Constraining the QCD critical point using active learning

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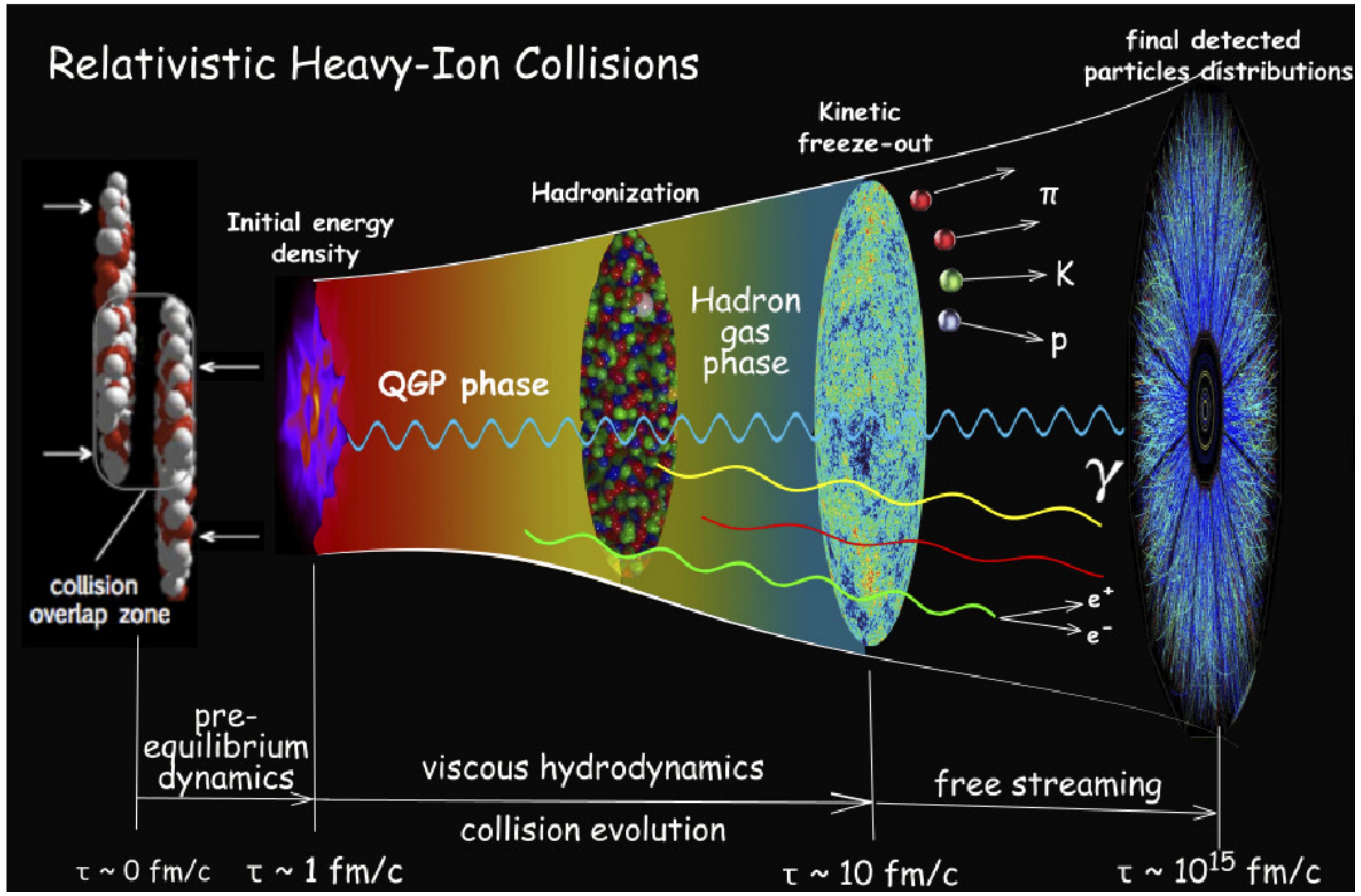
P. Parotto, D. Mroczek et. al PRC 101 (2020)
D. Mroczek, P. Parotto et. al PRC 103 (2021)
J.M. Karthein, D.Mroczek et. al EPJ+ 136 (2021)
D. Mroczek, M. Hjorth-Jensen, P. Parotto et. al — PRC 107 (2023)
T. Dore, J.M. Karthein, D. Mroczek et. al —PRD 106 (2022)

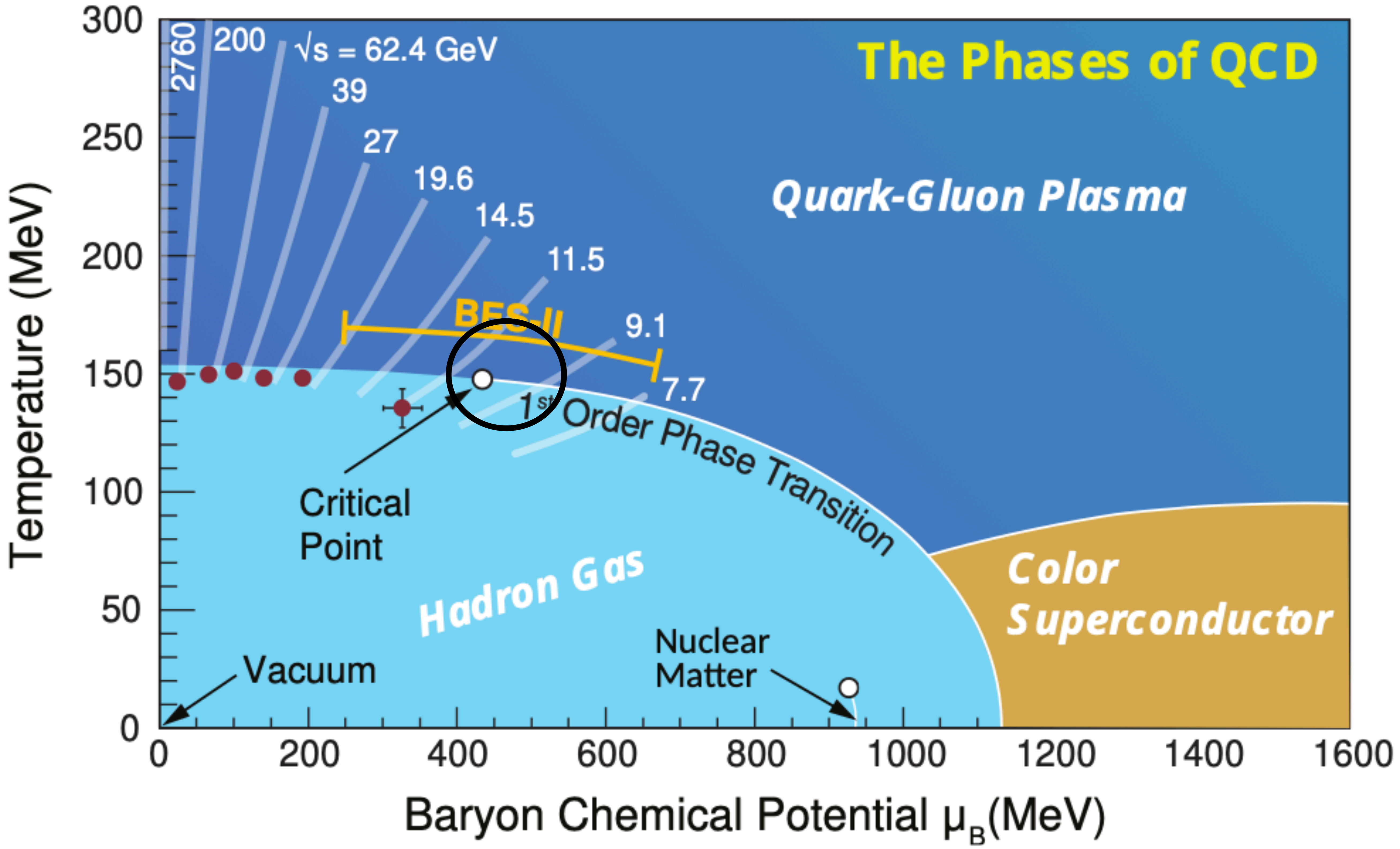
ISNET | Wash. U., May 2023

Ultra-relativistic heavy-ion collisions

What is the phase structure of QCD?



X. An et al, Nucl.Phys.A 1017 (2022)



Heavy-ions (Au, Pb) collided at relativistic speeds at the Relativistic Heavy-Ion Collider (RHIC) and LHC.

Ultra-relativistic heavy-ion collisions

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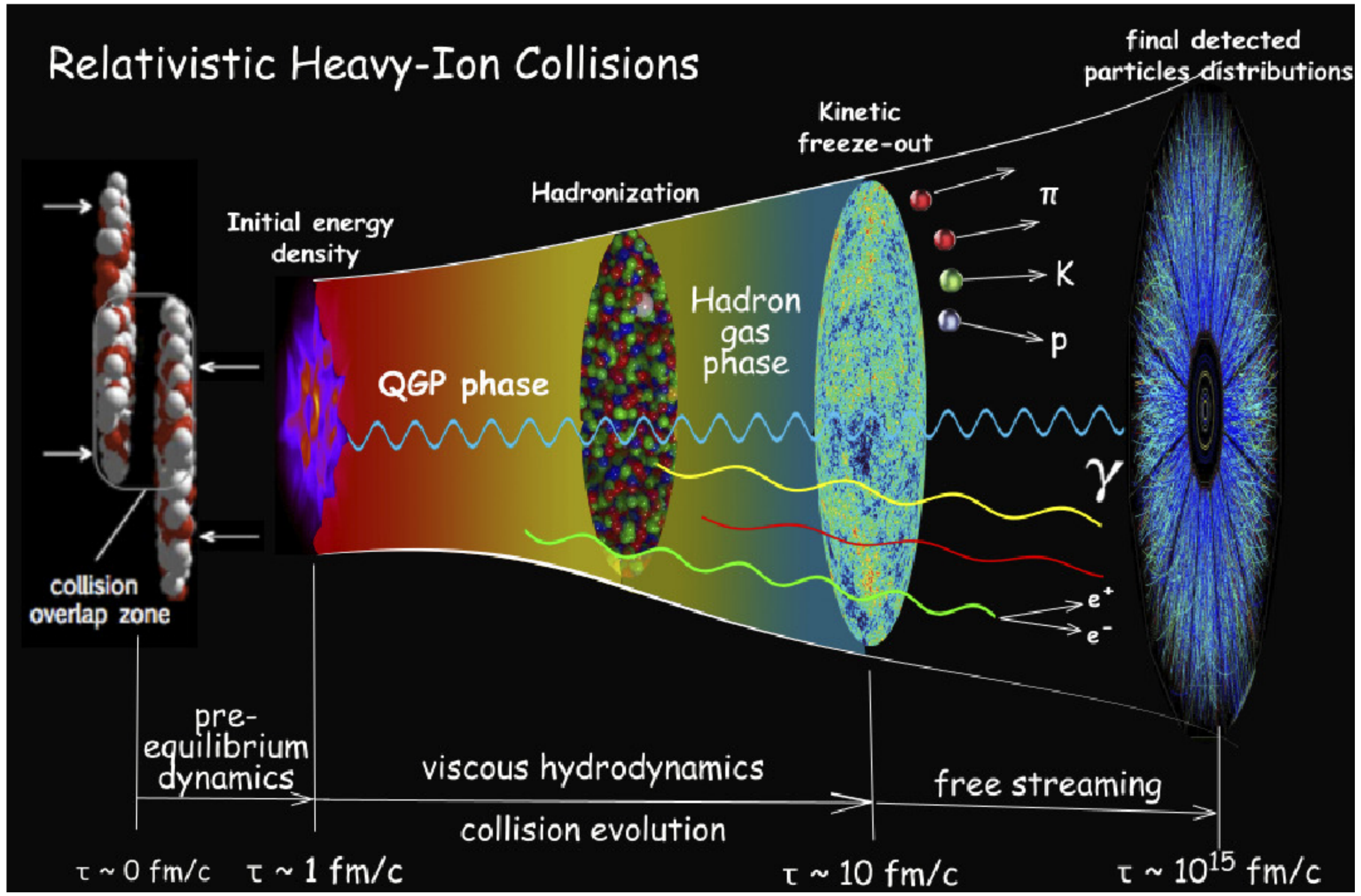

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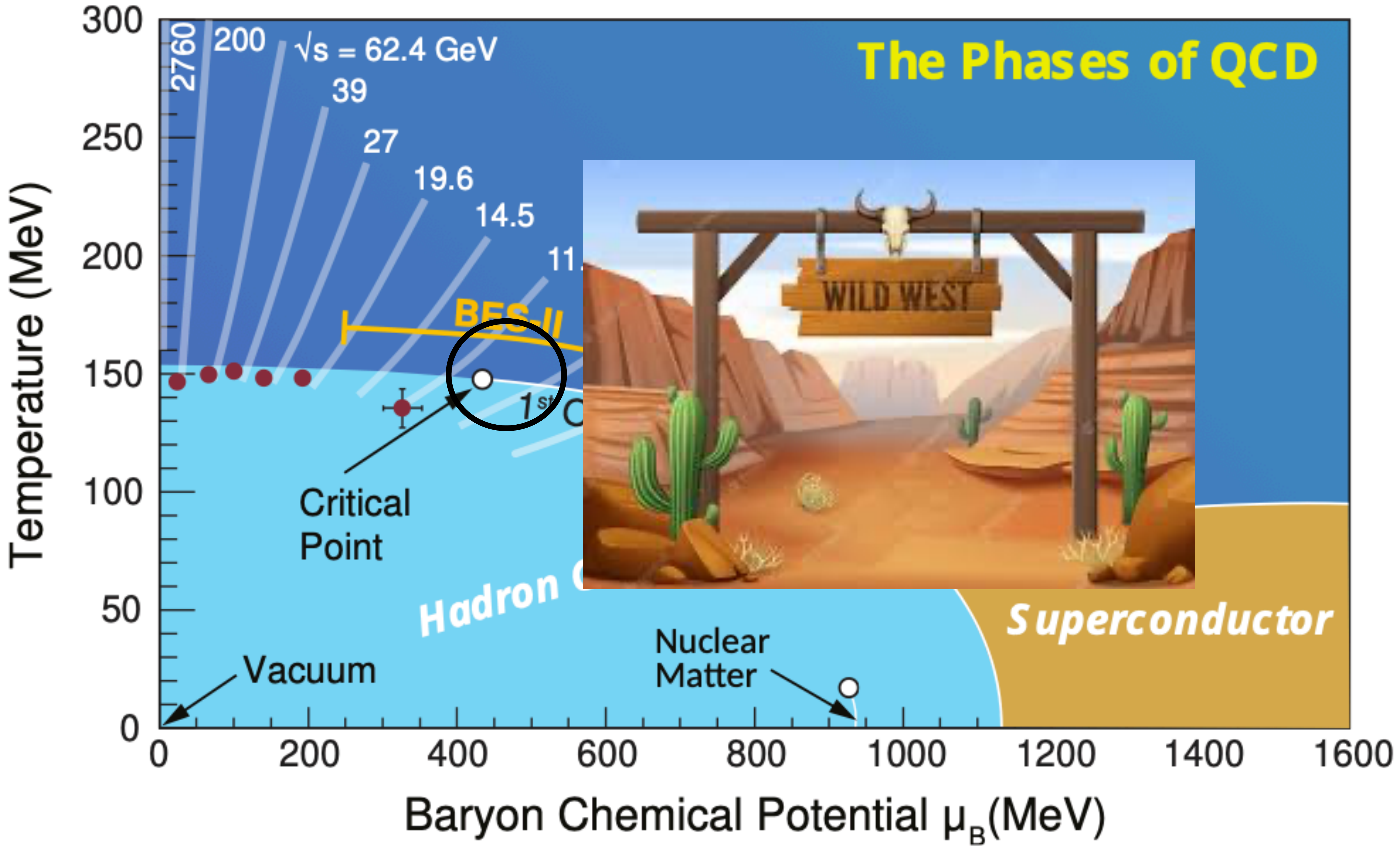


Heavy-ions (Au, Pb) collided at relativistic speeds at the Relativistic Heavy-Ion Collider (RHIC) and LHC.

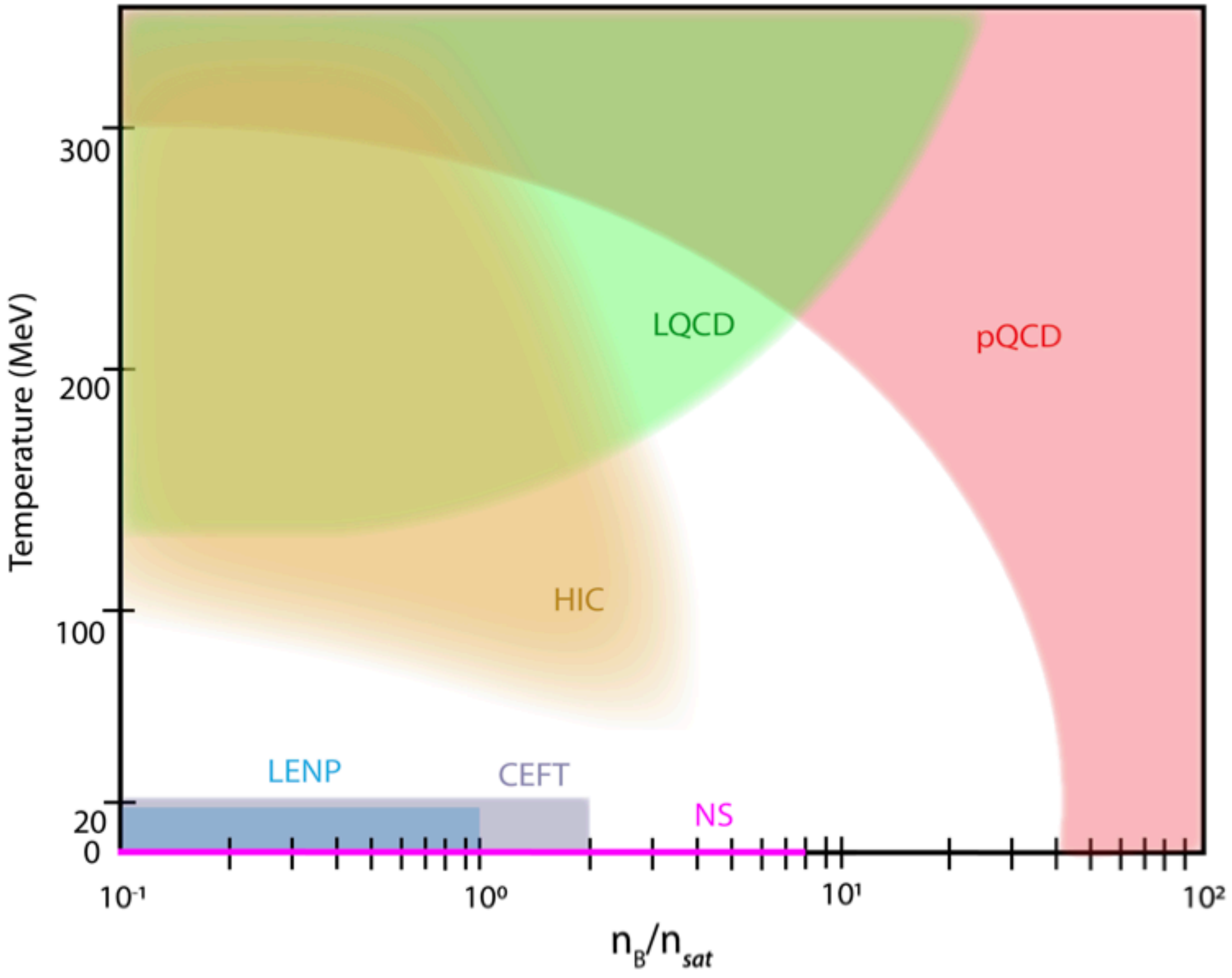
Ultra-relativistic heavy-ion collisions

Lattice QCD can only be computed at vanishing baryon densities due to the sign problem → expand to finite densities

Expansion cannot capture singular behavior: effective models / parameterizations

Large portion of the phase diagram only accessible in HIC's: model-to-data comparison

adapted from: 2303.17021



The Beam Energy Scan Program at RHIC

- Goal: Vary collision energy. General survey of QCD matter, but specifically: QCD critical point

- Requires: Quantitative description of heavy-ion collisions at BES energies

equilibrium quantities (e.g. EoS) + dynamical scheme

☑ Correlate observables

☑ Predict magnitude of expected effects

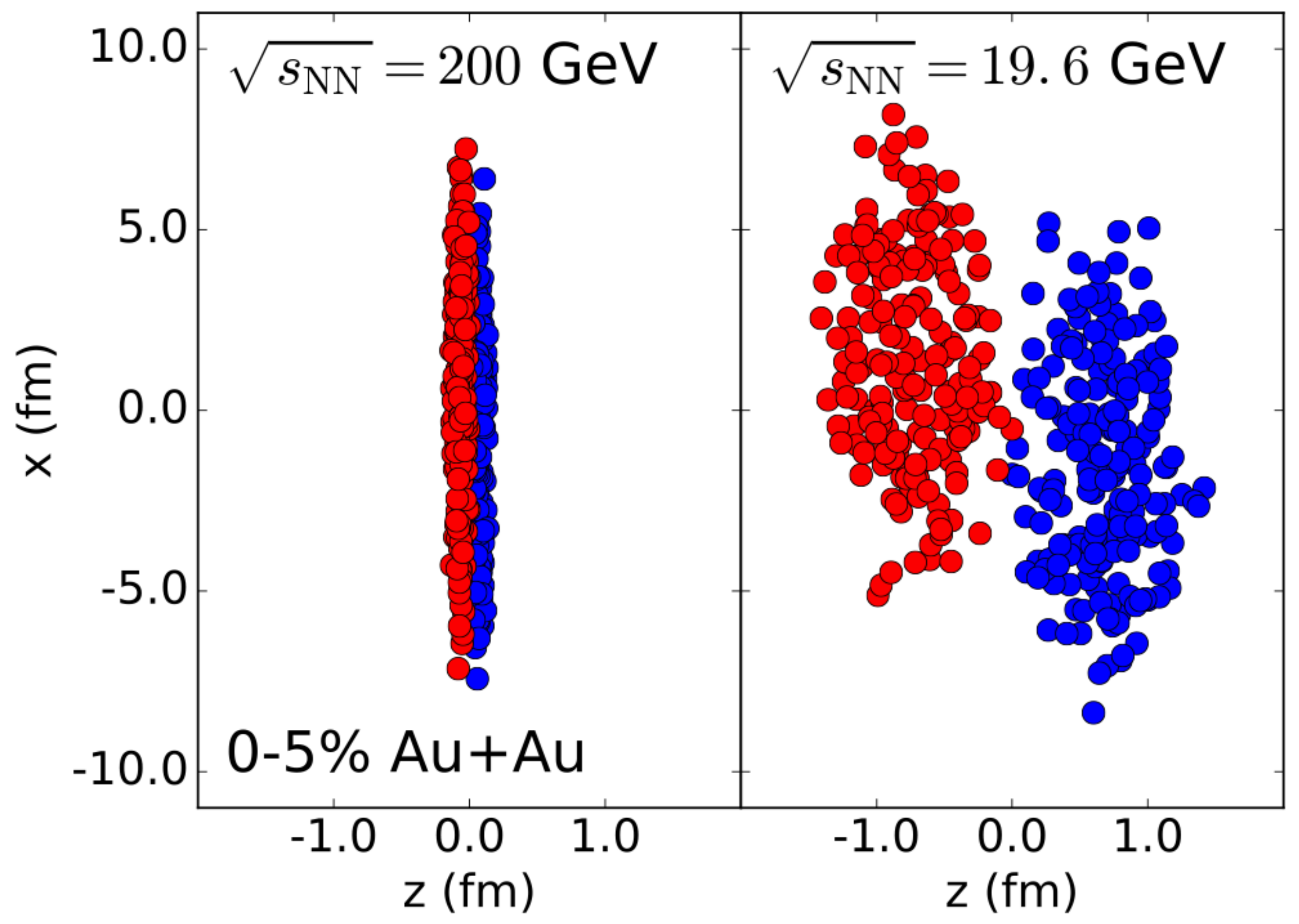
☑ Account for backgrounds

☑ Relates discovery at given beam energy + nuclear species + impact parameter to phase boundary/CP at a specific (T, μ_B)

See also: BEST collaboration summary paper: X. An et al, Nucl.Phys.A 1017 (2022)

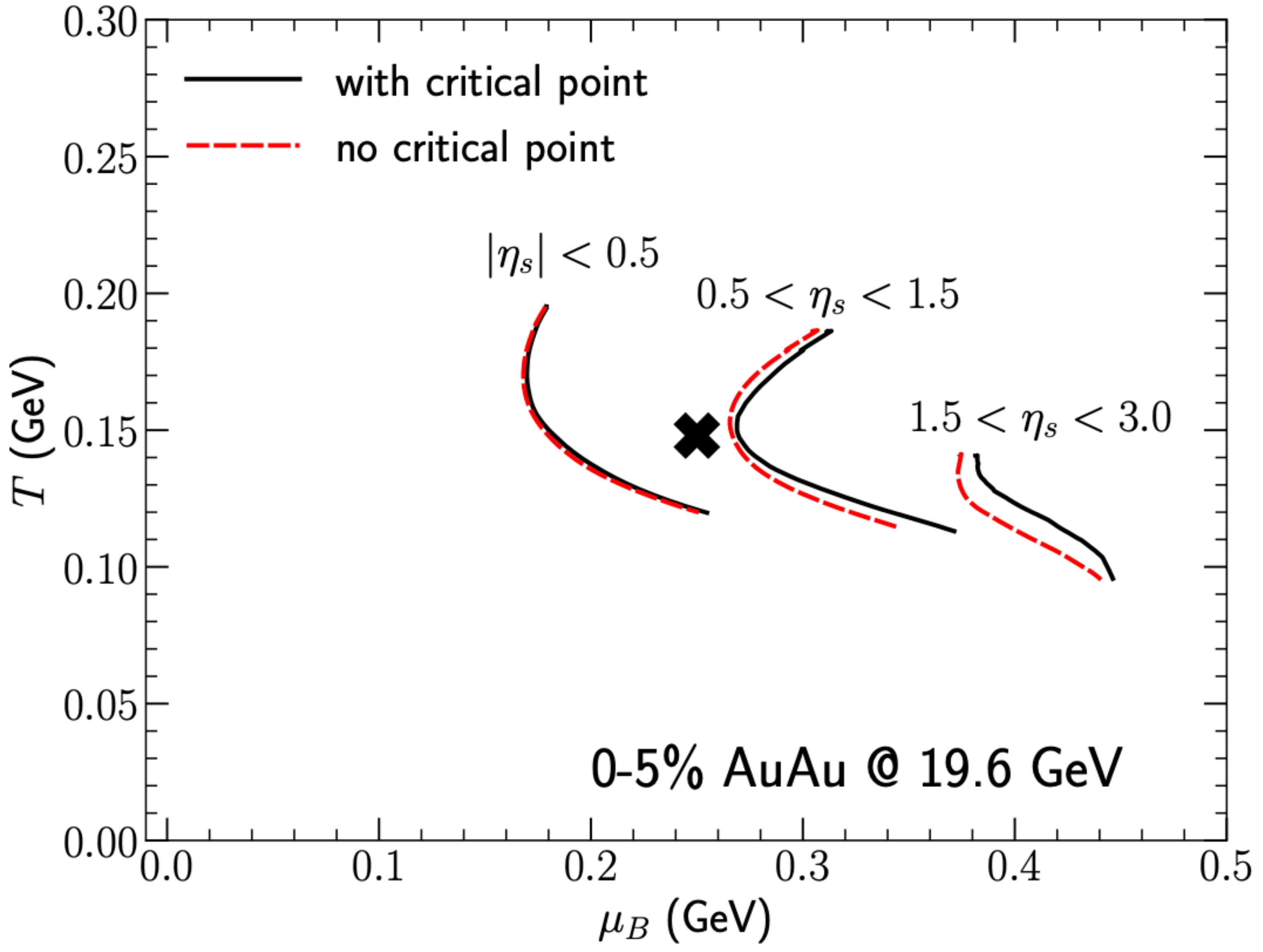
Challenges at BES energies

Initial Conditions
- Colliding nuclei not sufficiently contracted
- Transition to hydro over some interval
- Mix of hydro + pre-hydro subsystems
- Quarks + BSQ charges



Hydro. Evolution
- QCD currents: BSQ charge diffusion
- Critical fluctuations and correlations
- Critical slowing down
- Domain formation near 1st order P.T.

Equation of State
- Finite (large) μ_B + critical point
- Strangeness and electric charge dependence
- Match lattice QCD where it applies



Particlization + Hadronic Phase
- Particlization must preserve fluctuations + correlations
- Kinetic evolution: mean-field interactions reflecting phase transition/CP presence

Figs. and refs: BEST collaboration summary paper: X. An et al, Nucl.Phys.A 1017 (2022)

The EoS from lattice QCD — finite μ_B

Quantities can be calculated directly on the lattice only at $\mu_B = 0$

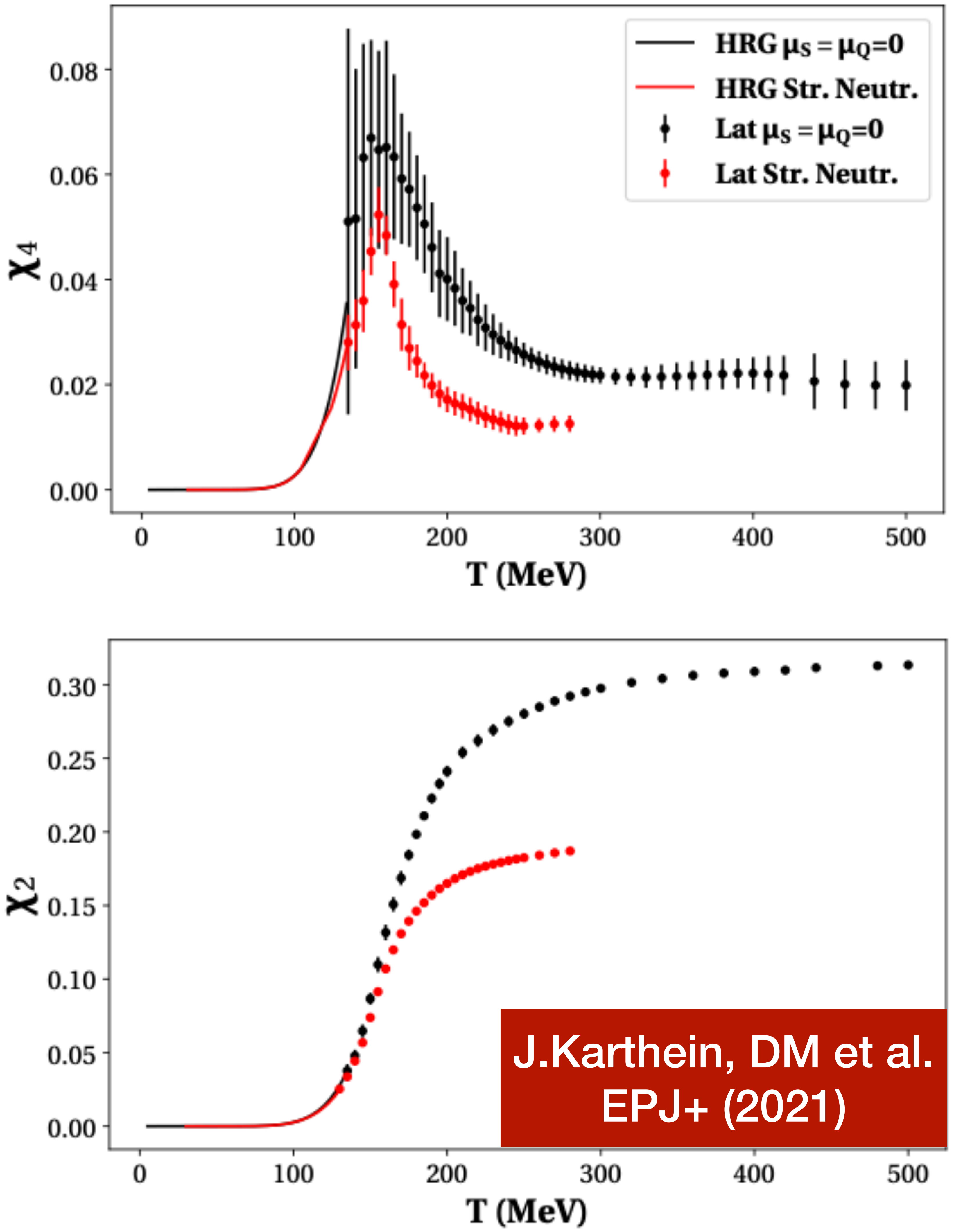
Expand to finite μ_B via Taylor expansion

$$P(T,\mu_B) = T^4 \sum_n c_{2n}(T) \left(\frac{\mu_B}{T}\right)^{2n} \qquad c_n(T) = \frac{1}{n!}\frac{\partial^n P/T^4}{\partial(\mu_B/T)^n} = \frac{1}{n!}\chi_n^B$$

We can impose $\mu_S = \mu_Q = 0$

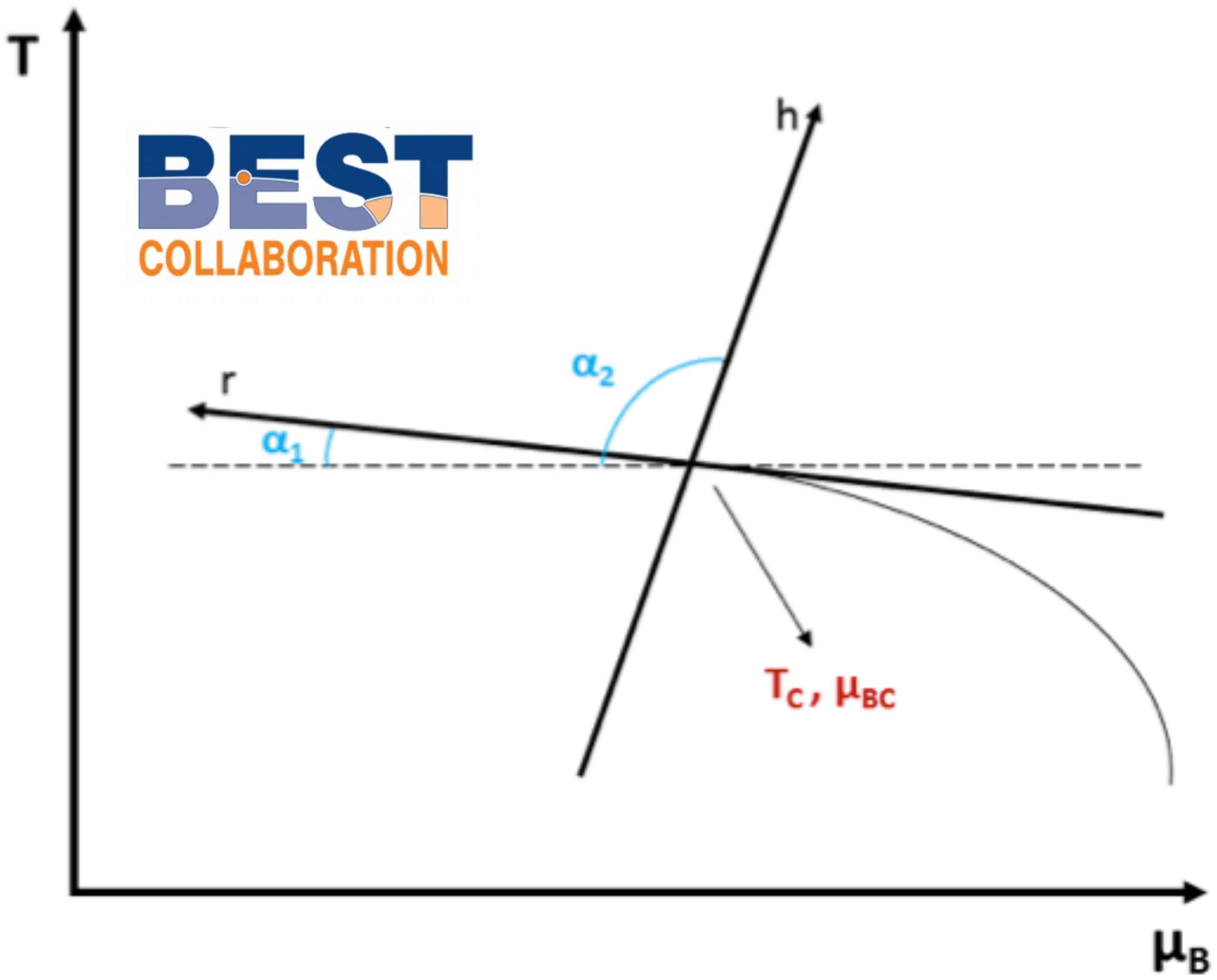
or charge density constraints from HIC

$$<\rho_S> = 0, <\rho_Q> = 0.4 <\rho_B>$$



Equation of state for QCD with a critical point

- Map a parameterization of the 3D Ising model critical point to QCD variables:



$$(\mathbf{r},\mathbf{h}) \longleftrightarrow (\mathbf{T},\mu_\mathbf{B}) : \quad \frac{T-\mathbf{T_C}}{\mathbf{T_C}} = \mathbf{w}\,(r\rho\,\sin\alpha_1 + h\,\sin\alpha_2)$$

$$\frac{\mu_B-\mu_\mathbf{BC}}{\mathbf{T_C}} = \mathbf{w}\,(-r\rho\,\cos\alpha_1 - h\,\cos\alpha_2)$$

Reconstruct QCD pressure:

$$T^4 c_n^{\mathrm{LAT}}(T) = T^4 c_n^{\mathrm{Non-Ising}}(T) + c_n^{\mathrm{Ising}}(T)$$

$$P(T,\mu_B) = T^4 \sum_n c_n^{\mathrm{Non-Ising}}(T)\left(\frac{\mu_B}{T}\right)^n + P_{\mathrm{crit}}^{\mathrm{QCD}}(T,\mu_B)$$

Reduce number of free parameters using input from LQCD:

$$T = T_0 + \kappa T_0\left(\frac{\mu_B}{T_0}\right)^2 + O(\mu_B^4), \qquad \alpha_1 = \tan^{-1}\left(2\frac{\kappa}{T_0}\mu_{BC}\right)$$

Up to $\mathcal{O}(\mu_B^4)$:

P. Parotto, DM, et al PRC (2020)

Up to $\mathcal{O}(\mu_B^4)$ + strangeness neutrality:

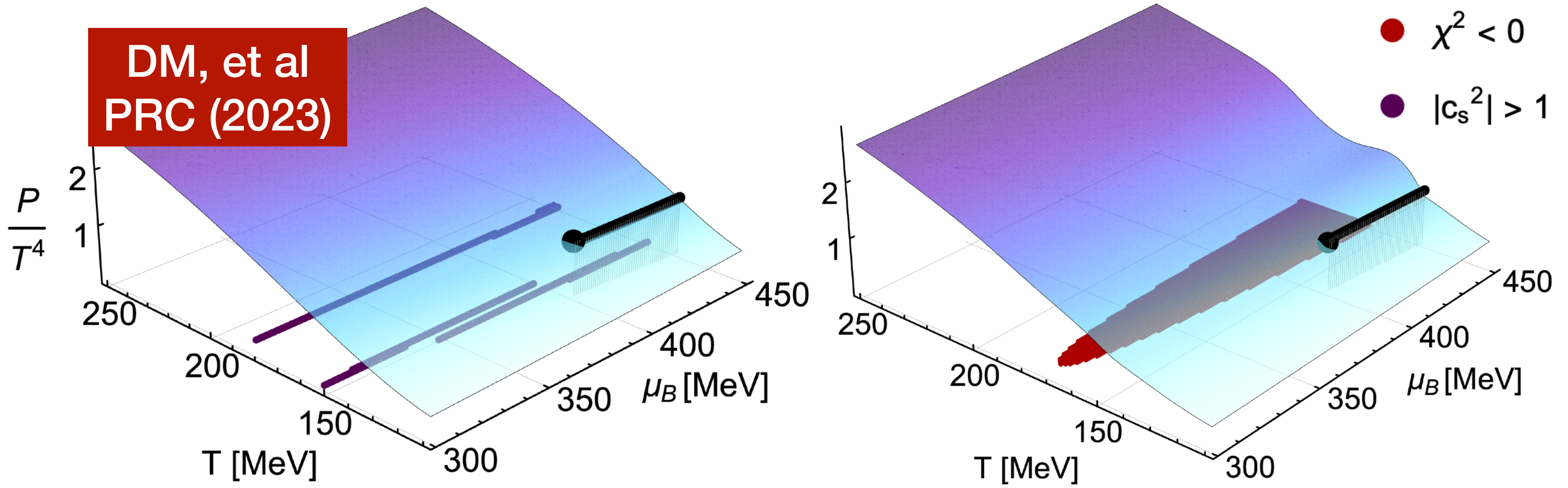
J.M. Karthein, DM, et al EPJ+ (2021)

The EoS parameter space

EoS meets important requirements:

- ✓ Critical point in the correct universality class
- ✓ Matched to lattice QCD at $\mu_B = 0$

Remaining free parameters $\mu_{BC}, w, \rho, \alpha_{diff} = \alpha_1 - \alpha_2$ can produce **acausal and unstable realizations** due to tension with lattice coefficients at $\mu_B = 0$



Traditionally: compute all relevant thermodynamic derivatives and check every point for stability/causality → Computationally costly and ineffective.

Use machine learning to recognize acceptable EoS, bypassing most or all calculations.

1) Which realizations to learn from?
2) How to learn?

Generating a training set

1.1) Learn from input parameters?

Option 1 (traditional): Once lattice data and parameters are chosen the map is deterministic:

Learn: $\{\mu_{BC}, w, \rho, \alpha_{diff}\} \rightarrow$ **{acceptable, acausal, unstable}**

<u>or</u>

Option 2: Stability and causality are encoded in the pressure:

$$P, s, \varepsilon, n_B, \chi_2^B, \left(\frac{\partial S}{\partial T}\right)_{n_B} > 0$$

$$0 < c_s^2 < 1$$

Learn: $P(T, \mu_B) \rightarrow$ **{acceptable, acausal, unstable}**

- No dimension-reduction required
- Does not generalize quantitatively beyond current EoS
- Bypasses all calculations: maps input parameters to stability / causality

- Requires dimension reduction: $P(T, \mu_B) \rightarrow P*$
- Smaller computational advantage: requires the pressure
- <u>Potentially generalizes beyond current EoS?</u>

Generating a training set

1.2) Which EoS to learn from?

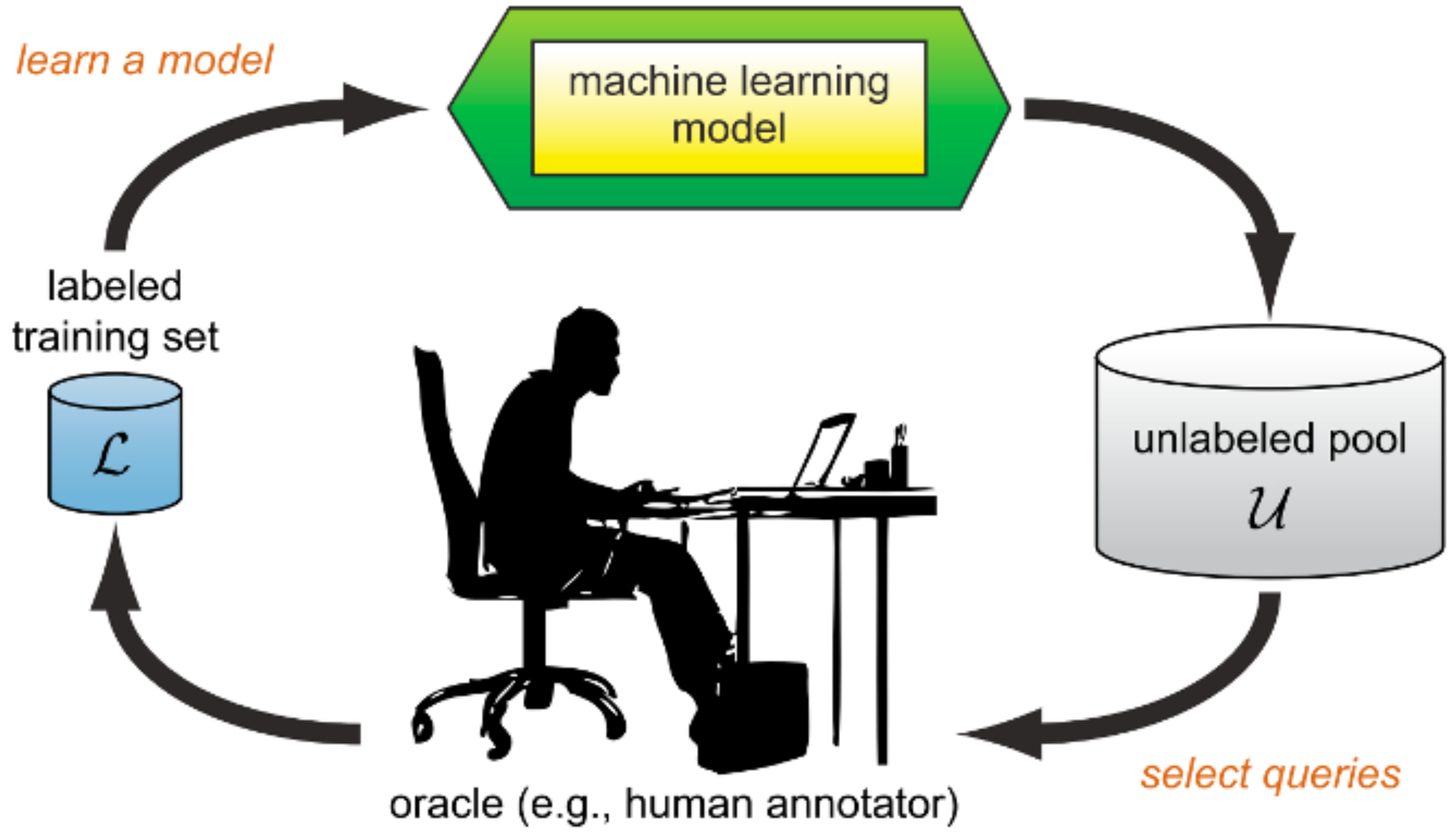
❌ Traditional machine learning: assumes all realizations are equally important. Not always true!

✔ **Active learning: ranks EoS realizations from most to least informative**

→ speed up learning the boundary between acceptable and acausal/unstable EoS.

Sampling method
(active learning v. random sampling)

Where in the parameter space should I sample?



B. Settles, Active Learning Lit. Survey (2009)

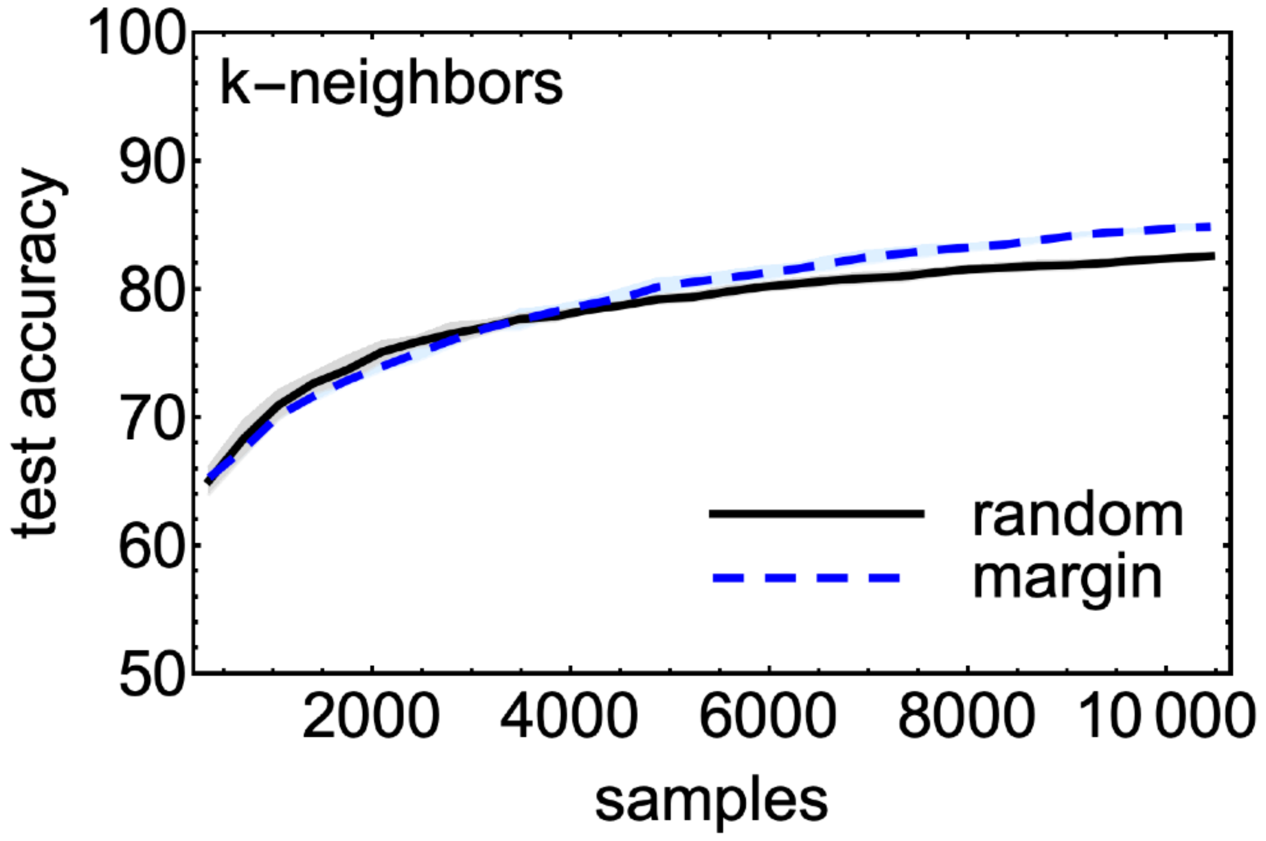
Margin-based ranking:
$M = P(\mathrm{A}) - P(B)$

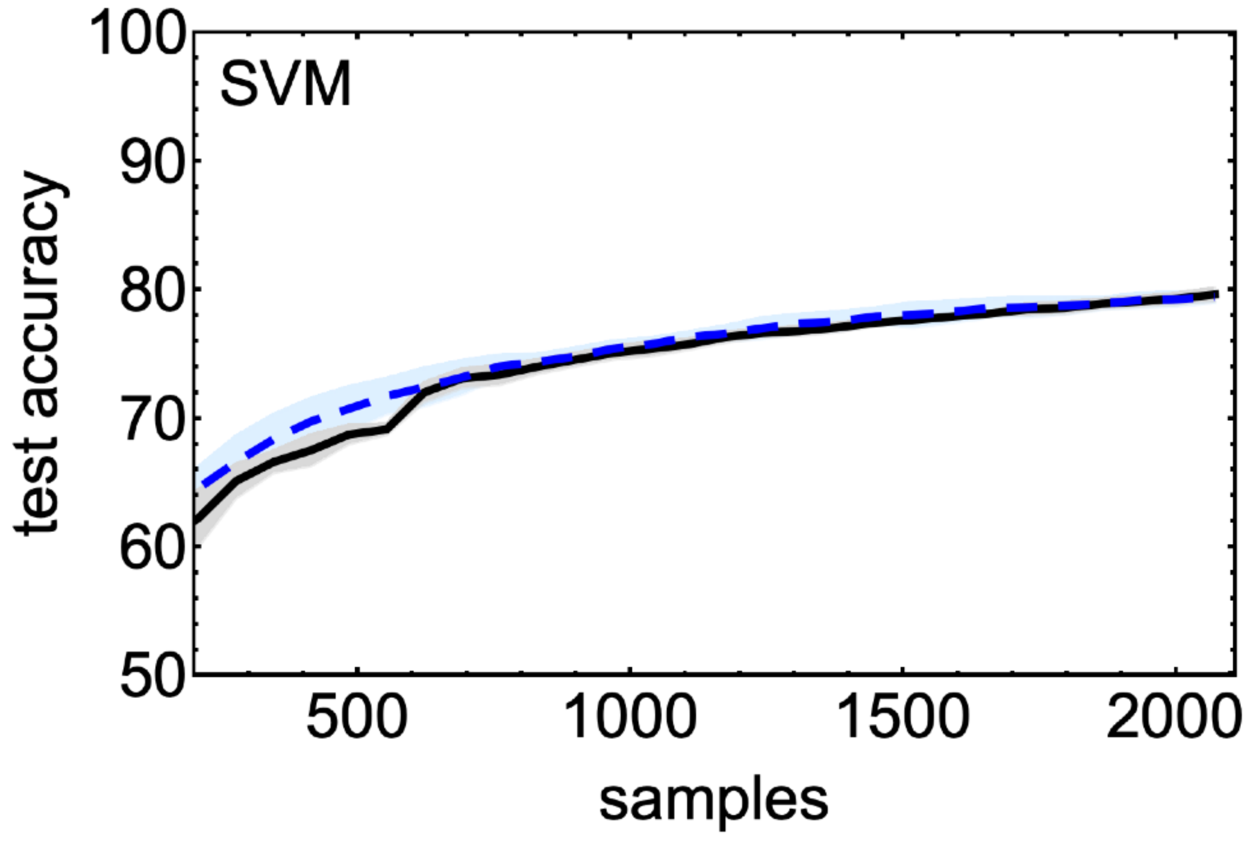
Large margin = high confidence in classification

Small margin = ambiguous sample → **prioritized**

Choosing a classifier

2) How do we know what algorithm to use? We don't… try several candidates

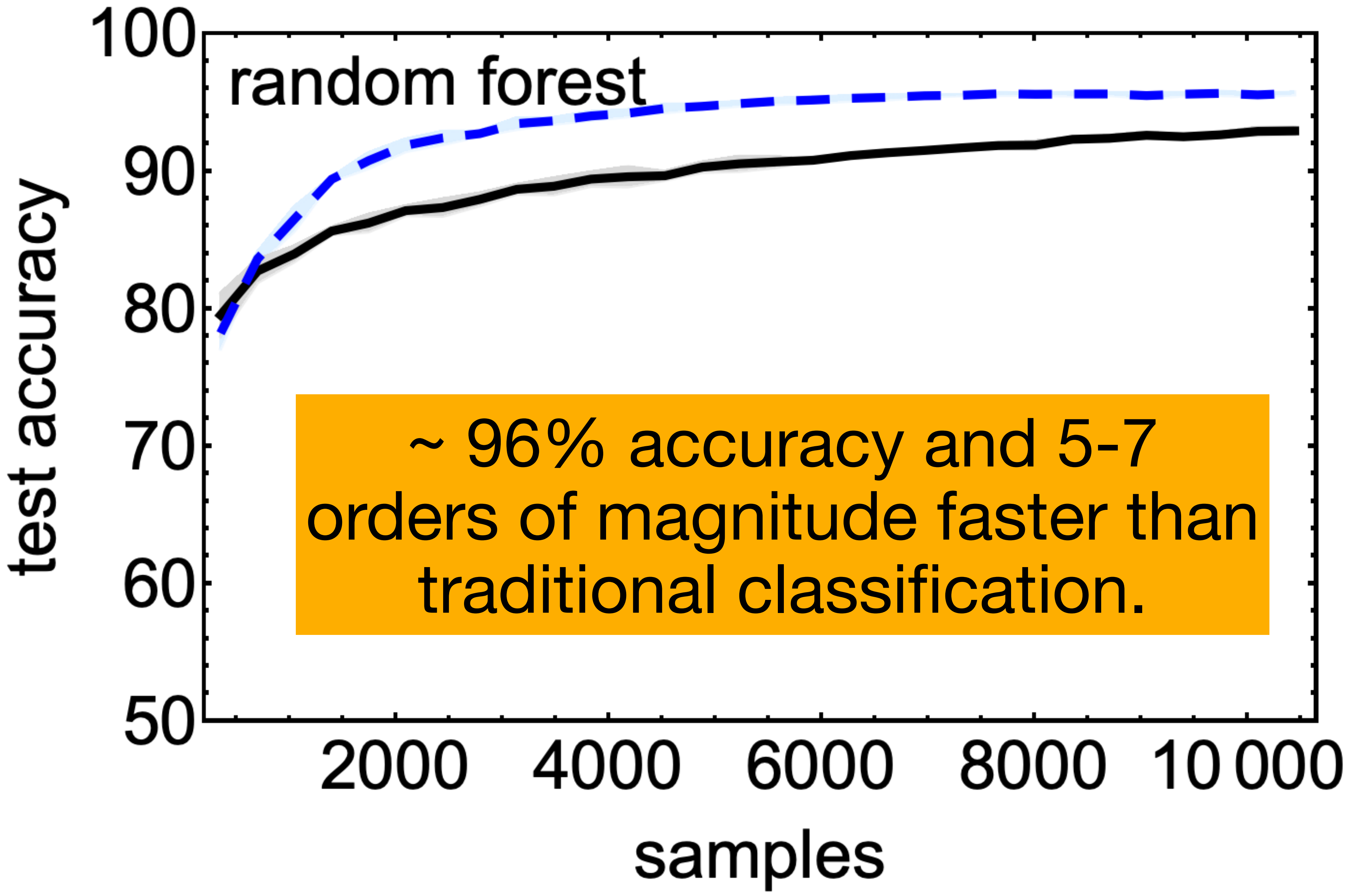


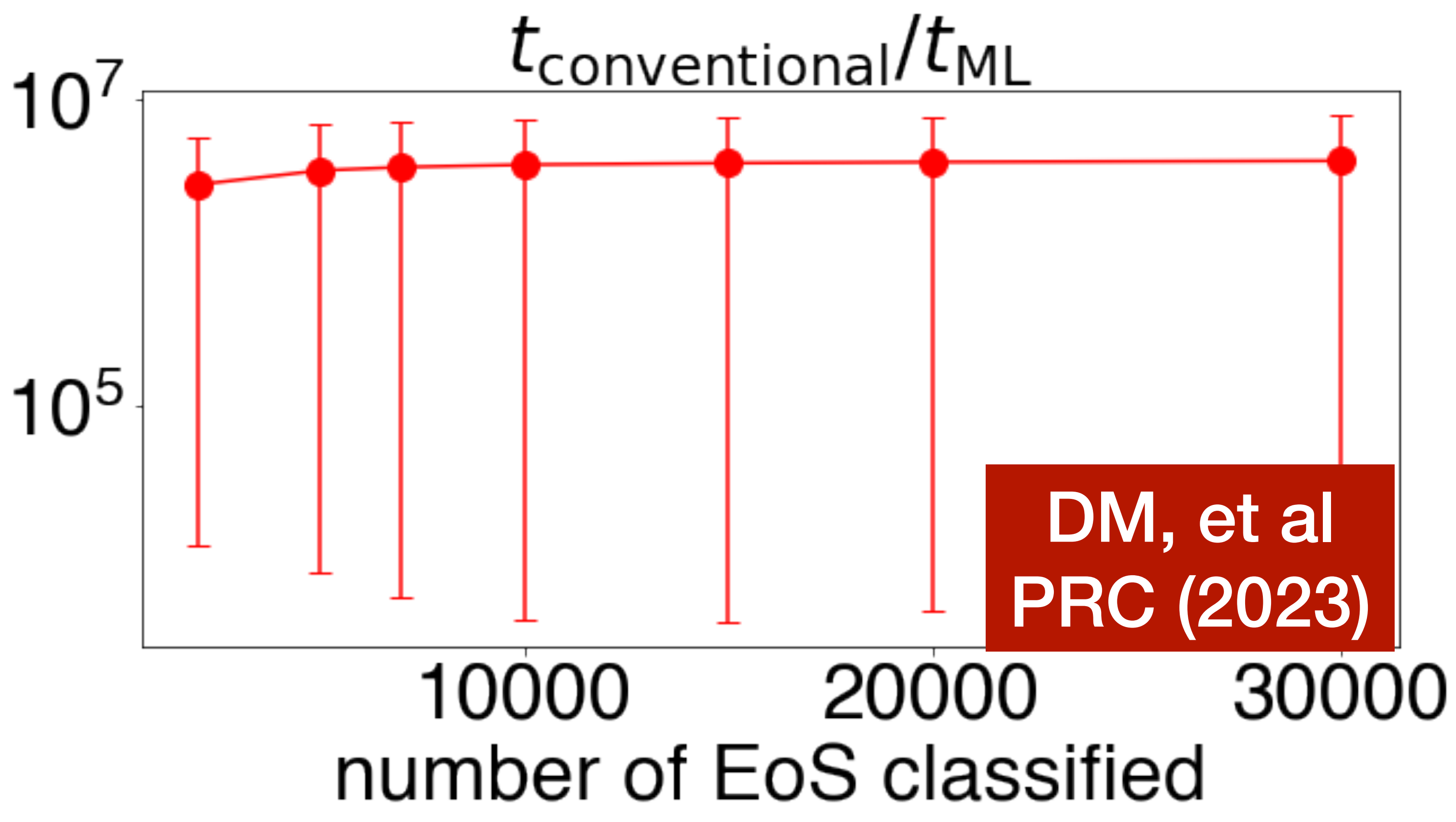


Considering:

- Final accuracy + confusion matrix
- Implementation
- Speed gain

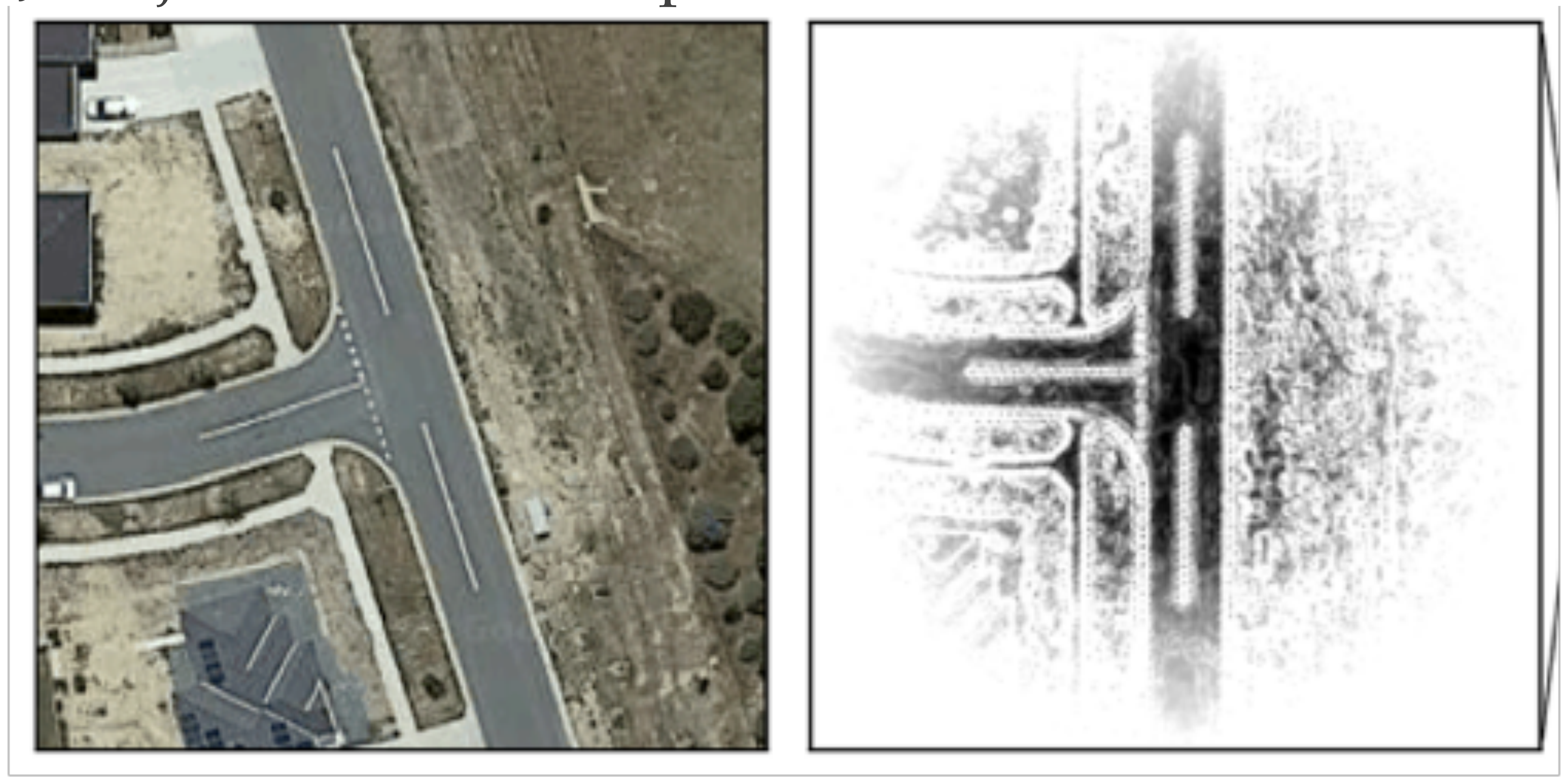
Top algorithm: random forest classifier trained with margin-based sampling

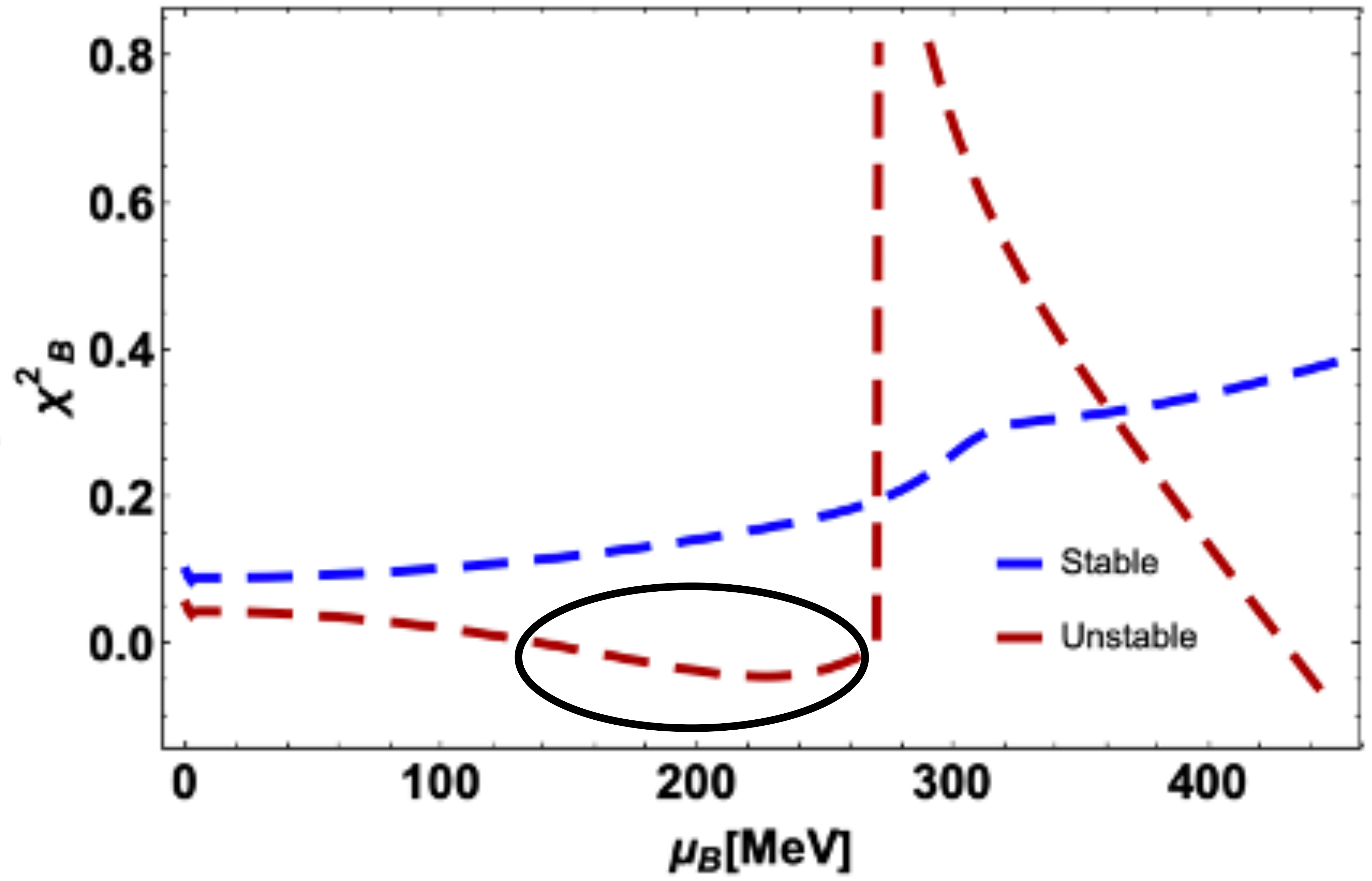


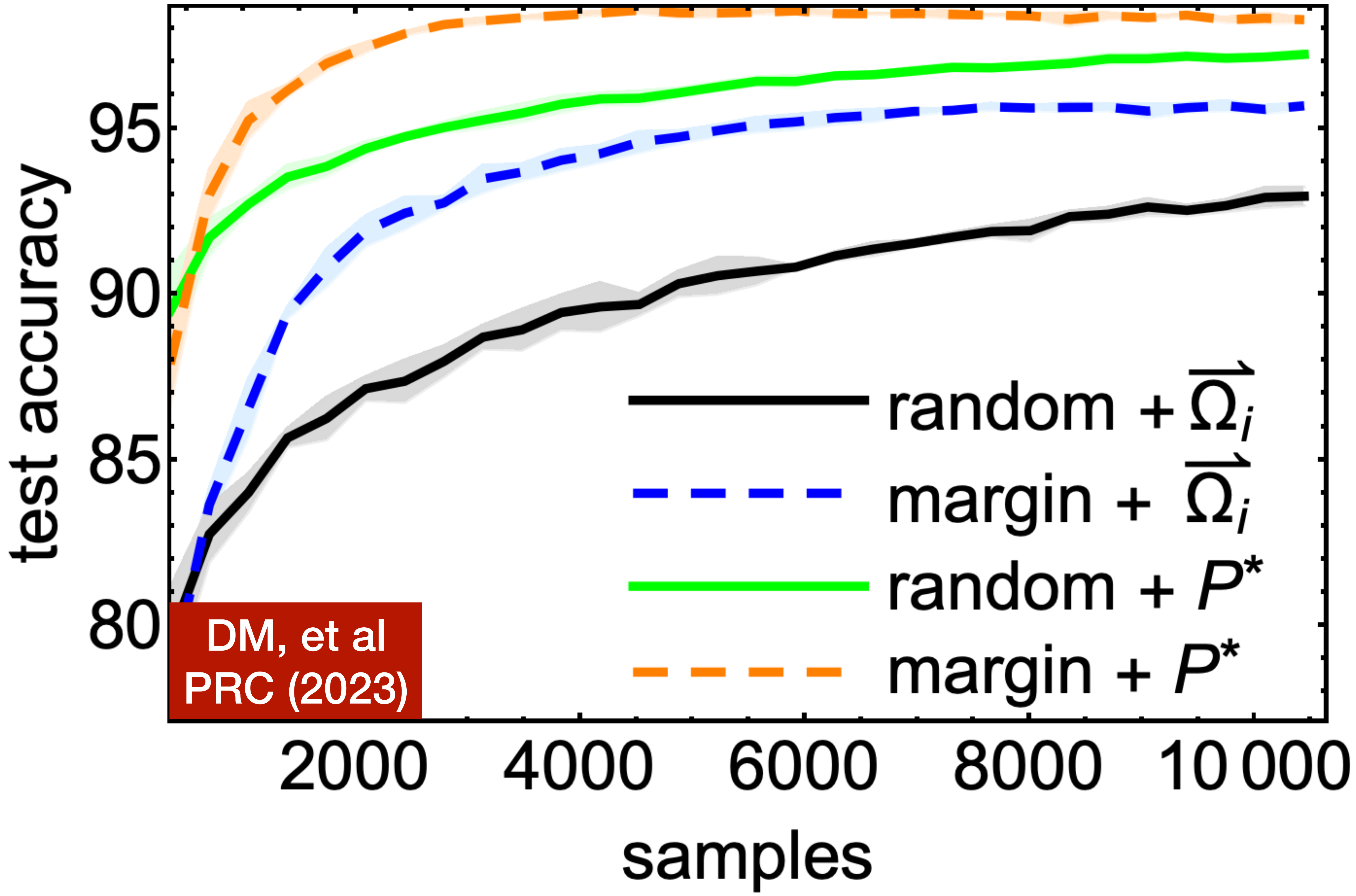


Performance using $P*$

J. Wijnands et al Comput. Aided Civ. Inf. (2020)







Preprocessing filters out irrelevant features

2-component PCA:

750 x 450 grid → ~1500 features

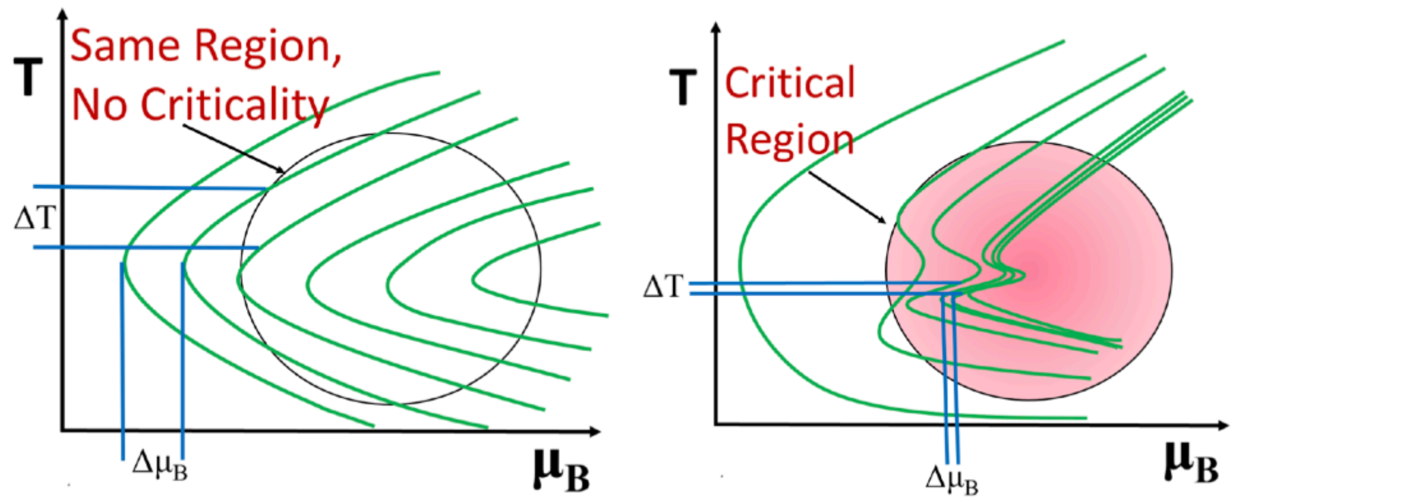
Main takeaways

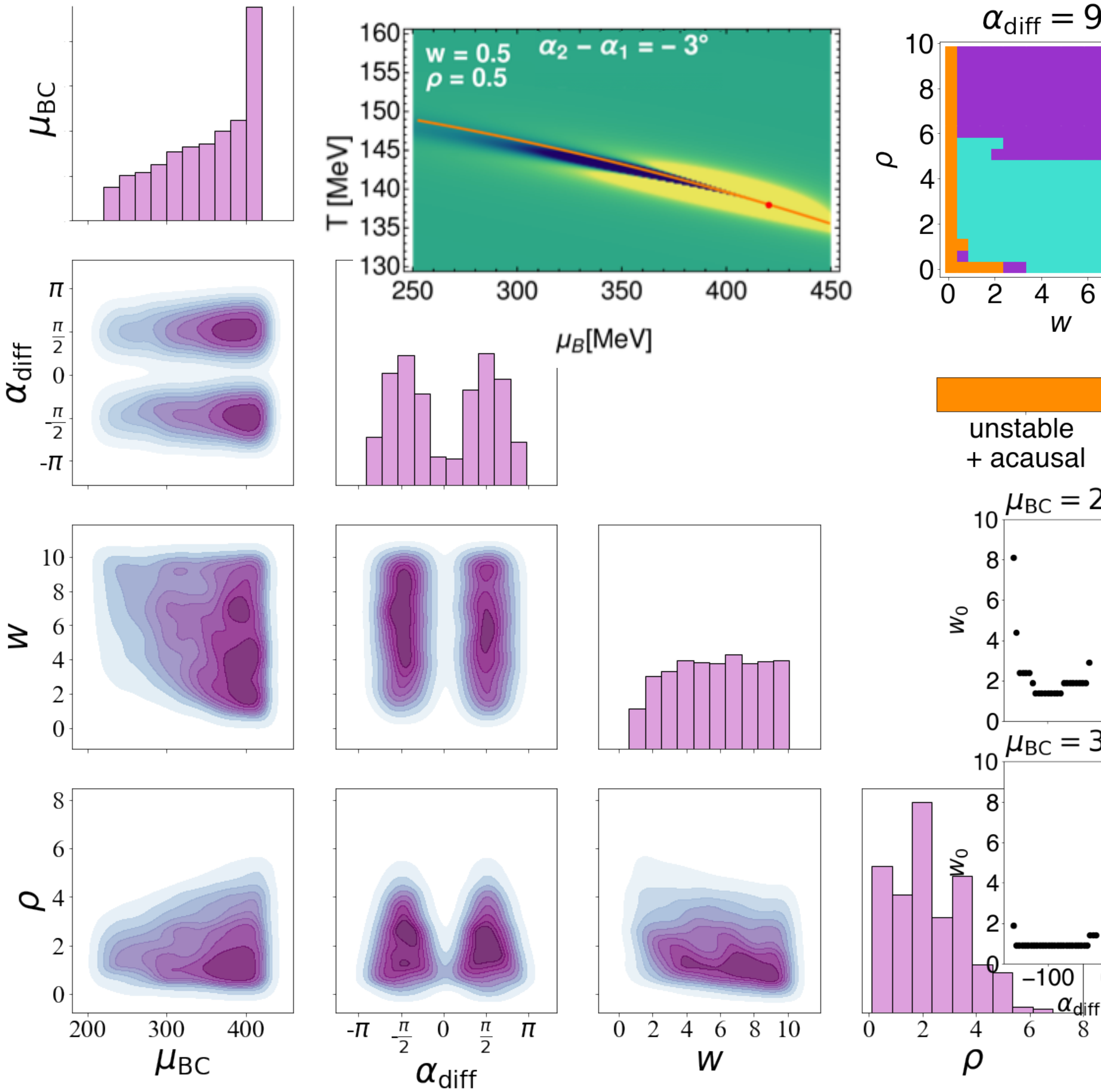
The Ising-to-QCD map determines the size and shape of the critical region and thus, how heavy-ion collisions are affected by a critical point.

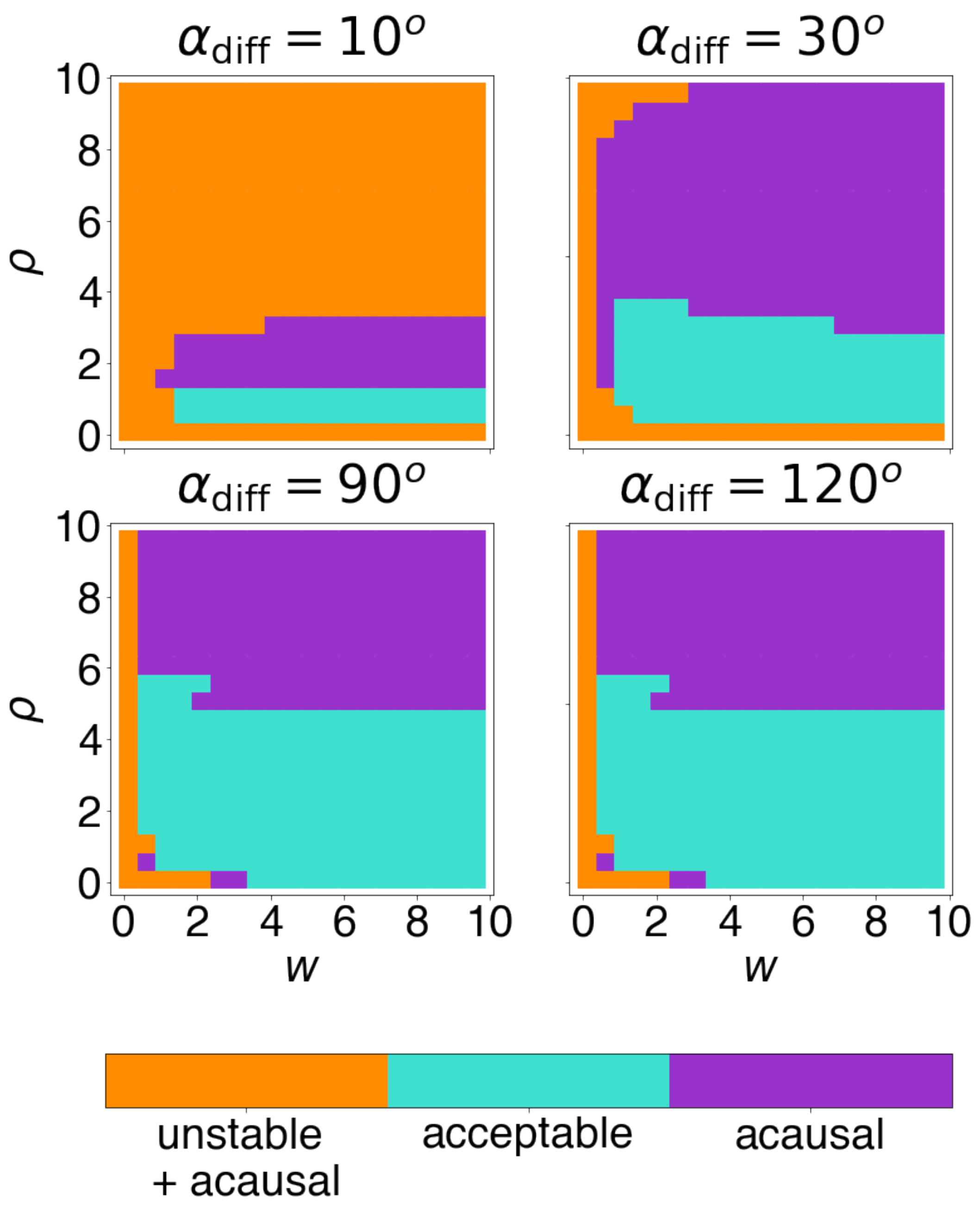
1. Same universal behavior, very different EoS.
2. Studies of critical effects should account for different CP location/size/shape systematically **within allowed parameter space**.
3. Theoretical models require further improvement: BSQ **EoS** with a CP + relativistic, viscous event-by-event + BSQ diffusion **hydro** + hadronic **transport**

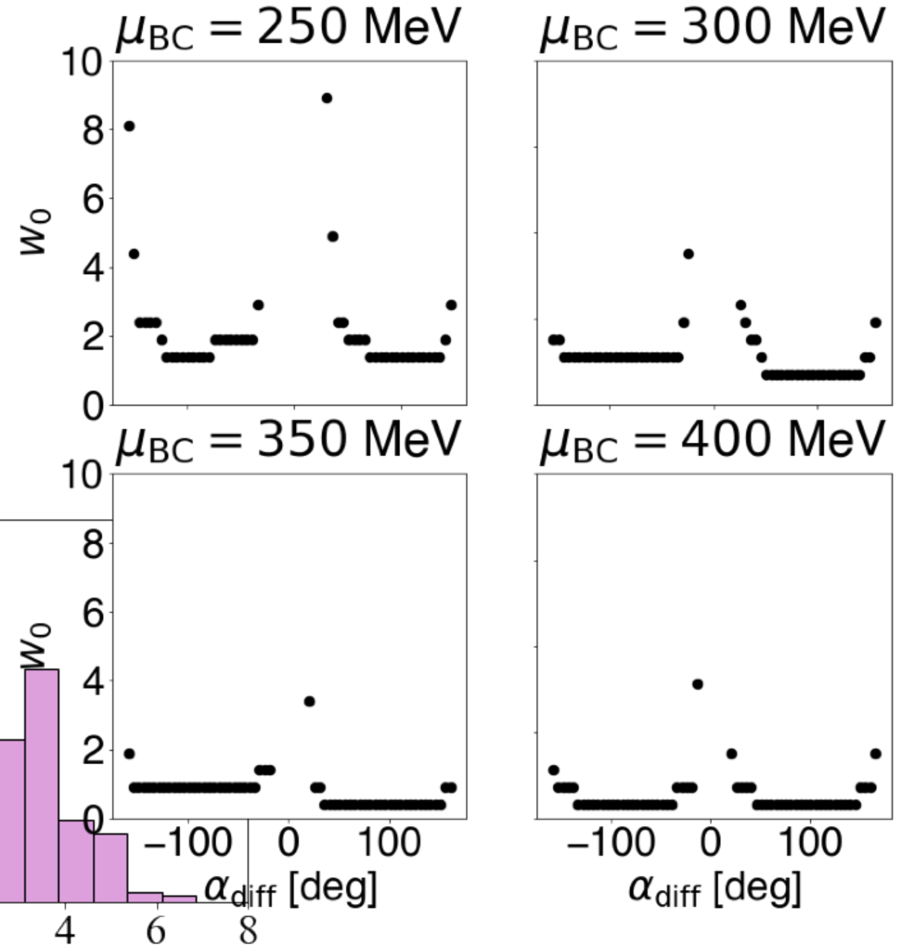
And then… physics

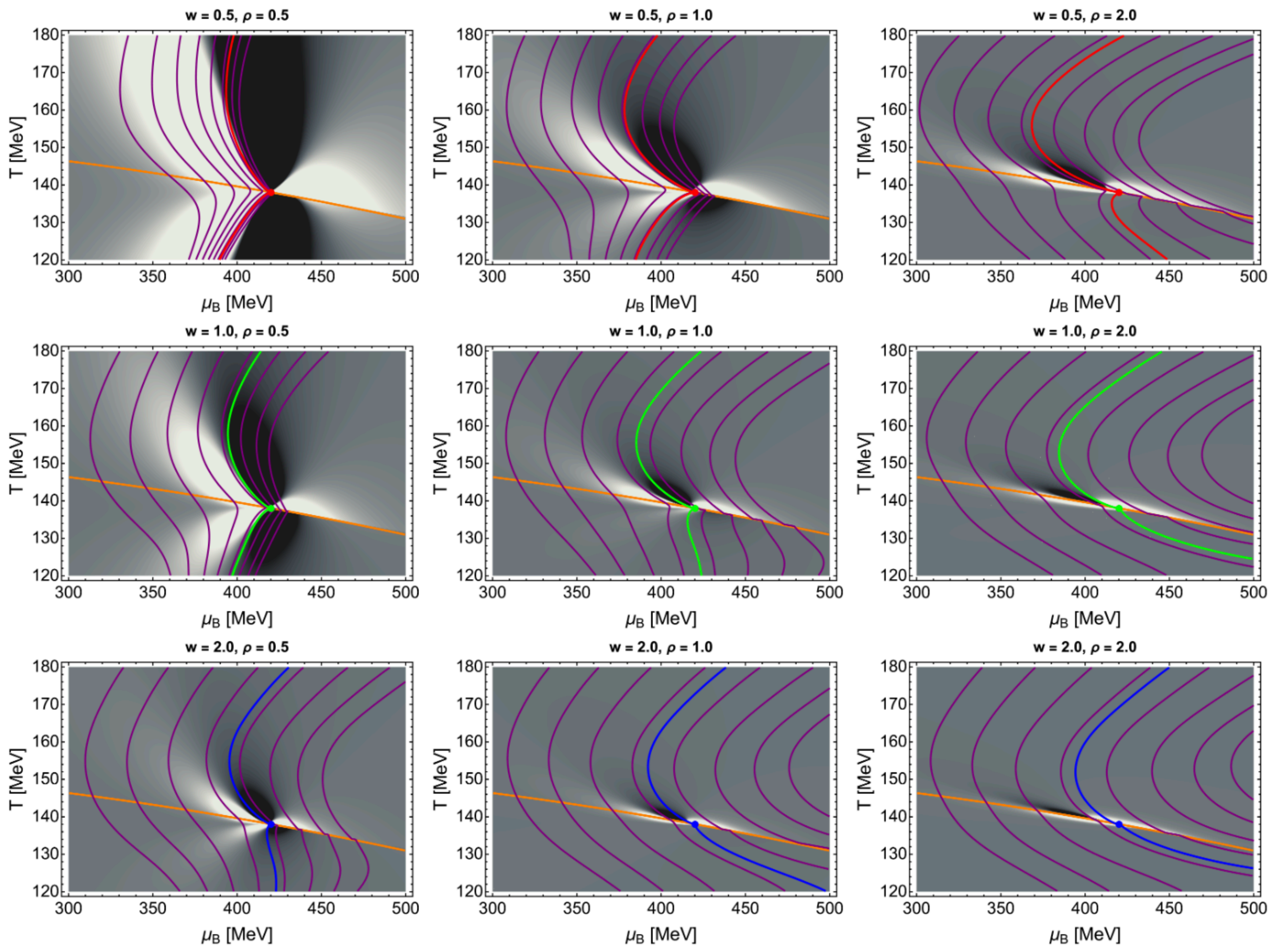
DM, et. al PRC (2021) T. Dore, DM et. al PRD (2022), DM et. al PRC (2023)

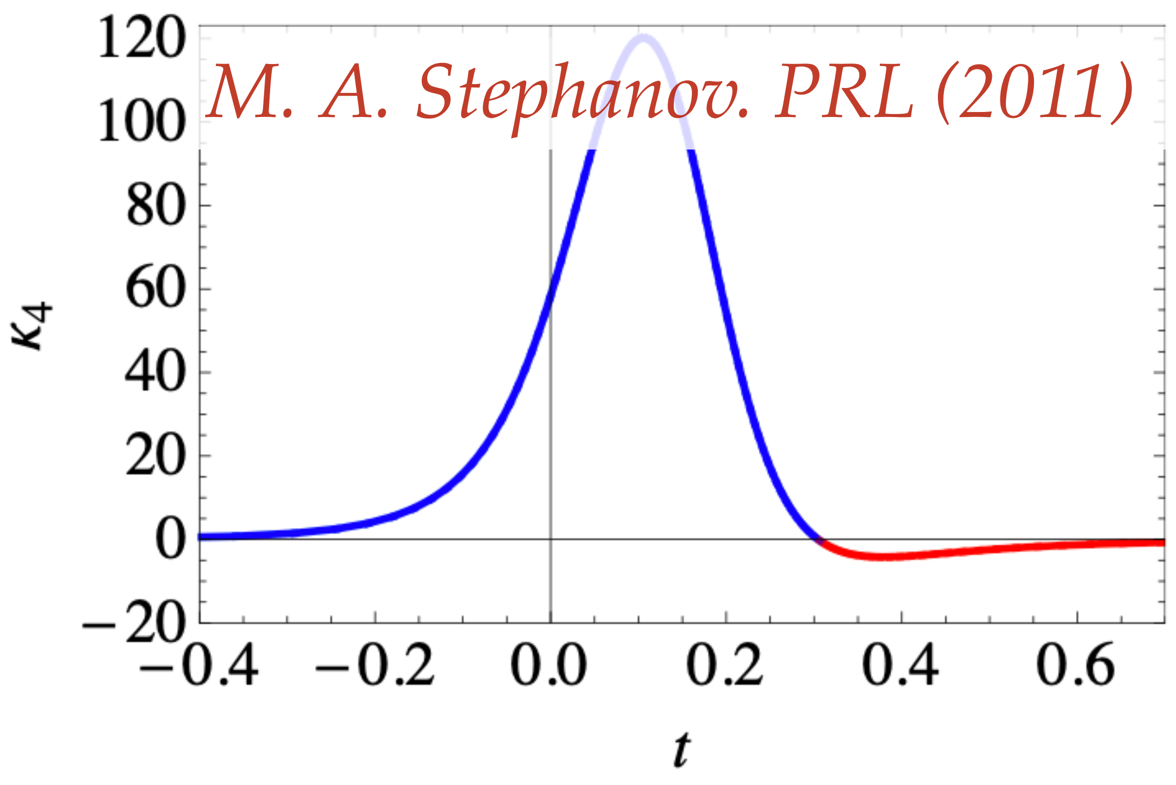


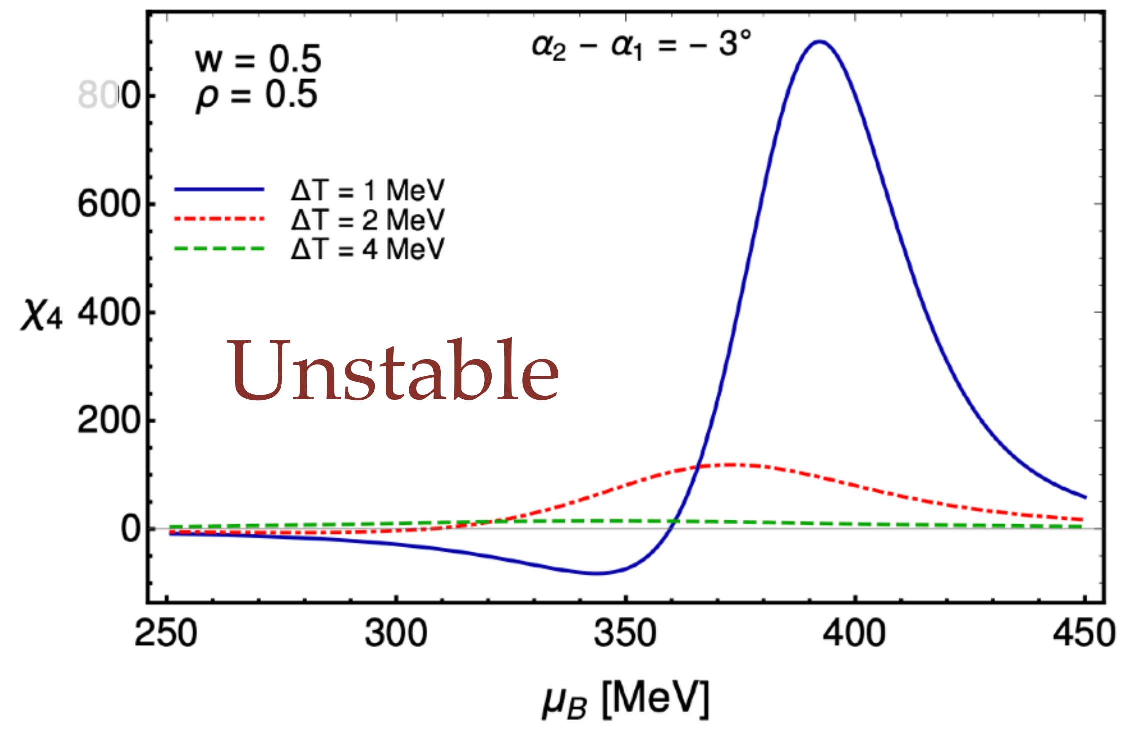












Physics-informed, model-agnostic

Agnostic sampling of the possible EoS

effective parameters: $p(T_i, n_{(B,S,Q),i}, Y_{Q,i})$, prior dictated by **most general set of physical constraints** (e.g. causality, stability, scaling, matching to effective theories)

In NS EoS inference — already implemented (GPs, piecewise polytopes, linear segments…), mapping the EoS to observables does not require emulators

In HIC's — event generation pipelines are complicated + need millions of events

Emulators need a "knob" to turn (typically parameters), but

results shown here: **working in model-agnostic space works**!

Model-agnostic description of the EoS over limited domain → expand to required domain → observables

Model-agnostic NS merger EoS: work in progress with Nanxi Yao + Katie Zine (UIUC)

EoS in different regimes: modeling challenges

Coming up with an EoS that meets a set of requirements is hard

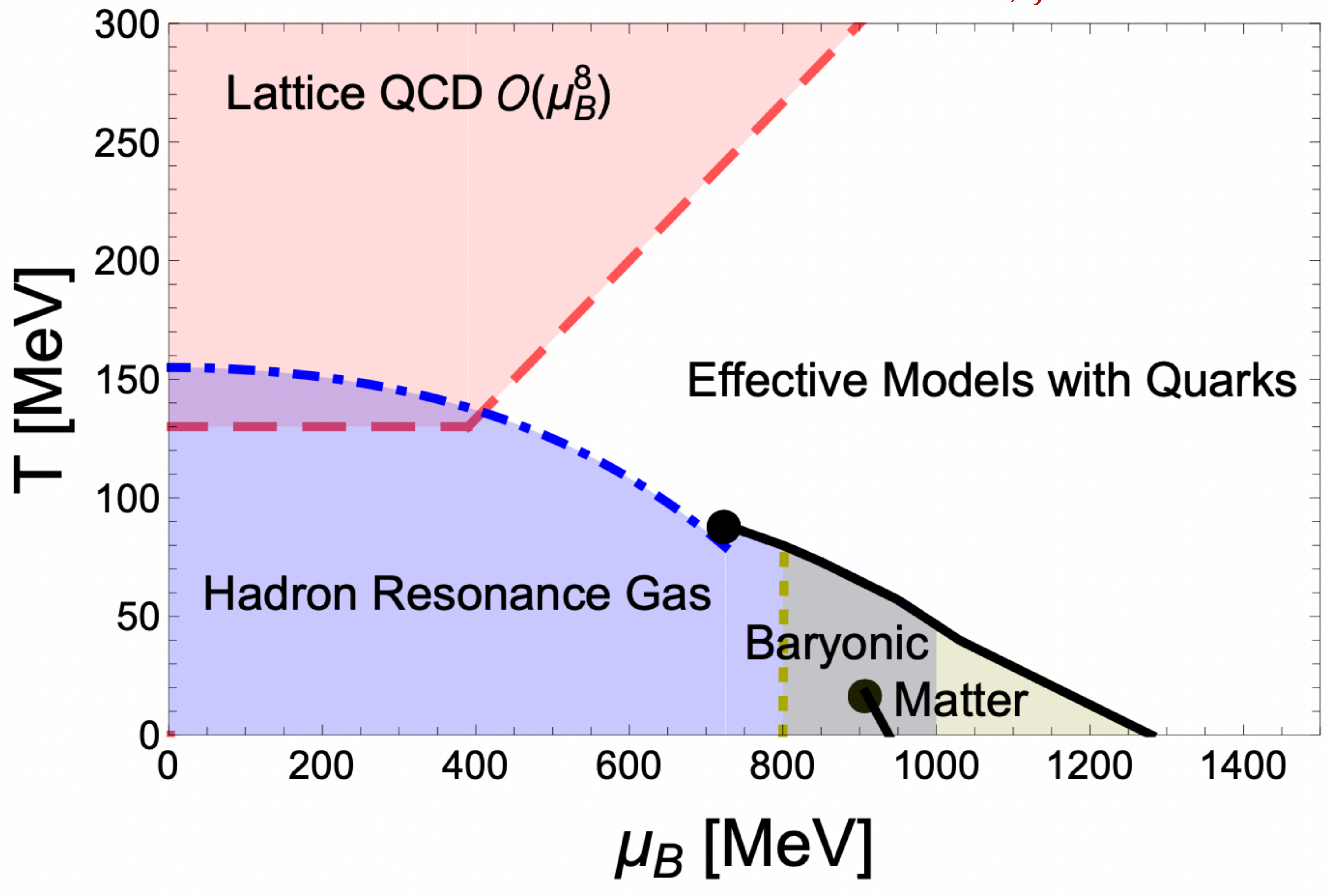
If you succeed: EoS will not be valid across the entire phase diagram

Dynamic simulations require large coverage of the phase diagram

e.g.: lattice QCD at low μ_B, HRG at low T, SB limit at high T, pQCD, liquid-gas phase transition, χEFT…

+ different models may or may not go to finite n_S, n_Q, Y_Q, $Y_S \ldots$

Dexheimer et al, JPG (2021)



MUSES — Cyberinfrastructure

Modular Unified Solver of the Equation of State

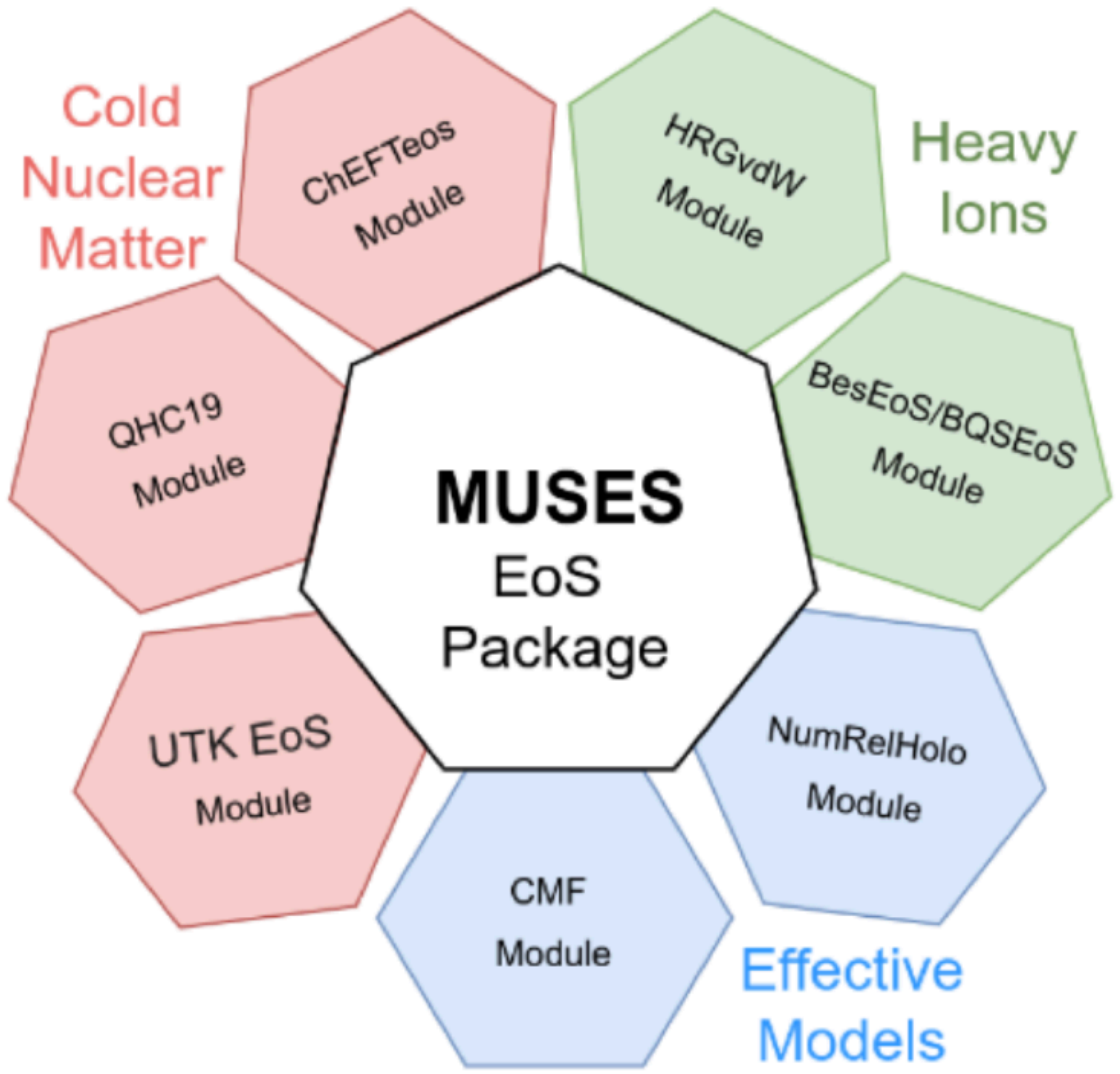
An open-source **cyberinfrastructure** that provides key **computational tools** to (i) create a unified equation of state for matter in all of the phase space, and (ii) to use this equation of state in astrophysical and heavy-ion data analysis and in the modeling of relativistic fluid dynamics, gravitational waves and compact objects.

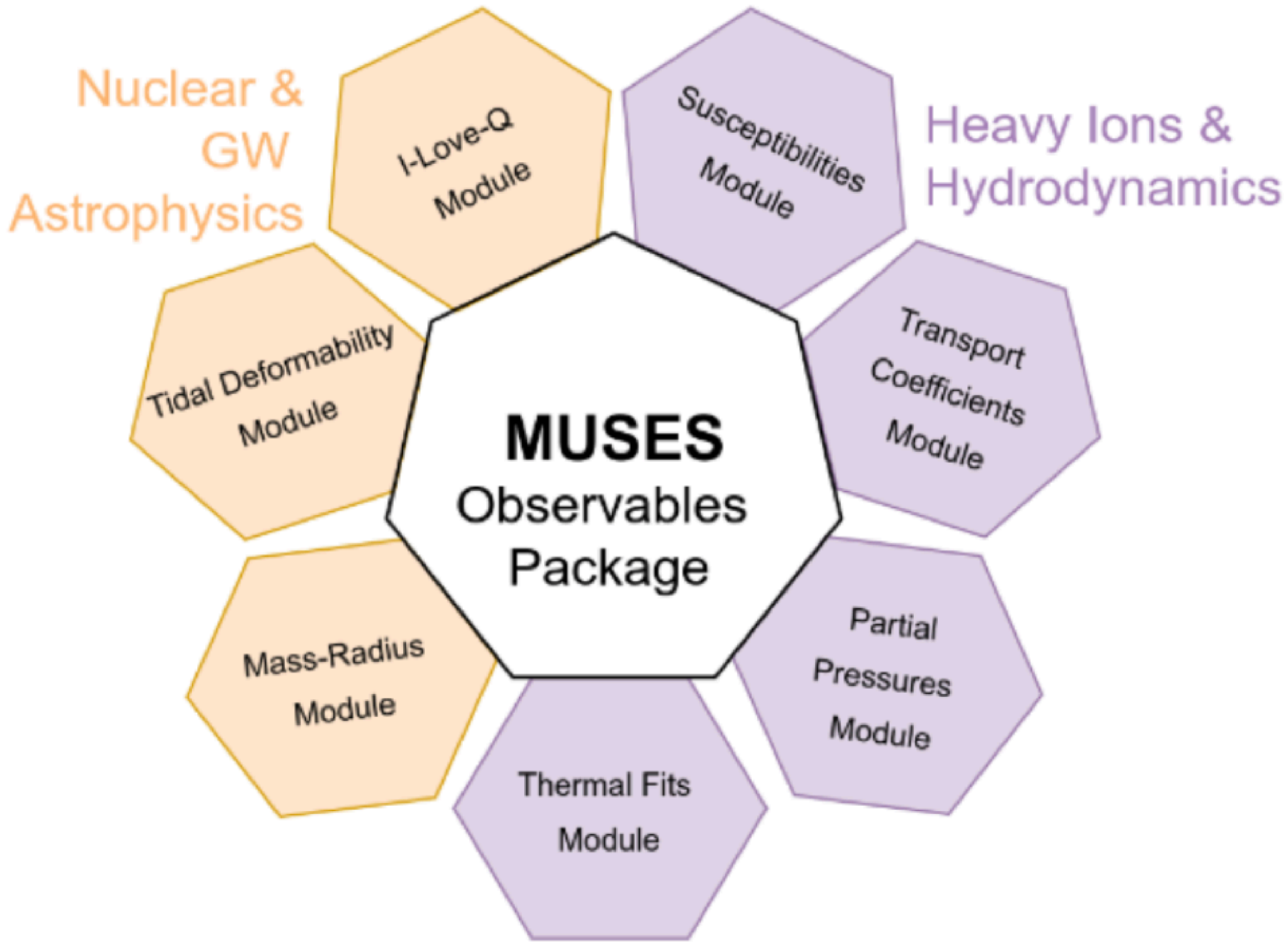
- Modular: different EoS (modules) are applicable to different regions of the QCD phase diagram
- Unified: Smooth merging of different modules to create one unified EoS which (i) maximizes phase-space coverage (ii) respects thermodynamic/observational/experimental constraints
- ML pipeline will be used to maintain EoS parameter spaces up-to-date with theoretical + experimental + observational constraints

MUSES

developers + users

- Upgrade of existing calculation tools to modern programming languages
- **Equation of State (EoS) package** that combines all the EoS modules using smooth transition functions
- **Web-based tools and services** that provide interactive interfaces to the calculation engine
- **Job management system** that executes client-requested calculations using the best available processing system
- Scalable, high-availability **deployment system** that can be reproduced in other computing environments





Summary

1. Mapping CP from the 3D Ising model to QCD phase diagram: allows for **systematic study of critical signatures**.

2. Active learning implemented to create a **fast and accurate tool** for studying EoS parameter space.

3. Working in model-agnostic space is possible with dimension-reduction techniques.

4. Large-scale cyberinfrastructure: key component for collaboration across communities/disciplines → **requires organization, funding, personnel.**