First Summit results
Lattice QCD at non-zero baryon density
Quantum Chromodynamics (QCD)

- Proton
- Quarks
- Gluons

1% of proton mass = quark mass
99% of proton mass = kinetic energy of gluons & quarks

Color Charge
Strong Force
Confinement
What happens if you make things hotter and hotter?

What happens if you keep squeezing and squeezing?
Phases of Water

Pressure

Solid

Liquid

Gas

Temperature
The QCD phase diagram
Relativistic Heavy Ion Collider
Beam Energy Scan Theory

- HotQCD is part of BEST and its mission is to provide critical input for the **Beam Energy Scan II** which is performed now.
Simulating Quantum Chromodynamics from first principles

- discretize Dirac equation
  \[
  (i\gamma^\mu \partial_\mu - m) \psi = 0
  \]
- calculate path integral using monte carlo methods
  \[
  \langle O \rangle = \frac{1}{Z} \int D U \quad O \exp (-S)
  \]

Lattice QCD

\[
V = (aN_\sigma)^3
\]
\[
T = \frac{1}{aN_\tau}
\]

e.g. 4-dimensional Lattice \( N_\sigma^3 \times N_\tau \)
The Lattice QCD Kernel

\[
\text{Tr } M^{-1} = \lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} M^{-1} \eta_k \eta_k^\dagger
\]

- evaluate traces using \( N \) random noise vectors \( \eta \)
- solve \( M^{-1} \eta_k \) using Conjugate Gradient

condition:
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} \eta^*_k \eta_k = \delta_{ij}
\]

99% of runtime
Conjugate Gradient

1. calculate stencil operator  
   (66% of runtime)
2. call multiple STREAM kernels  
   (33% of runtime)
3. repeat

- no optimizations possible for 2.
  - performance determined by memory bandwidth
Stencil Operator

\[ w_n = \sum_{\mu=0}^{4} \left[ (U_{n,\mu} v_{n+\mu} - U_{n-\mu,\mu}^\dagger v_{n-\mu}) + (N_{n,\mu} v_{n+3\mu} - N_{n-3\mu,\mu}^\dagger v_{n-3\mu}) \right] \]

- complex 3-dim vector
- complex 3x3 matrix
- U(3) matrix
- reconstruct from 14 floats
- matrix
- vector
Stencil Operator

\[ w_n = \sum_{\mu=0}^{4} \left[ (U_{n,\mu} v_{n+\mu} - U_{n-\mu,\mu}^{\dagger} v_{n-\mu}) + (N_{n,\mu} v_{n+3\mu} - N_{n-3\mu,\mu}^{\dagger} v_{n-3\mu}) \right] \]

complex 3-dim vector
complex 3×3 matrix

\[ U(3) \text{ matrix} \]
reconstruct from 14 floats

\[ w = \text{standard} \]
Stencil Operator

\[ w_n = \sum_{\mu=0}^{4} \left[ \left( U_{n,\mu} v_{n+\mu} - U_{n-\mu,\mu}^{\dagger} v_{n-\mu} \right) + \left( N_{n,\mu} v_{n+3\mu} - N_{n-3\mu,\mu}^{\dagger} v_{n-3\mu} \right) \right] \]

- complex 3-dim vector
- complex 3×3 matrix
- \( U(3) \) matrix
- reconstruct from 14 floats

\[ W \begin{cases} = \text{standard} \\ + \text{naik} \end{cases} \quad \text{preccalculated three-link term} \]
Stencil Operator

\[
    w_n = \sum_{\mu=0}^{4} \left[ \left( U_{n,\mu} v_{n+\mu} - U_{n-\mu,\mu}^\dagger v_{n-\mu} \right) + \left( N_{n,\mu} v_{n+3\mu} - N_{n-3\mu,\mu}^\dagger v_{n-3\mu} \right) \right]
\]

complex 3-dim vector

complex 3×3 matrix

\( U(3) \) matrix

\( \mapsto \) reconstruct from 14 floats

\( \uparrow \) matrix

\( \bullet \) vector

\( w_n = \) standard + naik

\( \leftarrow \) precalculated three-link term

1146 Flop/site

0.8 Flop/byte

\( \mapsto \) single-precision
# Multiple right-hand sides

<table>
<thead>
<tr>
<th>constant matrices</th>
<th>Memory</th>
</tr>
</thead>
</table>

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Multiple right-hand sides

| constant matrices | \( \eta_0 \) | \( \eta_1 \) | \( \eta_2 \) | \( \eta_3 \) | \( \eta_4 \) | \( \eta_5 \) | \( \eta_6 \) | \cdots | Memory |

random vectors
Multiple right-hand sides

| constant matrices | \( \eta_0 \) | \( \eta_1 \) | \( \eta_2 \) | \( \eta_3 \) | \( \eta_4 \) | \( \eta_5 \) | \( \eta_6 \) | \cdots | Memory

\[ \text{SO}(\quad) \]
Multiple right-hand sides

constant matrices

$\text{SO}(\cdot)$

random vectors

$\eta_0, \eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, \ldots$ Memory
Multiple right-hand sides

constant matrices

$\mathbf{SO}(\, ,)$

random vectors

$\eta_0 \eta_1 \eta_2 \eta_3 \eta_4 \eta_5 \eta_6$
Multiple right-hand sides

constant matrices

\[ \eta_0, \eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, \ldots \]

random vectors

\[ \mathfrak{so}(\cdot, \cdot) \]
Multiple right-hand sides

- Constant matrices
- Memory
- Random vectors

\[ \eta_0 \eta_1 \eta_2 \eta_3 \eta_4 \eta_5 \eta_6 \cdots \]

\[ \text{SO} \left( \text{multi3} \right) \]
Multiple right-hand sides

- Constant matrices
- $\eta_0, \eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, \ldots$

Random vectors

$SO(\cdot, \cdot)$

$SO\text{-multi3}(\cdot, \cdot, \cdot, \cdot, \cdot, \cdot)$

Memory
Multiple right-hand sides

- Memory
- Random vectors

Constant matrices

SO( )

SO\_multi3( )

Memory
Multiple right-hand sides

constant matrices

\[ \eta_0, \eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, \ldots \]

random vectors

**pro:** much better arithmetic intensity

**con:** higher register pressure
Multiple right-hand sides

Flop/byte

#right-hand sides

Stencil Operator
Single-node Performance

![Graph showing the performance of Conjugate Gradient in GFlop/s for different architectures.

- Volta V100
- Knights Landing
- Skylake
- Haswell
- K40
- K20X
- Ivy Bridge

The graph plots the number of right-hand sides against GFlop/s for fp32, single node performance.]
Multi-node Performance

- short setup phase assigns local problems to each GPU
  - e.g. inversions of different matrices
  - performance scales linearly with number of nodes

- maximize number of nodes to reduce time to solution

- largest Summit job used 2k nodes
  - achieved 23 PFlop/s

- largest Titan job used 14k nodes
  - achieved 5 PFlop/s
  - using both GPU and CPU
The QCD phase diagram
Critical point from Taylor expansions

- expansion of QCD pressure

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

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

\[
r_{2n}^P = \left| \frac{(2n + 2)(2n + 1)\chi_{2n}^B}{\chi_{2n+2}^B} \right|^{1/2}
\]

- only if coefficients are positive for all \( n \geq n_0 \)
  - if not \( \rightarrow \) no critical point on real axis
Radius of convergence

- complex function
  \[ f(z) = \frac{1}{1+z^2} \]

- series expansion
  \[ f(z) = \sum_{n=0}^{\infty} (-1)^n z^{2n} \]

- convergence determined by nearest singularity from the origin
Comparison to experiment

only at freeze-out \((\mu_f, T_f)\)

<table>
<thead>
<tr>
<th>Moment</th>
<th>Symbol</th>
<th>Experiment</th>
<th>Lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>mean</td>
<td>(M_X)</td>
<td>(\langle N_X \rangle)</td>
<td>(VT^3 \chi_1^X)</td>
</tr>
<tr>
<td>variance</td>
<td>(\sigma_X^2)</td>
<td>(\langle (\delta N_X)^2 \rangle)</td>
<td>(VT^3 \chi_2^X)</td>
</tr>
<tr>
<td>skewness</td>
<td>(S_X)</td>
<td>(\left(\frac{\langle (\delta N_X)^3 \rangle}{\sigma_X^3}\right))</td>
<td>(VT^3 \chi_3^X)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\frac{\langle (\delta N_X)^4 \rangle}{\sigma_X^4} - 3)</td>
<td>(\frac{VT^3 \chi_4^X}{(VT^3 \chi_2^X)^2})</td>
</tr>
</tbody>
</table>

- volume independent ratios

\[
\frac{\sigma_X^2}{M_X} = \frac{\chi_2^X}{\chi_1^X}, \quad S_X \sigma_X = \frac{\chi_3^X}{\chi_2^X}, \quad k_X \sigma_X^2 = \frac{\chi_4^X}{\chi_2^X}
\]
First results from Summit

![Graph showing data points and error bars for different moments and temperature.](image)
The QCD crossover line

\[
T_c [\text{MeV}] \quad \mu_B [\text{MeV}]
\]

\[n_S = 0, \quad \frac{n_Q}{n_B} = 0.4\]

crossover line: \(O(\mu_B^4)\)
constant: \(\epsilon\)
freeze-out: STAR, ALICE

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No signs for a QCD critical point along $T_c(\mu_B)$

- no deviations from HRG
- no increased fluctuations
- no narrowing crossover
Summary

- constrains on location of QCD critical point
  - upper bound from crossover line and radius of convergence
  - negative 6th and 8th order Taylor coefficients of $P$
  - no increased fluctuations along crossover
- possible existing critical point may be found only for
  \[ \mu_B > 400 \text{ MeV} \quad \text{and} \quad T < (130 - 140) \text{ MeV} \]
- provides important input for Beam Energy Scan II currently performed at the Relativistic Heavy Ion Collider
- CG sustained 23 Pflop/s on Summit using 2k nodes
Thank you for your attention!