The QCD transition temperature from simulations on BlueGene L supercomputer at LLNL

Rajan Gupta

T-8, Los Alamos National Lab

The HotQCD collaboration

(All HotQCD data are preliminary)
RHIC: What we don’t know a priori

- The nature (order) of the transition between hadronic matter and QGP
- The transition temperature $T_c$
- The equation of state (at $< T_c - 5 T_c$)
- The transport properties of the QGP
- Behavior of bound states (onia) in the QGP
- Collective excitations
- The process of hadronization
- The process of thermalization
# QCD at finite temperature

**HotQCD Collaboration:** A unique US wide opportunity for simulating QCD at finite temperature using the BlueGene L Supercomputer at LLNL

<table>
<thead>
<tr>
<th>T. Battacharya (LANL)</th>
<th>L. Levkova (Utah)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M. Cheng (Columbia)</td>
<td>T. Luu (LLNL)</td>
</tr>
<tr>
<td>N. Christ (Columbia)</td>
<td>R. Mawhinney (Columbia)</td>
</tr>
<tr>
<td>C. DeTar (Utah)</td>
<td>P. Petreczky (BNL)</td>
</tr>
<tr>
<td>S. Gottlieb (Indiana)</td>
<td>D. Renfrew (Columbia)</td>
</tr>
<tr>
<td>R. Gupta (LANL)</td>
<td>C. Schmidt (BNL)</td>
</tr>
<tr>
<td>U. Heller (APS)</td>
<td>R. Soltz (LLNL)</td>
</tr>
<tr>
<td>K. Huebner (BNL)</td>
<td>W. Soeldner (BNL)</td>
</tr>
<tr>
<td>C. Jung (BNL)</td>
<td>R. Sugar (UCSB)</td>
</tr>
<tr>
<td>F. Karsch (BNL/Bielefeld)</td>
<td>D. Toussaint (Arizona)</td>
</tr>
<tr>
<td>E. Laermann (Bielefeld)</td>
<td>P. Vranas (LLNL)</td>
</tr>
</tbody>
</table>
Timeline

• Developed collaboration with Ron Soltz and formulated project for Blue Gene L at LLNL (Nov-Dec 2005)
• Organized US wide meeting to explore doing RHIC phenomenology and Lattice QCD at LLNL (Feb 06)
• Developed white paper for calculation of $T_c$ and EOS on the Blue Gene L (Feb – May 06)
• Got NNSA approval to run on Blue Gene L (July 06)
• Ported Asqtad and p4fat codes to Blue Gene L (Sept 06)
• Started $N_T=8$ lattice QCD simulations (Oct 06)
• Continual code Optimization
• ~10,000 trajectories simulated at $15\beta$ for AsqTad & p4
Restrictive Environment

• Only T. Luu, R. Soltz and R. Gupta can access the machine or the data
• Minimal data can be brought into open
  – Print results in ASCII or print figures
  – Declassify
  – Scan to convert to digital for distribution

Blue Gene L at LLNL represents a 4-6 Teraflops sustained resource
HotQCD Collaboration: Goals

- **Nature of the transition**
  - Do deconfinement and $\chi S$ restoration "coincide"?

- **Transition temperature $T_c$**

- **Equation of State (EOS) at ($\mu = 0, \mu \neq 0$)**

- **Spectral Functions**

- **Spatial and temporal correlators versus $T$**

- **Transport coefficients of the quark gluon plasma**
Order of the transitions and $T_c$

- Look for discontinuities, singularities, peaks in thermodynamics quantities
  - Polyakov line and its susceptibility
  - Chiral condensate $\langle \bar{\psi} \psi \rangle$ and its susceptibility
  - Quark number $\langle \bar{\psi} \gamma_0 \psi \rangle$ and its susceptibility

- Finite size scaling analysis (1$^{\text{st}}$ versus 2$^{\text{nd}}$)

Previous Staggered simulations →
For 2+1 (ud, s) quark flavors the transition is a crossover
Observables

Polyakov loop
Quark number susceptibility
Chiral condensate
Chiral susceptibility

\[ \chi_S \text{ Restoration} \]

\[ \text{Deconfinement} \]
Issues with previous calculations (in 2005)

• Calculations on coarse lattices: $N_T=4,6$ and/or small volumes. ($a \sim 0.2$- 0.13 fermi).
  – Simulate $N_T=4,6,8, \ldots$ and do $a\rightarrow0$ extrapolation

• $T_c$ with different actions (different observables) differ by $\sim 20$ MeV
  – Reduce uncertainty to $\sim 5$ MeV if transition $T$ is unique

• Need simulations with 2+1 flavors with realistic light (up, down) quark masses holding strange quark mass fixed
  – $M_{ud} / m_s = 0.5, 0.2, 0.1 \rightarrow$ (physical $\sim 0.04$)

• Staggered fermions ($\det M^{1/4}$): Creutz/Kronfeld at LAT07
Improving continuum limit results

• Control discretization errors (compare 2 different improved staggered actions)
  – Asqtad Staggered (MILC collaboration)
  – p4 staggered (RBC-Bielefeld collaboration)
  – Explore Domain wall fermions

• New simulations at $N_T=8$ with 2+1 flavors ($m_{\text{light}} \approx 0.1 \ m_s$)

• Combine with ongoing/previous $N_T = 4,6$ simulations to perform $a \rightarrow 0$ extrapolation

• Precise determination of lattice scale
Status report: HOTQCD data sets
**P4 action $N_\tau$=8 simulations:** Status 7/21/07

- Lattice Size $8\times32\times32\times32$
- Quark mass $m_l/m_s = 0.1$

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$a m_l$</th>
<th>$T$ [MeV]</th>
<th># trajectories</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.460</td>
<td>0.00313</td>
<td>154</td>
<td>10000</td>
</tr>
<tr>
<td>3.490</td>
<td>0.00290</td>
<td>169</td>
<td>10000</td>
</tr>
<tr>
<td>3.510</td>
<td>0.00259</td>
<td>179</td>
<td>11280</td>
</tr>
<tr>
<td>3.540</td>
<td>0.00240</td>
<td>194</td>
<td>11440</td>
</tr>
<tr>
<td>3.570</td>
<td>0.00212</td>
<td>209</td>
<td>12460</td>
</tr>
<tr>
<td>3.600</td>
<td>0.00192</td>
<td>225</td>
<td>11790</td>
</tr>
<tr>
<td>3.630</td>
<td>0.00170</td>
<td>241</td>
<td>12070</td>
</tr>
<tr>
<td>3.660</td>
<td>0.00170</td>
<td>256</td>
<td>11190</td>
</tr>
<tr>
<td>3.690</td>
<td>0.00150</td>
<td>271</td>
<td>10760</td>
</tr>
<tr>
<td>3.760</td>
<td>0.00139</td>
<td>313</td>
<td>10920</td>
</tr>
<tr>
<td>h3.525</td>
<td>0.00240</td>
<td>186</td>
<td>6510</td>
</tr>
<tr>
<td>h3.530</td>
<td>0.00240</td>
<td>189</td>
<td>5450</td>
</tr>
<tr>
<td>h3.535</td>
<td>0.00240</td>
<td>191</td>
<td>5140</td>
</tr>
<tr>
<td>h3.540</td>
<td>0.00240</td>
<td>194</td>
<td>5410</td>
</tr>
<tr>
<td>h3.545</td>
<td>0.00240</td>
<td>196</td>
<td>6280</td>
</tr>
<tr>
<td>h3.550</td>
<td>0.00240</td>
<td>199</td>
<td>5790</td>
</tr>
<tr>
<td>c3.525</td>
<td>0.00240</td>
<td>186</td>
<td>6120</td>
</tr>
<tr>
<td>c3.530</td>
<td>0.00240</td>
<td>189</td>
<td>5530</td>
</tr>
<tr>
<td>c3.535</td>
<td>0.00240</td>
<td>191</td>
<td>5750</td>
</tr>
<tr>
<td>c3.540</td>
<td>0.00240</td>
<td>194</td>
<td>6260</td>
</tr>
<tr>
<td>c3.545</td>
<td>0.00240</td>
<td>196</td>
<td>6250</td>
</tr>
<tr>
<td>c3.550</td>
<td>0.00240</td>
<td>199</td>
<td>6520</td>
</tr>
</tbody>
</table>
Asqtad action data set as of 7/21/07

Lattice Size $8 \times 32 \times 32 \times 32$; Quark mass $m_l/m_s = 0.1$

<table>
<thead>
<tr>
<th>$\beta=6/g^2$</th>
<th>$\delta t$</th>
<th>Acceptance</th>
<th>$&lt;\Delta s \exp(-\Delta s/2)&gt;10^3$</th>
<th>Total # trajectories</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.4580</td>
<td>0.04170</td>
<td>0.66</td>
<td>-4.9 +/- 9.4</td>
<td>12965</td>
</tr>
<tr>
<td>6.5000</td>
<td>0.04170</td>
<td>0.72</td>
<td>3.7</td>
<td>12990</td>
</tr>
<tr>
<td>6.5500</td>
<td>0.04170</td>
<td>0.76</td>
<td>-4.5</td>
<td>12720</td>
</tr>
<tr>
<td>6.6000</td>
<td>0.04170</td>
<td>0.78</td>
<td>-1.5</td>
<td>12405</td>
</tr>
<tr>
<td>6.6625</td>
<td>0.04170</td>
<td>0.79</td>
<td>8.1</td>
<td>12365</td>
</tr>
<tr>
<td>6.6500</td>
<td>0.04540</td>
<td>0.76</td>
<td>2.8</td>
<td>12445</td>
</tr>
<tr>
<td>6.6675</td>
<td>0.04540</td>
<td>0.75</td>
<td>3.9</td>
<td>12660</td>
</tr>
<tr>
<td>6.7000</td>
<td>0.04540</td>
<td>0.81</td>
<td>-9.7</td>
<td>12320</td>
</tr>
<tr>
<td>6.7600</td>
<td>0.04540</td>
<td>0.83</td>
<td>2.0</td>
<td>12530</td>
</tr>
<tr>
<td>6.8000</td>
<td>0.04540</td>
<td>0.84</td>
<td>-3.4</td>
<td>12195</td>
</tr>
<tr>
<td>6.8500</td>
<td>0.04540</td>
<td>0.86</td>
<td>2.2</td>
<td>12405</td>
</tr>
<tr>
<td>6.9000</td>
<td>0.04540</td>
<td>0.86</td>
<td>3.4</td>
<td>12470</td>
</tr>
<tr>
<td>6.9500</td>
<td>0.04540</td>
<td>0.86</td>
<td>1.5</td>
<td>12625</td>
</tr>
<tr>
<td>7.0000</td>
<td>0.04540</td>
<td>0.87</td>
<td>-2.9</td>
<td>12595</td>
</tr>
<tr>
<td>7.0800</td>
<td>0.04540</td>
<td>0.86</td>
<td>3.6</td>
<td>12790</td>
</tr>
</tbody>
</table>

About 70% of target 15000 trajectories (statistics) achieved
AsqTad calculations and deductions
R algorithm and finite size effects

(Connected Chiral Susceptibility)

- Errors in data with R algorithm are small (below resolution)
- Finite size effects are most pronounced at low T
Finite volume correction:
(Disconnected chiral susceptibility)

Large spatial volume is important.

\[ N_\text{s} = 4 N_\tau \approx \text{infinite volume} \]
Singlet chiral susceptibility

Finite size effect tends to decrease $T_c$ slightly

$16^3$: 184(2) MeV

$32^3$: 186(2)

Errors shown are only statistical for this fit ansatz!

Systematic errors yet to be determined.
Renormalized singlet susceptibility (Raw versus Wuppertal-Budapest method)

Small (few MeV) difference in peak position
Strange quark number susceptibility

It is more difficult to estimate $T_c$ from fits to determine the inflection point than from a peak.
Polyakov Loop Data

Inflection point in $P$ is difficult to locate accurately.

Peak in susceptibility of $P$ hard to distinguish from a plateau/shoulder by $N_\tau=8$. 
Data with p4 action
P4: Line of constant physics (LCP)

- Use $T=0$ simulations
- $M_{ss} \, r_0 = 1.58 \quad (M_\pi \, r_0 \approx 0.52 \rightarrow M_\pi \approx 220 \text{ MeV})$
- Quark mass $m_l/m_s = 0.1$ (real world $\sim 0.04$)
- Take $a \rightarrow 0$ along this LCP varying just the gauge coupling $\beta$
P4: Setting the lattice scale

Jan van der Heide at LAT2007

\[
\left( r^2 \frac{dV_{\bar{q}q}(r)}{dr} \right)_{r=r_0} = 1.65, \quad \left( r^2 \frac{dV_{\bar{q}q}(r)}{dr} \right)_{r=r_1} = 1.0
\]

\[
r_0 = 0.469(7) \text{ fm}, \quad r_0 \sigma^{0.5} = 1.104(5), \quad r_0/r_1 = 1.463(7)
\]
Renormalized Polyakov Loop

\[ \langle L_R \rangle = Z(\beta)^{N_\tau} \langle L_{\text{Bare}} \rangle \]

(Kostya Petrov at LAT07)

- Smooth behavior
- \( N_\tau = 4, 6, 8 \) don’t show large \( O(a^2) \) effects

In all figures the band corresponds to the range \( T=185-195 \text{ MeV} \)
Chiral Condensate: $\chi S$ restoration

$$\Delta_l = \frac{\langle \bar{l}l \rangle_T - \frac{m_l}{m_s} \langle \bar{s}s \rangle_T}{\langle \bar{l}l \rangle_{T=0} - \frac{m_l}{m_s} \langle \bar{s}s \rangle_{T=0}}$$

- Subtraction to eliminate additive renormalization
- Sharp decrease in $\Delta$ reflects $\chi S$ restoration
\( N_\tau = 8 \): P4 consistent with AsqTAD
$T_{\chi S} \text{ Restoration} \approx T_{\text{Deconfinement}}$
Quark Number Susceptibility

\[ \frac{\chi_{l,s}}{T^2} = \frac{1}{TV} \frac{\partial^2 \log Z}{\partial \mu^2_{l,s}} \]

- States carrying such quantum numbers (\( \langle \bar{\psi}\gamma_0\psi \rangle \rightarrow \text{baryon number/strangeness} \)) are heavy at low \( T \) and light at high \( T \). Probe confinement
- Do not require renormalization at \( V=\infty \)
- Peak in fourth derivative!
Quark Number Susceptibility

P4 data consistent with AsqTAD

Determination of Tc from inflection point sensitive to
- Range of data points included in the fit (8 points)
- Fit function
\[ \Delta_{s,l} \text{ and } \chi_s/T^2 \]

- Smooth behaviour
- \( N_\tau = 4,6,8 \) don’t show large \( O(a^2) \) effects
- Crossover at roughly the same \( T \)
Chiral Susceptibility: $N_\tau = 4, 6, 8$

One flavor susceptibility for light ($l = u,d$) and strange ($s$) quarks:

$$\frac{\chi_{l,s}}{T^2} = \frac{T}{V} \frac{\partial^2 \log Z}{\partial^2 m_{l,s}^2} = \left\langle \text{Tr}(M_{l,s}^{-2}) \right\rangle + \frac{1}{4} \left( \left\langle \text{Tr}M_{l,s}^{-1} \right\rangle^2 - \left\langle \text{Tr}M_{l,s}^{-1} \right\rangle^2 \right)$$

Connected

Disconnected

Note: Isosinglet $\chi = \chi_{\text{disconnected}} + 2\chi_{\text{connected}}$

One flavor $\chi = \chi_{\text{disconnected}} + 4\chi_{\text{connected}}$
p4 (RBC-B) analysis

- Very Weak Volume dependence → Crossover
- Peaks become sharper with increasing V and decreasing quark mass
- Peak shift towards smaller $\beta$
Chiral Susceptibility: $N_\tau = 8$

Connected

Disconnected
Chiral Susceptibility $\chi$: $N_\tau = 8$

Total Susceptibility for light ($l = u,d$) quarks:

Unrenormalized $\Rightarrow$ only examine shape not value

Need more $N_\tau=8$ data to quantify [dis]agreement in the region of the peak before combining with $N_\tau=4, 6$ to extract $T_c(a=0)$
HotQCD: Future

- Complete $N_\tau = 8$ simulations
- Finish analysis of all the variables
- Combine $N_\tau = 4, 6, 8$ calculations
- Extract transition temperature at which bulk quantities show largest fluctuations
- Resolve Deconfinement versus $\chi S$ restoration
Much progress with staggered 2+1 simulations in last 2 years

- Exact Algorithm -- RHMC
- Finite Volume
  - $N_s \geq 4 N_T$
  - Peaks become sharper with larger $V$
  - Height approx. independent of $V$ ($\to$ crossover)
- Renormalization of observables
- Improvement of action works
  - $(N_T = 6, 8)$ P4 and $A_{\text{sqTad}} \approx (N_T = 8, 10)$ Stout
- Reaching physical masses
  - P4 and $A_{\text{sqTad}}$ ($m_l = 0.1\,\text{ms}$); Stout ($m_l = 0.04\,\text{ms}$)
- Setting the scale with $T=0$ simulations
  - Using $r_0$, $f_K$ ($\sim 10\,\text{MeV}$ difference)
- Continuum extrapolations ($N_T = 4, 6, 8, \ldots$)
Remaining Issues

• Resolving $T_{\text{deconfinement}}$ and $T_{\chi_{SB}}$ in $a \rightarrow 0$
• Improve determination of lattice scale
Fodor etal: different observables give different $T_c$

\[\text{use } T=0\text{ scale: } r_0=0.469\text{fm}\]

$N_f=2$:  
(improved Wilson, $N_t=8$, 10; input: $r_0=0.5$ fm)  
(rescaled to $r_0$)

Y. Maezawa et al., hep-lat/0702005 (QM’2006)  
(improved Wilson, $N_t=4$, 6; input: $m$–rho)  
(no cont. exp. yet)

$N_f=2=1$:  
(improved staggered (asqtad), $N_t=4,6,8$, input r1)  
(rescaled to $r_0$)

(improved staggered (p4), $N_t=4,6$; input r0)

(staggered (stout), $N_t=4,6,8,10$; input fK)  
(converted to $r_0$)

Important for RHIC

$\epsilon_C \sim T_c^4$  
$\epsilon_C = (0.3 - 1.0)\text{GeV/fm}^3$
Issues with “best” calculations

Known shortcomings:

- too few data: 3-parameter fit to 4 data points for $T_c$ determined at $m_\pi > 550$ MeV
- no continuum extrapolation attempted yet; would like to see results in units of $r_0$
- $N_\tau = 4, 6, 8$, but small spatial volume for larger $N_\tau$; still large statistical errors on individual data points
- only $N_\tau = 4$ and 6
- only one quark mass; $T_c$ determination partly based on determination of inflection points

Karsch Lat07
Stout Action: Summary  (Fodor LAT2007)

Chiral susceptibility

\[ T_c = 151(3)(3) \text{ MeV} \]
\[ \Delta T_c = 28(5)(1) \text{ MeV} \]

Quark number susceptibility

\[ T_c = 175(2)(4) \text{ MeV} \]
\[ \Delta T_c = 42(4)(1) \text{ MeV} \]

Polyakov loop

\[ T_c = 176(2)(4) \text{ MeV} \]
\[ \Delta T_c = 38(5)(1) \text{ MeV} \]
Stout Action versus p4/AsqTad

- Main disagreement with p4 & AsqTad

- Chiral susceptibility
  \[ T_c = 151(3)(3) \text{ MeV} \]
  \[ \Delta T_c = 28(5)(1) \text{ MeV} \]

- Quark number susceptibility
  \[ T_c = 175(2)(4) \text{ MeV} \]
  \[ \Delta T_c = 42(4)(1) \text{ MeV} \]

- Polyakov loop
  \[ T_c = 176(2)(4) \text{ MeV} \]
  \[ \Delta T_c = 38(5)(1) \text{ MeV} \]

T_c determined from inflection point
Issues in Crossover phenomena
(emphasized by Y. Aoki etal.)

Away from a phase transition, different observables can show largest fluctuations (defining the transition point) at different $T$

Difference should vanish as $m_l \rightarrow 0$
P4 versus stout

Stout: Much Larger O(a^2) errors
T (stout) smaller by ~30 Mev T(p4)
Stout: Can normalization & scale explain the 25 MeV difference between $T_{\chi S \text{ Restoration}}$ and $T_{\text{deconfinement}}$?

Important Role of: Data at $N_\tau = 8, 10$

Lattice scale? (Is $a(f_K) \approx a(r_0)$ as $a \to 0$?)

Changes made:
- $m^2\chi / T^4 \to \chi / T^2$
- $a(f_K) \to a(r_0)$
What next?

- Improve p4 and AsqTad continuum extrapolation (Finalize $N_\tau=8$ HotQCD data)

- Final HotQCD data unlikely to change the current qualitative picture $T_{\text{deconfinement}} \approx T_{\chi_{SB}}$ and lying in the band 185-195 MeV

- Resolve difference in $T_{\chi_{SB}}$ between stout and hotQCD results