High-order cumulants near the critical point from molecular dynamics

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8 Apr 2025

QCD matter

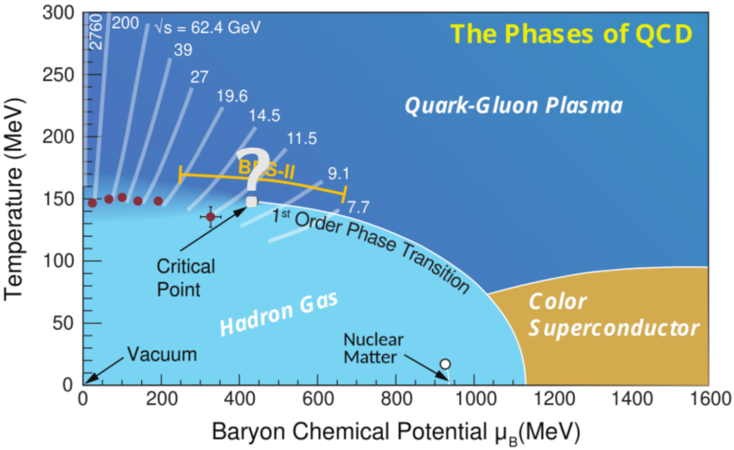


Figure from Bzdak et al., Phys. Rept. 2020 & 2015 Long Range plan

Fluctuations as CP signature

V. A. Kuznietsov et al., Phys. Rev. C 105, 044903 (2022)

In GCE density cumulants shows singularity behavior in the critical point.

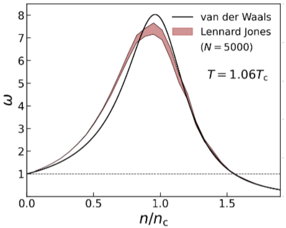
$$\ln Z^{\text{gce}}(T,V,\mu) = \ln\left[\sum_N e^{\mu N} Z^{\text{ce}}(T,V,N)\right],$$

$$\kappa_n \cong \frac{\partial^n(\ln Z^{\text{gce}})}{\partial(\mu_N)^n}.$$

The real expression for Z^{gce} is unknown in QCD matter.

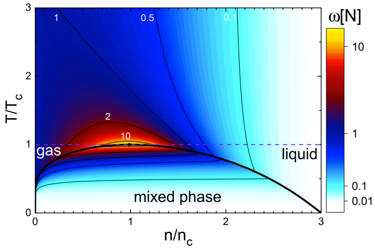
V. Vovchenko, D. V. Anchishkin, M. I. Gorenstein and R. V. Poberezhnyuk, Phys. Rev. C92 054901 (2015)

Scaled variance



$$\omega = \kappa_2/\kappa_1$$

$$\kappa_2 \sim \xi^2$$

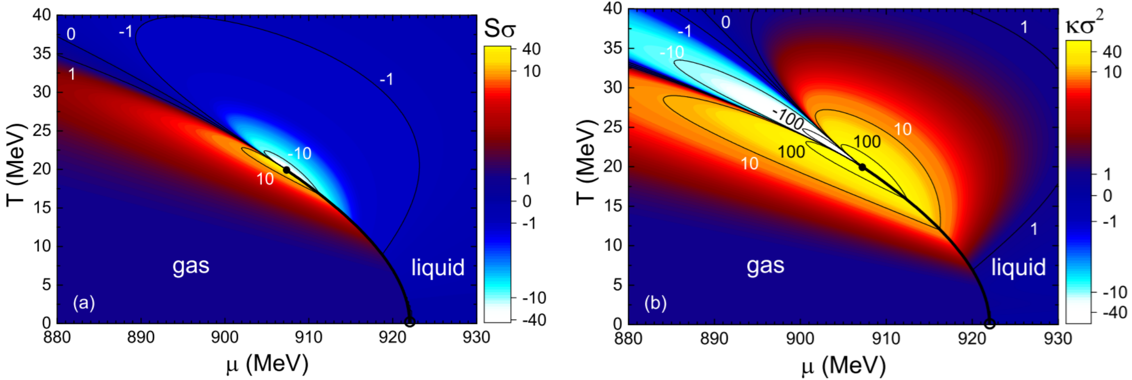


Fluctuations as CP signature

M.A. Stephanov, PRL, 102 (2009), 032301

$\kappa_3 \sim \xi^{9/2}$ $\kappa_4 \sim \xi^7$

Skewness $S\sigma = \kappa_3/\kappa_2$ **Kurtosis** $\kappa\sigma^2 = \kappa_4/\kappa_2$



V. Vovchenko et al, PRC 92 (2015) 5, 054901

Connection to the experiment

Theory	Experiment
Coordinate and/or momentum space	Momentum space
In contact with the heat bath	Expanding in vacuum
Conserved charges	Non-conserved charges
Uniform	Inhomogeneous
Fixed volume	Fluctuating volume
No CP at the transport models	3D Izing CP possibility

Need microscopic description of fluctuations

Lennard-Jones potential

The Lennard-Jones potential reads

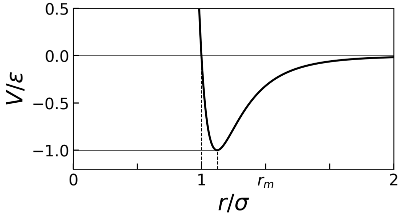
$$V_{\mathrm{LJ}} = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^6 - \left(\frac{\sigma}{r} \right)^{12} \right],$$

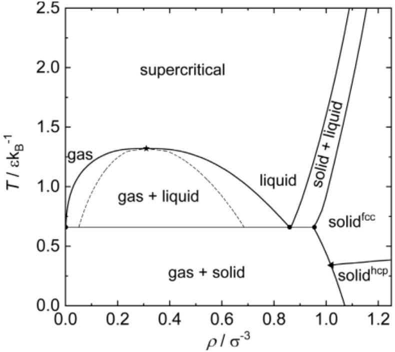
In reduced dimensionless variables it can be rewritten as

$$\tilde{V}_{\mathrm{LJ}} = 4[\tilde{r}^{-12} - \tilde{r}^{-6}],$$

where the reduced variables are used: $\tilde{r} = r/\sigma$ and $\tilde{V}_{\mathrm{LJ}} = V_{\mathrm{LJ}}/\varepsilon$.

The LJ fluid contains a critical point in the 3D Ising universality class.



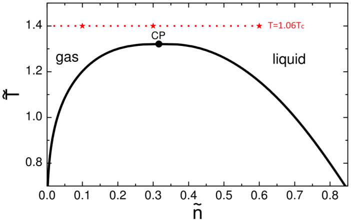


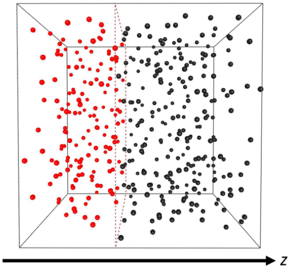
Simulation setup

$$m\frac{d^2\tilde{\mathbf{r}}_{\mathrm{ij}}}{d\tilde{t}^2} = -\vec{\nabla}\tilde{V}_{\mathrm{LJ}}(\tilde{\mathbf{r}}_{\mathrm{ij}})$$

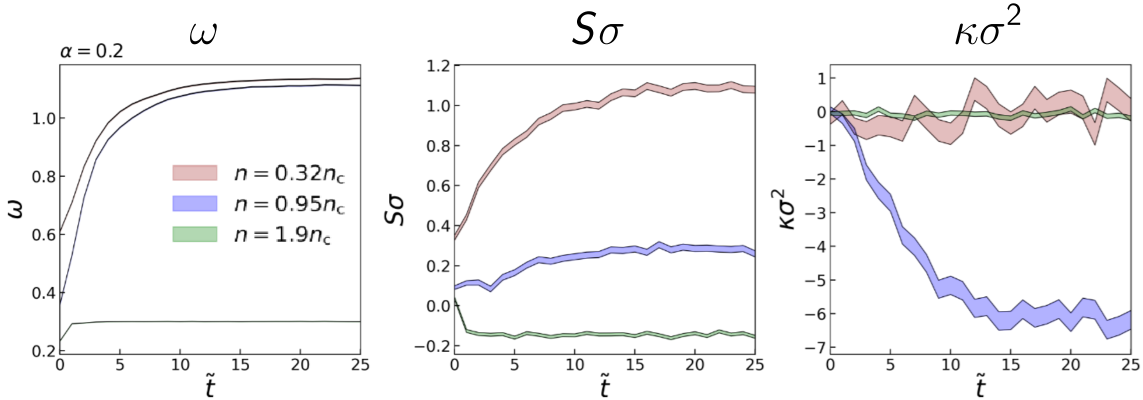
- Three points on the phase diagram, $\tilde{n} = 0.1 \approx 0.3n_c$, $\tilde{n} = 0.3 \approx 0.95n_c$, $\tilde{n} = 0.6 \approx 2n_c$, all for $T = 1.06T_c$
- $N_{\mathrm{ev}} \simeq 2$ million events at each density.
- Initialize each event with random initial coordinates and momenta
- Run each event for long time ($\tilde{t} = 50$), write snapshots to file at regular time intervals
- Calculate observables as event-by-event (ensemble) average

The simulations are performed on UH PhysGPU cluster.
Code is available at: **https://github.com/vlvovch/lennard-jones-cuda**





Cumulants equilibration

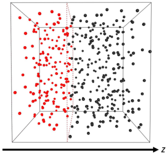


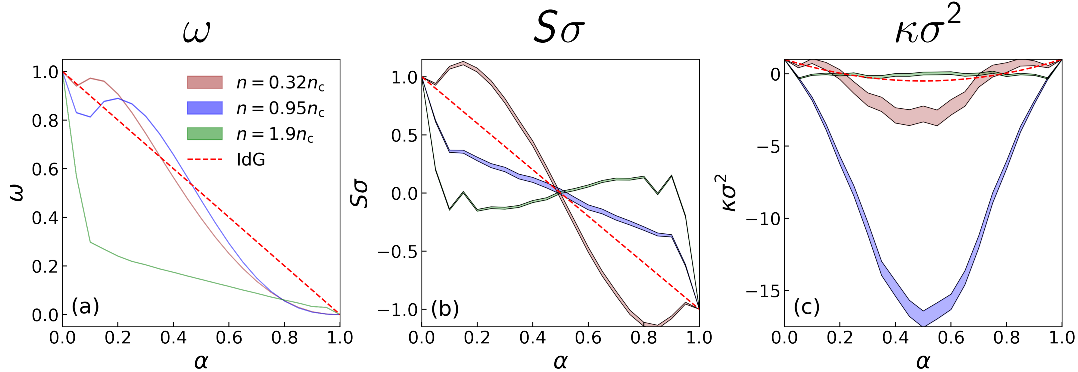
All three cumulant ratios equilibrate at comparable time scales

Acceptance dependence of cumulants

Large CP signal in the coordinate space for all cumulants.

$\alpha \sim$



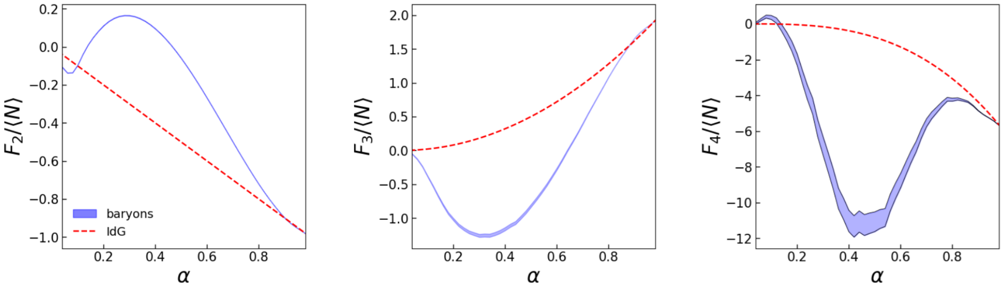


Factorial cumulants

One can express the factorial cumulants in terms of the mean density $\langle N \rangle = \kappa_1$ and standard cumulants κ_i

A. Bzdak, V. Koch, and N. Strodthoff, Phys. Rev. C 95, 054906 (2017)

$$F_2 = \kappa_2 - \langle N \rangle, \quad F_3 = \kappa_3 - 3\kappa_2 + 2\langle N \rangle,$$
$$F_4 = -6\langle N \rangle + 11\kappa_2 - 6\kappa_3 + \kappa_4.$$



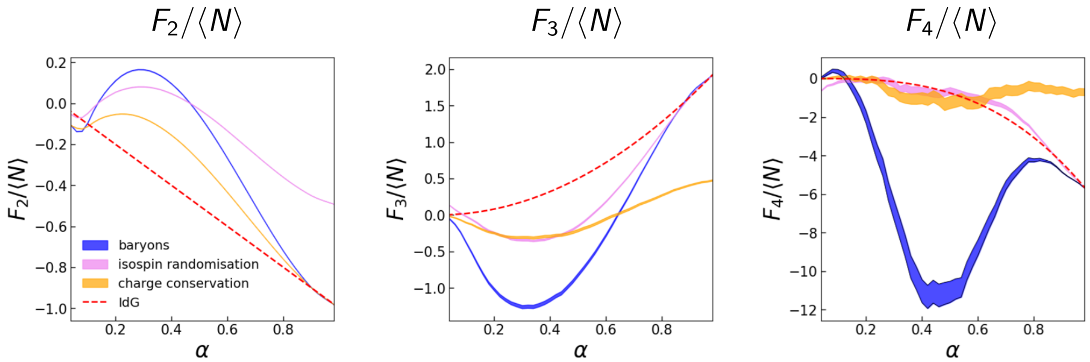
Protons

Experiments measure protons, rather than not all baryons. There are two ways to incorporate protons:

1. **Isospin randomisation:** Each time, randomly label a baryon as a proton with a probability of 50%. This implies isospin randomization expected to be valid for large collision energies (≥ 10 GeV). In this case, factorial cumulants scale as $F_k^{\text{baryon}} = 2^k F_k^{\text{proton}}$ for a symmetric system.
2. **Charge conservation (conserved proton number):** Neglect the production of pions: charge conservation implies conservation of proton number. Treat the first $N/2$ particles as protons. Expected to be appropriate for smaller energies (< 10 GeV).

M. Kitazawa and M. Asakawa, Phys. Rev. C 86, 024904 (2012)
M. Barej and A. Bzdak, Phys. Rev. C 102, 064908 (2020)

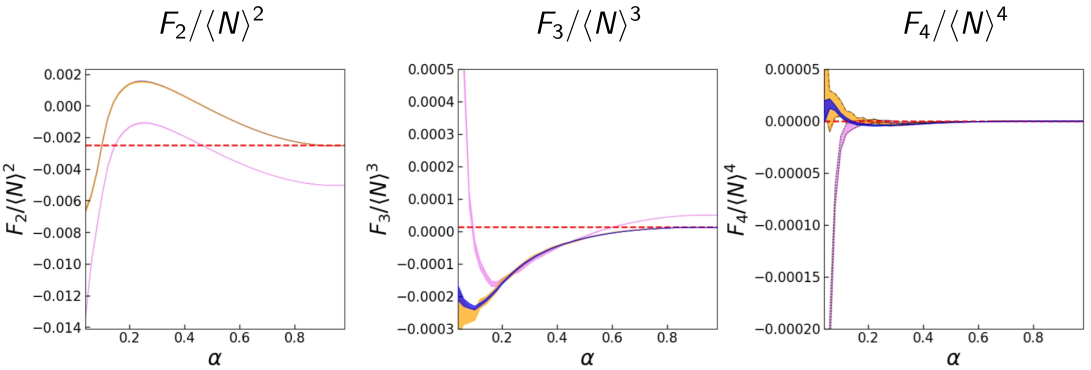
Factorial cumulants ($n = 0.95 n_c$)



Taking protons instead of baryons significantly reduces the signal, and no significant deviation from the ideal gas baseline seen for F_4 $\Longrightarrow$ may be relevant for RHIC-BES-II observations?

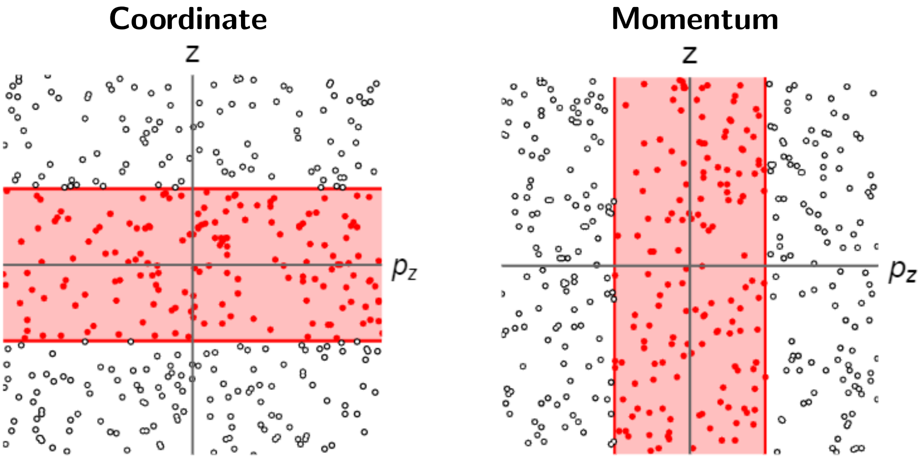
Normalised factorial cumulants ($n = 0.95n_c$)

Acceptance dependence of normalized FC suggested in **A. Bzdak et al., arXiv:2503.16405**



Normalized factorial cumulants show non-flat acceptance dependence, indicating short-range correlations, the signal is diluted in the case of protons

Momentum vs coordinate cuts



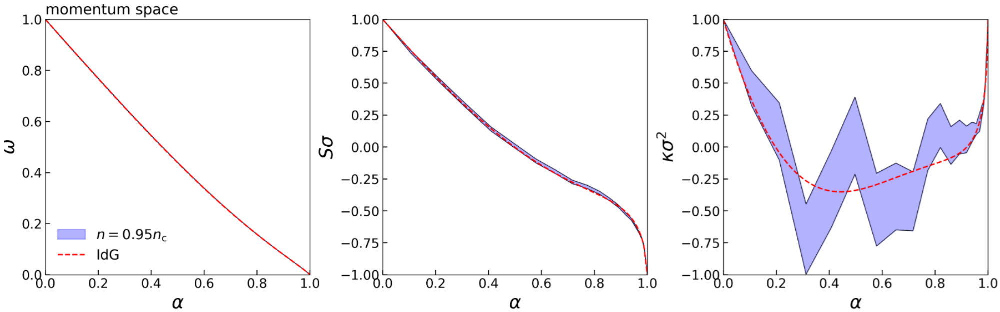
Fluctuations in the momentum space

Red dashed line corresponds to the large N limit formulas for the Ideal gas result with the energy conservation. For scaled variance such formula could be written in a compact form

V. A. Kuznietsov et al., PRC 105, 044903 (2022)

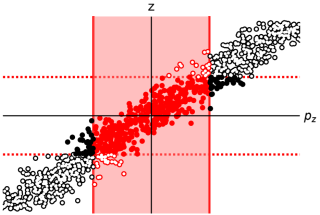
$$\omega^{\mathrm{mom}}_{\mathrm{IdG}} = 1 - \alpha - \frac{2e^{-2\mathrm{erf}^{-1}(\alpha)^2}\mathrm{erf}^{-1}(\alpha)^2}{3\pi\alpha}.$$

Similar results were found for skewness and kurtosis could, but the analytical form becomes more complicated.



Collective flow

We now add collective flow to the longitudinal velocity (rapidity) as follows



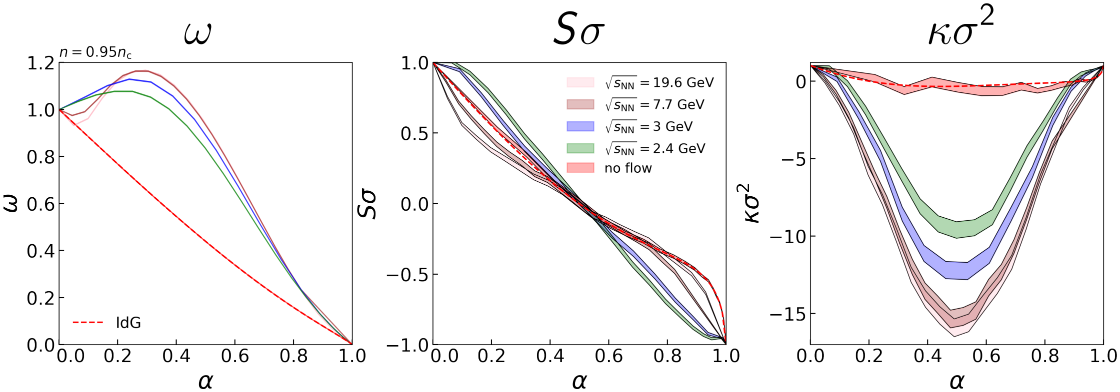
$$\tilde{v}_z = \tilde{v}_z^{\mathrm{LJ}} + \kappa\left(\frac{\tilde{z}}{\tilde{L}} - \frac{1}{2}\right)$$

thermal part collective flow part

$$y(\tilde{z}) = y_{\mathrm{th}} + \sqrt{\frac{T_{\mathrm{frz}}}{m\tilde{T}}}\kappa\left(\frac{\tilde{z}}{\tilde{L}} - \frac{1}{2}\right).$$

We map κ to the collision energies, using the heavy-ion inspired parameters: $T_{\mathrm{frz}} = 150$ MeV, $m = 938$ MeV.

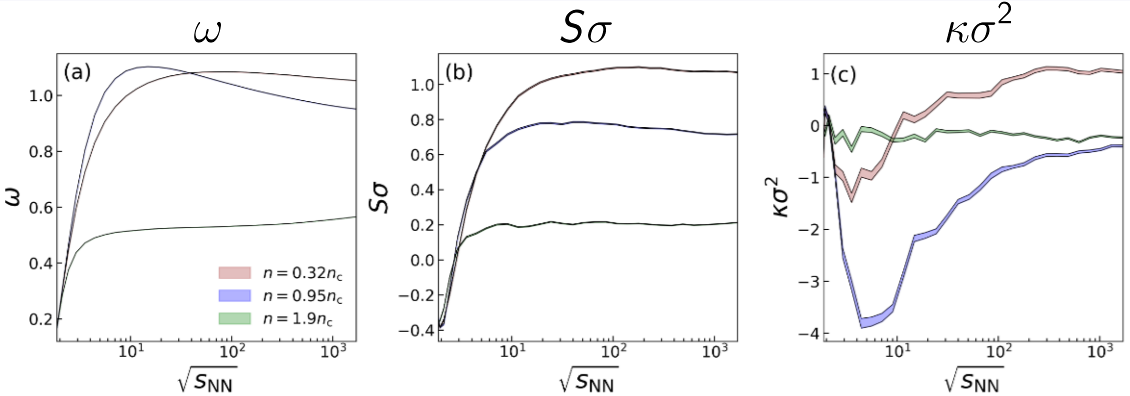
Flow at fixed acceptance



With correlation cumulants in the momentum space becomes notably non-Gaussian.[1]

[1]NB: This is not a prediction of $\sqrt{s_{\rm NN}}$ dependence but an estimation of the signal for a freeze-out at critical density.

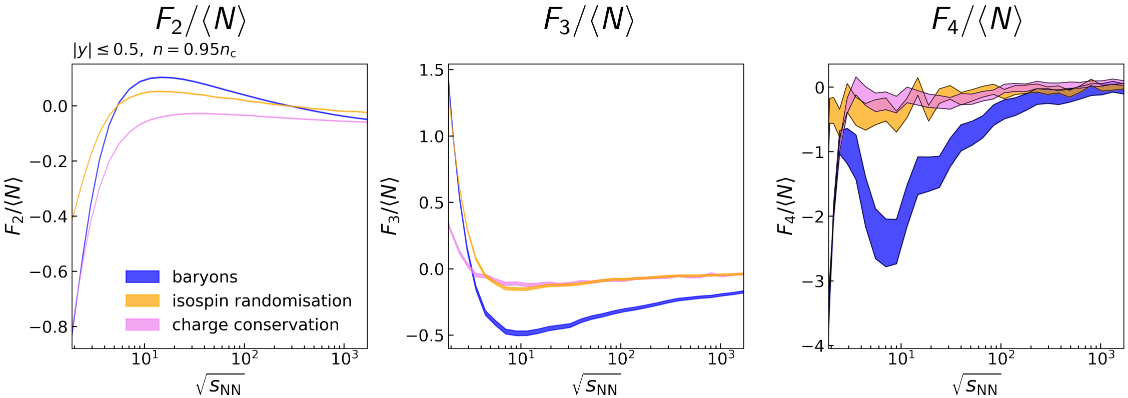
Cumulants at fixed $|y| < 0.5$ acceptance



The interplay between the increasing flow and the decreasing of subsystem fraction α gives a non-trivial dependence on $\sqrt{s_{\mathrm{NN}}}$.[2]

[2]NB: Once again, this is not a prediction of actual $\sqrt{s_{\mathrm{NN}}}$ dependence but an estimation of the signal for a freeze-out at critical density occurring at a given $\sqrt{s_{\mathrm{NN}}}$.

Factorial cumulants at fixed $|y| < 0.5$ acceptance ($n = 0.95 n_c$)



Proton factorial cumulants do not show as strong signal as observed for baryons.[3]

[3] NB: Once again, this is not a prediction of actual $\sqrt{s_{\mathrm{NN}}}$ dependence but an estimation of the signal for a freeze-out at critical density occurring at a given $\sqrt{s_{\mathrm{NN}}}$.

Summary

1. High-statistics (2 million events) simulations of the Lennard-Jones fluid have been performed to compute skewness and kurtosis of particle number for the **first time in a microscopic MD framework**.
2. Scaled variance, skewness, and kurtosis, have same equilibration rates and **show large deviations from Poisson baseline near the CP in coordinate space.** Same is true for the factorial cumulants.
3. Momentum-space fluctuations coincide with the analytical expectations for the Ideal gas with the energy conservation $\rightarrow$ *no effects of the CP in momentum space even for the higher cumulants in the system without collective flow.*
4. Implementing the Bjorken-like flow in the system recovers the CP signal in the momentum space. The results confirm the sensitivity of non-Gaussian fluctuations to criticality.

- **Future plans:** Implementation of multiple components (protons, neutrons, ...) and more realistic expansion dynamics, comparison with experimental data.

THANK YOU FOR ATTENTION!

Questions?

Cumulants definition

Scaled variance

$$\omega = \frac{\kappa_2}{\kappa_1} = \frac{\langle N^2\rangle - \langle N\rangle^2}{\langle N\rangle}.$$

Skewness

$$S\sigma = \frac{\kappa_3}{\kappa_2} = \frac{\langle N^3\rangle - 3\langle N^2\rangle\langle N\rangle + 2\langle N\rangle^3}{\langle N^2\rangle - \langle N\rangle^2}.$$

(Excess) kurtosis

$$\kappa\sigma^2 = \frac{\kappa_4}{\kappa_2} = \frac{\langle N^4\rangle - 4\langle N^3\rangle\langle N\rangle + 6\langle N^2\rangle\langle N\rangle^2 - 3\langle N\rangle^4}{\langle N^2\rangle - \langle N\rangle^2} - 3(\langle N^2\rangle - \langle N\rangle^2).$$

Subensemble method – correction for global conservation

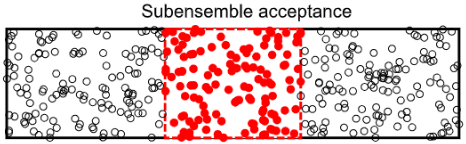
Cumulants, corrected for the baryon conservation reads (**V Vovchenko O. Savchuk, R. Poberezhnyuk, M. Gorenstein, V. Koch, Phys. Let. B, 2020**)

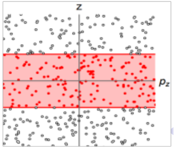
$$\tilde{\omega} \equiv \omega/(1-\alpha),$$

$$\tilde{s\sigma} \equiv s\sigma/(1-2\alpha),$$

$$\tilde{\kappa\sigma}^2 \equiv \frac{1}{(1-3\alpha(1-\alpha))}\kappa\sigma^2 - \frac{3\alpha(1-\alpha)}{1-3\alpha(1-\alpha)}(\tilde{s\sigma})^2,$$

where $\alpha = \langle N \rangle / N$ - subensemble fraction.
Unfortunately, higher corrected cumulants have pole at $\alpha = 0.5$, which leads to the artificial infinities because we compute the moments values with finite precision.





Collective flow

We can identify the boundary rapidity $y(\tilde{z} = \tilde{L}/2)$ with the center-of-mass rapidity

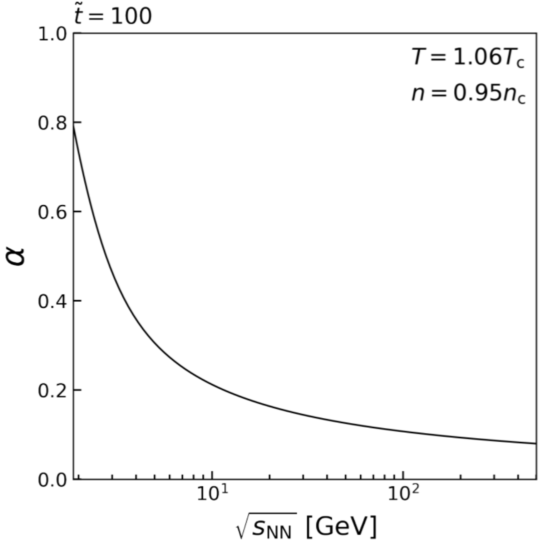
$$y_{\rm cm} = y_{\rm beam}/2 = \ln\left[\frac{\sqrt{s_{\rm NN}} + \sqrt{s_{\rm NN} - 4m_N^2}}{2m_N}\right].$$

$$\langle y(\tilde{z} = \tilde{L}/2)\rangle = \sqrt{\frac{T_{\rm frz}}{m\tilde{T}}}\kappa\frac{1}{2} = y_{\rm cm},$$

therefore

$$\kappa = 2y_{\rm cm}\sqrt{\frac{m\tilde{T}}{T_{\rm frz}}}, \quad \sqrt{s_{\rm NN}} = 2m\ {\rm ch}\left(\frac{\kappa}{2}\sqrt{\frac{T_{\rm fr}}{m\tilde{T}}}\right).$$

α as a function of $\sqrt{s_{\mathrm{NN}}}$ at $y_{\mathrm{cut}} = 0.5$



Flow at fixed $\alpha = 0.2$