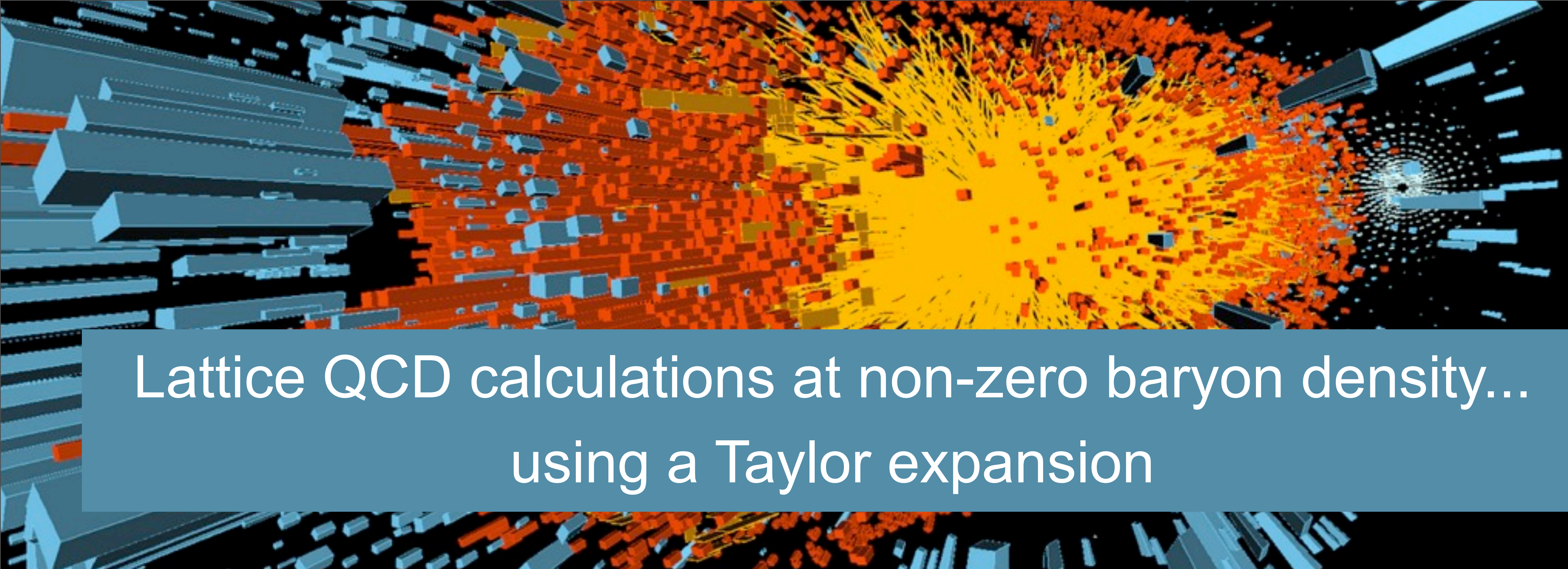


Lattice QCD calculations at non-zero baryon density...
using a Taylor expansion

Christian Schmidt

Universität Bielefeld

Motivation: Extending lattice QCD to $\mu_B \neq 0$

Phases of QCD ?

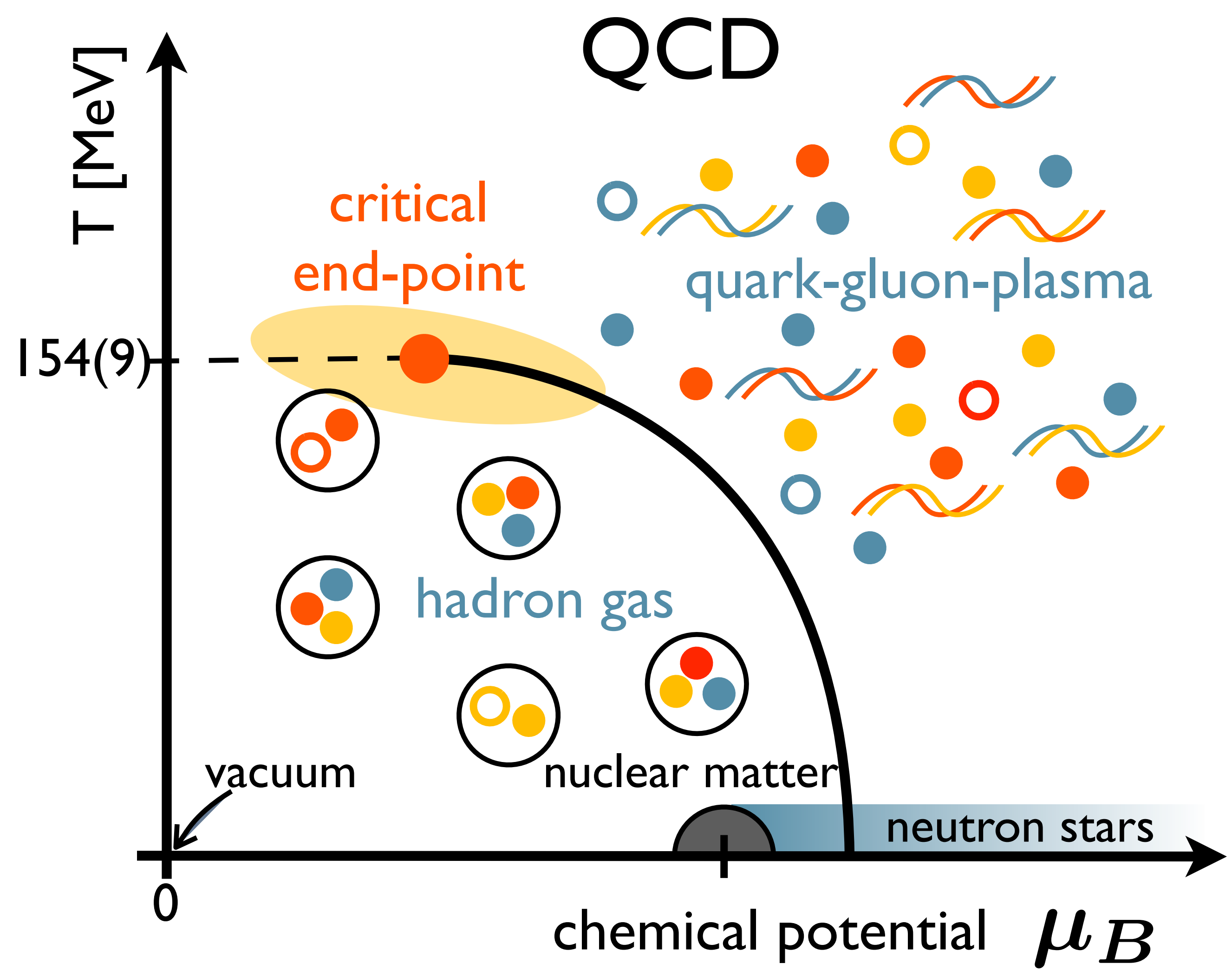
1) hadronic states at low T, low densities
2) quasi-free quarks and gluons at high T and/or high densities

Underlying Mechanisms ?

1) spontaneous chiral symmetry breaking
2) (de-)confinement

Critical end-point?

Expected phase diagram of QCD:



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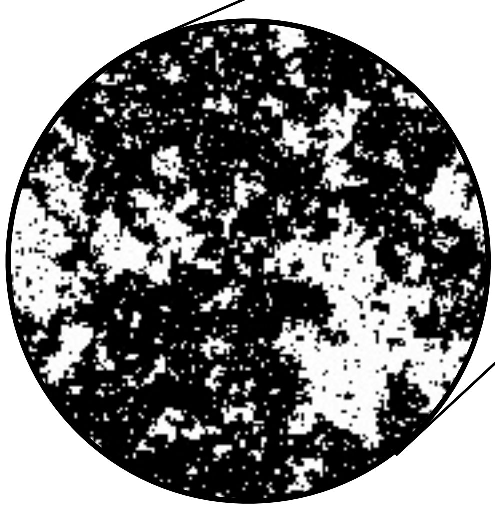
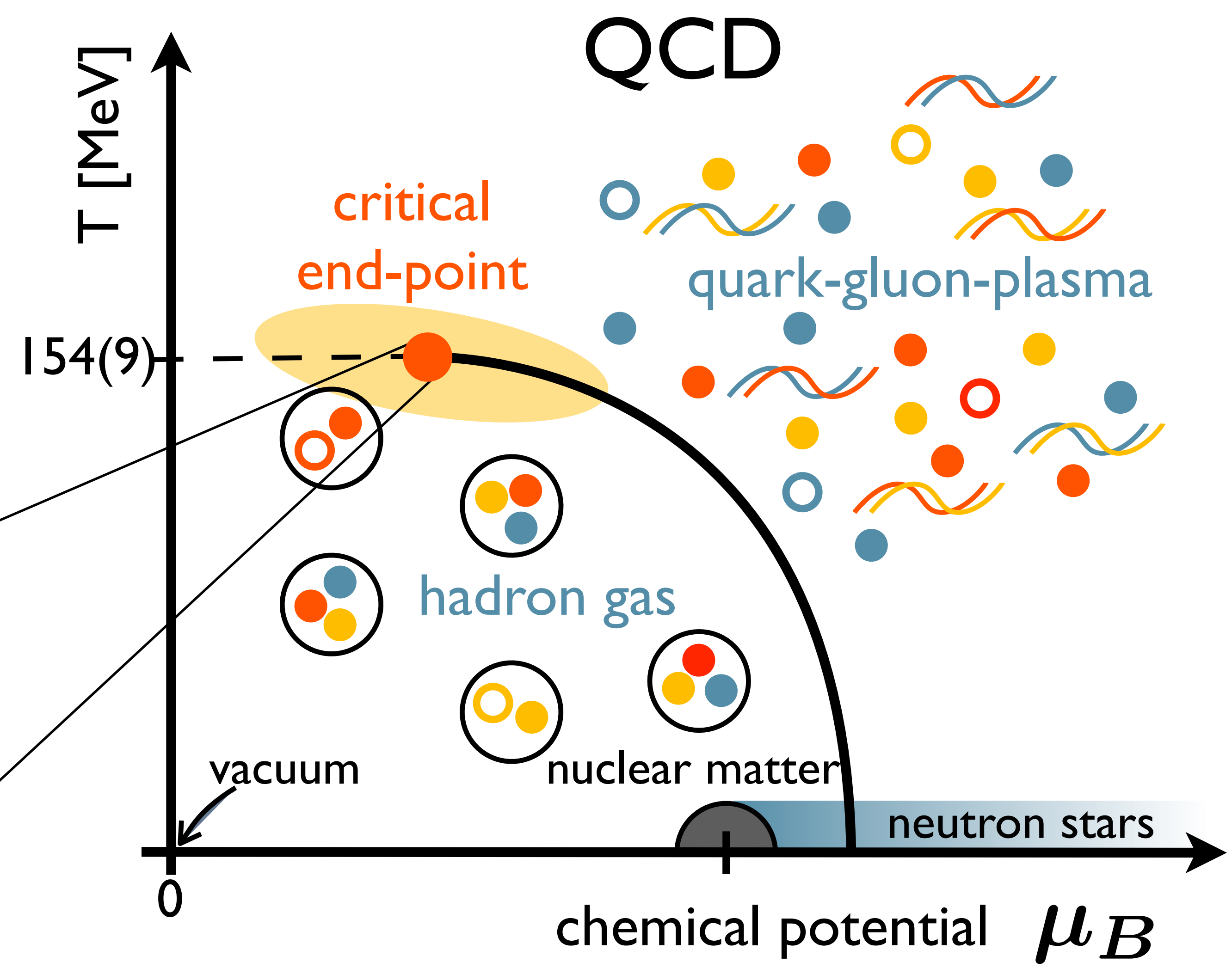




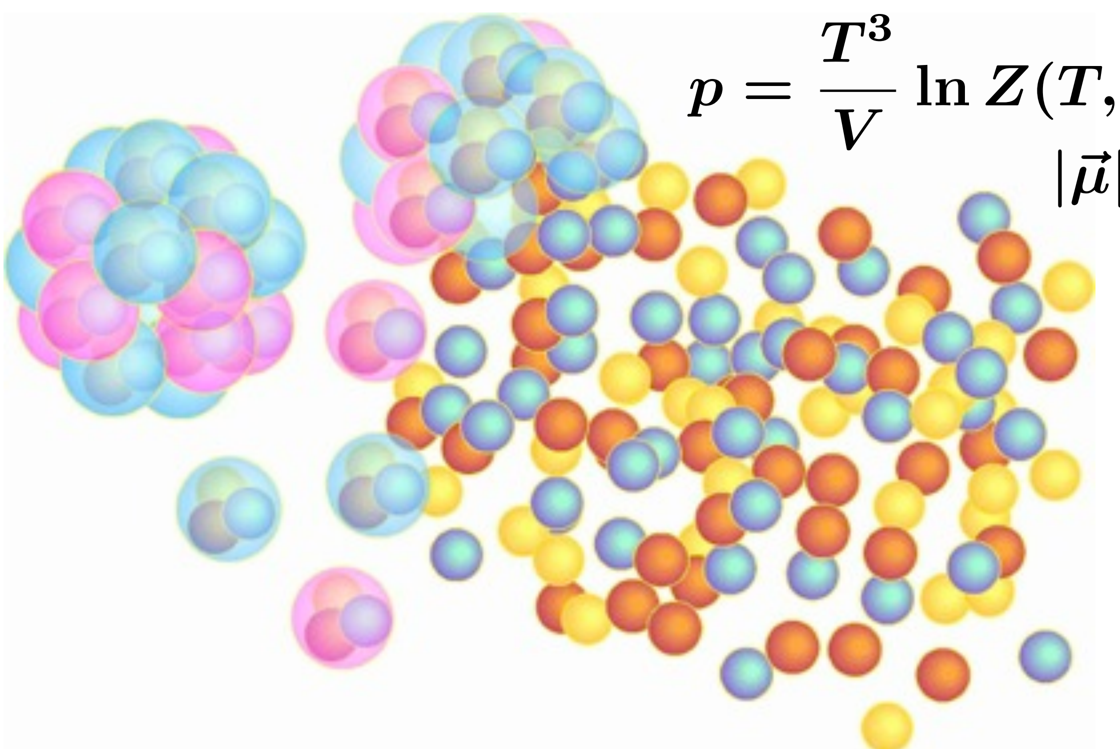
$\Rightarrow$ **Diverging correlation length and fluctuations. Universal behavior within a scaling region.**

Montag, 29. April 13

Methodology: Expanding *p/T⁴*

- Lattice QCD simulations at $\mu_B > 0$ **not** feasible by std. Monte Carlo methods (complex action, sign problem)

hot quarks and gluons in a box:



$$p = \frac{T^3}{V} \ln Z(T, V, \vec{\mu})$$
$$|\vec{\mu}| = 0$$

derivatives of ***lnZ*** are widely used quantities in thermodynamics

***T*-derivatives:**
used to calculate the equation of state (p,e,s,...)

***m*-derivatives:**
used to study chiral symmetry breaking

μ -derivatives:
used to study density fluctuations

$\Rightarrow$ study higher derivatives (*n*=2-6)

$$\frac{\partial^n \ln Z}{\partial(\mu_X/T)^n} \qquad X \in \{u, d, s, B, Q, S, \ldots\}$$

$\Rightarrow$ obtain **Taylor expansion** of ***lnZ***

Generalized Susceptibilites vs Cumulants

- derivatives of ***lnZ*** with respect to $\mu_{B,Q,S}$ can also be studied in **heavy ion collisions**

Expansion of the pressure:

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

$X = B, Q, S$: conserved charges

Lattice

$$\boxed{\chi_{n,0}^X} = \frac{1}{VT} \frac{\partial^n \ln Z}{\partial(\mu_X/T)^n}\bigg|_{\mu_X=0}$$

generalized susceptibilities

$\Rightarrow$ only at $\mu_X = 0$!

Experiment

$$\begin{aligned}
VT^3 \, \boxed{\chi_2^X} &= \langle (\delta N_X)^2 \rangle \\
VT^3 \, \boxed{\chi_4^X} &= \langle (\delta N_X)^4 \rangle - 3 \langle (\delta N_X)^2 \rangle^2 \\
VT^3 \, \boxed{\chi_6^X} &= \langle (\delta N_X)^6 \rangle \\
&\quad -15 \langle (\delta N_X)^4 \rangle \langle (\delta N_X)^2 \rangle \\
&\quad +30 \langle (\delta N_X)^2 \rangle^3
\end{aligned}$$

cumulants of net-charge fluctuations

$$\delta N_X \equiv N_X - \langle N_X \rangle$$

$\Rightarrow$ only at freeze-out $(\mu_f(\sqrt{s}), T_f(\sqrt{s}))$!

Content

1) Applications

- Freeze-out condition in heavy ion collisions
- The relevant (strange) degrees of freedom

2) The lattice setup

- Adopted numerical methods
- Lattice sizes and quark mass parameter

3) GPU Acceleration

- Performance of the code
- Computing strategy for Titan

4) Summary

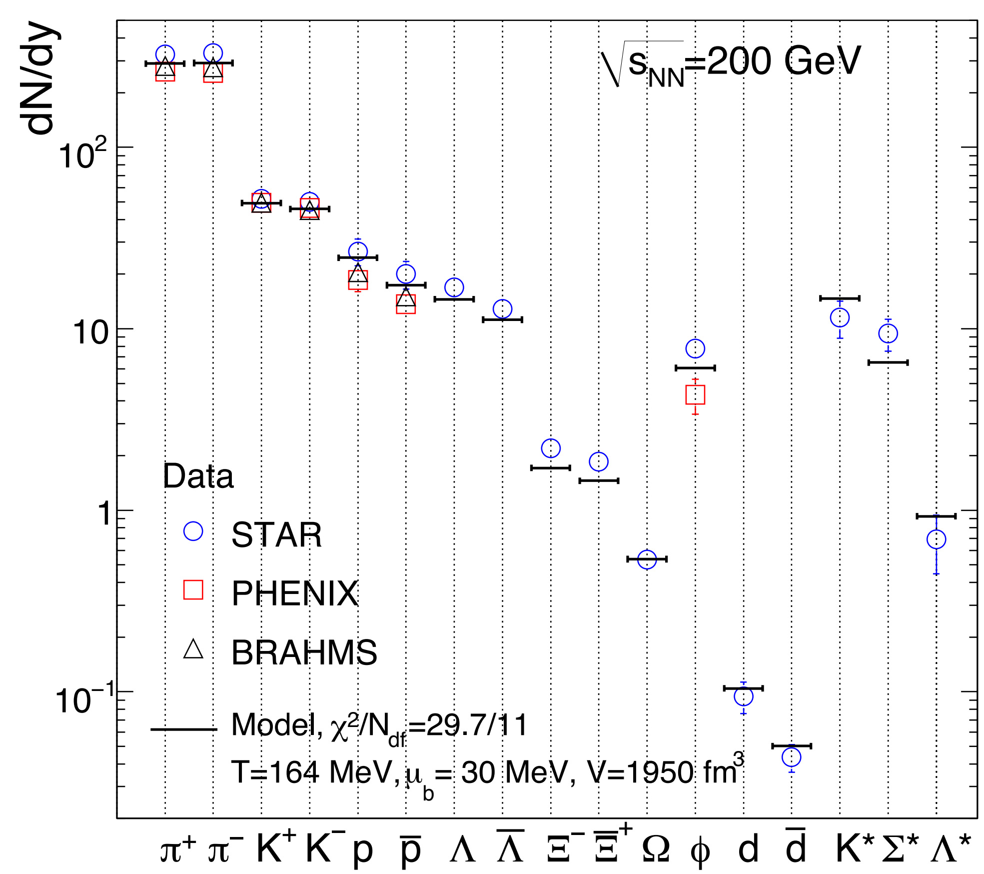
BNL-Bielefeld Collaboration:
A. Bazavov, H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, E. Laermann, S. Mukherjee, P. Petreczky, C. Schmidt, D. Smith, W. Soeldner, M. Wagner

HotQCD Collaboration:
A. Bazavov, T. Bhattacharya, M. Buchoff, M. Cheng, N. Christ, C. DeTar, H.-T. Ding, S. Gottlieb, R. Gupta, P. Hegde, U. Heller, C. Jung, F. Karsch, E. Laermann, L. Levkova, Z. Lin, R. Mawhinney, S. Mukherjee, P. Petreczky, D. Renfrew, C. Schmidt, C. Schroeder, W. Soeldner, R. Solz, R. Sugar, D. Toussaint, P. Vranas

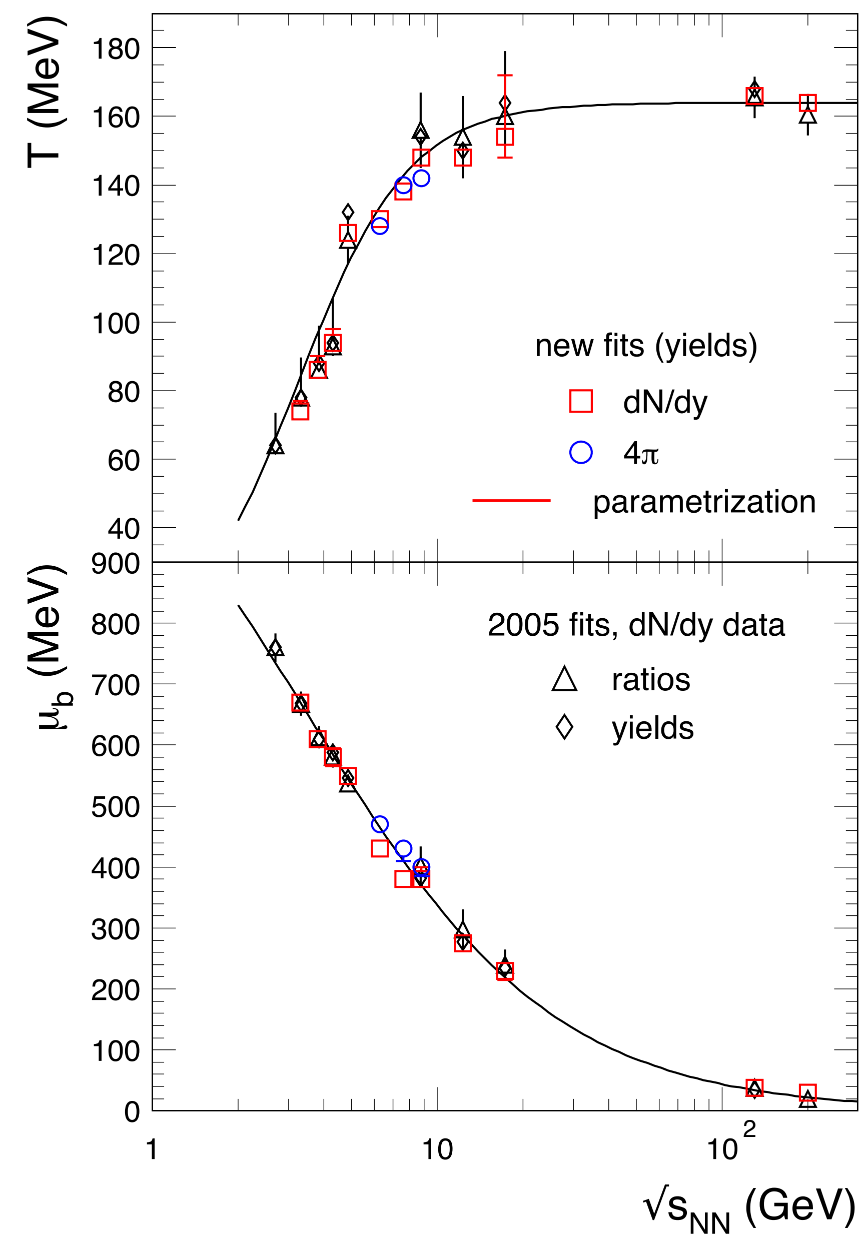
Applications

Application I: Probing freeze-out conditions

- **established method:** parse particle yields through the HRG model in order to extract freeze-out parameters as function of the collision energy.



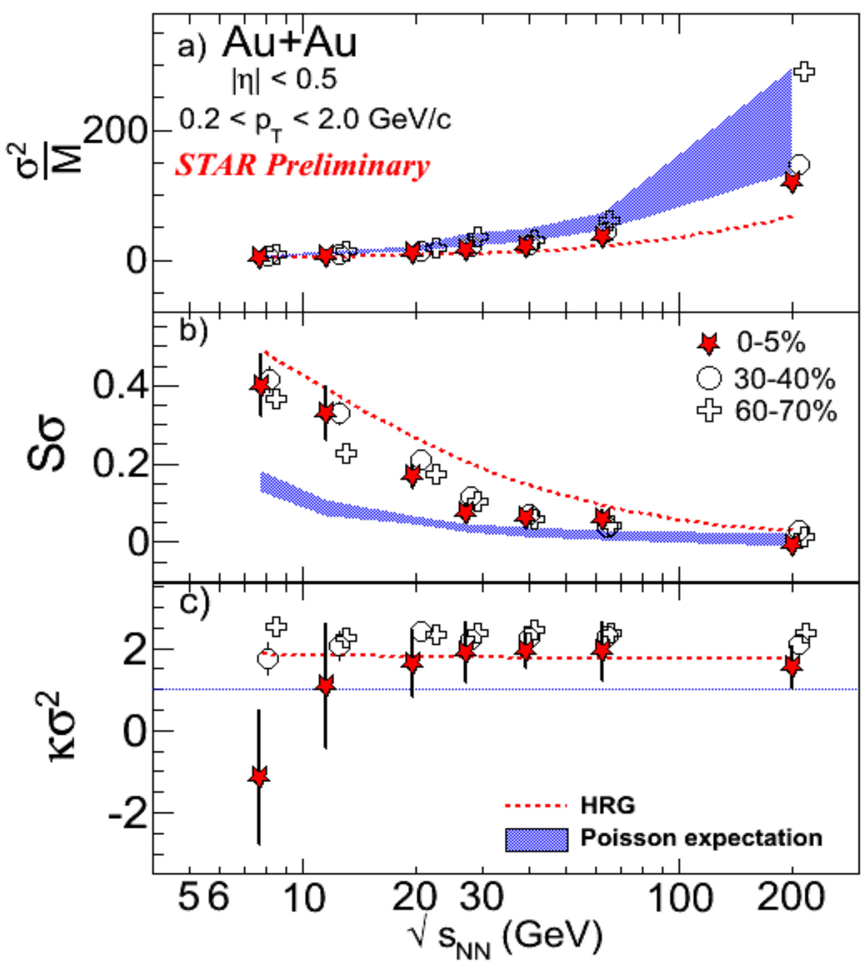
Andronic, Braun-Munzinger, Stachel, PLB 673 (2009) 142.



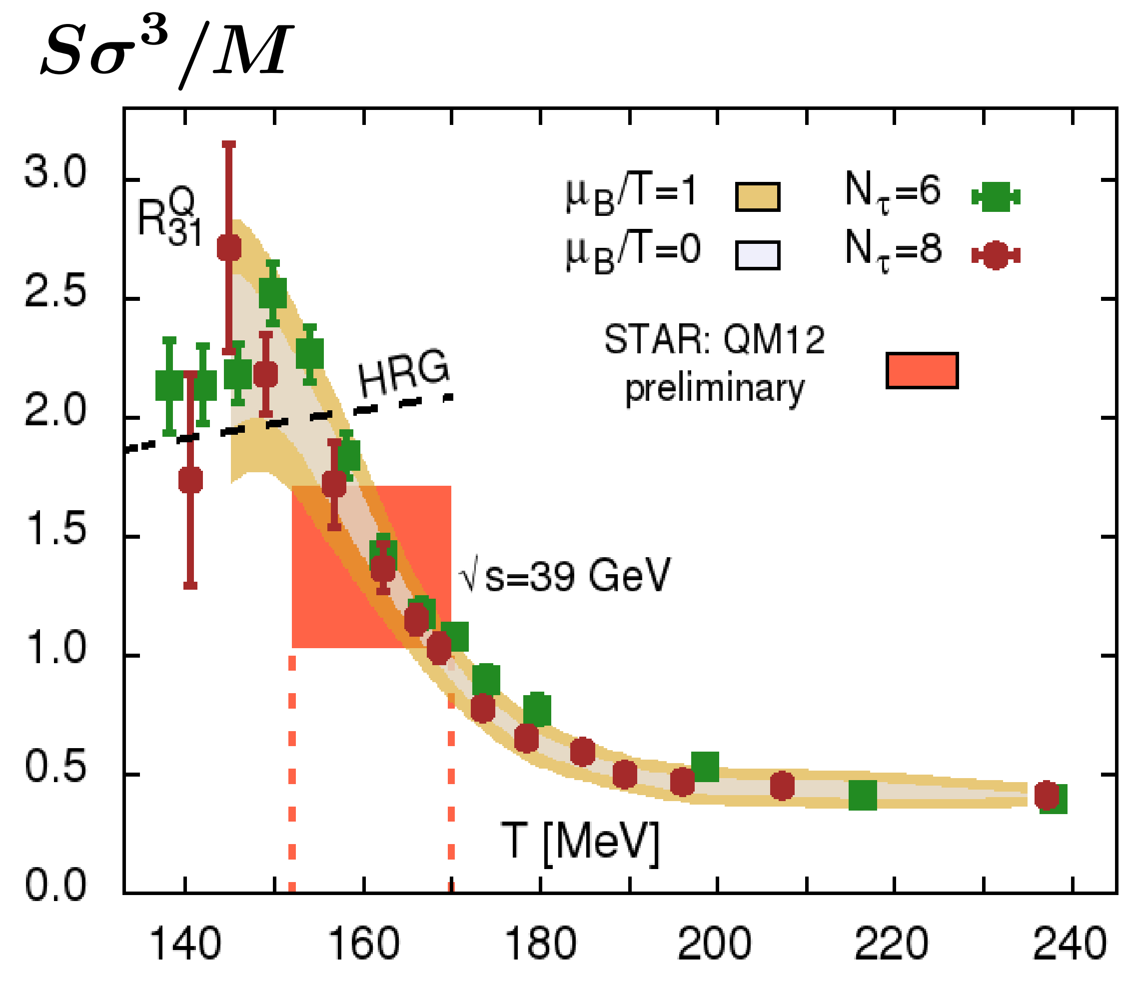
Application I: Probing freeze-out conditions

- **new method:** match measured cumulant ratios of electric charge fluctuations with first principle lattice QCD calculations to eliminate a model dependent analysis step.

BNL-Bielefeld, PRL 109 (2012) 192302



L. Kumar, QM'12



S. Mukherjee, CPOD'13

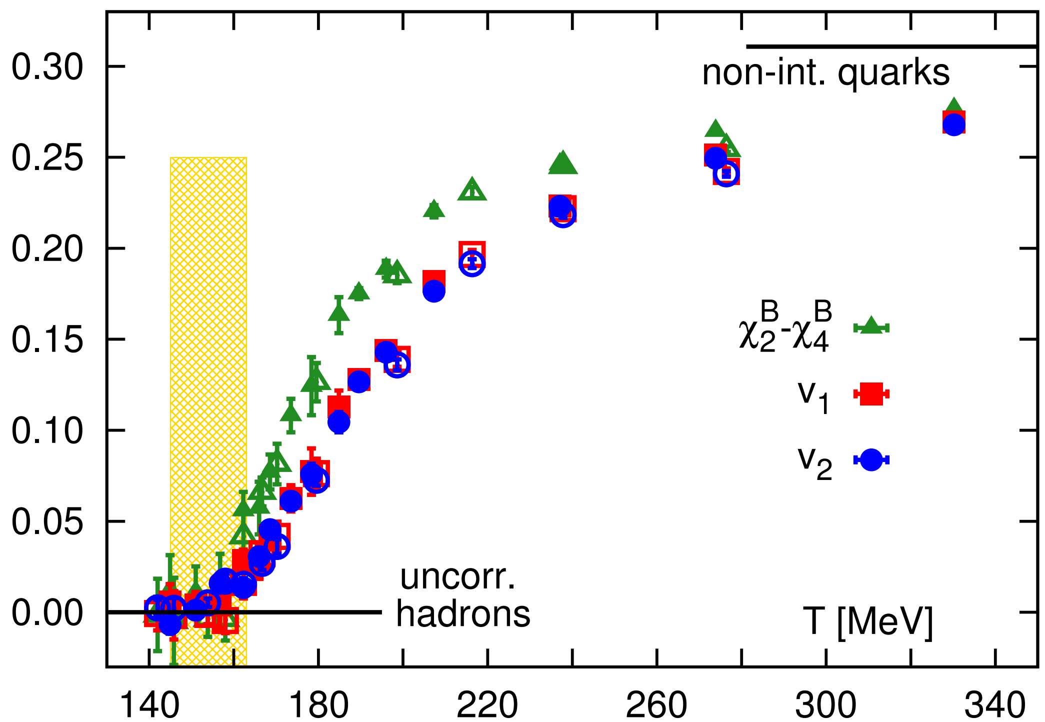
$\Rightarrow$ match at least to cumulant ratios to obtain μ_B^f and T^f, eventually more for thermodynamic consistency check

Application II: The relevant degrees of freedom

- **cumulants are sensitive to effective charges:** compare cumulants from non-perturbative (lattice) QCD calculations to other scenarios such as an uncorrelated gas of hadrons (HRG) or perturbative QCD *BNL-BI: arXiv:1304.7220*

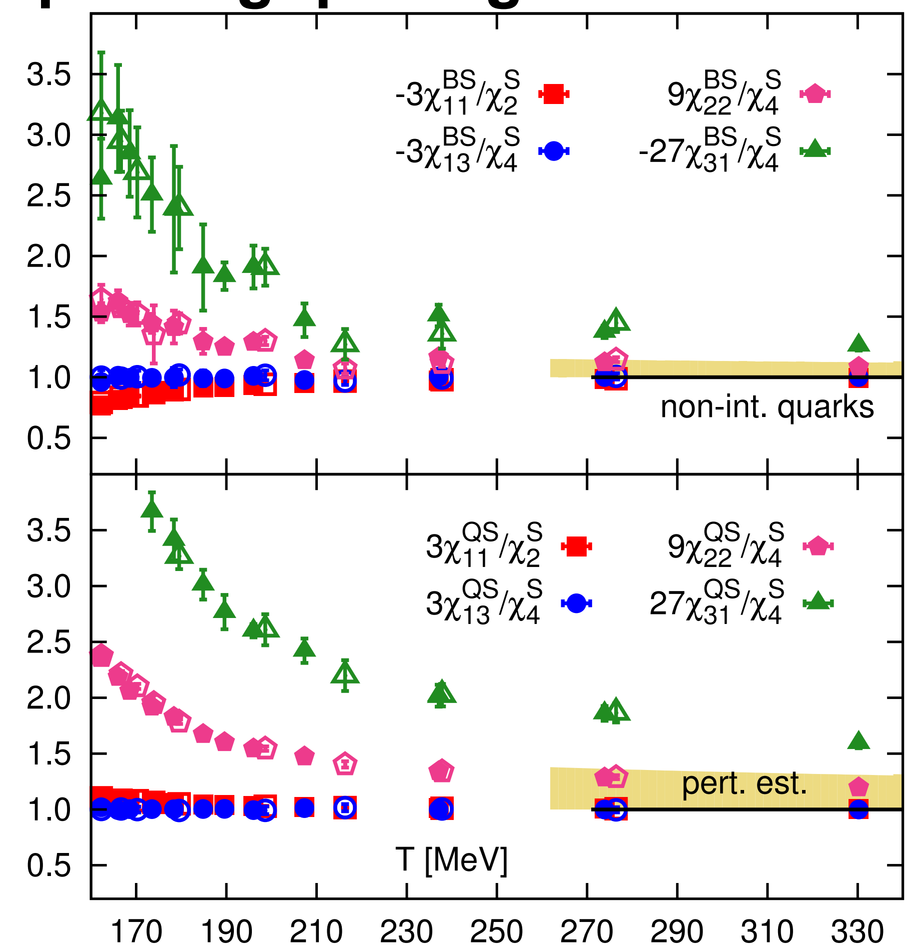
probing HRG DoFs:

$$v_1 = \chi_{31}^{BS} - \chi_{11}^{BS} \ ,$$
$$v_2 = \frac{1}{3}(\chi_2^S - \chi_4^S) - 2\chi_{13}^{BS} - 4\chi_{22}^{BS} - 2\chi_{31}^{BS}$$



$\Rightarrow$ relevant degrees of freedom are hadronic and uncorrelated for $T \lesssim T_c$

probing quark gas DoFs:



$\Rightarrow$ relevant degrees of freedom are that of a weakly interact. quark gas for $T \gtrsim 2T_c$

The lattice setup

Formulation of the operators

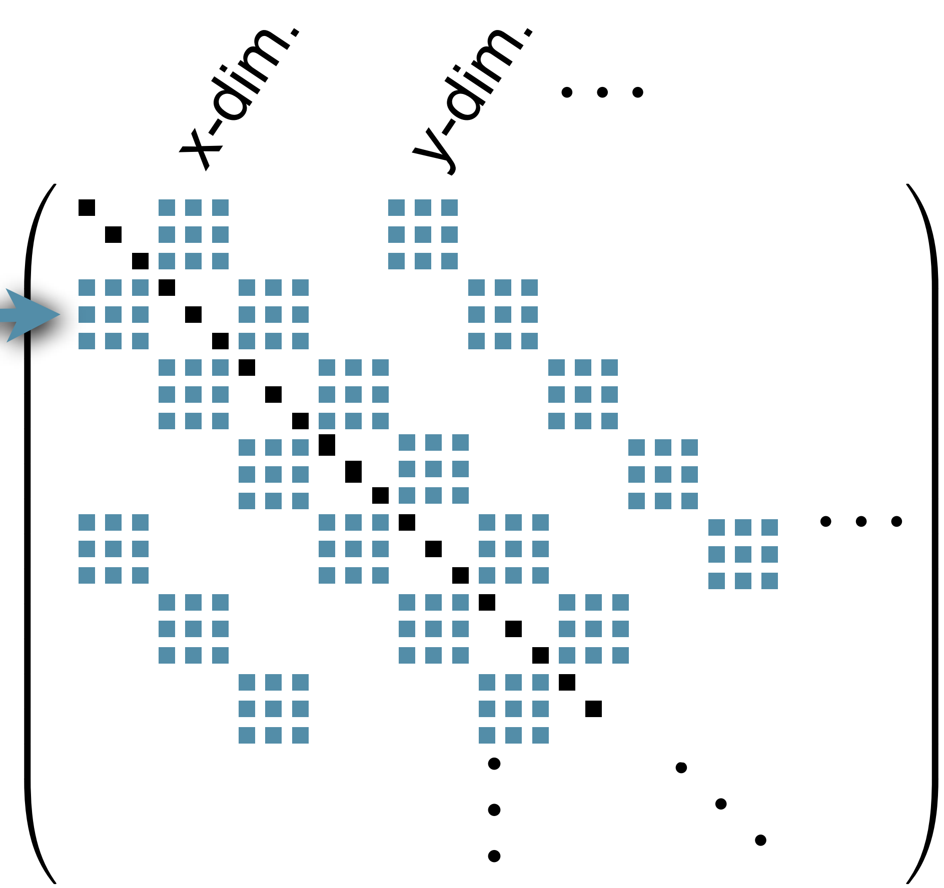
- path integral formulation of the partition function:

$$Z(\mu,\beta) = \int \mathcal{D}U \, \det M(U,\mu) \, e^{-\beta S_G(U)}$$
$$= \int \mathcal{D}U \, e^{\mathrm{Tr}\,\ln M(U,\mu)} \, e^{-\beta S_G(U)}$$

SU(3)-valued link variables

sparse fermion matrix

$M =$



band structure due to nearest neighbor interaction

Formulation of the operators

- path integral formulation of the partition function:

$$Z(\mu,\beta) = \int \mathcal{D}U \, \det M(U,\mu) \; e^{-\beta S_G(U)}$$
$$= \int \mathcal{D}U \; e^{\mathrm{Tr}\,\ln M(U,\mu)} \; e^{-\beta S_G(U)}$$

SU(3)-valued link variables

sparse fermion matrix

- taking the μ-derivative:

$$\frac{\partial \ln Z}{\partial \mu} = \frac{1}{Z}\int \mathcal{D}U \; \mathrm{Tr}\left[M^{-1}M'\right] \; e^{\mathrm{Tr}\,\ln M} e^{-\beta S_G}$$
$$= \left\langle \mathrm{Tr}\left[M^{-1}M'\right]\right\rangle$$

with $M' = \partial M/\partial\mu$, similar to M
but with less bands

Formulation of the operators

- taking further μ-derivatives:

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = \left\langle \mathrm{Tr}\left[M^{-1}M''\right]\right\rangle - \left\langle \mathrm{Tr}\left[M^{-1}M'M^{-1}\right]\right\rangle + \left\langle \mathrm{Tr}\left[M^{-1}M'\right]^2\right\rangle$$

quark line connected

quark line disconnected

$\Rightarrow$ **required operators for the 6th derivative:**
traces of 33 different matrices, each of which a combination of *up to 6* M^{-1} *with insertions of* $M^{(n)} = \partial^n M/\partial \mu^n$

$\Rightarrow$ **use noisy estimators to for the traces:**

$$\mathrm{Tr}\left[Q\right] \approx \frac{1}{N}\sum_{i=1}^{N} \eta_i^\dagger Q \eta_i$$

with η_i being a vector with uncorrelated random entries, normalized such that

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \eta_{i,x}^\dagger \eta_{i,y} = \delta_{x,y}$$

Formulation of the operators

- taking further μ-derivatives:

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = \left\langle \mathrm{Tr}\left[M^{-1}M''\right]\right\rangle - \left\langle \mathrm{Tr}\left[M^{-1}M'M^{-1}\right]\right\rangle + \left\langle \mathrm{Tr}\left[M^{-1}M'\right]^2\right\rangle$$

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$\Rightarrow$ **required operators for the 6th derivative:**
traces of 33 different matrices, each of which a combination of *up to 6* M^{-1} *with insertions of* $M^{(n)} = \partial^n M/\partial\mu^n$

$\Rightarrow$ **use noisy estimators to for the traces:**

$\Rightarrow$ **use Conjugate Gradient (CG) algorithm to solve:**

$$M\chi = M'\eta_i \;\Rightarrow\; \chi = M^{-1}M'\eta_i \;\Rightarrow\; \eta_i^\dagger\chi = \eta_i^\dagger M^{-1}M'\eta_i$$

and for other operators respectively. A recursive strategy allows to obtain estimators for all 33 traces with 10 CG calls per random source.

Lattice sizes and parameters

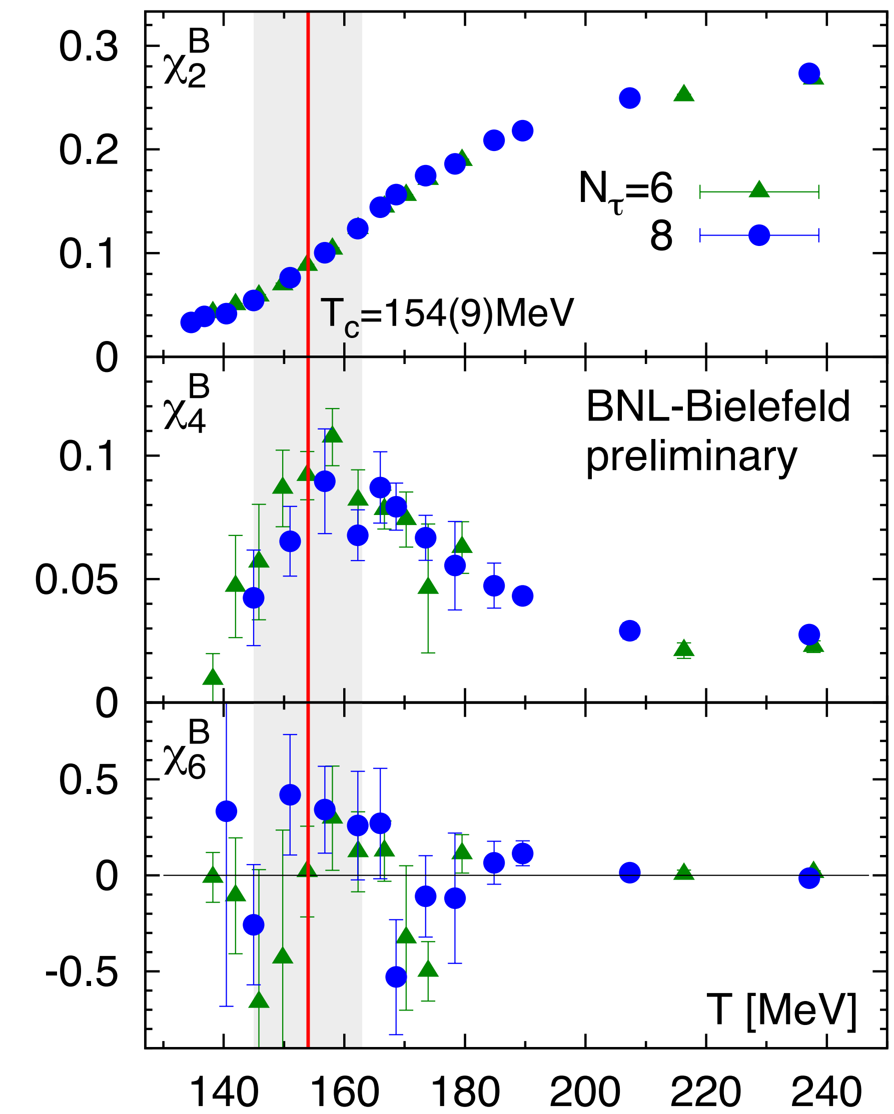
Current status:

Action: highly improved staggered quarks (HISQ)

Lattice size: $24^3 \times 6,\ 32^3 \times 8,\ 48^3 \times 12$

Mass: $m_q = m_s/20 \quad \longrightarrow m_\pi \approx 160\ \mathrm{MeV}$

Statistics: #confs=2000-8000, #sources=1500



Next goal:

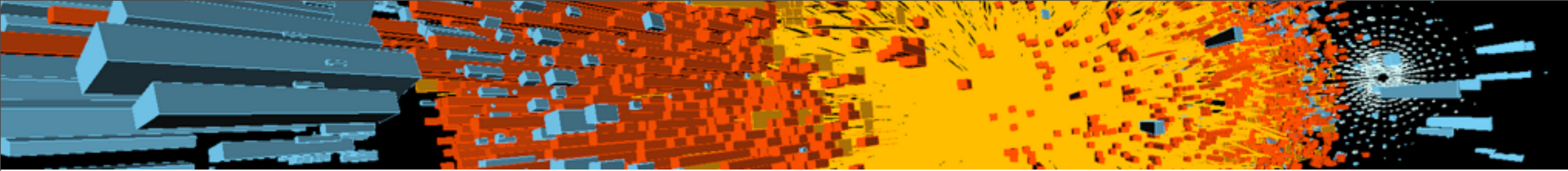
Action: highly improved staggered quarks (HISQ)

Lattice size: $24^3 \times 6,\ 32^3 \times 8,\ 48^3 \times 12,\ 64^3 \times 16$

Mass: $m_q = m_s/27 \quad \longrightarrow m_\pi \approx 138\ \mathrm{MeV}$

$\Longrightarrow$ generation of $64^3 \times 16$ is ongoing

$\Longrightarrow$ calculations of cumulants could be done on Titan



GPU acceleration

Fermion matrix application on the GPU

- runtime dominated by the CG-applications, which again are dominated by the applications of the fermion matrix applications $M(U) = \mathbb{1}m + D(U)$ (>80%)

$$w_x = D_{x,y} v_y = c_1 \sum_{\nu=0}^{3} \left\{ \left(U^{\text{fat}}_{x,\nu} \right) v_{x+\hat{\nu}} - \left(U^{\text{fat}}_{x-\hat{\nu},\nu} \right)^{\dagger} v_{x-\hat{\nu}} \right\}$$
$$+ c_3 \sum_{\nu=0}^{3} \left\{ \left(U^{\text{Naik}}_{x,\nu} \right) v_{x+3\hat{\nu}} - \left(U^{\text{Naik}}_{x-3\hat{\nu},\nu} \right)^{\dagger} v_{x-3\hat{\nu}} \right\}$$

low arithmetic intensity (flops/byte $\approx \mathbf{0.73}$ (32bit))

$\Longrightarrow$ **code is bandwidth limited:**
optimize memory access (coalescing)

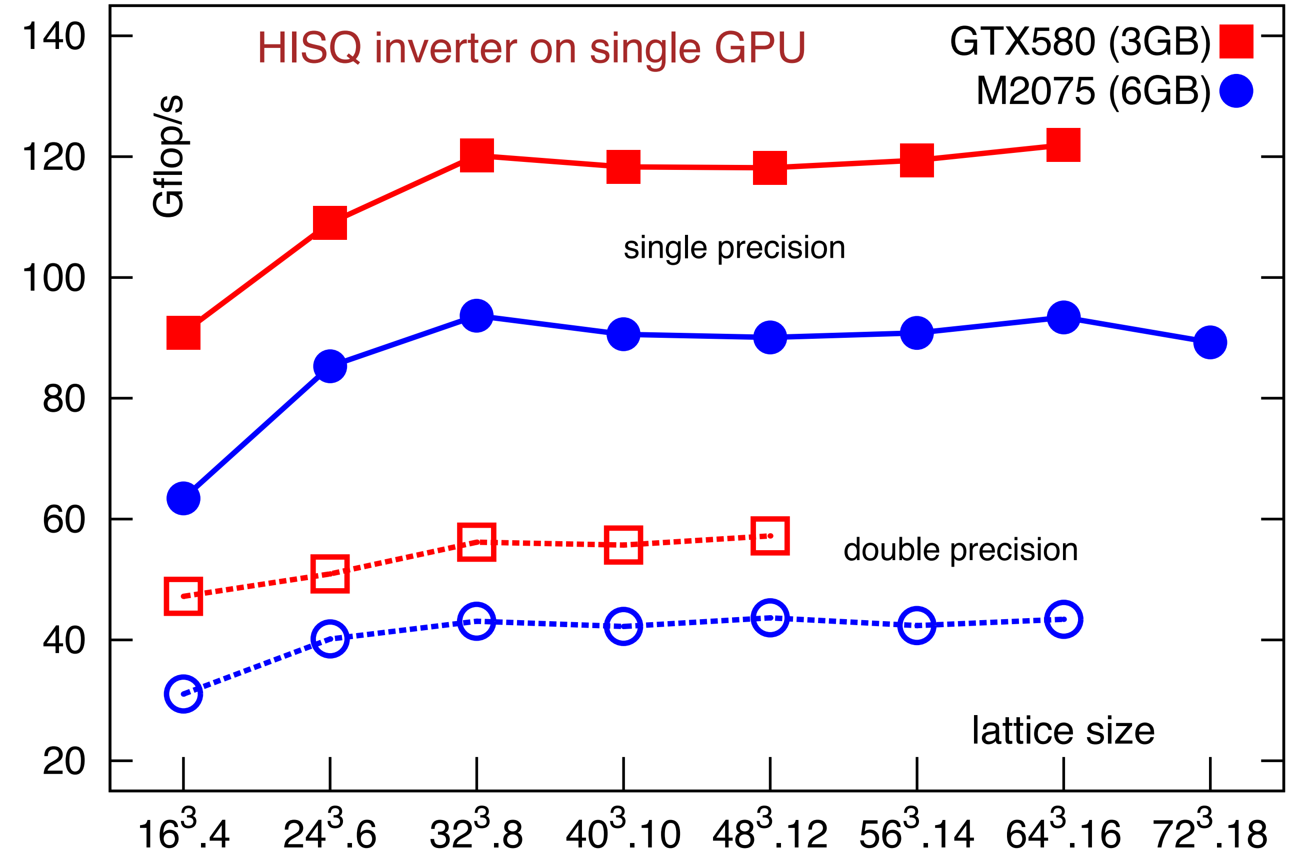
$\Longrightarrow$ keep fields on GPU to eliminate slow PCIe bandwidth and latencies

$\Longrightarrow$ theoretical performance (without further tricks):

M2075: 105 GFlops GTX Titan: 210 GFlops
GTX580: 140 GFlops

CG performance on the GPU

⇒ CG performance (10-15)% lower than Dslash performance (due to linear algebra which has even lower arithmetic intensity)



reduce transferred memory:

⇒ one possibility: use mixed precision inverter (M. Clark, R. Brower, *et al.*)

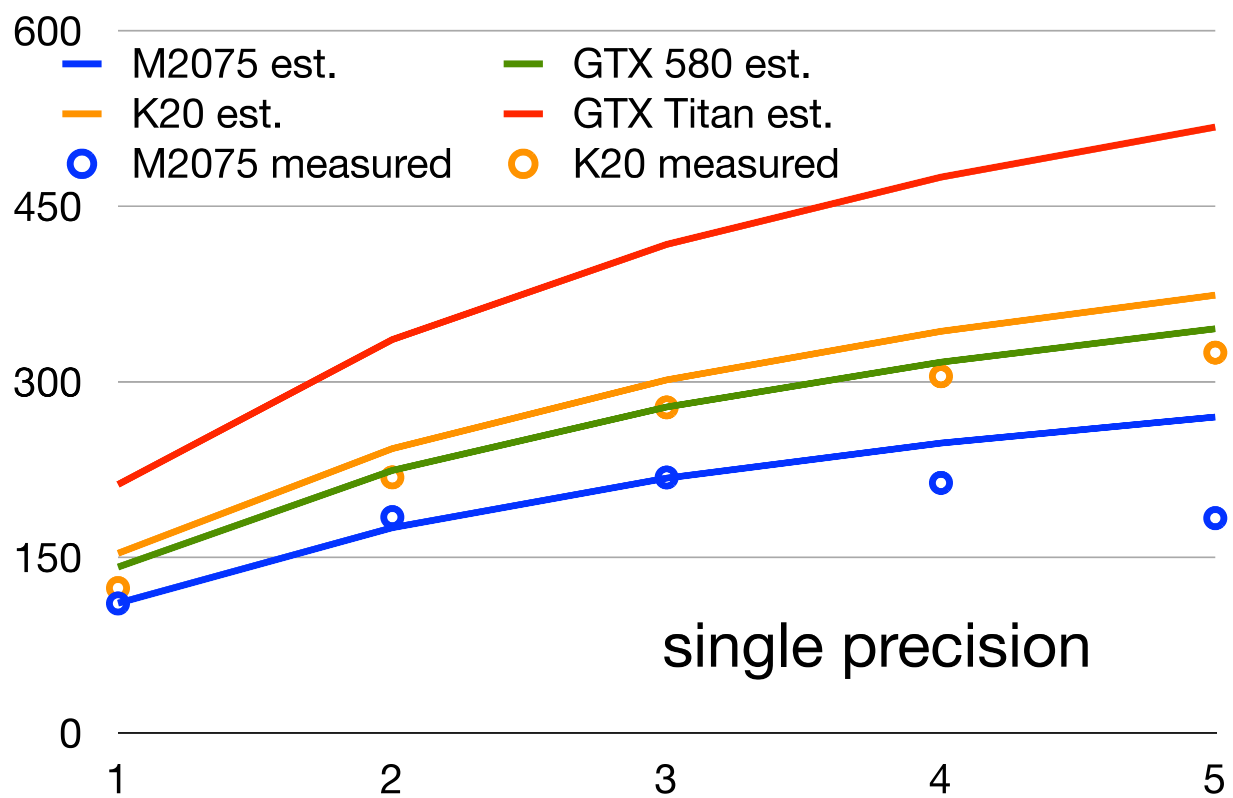
⇒ our strategy: use multiple right hand sites

# r.h.s.	1	2	3	4	5
flops/ byte	0.73	1.16	1.45	1.65	1.8

M. Wagner, GTC 2013

CG Performance on Titan

Dslash performance with multiple r.h.s:



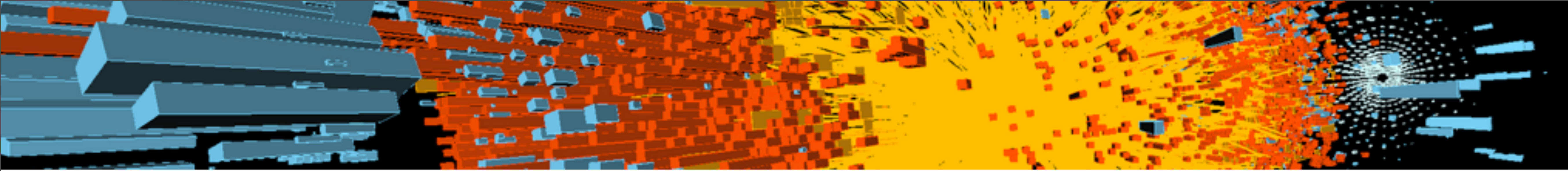
M. Wagner, GTC 2013

on the GTX Titan we can get the inverter with 3 r.h.s into GPU memory for the $64^3 \times 16$ lattices

$\Rightarrow$ Inverter should run with ca. 300 GFlops (ca. 25% penalty for LA and ECC)

Parallelize over random sources, need communication only after CG to collect the estimators of the traces

$\Rightarrow$ Performance will show good scaling: $\approx$ #nodes x 300 GFlops



Summary

Summary

- Cumulants of conserved charge fluctuations are interesting quantities to compute in (lattice) QCD, they can also be measured in heavy ion collision.

- Computational cost drastically increase with the order of the cumulant.

- Main computational cost got into the inversion of a space matrix (CG).

- On the GPU we can increase the performance by using inverters with support for multiple right hand sites.

- On Titan we can distribute the random source vectors over the GPUs, and in addition can fit a 3 r.h.s-inverter for the $64^3 \times 16$ lattices (this code is ready and tested).

Back up

Lattice sizes and parameters

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Statistics: #confs=2000-8000, #sources=1500

Properties of different staggered actions:

action	low T impr.	high T impr.	groups
naive	none	none	Mumbai
p4	not good	very good	BNL-BI
asqtad	good	good	HotQCD
stout	very good	none	WB
HISQ	excellent	good	HotQCD/BNL-BI

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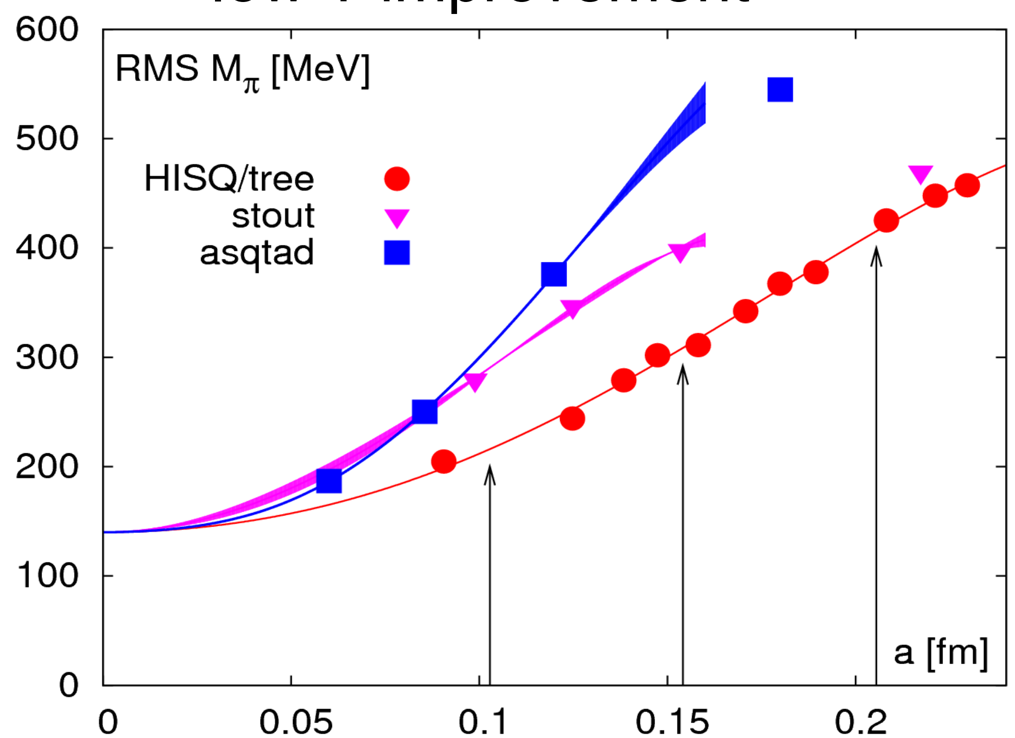
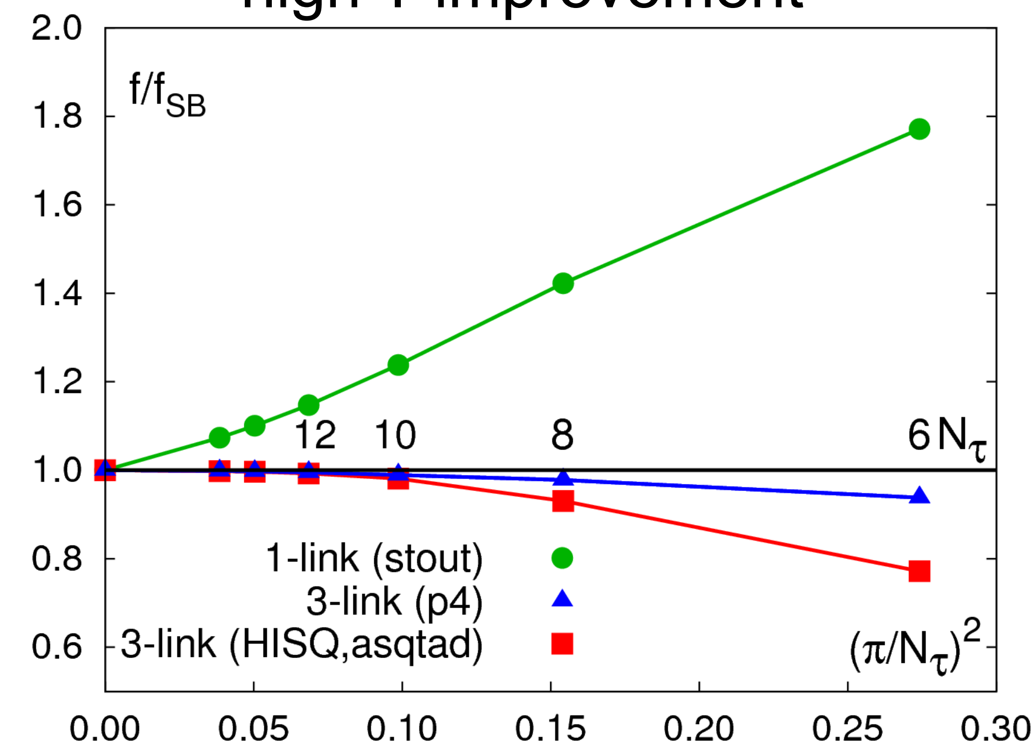
Properties of different staggered actions:

low T improvement



high T improvement



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