Study of Fluctuations by QMD

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FIAS, Frankfurt

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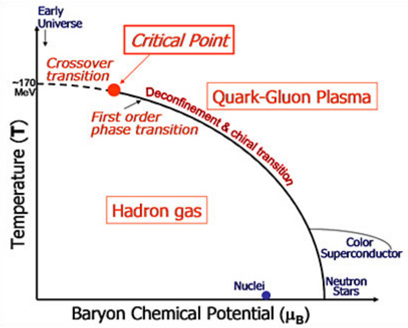
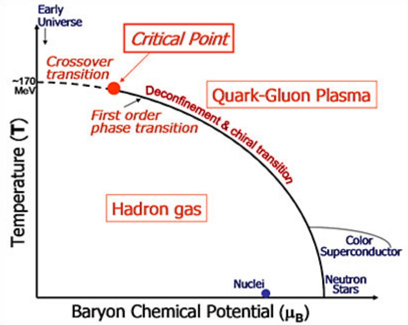


- Fluctuations of conserved quantities are thought to be a signal for phase transition and possible critical end point
- Recently it has been suggested that higher order cumulants would be more sensitive to the fluctuations associated with the phase transition
- Various other non-critical effects like global conservation laws in a subsystem, initial size fluctuations, experimental acceptance cuts etc, may contribute to the measured cumulants



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- For an ideal thermodynamic system, the number of particles is infinite and the statistical fluctuations are small and negligible
- Experiments deal with finite number of particles and therefore statistical fluctuations are not negligible
- Our aim is to Study the statistical fluctuation due to finite number of particles

QMD

The single-nucleon state is represented by a Gaussian wave packet:

$$\phi_i(\mathbf{r}) = \langle \mathbf{r} | \phi_i \rangle = \frac{1}{(2\pi L)^{3/4}} \exp\left[-\frac{(\mathbf{r} - \mathbf{R}_i)^2}{4L} + \frac{i}{\hbar}\, \mathbf{r} \cdot \mathbf{P}_i \right] ,$$

The N-nucleon wave function:

$$|\Phi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_N\rangle \; .$$

- We take 512 particles in the simulation box
- Choose their positions and velocities randomly
- Evolve according to

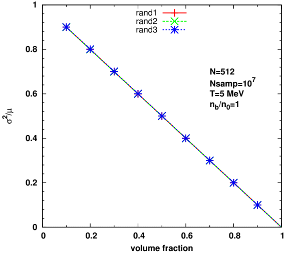
$$\mathcal{H} = T = \sum_i \frac{\mathbf{P}_i^2}{2m_i}$$

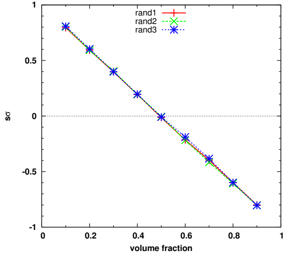
$$\dot{\mathbf{R}}_i = \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i}$$

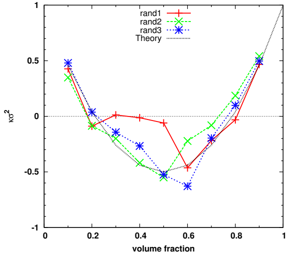
$$\dot{\mathbf{P}}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_i}$$

- Thermalize the system to have a temperature
- Divide the box in 10 equal bins
- Calculate number of particles for each bin
- Do this for millions of times
- Calculate cumulants

For speeding up the simulation to practical wall-times we have ported the QMD code to a GPU version







Message: Random number generator should be chosen very carefully

$$\mathcal{H} = T + V_{Pauli} + V_{local} + V_{sym} + V_{MD} + V_{Coul}$$

$$T = \sum_i \frac{\mathbf{P}_i^2}{2m_i} ,$$

$$V_{\rm Pauli} = \frac{1}{2}\, C_{\rm P} \left(\frac{\hbar}{q_0 p_0}\right)^3 \sum_{i,j(\neq i)} \exp\left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2}\right] \delta_{\tau_i\tau_j}\delta_{\sigma_i\sigma_j} ,$$

$$V_{\rm local} = \frac{\alpha}{2\rho_0} \sum_{i,j(\neq i)} \rho_{ij} + \frac{\beta}{(1+\tau)\ \rho_0^\tau} \sum_i \left[\sum_{j(\neq i)} \int d^3\mathbf{r}\ \tilde{\rho}_i(\mathbf{r})\ \tilde{\rho}_j(\mathbf{r})\right]^\tau ,$$

ρ_i and $\tilde{\rho}_i$ are single-nucleon densities and ρ_{ij} gives the overlap between nucleons

$$\rho_i(\mathbf{r}) = |\phi_i(\mathbf{r})|^2 = \frac{1}{(2\pi L)^{3/2}}\ \exp\left[-\frac{(\mathbf{r}-\mathbf{R}_i)^2}{2L}\right] ,$$

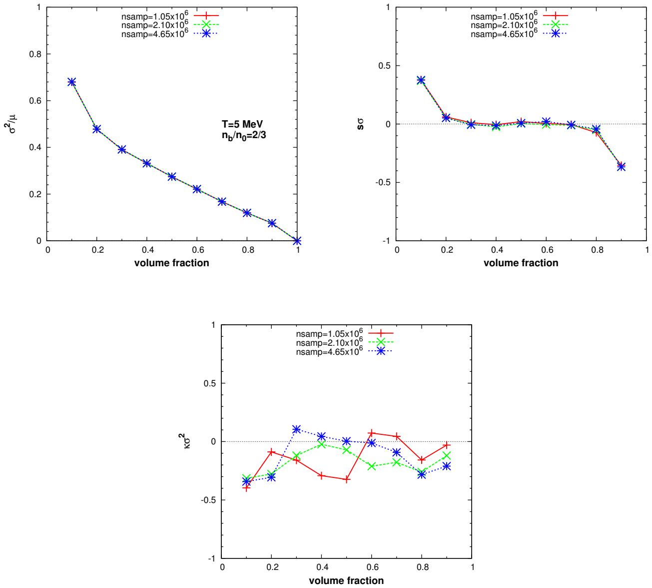
$$\tilde{\rho}_i(\mathbf{r}) = \frac{1}{(2\pi\tilde{L})^{3/2}}\ \exp\left[-\frac{(\mathbf{r}-\mathbf{R}_i)^2}{2\tilde{L}}\right], \quad \rho_{ij} = \int d^3\mathbf{r}\rho_i(\mathbf{r})\rho_j(\mathbf{r}), \quad \tilde{L} = \frac{(1+\tau)^{1/\tau}}{2} L$$

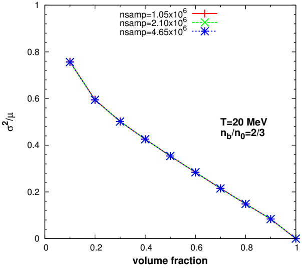
$$
\begin{aligned}
V_{\mathrm{sym}} &= \frac{C_{\mathrm{s}}}{2\rho_0} \sum_{i,j(\neq i)} (1 - 2|c_i - c_j|)\ \rho_{ij} \\
V_{\mathrm{MD}} &= V_{\mathrm{MD}}^{(1)} + V_{\mathrm{MD}}^{(2)} \\
&= \frac{C_{\mathrm{ex}}^{(1)}}{2\rho_0} \sum_{i,j(\neq i)} \frac{1}{1 + \left[\frac{\mathbf{P}_i - \mathbf{P}_j}{\hbar\mu_1}\right]^2}\ \rho_{ij} + \frac{C_{\mathrm{ex}}^{(2)}}{2\rho_0} \sum_{i,j(\neq i)} \frac{1}{1 + \left[\frac{\mathbf{P}_i - \mathbf{P}_j}{\hbar\mu_2}\right]^2}\ \rho_{ij}\ , \\
V_{\mathrm{Coulomb}} &= \frac{e^2}{2} \sum_{i,j(\neq i)} \left(\tau_i + \frac{1}{2}\right) \left(\tau_j + \frac{1}{2}\right) \iint d^3\mathbf{r}\, d^3\mathbf{r}'\, \frac{1}{|\mathbf{r} - \mathbf{r}'|}\ \rho_i(\mathbf{r})\rho_j(\mathbf{r}')\ ,
\end{aligned}
$$

$$
\begin{aligned}
c_i = 1 \quad &\text{and} \quad \tau_i = \frac{1}{2} \quad \text{for protons} \\
c_i = 0 \quad &\text{and} \quad \tau_i = -\frac{1}{2} \quad \text{for neutrons}
\end{aligned}
$$

Parameter set

C_{P} (MeV)	207
p_0 (MeV$/c$)	120
q_0 (fm)	1.644
α (MeV)	-92.86
β (MeV)	169.28
τ	1.33333
C_{s} (MeV)	25.0
$C_{\mathrm{ex}}^{(1)}$ (MeV)	-258.54
$C_{\mathrm{ex}}^{(2)}$ (MeV)	375.6
μ_1 (fm^{-1})	2.35
μ_2 (fm^{-1})	0.4
L (fm^2)	2.1


nsamp=1.05x10^6
nsamp=2.10x10^6
nsamp=4.65x10^6
T=5 MeV
n_b/n_0=2/3
σ^2/μ
sσ
κσ^2
volume fraction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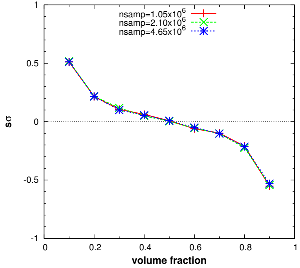
nsamp=2.10x10^6
nsamp=4.65x10^6
T=20 MeV
n_b/n_0=2/3
σ^2/μ
volume fraction


nsamp=1.05x10^6
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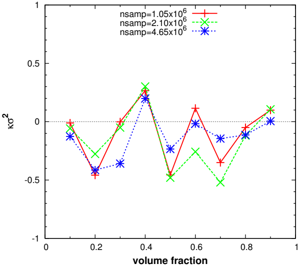
nsamp=4.65x10^6
sσ
volume fraction


nsamp=1.05x10^6
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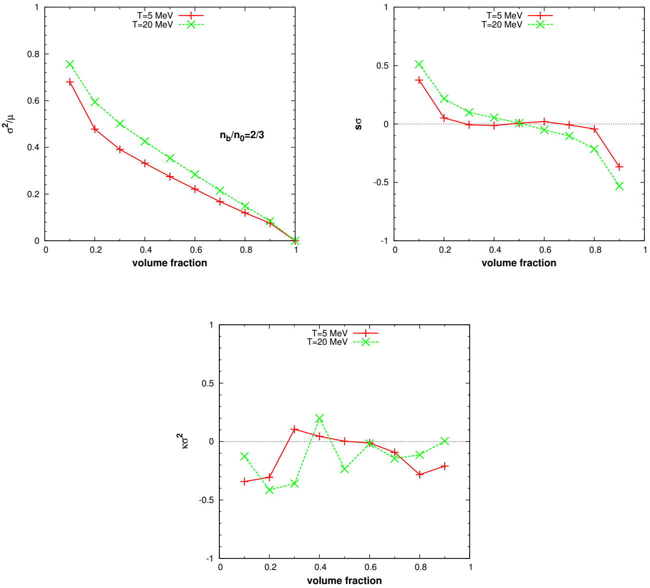
κσ^2
volume fraction



T=5 MeV
T=20 MeV
σ^2/μ
n_b/n_0=2/3
volume fraction
$s\sigma$
volume fraction
$\kappa\sigma^2$
volume fraction

- Need more statistics
- Need to explore the phase diagram with the interaction used here

Work in progress ....