Critical point particle number fluctuations from molecular dynamics

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based on V.A. Kuznietsov, O. Savchuk, M.I. Gorenstein (BITP, Kyiv), V. Koch, V.V. (LBNL), arXiv:2201.08486

BEST COLLABORATION

BES-Tea Seminar

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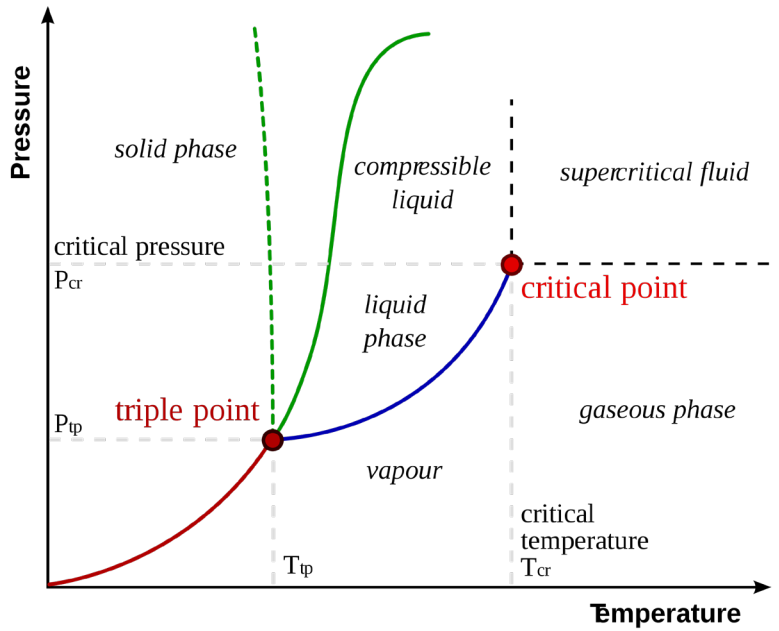
QCD critical point

Ordinary fluid (e.g. water)



QCD

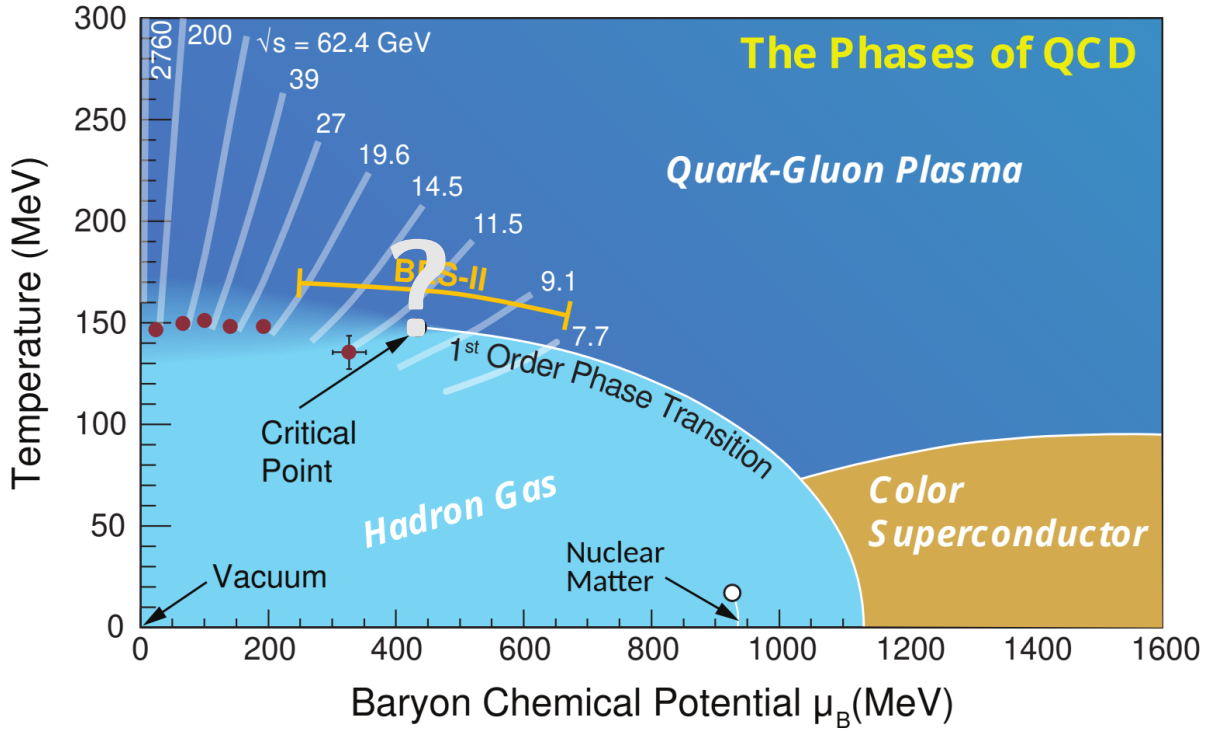


Figure from Bzdak et al., Phys. Rept. '20

What is the nature of the quark-hadron transition at finite baryon density?

*Is there a QCD phase transition and **critical point**? Where?*

Tackle these questions with event-by-event fluctuations in heavy-ion collisions

Event-by-event fluctuations and statistical mechanics

Consider a fluctuating number N

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

variance $\kappa_2 = \langle(\Delta N)^2\rangle = \sigma^2$

width

skewness $\kappa_3 = \langle(\Delta N)^3\rangle$

asymmetry

kurtosis $\kappa_4 = \langle(\Delta N)^4\rangle - 3\langle(\Delta N^2)\rangle^2$

peak shape

Experiment:

$$P(N) \sim \frac{N_{events}(N)}{N_{events}^{total}}$$

Statistical mechanics:

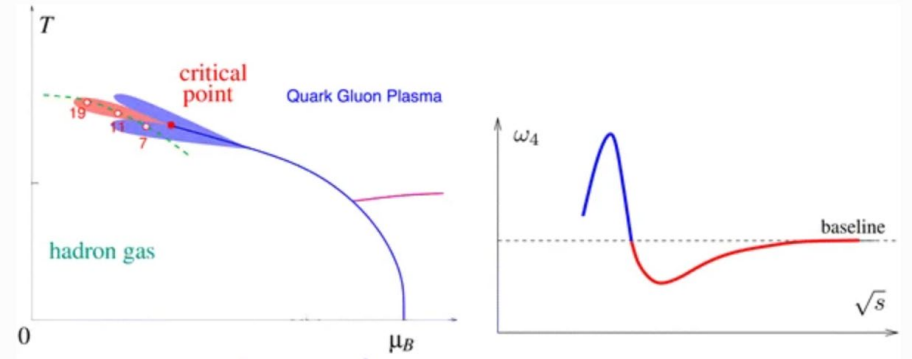
Grand partition function $ln\, Z^{\mathrm{gce}}(T, V, \mu) = ln\left[\sum_N e^{\mu N} Z^{\mathrm{ce}}(T, V, N)\right],$

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

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

Applications

- **(QCD) critical point** – large critical fluctuations of baryon (proton) number



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

Correlation length $\xi \to \infty$ diverges at the critical point

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

Looking for non-monotonic dependence of κ_4 vs $\sqrt{s_{NN}}$

- Test of (lattice) QCD at $\mu_B \approx 0$

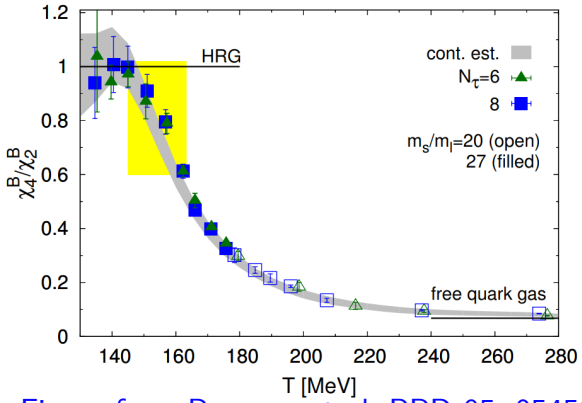
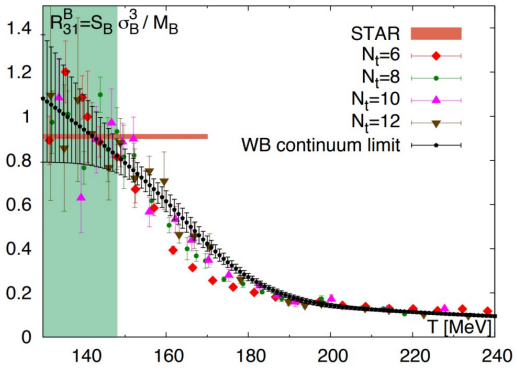
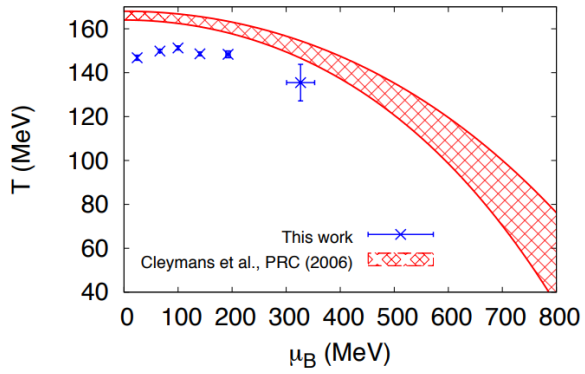


Figure from Bazavov et al. PRD 95, 054504 (2017)
Probed by LHC and top RHIC

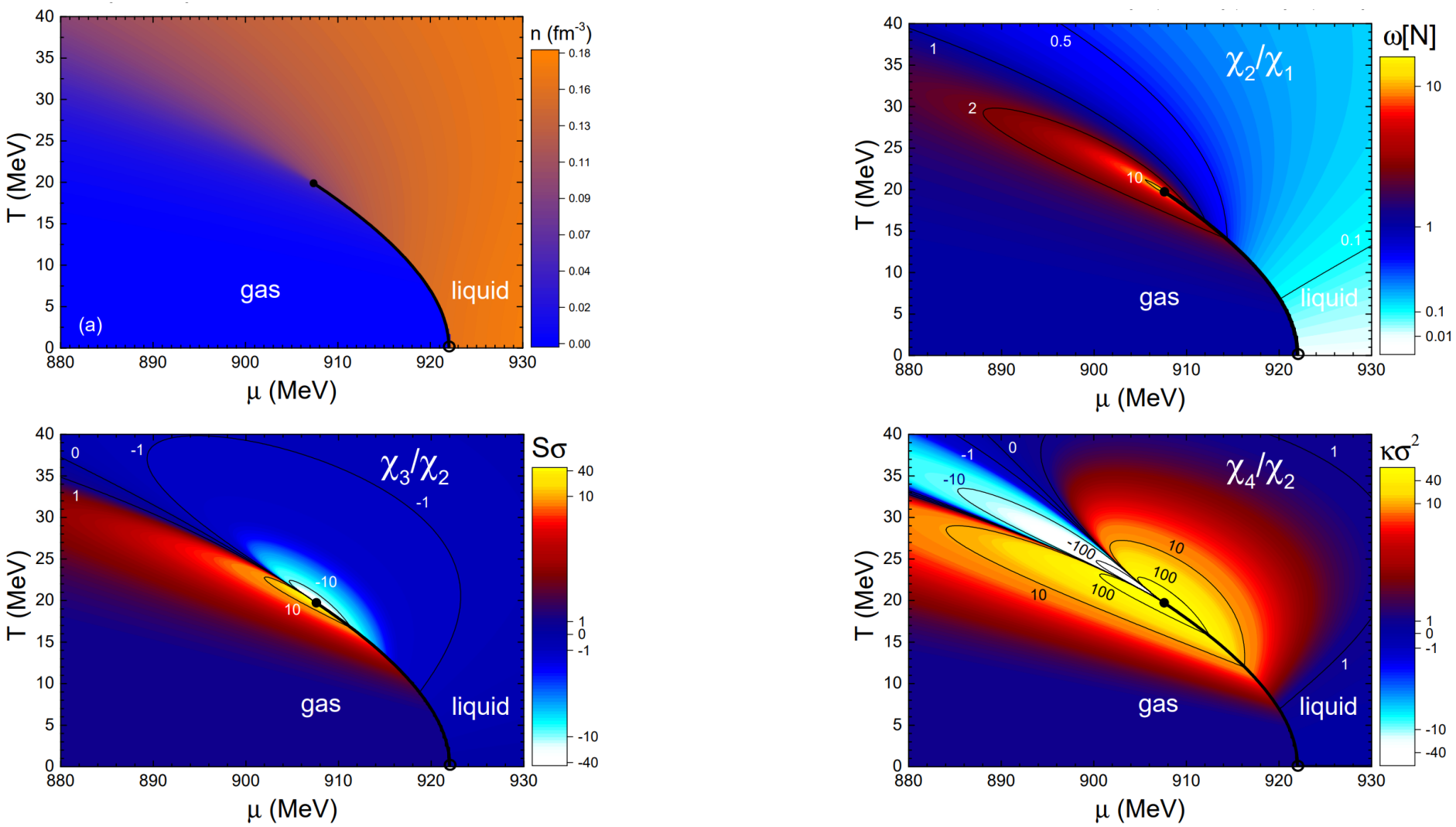
- Freeze-out from fluctuations





Borsanyi et al. PRL 113, 052301 (2014); Bazavov et al. PRL 109, 192302 (2012)

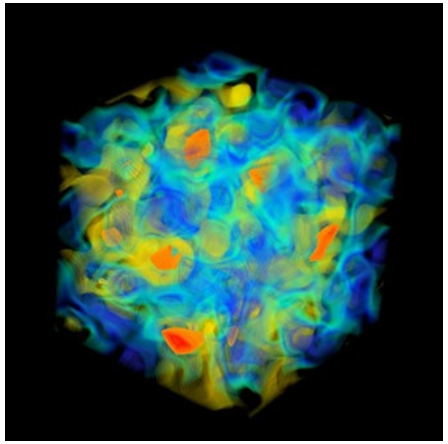
Example: Nuclear liquid-gas transition



VV, Anchishkin, Gorenstein, Poberezhnyuk, Phys. Rev. C 92, 054901 (2015)

Theory vs experiment

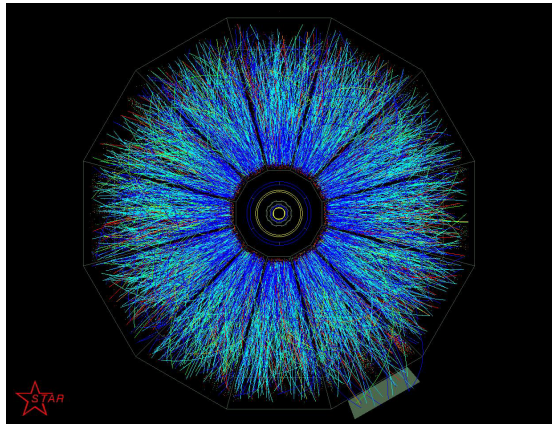
Theory



© Lattice QCD@BNL

- 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

Makes direct application of grand-canonical cumulants questionable

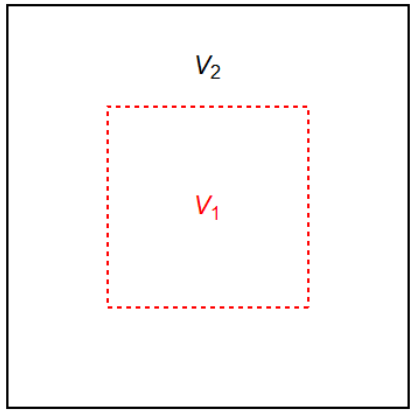
Subensemble acceptance method

VV, Savchuk, Poberezhnyuk, Gorenstein, Koch, Phys. Lett. B 811, 135868 (2020)

Subensemble acceptance method (SAM) – method to correct *any* EoS (e.g. *lattice QCD*) for **charge conservation** and extract the **susceptibilities**

Partition a thermal system with a globally conserved charge B *(canonical ensemble)* into two coordinate subsystems which can exchange the charge

$V_1 + V_2 = V$

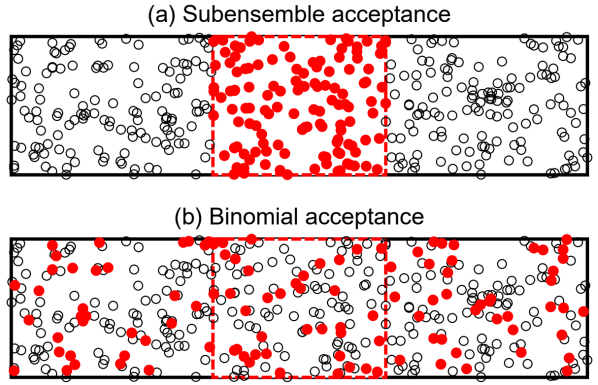


Fluctuations in a subsystem (acceptance):

scaled variance $$\frac{\kappa_2[B_1]}{\kappa_1[B_1]} = (1-\alpha)\,\frac{\chi_2^B}{\chi_1^B}, \qquad \frac{V_1}{V} = \alpha$$

skewness $$\frac{\kappa_3[B_1]}{\kappa_2[B_1]} = (1-2\alpha)\,\frac{\chi_3^B}{\chi_2^B},$$

kurtosis $$\frac{\kappa_4[B_1]}{\kappa_2[B_1]} = (1-3\alpha\beta)\,\frac{\chi_4^B}{\chi_2^B} - 3\alpha\beta\left(\frac{\chi_3^B}{\chi_2^B}\right)^2.$$



Assumptions: thermodynamic limit, coordinate space, $V_1, V_2 \gg \xi^3$, ξ = correlation length

Lennard-Jones fluid

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

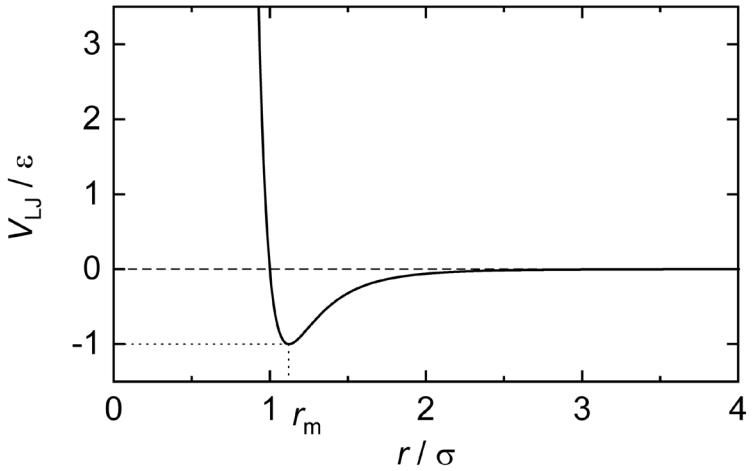
Reduced variables:

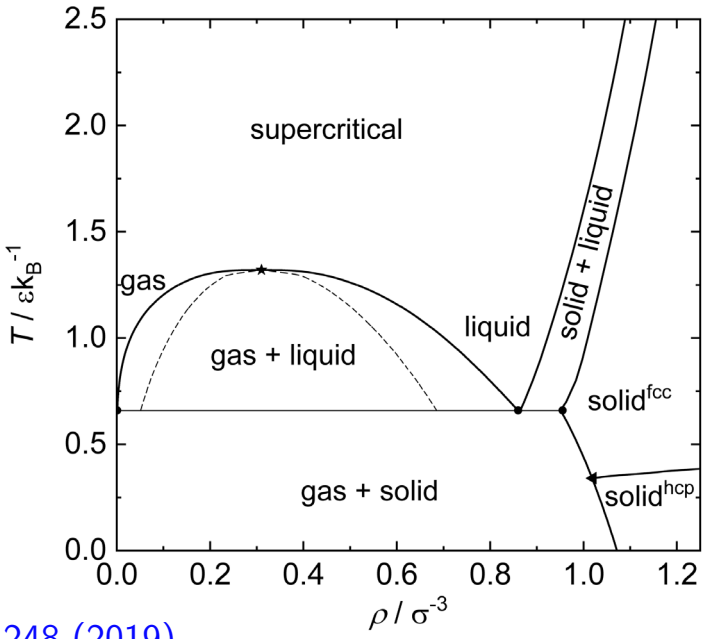
$$\tilde{r} = r/\sigma \qquad \tilde{T} = T/(k_B\varepsilon) \qquad \tilde{n} = n\sigma^3$$

Properties:

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

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





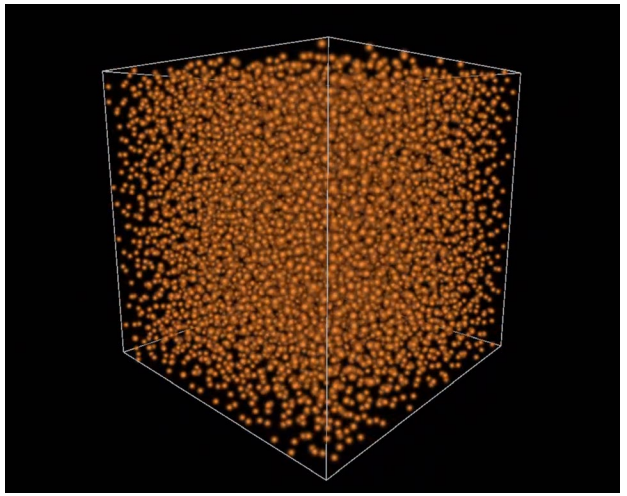
S. Stephan, M. Thol, J. Vrabec, H. Hasse, Journal of Chemical Information and Modeling 59, 4248 (2019)

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
- Ensembles
  - Microcanonical ensemble, const. UVN
  - Canonical-like ensemble, const. TVN
    - O.K. for simple averages, not o.k. for correlations and fluctuations



Implementation:

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

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

NVIDIA CUDA

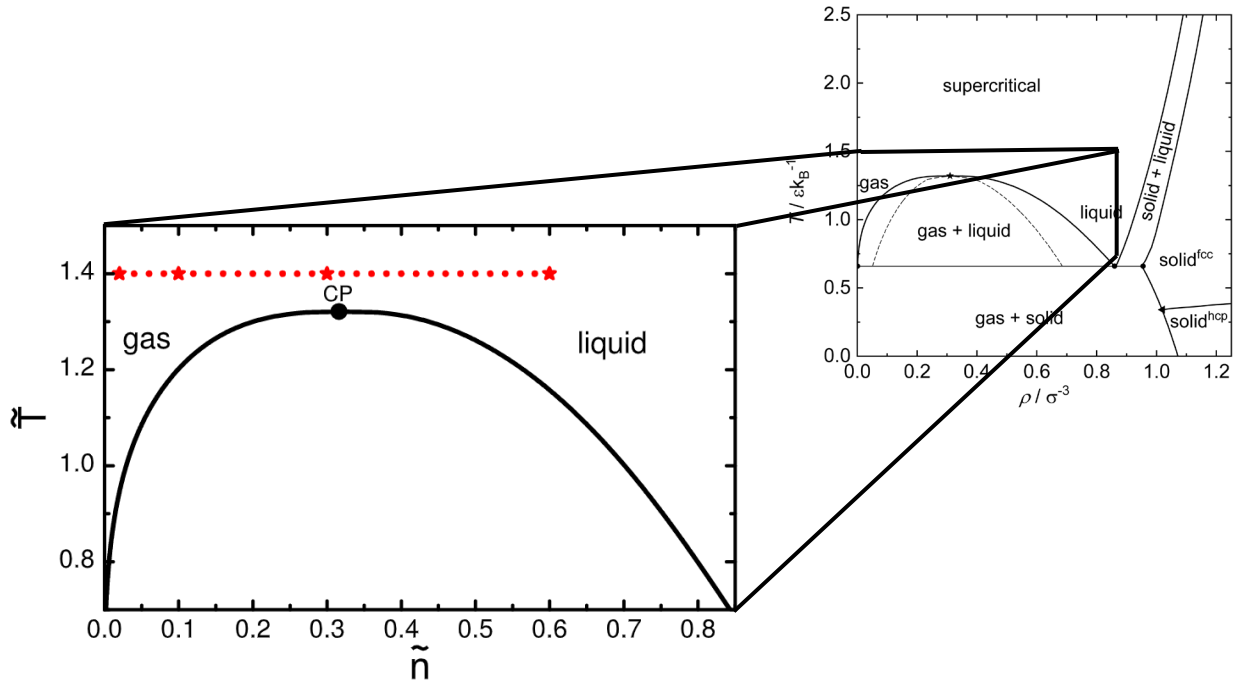
*This research used the Lawrencium computational cluster resource provided by the IT Division at the Lawrence Berkeley National Laboratory

Simulation strategy

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

Observables as time averages:

$$\langle A \rangle = \frac{1}{\tilde{\tau}} \int_{\tilde{t}_{\mathrm{eq}}}^{\tilde{t}_{\mathrm{eq}}+\tilde{\tau}} A(\{\tilde{\mathbf{r}}_i(\tilde{t}), \tilde{\mathbf{v}}_i(\tilde{t})\}) d\tilde{t}$$

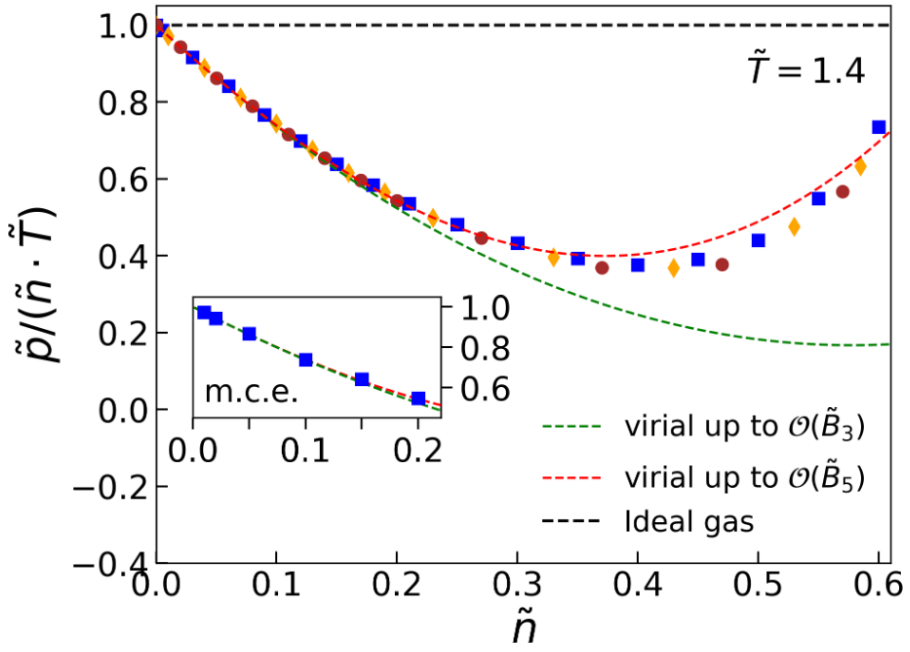


Two steps:

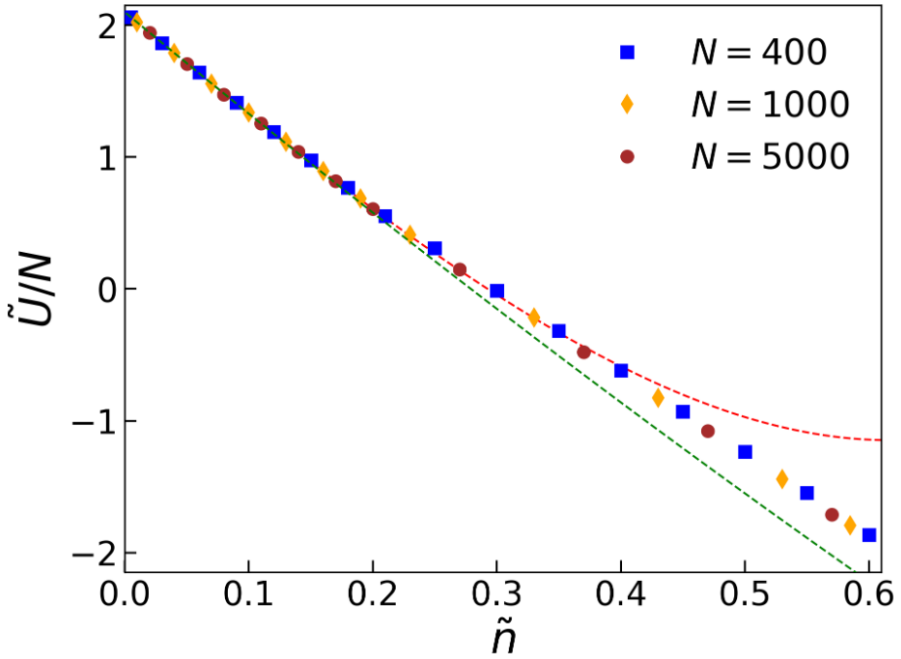
1. Equation of state properties (simple averages) via canonical-like ensemble
   - Establish the map $(\tilde{T}, \tilde{n}) \rightarrow (\tilde{u}, \tilde{n})$
2. Particle number fluctuations in the microcanonical ensemble

Equation of state

Compressibility factor $Z = \frac{\tilde{p}}{\tilde{n}\tilde{T}}$



Energy per particle $\tilde{u} = \frac{\tilde{U}}{N}$



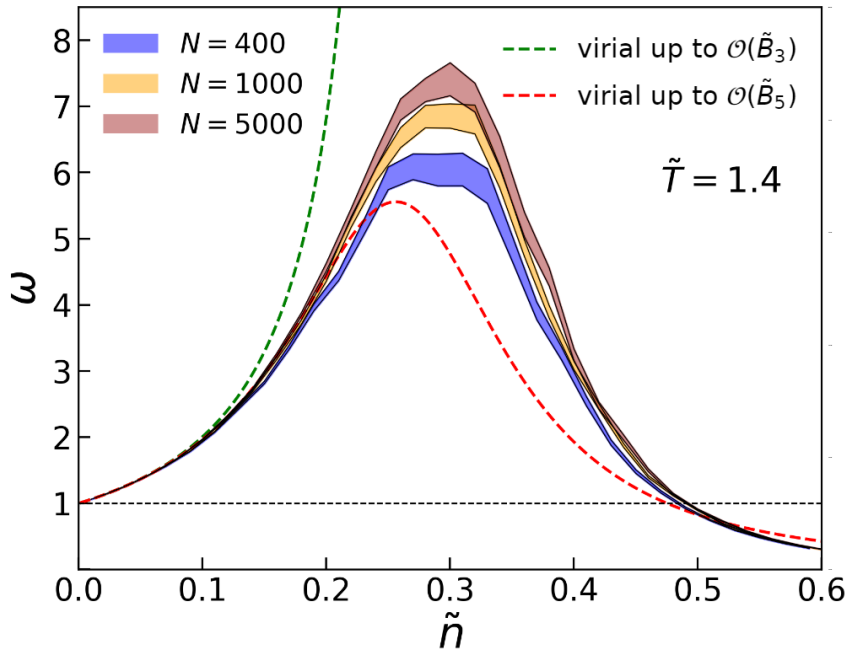
The low-density limit agrees with the virial expansion

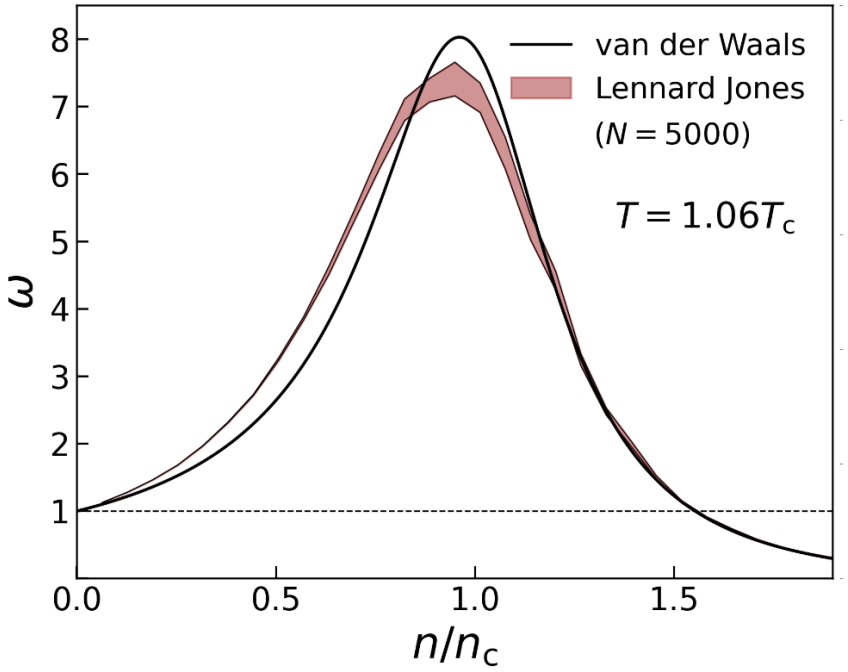
$$Z \equiv \frac{\tilde{p}}{\tilde{n}\,\tilde{T}} = 1 + \sum_{k=2}^{\infty} \tilde{B}_k\,(\tilde{T})\,\tilde{n}^{k-1}.$$

$$\frac{\tilde{U}}{N} = \frac{3}{2}\tilde{T} - \sum_{k=2}^{\infty} \frac{\tilde{T}^2\,\tilde{B}_k'(\tilde{T})}{k-1}\tilde{n}^{k-1}\ .$$

Grand-canonical fluctuations

Scaled variance of particle number in the GCE: $\omega^{\mathrm{gce}} = \dfrac{\Delta N}{\langle N \rangle} = \dfrac{T}{\langle N \rangle} \left(\dfrac{\partial \langle N \rangle}{\partial \mu} \right)_{T,V} = \dfrac{T}{\left(\frac{\partial p}{\partial n} \right)_T}$





In qualitative agreement with the van der Waals model

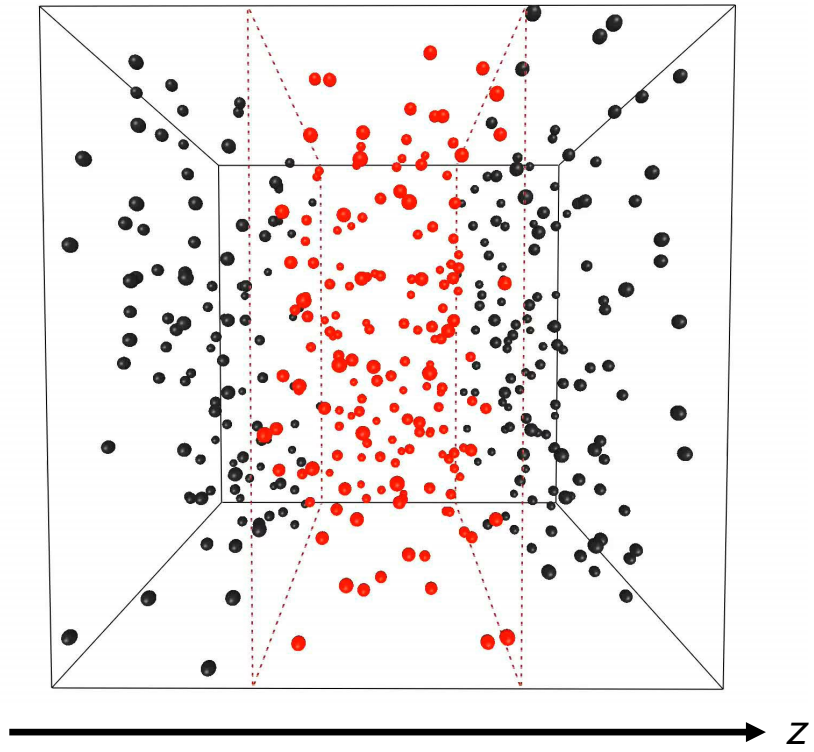
$$\omega_{\mathrm{vdW}}(T^*, n^*) = \frac{1}{9} \left[\frac{1}{(3 - n^*)^2} - \frac{n^*}{4T^*} \right]^{-1}$$

Fluctuations in molecular dynamics

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

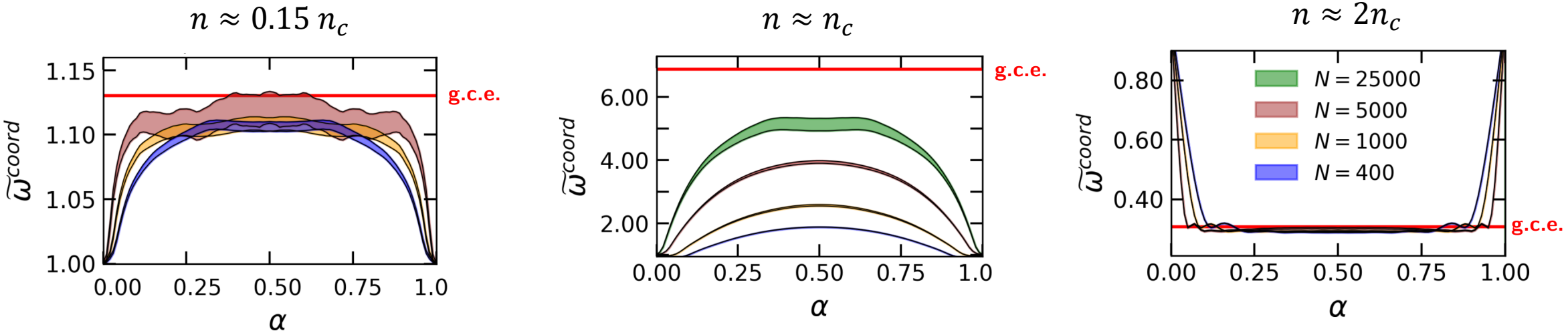
$$\tilde{\omega}^{\text{coord}} = \frac{1}{1-\alpha} \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle}$$

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



Much longer simulations needed to control the statistical error for the variance relative to simple averages

Fluctuations in molecular dynamics: coordinate space



- The results approach the expected thermodynamic limit as N (i.e. volume) increases
- Provides access to the grand-canonical susceptibilities
- Large finite-size effects near the critical point
- Enhancement of fluctuations in coordinate space subvolume is a critical point signature

Fluctuations in molecular dynamics: momentum space

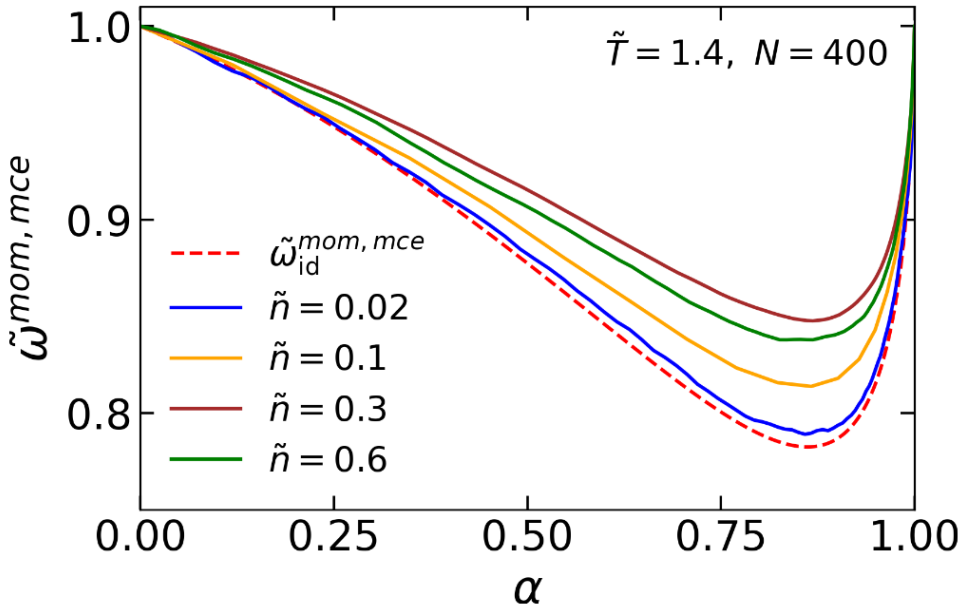
Experiments measure momenta, not coordinates → consider momentum subvolume instead

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

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

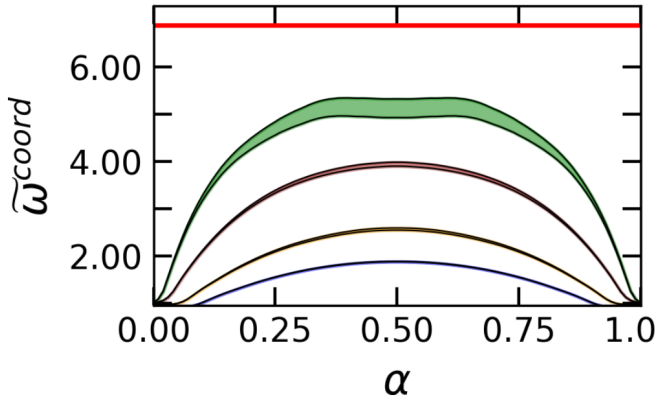
Large fluctuations near the CP are washed out when momentum cuts imposed instead of coordinates

NB: here no collective flow and expansion

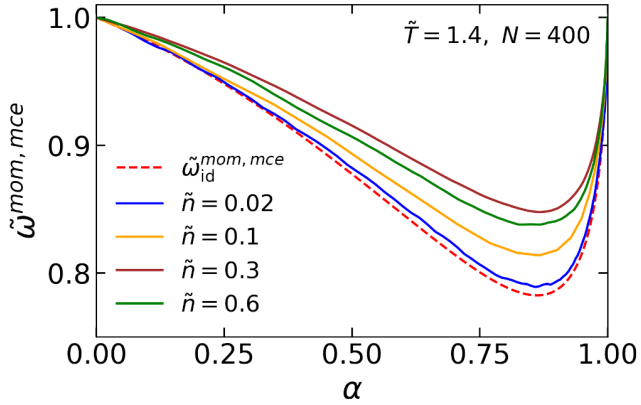


Summary and outlook

- Molecular dynamics of the Lennard-Jones fluid provide a microscopic approach to study system with a critical point



- Variance of particle number fluctuations
  - Is large as advertised near the CP when measured in coordinate space
  - …but the signal is washed out in the momentum space



- Outlook:
  - Collective flow and expansion
  - Ensemble averaging instead of time averaging
  - High-order cumulants

Thanks for your attention!

Backup slides

Virial expansion coefficients

$$Z \equiv \frac{\tilde{p}}{\tilde{n}\tilde{T}} = 1 + \sum_{k=2}^{\infty} \tilde{B}_k\left(\tilde{T}\right) \tilde{n}^{k-1}.$$

2nd virial coefficient known analytically

$$\tilde{B}_2(\tilde{T}) = \frac{\pi^2\sqrt{2}e^{1/2\tilde{T}}}{3\tilde{T}}\left[I_{3/4}\left(\frac{1}{2\tilde{T}}\right) + I_{-3/4}\left(\frac{1}{2\tilde{T}}\right) - I_{1/4}\left(\frac{1}{2\tilde{T}}\right) - I_{-1/4}\left(\frac{1}{2\tilde{T}}\right)\right]$$

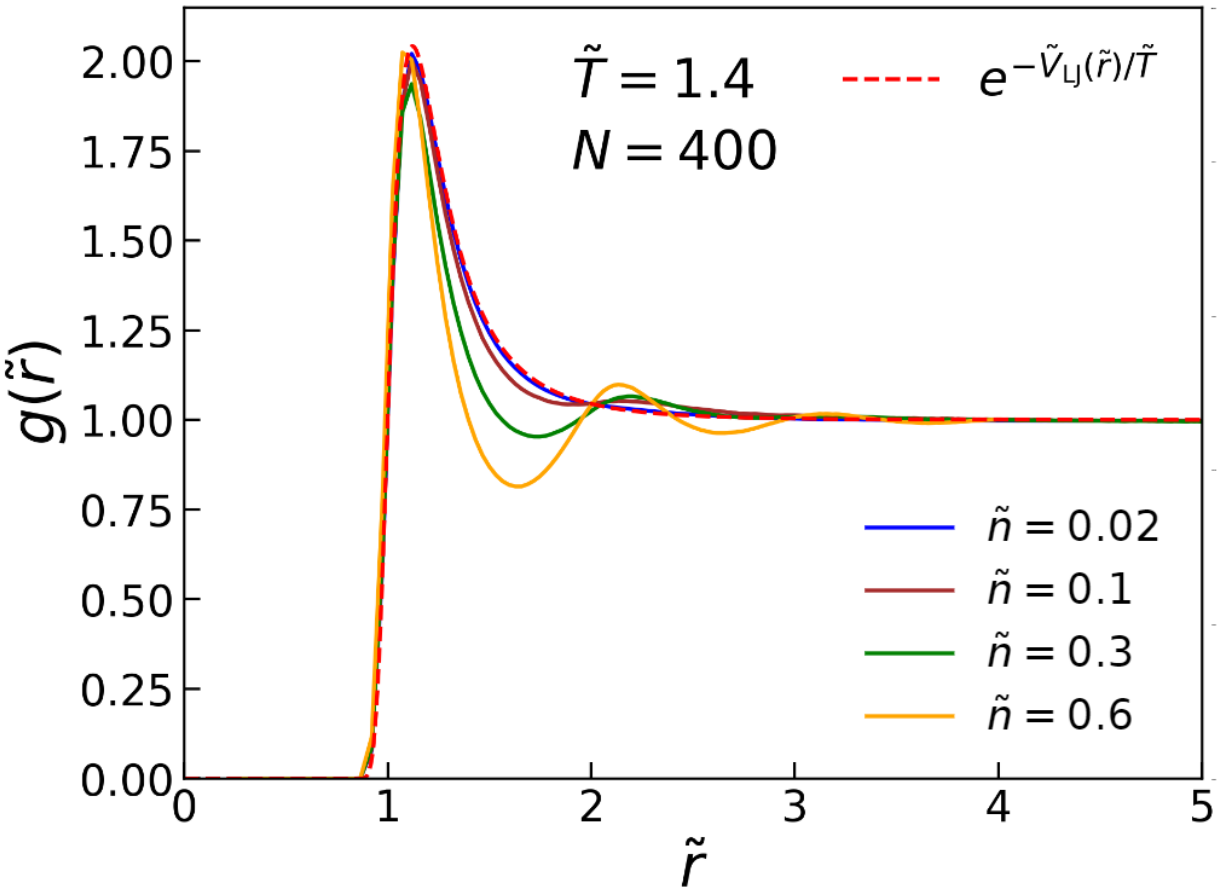
P. Vargas, E. Muoz, L. Rodriguez, Physica A 290, 92 (2001)

Parametrized Monte Carlo data for high-order coefficients up to $\tilde{B}_6(\tilde{T})$

M. Gottschalk, AIP Advances 9, 125206 (2019)

Radial distribution function

The radial distribution function $g(\tilde{r})$ describes how the (time-averaged) density of particles varies around a reference particle at the origin relative to the expectation based on the mean particle number density



Lennard-Jones vs van der Waals

$$\omega_{\mathrm{vdW}}(T^*, n^*) = \frac{1}{9}\left[\frac{1}{(3-n^*)^2} - \frac{n^*}{4T^*}\right]^{-1}$$