Lattice QCD at finite temperature using C2PAP

J. Weber[1]

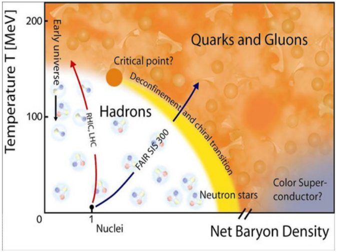
[1]Physik Department, Technische Universität München, Garching

Science Week 2014,
Universe Cluster, Garching

Overview

The QCD phase diagram

QCD phase diagram



'Plasma liquid'

Quarks and gluons are deconfined with **screened** potential.

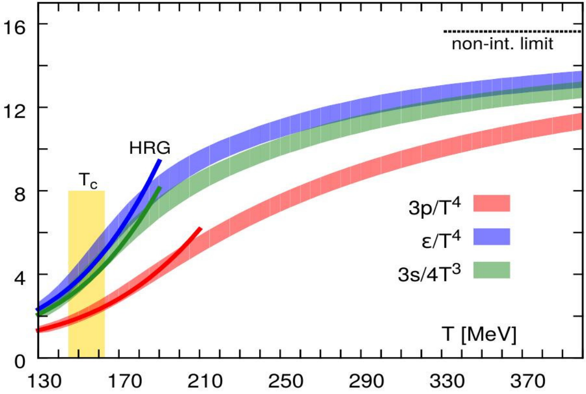
'Hadron gas'

Quarks and gluons are confined into colourless **hadrons**.

Does the QCD medium behave as a liquid?

The equation of state in (2+1)-flavor QCD

A. Bazavov et.al., Phys. Rev. D 90 (2014)



$$\frac{\Theta^{\mu\mu}(T)}{T^4} = \frac{\epsilon - 3p}{T^4} = T\frac{d}{dT}\left(\frac{p}{T^4}\right)$$

Quantum chromodynamics...

on Euclidean space-time...

$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{4g^2}\mathrm{Tr}_c\, F_{\mu\nu}F_{\mu\nu} + \sum_{f=1}^{n_f} \bar{\psi}_f \underbrace{\left[\gamma_\mu D_\mu[A] + m_f\right]} \psi_f$$

Integrate out the fermions

Partition function...

$$\mathcal{Z}_{\mathrm{QCD}} \propto \int \mathcal{D}A \prod_f \overbrace{\det M[A; m_f]}\, e^{-S^g[A,g]}$$

Quantum chromodynamics. . .

on Euclidean space-time. . .

$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{4g^2}\mathrm{Tr}_c\, F_{\mu\nu}F_{\mu\nu} + \sum_{f=1}^{n_f} \bar{\psi}_f \left[\gamma_\mu D_\mu[A] + m_f\right]\psi_f$$

Observables. . .

$$\langle \mathcal{O} \rangle \propto \int \mathcal{D}A\ \mathcal{O}[A] \prod_f \det M[A; m_f] e^{-S^g[A,g]}$$

Quantum chromodynamics. . .

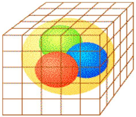
on Euclidean space-time. . .

$$\mathcal{L}_{\mathrm{QCD}} = \frac{\beta}{6}\mathrm{Re\ Tr}\, e^{i\widehat{F_{\mu\nu}}} + \sum_{f=1}^{n_f} \bar{\psi}_f \left[\gamma_\mu \widehat{D_\mu[U]} + m_f\right] \psi_f$$

Observables. . .

$$\langle \mathcal{O} \rangle \propto \frac{1}{N_U} \sum_U \mathcal{O}[U] \prod_f \det M[U; m_f] e^{-S^g[U,\beta]}$$

in a box, on a grid



$4d : N_s^3 \times N_t$

- States must fit into the box

$$a N_s M_\pi \gtrsim 3 - 4$$

Quantum chromodynamics. . .

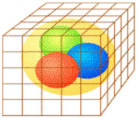
on Euclidean space-time. . .

$$\mathcal{L}_{\text{QCD}} = \frac{\beta}{6} \text{Re Tr}\, e^{i\widehat{F_{\mu\nu}}} + \sum_{f=1}^{n_f} \bar{\psi}_f \left[\gamma_\mu \widehat{D_\mu[U]} + m_f\right] \psi_f$$

Observables. . .

$$\langle \mathcal{O} \rangle \propto \frac{1}{N_U} \sum_U \mathcal{O}[U] \prod_f \det M[U; m_f] e^{-S^g[U,\beta]}$$

in a box, on a grid



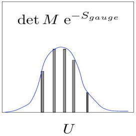
$4d : N_s^3 \times N_t$

- States must fit into the box

$$aN_s M_\pi \gtrsim 3-4$$

- **Finite sample** of gauge fields $\Rightarrow$ give preference to important configurations

Importance sampling



Lattice QCD at finite temperature

Finite temperature comes in here: **1/T**

Finite temperature partition function . . .

$$\mathcal{Z}_{\mathrm{QCD}} \propto \int \mathcal{D}U \prod_f \det M[U; m_f] \exp\left(- \int_0^{1/T} dt \int_{\mathbb{R}^3} d^3x\, \mathcal{L}^g[U(x), \beta] \right)$$

Simulations at fixed temperature

- **Temperature is fixed** by temporal extent of lattice: $T = \frac{1}{a_t N_t}$.
- Lattice simulation always in **thermal equilibrium**.
- Lattice spacing is function of gauge coupling (and quark masses).
- Change temperature by either varying gauge coupling or lattice size.
- **Continuum limit** at fixed temperature: vary both lattice spacing and size.

Lattice QCD simulations step by step

Production requires supercomputers!

- Generate (and store) gauge configurations according to distribution

$$\det M[U;m_f]e^{-S^g[U,\beta]} = e^{-S^g[U,\beta]+\mathrm{Tr}\,\log M[U;m_f]}$$

- Production of gauge configurations exceeds 95% of total computational cost
- Multi-purpose gauge configurations are highly desirable!
- We **recycle Hot QCD configurations** worth $\mathcal{O}(10^8)$ core hours!

Observables are better on supercomputers!

- Preprocess gauge configuration (e.g. gauge fixing, smearing, Wilson flow, . . .)
- Compute observables on preprocessed gauge configuration

Analysis on laptop/desktop/. . .

- Combine ensemble of observables from different gauge configurations
- Extract QCD parameters by fitting the data

Requirements of Lattice QCD simulations

Memory requirements are fairly small

- Aspect ratio 4 – lattice volume V=$N_t \times (4N_t)^3$ – we use $N_t = 4, 6, 8, 12$
- Four gauge fields each site, each SU(3) matrix – 18 Reals per matrix
- Fermion fields, each (four-spinor of) SU(3) vectors – (4 ×) 6 Reals each

Mostly local operations

- Most operations involve only local variables – ideal for parallelisation
- Elementary steps – SU(3) matrix times vector 66 FP operations each
- Fermion matrix is expensive: $V \overset{N_t=12}{\Longrightarrow} 1.3 \times 10^6$ times matrix × vector

Global operations

- Exchange of information between all sublattices – bad for parallelisation
- Updating of gauge fields – accept-reject steps depend on global changes
- Gauge fixing – globally maximise $\sum_n \mathrm{Tr}(U_n + U_n^\dagger)$

What is calculated on C2PAP?

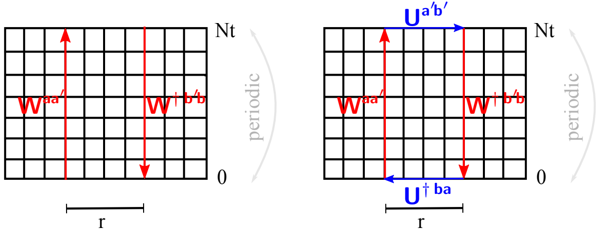
Static quark correlators

- Approximate heavy quarks as **static quarks** Q – no spin, only time evolution
- Represent Q as temporal **Wilson line** (gauge transporter from t=0 to t=τ)

$$W(\mathbf{x},\tau) = \mathcal{P}\exp\left(ig\int_0^\tau dt A_0(t,\mathbf{x})\right)$$

- We compute two types of correlators related to the **static quark potential**

Wilson line correlators | Cyclic Wilson loops

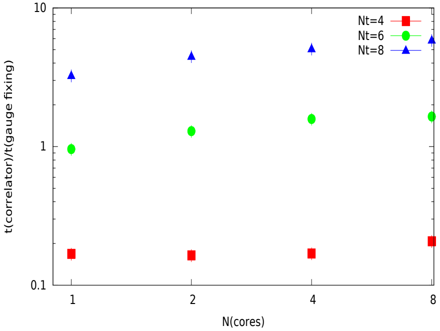


Unless all colour indices are contracted locally & pairwise: **gauge-fixing** required!

Scaling behaviour (I)

Gauge fixing vs correlators

- Different steps of simulations scale differently with number of cores.



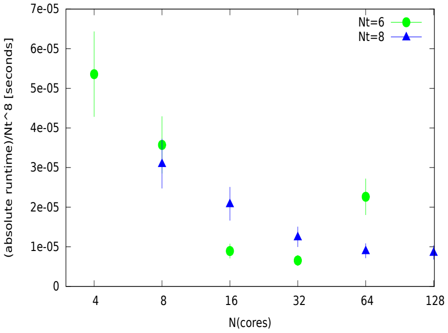
- Global operations (e.g. gauge fixing) relatively less costly for larger N_t

  e.g. Gauge fixing scales approximately as $N_t^{4.6}$

Scaling behaviour (II)

Volume dependence

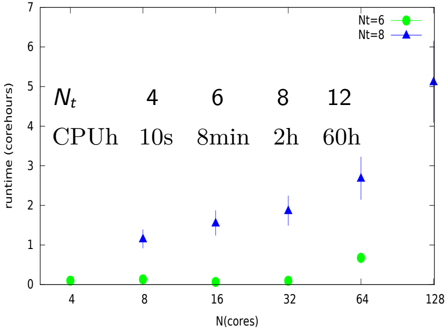
- Number of sites scales as N_t^4 $\Rightarrow$ both ends of paths each scale as N_t^4



- Optimal conditions: $N_t = 6$: 16 cores, $N_t = 8$: 32 cores, ...

total scaling behaviour is approximately N_t^8

Scaling behaviour (III)



N_t	4	6	8	12
CPUh	10s	8min	2h	60h

Corehours

- Runtime in corehours: logarithmic rise or less for single node island
- Significant increase due to communication between node islands

Analysis of finite temperature Lattice QCD simulations

Controlling the cutoff effects

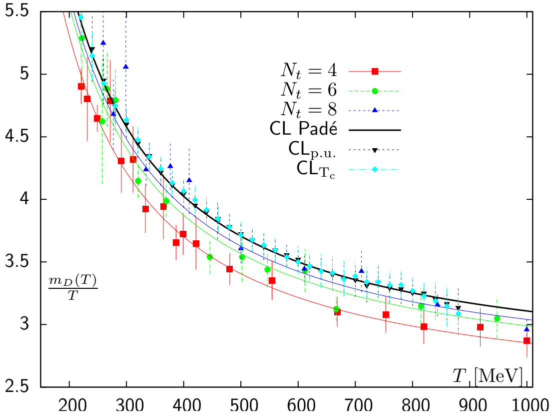
- Vary temperature: repeat "same" simulation with different β (10-25 times)
- Probe cutoff effects: repeat "same" simulations with different N_t (4,6,8,12)
- Currently $\sim$ 90 different ensembles being processed using C2PAP
- About 250.000 configurations were processed within 5 months

Continuum limit

- Interpolate in temperatures (different β) at fixed N_t
- Extrapolate lattice size $N_t \to \infty$ on lines of constant physics
  $\Rightarrow$ need at least 3 different N_t
- For highly improved staggered quarks (HISQ): leading corrections $\mathcal{O}(\alpha_s N_t^{-2})$
- Simultaneous fit in both T and N_t

Taking the continuum limit – an example

Screening mass



Summary

- C2PAP is an excellent device for Lattice QCD simulations
- We observe good scaling of our codes on C2PAP
- We are running both production and measurement codes on C2PAP

- QCD at fixed temperature can be studied in lattice QCD
- Need ~ 10 or more different gauge couplings for varying T at each N_t
- Need at least 3 different lattice sizes N_t for continuum limit

- Static quarks are represented by Wilson lines in lattice QCD
- Fractional cost of preprocessing decreases with increasing lattice size
- Computational cost of static quark correlators scales as N_t^8