Fluctuations of conserved charges in hydrodynamics and molecular dynamics

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Acknowledgements:

M.I. Gorenstein, V. Koch, V.A. Kuznietsov, R. Poberezhnyuk, O. Savchuk, J. Steinheimer, H. Stoecker

QCD phase structure

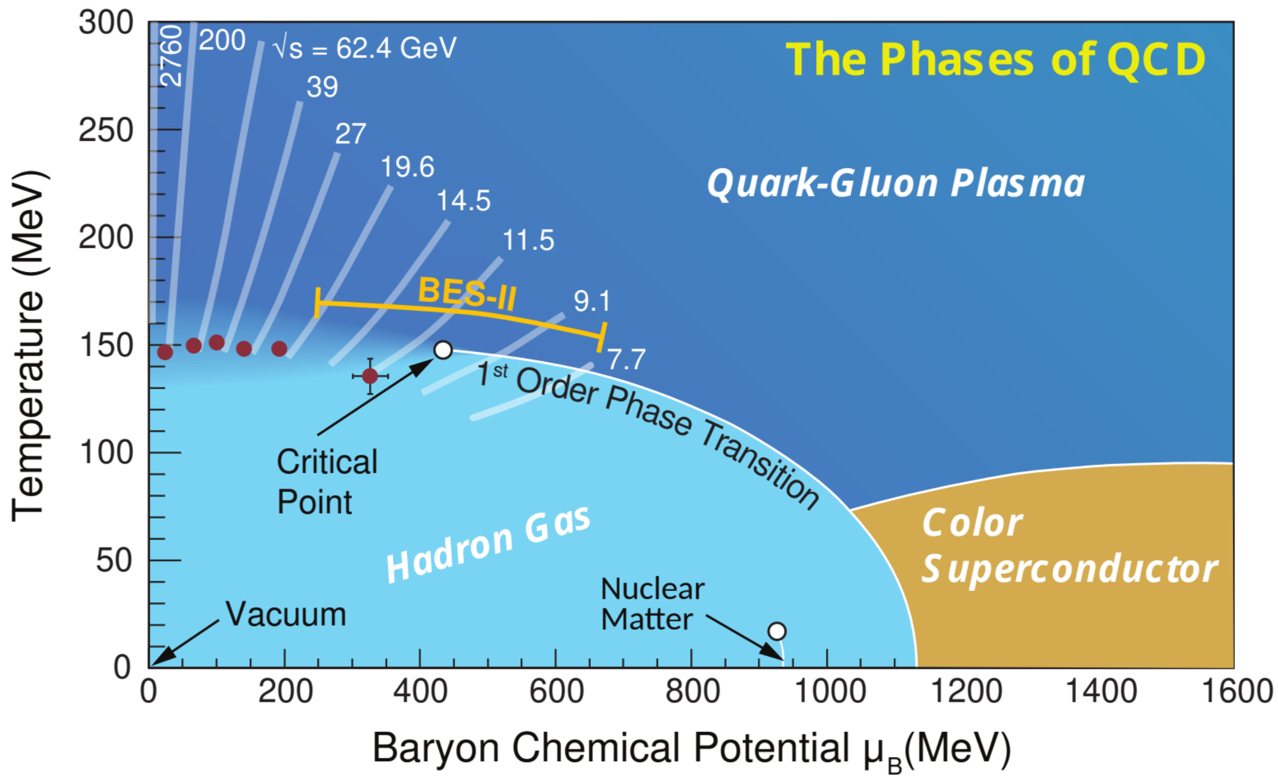


Figure from Bzdak et al., Phys. Rept. '20

- Dilute hadron gas at low T & ρ_B due to confinement, quark-gluon plasma high T & ρ_B
- Nuclear liquid-gas transition in cold and dense matter, lots of other phases conjectured

Is there a critical point and how to find it with heavy-ion collisions?

Event-by-event fluctuations and statistical mechanics

Cumulant generating function

$$K_N(t) = \ln\langle e^{tN}\rangle = \sum_{n=1}^{\infty} \kappa_n \frac{t^n}{n!}$$

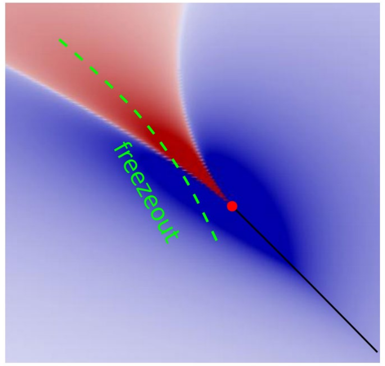
Grand partition function

$$\ln Z^{\mathrm{gce}}(T,V,\mu) = \ln\left[\sum_N e^{\mu N/T} Z^{\mathrm{ce}}(T,V,N)\right]$$

$$\kappa_n \propto \frac{\partial^n(\ln Z^{\mathrm{gce}})}{\partial\mu^n}$$

Cumulants measure chemical potential derivatives of the (QCD) equation of state

- **(QCD) critical point** – large correlation length, critical fluctuations of baryon number



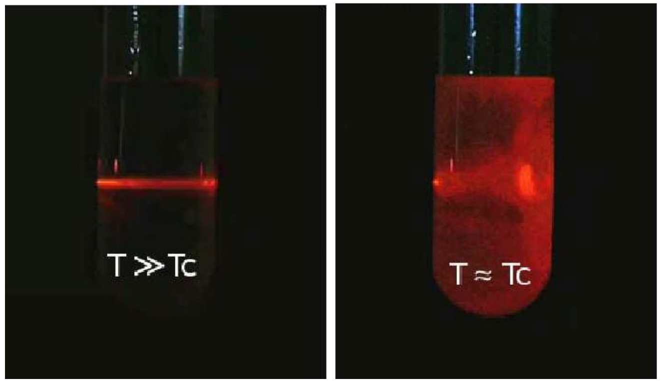
M. Stephanov, PRL '09, '11
Energy scans at RHIC (STAR)
and CERN-SPS (NA61/SHINE)

$$\kappa_2 \sim \xi^2, \quad \kappa_3 \sim \xi^{4.5}, \quad \kappa_4 \sim \xi^7$$

$$\xi \to \infty$$

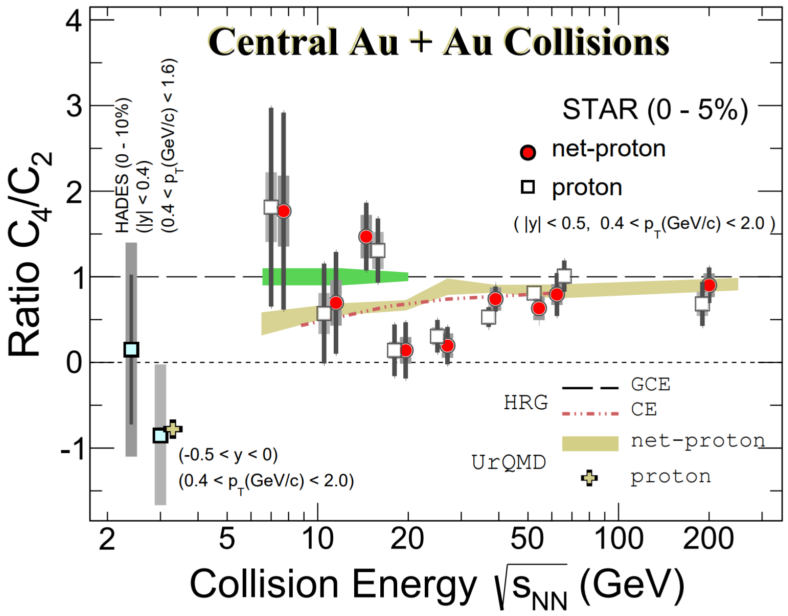
Looking for enhanced fluctuations
and non-monotonicities

Critical opalescence

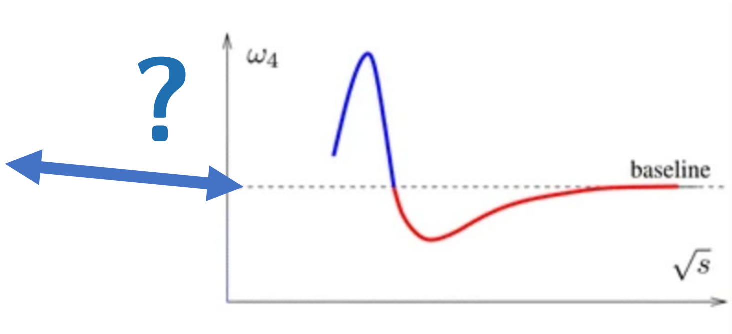


Experimental measurements

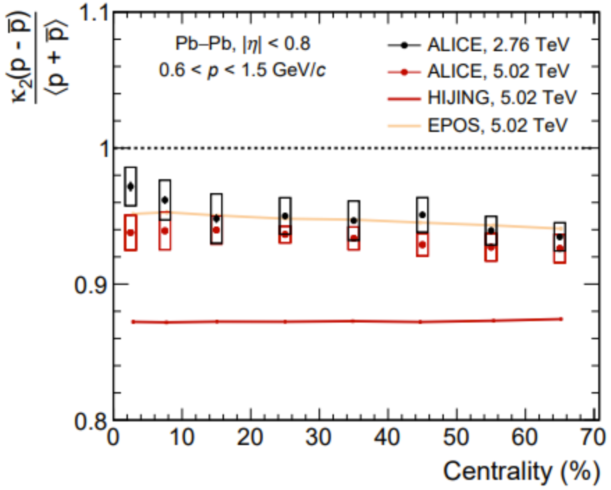
Beam energy scan in search for the critical point (STAR Coll.)



STAR Coll., Phys. Rev. Lett. 126, 092301 (2021); arXiv:2112.00240



M. Stephanov, Phys. Rev. Lett. (2011)



ALICE Coll., arXiv:2206.03343

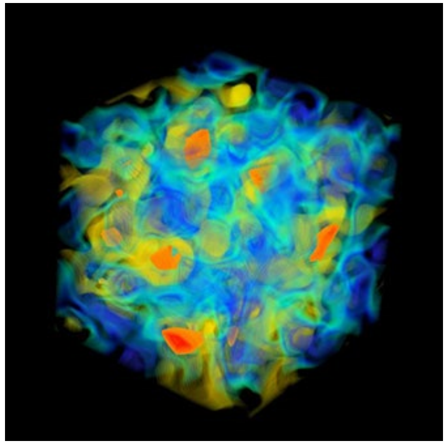
Reduced errors (better statistics), more energies, to come soon from RHIC-BES-II program, STAR-FXT etc.

Can we learn more from the more accurate data available for κ_2 and κ_3?

Other measurements: LHC-ALICE, GSI-HADES & CERN-NA61/SHINE Collaborations

Theory vs experiment: Challenges for fluctuations

Theory



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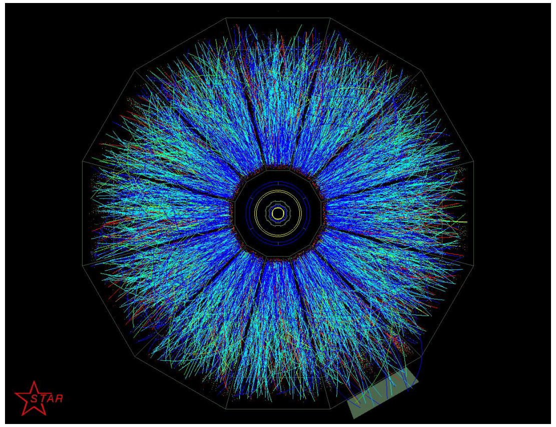
- Coordinate space
- In contact with the heat bath
- Conserved charges
- Uniform
- Fixed volume

Experiment



STAR event display

- Momentum space
- Expanding in vacuum
- Non-conserved particle numbers
- Inhomogenous
- Fluctuating volume

Need dynamical description

Theory vs experiment: Challenges for fluctuations

- canonical ensemble effects
  - subensemble acceptance method (SAM) **R. Poberezhnyuk, talk Wed 11:10**

    VV, Savchuk, Poberezhnyuk, Gorenstein, Koch, PLB 811, 135868 (2020); JHEP 089(2020); PRC 105, 014903 (2022)
  - ideal gas limit **A. Rustamov, talk Mon 17:35**

    Bzdak, Koch, Skokov, PRC 87, 014901 (2013); Braun-Munzinger et al., NPA 1008, 122141 (2021)

- coordinate vs momentum space

  Ling, Stephanov, PRC 93, 034915 (2016); Ohnishi, Kitazawa, Asakawa, PRC 94, 044905 (2016)

- proxy observables in experiment (net-proton, net-kaon) vs conserved charges in QCD (net-baryon, net-strangeness) **M. Kitazawa, talk Mon 16:45**

  Kitazawa, Asakawa, PRC 85, 021901 (2012); VV, Jiang, Gorenstein, Stoecker, PRC 98, 024910 (2018)

- volume fluctuations

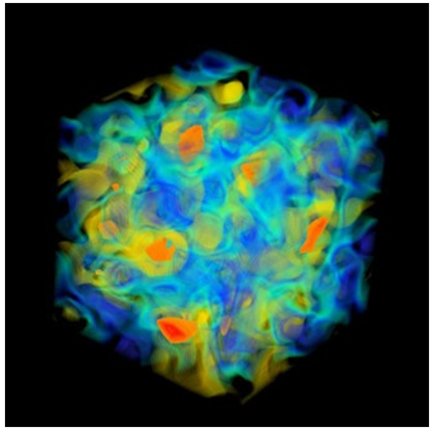
  Gorenstein, Gazdzicki, PRC 84, 014904 (2011); Skokov, Friman, Redlich, PRC 88, 034911 (2013)
  X. Luo, J. Xu, B. Mohanty, JPG 40, 105104 (2013); Braun-Munzinger, Rustamov, Stachel, NPA 960, 114 (2017)

- hadronic phase

  Steinheimer, VV, Aichelin, Bleicher, Stoecker, PLB 776, 32 (2018)
  Savchuk, VV, Koch, Steinheimer, Stoecker, PLB 827, 136983 (2022)

- non-equilibrium (memory) effects

  Mukherjee, Venugopalan, Yin, PRC 92, 034912 (2015)
  Asakawa, Kitazawa, Müller, PRC 101, 034913 (2020)



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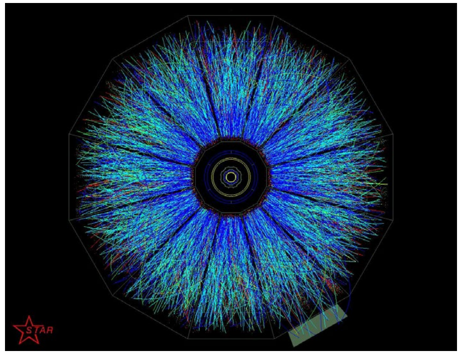


STAR event display

Dynamical approaches to the QCD critical point search

1. **Deviations from precision calculations of non-critical fluctuations**
   - Include essential non-critical contributions to (net-)proton number cumulants
   - Exact baryon conservation + hadronic interactions* (hard core repulsion)
   - Based on realistic hydrodynamic simulations tuned to bulk data

   [VV, C. Shen, V. Koch, Phys. Rev. C 105, 014904 (2022)]

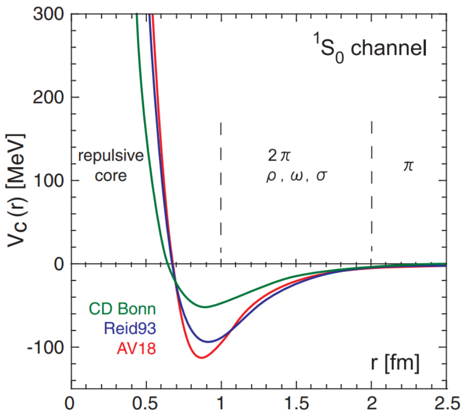


Figure from Ishii et al., PRL '07

2. **Molecular dynamics with a critical point**

   [V.A. Kuznietsov, O. Savchuk, M.I. Gorenstein, V. Koch, VV, Phys. Rev. C 105, 014904 (2022)]

3. Dynamical model calculations of critical fluctuations
   - Fluctuating hydrodynamics
   - Equation of state with tunable critical point [P. Parotto et al, Phys. Rev. C 101, 034901 (2020)]

   Under development within the Beam Energy Scan Theory (BEST) Collaboration

   [X. An et al., Nucl. Phys. A 1017, 122343 (2022)]

*J. Karthein, talk Tue 09:40

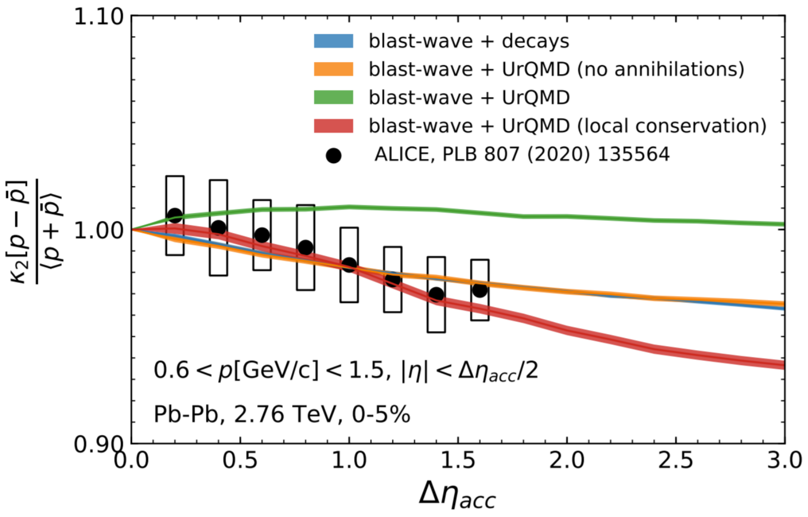
Hydrodynamics based analysis of (net-)particle fluctuations and constraints on the QCD critical point

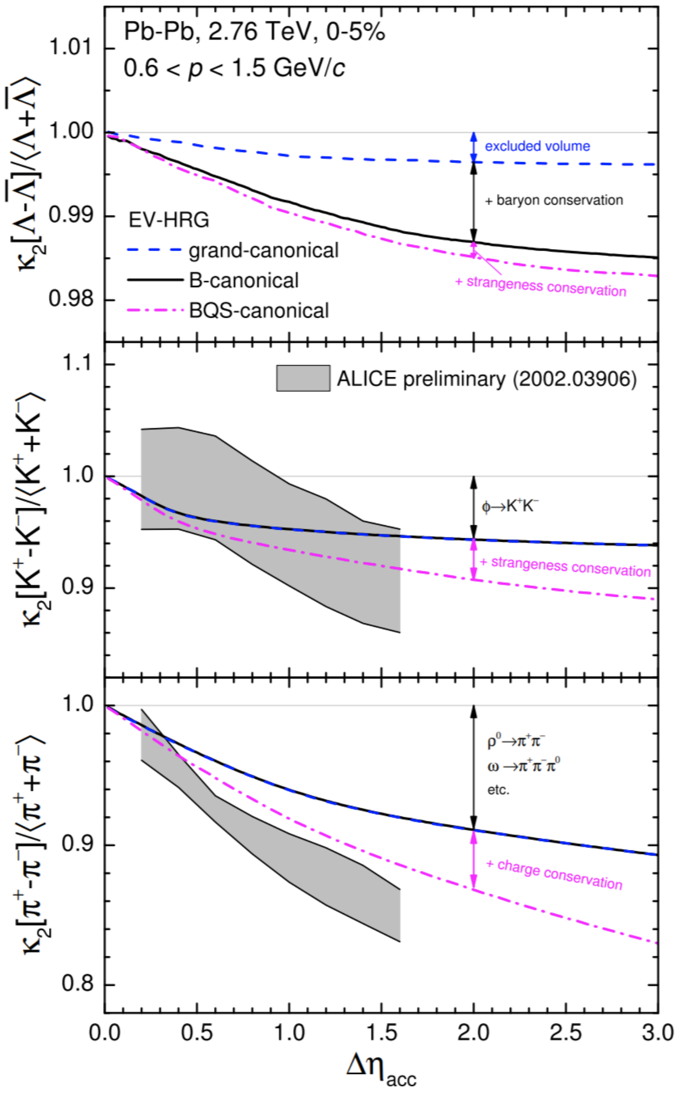
Net-particle fluctuations at the LHC

- Net protons described within errors and consistent with either
  - global baryon conservation without $B\bar{B}$ annihilations

    see e.g. ALICE Coll. arXiv:2206.03343
  - or local baryon conservation with $B\bar{B}$ annihilations

    O. Savchuk et al., Phys. Lett. B 827, 136983 (2022)



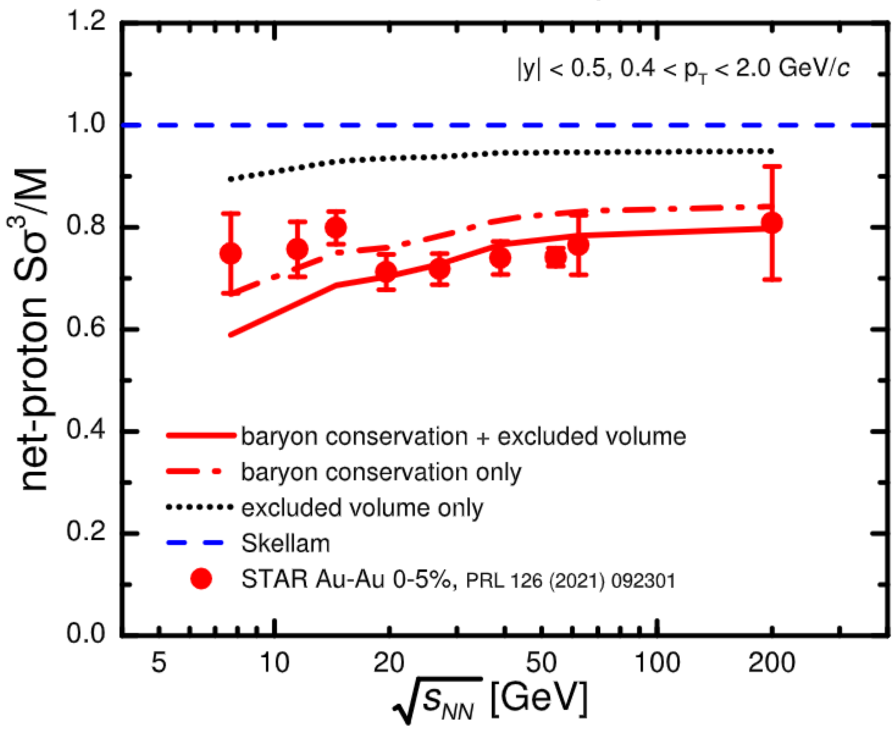


VV, Koch, Phys. Rev. C 103, 044903 (2021)

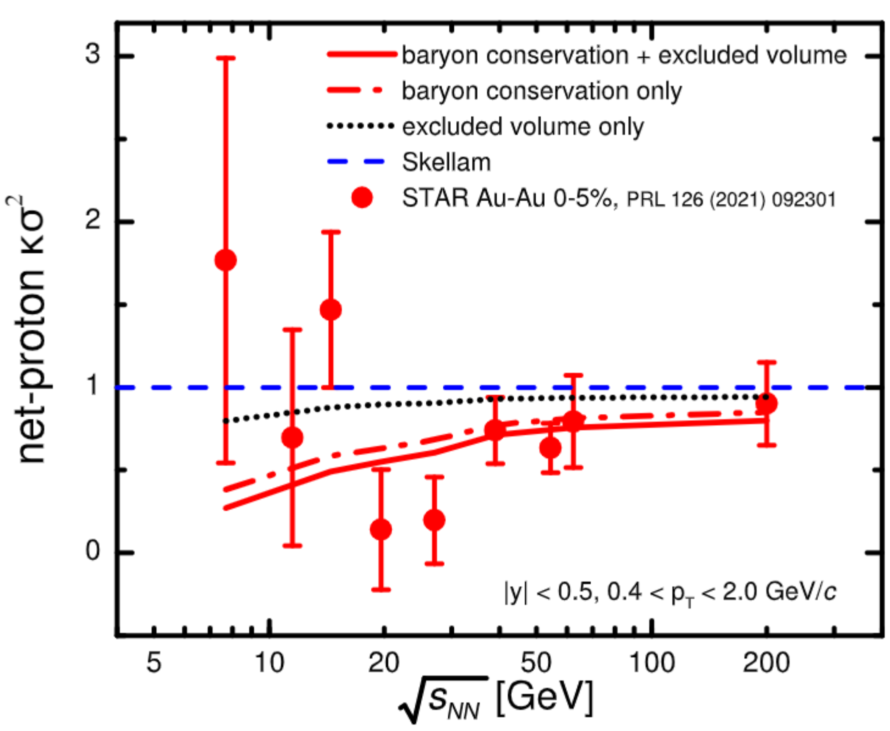
- Large effect from resonance decays for pions and kaons + exact conservation of electric charge/strangeness

RHIC-BES: Net proton cumulant ratios (MUSIC)

κ_3/κ_1



κ_4/κ_2



- Data at $\sqrt{s_{NN}} \geq 20$ GeV consistent with non-critical physics (baryon conservation and repulsion)
- Effect from baryon conservation is larger than from repulsion
- Excess of skewness in data at $\sqrt{s_{NN}} < 20$ GeV – *hint of attractive interactions?*

VV, V. Koch, C. Shen, Phys. Rev. C 105, 014904 (2022)

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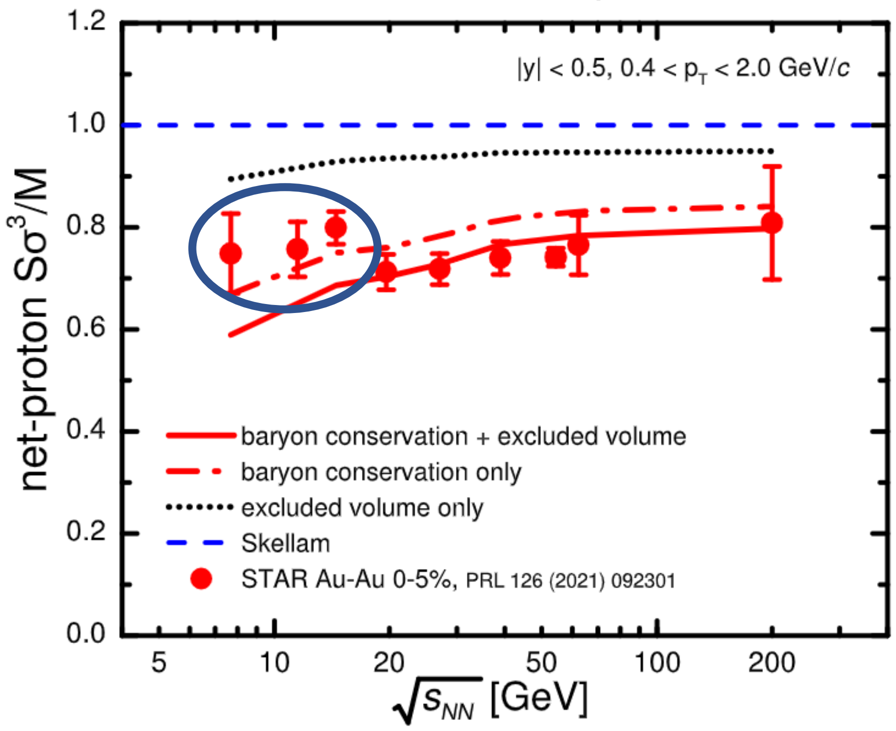
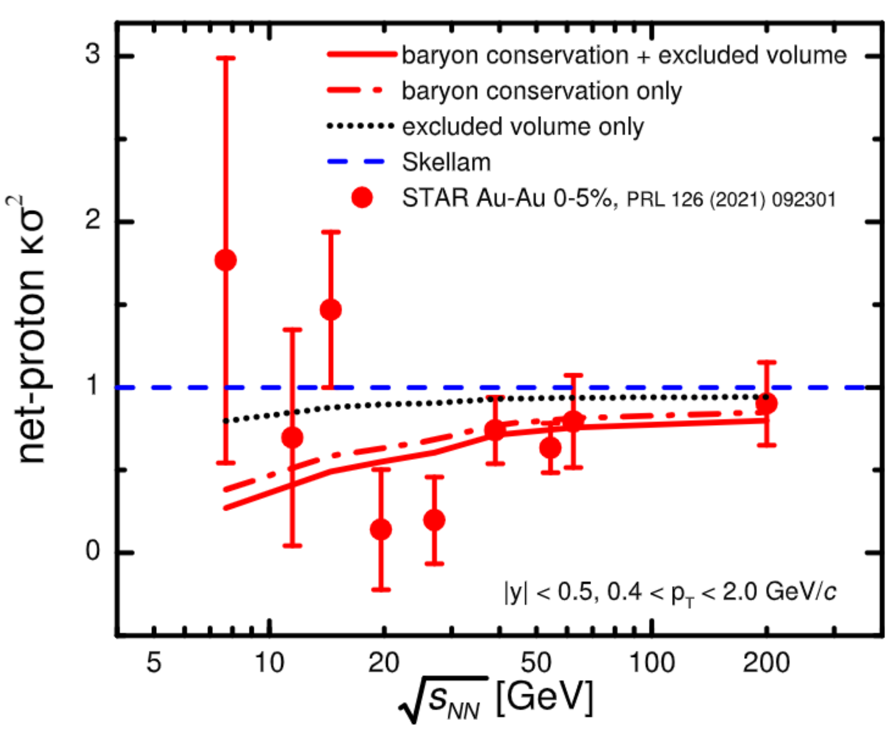


κ_4/κ_2



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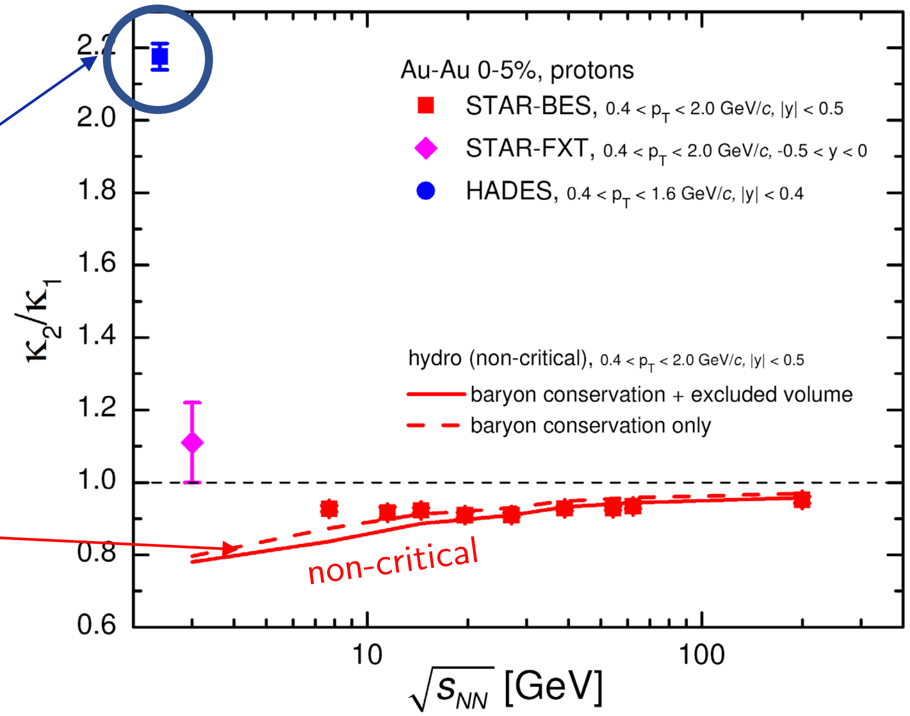
VV, V. Koch, C. Shen, Phys. Rev. C 105, 014904 (2022)

Second order proton cumulants and $\sqrt{s_{NN}} \leq 7.7$ GeV

- Second order cumulants measured with much higher precision
- Intriguing hint from HADES @ $\sqrt{s_{NN}} = 2.4$ GeV: huge excess of two-proton correlations!
  [HADES Collaboration, Phys. Rev. C 102, 024914 (2020)]
- No change of trend in the non-critical hydro
- Additional mechanisms:
  - Nuclear liquid-gas transition
  - Light nuclei formation
- Fill the gap with data from STAR-FXT (e.g. Phys.Rev.Lett. 128 (2022) 202303), future experiments like CBM-FAIR



A closer look at the HADES data

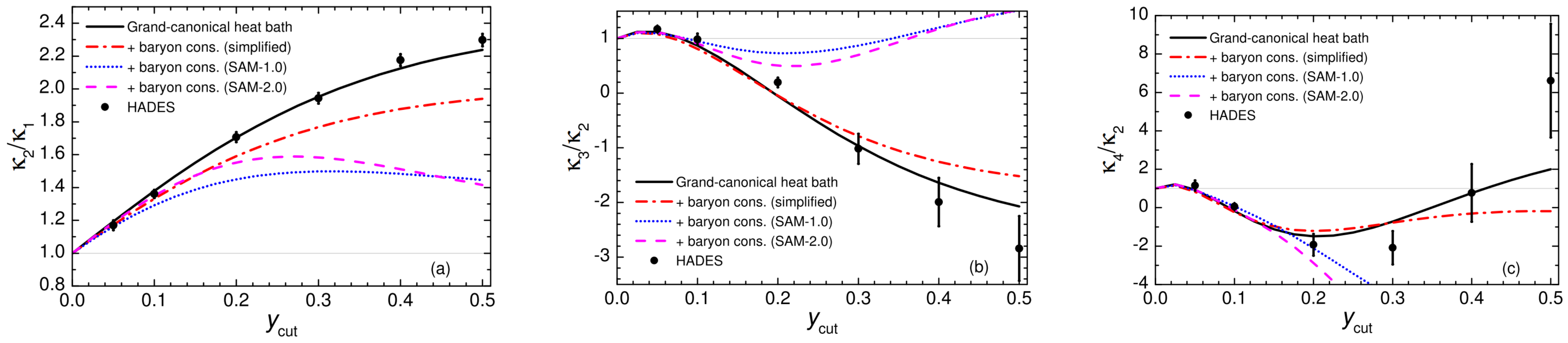
VV, Koch, arXiv:2204.00137

- Fit baryon susceptibilities to data within a fireball model (Siemens-Rasmussen*)

- In the grand-canonical limit (no baryon conservation, small y_{cut}) the data are described well with

$$\frac{\chi_2^B}{\chi_1^B} = 9.35 \pm 0.40, \qquad \frac{\chi_3^B}{\chi_2^B} = -39.6 \pm 7.2, \qquad \frac{\chi_4^B}{\chi_2^B} = 1130 \pm 488 \qquad \text{i.e.} \qquad \chi_4^B \gg -\chi_3^B \gg \chi_2^B \gg \chi_1^B$$

- Could be indicative of a *critical point* near the HADES freeze-out at $T \sim 70$ MeV, $\mu_B \sim 875$ MeV
- However, the results for $y_{cut} > 0.2$ are challenging to describe with baryon conservation included



*Fireball parameters from Harabasz et al., PRC 102 (2020) 054903 and Motornenko et al., PLB 822 (2021) 136703

Critical point particle number fluctuations from molecular dynamics

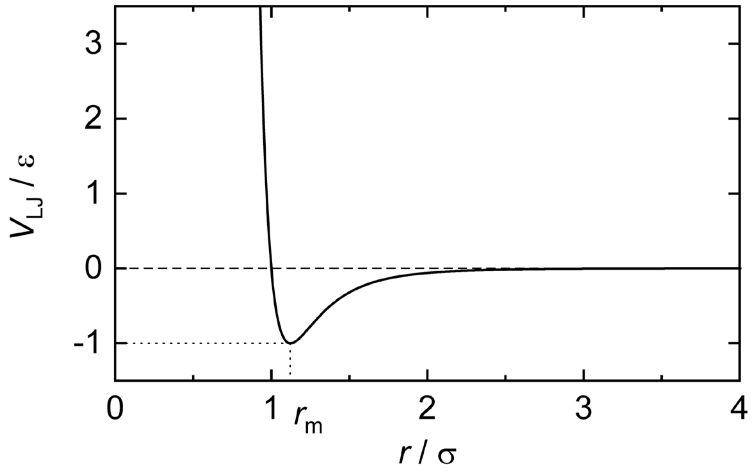
V.A. Kuznietsov, O. Savchuk, M.I. Gorenstein, V. Koch, VV, Phys. Rev. C 105, 044903 (2022)

For non-critical fluctuations in molecular dynamics see Hammelmann et al., arXiv:2202.11417

Lennard-Jones fluid

S. Stephan, M. Thol, J. Vrabec, H. Hasse, Journal of Chemical Information and Modeling 59, 4248 (2019)

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



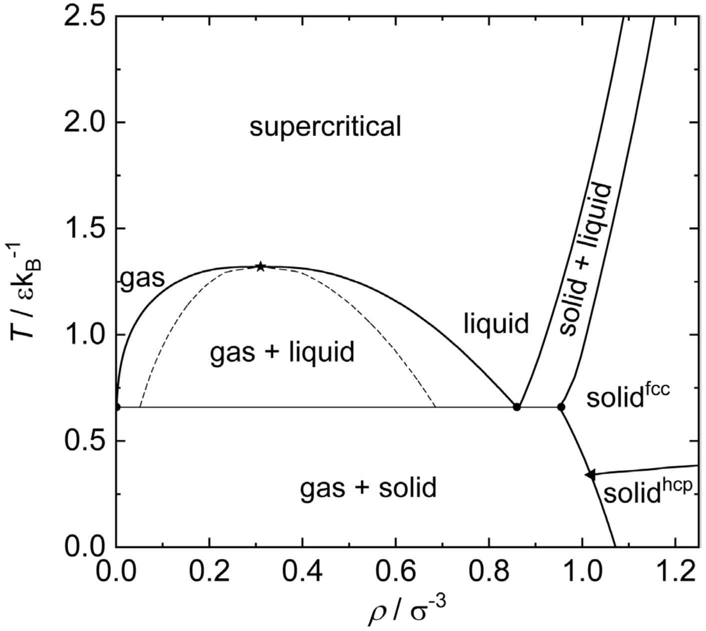
Reduced variables:

$$\tilde{r} = r/\sigma \qquad \tilde{T} = T/(k_B\varepsilon) \qquad \tilde{n} = n\sigma^3$$

Properties:

- Multiple phase transitions, including critical point
- Tractable with molecular dynamics simulations
- Critical point in 3D-Ising universality class at

$$\tilde{T}_c = 1.321 \pm 0.007\ , \quad \tilde{n}_c = 0.316 \pm 0.005$$

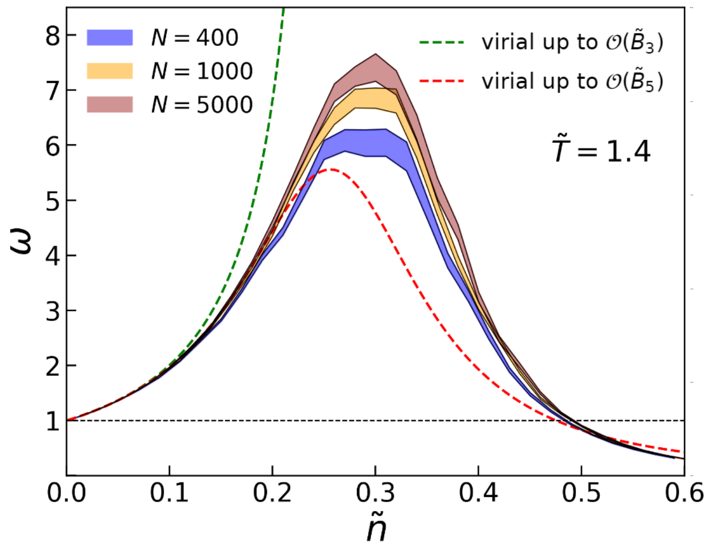


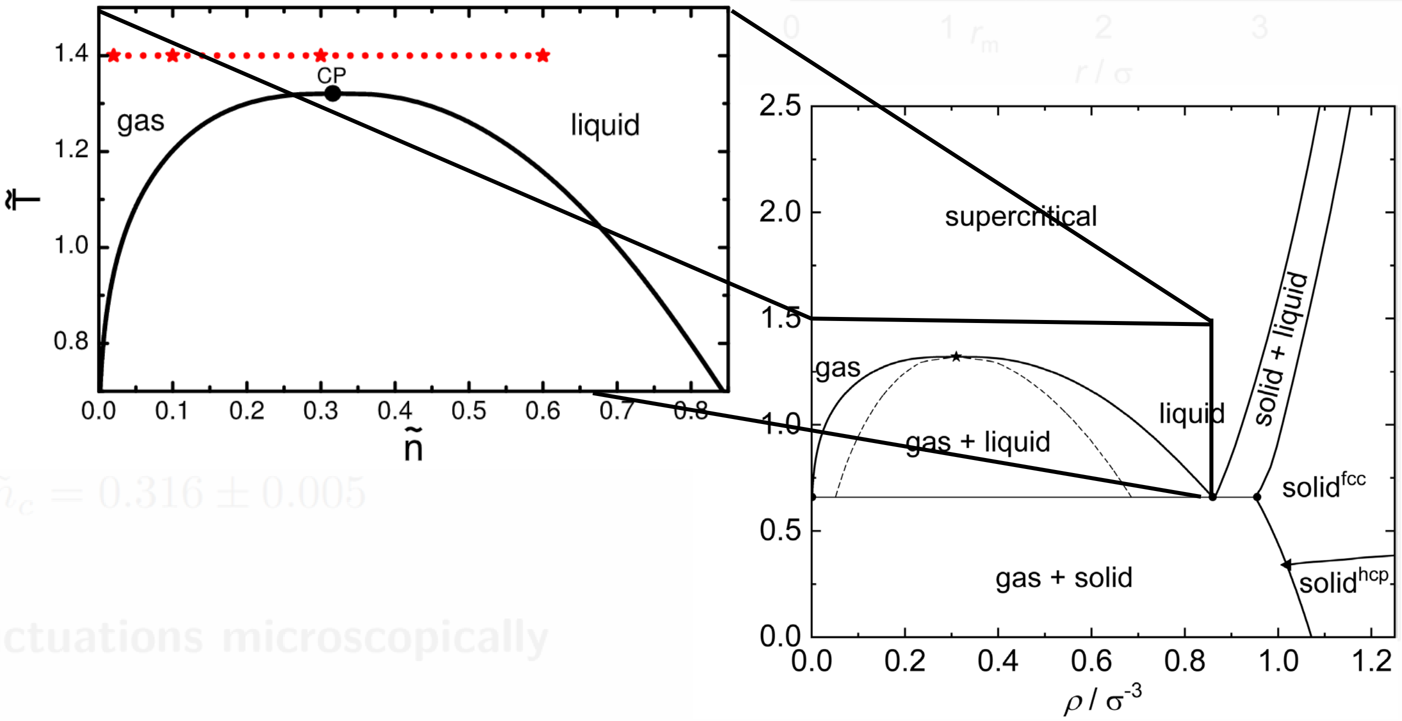
Toy model to study critical point fluctuations microscopically

Lennard-Jones fluid

Study the supercritical isotherm $\tilde{T} = 1.4 = 1.06\,\tilde{T}_C$ in density range $0.05\tilde{n}_C < \tilde{n} < 2\tilde{n}_C$

Large fluctuations

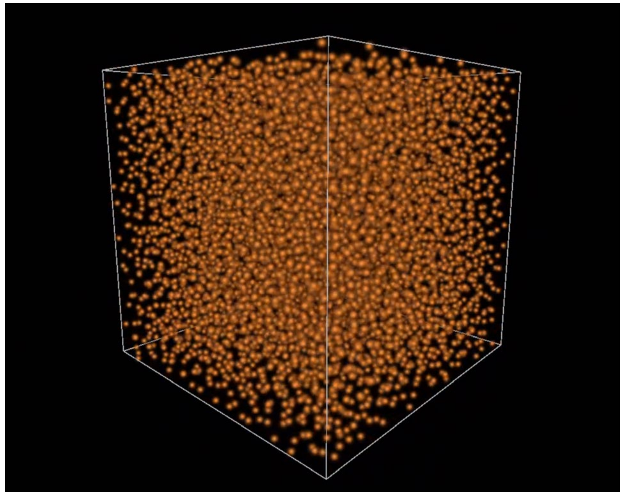




Molecular dynamics setup

- Newton's equations of motion (classical N-body problem)

$$m\ddot{\mathbf{r}}_\mathbf{i} = -\sum_j \nabla_i V_{\mathrm{LJ}}^{ij}(|\mathbf{r}_\mathbf{i} - \mathbf{r}_\mathbf{j}|)$$



- Box simulation
  - Periodic boundary conditions
  - Minimum-image convention
- Microcanonical (UVN) and canonical-like (TVN) ensembles
- Observables as time averages $\langle A \rangle = \frac{1}{\tilde{\tau}} \int_{\tilde{t}_{\mathrm{eq}}}^{\tilde{t}_{\mathrm{eq}}+\tilde{\tau}} A(\{\tilde{\mathbf{r}}_i(\tilde{t}), \tilde{\mathbf{v}}_i(\tilde{t})\}) d\tilde{t}$

Implementation:

Velocity Verlet integration scheme implemented on CUDA-GPU (x100-200 speed-up*)

open source: https://github.com/vlvovch/lennard-jones-cuda

NVIDIA CUDA

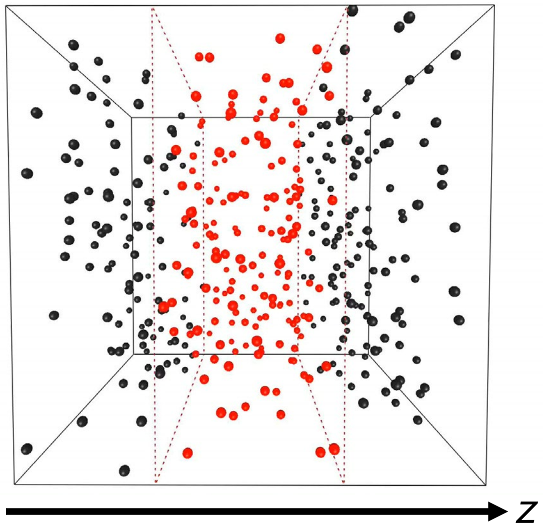
*This research used the Lawrencium computational cluster resource provided by the IT Division at the Lawrence Berkeley National Laboratory

Fluctuations in molecular dynamics

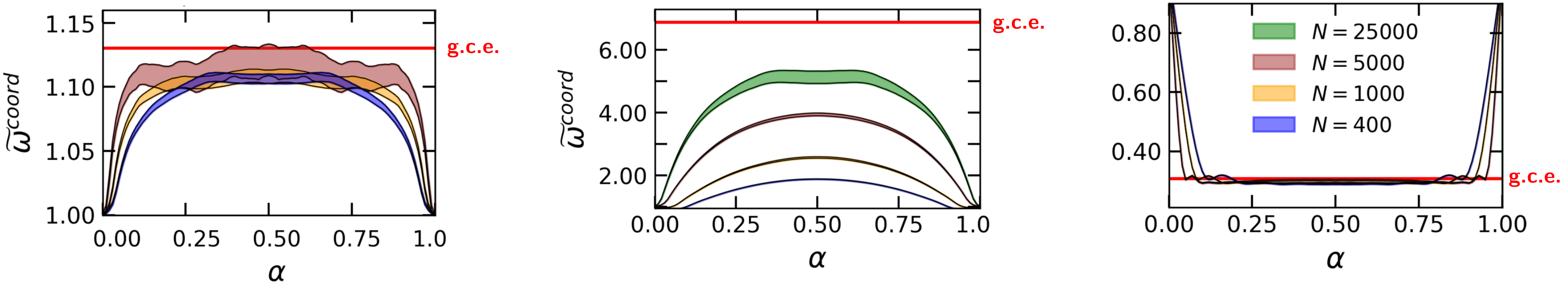
Variance of conserved particle number distribution inside coordinate space subvolume $|z| < z^{max}$ as time average

- $\langle N \rangle$, $\langle N^2 \rangle$ as time averages
- Microcanonical ensemble
- $1 - \alpha$ factor to cancel out global conservation
- $\widetilde{\omega}^{coord} \to \omega^{gce}$ expected as $\langle N \rangle \to \infty$

$$\tilde{\omega}^{\text{coord}} = \frac{1}{1-\alpha} \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle}$$



$n \approx 0.15\, n_c$ $n \approx n_c$ $n \approx 2 n_c$



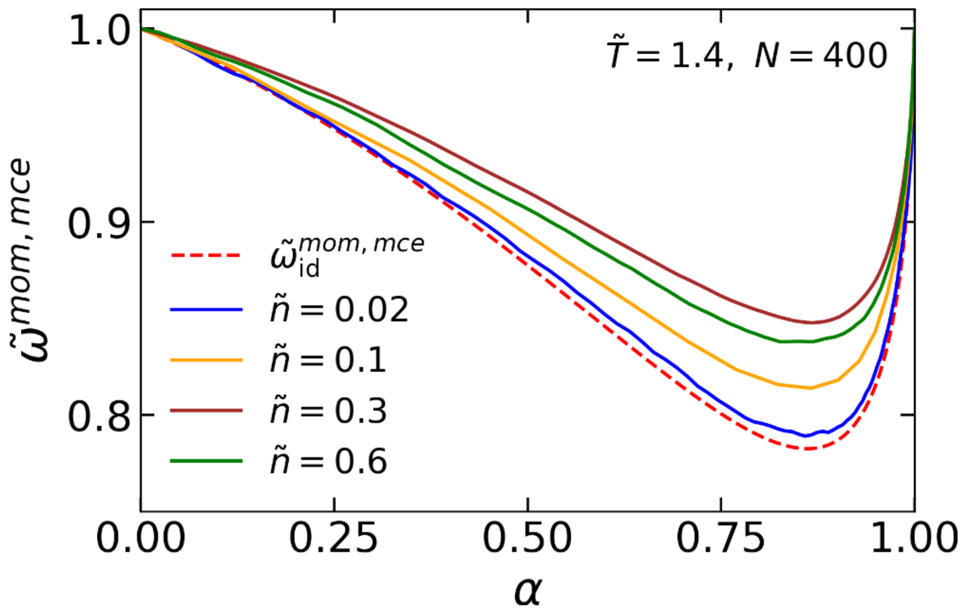
Fluctuations in molecular dynamics: momentum space

Experiments measure momenta, not coordinates → consider momentum space subvolume instead

$|v_z| < v_z^{\text{cut}}$ (à la $|y| < y^{\text{cut}}$) $\qquad \alpha = \langle N^{\text{acc}} \rangle / N$

total energy conservation effect

Ideal gas limit: $\tilde{\omega}_{\text{id}}^{\text{mom,mce}} = 1 - \frac{2[\text{erf}^{-1}(\alpha)]^2 e^{-2[\text{erf}^{-1}(\alpha)]^2}}{3\pi\alpha(1-\alpha)}$



Large fluctuations near the CP are washed out when momentum cuts imposed instead of coordinates

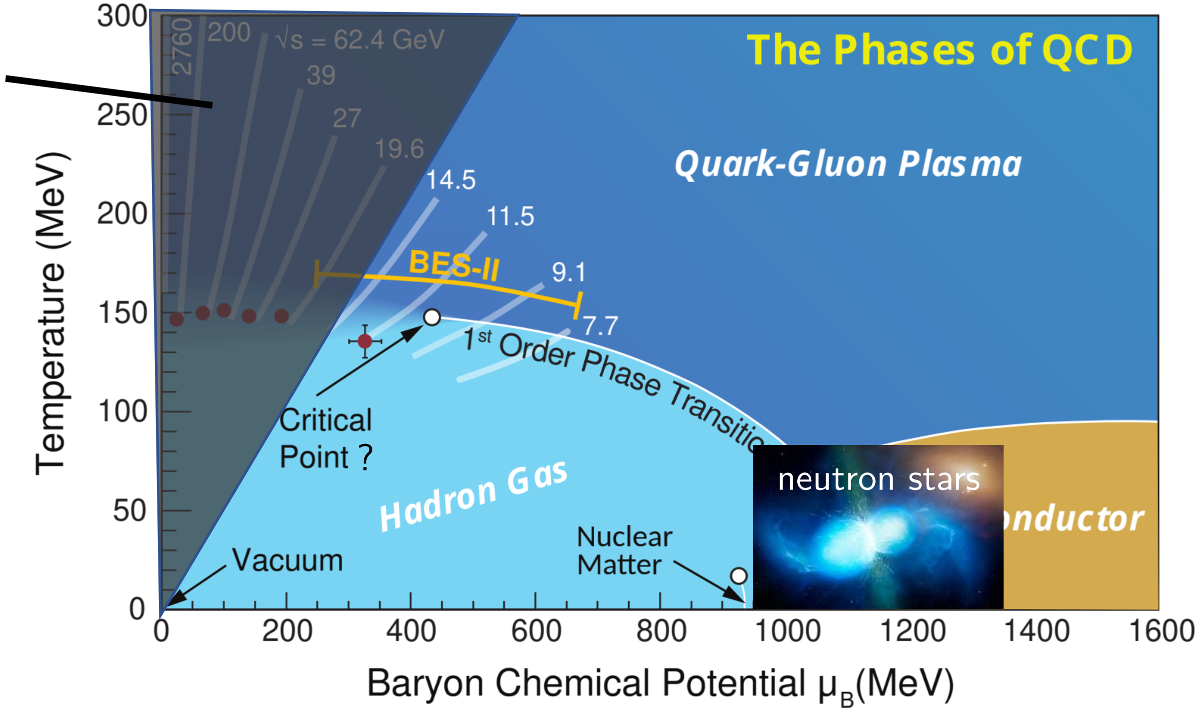
NB: here no collective flow and expansion

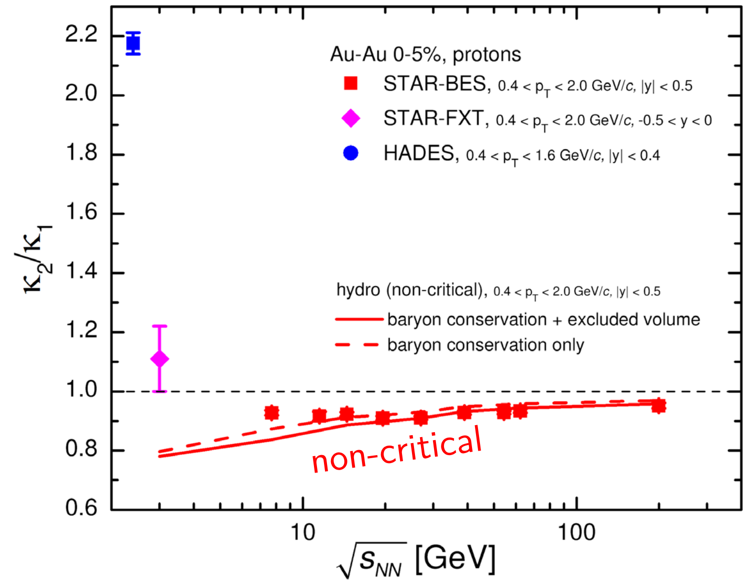
Outlook:

- Collective flow and expansion, clustering
- Ensemble averaging instead of time averaging
- High-order cumulants

Summary: What we learned so far from fluctuations

Critical point disfavored





- Data at high energies ($\sqrt{s_{NN}} \geq 20$ GeV) consistent with "non-critical" physics
- Interesting indications for (multi)-proton correlations at $\sqrt{s_{NN}} \leq 7.7$ GeV
- Critical point: Promising developments in hydrodynamics and molecular dynamics

Thanks for your attention!

Backup slides

Hydrodynamic description

- Collision geometry based 3D initial state [Shen, Alzhrani, PRC '20]
  - Constrained to net proton distributions

- Viscous hydrodynamics evolution – MUSIC-3.0

  - Energy-momentum and baryon number conservation
  - NEOS-BSQ equation of state [Monnai, Schenke, Shen, PRC '19]
  - Shear viscosity via IS-type equation

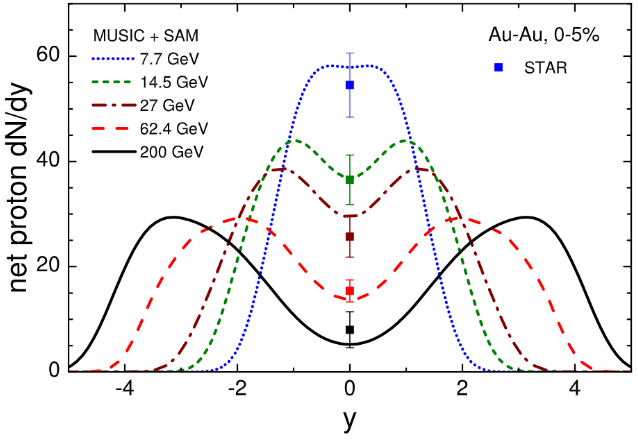
- Cooper-Frye particlization at $\epsilon_{sw} = 0.26$ GeV/fm^3

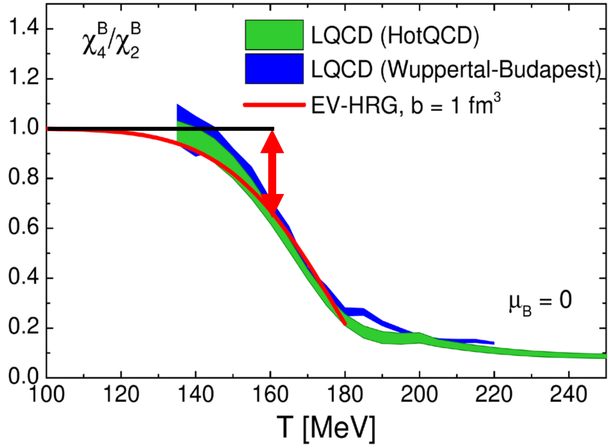
$$\omega_p \frac{dN_j}{d^3p} = \int_{\sigma(x)} d\sigma_\mu(x)\, p^\mu \, \frac{d_j\, \lambda_j^{\rm ev}(x)}{(2\pi)^3} \, \exp\left[\frac{\mu_j(x) - u^\mu(x) p_\mu}{T(x)}\right].$$

- Particlization includes QCD-based baryon number distribution
  - Here incorporated via baryon excluded volume

[VV, Pasztor, Fodor, Katz, Stoecker, PLB 775, 71 (2017)]

VV, C. Shen, V. Koch, in preparation





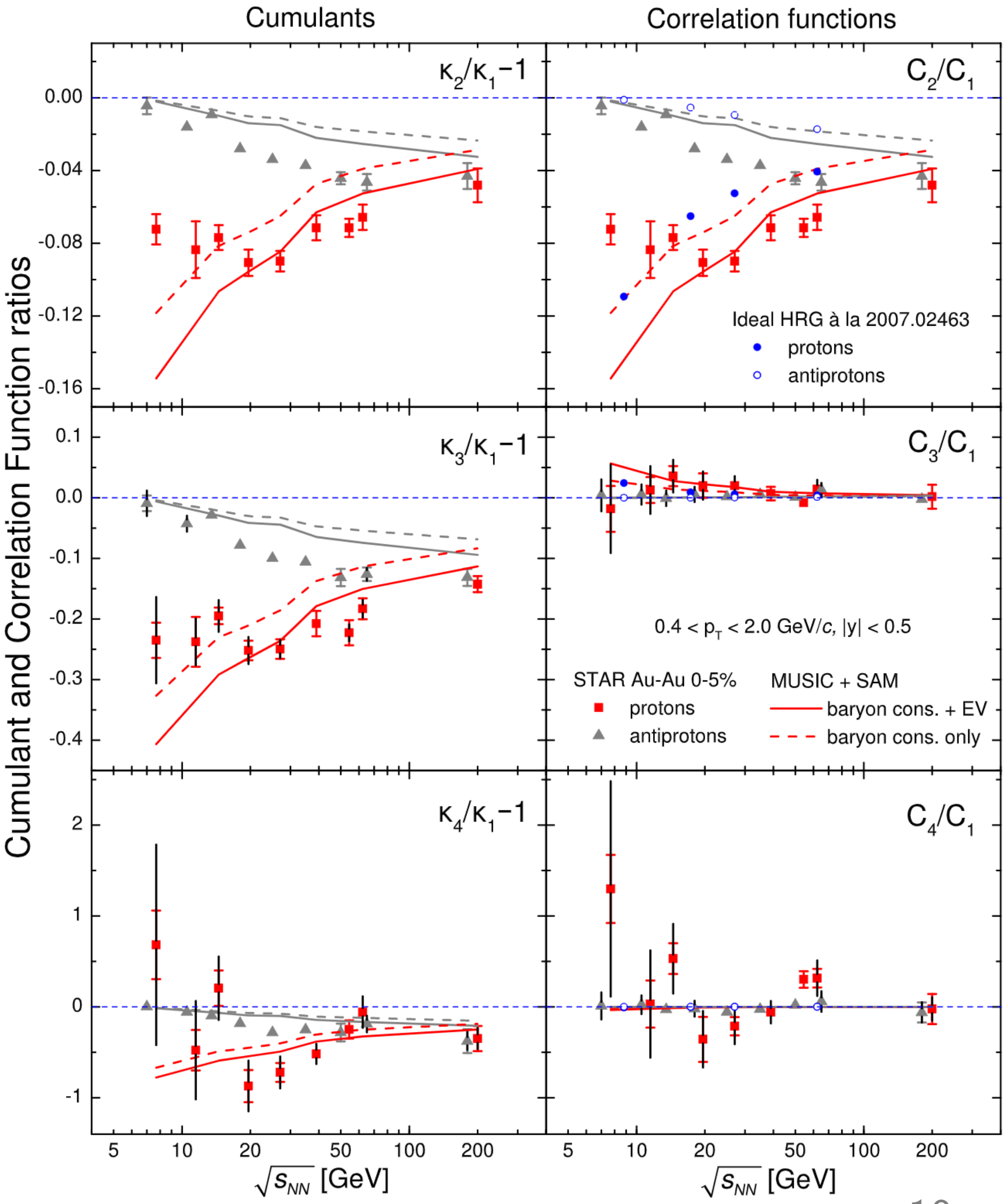
Cumulants vs Correlation Functions

- Analyze genuine multi-particle correlations via **factorial cumulants** [Bzdak, Koch, Strodthoff, PRC '17]

$$\hat{C}_1 = \kappa_1, \qquad \hat{C}_3 = 2\kappa_1 - 3\kappa_2 + \kappa_3,$$
$$\hat{C}_2 = -\kappa_1 + \kappa_2, \qquad \hat{C}_4 = -6\kappa_1 + 11\kappa_2 - 6\kappa_3 + \kappa_4.$$

- Three- and four-particle correlations are small
  - Higher-order cumulants are driven by two-particle correlations
  - Small positive $\hat{C}_3/\hat{C}_1$ in the data is explained by baryon conservation + excluded volume
  - Strong multi-particle correlations would be expected near the critical point [Ling, Stephanov, 1512.09125]

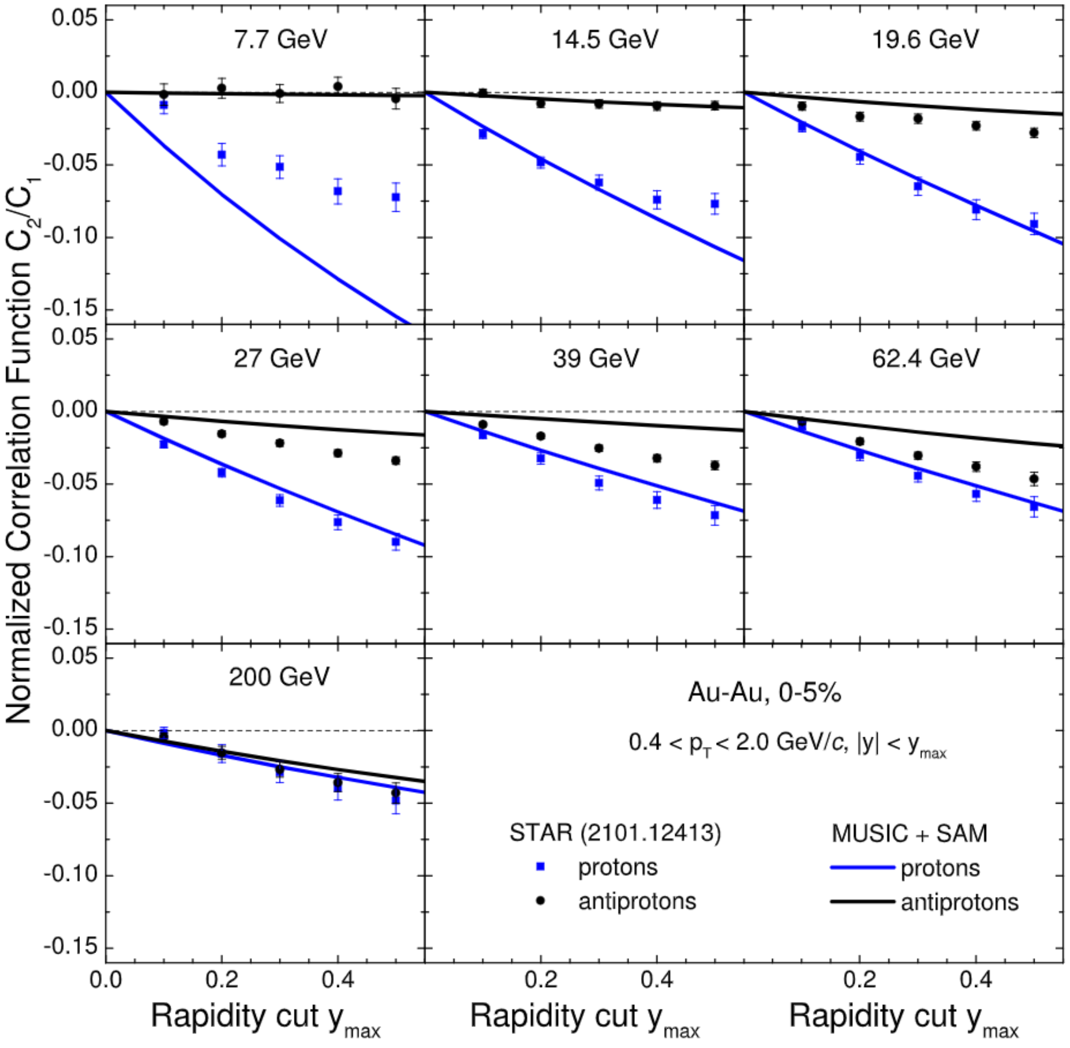
- Two-particle correlations are negative
  - Protons at $\sqrt{s_{NN}} \leq 14.5$ GeV overestimated
  - Antiprotons at $19.6 \leq \sqrt{s_{NN}} \leq 62.4$ GeV underestimated



*We use the notation for (factorial) cumulants from Bzdak et al., Phys. Rept. '20. This is different from STAR's 2101.12413 where it is reversed

Acceptance dependence of two-particle correlations

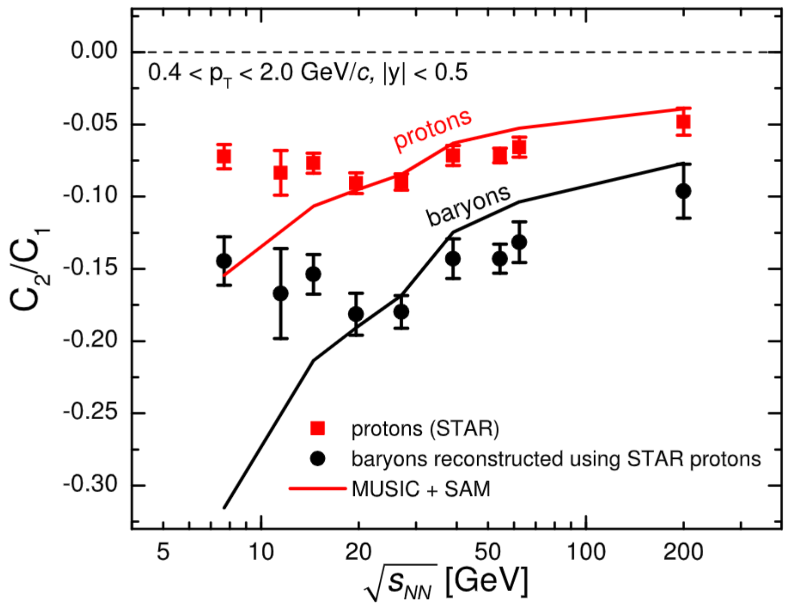
- Qualitative agreement with the STAR data
- Data indicate a changing y_{max} slope at $\sqrt{s_{NN}} \leq 14.5$ GeV
- Volume fluctuations? [Skokov, Friman, Redlich, PRC '13]
  - Can improve low energies but spoil high energies?
- Exact electric charge conservation?
  - Worsens the agreement at $\sqrt{s_{NN}} \leq 14.5$, higher energies virtually unaffected (see backup)
- Attractive interactions?
  - Could work if baryon repulsion switches to attraction in the high-μ_B regime



Net baryon vs net proton

- **net baryon** $\neq$ **net proton**

- Baryon cumulants can be reconstructed from proton cumulants via binomial (un)folding based on isospin randomization [Kitazawa, Asakawa, Phys. Rev. C 85 (2012) 021901]
  - Requires the use of joint factorial moments, only experiment can do it model-independently



$$\frac{\hat{C}_2^B}{\hat{C}_1^B} \approx 2\,\frac{\hat{C}_2^p}{\hat{C}_1^p}$$