Lattice QCD, Charge Fluctuations, and Bootstrap Algebraic Multigrid

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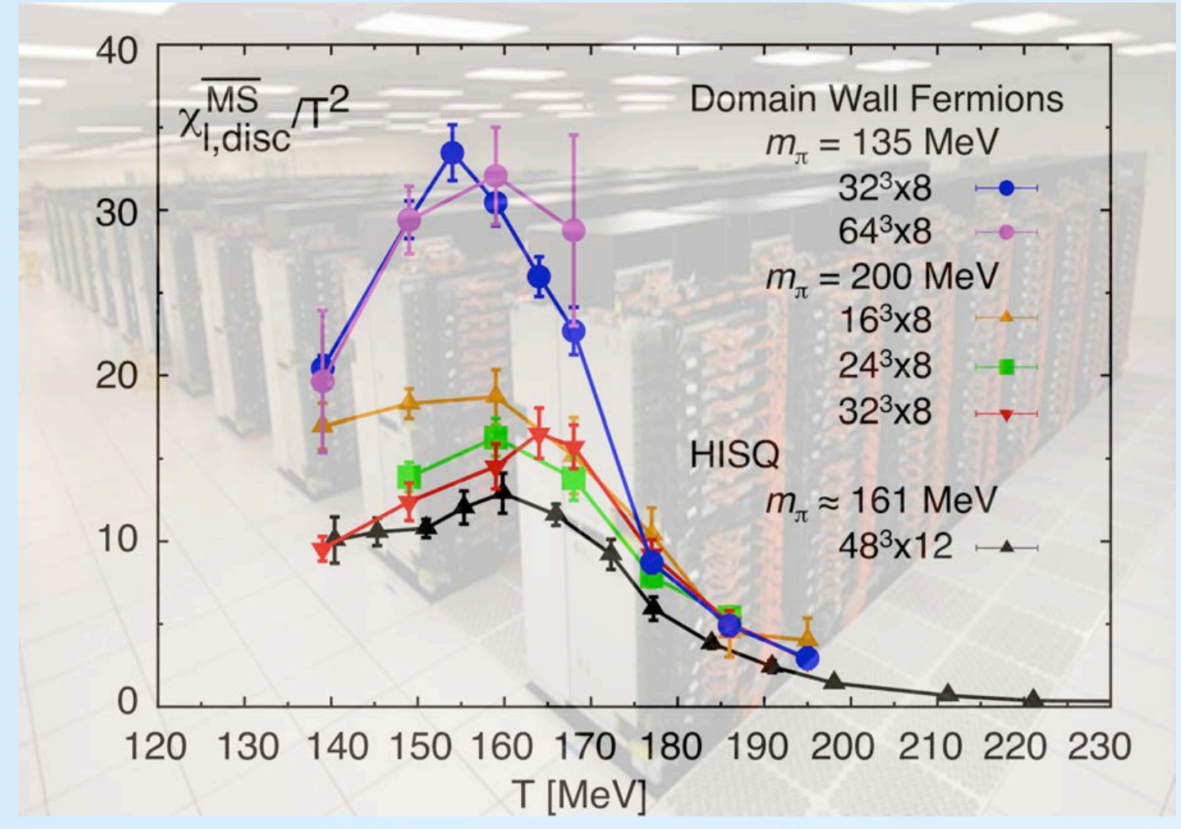
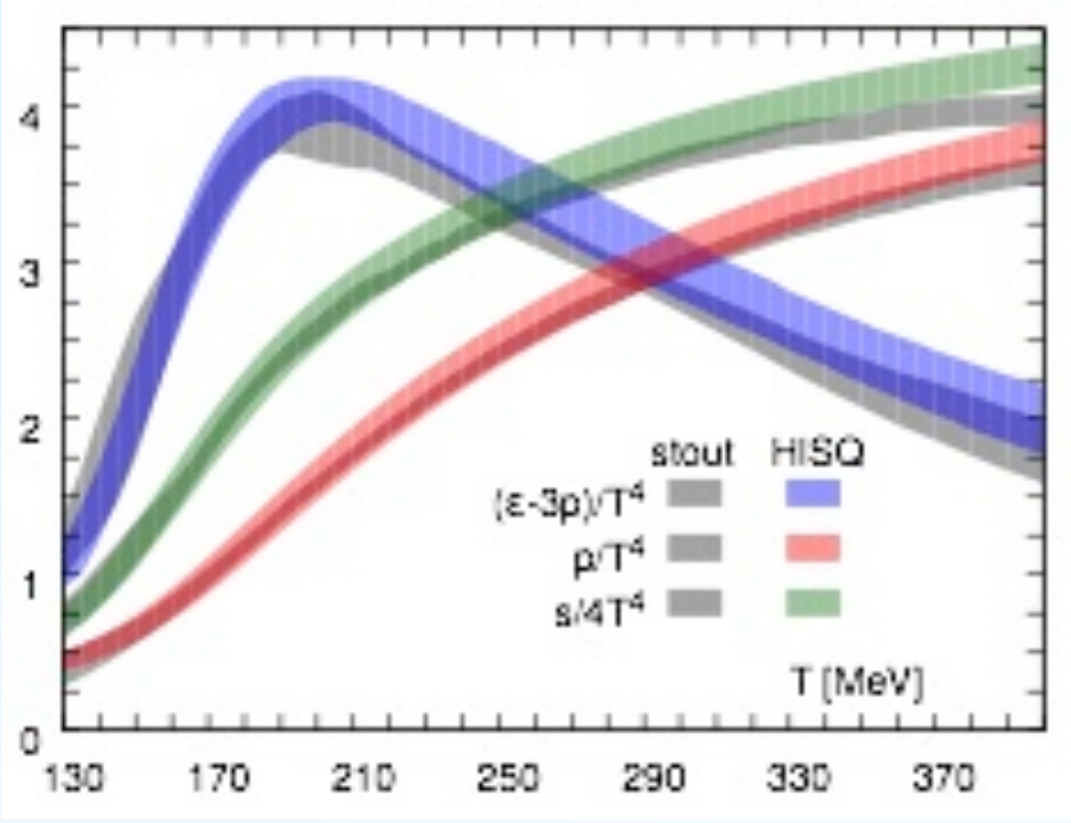


Calculation of cross-over temperature with chiral quarks, HotQCD, arxiv:1402.5175

Lattice gauge techniques have greatly improved our understanding of the properties of Quantum Chromodynamics (QCD) at finite temperature. Recent results confirm the presence of a crossover transition from hadrons to quarks and gluons above about 155 MeV using several different methods, and the QCD Equation of State has been determined in the continuum limit, as required for precision hydrodynamic modeling of the zero baryon density regions created in full-energy heavy ion collisions at RHIC and the LHC. The next great challenge in Lattice QCD thermodynamics is to extend the calculations into regions of finite baryon density that will be probed by FAIR and the beam energy scan at RHIC to identify and study the critical end point that must exist if there is a first order transition at high baryon density.



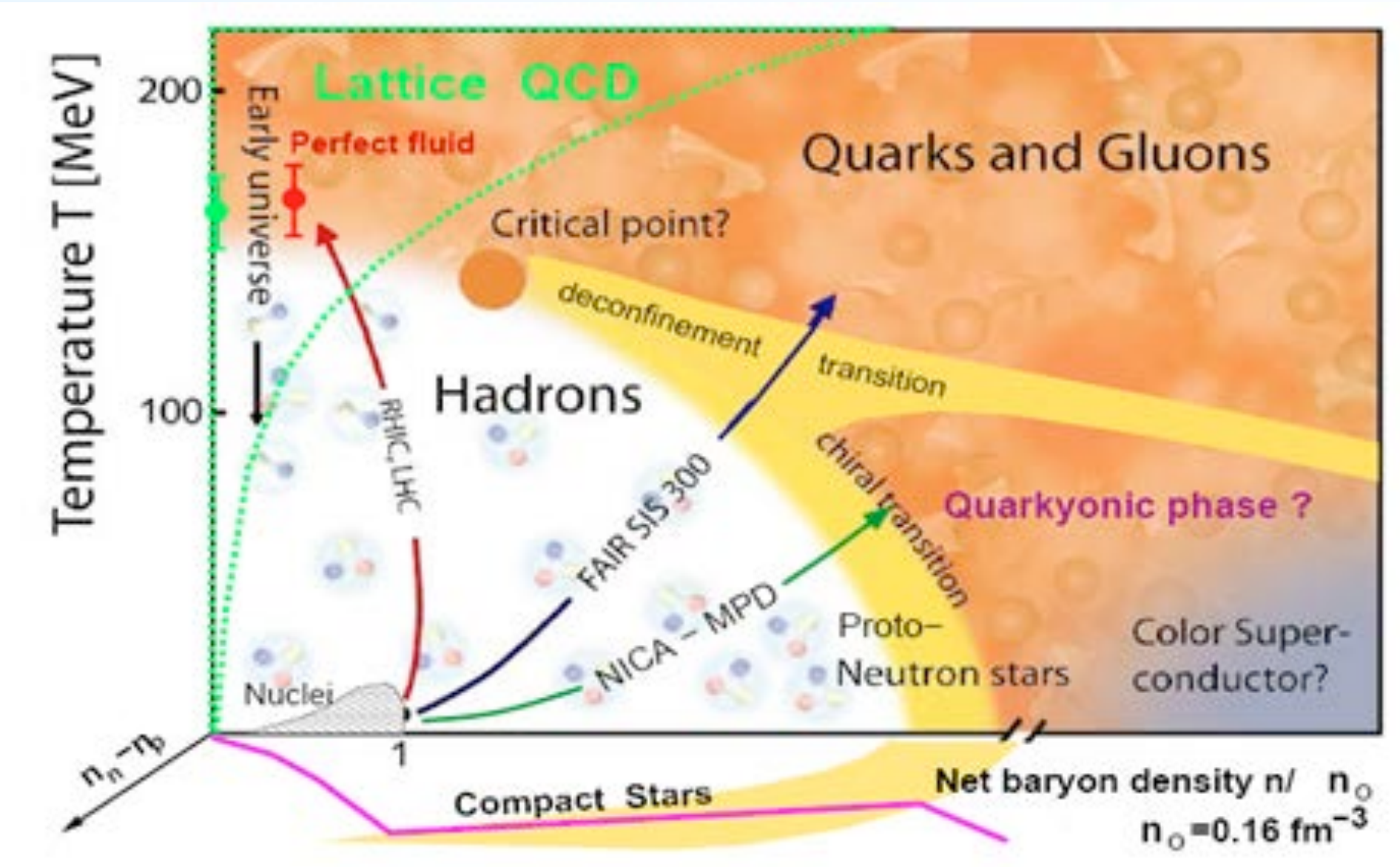
Lattice QCD EoS for two fermion actions B-W & HotQCD arxiv: 1309.5258,1407.6387

The most promising approach for extending lattice techniques into regions of finite baryon density involves the calculation of susceptibilities, which if calculated to sufficient order, provide an estimate for the location of the critical end point [Gavai and Gupta (05)].

$$\chi_{lmn}^{BSQ} = \frac{\partial^{l+m+n}(p/T^4)}{\partial(\mu_B/T)^l\partial(\mu_S/T)^m\partial(\mu_Q/T)^n}$$

The baryon susceptibility will diverge at the location of the critical point (if it exists), and it's location can be determined by Taylor series expansion through the radius of convergence,

$$r_n = \lim_{n\to\infty}\sqrt{\frac{\chi_B^{(n+1)}}{\chi_B^{(n+3)}}}\,, \quad \text{or} \quad r_n = \lim_{n\to\infty}\left[\frac{\chi_B^{(2)}}{\chi_B^{(n+2)}}\right]^{1/n}$$

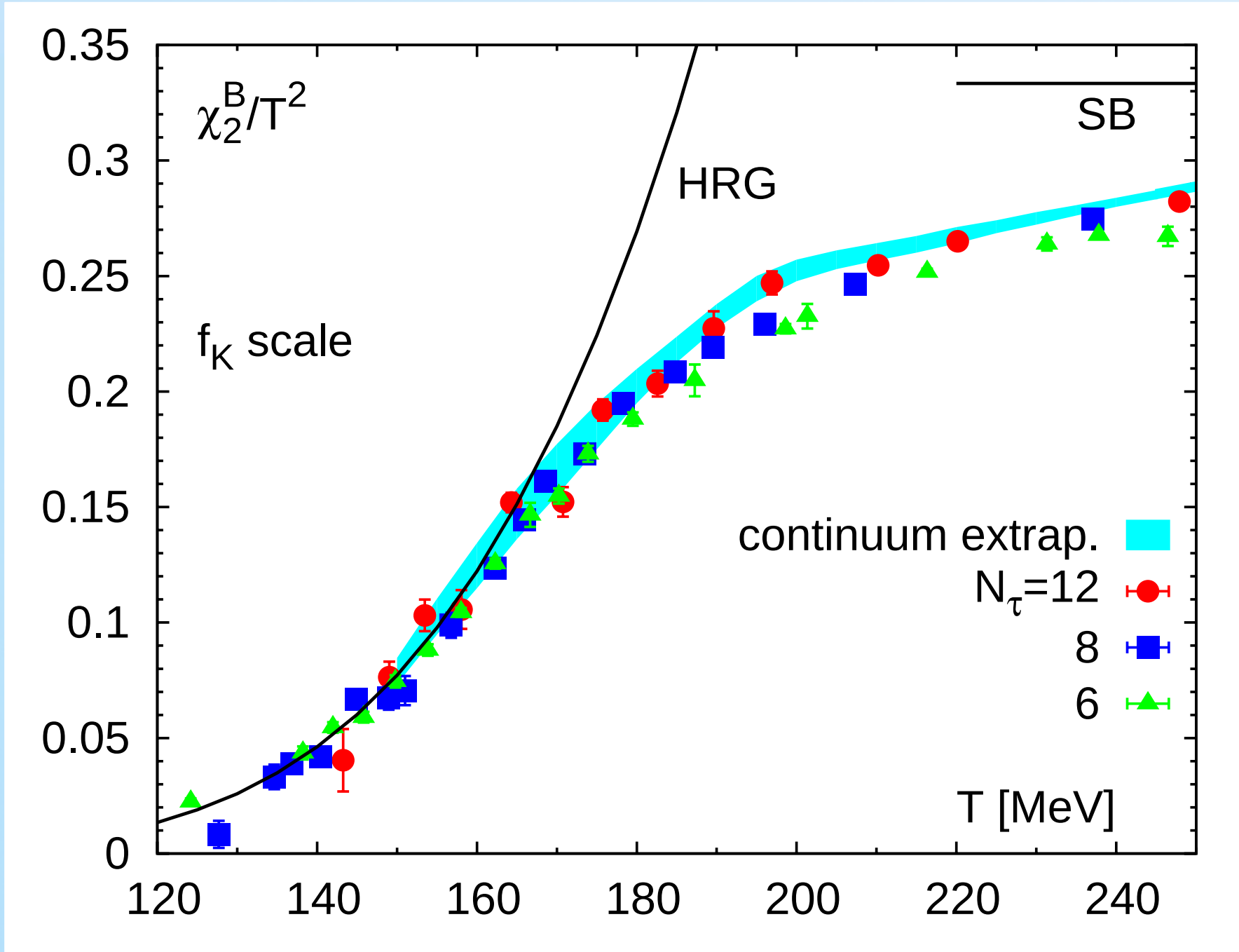


Schematic phase diagram for QCD with critical end point separating cross-over from first order transition at high baryon density.

Estimates of the radius of convergence will need to be computed in the continuum limit and will require higher order susceptibilities, eighth order or higher. These calculations are computationally intensive and will not be feasible without significant advances in hardware as well as more powerful numerical methods. A speedup of at least an order of magnitude is needed for such a calculation to be possible on a 1-year timescale. Algebraic multigrid (AMG) has the potential to provide this speedup and benefit many other Lattice QCD calculations as well.

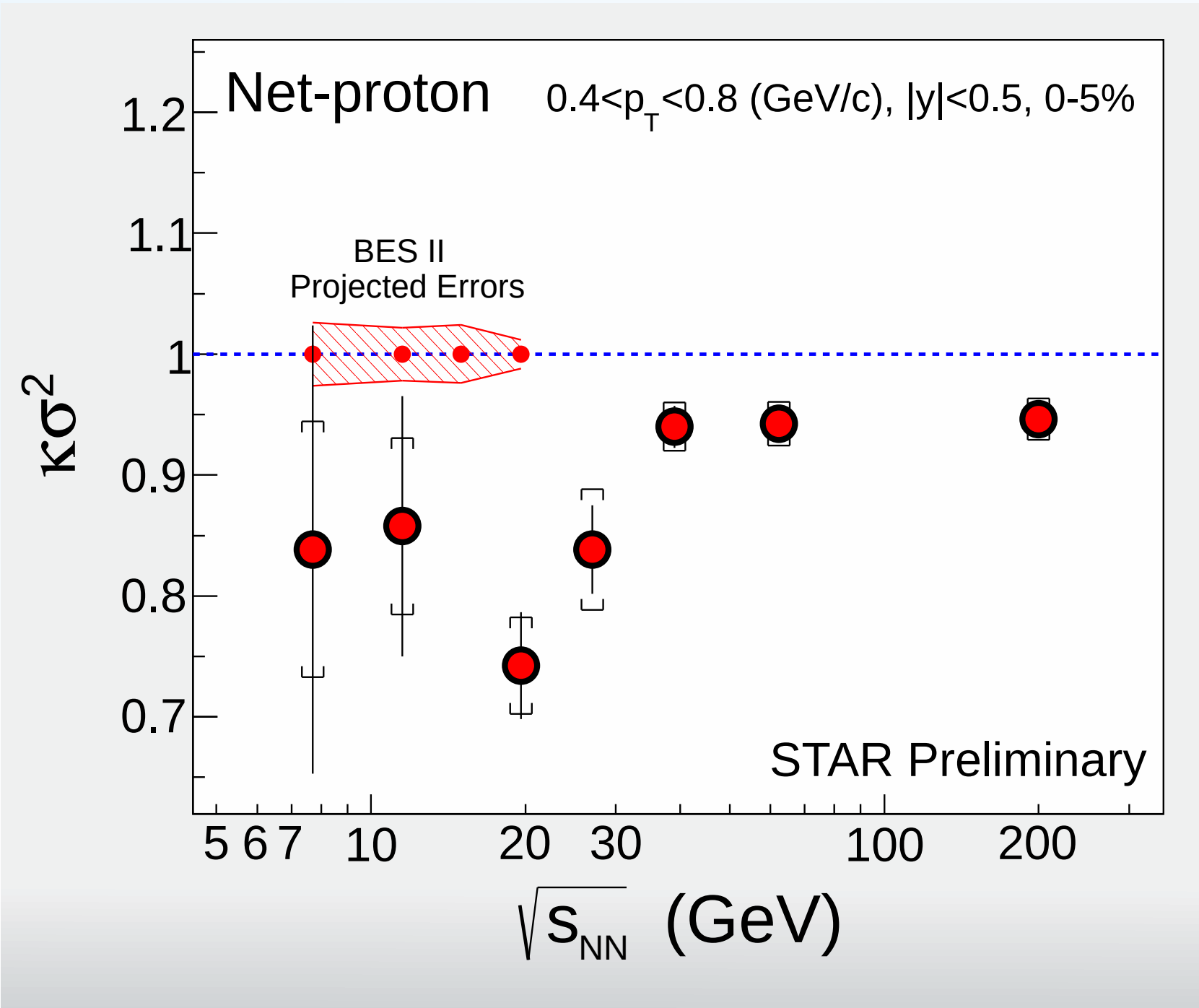
The susceptibilities with respect to charge, strangeness, and baryon number also provide information on fluctuations, which can be compared directly to experimental measurements at freeze-out [Karsch and Redlich (11)], as well as to calculations of a non-interacting Hadron Resonance Gas (HRG). Therefore, at zero baryon density, the lattice susceptibilities can be benchmarked against experimental data and HRG calculations in order to understand the freeze-out conditions. The higher order susceptibilities can be used to study higher order moments of the charge, strangeness, and baryon number fluctuations measured by experiments.

moments	experimental definitions	lattice susceptibilities
$\frac{\sigma_q^2}{M_q}$	$\frac{\langle(\delta N_q)^2\rangle}{\langle N_q\rangle}$	$\frac{\chi_q^{(2)}}{\chi_q^{(1)}}$
$S_q\sigma_q$	$\frac{\langle(\delta N_q)^3\rangle}{\sigma^2}$	$\frac{\chi_q^{(3)}}{\chi_q^{(2)}}$
$\kappa_q\sigma_q^2$	$\frac{\langle(\delta N_q)^4\rangle}{\sigma^2} - 3\sigma^2$	$\frac{\chi_q^{(4)}}{\chi_q^{(2)}}$



Comparison of continuum extrapolation of baryon number susceptibility and Hadron Resonance Gas, PRD 86, 023509.

Calculations of sixth order susceptibilities are being carried out by both the HotQCD and B-W collaborations. These calculations will be sufficient to understand experimental freeze-out conditions and deviations from the Hadron Resonance Gas calculations; however, reliable predictions for the location of a critical end point in the QCD phase diagram are beyond state-of-the-art capabilities of the lattice community. Work on AMG offers the best possibility for achieving significant speedups in lattice QCD calculations. A reliable prediction for the location of the critical endpoint would have an enormous impact on the experimental program at RHIC and other heavy ion colliders.



Net proton normalized kurtosis measured by STAR, PRL 112, 302032, and projected errors for RHIC Beam Energy Scan (2018/19).

Joining forces: *hypre* and QLua

The *hypre* package is an advanced and growing suite of parallel linear solvers and preconditioners scalable on massively parallel architectures, including the LLNL/IBM Sequoia Blue Gene/Q.

It was developed at LLNL's Center for Applied Scientific Computing (CASC) under the direction of Rob Falgout, a leader in the field of algebraic multigrid.

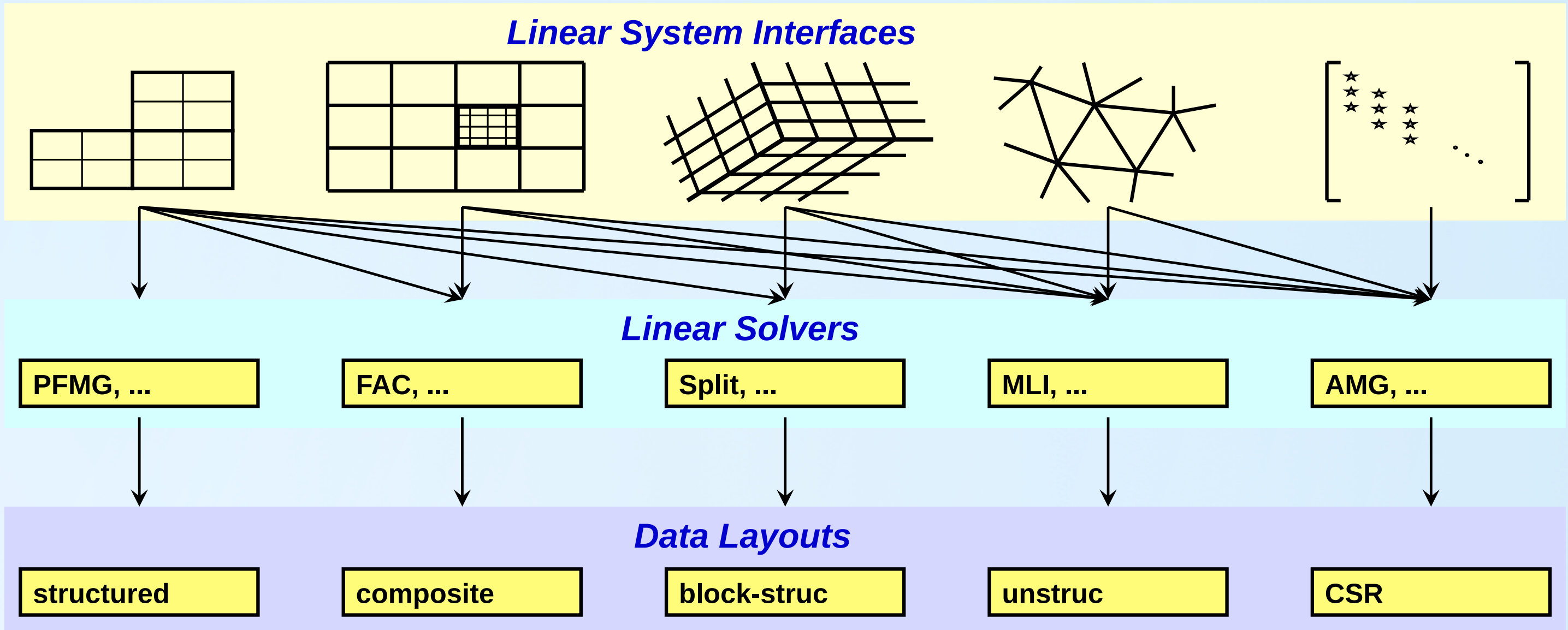
hypre is a vital component of a broad array of application codes both at LLNL and worldwide; it's been downloaded over 10,000 times in more than 70 countries.

QLua is a domain-specific language for lattice QCD based on the Lua scripting language, being developed principally by Andrew Pochinsky at MIT.

QLua combines the ease and convenience of a high-level scripting language with the extensive set of parallel capabilities contained in the USQCD software stack.

By interfacing *hypre* and QLua with the new, aptly named *hypre*-QLua Layer (HQL), we aim to bring the advanced AMG methods of *hypre* to bear on lattice gauge theory, specifically for our work with the HISQ and Domain Wall fermion discretizations.

At the same time, we are working closely with the HEP and CalLat teams to make substantial extensions to *hypre* that will benefit its non-lattice user community, such as higher dimensions, complex numbers, and development of new adaptive multigrid methods starting with Bootstrap AMG. Refer to posters by Rich Brower (USQCD HEP) and Evan Berkowitz (CalLat).



Linear System Interfaces

Linear Solvers

PFMG, ...
FAC, ...
Split, ...
MLI, ...
AMG, ...

Data Layouts

structured
composite
block-struc
unstruc
CSR

Of *hypre*'s four system interfaces, the semi-structured grid is the most efficient for lattice QCD, and provides access to most of the solvers in *hypre*.

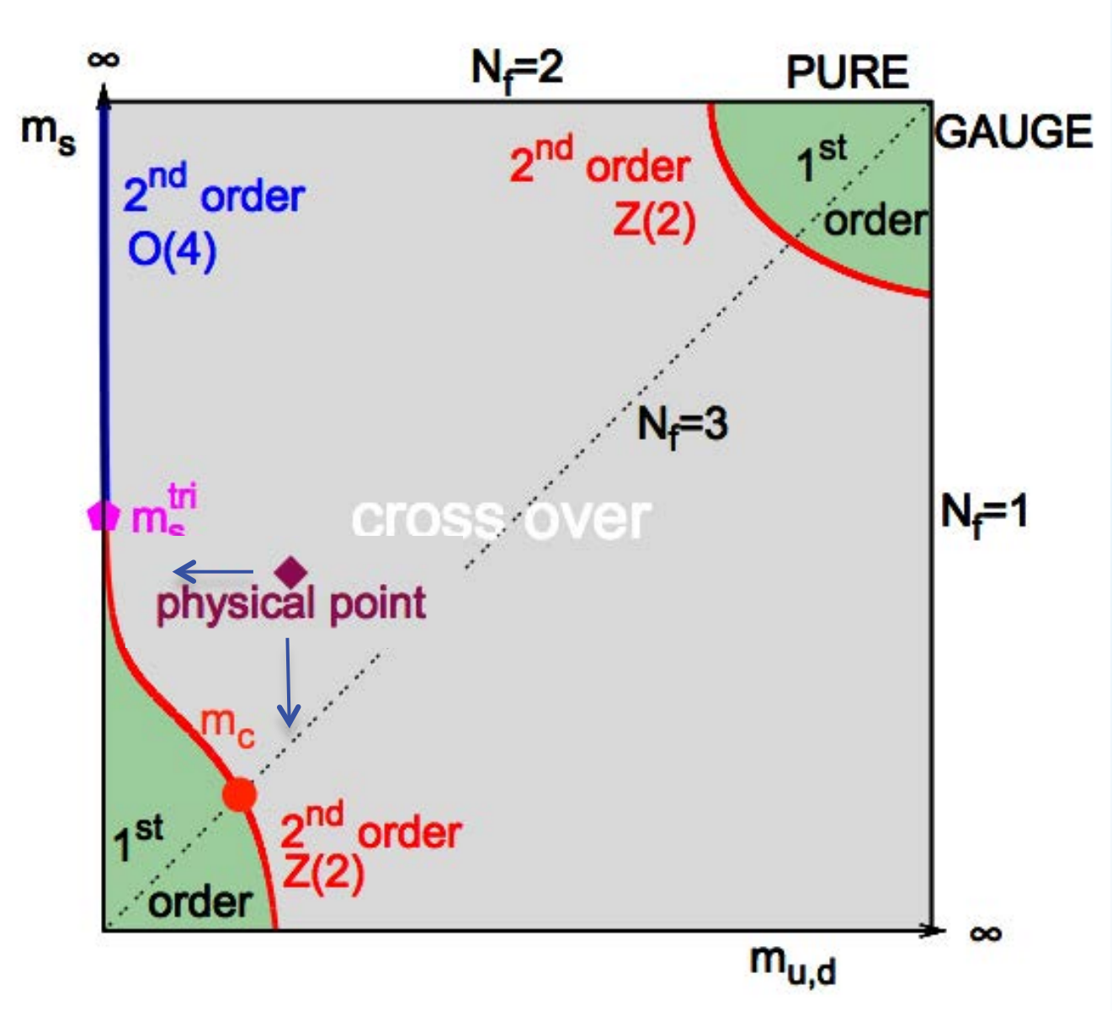
Translating the lattice QCD language of pseudofermions, spins, colors, gauge links and so on into the *hypre* language of parts and stencils was not simple but was not a tremendous challenge.

At present functionality includes:

- passing pseudofermion "vectors" between QLua and *hypre*
- converting gauge fields and arbitrary Dirac operators, defined fairly simply in QLua, into *hypre* SStruct matrices
- providing access to native linear algebra operations in *hypre*

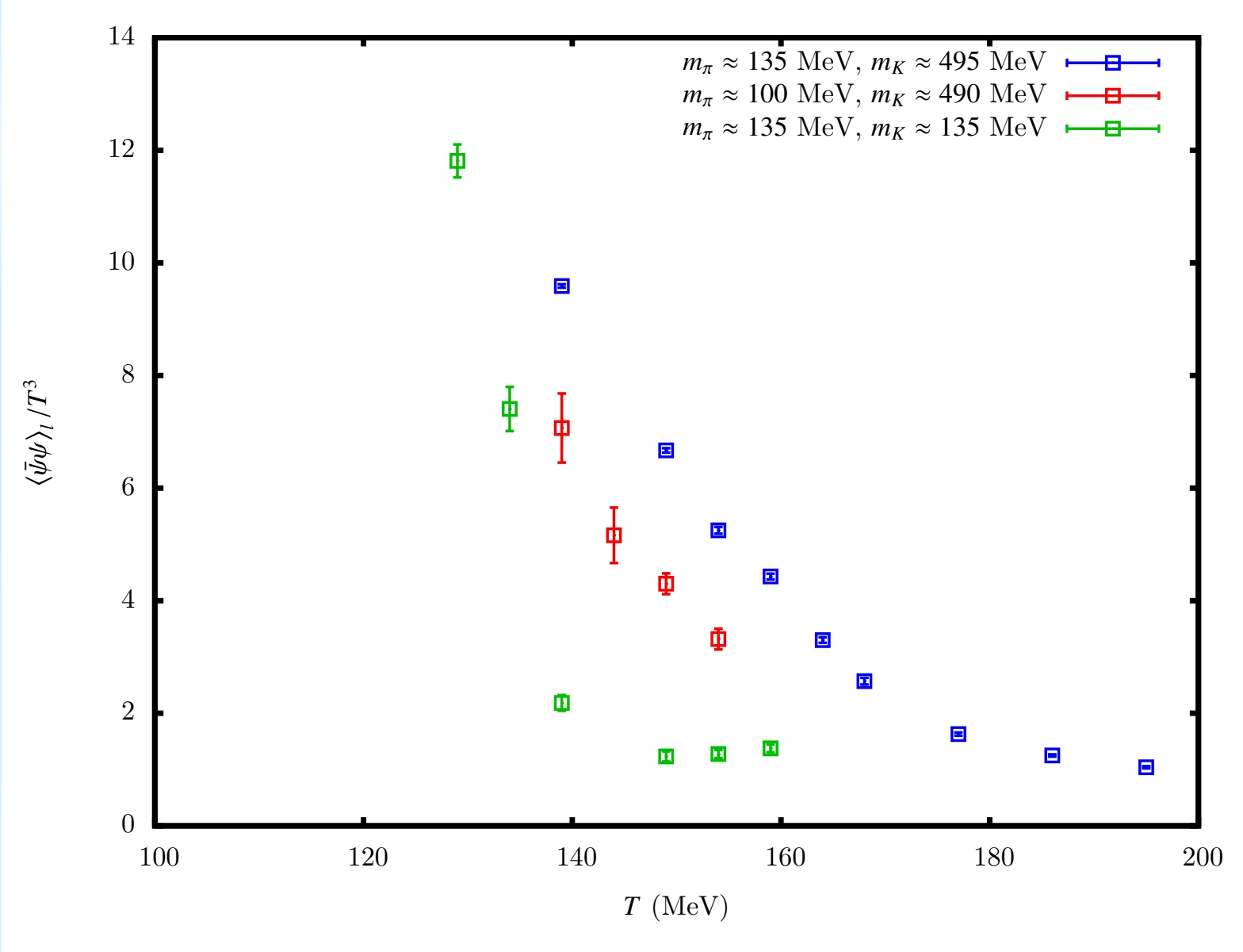
All that remains is to provide access to the adaptive methods which are currently being developed. As these become available, we will extend the interface and begin to use *hypre* to develop the methods needed to accomplish our physics goals.

Searching for First Order Phase Transitions at Zero Chemical Potential



The LLNL Lattice subgroup and HotQCD collaborators are also extending the recently completed most accurate calculation of the critical temperature to date using physical pion masses and chiral Domain Wall Fermions both by exploring the region of the "Columbia plot" near the physical point.

We have performed temperature scans for the [pseudo-]critical temperature for 1) 100 MeV pions and "physical" strange quark mass and 2) 135 MeV pions and a strange quark mass equal to the light quark mass. In both cases, we have bracketed the transition temperature, and in the $m_s = m_l$ case, we see a substantial sharpening in the rise of the chiral condensate, which may be a hint that we are approaching a true transition.



Acknowledgements

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