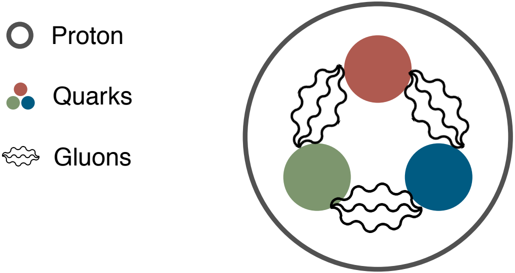
First Summit results

Lattice QCD at non-zero baryon density

April 26, 2019 | Patrick Steinbrecher, HotQCD

Quantum Chromodynamics (QCD)



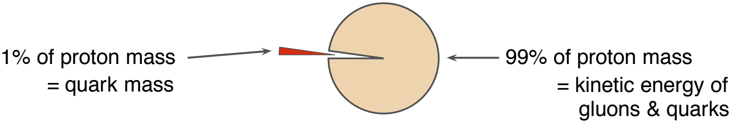
Color Charge

↓

Strong Force

↓

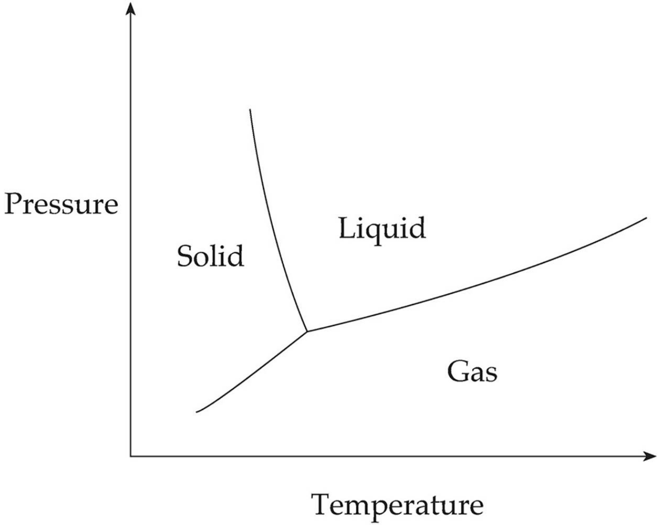
Confinement



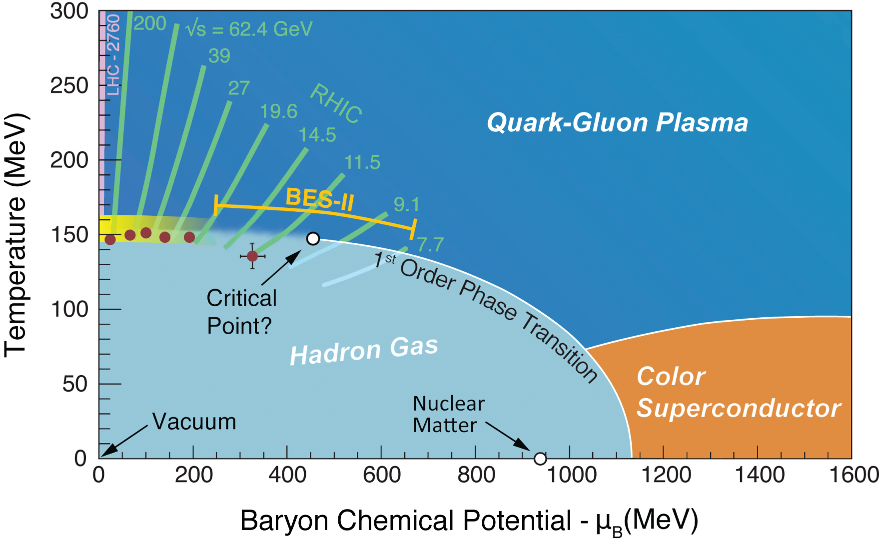
What happens if you make things hotter and hotter?

What happens if you keep squeezing and squeezing?

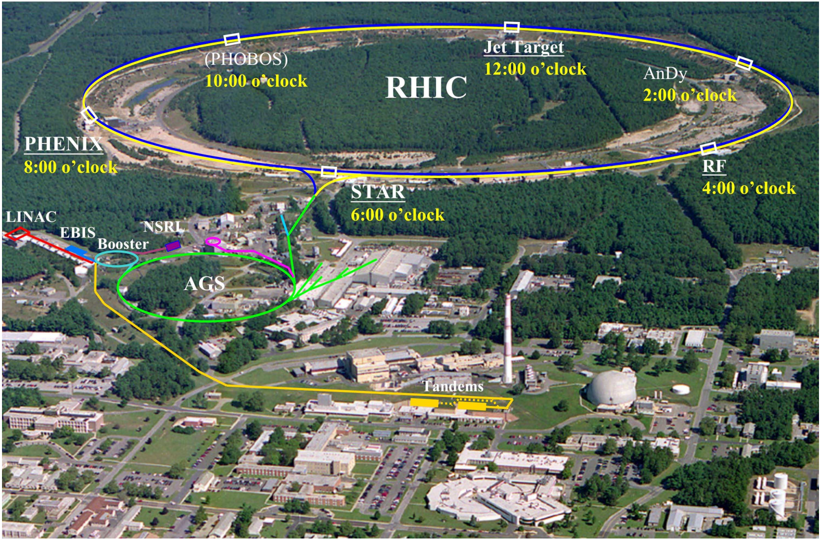
Phases of Water



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

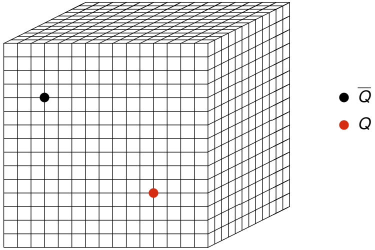
$$(i\gamma^\mu \partial_\mu - m)\,\Psi = 0$$

- calculate path integral using monte carlo methods

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \;\; \mathcal{O} \;\, \exp\left(-S\right)$$

→ Lattice QCD

e.g. 4-dimensional Lattice $N_\sigma^3 \times N_\tau$



$$V = (aN_\sigma)^3$$

$$T = \frac{1}{aN_\tau}$$

The Lattice QCD Kernel

condition:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \eta_{ki}^{*} \eta_{kj} = \delta_{ij}$$

99% of runtime

$$\mathrm{Tr}\, M^{-1} = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \eta_k^{\dagger} M^{-1} \eta_k$$

- evaluate traces using N random noise vectors η

  up to 2000 η per gauge field configuration

- solve $M^{-1}\eta_k$ using Conjugate Gradient

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

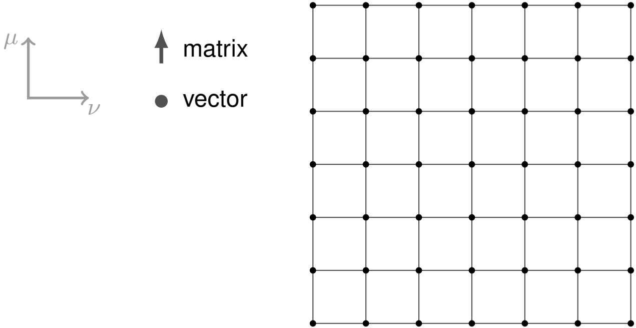
Stencil Operator

complex 3-dim vector

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

complex 3×3 matrix

$U(3)$ matrix
↪ reconstruct from 14 floats



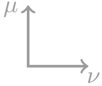
Stencil Operator

complex 3-dim vector

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

complex 3×3 matrix

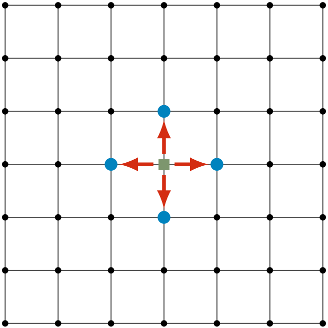
$U(3)$ matrix
↪ reconstruct from 14 floats



↑ matrix

● vector

$w_{\blacksquare}$ = standard



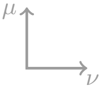
Stencil Operator

complex 3-dim vector

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

complex 3×3 matrix

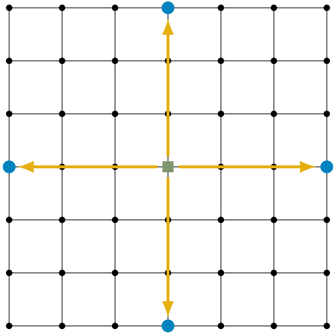
$U(3)$ matrix
$\hookrightarrow$ reconstruct from 14 floats



↑ matrix

● vector

$w_{\blacksquare}$ = standard
\+ naik
↼ precalculated three-link term



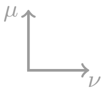
Stencil Operator

complex 3-dim vector

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

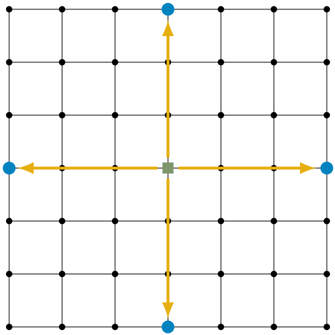
complex 3×3 matrix

$U(3)$ matrix
↪ reconstruct from 14 floats



matrix

vector



1146 Flop/site

0.8 Flop/byte
↪ single-precision

$w_{\blacksquare}$ = standard
+ naik
↰ precalculated three-link term

Multiple right-hand sides

Memory

Memory

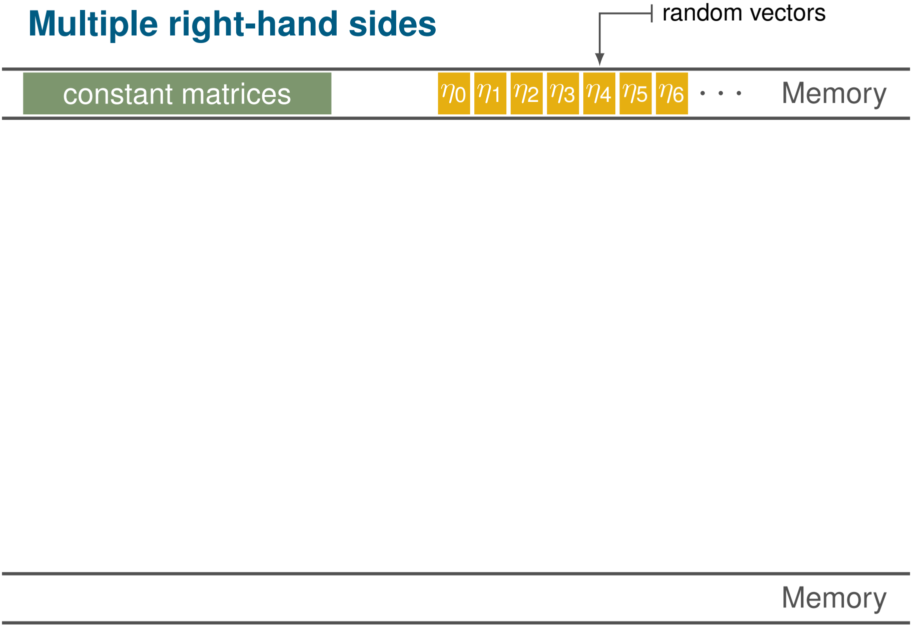
Multiple right-hand sides

constant matrices

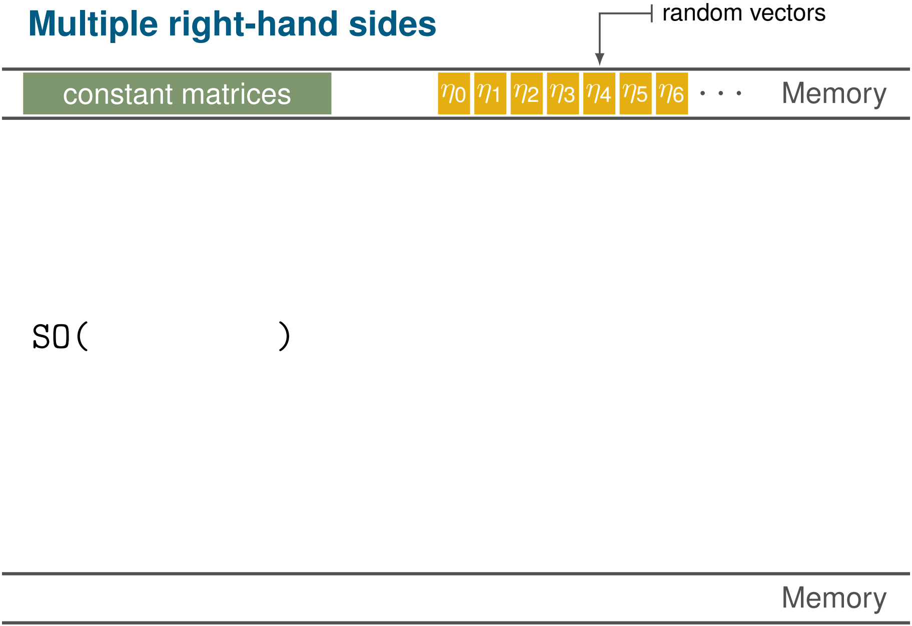
Memory

Memory

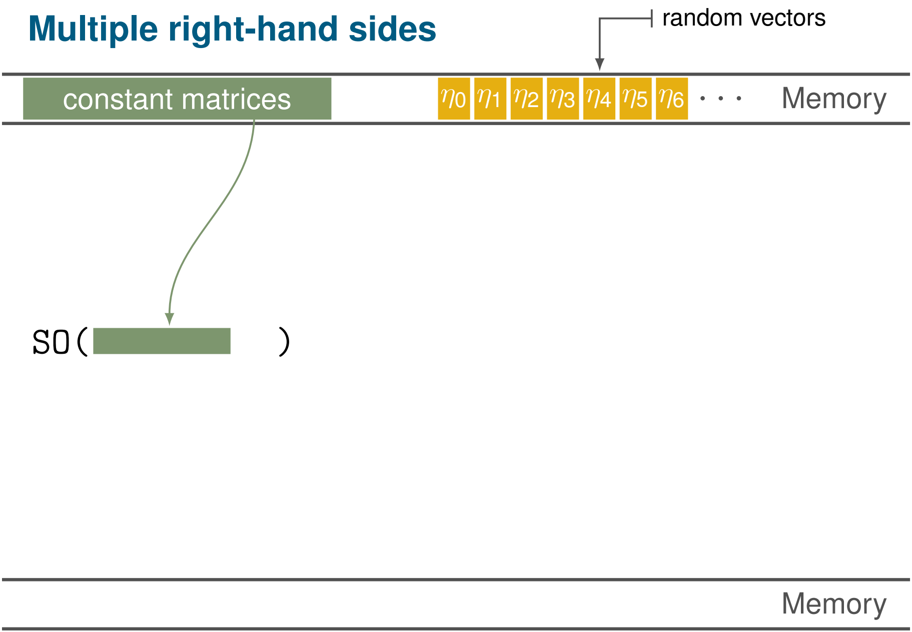
Multiple right-hand sides



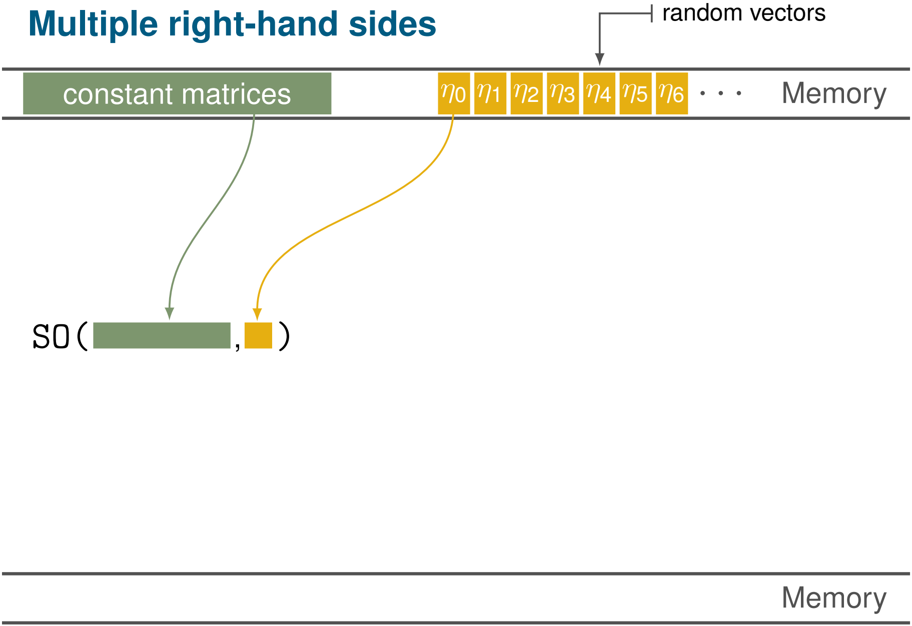
Multiple right-hand sides



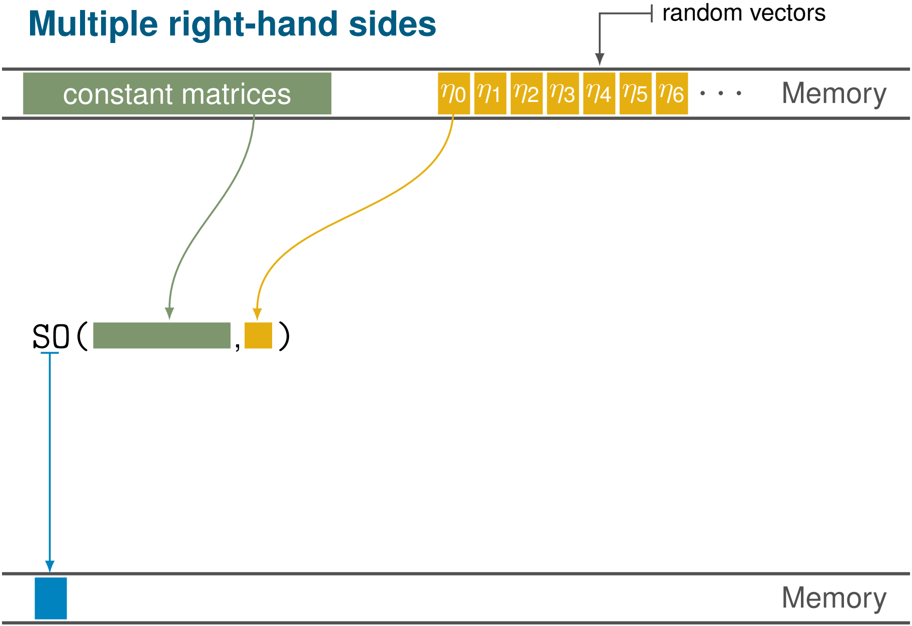
Multiple right-hand sides



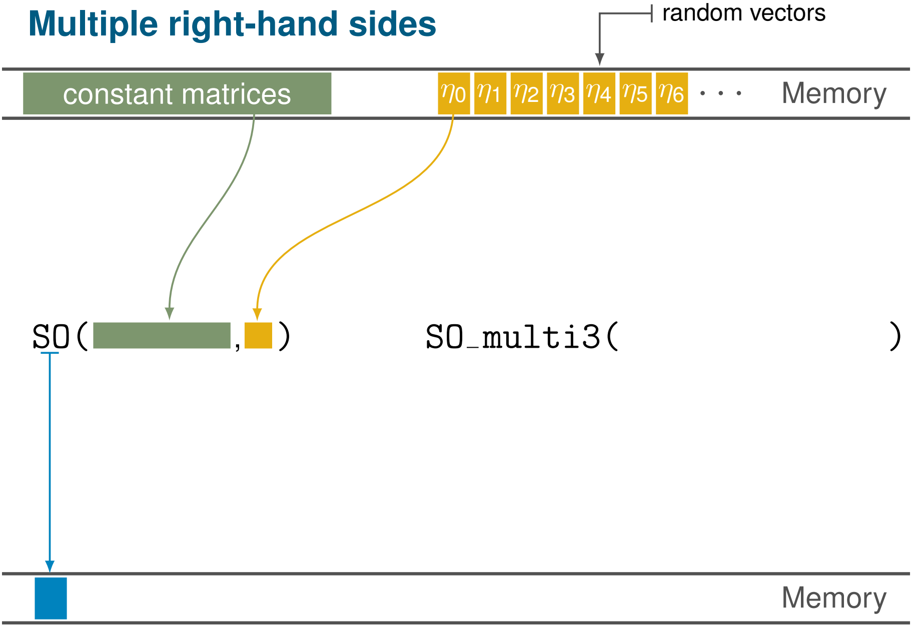
Multiple right-hand sides



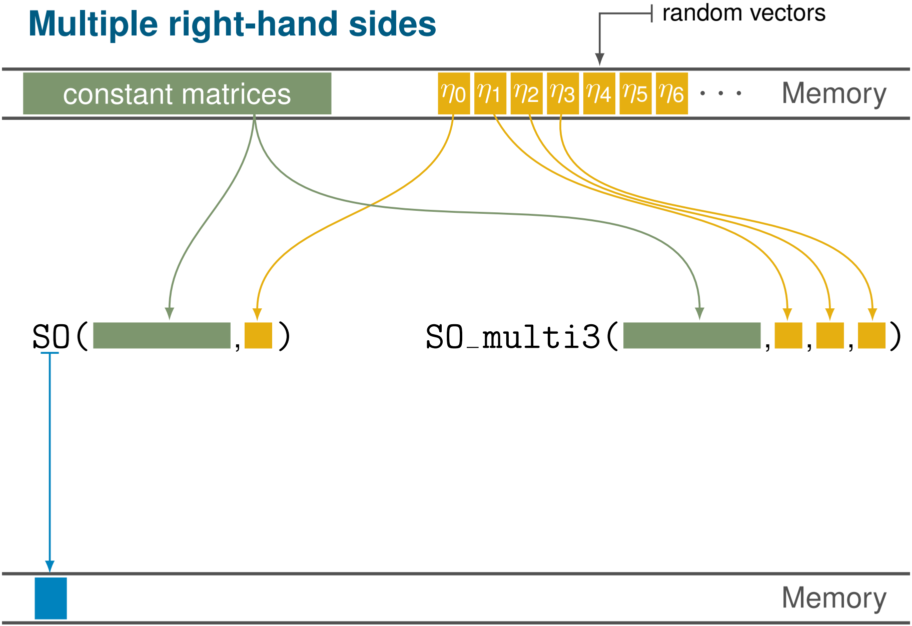
Multiple right-hand sides



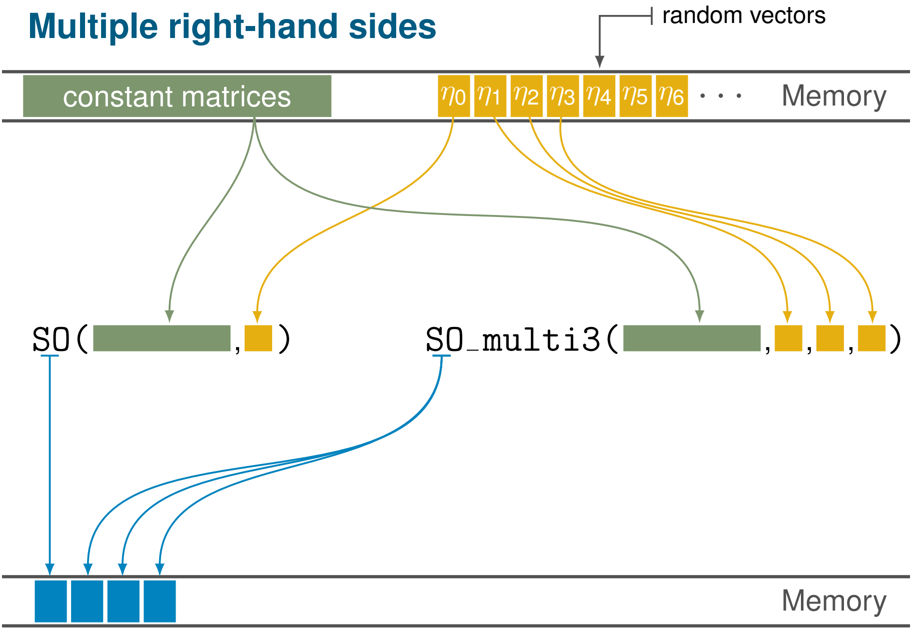
Multiple right-hand sides



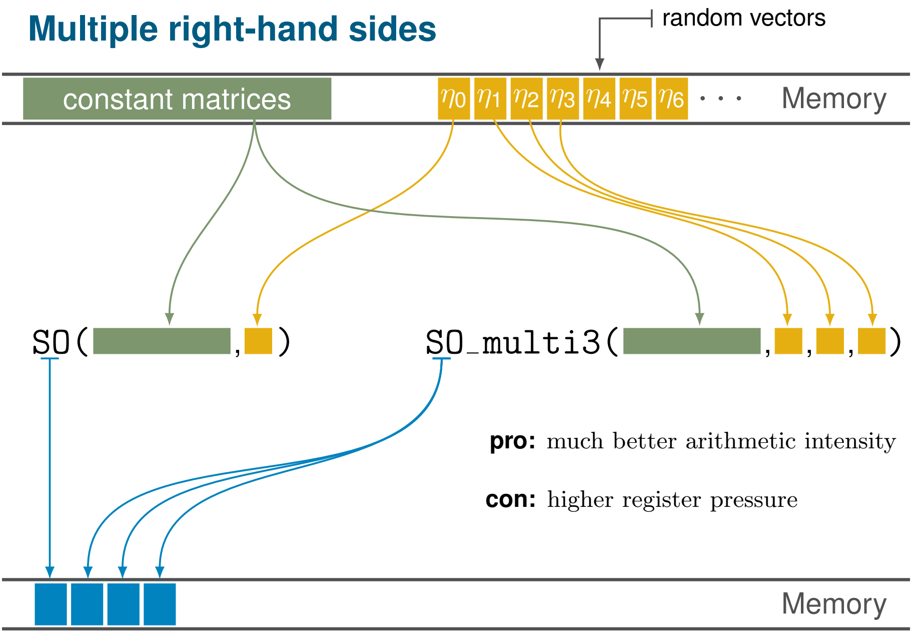
Multiple right-hand sides



Multiple right-hand sides



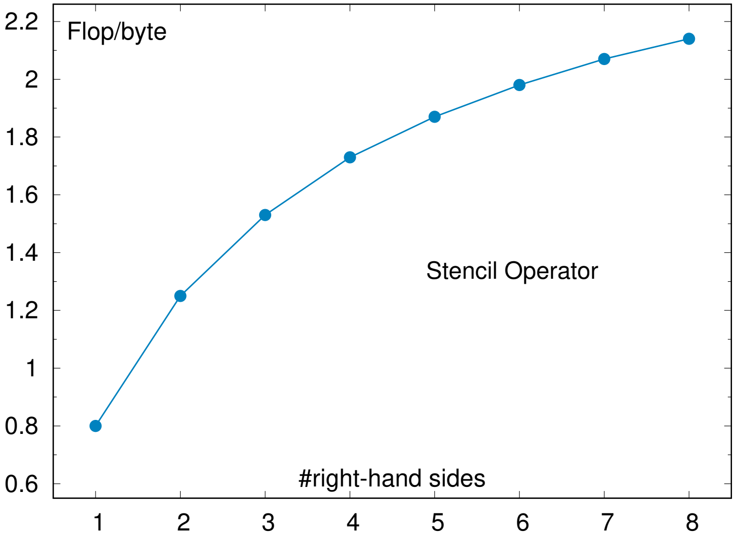
Multiple right-hand sides



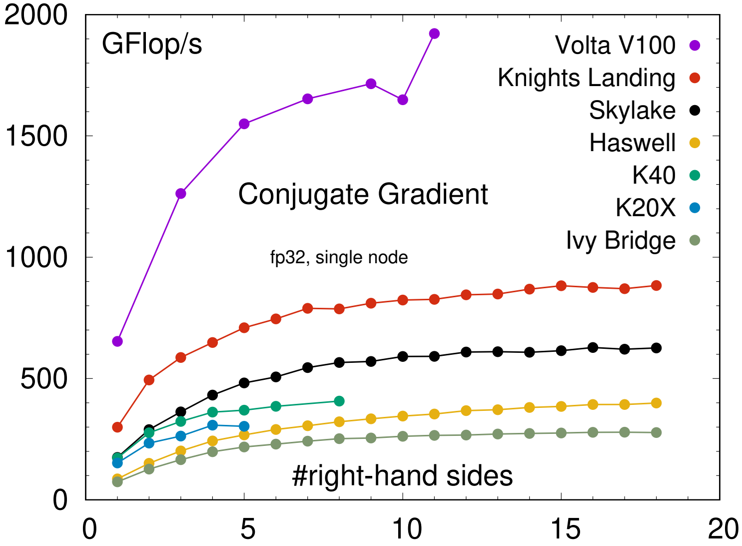
pro: much better arithmetic intensity

con: higher register pressure

Multiple right-hand sides



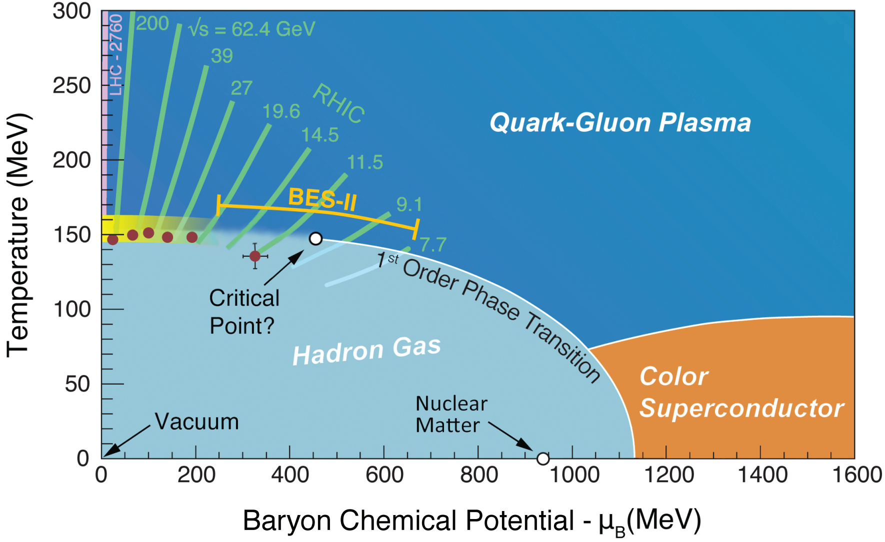
Single-node Performance



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 $\mathrm{PFlop/s}$
- largest Titan job used 14k nodes
  - achieved 5 $\mathrm{PFlop/s}$
  - using both GPU and CPU

The QCD phase diagram



Critical point from Taylor expansions

- expansion of QCD pressure

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

- 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

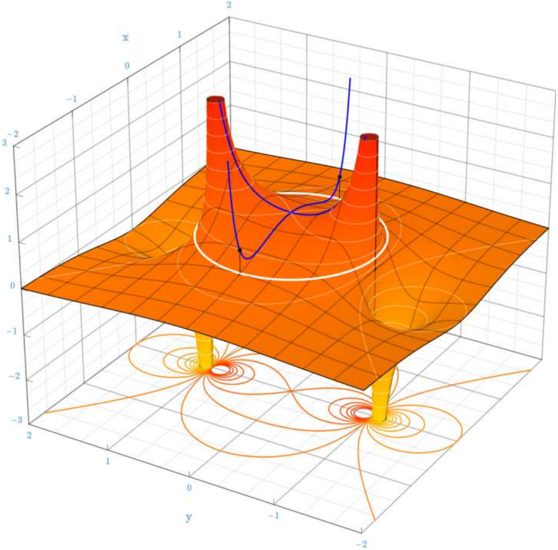
- complex function

  $$f(z) = \frac{1}{1+z^2}$$

- series expansion

  $$f(z) = \sum_n^{\infty} (-1)^n z^{2n}$$

- convergence determined by nearest singularity from the origin



Comparison to experiment

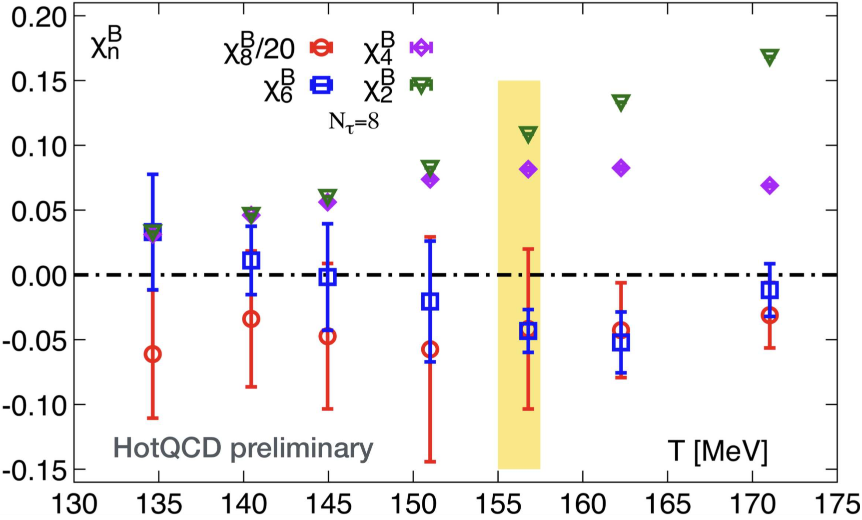
only at freeze-out $(\mu_f,\ T_f)$

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	$\dfrac{\left\langle (\delta N_X)^4 \right\rangle}{\sigma_X^4} - 3$	$\dfrac{VT^3\chi_4^X}{\left(VT^3\chi_2^X\right)^2}$

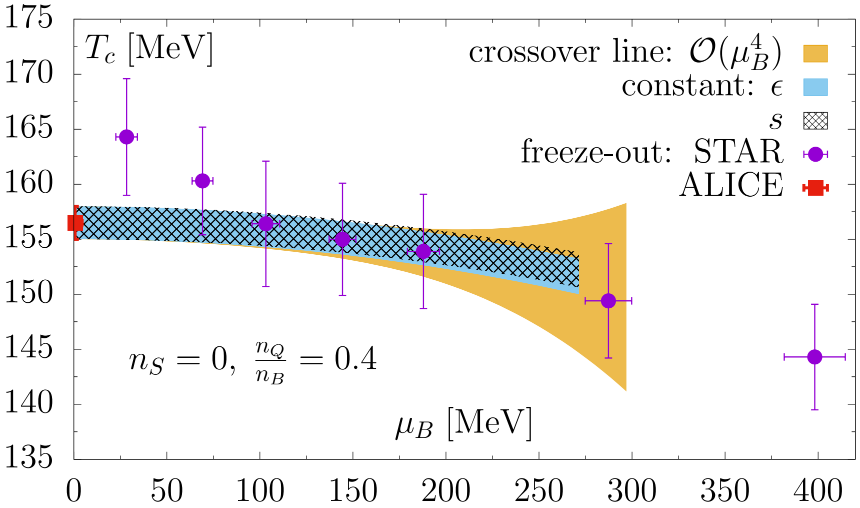
- volume independent ratios

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

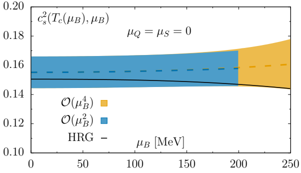
First results from Summit

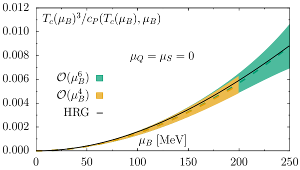


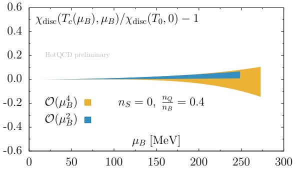
The QCD crossover line

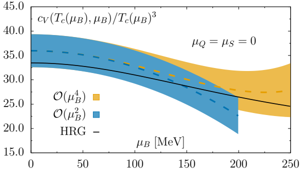


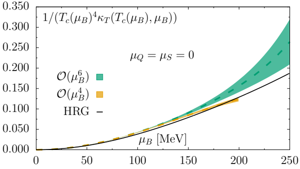
No signs for a QCD critical point along $T_c(\mu_B)$

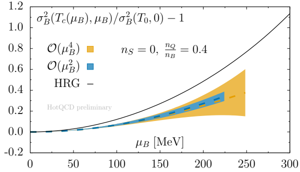




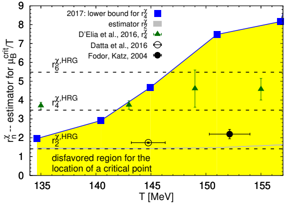


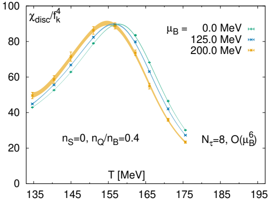






- no deviations from HRG
- no increased fluctuations
- no narrowing crossover





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

$$\mu_B > 400\ \mathrm{MeV} \quad \text{and} \quad T < (130 - 140)\ \mathrm{MeV}$$

- provides important input for Beam Energy Scan II currently performed at the Relativistic Heavy Ion Collider
- CG sustained 23 $\mathrm{PFlop/s}$ on Summit using 2k nodes

Thank you for your attention!