Charge Fluctuations

from Lattice QCD

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Bielefeld-BNL-CCNU collaboration

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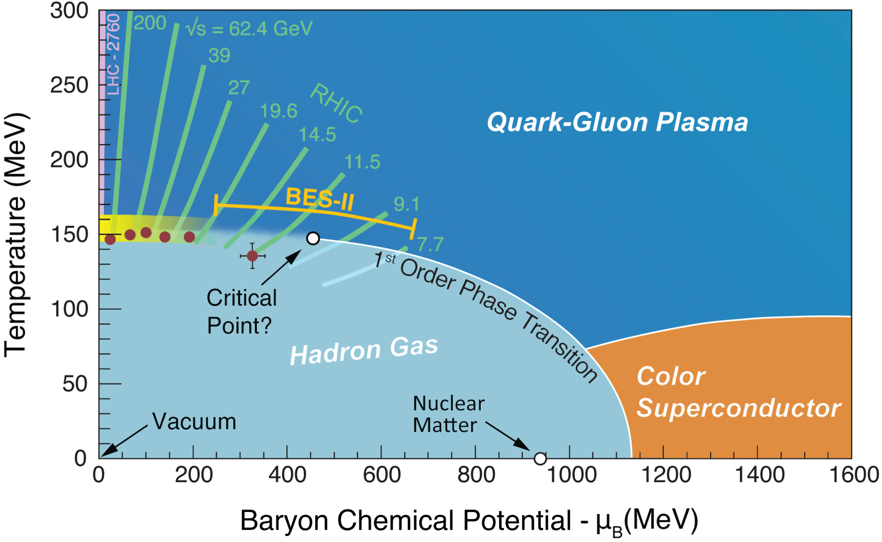
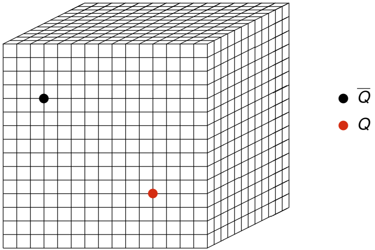
The QCD phase diagram



Outline

- Charge fluctuations
  - chemical freeze-out
  - critical point
  - equation of state

- Computational challenges
  - required resources
  - software development



Fluctuations of conserved charges

$$\chi_i^X = \frac{1}{T^4} \frac{\partial^i}{\partial \hat{\mu}_X^i} P_{\mathrm{QCD}} \ , \qquad \chi_{ij}^{XY} = \frac{1}{T^4} \frac{\partial^{i+j}}{\partial \hat{\mu}_X^i \partial \hat{\mu}_Y^j} P_{\mathrm{QCD}} \ , \quad \hat{\mu}_X = \frac{\mu_X}{T}$$

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- on the Lattice
  - only at $\mu = 0$
  - accessible through quark number fluctuations

$$\begin{aligned} B &= (N_u + N_d + N_s)/3 & & \mu_B = \mu_u + 2\mu_d \\ Q &= (2N_u - N_d - N_s)/3 & \Longrightarrow \quad & \mu_Q = \mu_u - \mu_d \\ S &= -N_s & & \mu_S = \mu_d - \mu_s \end{aligned}$$

Comparison to low and high T limit

- gas of free quarks and gluons

$$\frac{P_{SB}}{T^4} = \frac{8\pi^2}{45} + \sum_f \left(\frac{7\pi^2}{60} + \frac{1}{2} \left(\frac{\mu_f}{T} \right)^2 + \frac{1}{4\pi^2} \left(\frac{\mu_f}{T} \right)^4 \right)$$

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- gas of hadrons and possible resonances

$$\frac{P_{HRG}}{T^4} = \frac{1}{VT^3} \sum_{i \in \mathrm{baryons}} \ln Z_i^B \ + \frac{1}{VT^3} \sum_{i \in \mathrm{mesons}} \ln Z_i^M$$

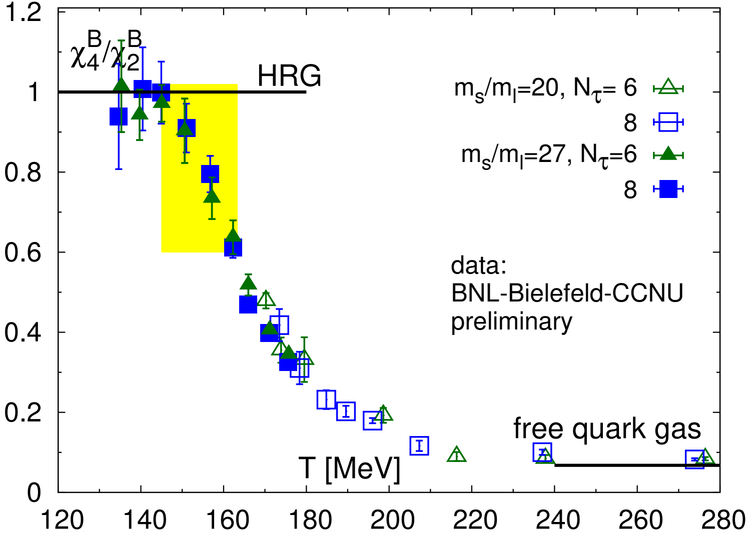
$$\ln Z_i^{M/B} = \frac{VT^3}{\pi^2} d_i \left(\frac{m_i}{T}\right)^2 \sum_{k=1}^{\infty} \frac{(\pm 1)^{k+1}}{k^2} K_2(km_i/T) \cosh\left(k(B_i\mu_B + Q_i\mu_Q + S_i\mu_S)/T\right)$$

Comparison to low and high T limit

$$\left(\frac{\chi_4^B}{\chi_2^B}\right)_{HRG} = \frac{\sum\limits_{i\in\text{baryons}} d_i \left(\frac{m_i}{T}\right)^2 K_2(m_i/T)\, B_i^4}{\sum\limits_{i\in\text{baryons}} d_i \left(\frac{m_i}{T}\right)^2 K_2(m_i/T)\, B_i^2} = 1$$

$$\left(\frac{\chi_4^B}{\chi_2^B}\right)_{SB} = \frac{\frac{6N_f}{81\pi^2}}{\frac{N_f}{9}} = \frac{2}{3\pi^2}$$

Comparison to low and high T limit



From zero to finite chemical potential

- Lattice simulations not possible at real finite μ
  - sign problem

- Taylor expand observables around $\mu = 0$
  - simplest case $\mu_Q \equiv 0, \ \mu_S \equiv 0$

$$\chi_i^X(\mu_B) = \sum_k \frac{1}{k!} \chi_{k+i}^X \, \hat{\mu}_B^k \, , \qquad \text{with} \qquad \chi_i^X = \frac{1}{T^4} \left. \frac{\partial^i P_{\mathrm{QCD}}}{\partial \hat{\mu}_X^i} \right|_{\mu_X = 0}$$

- coefficients defined at vanishing chemical potential
  - Lattice QCD techniques work

Comparison to experiment

only at freeze-out $(\mu_f,\ T_f)$ → Experiment

Moment	Symbol	Experiment	Lattice
mean	M_X	$\langle N_X \rangle$	$VT^3\chi_1^X$
variance	σ_X^2	$\left\langle (\delta N_X)^2 \right\rangle$	$VT^3\chi_2^X$
skewness	S_X	$\dfrac{\left\langle (\delta N_X)^3 \right\rangle}{\sigma_X^3}$	$\dfrac{VT^3\chi_3^X}{\left(VT^3\chi_2^X\right)^{3/2}}$
kurtosis	k_X	$\dfrac{\left\langle (\delta N_X)^4 \right\rangle}{\sigma_X^4} - 3$	$\dfrac{VT^3\chi_4^X}{\left(VT^3\chi_2^X\right)^2}$

- volume independent ratios

$$\frac{\sigma_X^2}{M_X} = \frac{\chi_2^X}{\chi_1^X}, \qquad S_X\sigma_X = \frac{\chi_3^X}{\chi_2^X}, \qquad k_X\sigma_X^2 = \frac{\chi_4^X}{\chi_2^X}$$

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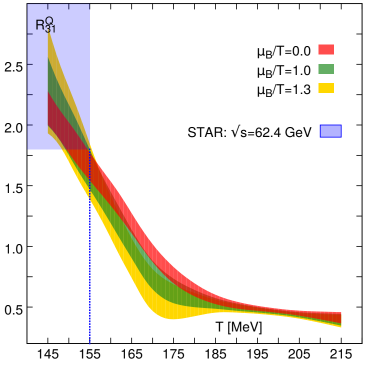
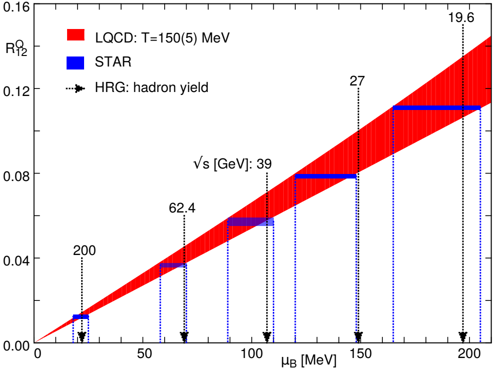
$$R_{31}^Q \equiv \frac{\chi_3^Q}{\chi_1^Q} = R_{31}^{Q,0} + \mathcal{O}(\hat{\mu}_B^2) \, , \quad R_{12}^Q \equiv \frac{\chi_1^Q}{\chi_2^Q} = \hat{\mu}_B \left(R_{12}^{Q,1} + \mathcal{O}(\hat{\mu}_B^2) \right)$$

Chemical freeze-out





$$R_{31}^{Q}\Big|_{\mathrm{exp}}\left(\sqrt{s}\right) = R_{31}^{Q}\Big|_{\mathrm{lat}}\left(T_f\right)$$

$$R_{12}^{Q}\Big|_{\mathrm{exp}}\left(\sqrt{s}\right) = R_{12}^{Q}\Big|_{\mathrm{lat}}\left(\mu_B^f/T_f\right)$$

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- e.g. expansion of the pressure around $\mu_B = 0$ (for $\mu_Q \equiv \mu_S \equiv 0$)

$$\frac{P_{\mathrm{QCD}}}{T^4} = \sum_n \frac{1}{n!} \chi_n^B \, \hat{\mu}_B^n \,, \quad \chi_n^B = \frac{1}{VT^3} \left. \frac{\partial^n \ln Z}{\partial \hat{\mu}_B^n} \right|_{\mu_B = 0}$$

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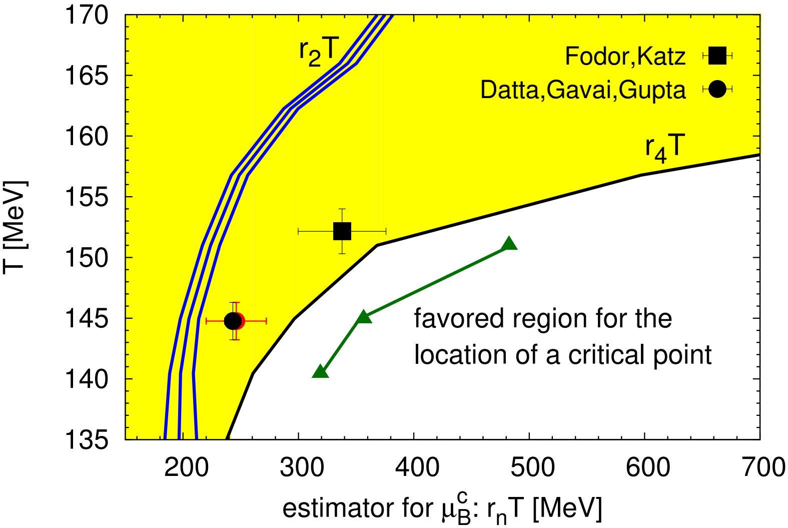
- analysis of convergence radius can determine bound on the location of a critical point:

$$r_{2n} = \sqrt{2n(2n-1) \left| \frac{\chi_{2n}^B}{\chi_{2n+1}^B} \right|}$$

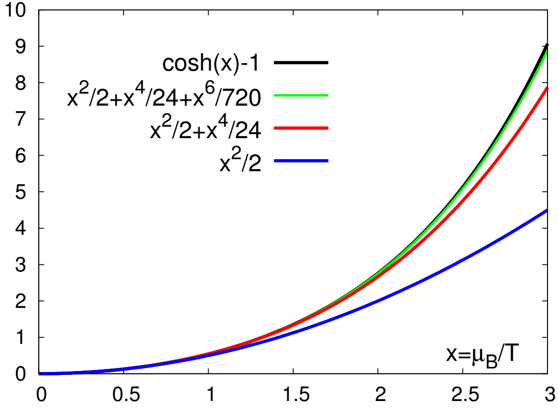
- only if $\chi_n > 0$ for all $n \geq n_0$

Critical point from Taylor expansions



Equation of State of (2+1)-flavor QCD

- when does HRG break down? onset of criticality?



- including 6th order should be accurate up to $\mu_B/T = 3$

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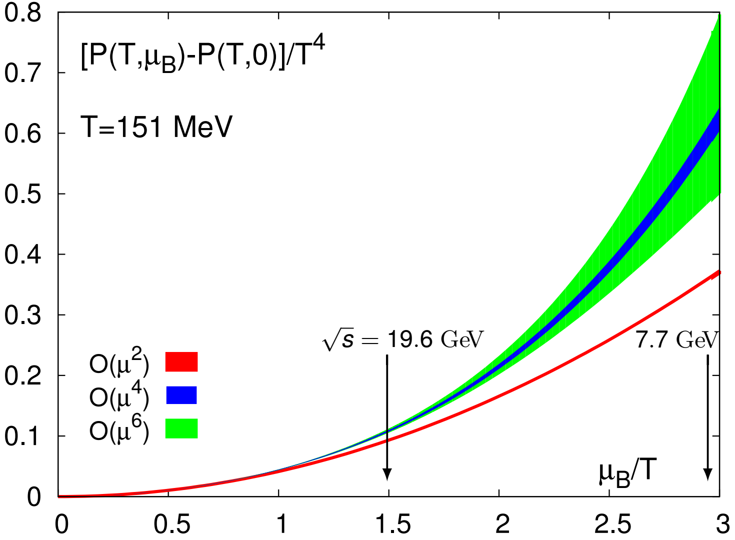
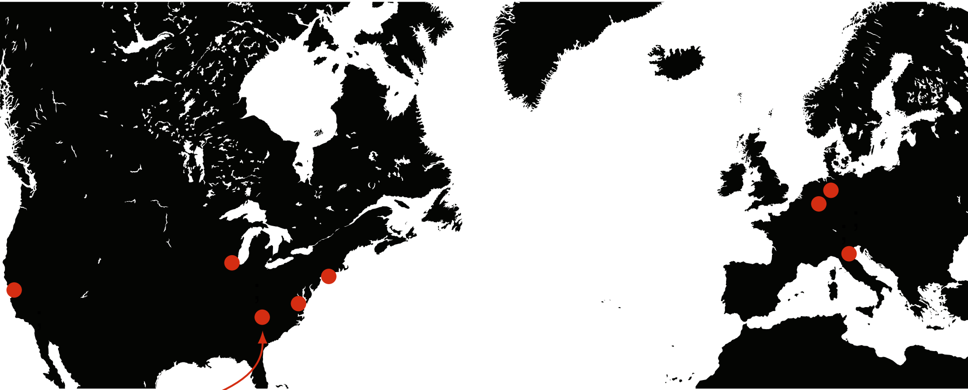


Project status & plans

- all simulations done with physical quark masses
- EoS is under control up to $\mu_B/T = 1.5$
- higher orders important for $\mu_B/T > 1.5$
  - observe breakdown of HRG?
  - relevant region for BESII
- need more statistics for higher orders and larger lattices
  - requires a lot of computing time

Computing resources



OLCF
OAK RIDGE LEADERSHIP COMPUTING FACILITY

- current Titan allocation
  - 200M core-hours (exceptional good year)
    - equivalent to 5% of Titan for one year
    - or full Titan machine for $\sim$16 days
  - largest jobs use 14k nodes and sustain 5 $\mathrm{PFlop/s}$

Algorithmic improvements

- Lattice simulations dominated by Conjugate Gradient (CG)
  - CG frequently used solver in many scientific fields
  - many improvements known
    - time consuming to validate all

	method	speed-up
CG		
	deflation	10x
	noise reduction	2x
	multi right-hand side	4x
	pipelined formulation	1.2x
-		
	linear-μ formulation	4x
total		384x

more to come: truncated solver, block CG, multi pseudo-fermion RHMC

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- need to write low-level code hidden behind a high-level interface
  - can be designed in a future-proof way

Required computing time

- for extending our simulations up to 8th order
  - e.g. on a $48^3 \times 12$ lattice in the low temperature region

code	core-hours/temperature
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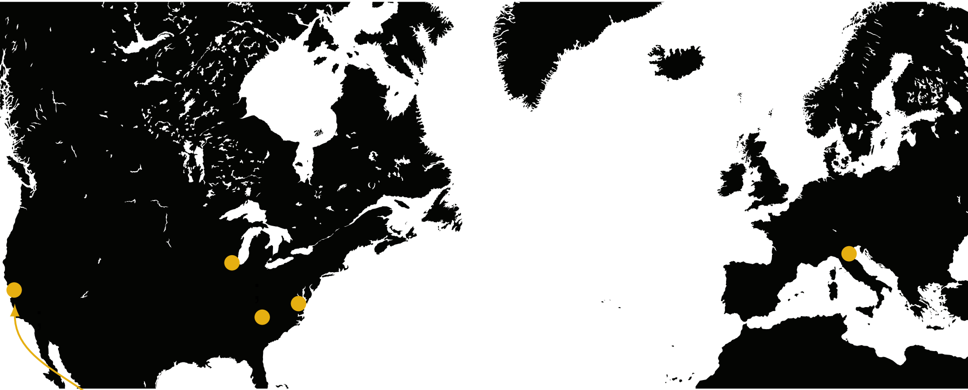
- our project is just not possible with unoptimized code
- still, 180M core-hours is a lot
  - need to further improve our codes and algorithms

New Supercomputers in 2016/17



- Intel® Xeon Phi™ KNL and NVIDIA® Pascal™ based
- GPU code is ready for next machines
- software development focused on KNL
  - our codes are part of NERSC's exascale program

Thank you for your attention!

Performance gains on Haswell

(dual-socket E5-2698V3, 2.3 GHz, 32 cores)

Dslash, $32^3 \times 8$, 16 right-hand sides