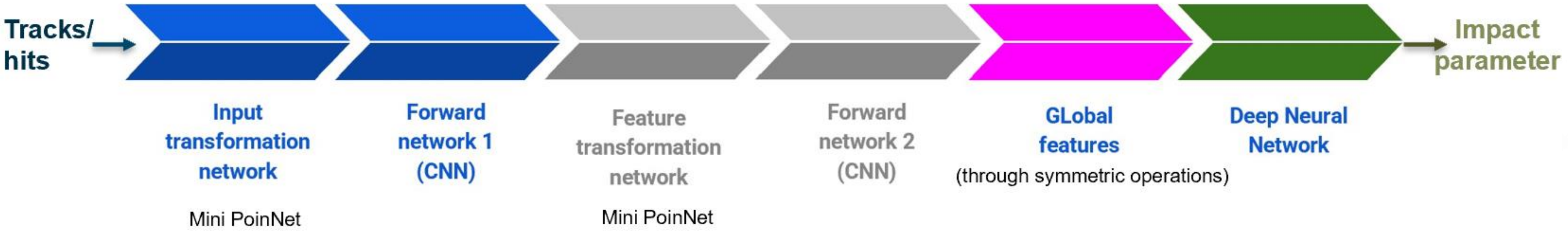
end-to-end online b-meter: **PointNet**



Impact Parameter



Models

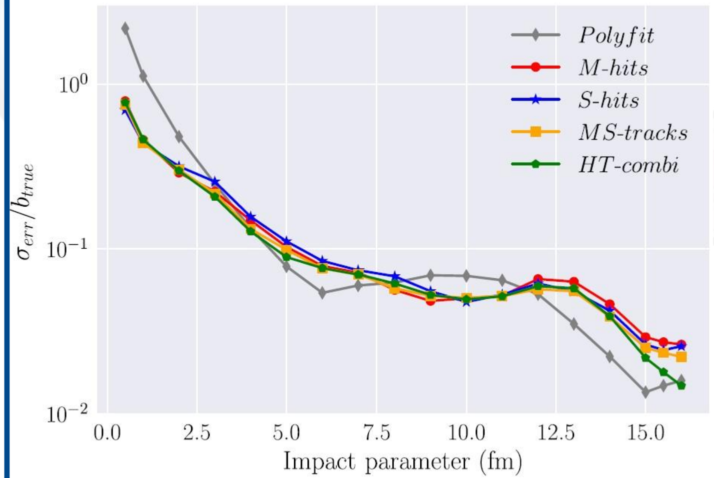


01	**M-hits**	(x,y,z) of all Hits in MVD
02	**S-hits**	(x,y,z) of all hits in STS
03	**MS-tracks**	(x,y,z,dx/dz,dy/dz,q/P) of all tracks in first and last plane from MVD+ STS
04	**HT-combi**	Hits from MVD and tracks from MVD+STS
05	**Polyfit (non-ML baseline)**	Third order polynomial fit to multiplicity vs. impact parameter curve

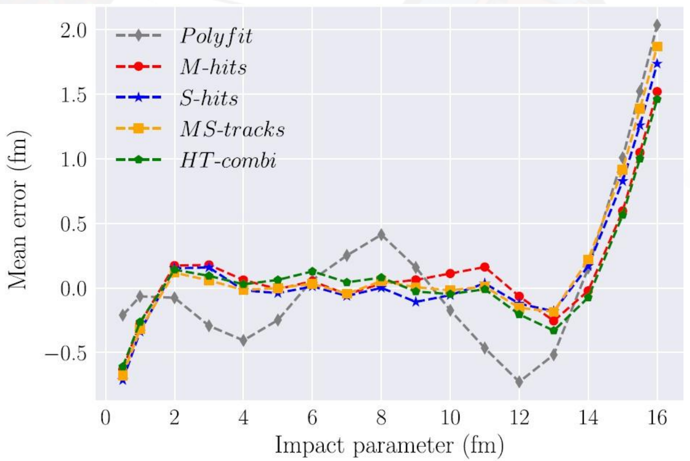
- Works on direct exp. output
- Event-by-event online possible
- Training data generated by **'UrQMD → CbmRoot'** 10^5 Au+Au 10 AGeV events b ~ (0-16)fm

Test Result : resolution, accuracy, more actual case ?

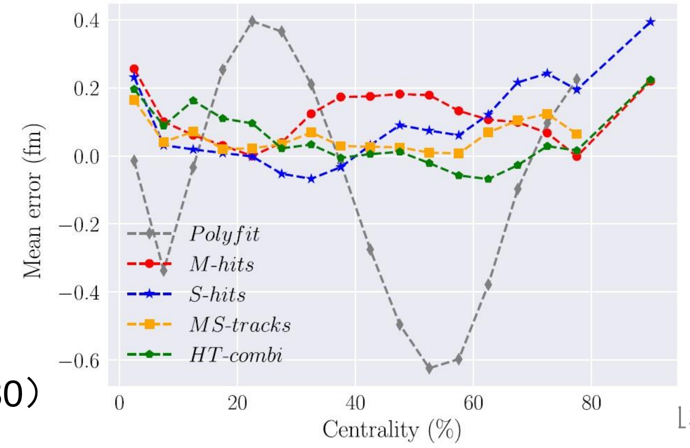
- Quantifies precision in predictions
- Polyfit fails for central events!
- Similar precision for b>3 fm



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



- For realistic bdb distributed testing collision events →
- Fast online event selection ~ 1k events/s on 1 game GPU（RT2080）



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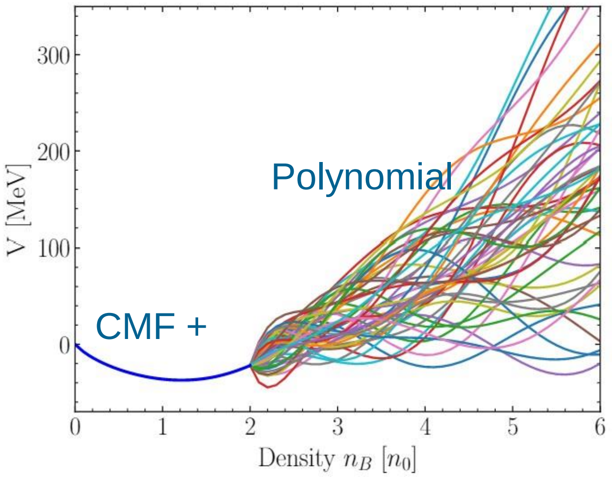
1.3, Bayesian inference of high density EoS from low energy heavy ion collisions

With **Manjunath O.K**, Jan Steinheimer, Horst Stoecker

To be online soon

The EoS parameterization, the flow and transverse kinetic energy measurements



$$V(n_B) = \sum_{i=1}^{7} \theta_i \left(\frac{n_B}{n_0} - 2\right)^i + h$$

$$P(n_B) = P_{\rm id}(n_B) + \int_0^{n_B} n' \frac{\partial U(n')}{\partial n'} dn'$$

$$U(n_B) = \frac{\partial(n_B \cdot V(n_B))}{\partial n_B}$$

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

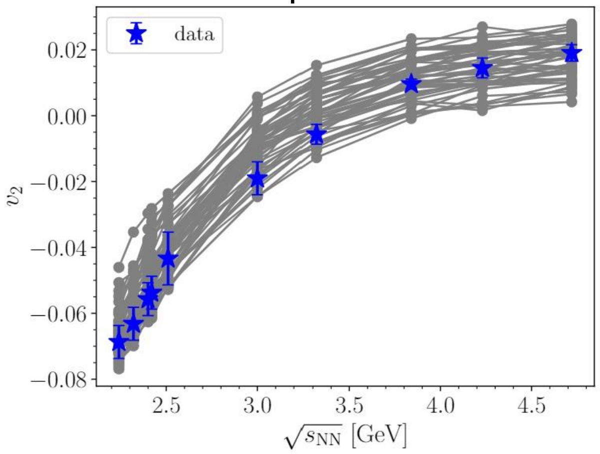
Eur.Phys.J.C82(2022)5,417

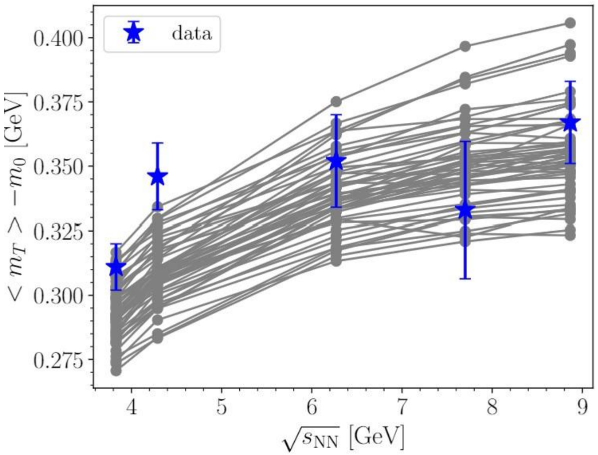
$$\dot{\mathbf{r}}_i = \frac{\partial \mathbf{H}}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i = -\frac{\partial \mathbf{H}}{\partial \mathbf{r}_i}$$

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

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

Evidence : proton's v2 and mT



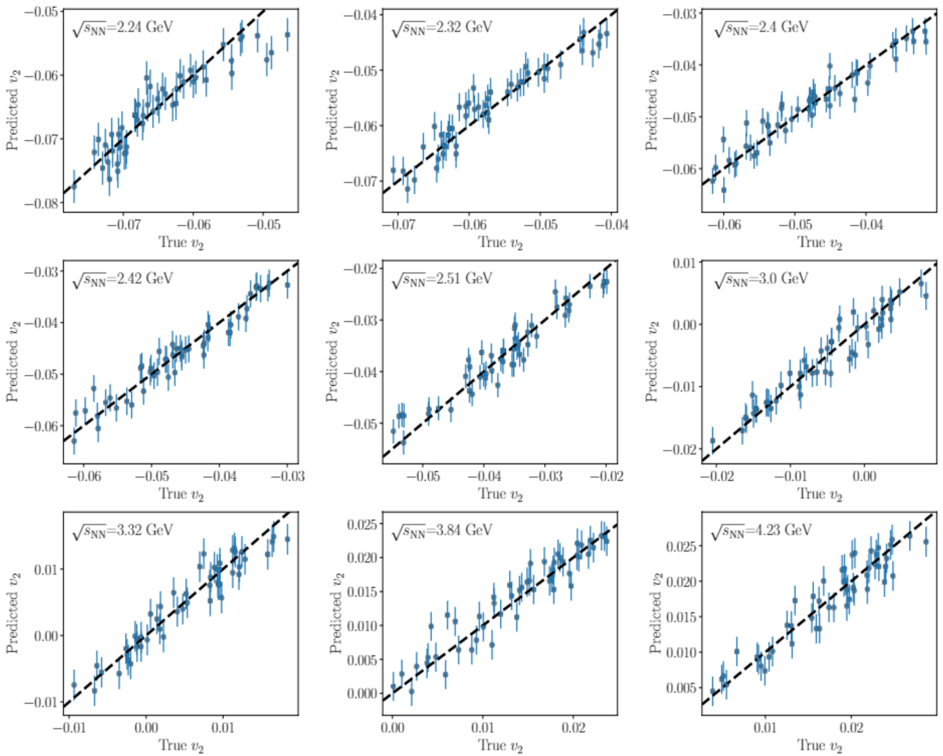


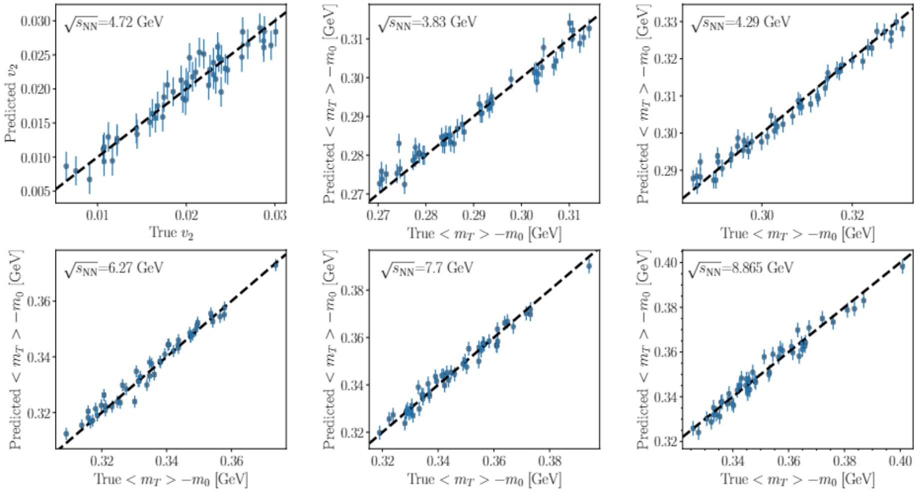
Emulator with Gaussian Process

- $Obs_i(\boldsymbol{\theta}) \sim GP(\mu(\boldsymbol{\theta}), \kappa(\boldsymbol{\theta}, \boldsymbol{\theta}'))$

- Performance of the trained GP Models :

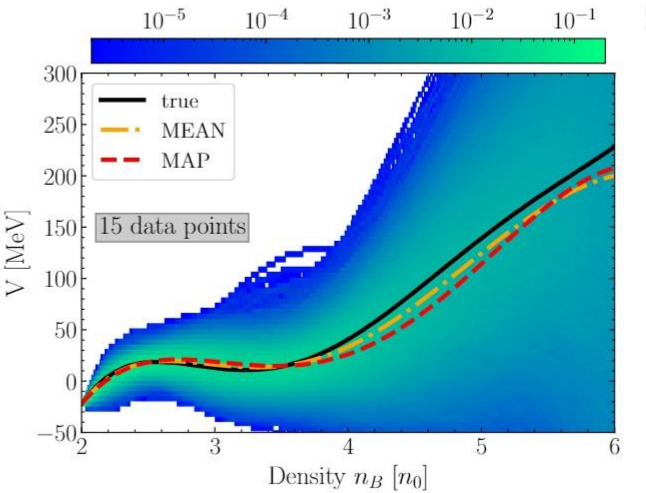
  $R^2 \sim 0.9$

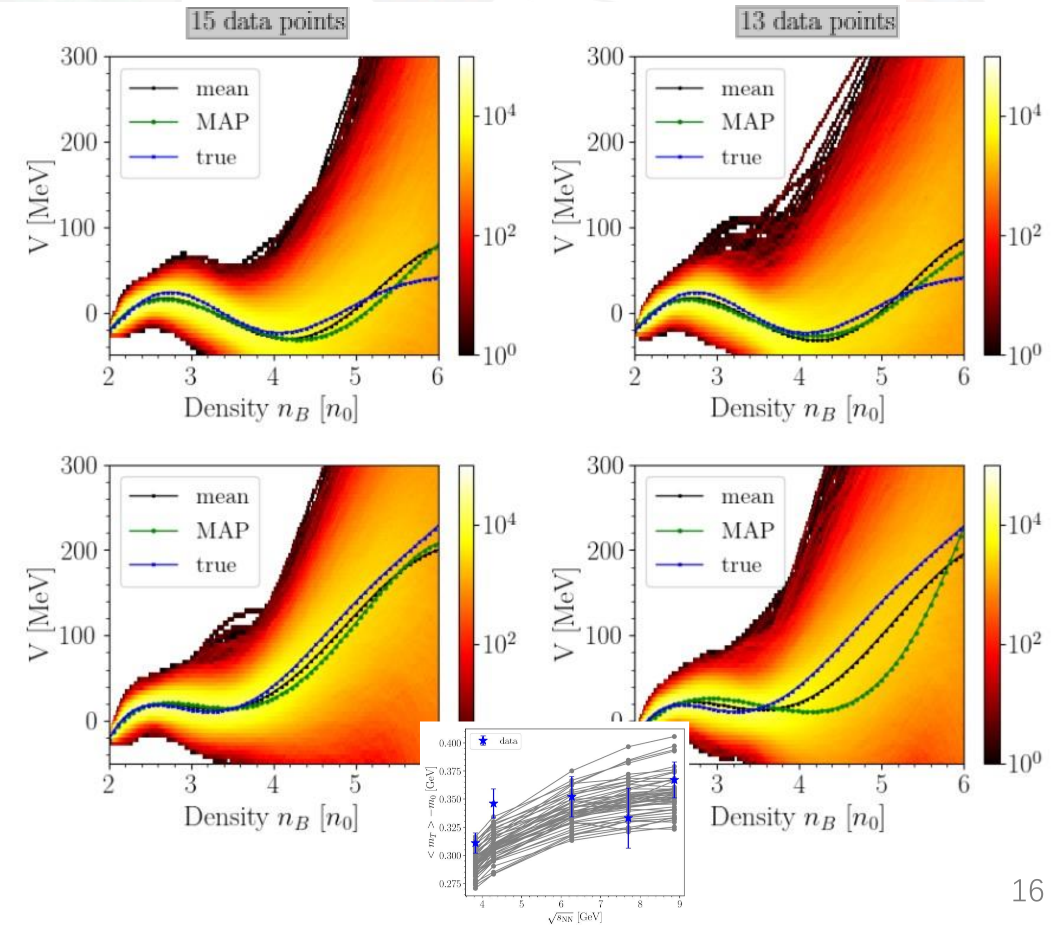




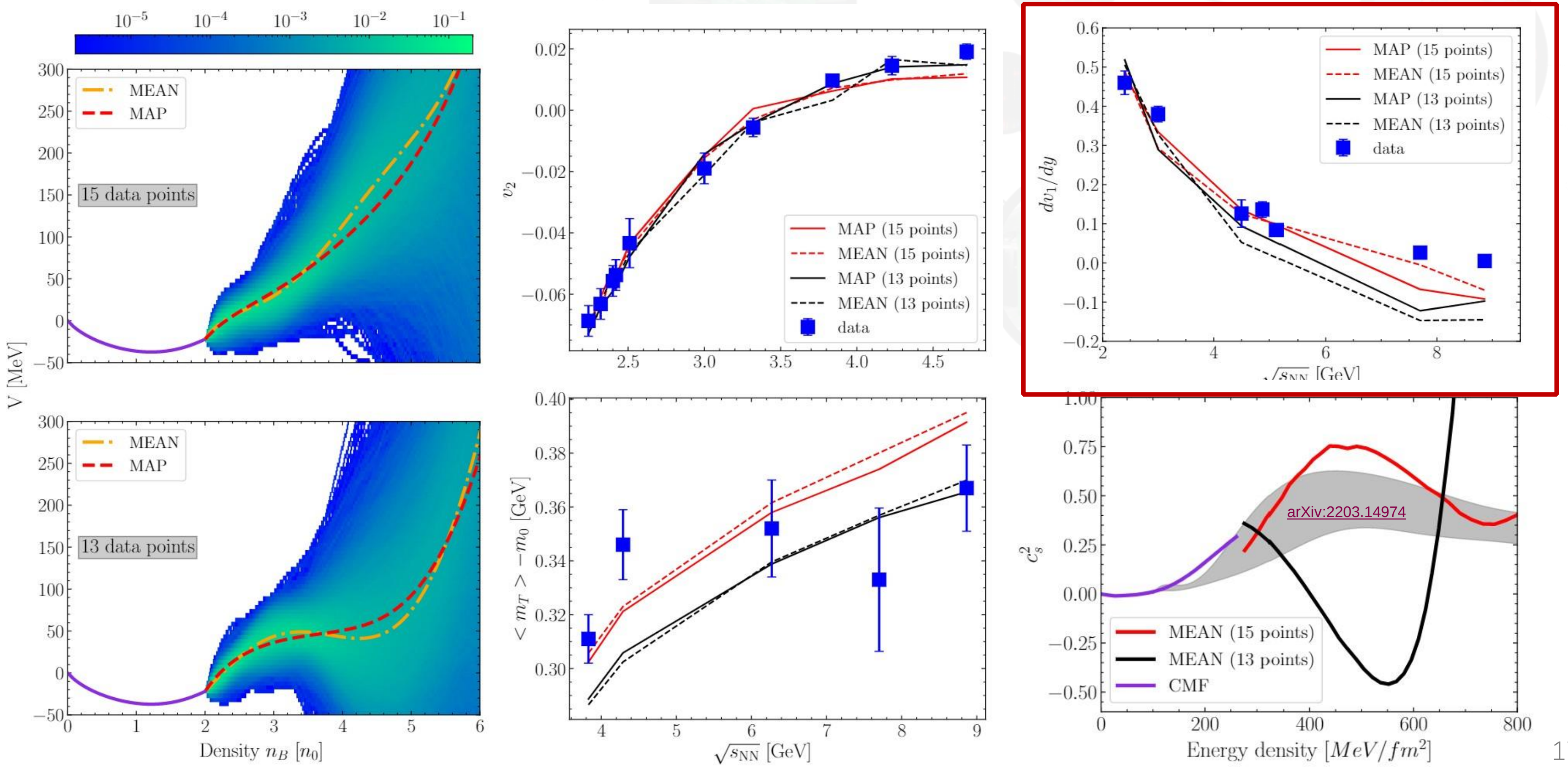
Closure tests

- Posterior ~ Likelihood * Prior
- Reconstruct well the EoS to 4-6 n_0
- Drop the first 2 points of m_T ?
  not influence 2-3.5 n_0
  but matters for 4-6 n_0





Inference results with experimental data, and **predictability**



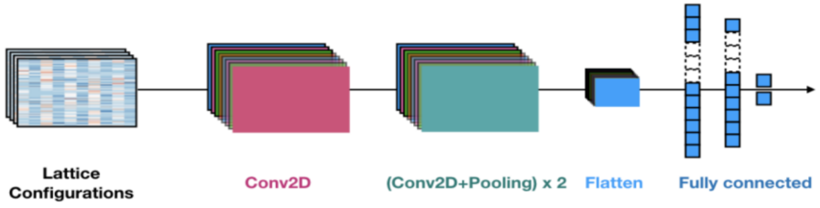
2.1 Basic applications in Lattice calculation for QFT or many-body system

With Gergely Endroedi, Long Pang, Horst Stoecker,
Lingxiao Wang, Yin Jiang, Shile Chen, Oleg Savchuk, Lianyi He

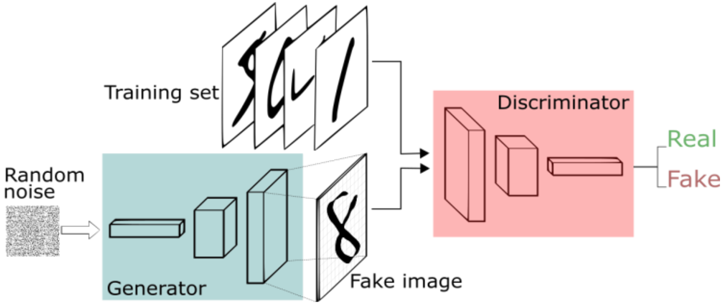
Phys.Rev.D 100,011501(R) (2019)
arXiv:2005.04857
arXiv:2007.01037

DNN into Quantum Field Theory

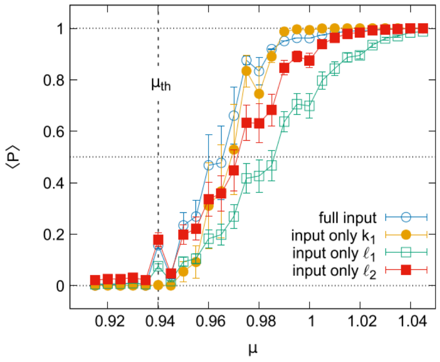
- Discriminative DL methods for phase classification and physics regression:

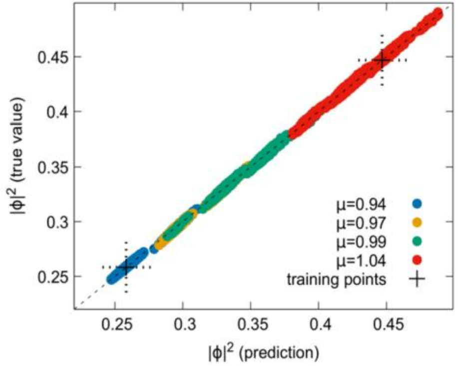


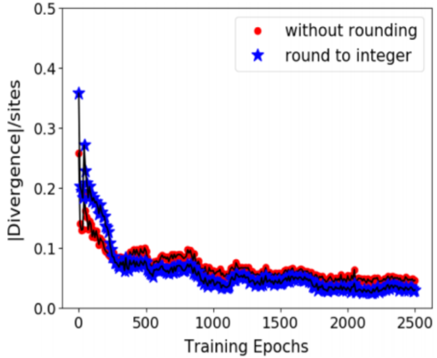
- Generative models for more efficient config sampling and physics decoding:

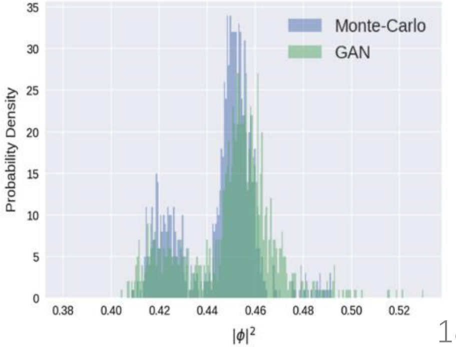


K. Zhou, et.al, **Phys.Rev.D 100,011501(R) (2019)**









Exploring Many-Body System Phase Structure Unsupervisedly

- **Boltzmann** distribution for statistical svstem (e.g. Field, or simply XY model)

$$p(\phi) = \frac{1}{Z} e^{-S(\phi)} \qquad p(\mathbf{s}) = \frac{e^{-\beta E(\mathbf{s})}}{Z}$$

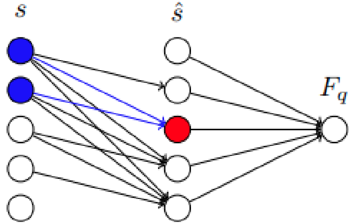
- Variational approach (e.g. mean field theory) : minimize **variational Free Energy**

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

- Introduce more expressive Ansatz with neural network : <u>**autoregressive net**</u> or Flow model

D. Wu, et.al., PRL122,080602(2019)

$$q_\theta(\mathbf{s}) = \prod_{i=1}^{N} q_\theta(s_i \mid s_1, \ldots, s_{i-1}) \qquad \hat{s}_i = \sigma\left(\sum_{j<i} W_{ij} s_j\right) = q(s_i = +1 \mid \mathbf{s}_{<i})$$



- generalize to continuous variable systems? Like, for XY model :

$$H = -J \sum_{<i,j>} s_i s_j = -J \sum_{<i,j>} \cos(\phi_i - \phi_j)$$

- **Continuous-mixture Autoregressive Network**

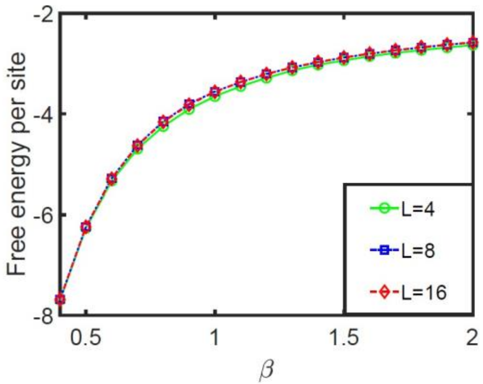
$$f_\theta(s_i | s_1, \ldots, s_{i-1}) = \frac{\Gamma(a_i + b_i)}{\Gamma(a_i)\Gamma(b_i)} s_i^{a_i - 1} (1 - s_i)^{b_i - 1}$$

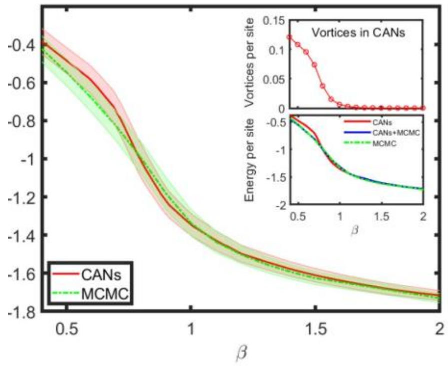
*L.Wang, Y. Jiang, L.He, **K.Zhou***
arXiv:2005.04857

Continuous-mixture Autoregressive Network

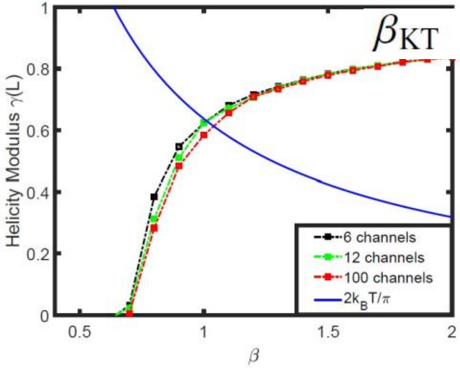
- Thermodynamics and transition estimate come out from CAN agrees well with MCMC

*L.Wang, Y. Jiang, L.He, **K.Zhou***
arXiv:2005.04857

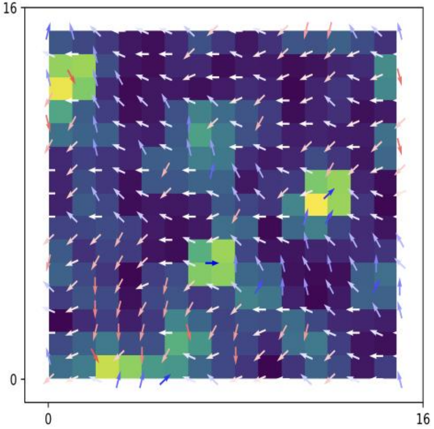


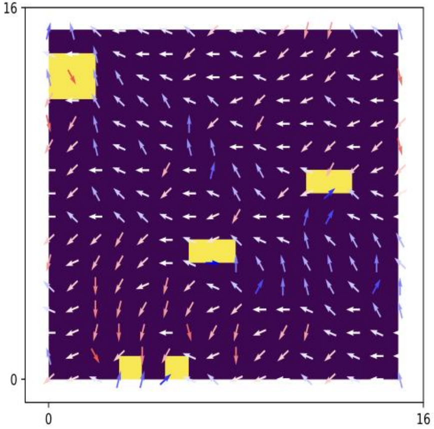


$\beta_{\rm KT} \approx 1.12.$



conditional probability from CAN





Vorticity density map

The trained CAN network captures the physics of vortex automatically!

2.1 From lQCD to in-medium HQ interactions

With **Shuzhe Shi**, Jiaxing Zhao, Swagato Mukherjee, Pengfei Zhuang

Phys. Rev. D 105 (2022) 1, 1

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

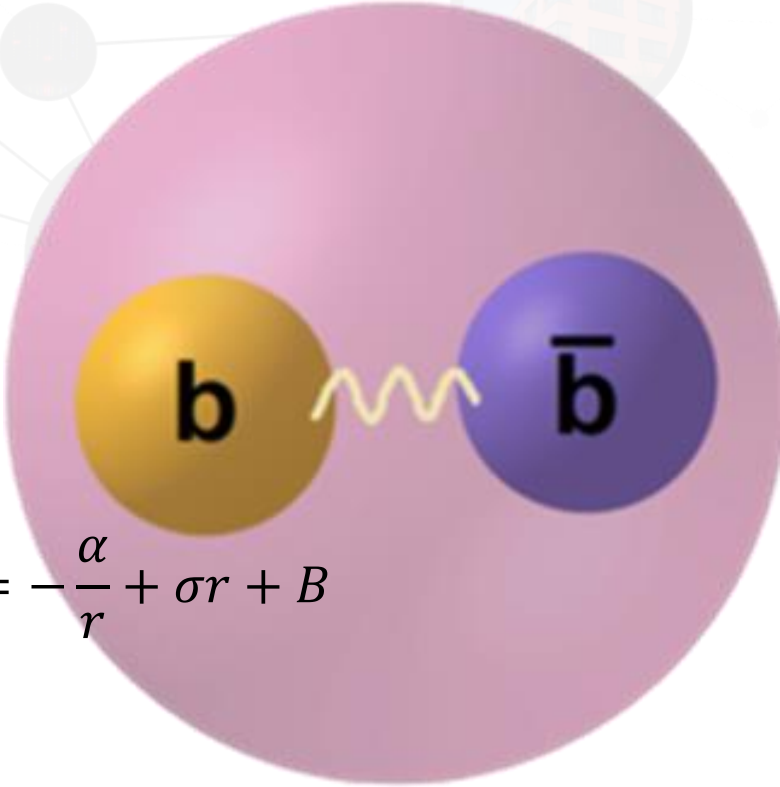
- Produced via Hard Processes from early stage
- 'Calibrated' QCD Force – HQ interaction

In Vacuum : NR potential (NRQCD) , Cornell-like

$$V(r) = -\frac{\alpha}{r} + \sigma r + B$$

In Medium : Color Screening , Thermal Width

Laine, et.al, JHEP(2007)

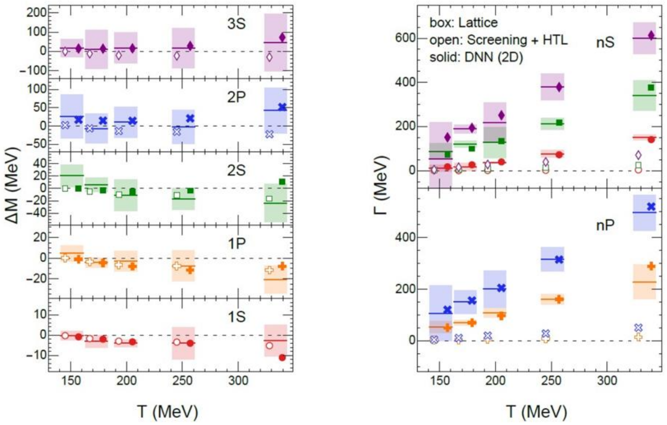


Potential model : Inverse Schrödinger equation

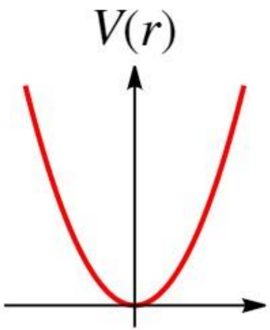
$$\hat{H}\psi_n = -\frac{\nabla^2}{2m_\mu}\psi_n + V(r)\psi_n = E_n\psi_n$$

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

New lQCD results cannot be explained by HTL-inspired potentials



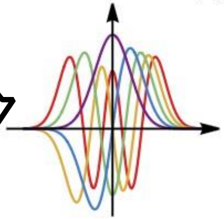
R. Larsen, et.al, PRD(2019), PLB(2020), PRD(2020)



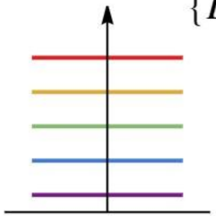
Inverse Power method

H.W.Crater, JCP(1994)

$\{\psi_n(r)\}$



$\{E_n\}$



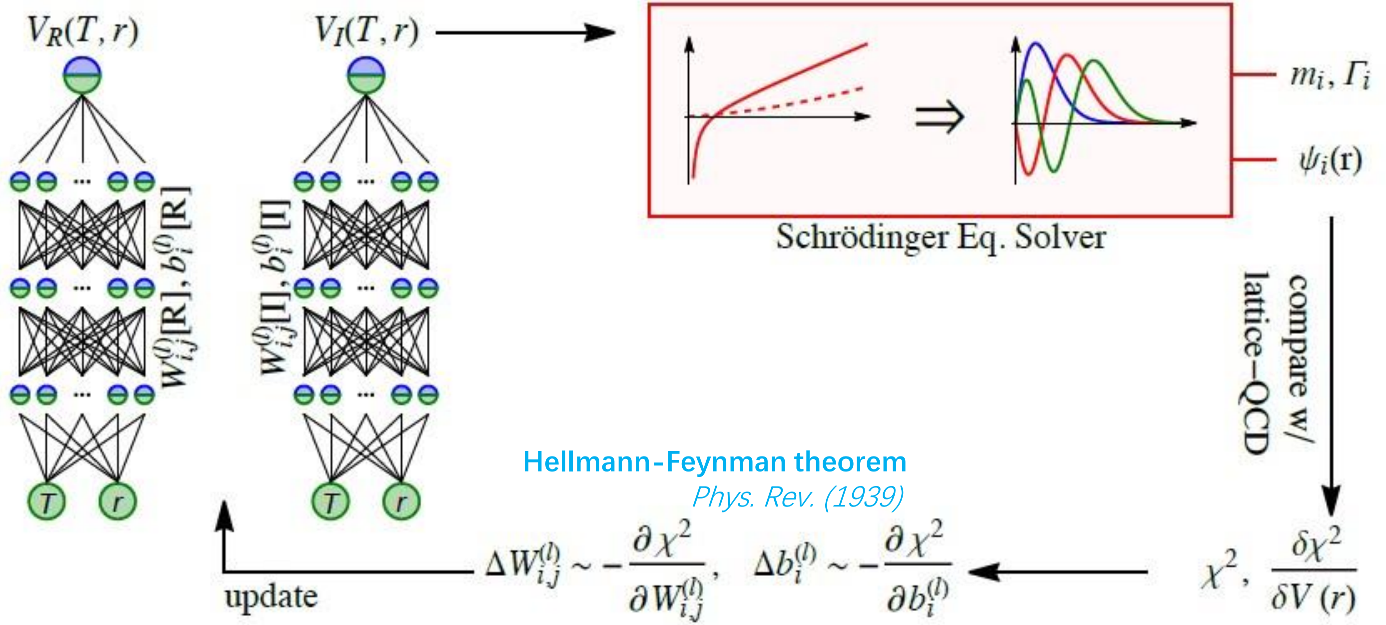
$$\begin{cases} \mathrm{Re}[E_n] = m - 2m_b \\ \mathrm{Im}[E_n] = -\Gamma \end{cases}$$

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

?

How to extract potential in a model-independent way given spectroscopy?

Flow chart for “DNN + Schrödinger Eq.”



Hellmann-Feynman theorem
Phys. Rev. (1939)

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

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

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

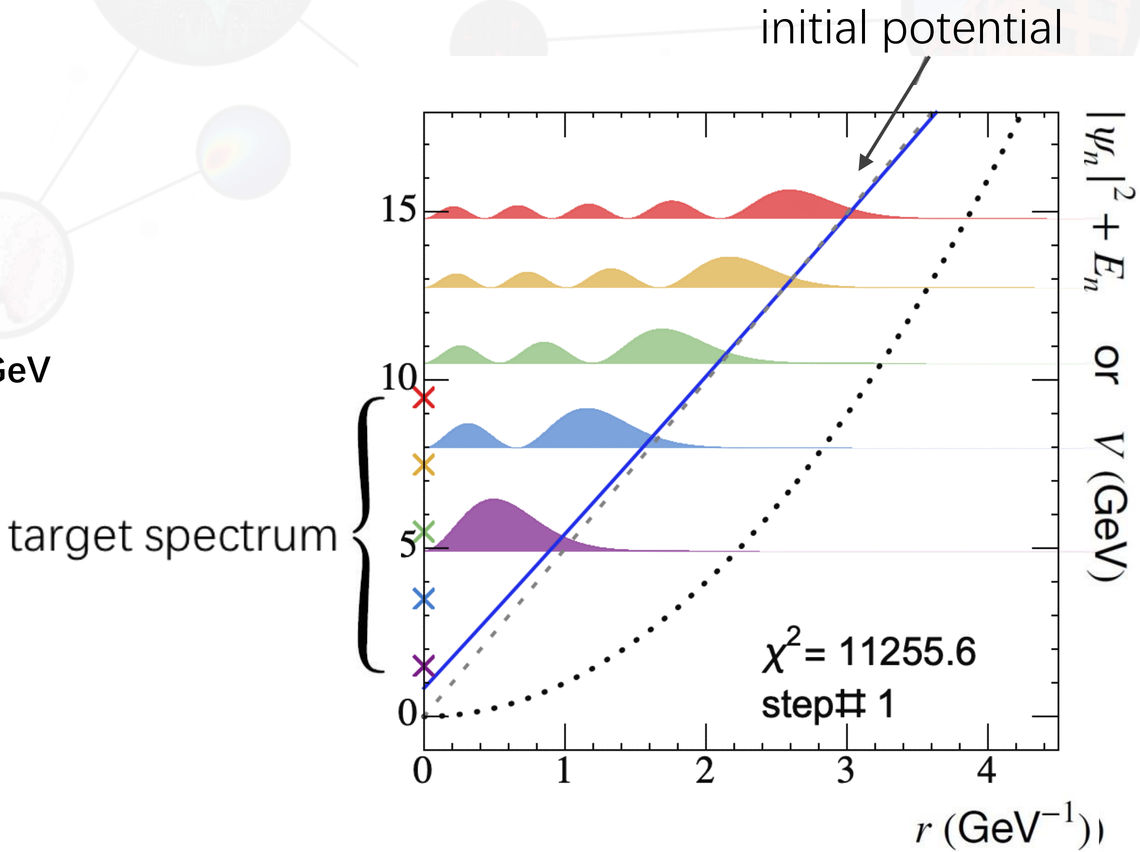
Phys. Rev. D 105 (2022) 1, 1

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



Proof of Concept

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

-- Yes! To certain range decided by the provided states.

Learn V(r) from 5 eigenvalues :

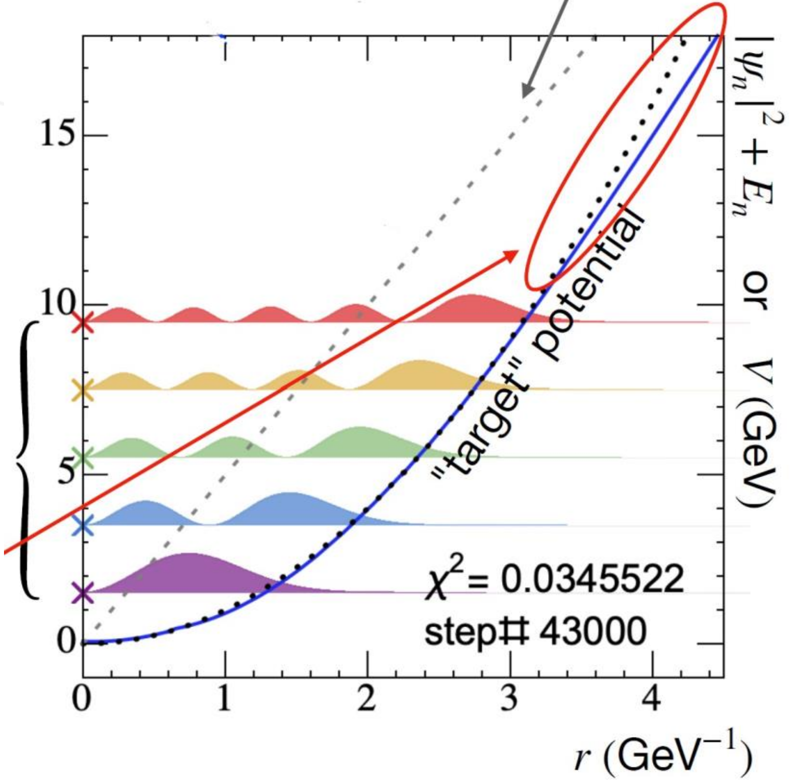
{ En } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV

Deviation @ given states' wavefunction vanishes

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

initial potential

target spectrum



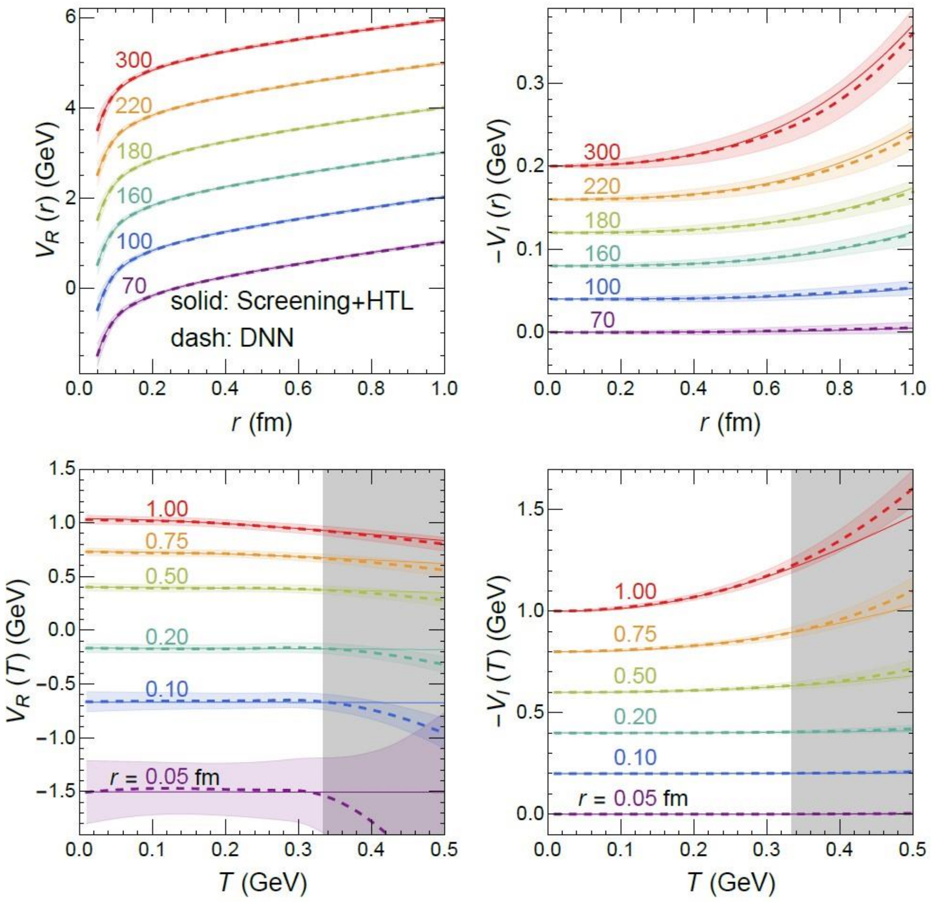
Closure Test – reconstruct HTL potential

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

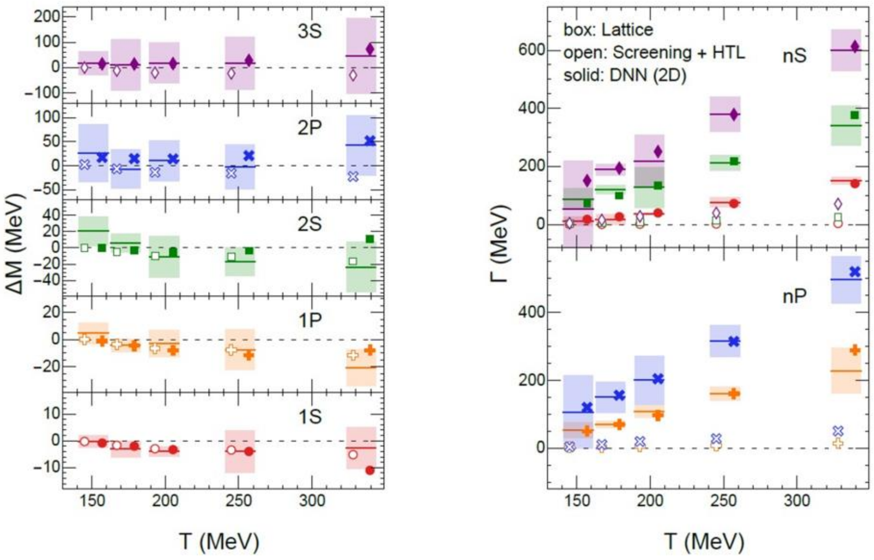
$$V_I(T,r) = -\frac{\sqrt{\pi}}{4}\mu_D T\sigma r^3 G^{2,2}_{2,4}\left(\begin{matrix}-\frac{1}{2},-\frac{1}{2}\\ \frac{1}{2},\frac{1}{2},-\frac{3}{2},-1\end{matrix}\middle|\frac{\mu_D^2 r^2}{4}\right) - \alpha T\,\phi(\mu_D r)\,,$$

$m_b = 4.676$ 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

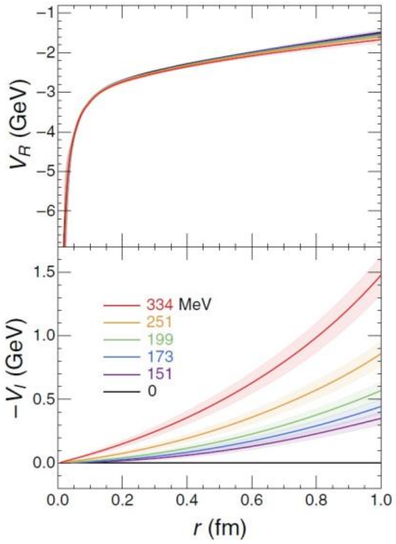


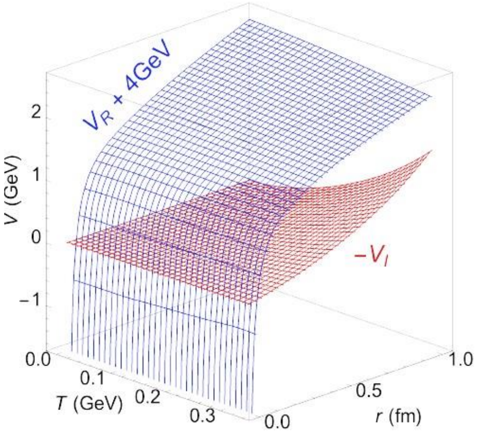
Results with lattice data for HQ potential



Chi2-per-data=16.5/30

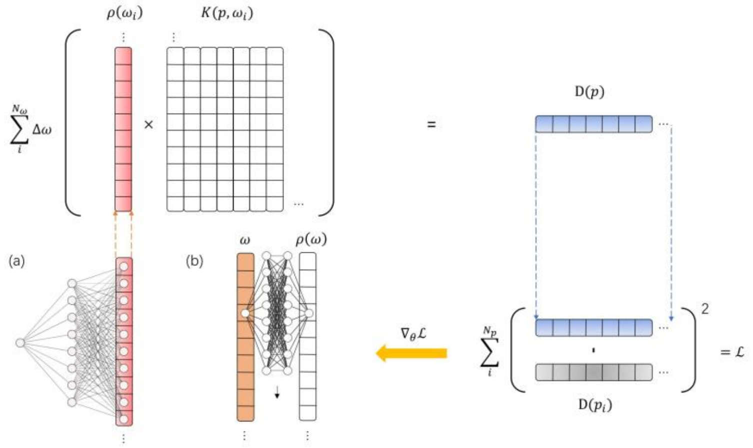
The reconstructed T, r dependent potential

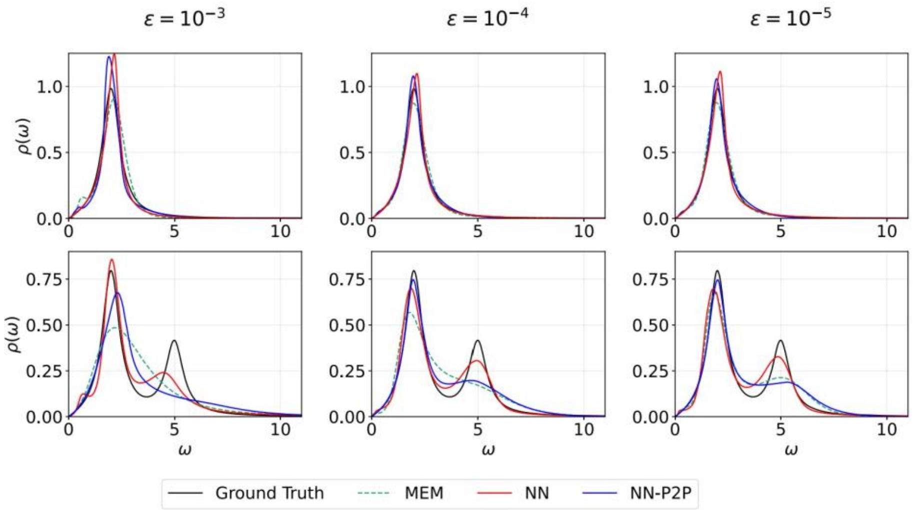




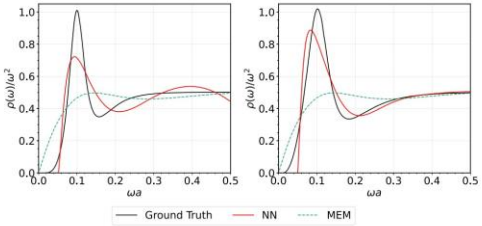
2.3 Spectral function reconstruction from Euclidean correlator

With **Lingxiao Wang** and **Shuzhe Shi**





NeurIPS2021 ''Machine learning and the Physical Science'', arXiv:2112.06206
Phys. Rev. D 106, L051502 (Letter), arXiv: 2111.14760
Computer Physics Communications (2022) 108547, arXiv: 2201.02564



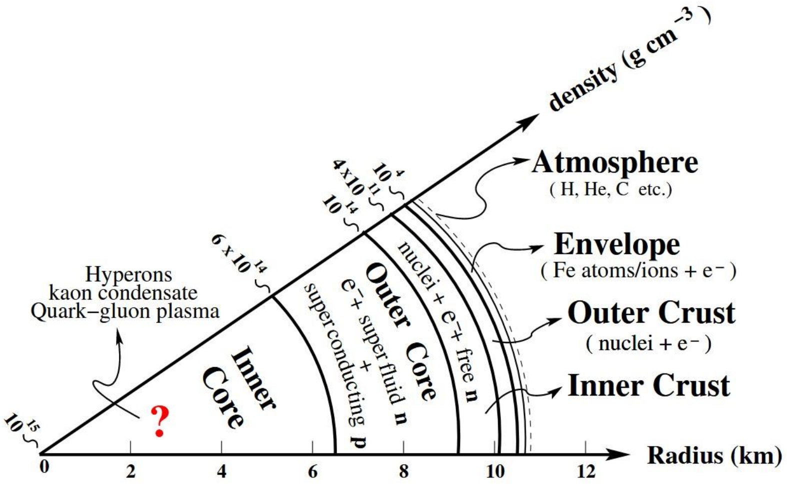
3, Dense matter EoS reconstruction for Neutron Star from M-R observation

With **Shriya Soma**, Lingxiao Wang, Shuzhe Shi and Horst Stoecker

JCAP08(2022)071 (arXiv:2201.01756)
arXiv:2209.08883

From EoS to Stellar Structure (MR)

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



- Gravity ← → Pressure

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

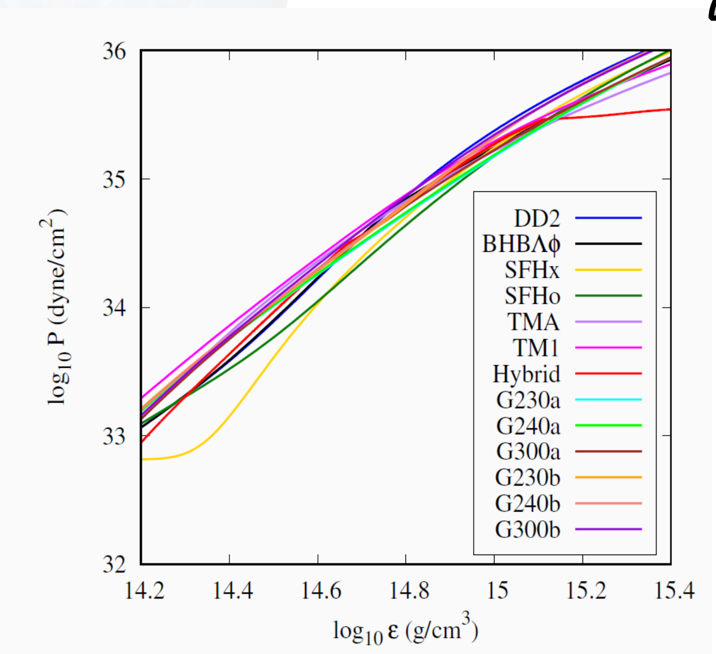
$$M = m(R) = \int_0^R 4\pi r^2 \rho \, dr$$

- Dense matter Equation of State

$$P(\rho)$$

1-to-1 mapping from EoS to M(R)

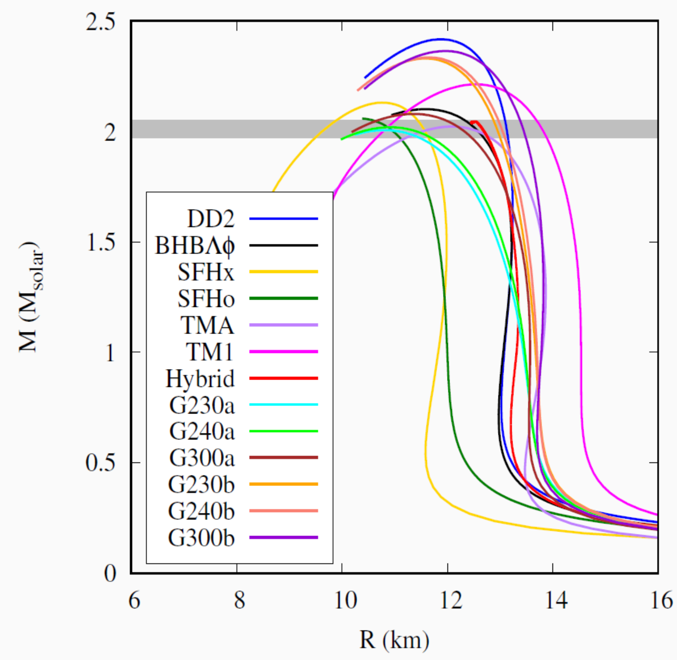
Micro to Macro



TOV solver

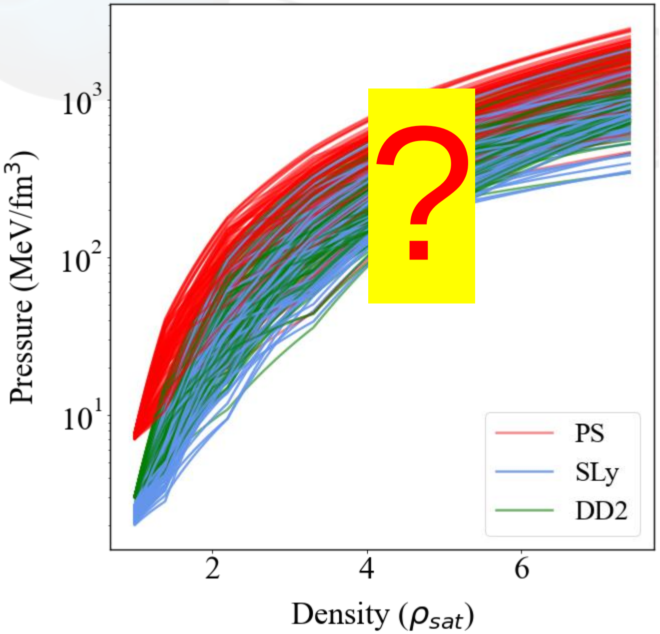
$$-\frac{dP}{dr} = \frac{[\epsilon(r) + P(r)]\,[M(r) + 4\pi r^3 P(r)]}{r[r - 2M(r)]}$$

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



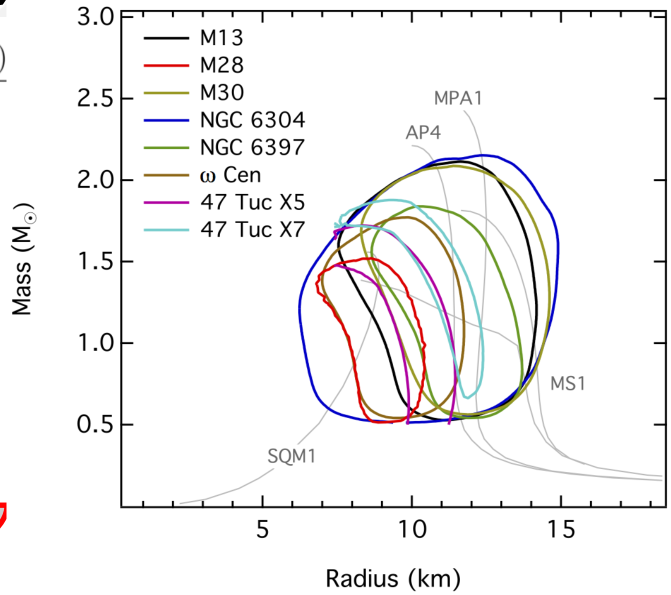
Noisy NS Observables to Equation of State ?

TOV solver

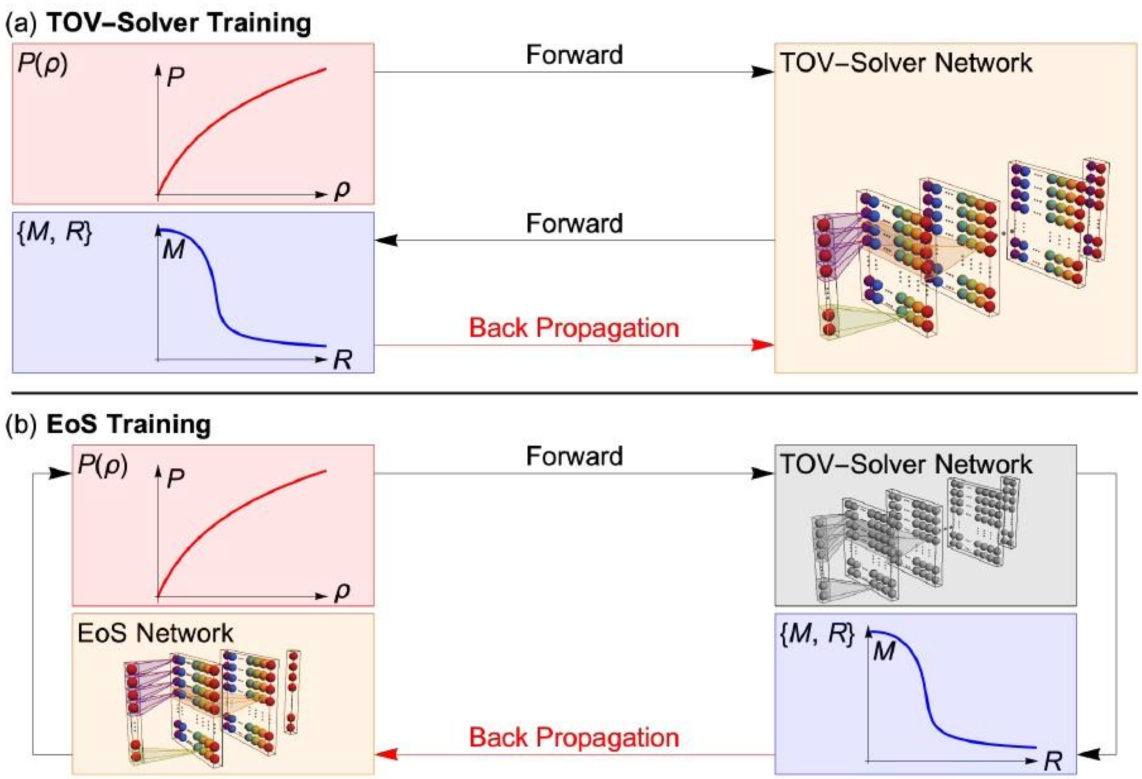


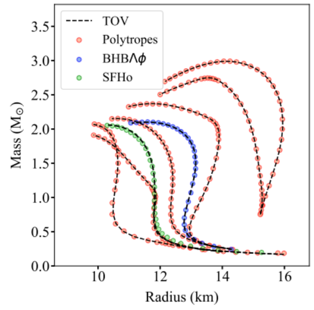
$$-\frac{dP}{dr} = \frac{[\epsilon(r) + P(r)]\,[M(r) + 4\pi r^3 P(r)]}{r[r - 2M(r)]}$$

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



Infer matter's EoS inside NS from M(R)



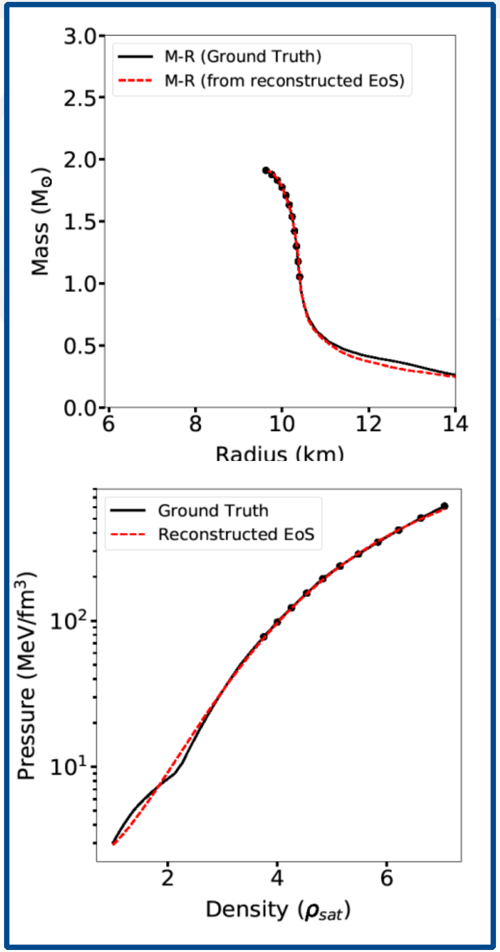


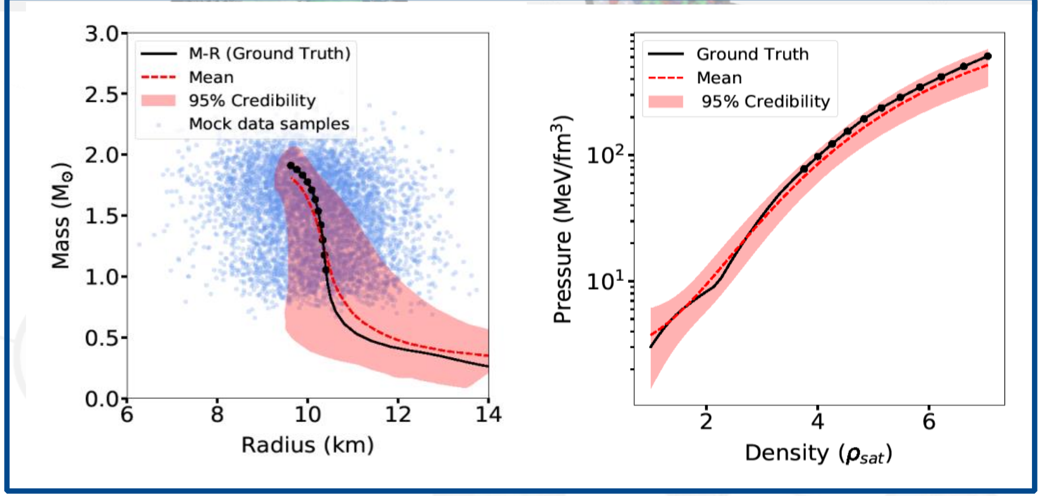
Generalized Bayesian Inference :

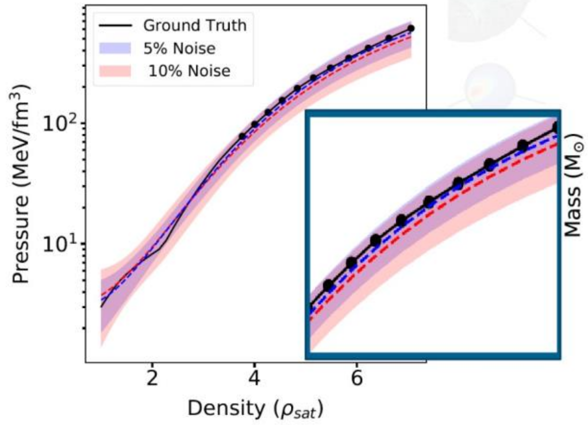
- The EoS is represented by DNN universal, unbiased, but more params
- The TOV eqs solving is replaced by a well-trained DNN
- Gradient based optimization and sa mpling for M-R data

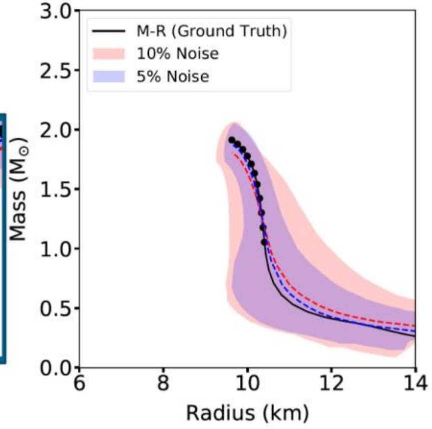
S.Soma, L.Wang, S.Shi, H. Stoecker, and K. Zhou, **JCAP08(2022)071**

Validate on closure tests w/o and with noise

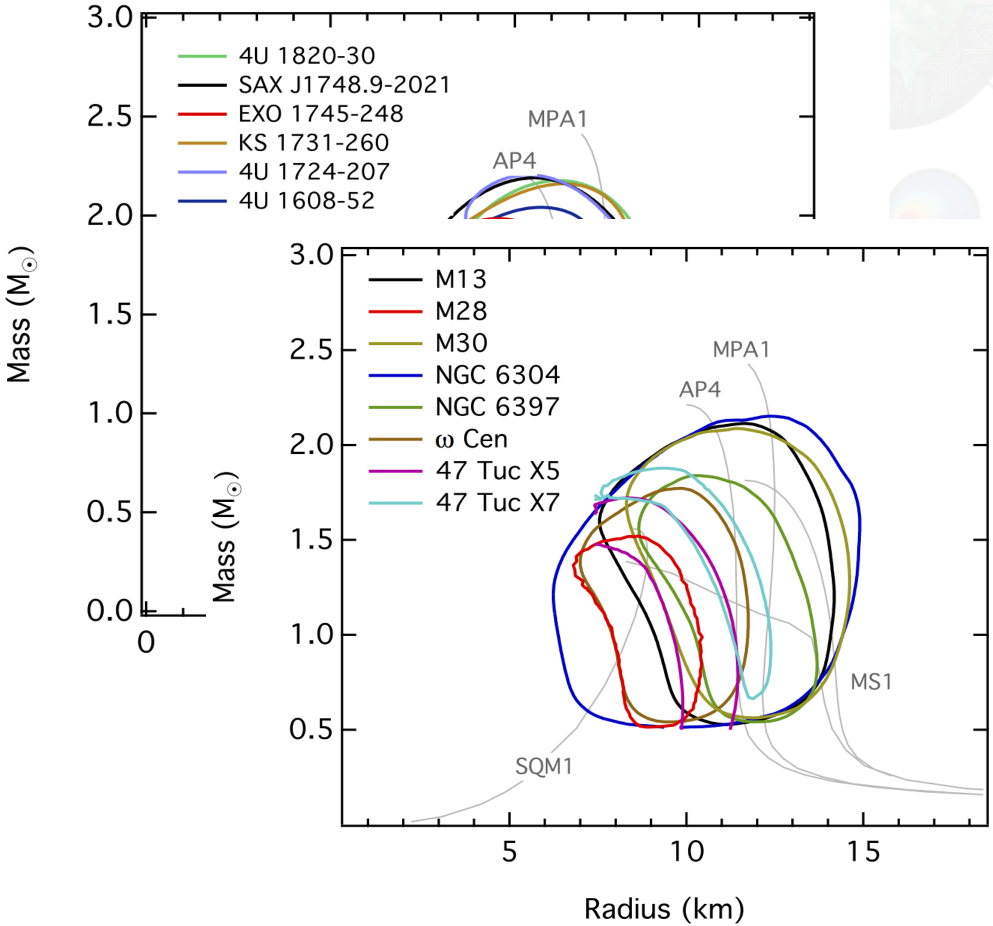


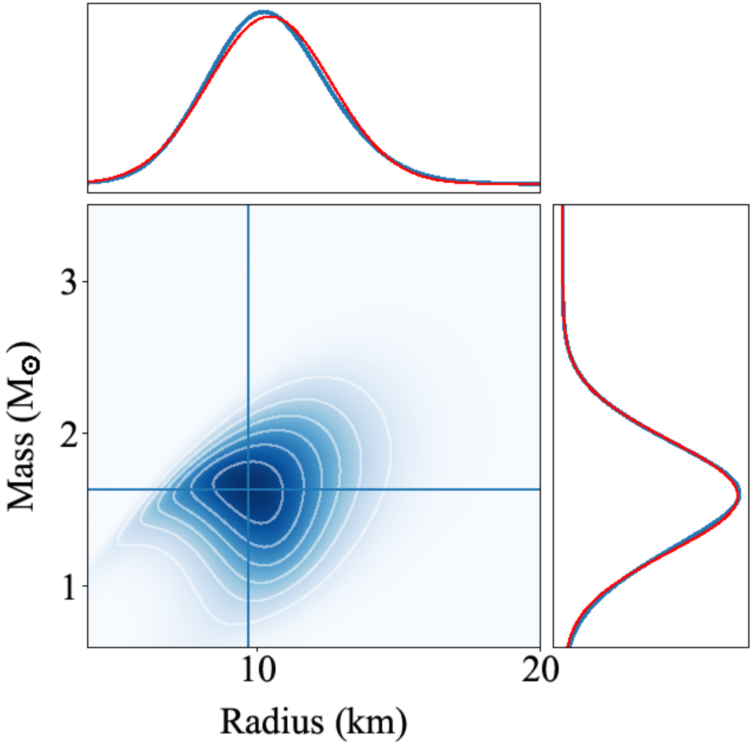




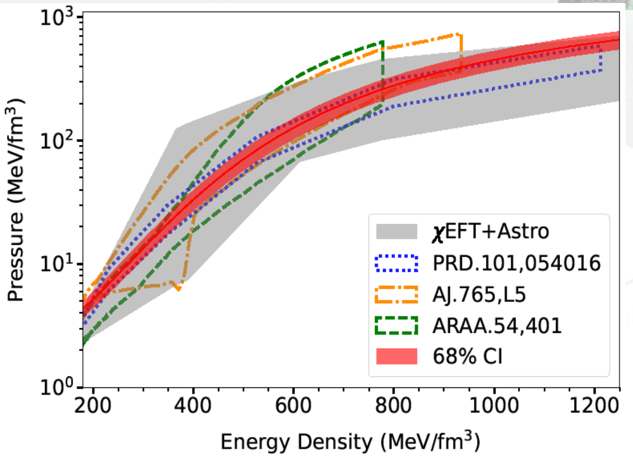


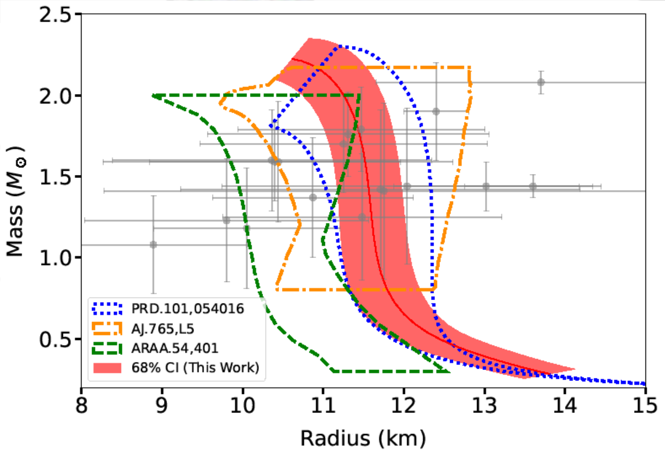
Neutron Star Observables

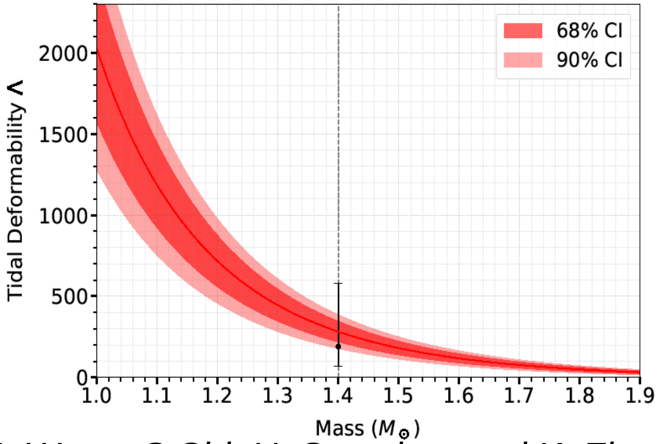


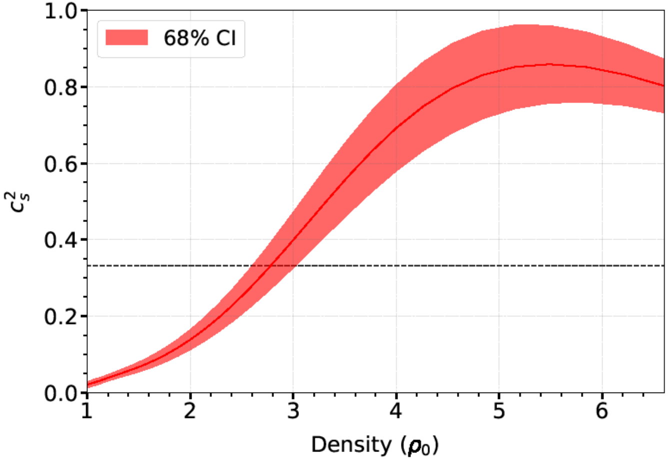


With real observables









S.Soma, L.Wang, S.Shi, H. Stoecker, and K. Zhou, **arXiv:2209.08883**

Conclusion

We demonstrated that physics of early dynamics (e.g. EoS, CME, centrality info.) in heavy ion collisions can survive into final states, with its signal can be decoded by machine learning and immune to model uncertainties. <u>ML thus constructs an efficient bridge in connecting theory to experiment for physics exploration!</u>

Inverse Problems happened in nuclear physics can be well handled/improved by deep learning based solving, e.g. for real-time potential, spectral function reconstruction, neutron star EoS constraining.

Generative deep learning models can help many-body physics in efficient sampling, mitigating critical slowing-down, represent ensemble of configs in one setup (Net)

Summary : Inverse Problems

Thanks !

Explicit 1-to-1 mapping

Quantity of Interest

Accessible Observation

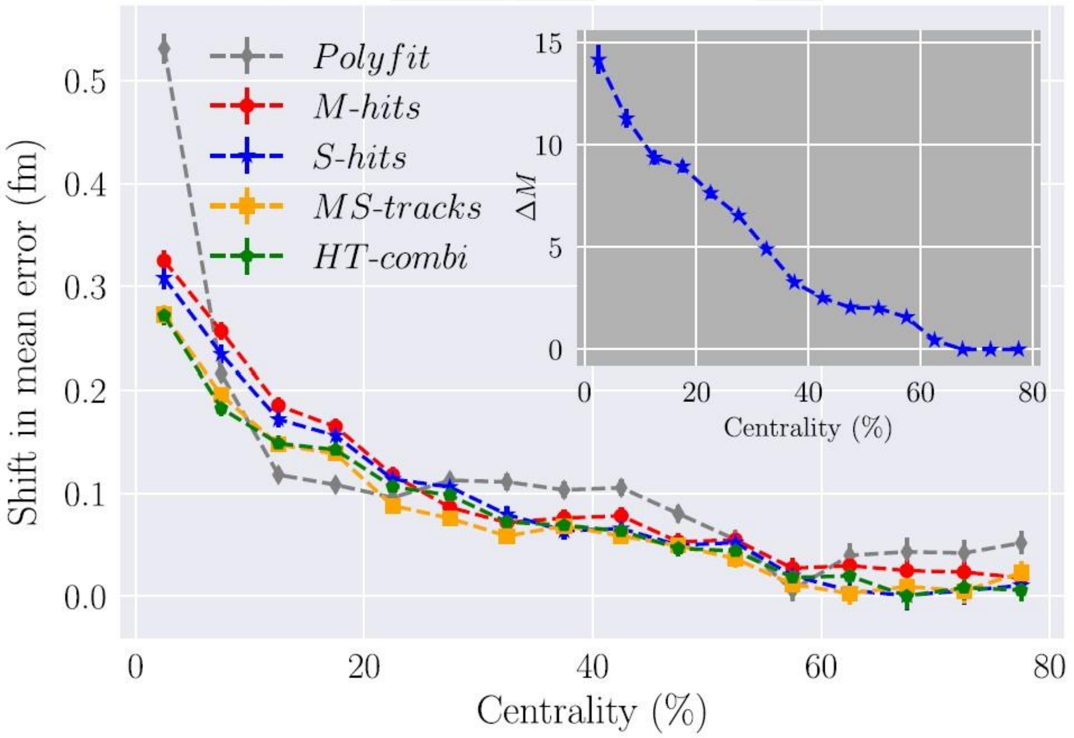
Exist, but implicit

- Physics Priors are needed for solving the inverse problem , coult be put into :

1, **training data** **(Implicit) :** train **proper DNN** to learn the inverse mapping
can learn directly the general mapping, avoid case-specific retraining

2, **inference process** **(Explicit) :** Chi2 fit+**Bayesian** inference+Gradient Descent
Automatic differentiation and Network representation

Result : model dependency ?



Perturbation on Schroedinger Eq.

$$\boxed{\begin{aligned}&\left(\frac{\widehat{p}^2}{2m}+V(r)\right)|\psi_i\rangle = E_i|\psi_i\rangle,\\ &\left(\frac{\widehat{p}^2}{2m}+V(r)+\delta V(r)\right)|\psi_i'\rangle = (E_i+\delta E_i)|\psi_i'\rangle.\end{aligned}}$$

$$\Longrightarrow \quad \begin{aligned}\delta m_i &= \langle\psi_i|\delta V_R(r)|\psi_i\rangle,\\ \delta\Gamma_i &= -\langle\psi_i|\delta V_I(r)|\psi_i\rangle.\end{aligned}$$

$$|\psi_i'\rangle = |\psi_i\rangle + \sum_{j\neq i}\frac{\langle\psi_j|\delta V(r)|\psi_i\rangle}{E_i-E_j}|\psi_j\rangle.$$

Hellmann-Feynman theorem

Phys. Rev. (1939)

$$\delta V(r) = v\,\delta(r-r_k), \quad \Longrightarrow \quad \boxed{\begin{aligned}&\frac{\delta m_i}{\delta V_R(r)} = -\frac{\delta\Gamma_i}{\delta V_I(r)} = |\psi_i(r)|^2,\\ &\frac{\delta m_i}{\delta V_I(r)} = \frac{\delta\Gamma_i}{\delta V_R(r)} = 0.\end{aligned}}$$

Uncertainty Estimation – Bayesian Inference

$$\boxed{\text{Posterior}(\boldsymbol{\theta}|\text{data}) \propto L(\boldsymbol{\theta}|\text{data}) \cdot \text{Prior}(\boldsymbol{\theta}).}$$

$$L(\boldsymbol{\theta}|\text{data}) = P(\text{data}|\boldsymbol{\theta}) \propto \exp[-\chi^2(\boldsymbol{\theta})/2].$$

$$\text{Prior}(\boldsymbol{\theta}) \propto \exp[-\frac{\lambda}{2}\boldsymbol{\theta} \cdot \boldsymbol{\theta}].$$

$$\boxed{\text{Posterior}(\boldsymbol{\theta}|\text{data}) = N_0 \exp\left[-\frac{\chi^2(\boldsymbol{\theta})}{2} - \frac{\lambda}{2}\boldsymbol{\theta} \cdot \boldsymbol{\theta}\right]}$$

Sample potentials ~ $P(V_{\boldsymbol{\theta}}(T,r)) = \text{Posterior}(\boldsymbol{\theta}|\text{data})\,.$

Reference Sampler ~ $$\widetilde{P}(\boldsymbol{\theta}) = (2\pi)^{-N_\theta/2}\sqrt{\det[\Sigma^{-1}]} \times \exp\left[-\frac{\Sigma_{ab}^{-1}}{2}(\theta_a - \theta_a^{\text{opt}})(\theta_b - \theta_b^{\text{opt}})\right]$$

$$\left(\Sigma_{ab}^{-1} \equiv \frac{\partial^2 J(\boldsymbol{\theta})}{\partial\theta_a \partial\theta_b}\right)$$

re-weighting with :

$\omega(\theta) = p\left(V_\theta(T,r)\right)/\tilde{p}\,(\theta)$ to grantee posterior sampling