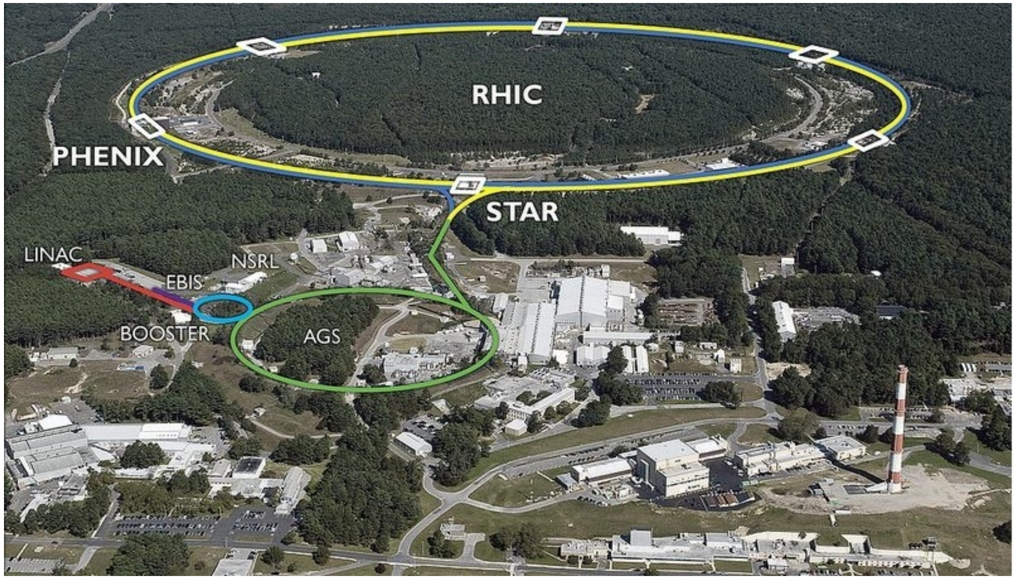
Supercomputing the phase diagram of strongly interacting matter

Frithjof Karsch

UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC-TR 211
Strong-interaction matter under extreme conditions

BEST COLLABORATION



Relativistic Heavy Ion Collider @ BNL

Summit @ ORNL
~200 PetaFlops

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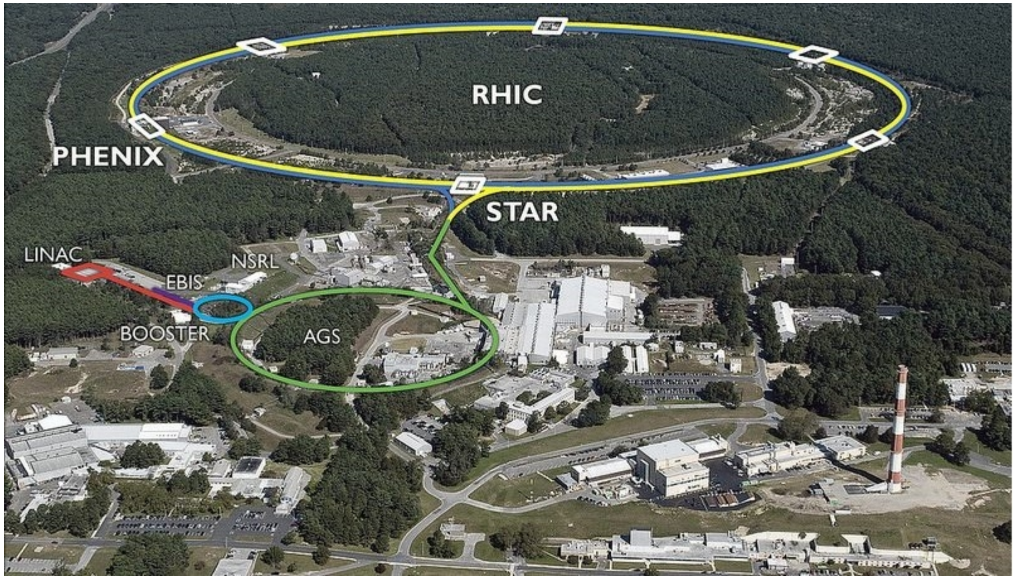

Relativistic Heavy Ion Collider @ BNL

OUTLINE

– the physics case:
strongly interacting matter at high temperature and density

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JUWELS Booster @ FZ Jülich, Germany, 2020
~ 70 Petaflops

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– the physics case:
strongly interacting matter at high temperature and density

– the computational needs:
High Performance Computing; the need of Exascale Performance

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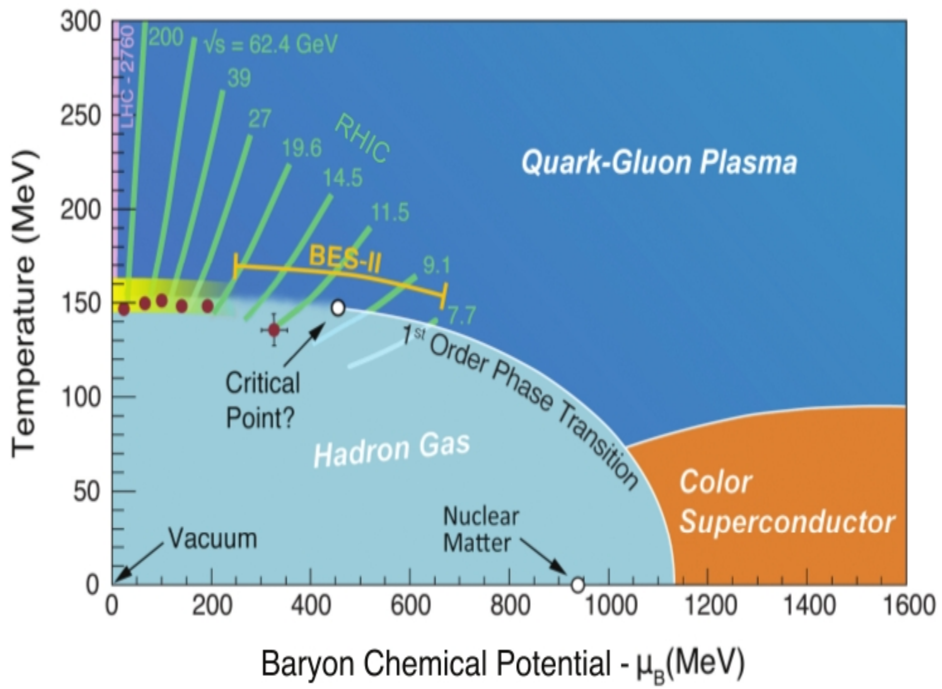


OUTLINE

– the physics case:
strongly interacting matter at high temperature and density

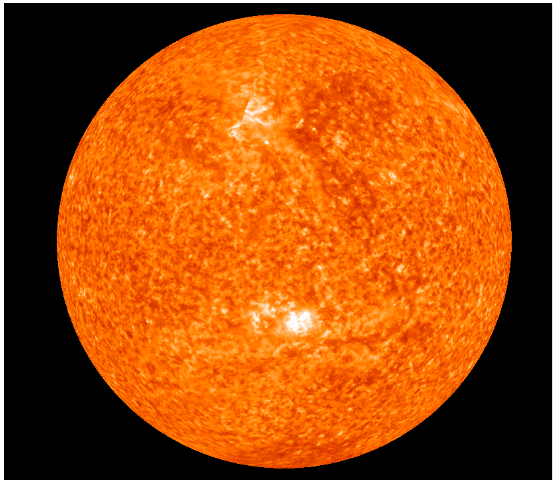
– the computational needs:
High Performance Computing; the need of Exascale Performance

– some physics results:
the structure of strong interaction matter; its phase diagram & equation of state

the sun

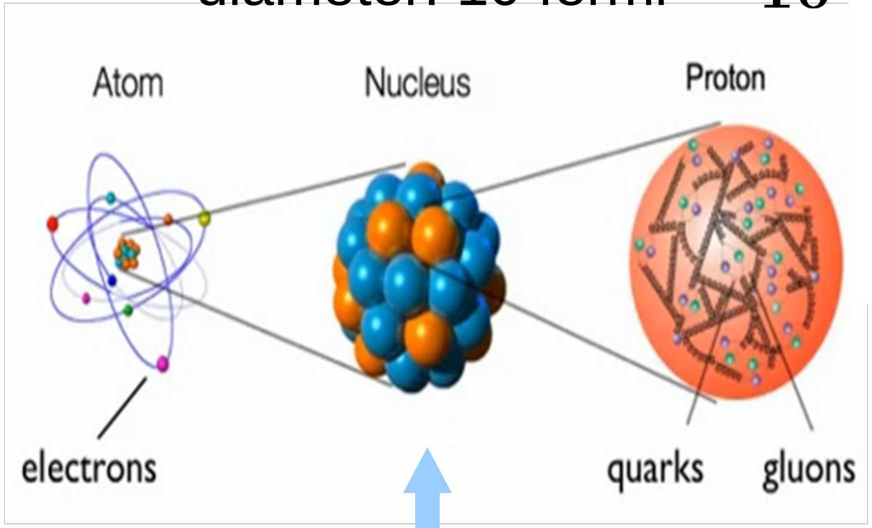
diameter: 1 million km = 10^9 m

temperature: 10 million degree = $10^7\ ^oC$



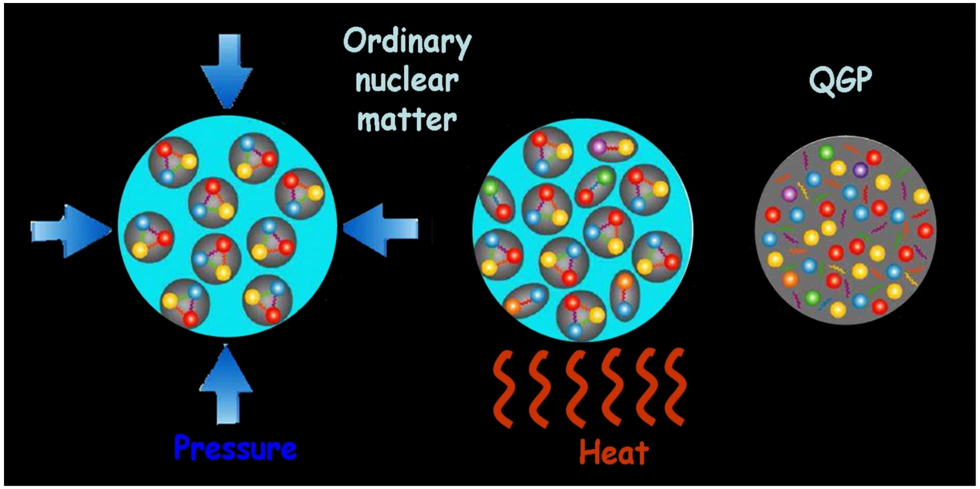
the atomic nucleus

diameter: 10 fermi = 10^{-9} m



the Quark-Gluon Plasma

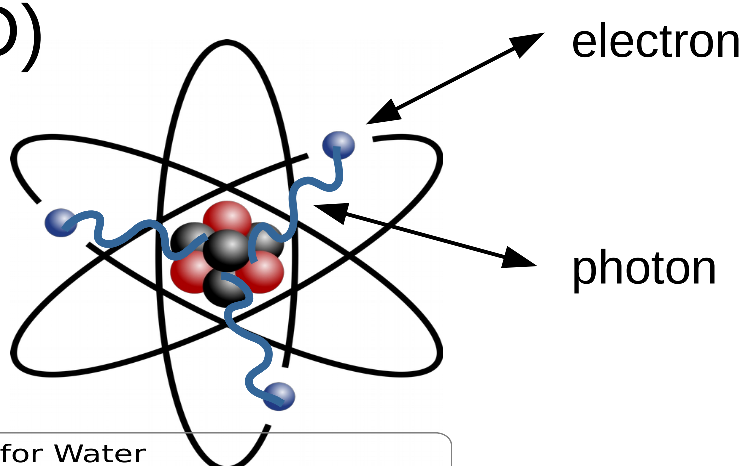
temperature: $10^{12}\ ^oC$

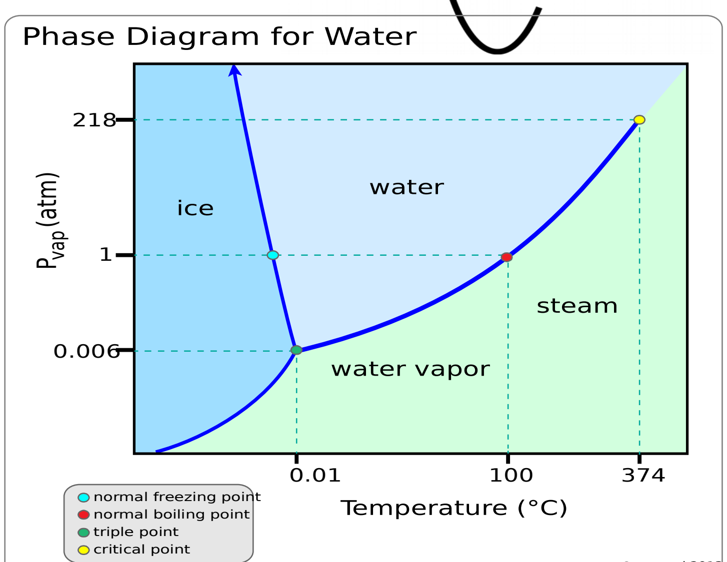


The electromagnetic force

electron
photon
↔ electric charge

Quantumelectrodynamics
(QED)

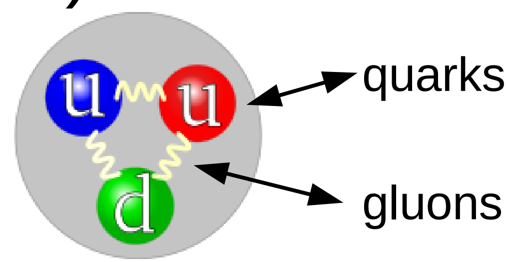


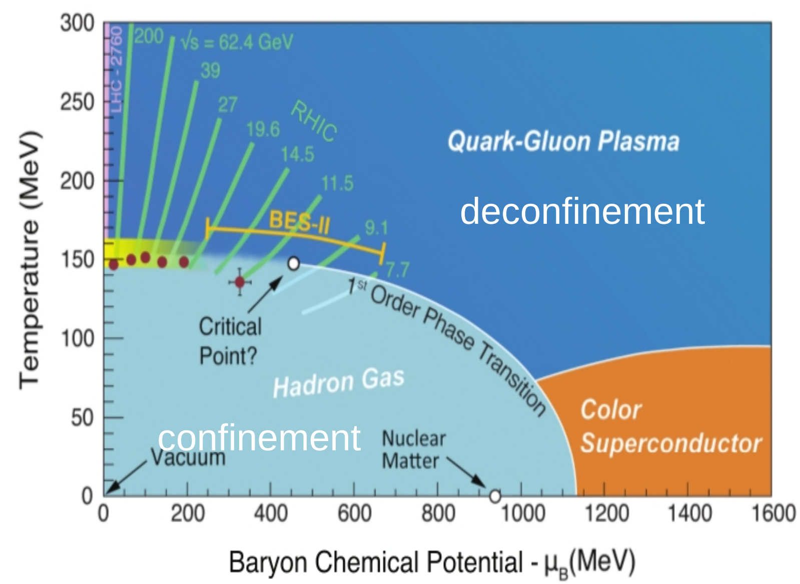


The strong force

quark
gluon
↔ color

Quantumchromodynamics
(QCD)





The electromagnetic force

electron
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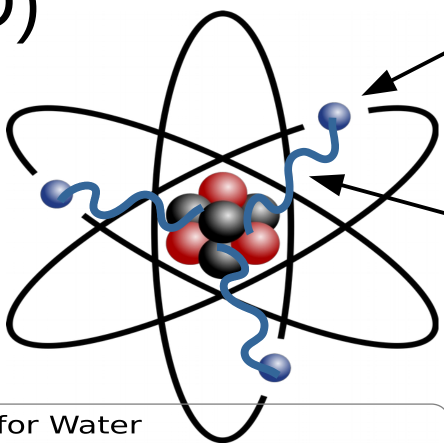
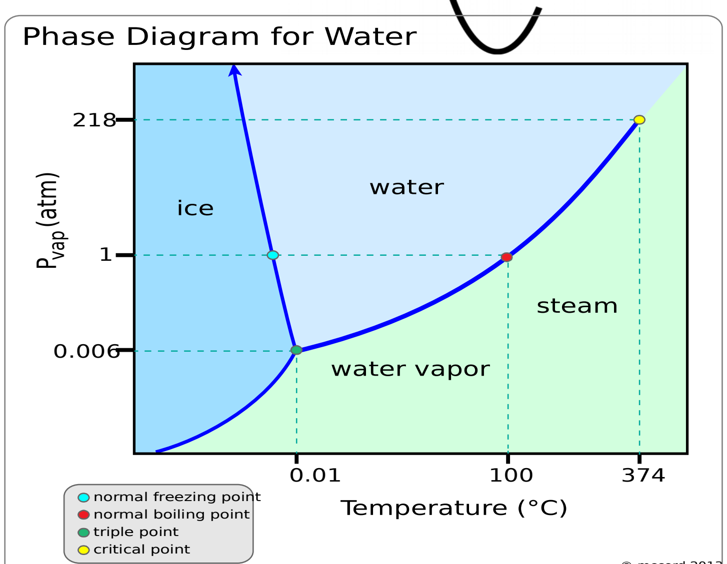


electron

photon



The strong force

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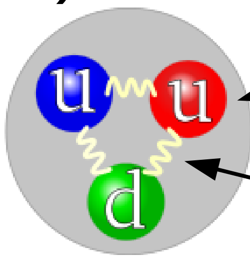


quarks

gluons

key properties:

chiral symmetry breaking
– light Goldstone particle → **pion**

confinement
– colorless bound states → **hadrons**

asymptotic freedom
– weakly interacting at short distances
→ **quark-gluon plasma**

The confinement – deconfinement transition

confinement ⇔ hadrons

– stick together, find a comfortable distance
– controlled by the "confinement potential"

$$V_{\bar{q}q}(r) = -\frac{4}{3}\frac{\alpha(r)}{r} + \sigma\, r$$

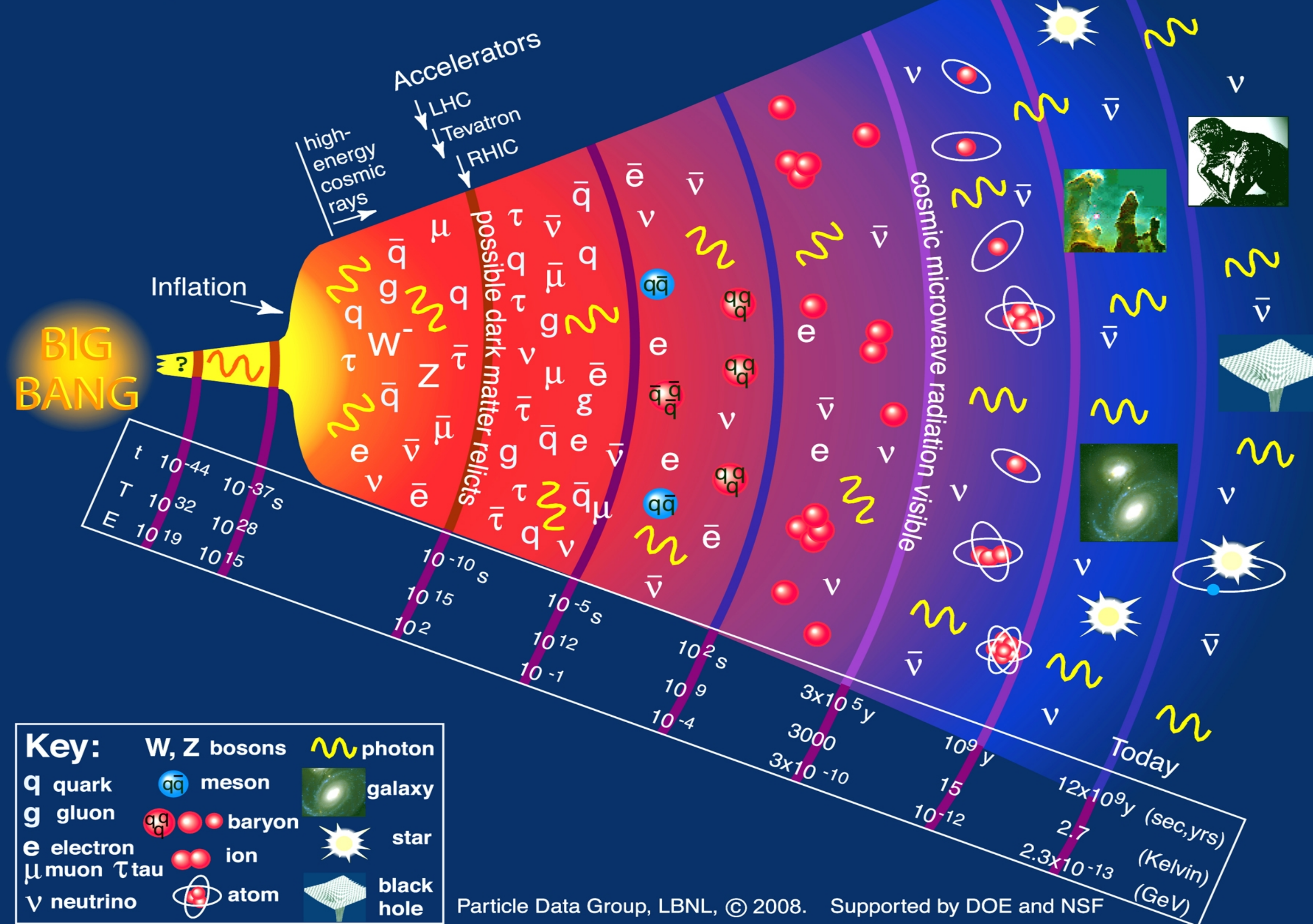
deconfinement ⇔ quarks&gluons

– freely floating in the crowed
– do not care what color your neighbor has

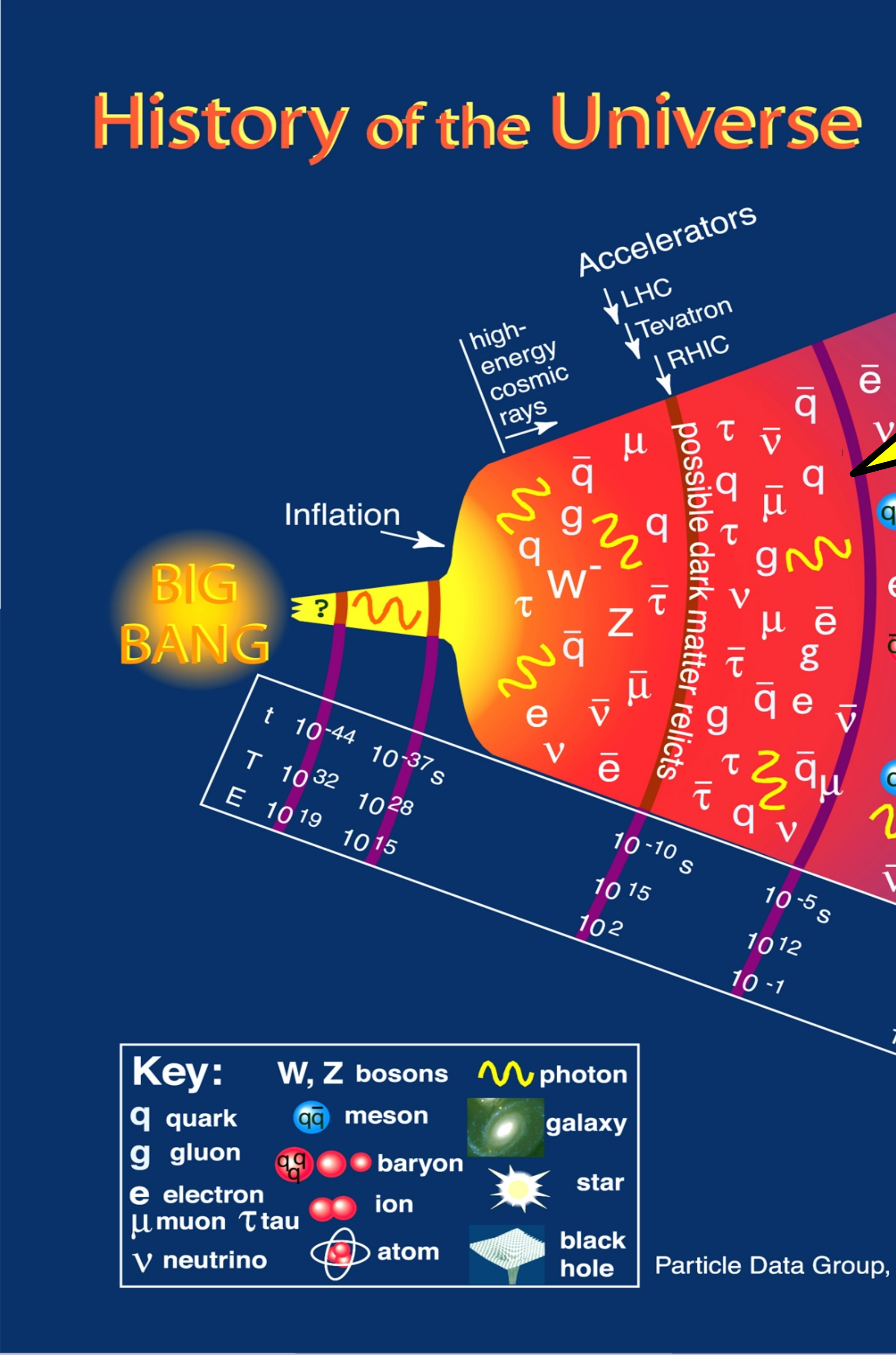
screening, color is neutralized on the average over a (short) distance

This transition happens abruptly: (almost a) PHASE TRANSITION

History of the Universe



Particle Data Group, LBNL, © 2008. Supported by DOE and NSF



The "phase" transition from the quark - gluon plasma to ordinary (hadronic) matter

1/100.000 seconds after the big bang quarks and gluons recombine to hadrons

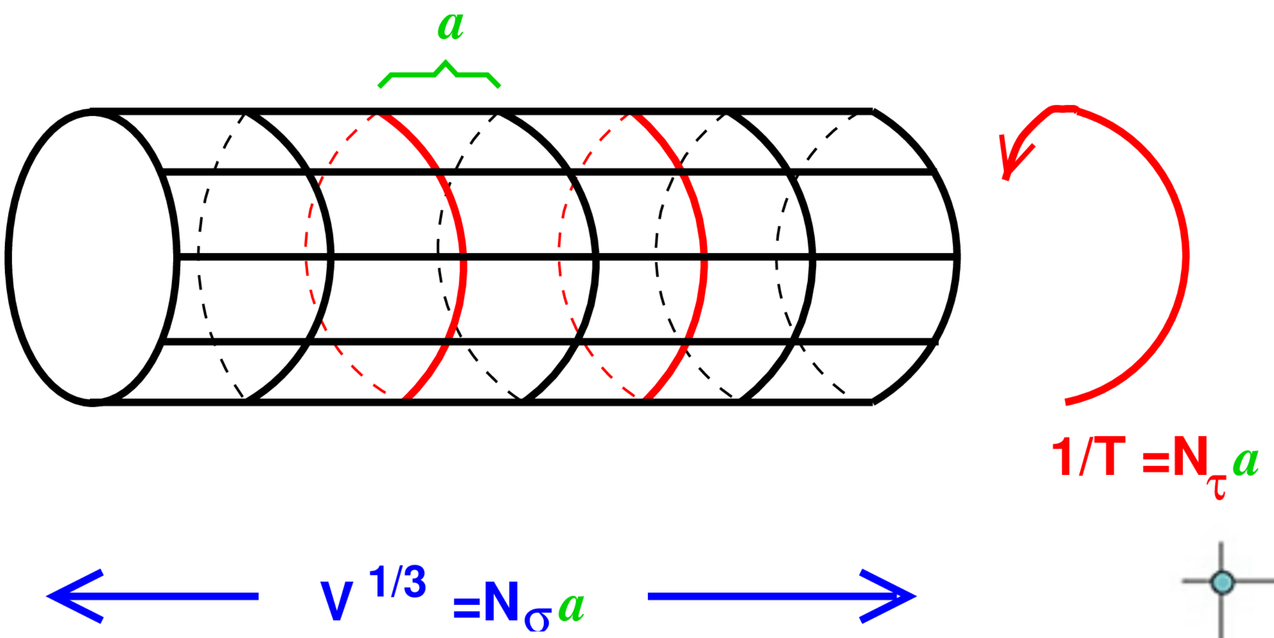
"freeze-out" of hadrons (protons, neutrons,..)

the temperature at this time was about 100.000 times that of the interior of the sun

the confinement of quarks and gluons happened "suddenly", i.e. "almost in a phase" transition

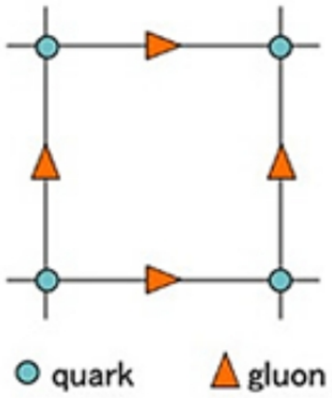
Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)

Kenneth G. Wilson
1974



Monte Carlo simulation 1979

partition function:



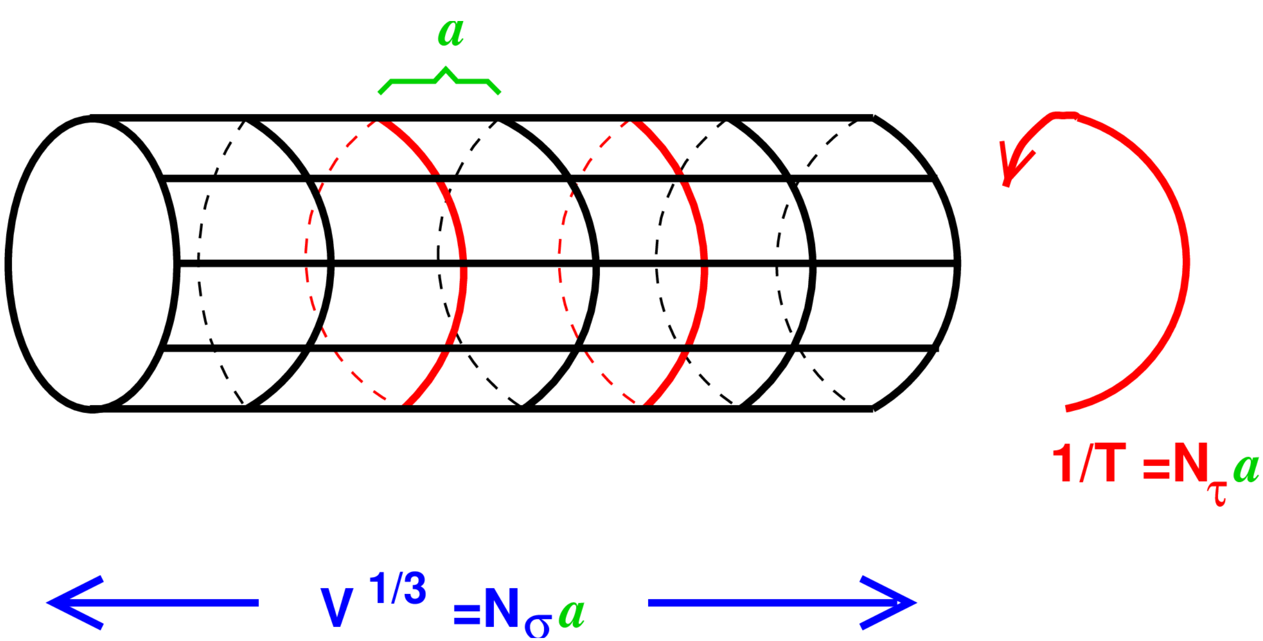
$$Z(V,T,\mu) = \int \mathcal{D}\mathcal{A}\mathcal{D}\psi\mathcal{D}\bar{\psi}\; \mathrm{e}^{-S_E}$$

$$S_E = \int_0^{1/T} dx_0 \int_V d^3x\; \mathcal{L}_E(\mathcal{A},\psi,\bar{\psi},\mu)$$

Mike Creutz, 1979

T: temperature V: volume μ : chemical potential

Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)



the lattice: $N_\sigma^3 \times N_\tau$

lattice spacing: a

THE fermion determinant: source of all problems

partition function:

$$Z(V,T,\mu) = \int \mathcal{D}\mathcal{A}\; Det M(\mathcal{A},\mu)\; \mathrm{e}^{-S_G}$$

$\mathcal{O}\left(10^6\right)$ grid points

$\mathcal{O}\left(10^8\right)$ d.o.f.

Dealing with the fermion determinant

partition function again:

$$Z(V,T) = \int \mathcal{D}\mathcal{A} \int \prod_n \mathrm{d}\psi_n \mathrm{d}\bar{\psi}_n \; \mathrm{e}^{\bar{\psi}_n M(A,m_q)_{nm}\psi_m} \; \mathrm{e}^{-S_G}$$

fermions (anti-commuting)

"fermion matrix"

$$= \int \mathcal{D}\mathcal{A} \; DetM(\mathcal{A}, m_q) \; \mathrm{e}^{-S_G}$$

"importance sampling"

$$DetM(\mathcal{A}, m_q) = \int \prod_n \mathrm{d}\phi_n \; \mathrm{e}^{-\sum_{nm} \phi_n^* M_{nm}^{-1}(\mathcal{A},m_q)\phi_m}$$

bosons (commuting)

– need $x_n = M_{nm}^{-1}\phi_m$

– solve $M_{nm}x_m = \phi_n$

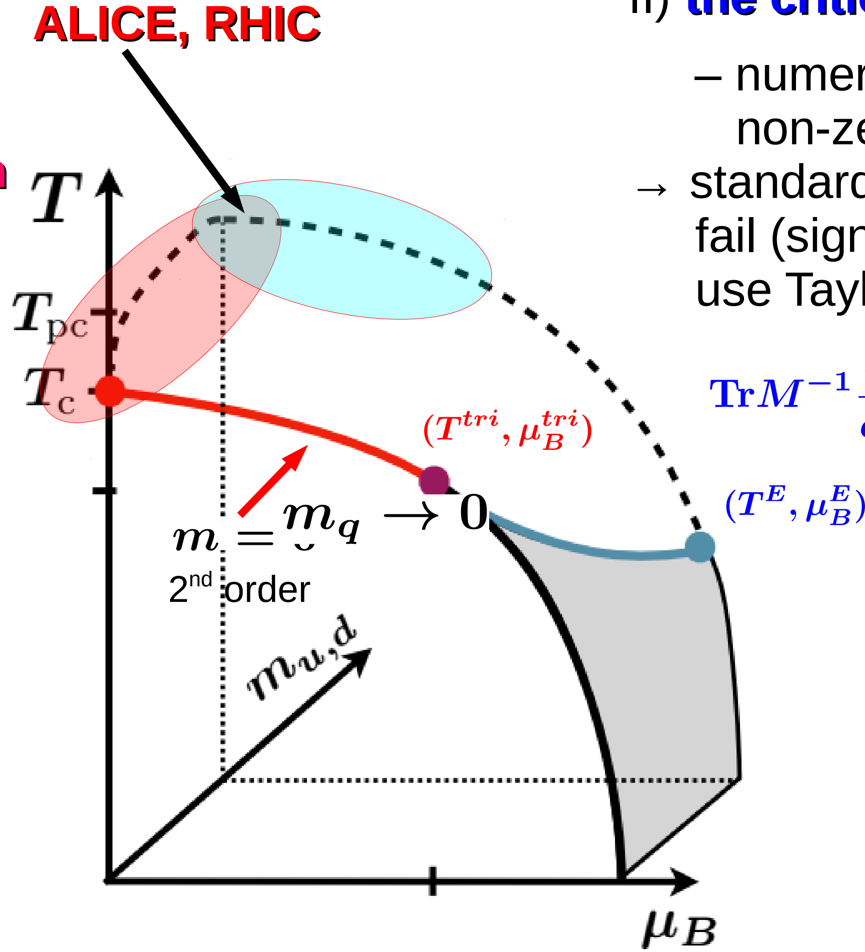
Exploring the phase diagram --- two major challenges--

I) **the chiral phase transition**

– need to approach vanishing quark masses

$$\mathrm{Tr} M^{-1}$$

→ computational cost for matrix inversion diverges for $m_q \to 0$



II) **the critical point at high density**

– numerical calculations at non-zero baryon density

→ standard numerical algorithms fail (sign-problem); use Taylor expansion techniques

$$\mathrm{Tr} M^{-1} \frac{\partial M}{\partial \mu_B} M^{-1} \frac{\partial M}{\partial \mu_B} \ldots M^{-1} \frac{\partial M}{\partial \mu_B}$$

Random Matrix Model	A. Halasz, A.D. Jackson, R.E. Shrock, M.A. Stephanov, J.J.,M. Verbaarschot, Phys. Rev. D58 (1998) 096007
QCD	M. Stephanov, Phys. Rev. D73 (2006) 094508
NJL	M. Buballa, S. Carignano, Phys. Lett. B791 (2019) 361

Computational cost of a QCD calculation is dominated by the cost to invert the fermion matrix M, using e.g. the CG-algorithm

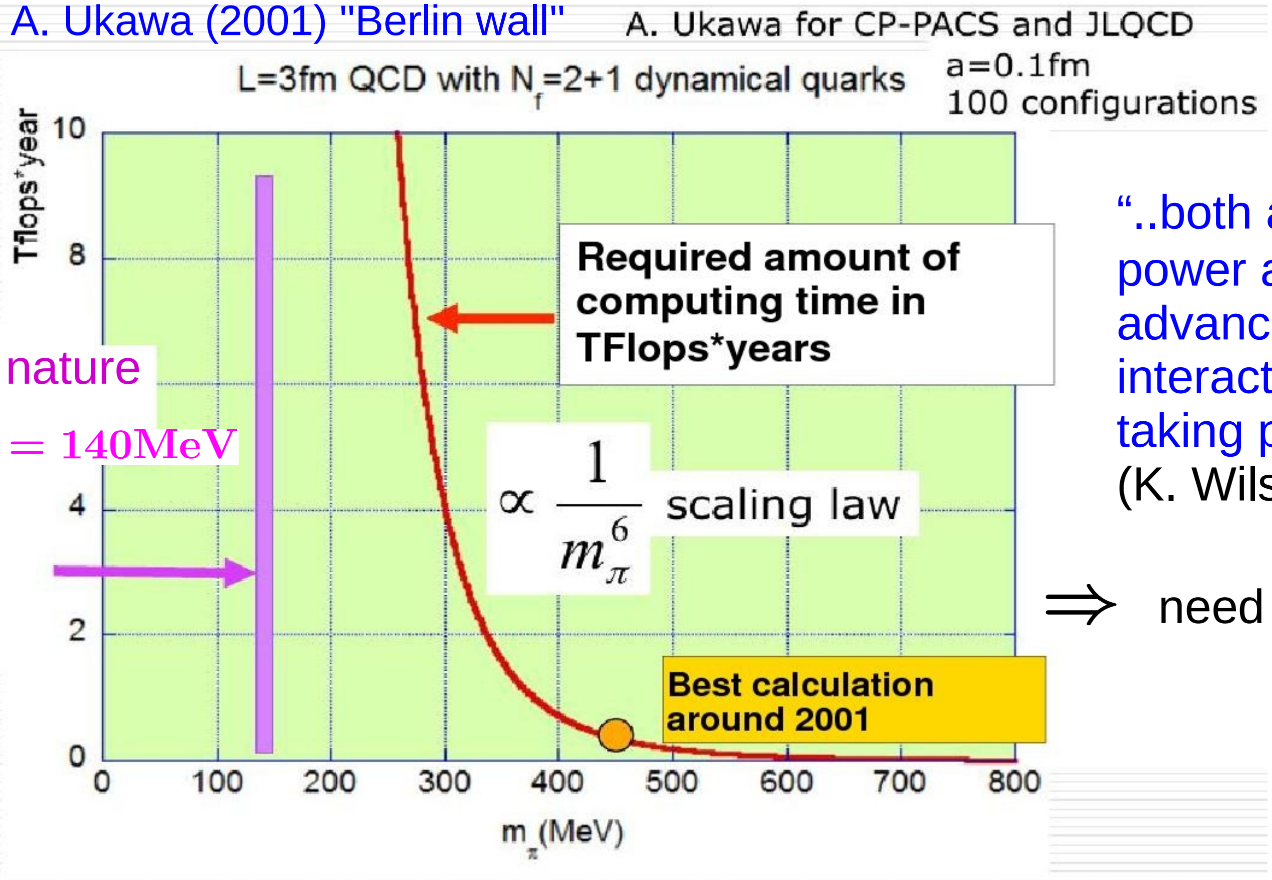
$$\text{cost} \sim m_\pi^{-z_\pi} V^{5/4} a^{-7}$$

$m_\pi \sim m_q^{1/2}$ pion

m_q : quark mass

$\sim 2000 \; : \quad z_\pi \simeq 6$

A. Ukawa (2001) "Berlin wall"



nature

$m_\pi = 140\text{MeV}$

"..both a 10^8 increase in computing power and spectacular algorithmic advances are needed before a useful interaction with experiments starts taking place.."
(K. Wilson, 1989)

$\Rightarrow$ need Exaflop computers

Computational cost of a QCD calculation is dominated by the cost to invert the fermion matrix, using e.g. the CG-algorithm

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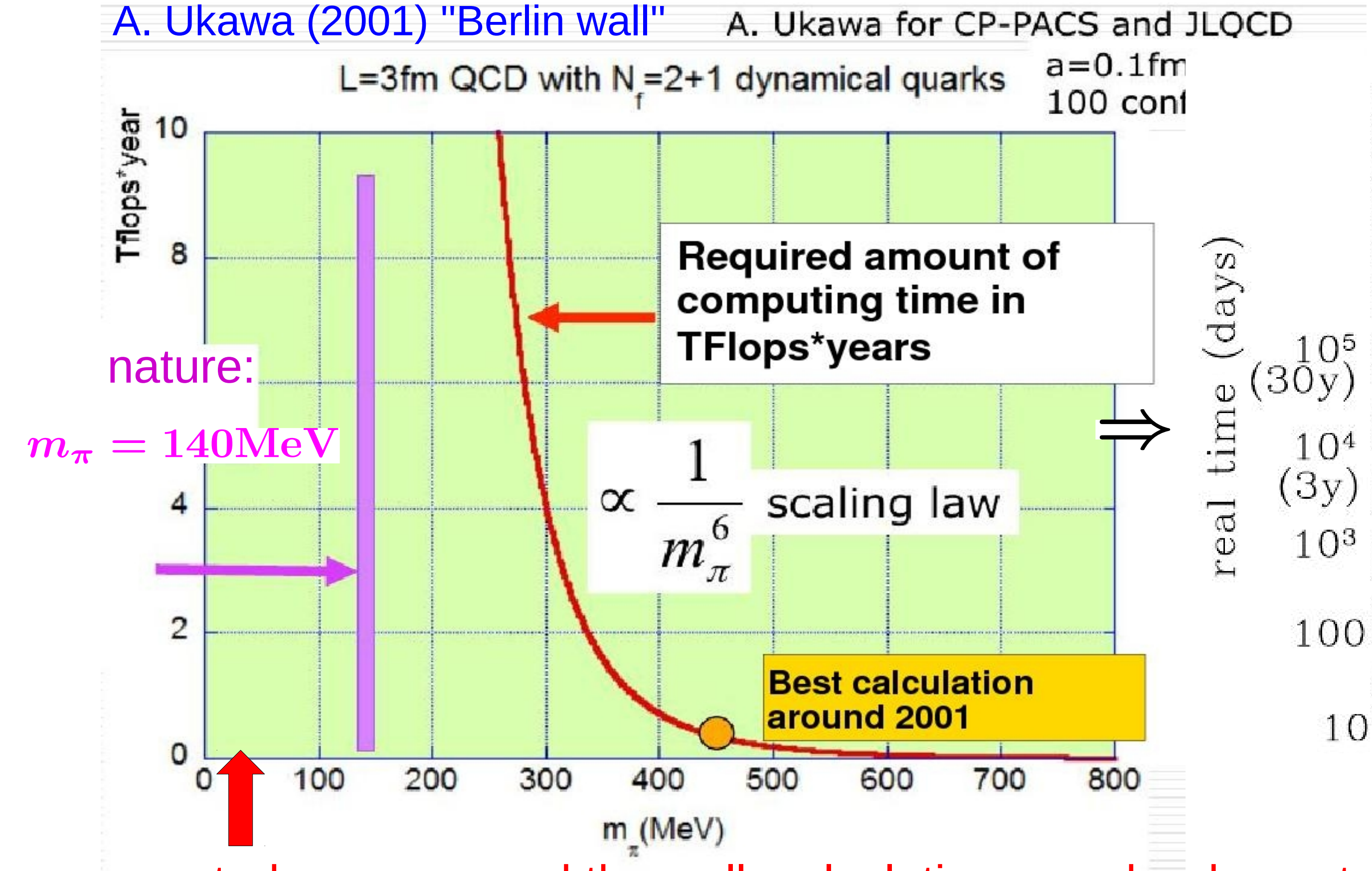
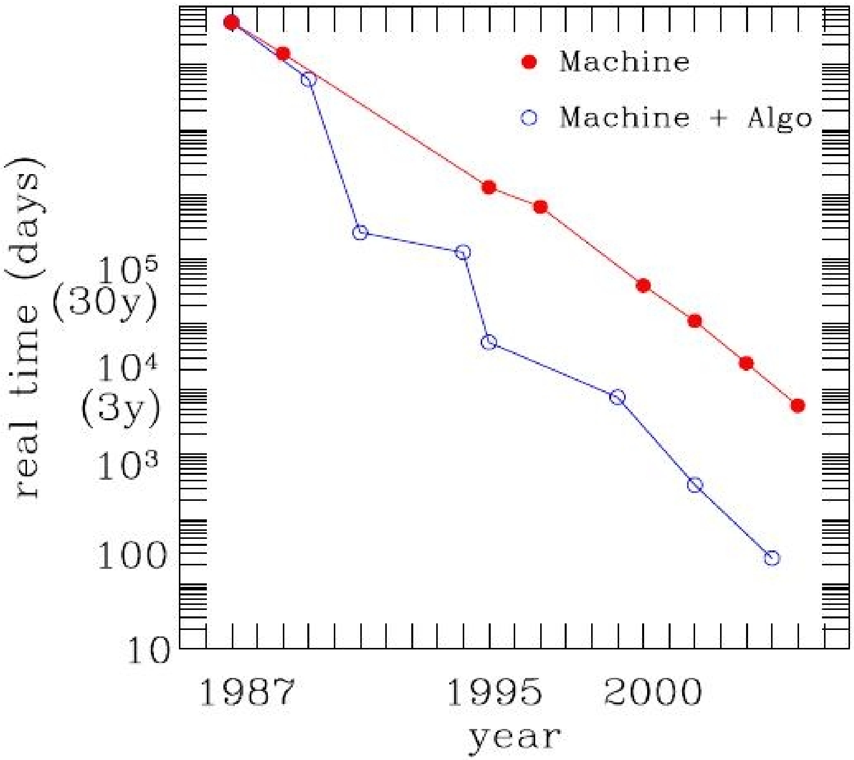


$\Rightarrow$

improvement with time



today we passed the wall: calculations can be done at $m_\pi \sim m_\pi^{phys}/3$

K. Jansen

need to solve: $M \cdot \vec{x} = \vec{b}$ use, e.g. the Conjugate Gradient algorithm

preconditioned CG

$$r_0 = b - Mx_0$$
$$z_0 = P^{-1} r_0$$
$$p_0 = z_0$$
$$k = 0$$

repeat

$$\alpha_k = \frac{r_k^T z_k}{p_k^T M p_k}$$
$$x_{k+1} = x_k + \alpha_k p_k$$
$$r_{k+1} = r_k - \alpha_k M p_k$$
$$if(r_{k+1} < rtoll) \text{ exit}$$
$$z_{k+1} = P^{-1} r_{k+1}$$
$$\beta_k = \frac{z_{k+1}^T r + k + 1}{z_k^T r_k}$$
$$p_{k+1} = z_{k+1} + \beta_k p_k$$
$$k = k + 1$$

end repeat

condition number κ controls #iterations needed for CG to converge:

κ = (max. eigenvalue) / (min. eigenvalue)

$$\kappa = \frac{\lambda_{max}}{\lambda_{min}}$$

improvement of the CG solver

⇔ try to reduce condition number

– preconditioning, solve $P^{-1}(b - Mx) = 0$
– multigrid
– multi-boson algorithms
– deflation
– ….

https://en.wikipedia.org/wiki/Conjugate_gradient_method need to solve: $M \cdot \vec{x} = \vec{b}$

use, e.g. the Conjugate Gradient algorithm

preconditioned CG

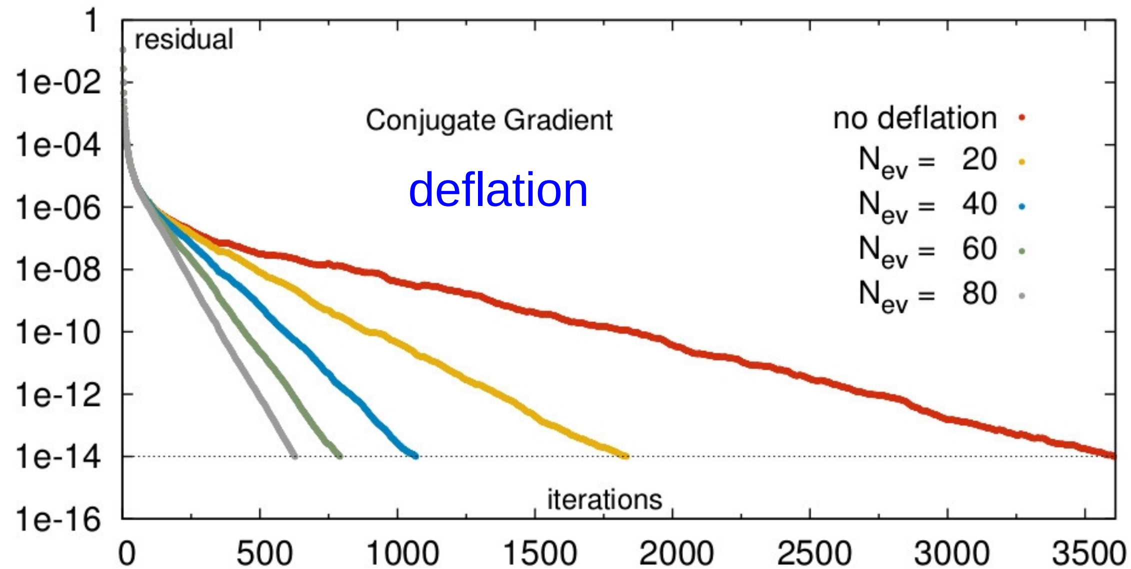
$$
\begin{aligned}
r_0 &= b - M x_0 \\
z_0 &= P^{-1} r_0 \\
p_0 &= z_0 \\
k &= 0
\end{aligned}
$$

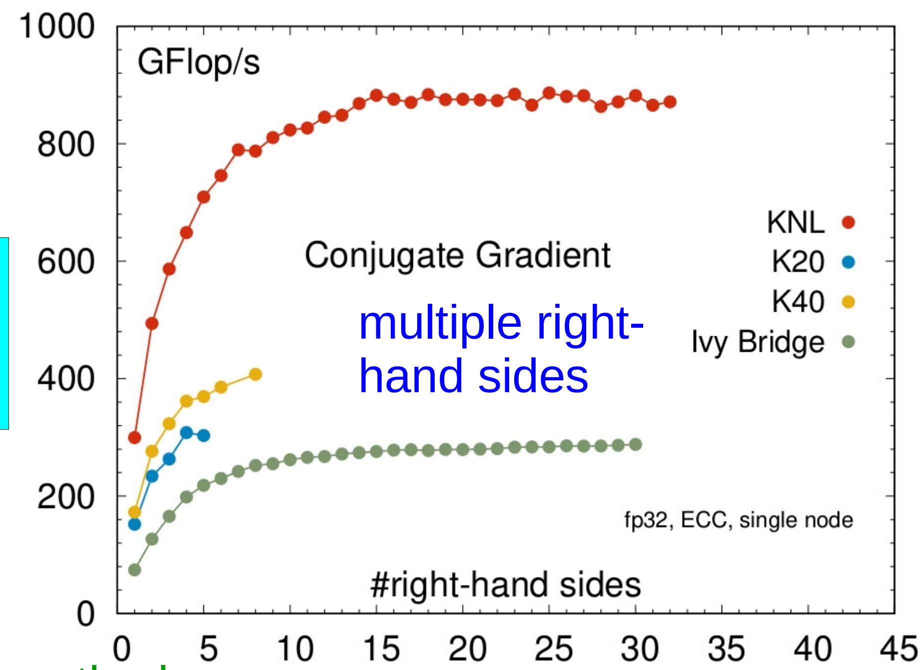
repeat

$$
\begin{aligned}
\alpha_k &= \frac{r_k^T z_k}{p_k^T M p_k} \\
x_{k+1} &= x_k + \alpha_k p_k \\
r_{k+1} &= r_k - \alpha_k M p_k \\
& if(r_{k+1} < rtoll)\ \text{exit} \\
z_{k+1} &= P^{-1} r_{k+1} \\
\beta_k &= \frac{z_{k+1}^T r + k + 1}{z_k^T r_k} \\
p_{k+1} &= z_{k+1} + \beta_k p_k \\
k &= k + 1
\end{aligned}
$$

end repeat

O(100) speed-up





https://en.wikipedia.org/wiki/Conjugate_gradient_method

Critical behavior and higher order cumulants
– Taylor expansion –

Taylor expansion of the **QCD** pressure: $\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \mu_B, \mu_Q, \mu_S)$

$$\frac{P}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk}^{BQS}(T) \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

cumulants of net-charge fluctuations and correlations:

$$\chi_{ijk}^{BQS} = \left. \frac{\partial^{i+j+k} P/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k} \right|_{\mu_{B,Q,S}=0} \quad , \quad \hat{\mu}_X \equiv \frac{\mu_X}{T}$$

cumulants at vanishing chemical potential provide information on the equation of state at small non-zero chemical potential

chiral order parameter and its susceptibility:

$$\langle \bar{\psi}\psi \rangle = \langle \mathrm{Tr} M^{-1} \rangle \quad , \quad \chi_{dis} = \langle (\mathrm{Tr} M^{-1})^2 \rangle - \langle \mathrm{Tr} M^{-1} \rangle^2$$

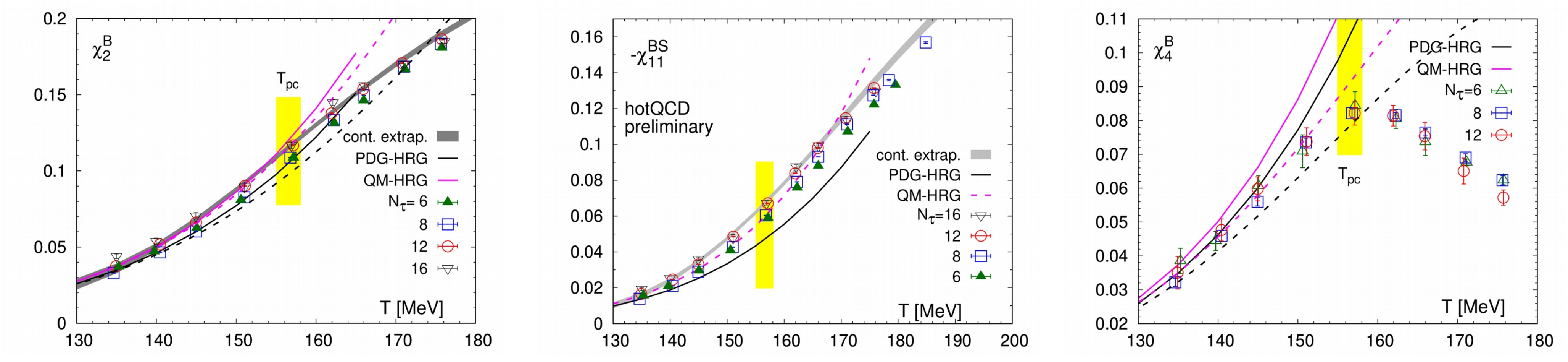
$$\sim m_l^{-(1-1/\delta)}$$

divergence signals phase transition

Critical behavior and higher order cumulants
– Taylor expansion and universality –

Taylor expansion of the **QCD** pressure: $\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \mu_B, \mu_Q, \mu_S)$

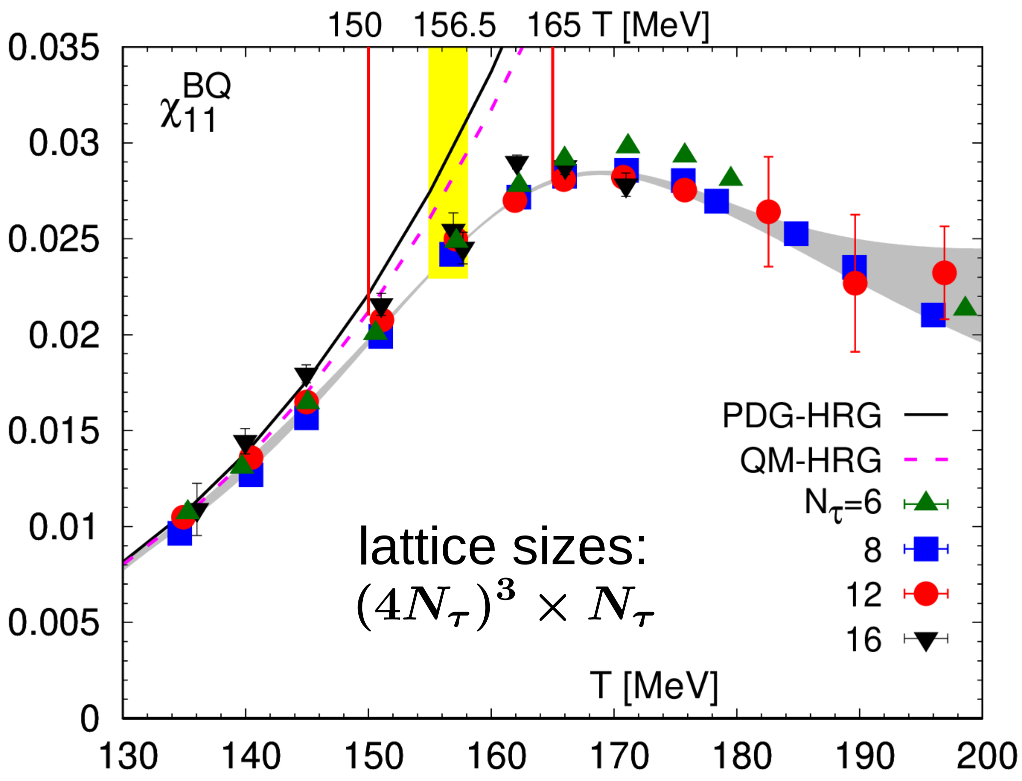
$$\frac{P}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk}^{BQS}(T) \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$



– some 2[nd] and 4[th] order cumulants in (2+1)-flavor QCD

Calculation of cumulants of conserved charge fluctuations

state-of-the-art calculations on GPUs



each data point requires

$\mathcal{O}(10\ \text{Million})$

matrix inversions

matrix size: $\sim 10^6 \times 10^6$

~100 non-zero entries per column

20 PFlops=20x10^{15} Flops

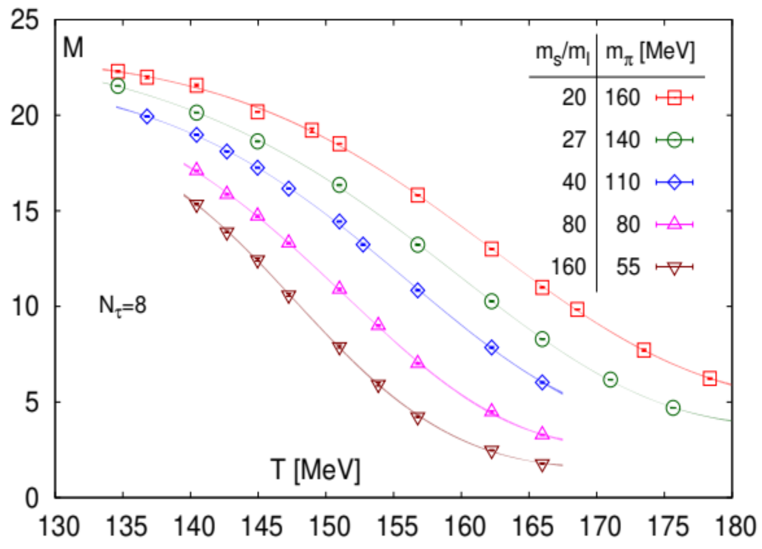
18688 GPUs

~ 2 million GPU-hours = 230 GPU-years

= 6 days on Titan

The Chiral PHASE TRANSITION in (2+1)-flavor QCD

$$\langle\bar\psi\psi\rangle \sim m_s \frac{\partial \ln Z}{\partial m_l}$$



$m_l = (m_u + m_d)/2 \Rightarrow 0$

m_s fixed, physical

$m_s \partial\langle\bar\psi\psi\rangle/\partial m_l$

"magnetic" susceptibility

$\sim (m_s/m_l)^{0.79}$

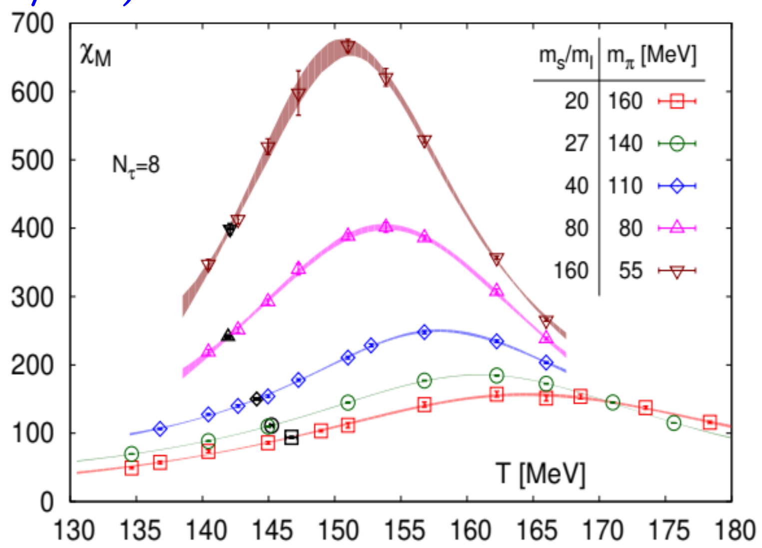
$(160/27)^{0.79} \sim 4$

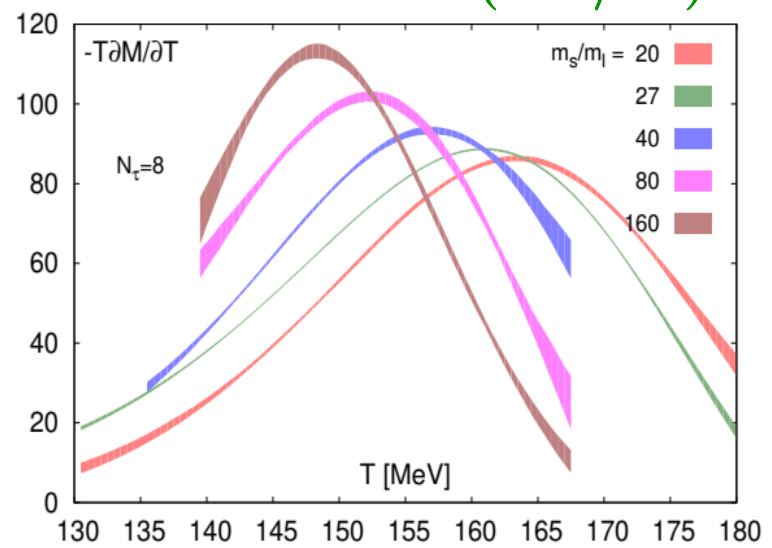
$T\partial\langle\bar\psi\psi\rangle/\partial T$

"mixed" susceptibility

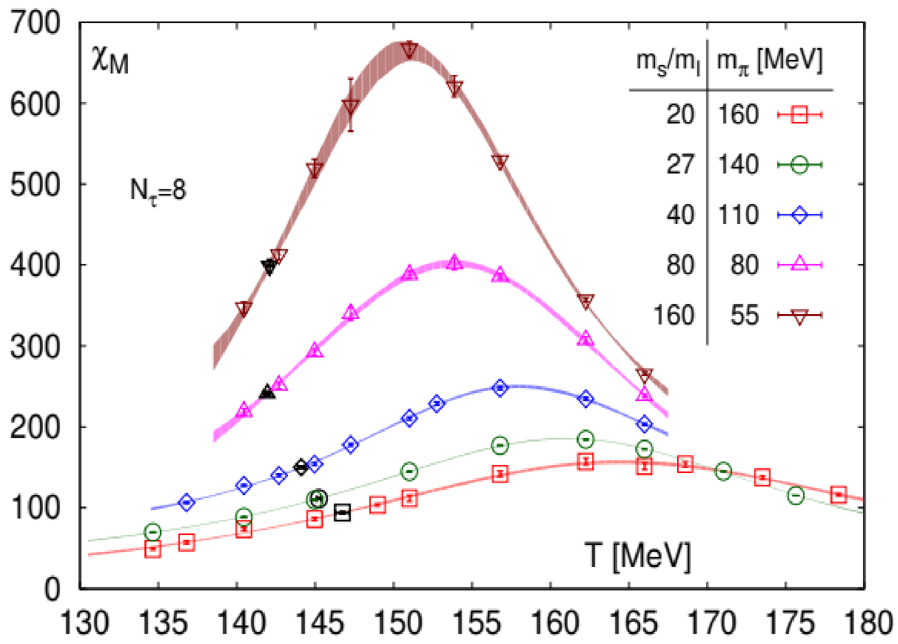
$\sim (m_s/m_l)^{0.34}$

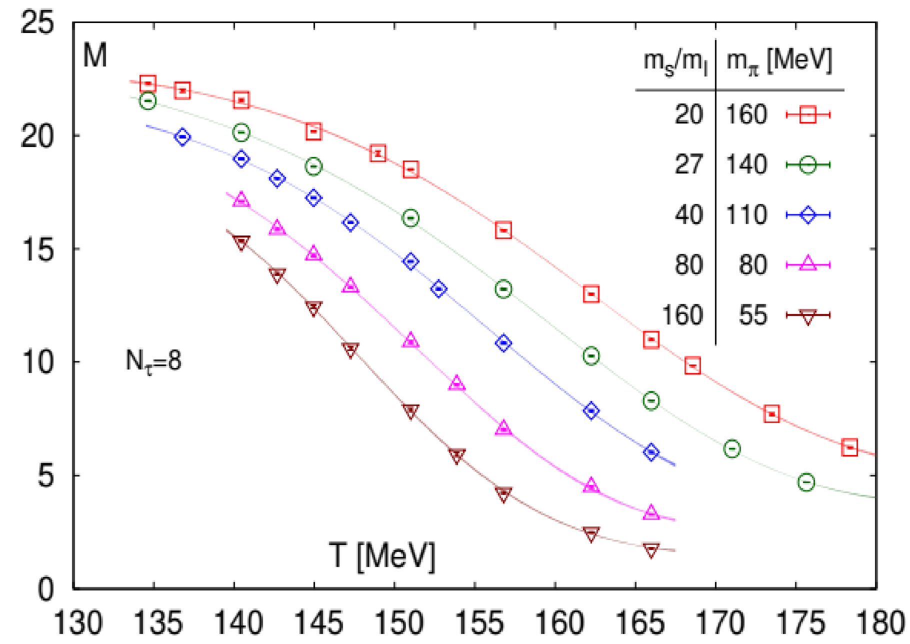
$(160/27)^{0.34} \sim 1.8$

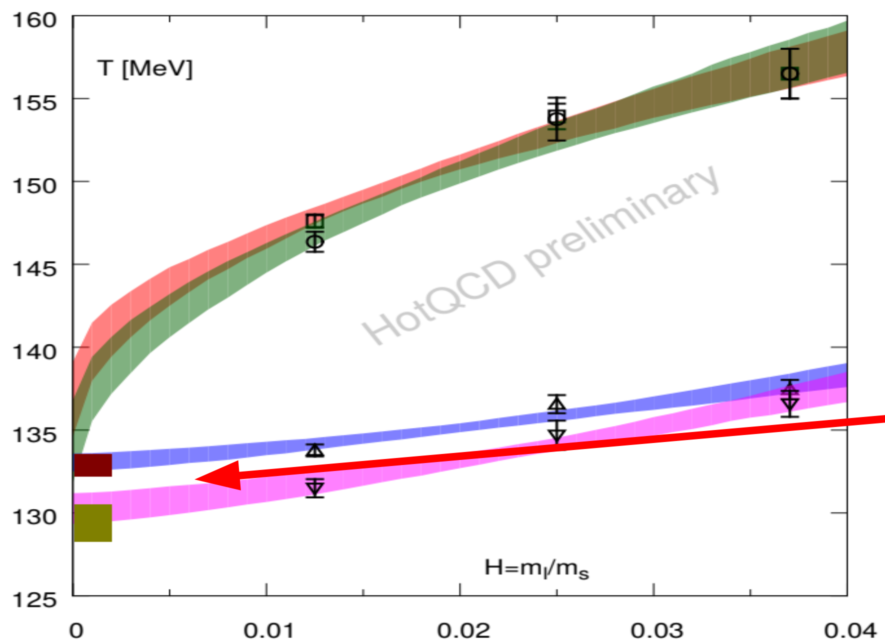




Chiral PHASE TRANSITION temperature







$$T_{pc}^{phys} = (156.5 \pm 1.5)\ \mathrm{MeV}$$

A. Bazavov et al [HotQCD], arXiv:1812.08235

chiral limit extrapolation

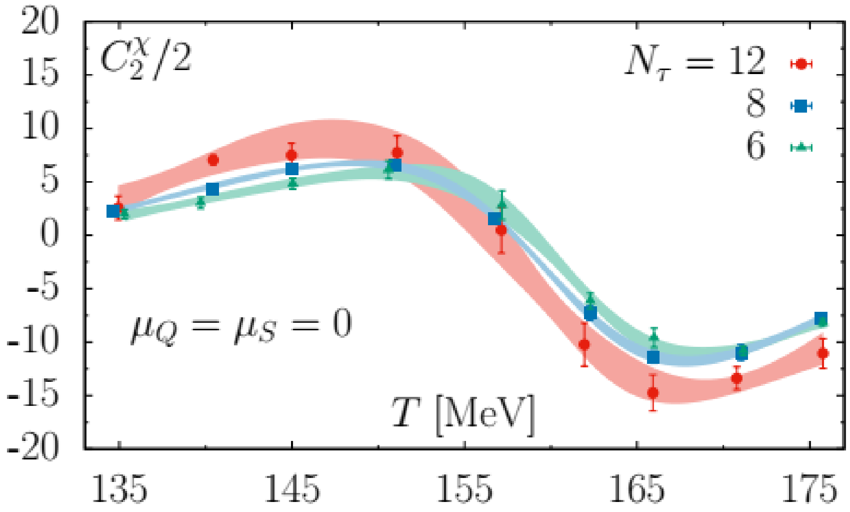
$$T_c^0 = 132^{+3}_{-6}\ \mathrm{MeV}$$

H.-T. Ding et al [HotQCD], arXiv:1903.04801

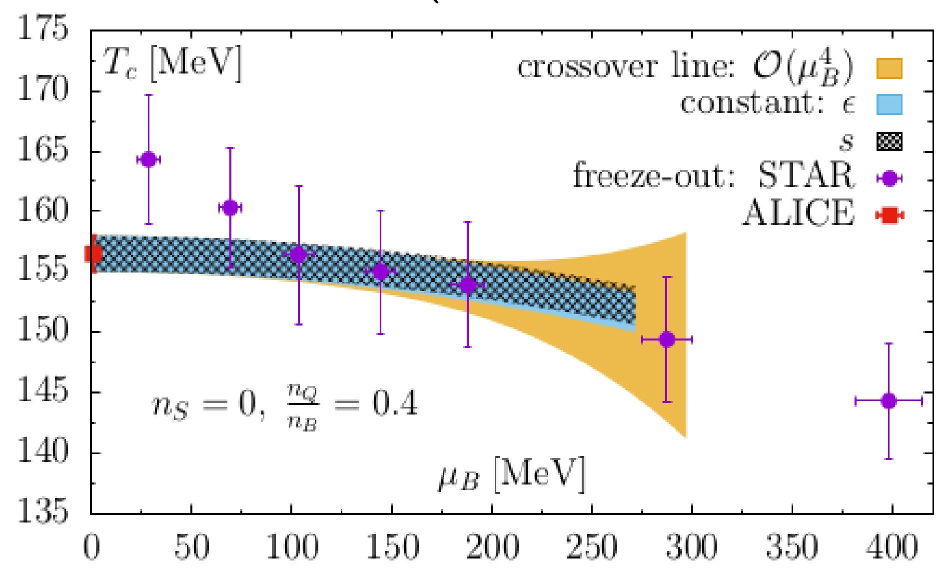
Pseudo-critical (crossover) temperature

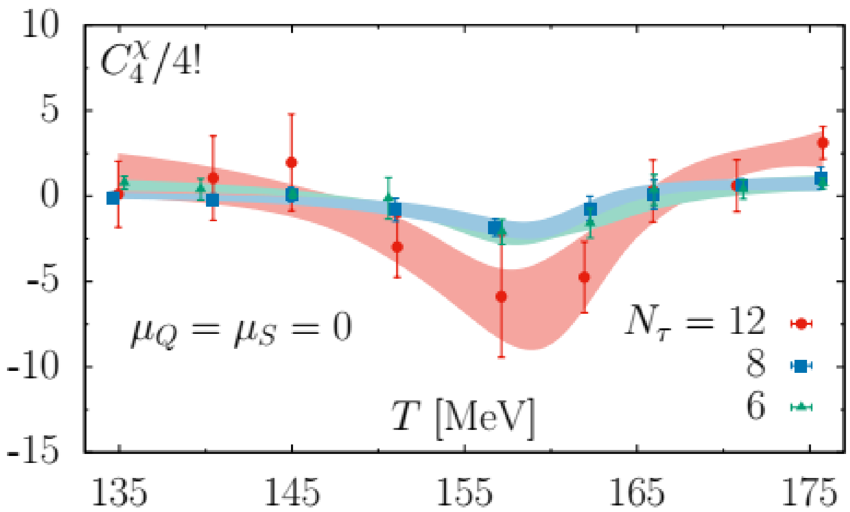
Taylor expansion of chiral susceptibility:

$$\chi_M(T,\mu_B) = m_s \frac{\partial \langle \bar{\psi}\psi \rangle}{\partial m_l} = \chi_M(T,0) + \frac{1}{2} c_2^{\chi}(T) \left(\frac{\mu_B}{T}\right)^2 + \mathcal{O}(\mu_B^4)$$



$$T_{pc}(\mu_B) = T_{pc}\left(1 + \kappa_2 \left(\frac{\mu_B}{T_{pc}}\right)^2 + \ldots\right)$$

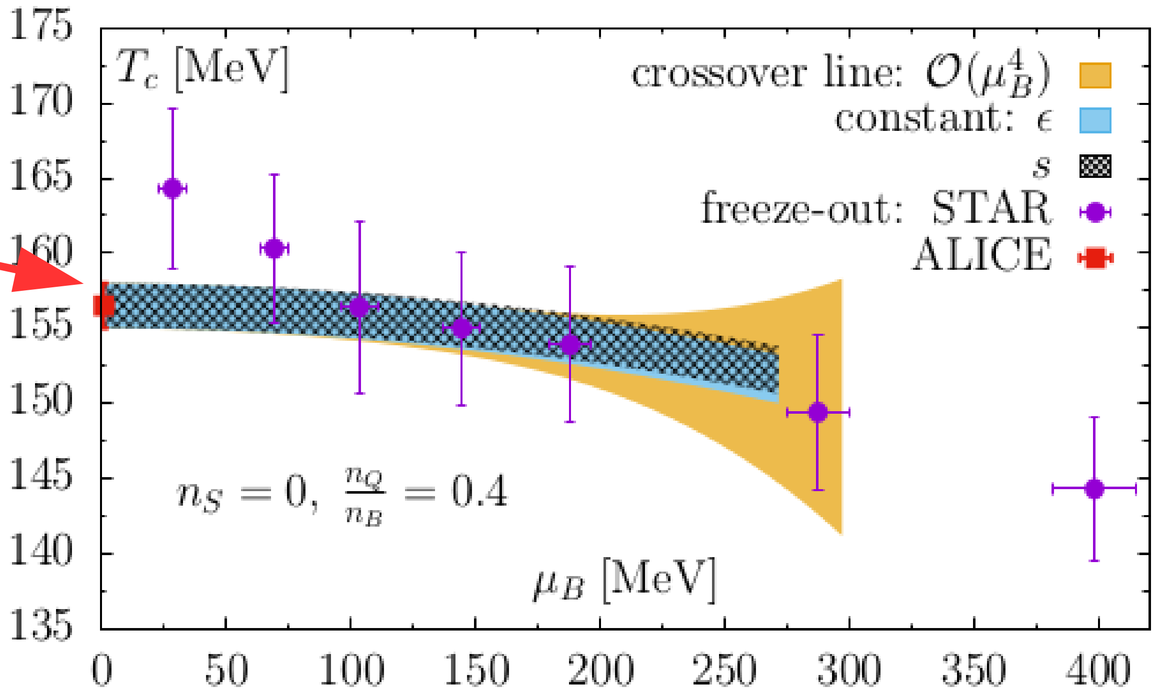




Pseudo-critical (crossover) temperature

$$T_{pc}(\mu_B) = T_{pc}\left(1 + \kappa_2\left(\frac{\mu_B}{T_{pc}}\right)^2 + \ldots\right)$$

A. Andronic et al., Nature 561 (2018) 321



hadrons freeze-out on the pseudo-critical line of the QCD phase transition

$$T_{pc} = (156.5 \pm 1.5)\ \mathrm{MeV} \qquad (158.0 \pm 0.6)\ \mathrm{MeV}$$

$$\kappa_2 = 0.012(4) \qquad 0.0153(18)$$

A. Bazavov et al [HotQCD], arXiv:1812.08235

S. Borsanyi et al., arXiv:2002.02821

Explore the **structure of matter** close to the QCD transition temperature using **fluctuations of conserved charges**

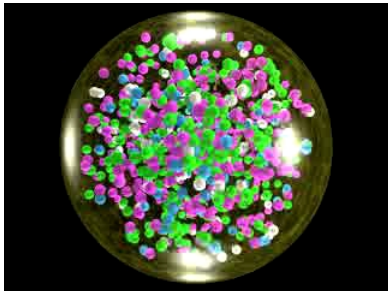
baryon number, strangeness, electric charge

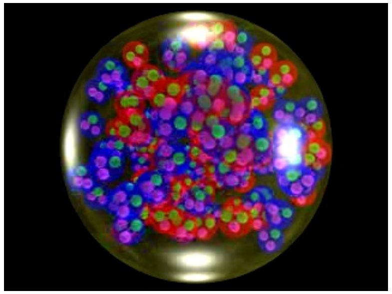
High T: ideal gas

Low T: HRG

ideal quark (fermi) gas, m=0

hadron resonance gas





fractional charges

baryon number: B= +/- 1/3

electric charge: Q= +/- 1/3, +/- 2/3

strangeness: S= +/- 1

integer charges

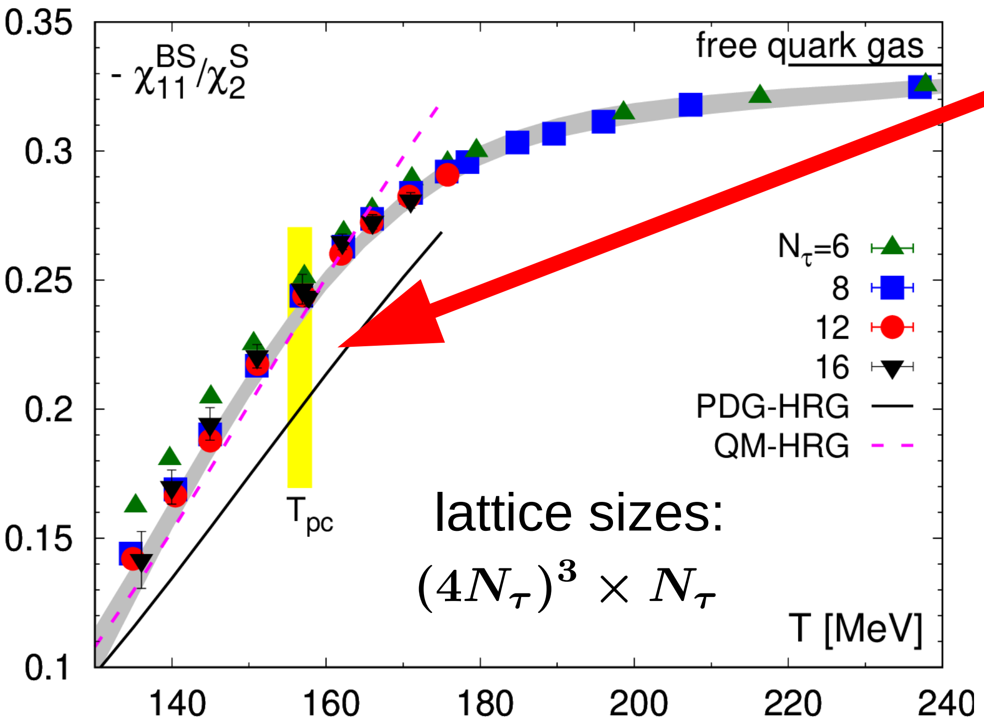
baryon number: B= +/-1

electric charge: Q= 0 =+/- 1, +/- 2

strangeness: S= 0, +/- 1, +/- 2, +/- 3

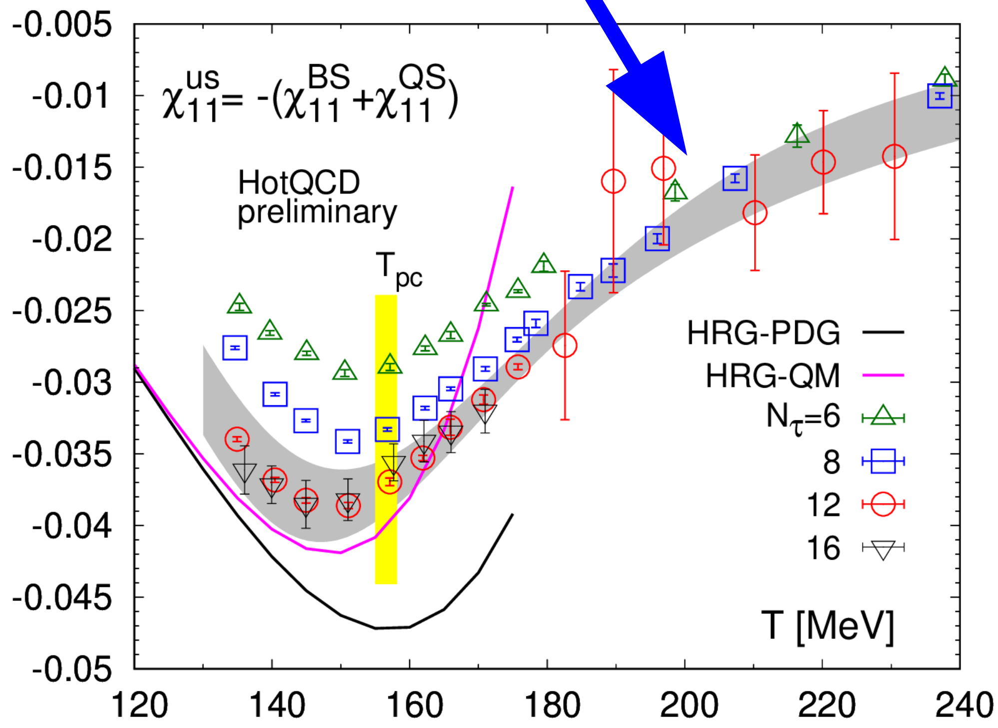
Ratio of baryon number – strangeness correlation and net strangeness fluctuations

state-of-the-art calculations on GPUs



change from **correlated quark flavors inside hadrons**

to almost **uncorrelated quark flavors in the quark gluon plasma**



$$-\frac{\chi_{11}^{BS}}{\chi_2^S} = \frac{1}{3} + \frac{2}{3}\frac{\chi_{11}^{us}}{\chi_2^s}$$

Equation of state of (2+1)-flavor QCD: $\mu_B/T > 0$

Taylor expansion in the chemical potentials

$$\frac{P}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{i,j,k}^{BQS}(T) \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

constrained by external (boundary) conditions, e.g.

- vanishing strangeness
- fixed electric charge to baryon number ratio

$$\frac{P(T,\mu_B)}{T^4} = \frac{P(T,\mu_B=0)}{T^4} + \sum_{n=2}^{\infty} \frac{1}{n!} \bar{\chi}_n^B(T) \left(\frac{\mu_B}{T}\right)^n$$

n-th order coefficients require n inversions of the fermion matrix,e.g.

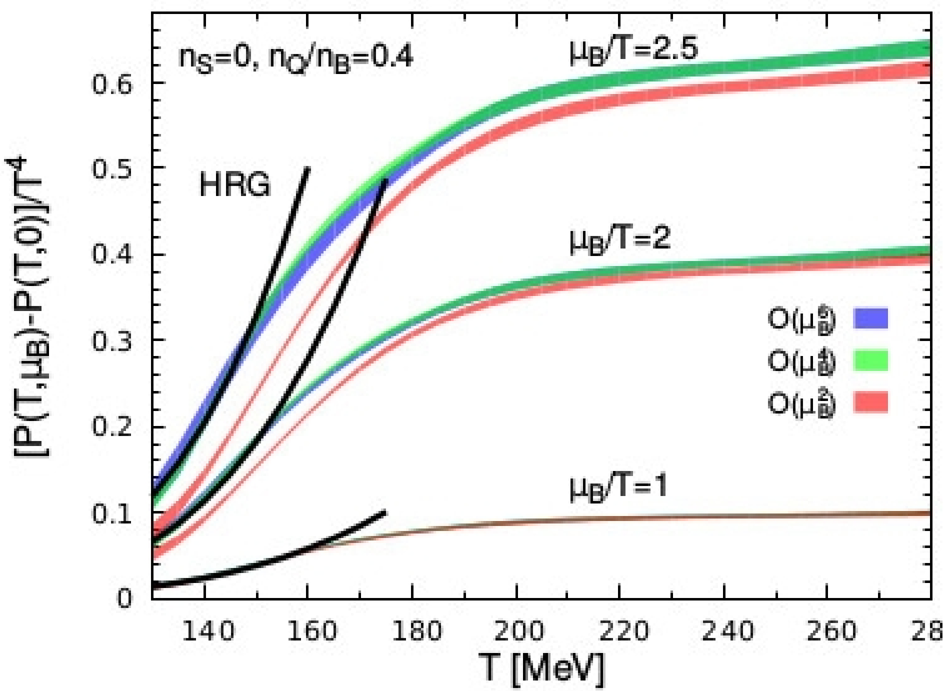
$$\bar{\chi}_n^B \sim \mathrm{Tr} M^{-1} \frac{\partial M}{\partial \mu_B} M^{-1} \frac{\partial M}{\partial \mu_B} ... M^{-1} \frac{\partial M}{\partial \mu_B}$$

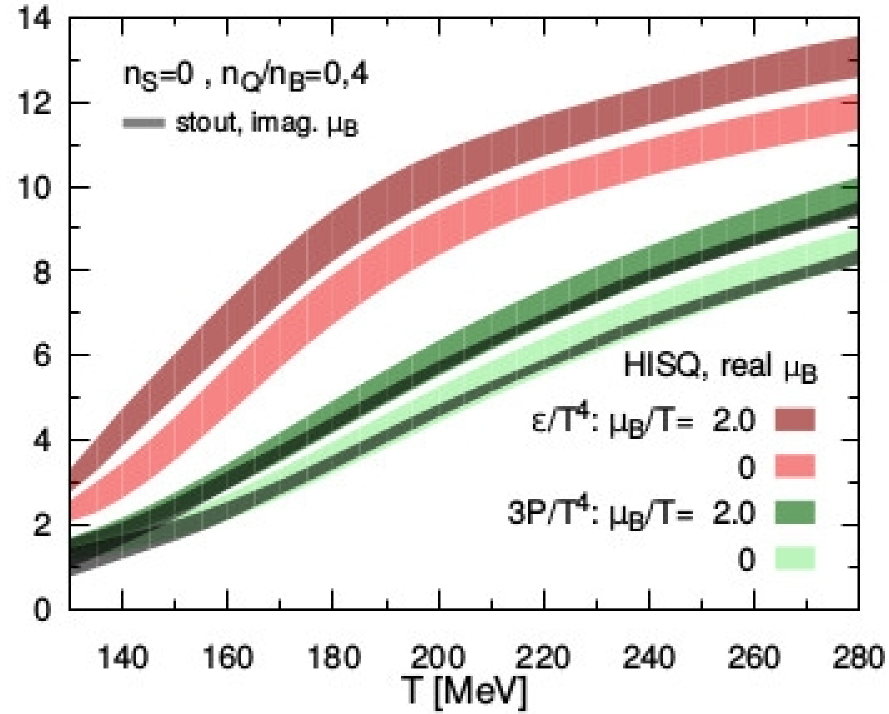
Equation of state of (2+1)-flavor QCD: $\mu_B/T > 0$

$$\frac{P(T,\mu_B)}{T^4} = \frac{P(T,0)}{T^4} + \frac{\chi_2^B}{2}\left(\frac{\mu_B}{T}\right)^2 \Bigg(1 + \frac{1}{12}\frac{\chi_4^B}{\chi_2^B}\left(\frac{\mu_B}{T}\right)^2 + \frac{1}{360}\frac{\chi_6^B}{\chi_2^B}\left(\frac{\mu_B}{T}\right)^4 + \mathcal{O}(\mu_B^6)\Bigg)$$

variance of net-baryon number distribution

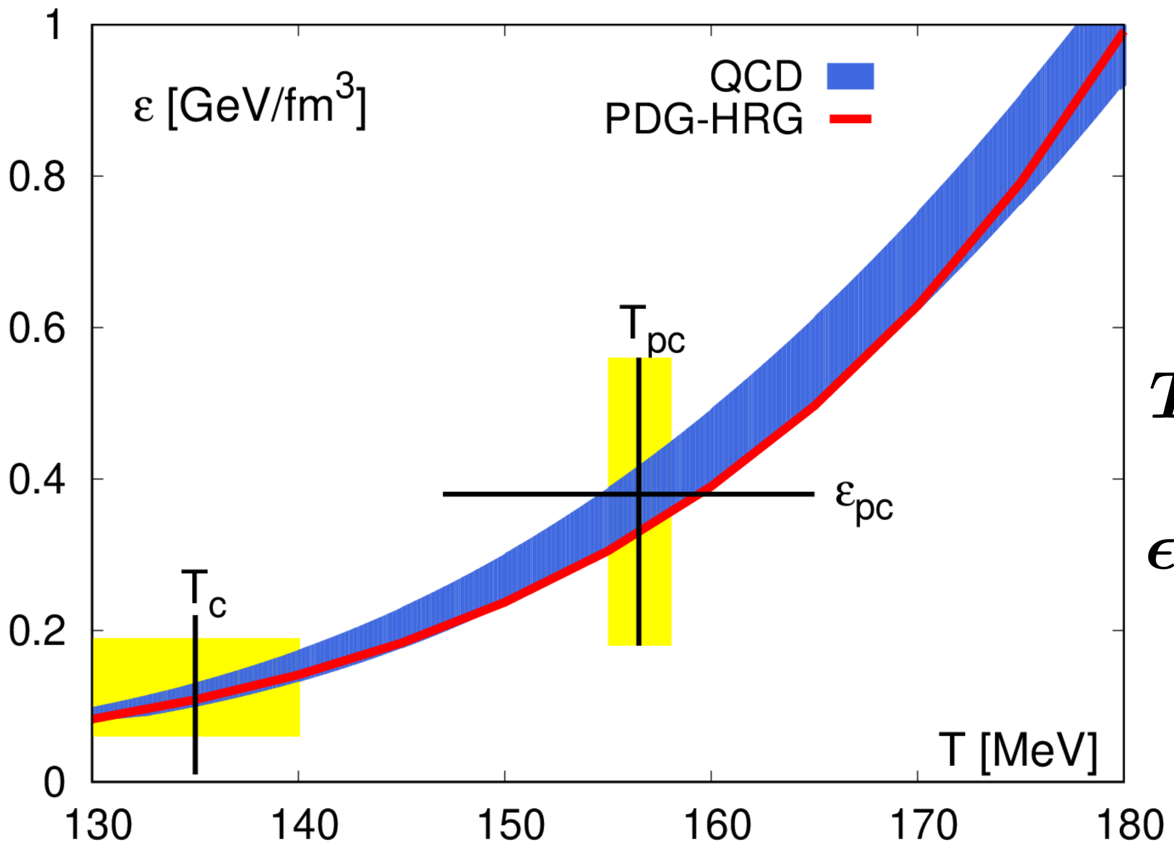
kurtosis*variance





Crossover transition parameters

PDG: Particle Data Group hadron spectrum



$$T_c = (156.5 \pm 1.5)\ \mathrm{MeV}$$

$$\epsilon_c = (380 \pm 120)\mathrm{MeV/fm^3}$$

compare with:

$$\epsilon^{\mathrm{nucl.\ mat.}} \simeq 150\ \mathrm{MeV/fm^3}$$

$$\epsilon^{\mathrm{nucleon}} \simeq 450\ \mathrm{MeV/fm^3}$$

A. Bazavov et al. (HotQCD) ,
Phys. Rev. D90 (2014) 094503

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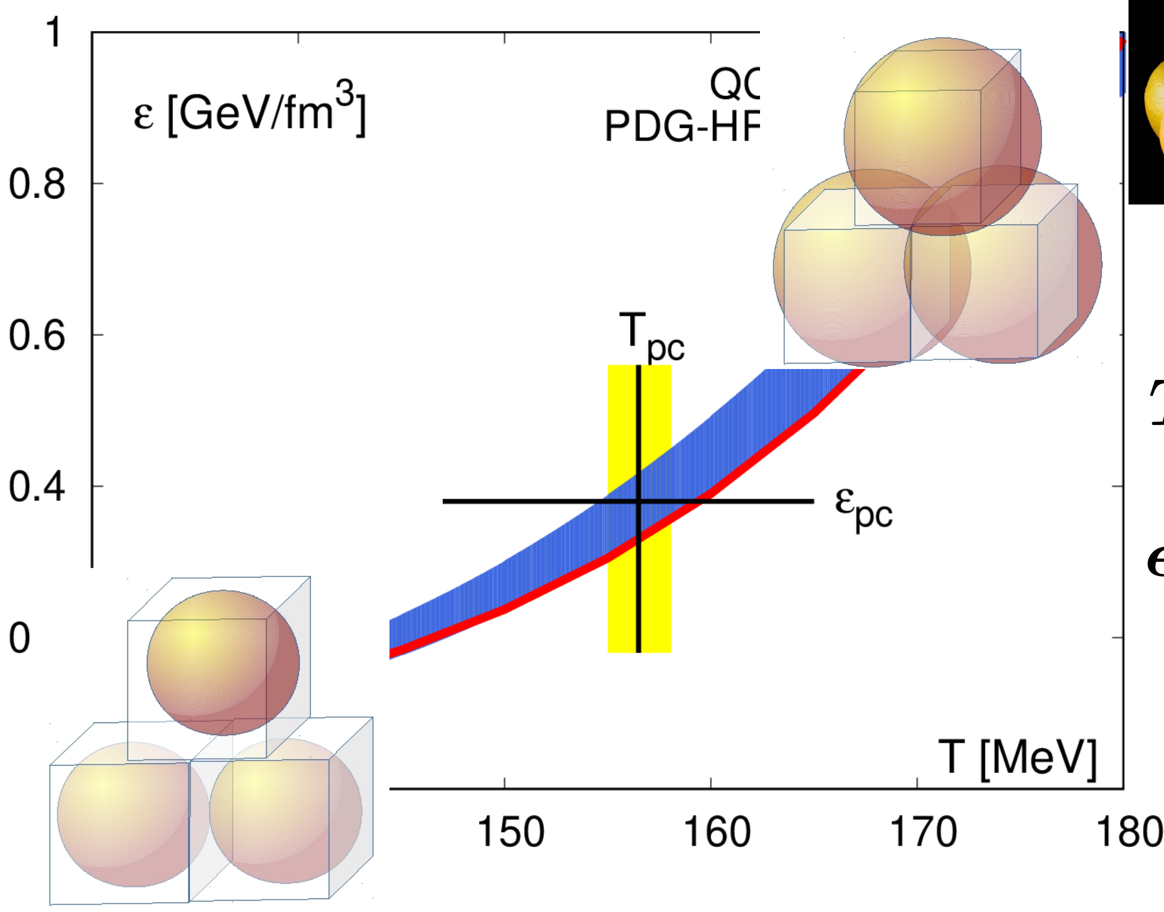

dense packing of spheres (DPS)

$$\epsilon^{\mathrm{DPS}} = 0.74\epsilon^{\mathrm{nucleon}} \simeq 330\ \mathrm{MeV/fm^3}$$

$$(R_p \simeq 0.8\mathrm{fm})$$

overlapping hadrons = QGP ??

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compare with:

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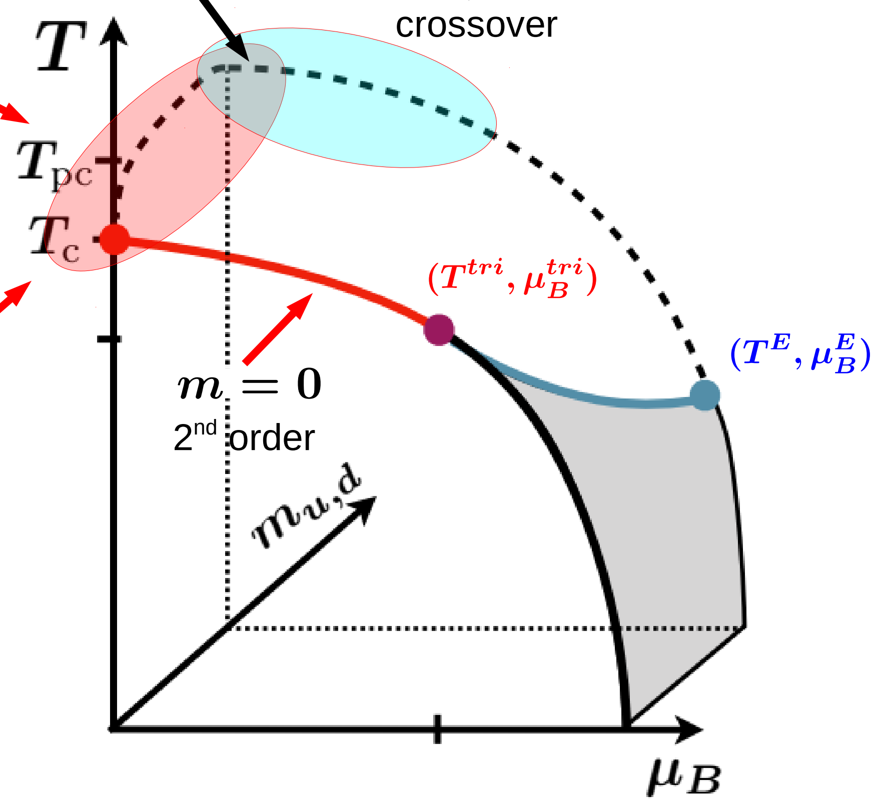
Phase diagram of strongly interacting matter

pseudo-critical temperature drops by 15% when approaching the chiral limit

ALICE, RHIC

pseudo-critical temperature
(156.5 ± 1.5) MeV



the critical point is likely to be located at
$T < 130$ MeV

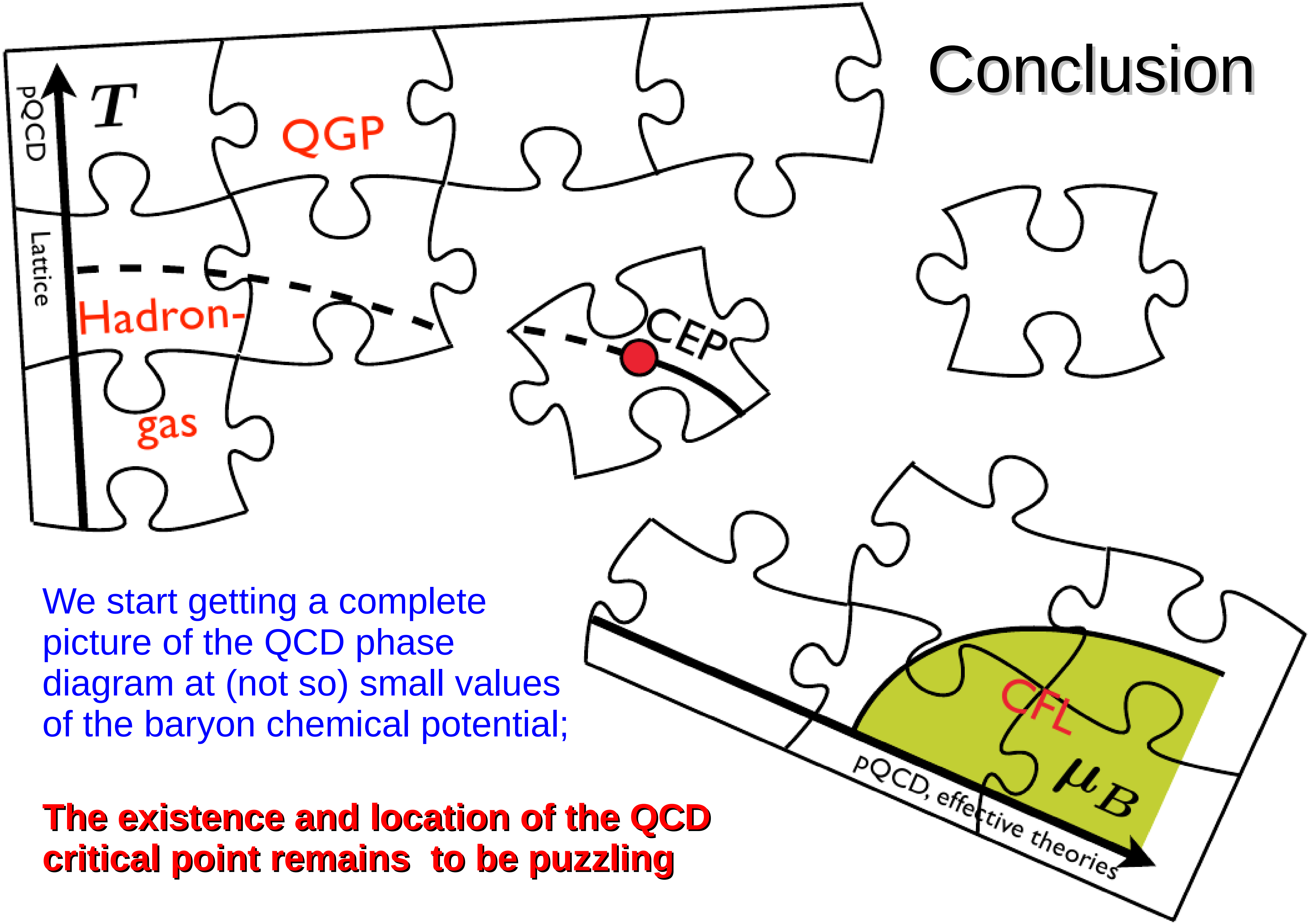
chiral phase transition temperature
132^{+3}_{-6} MeV

"critical" energy density

$$\epsilon_c = (380 \pm 120)\mathrm{MeV/fm}^3$$

transition occurs at roughly constant pion number density $n_\pi \simeq 0.12/\mathrm{fm}^3$

Conclusion



We start getting a complete picture of the QCD phase diagram at (not so) small values of the baryon chemical potential;

The existence and location of the QCD critical point remains to be puzzling

all data shown are based on work done by the HotQCD Collaboration

A. Bazavov, D. Bollweg, H.-T. Ding, P. Enns, J. Goswami, P. Hegde, O. Kaczmarek, F. Karsch, N. Karthik, E. Laermann, A. Lahiri, R. Larsen, S.-T. Li, Swagato Mukherjee, **H. Ohno**, P. Petreczky, H. Sandmeyer, C. Schmidt, S. Sharma, P. Steinbrecher.......

BEST COLLABORATION

CRC-TR 211 Strong-interaction matter under extreme conditions