Computing requirements of the HotQCD Collaboration

C. Schmidt for the Collaboration

UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC–TR 211
Strong-interaction matter under extreme conditions

Plan

- The Collaboration
- The physics program
- Some research highlights
- Current resources
- Future plans
- Exascale readiness
- Conclusion

The HotQCD Collaboration

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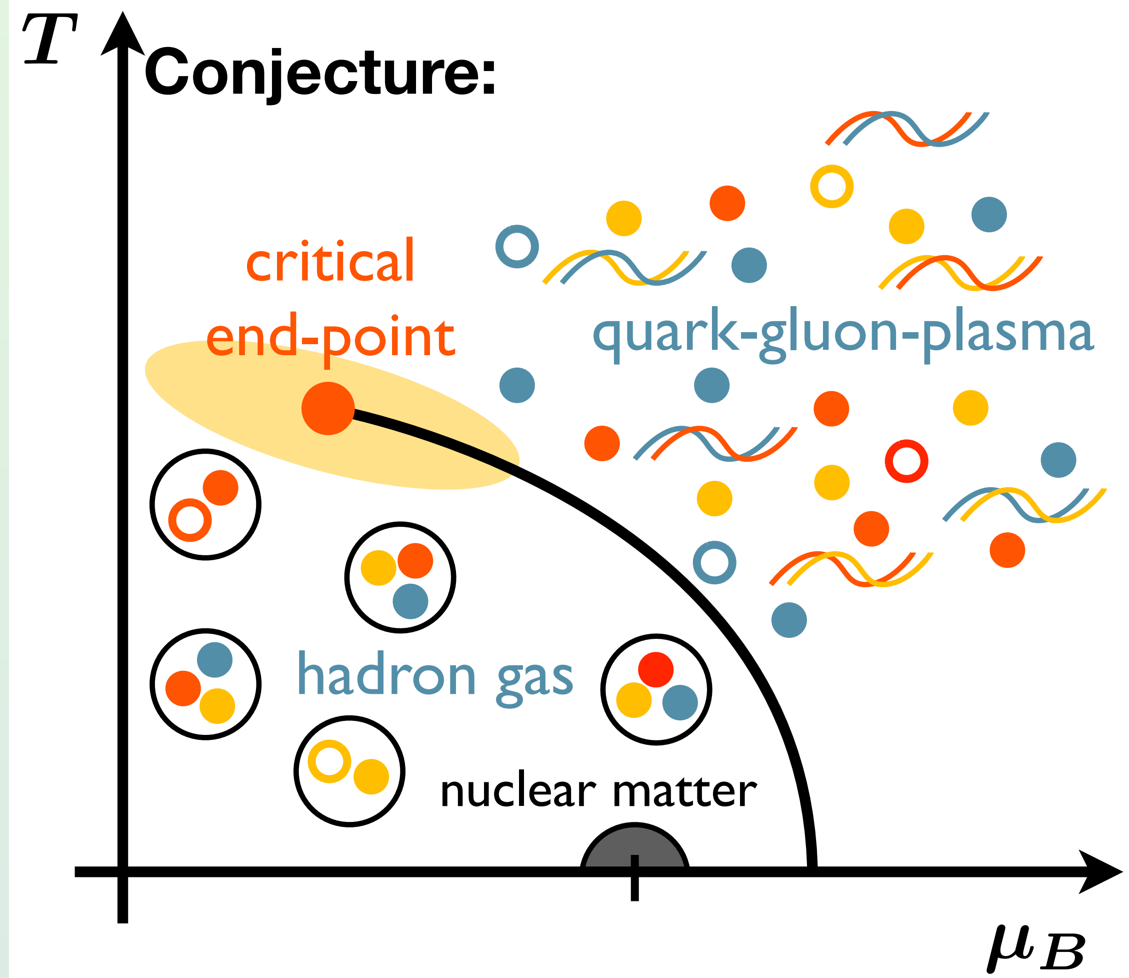
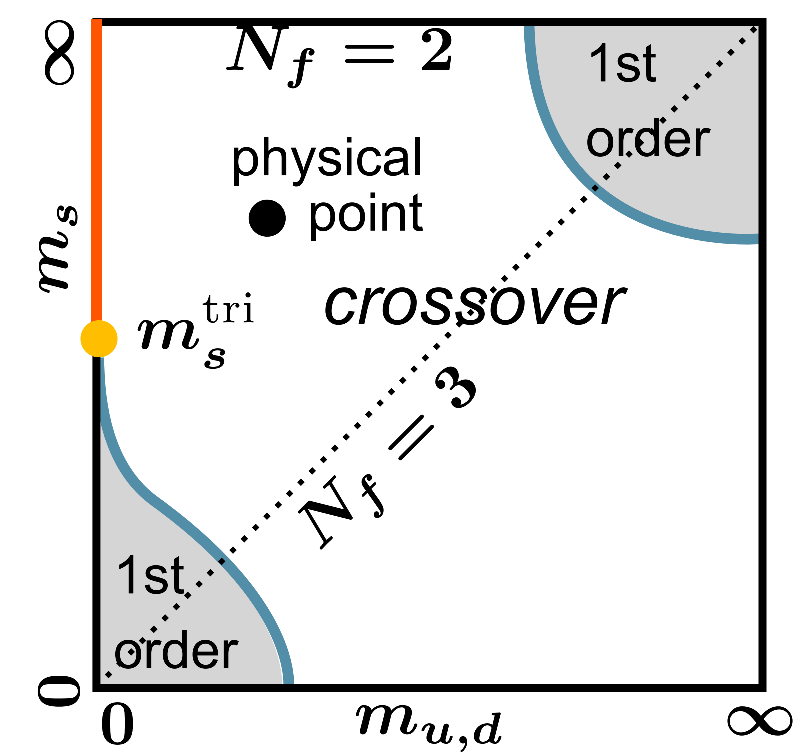
Topics of interest

- **The QCD Phase diagram**
  - ➡ The existence/location of the QCD critical point
  - ➡ The nature of the chiral transition in the chiral limit and the role of the chiral anomaly
  - ➡ QCD in external fields (constant magnetic background field, imaginary chemical potential)

- **The QCD equation of state (EoS)**
  - ➡ Isentropic EoS as input for hydrodynamic calculations
  - ➡ The relevant degrees of freedom at low and high temperatures, thermal modifications of hadrons





Pisarski, Wilczek (1984)

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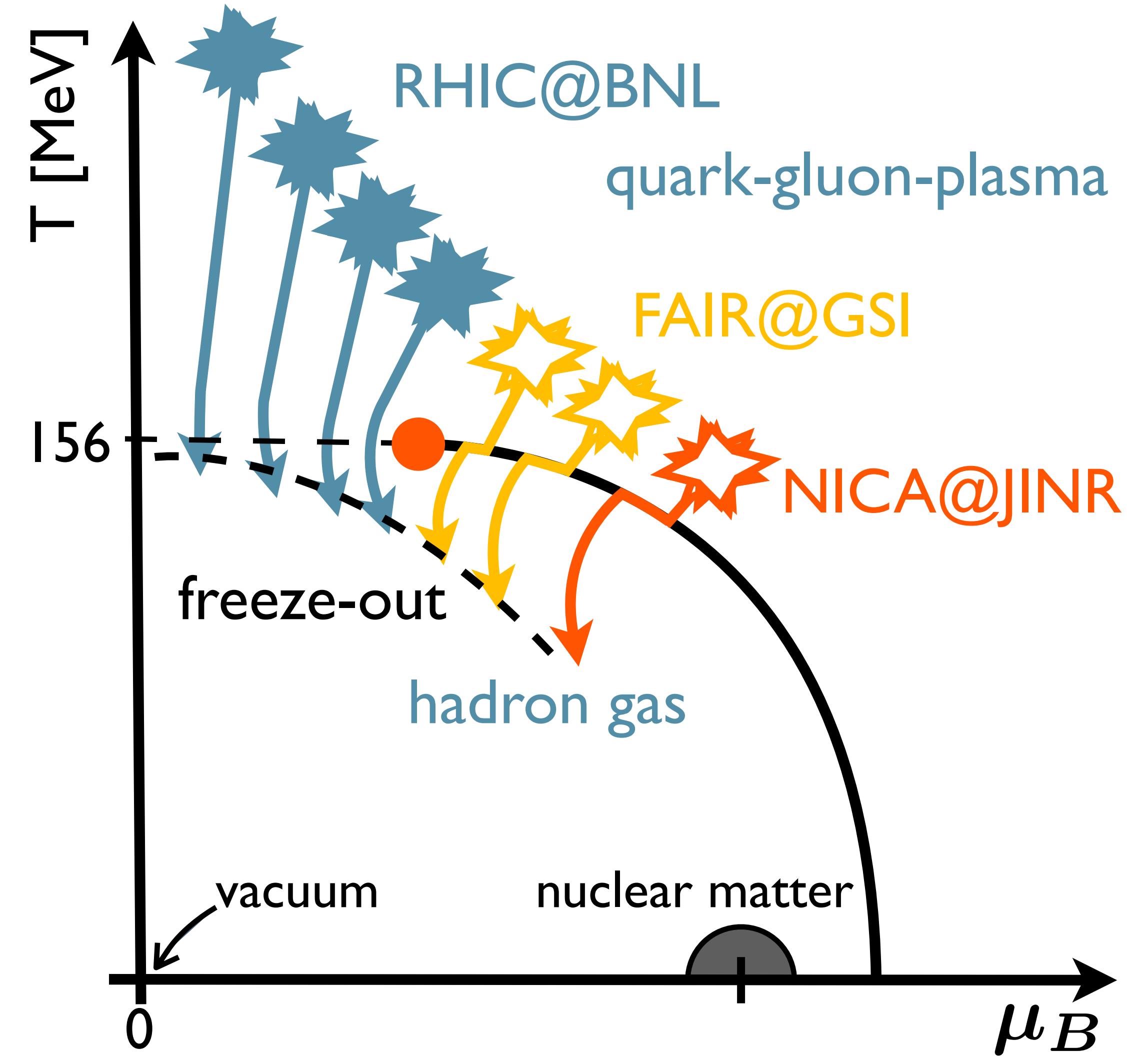
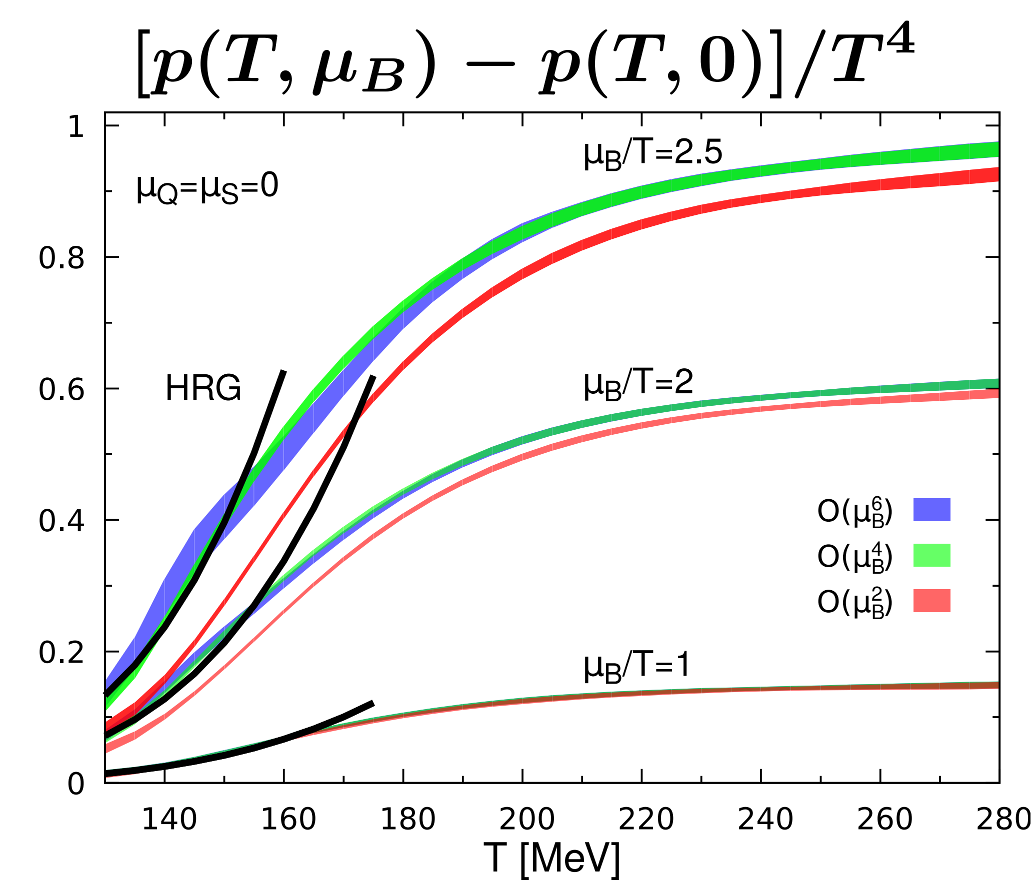
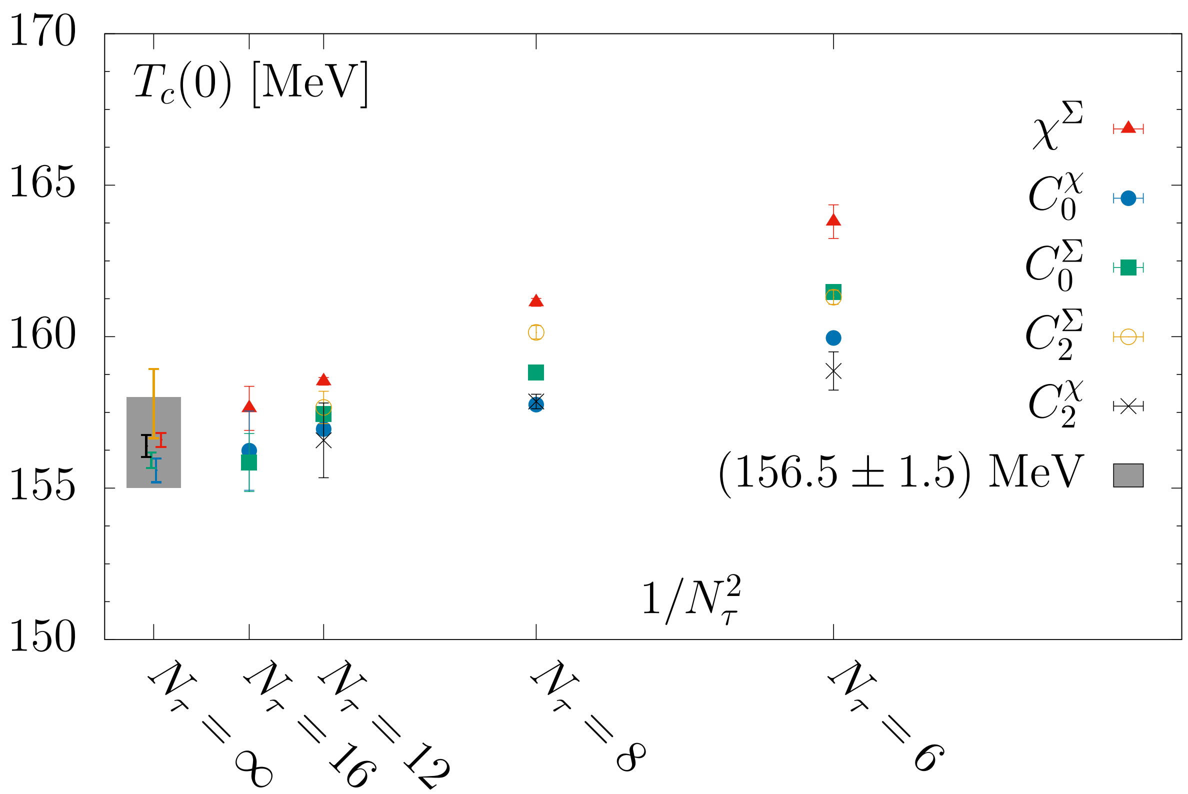


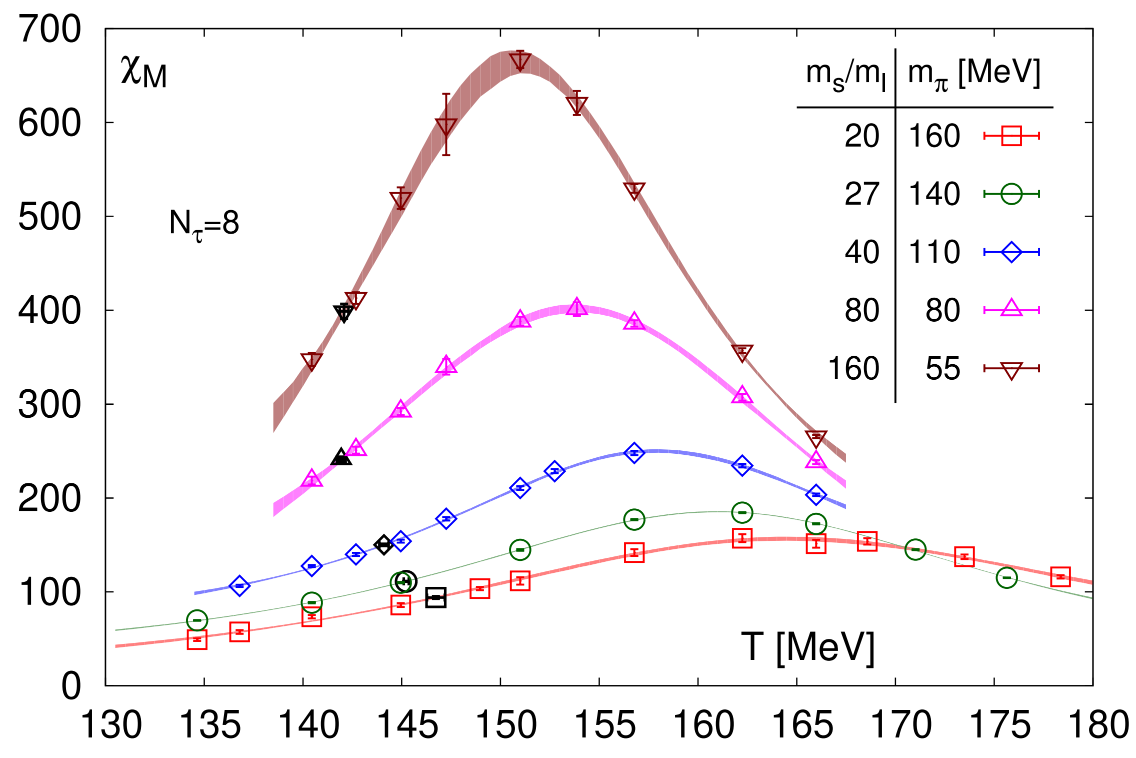


Highlighting some results

- **The chiral crossover of (2+1)-flavor QCD at physical quark masses**
  - New estimate of the pseudo critical temperature $T_{pc} = 156.5 \pm 1.5$ MeV
  - The curvature of the pseudo critical line $\kappa_2^B = 0.012(4)$
- **Universal scaling towards the chiral limit of (2+1)-flavor QCD**
  - Consistency with an O(4) critical point in the chiral limit is found
  - The chiral transition temperature is estimated to $T_c = 132^{+3}_{-6}$ MeV



HotQCD, PLB 795 (2019)



HotQCD, PRL 123 (2019)

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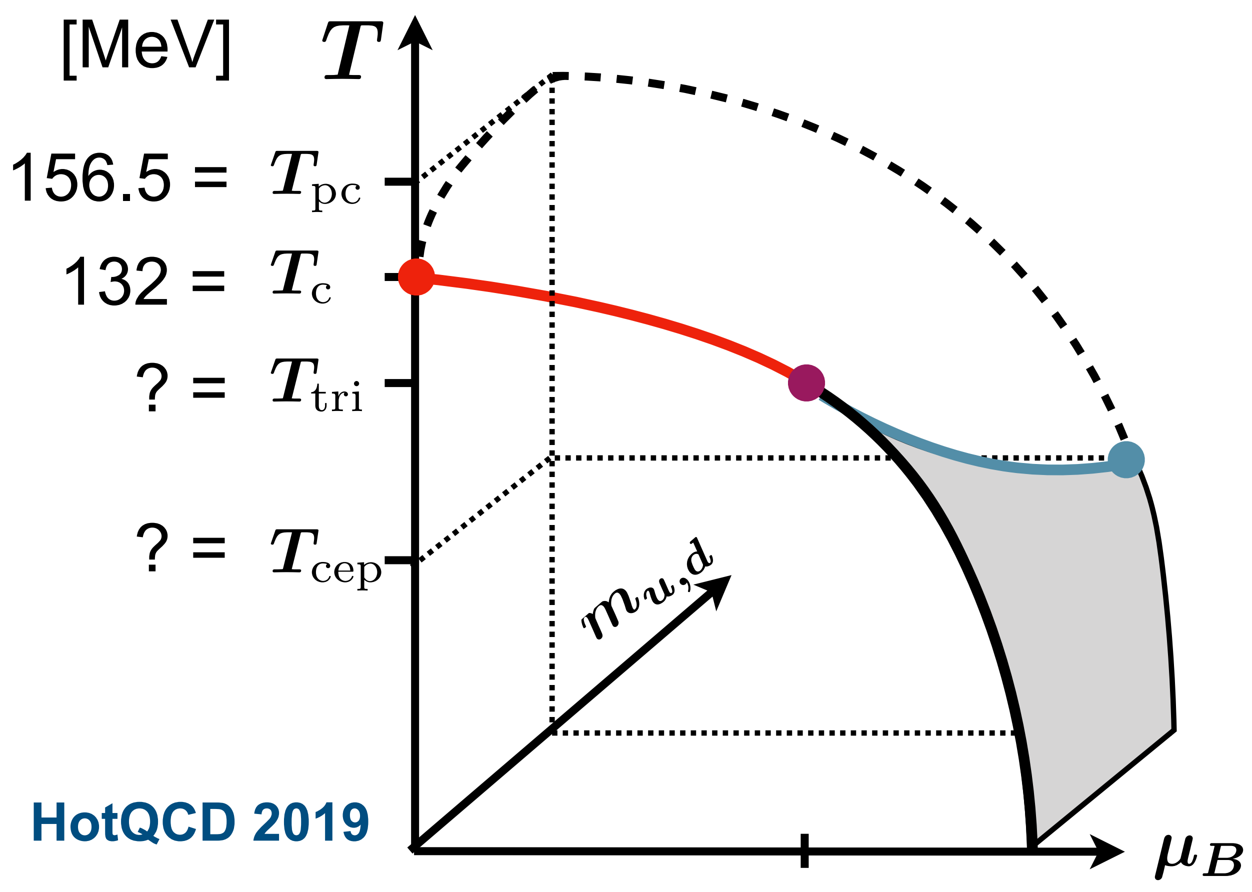
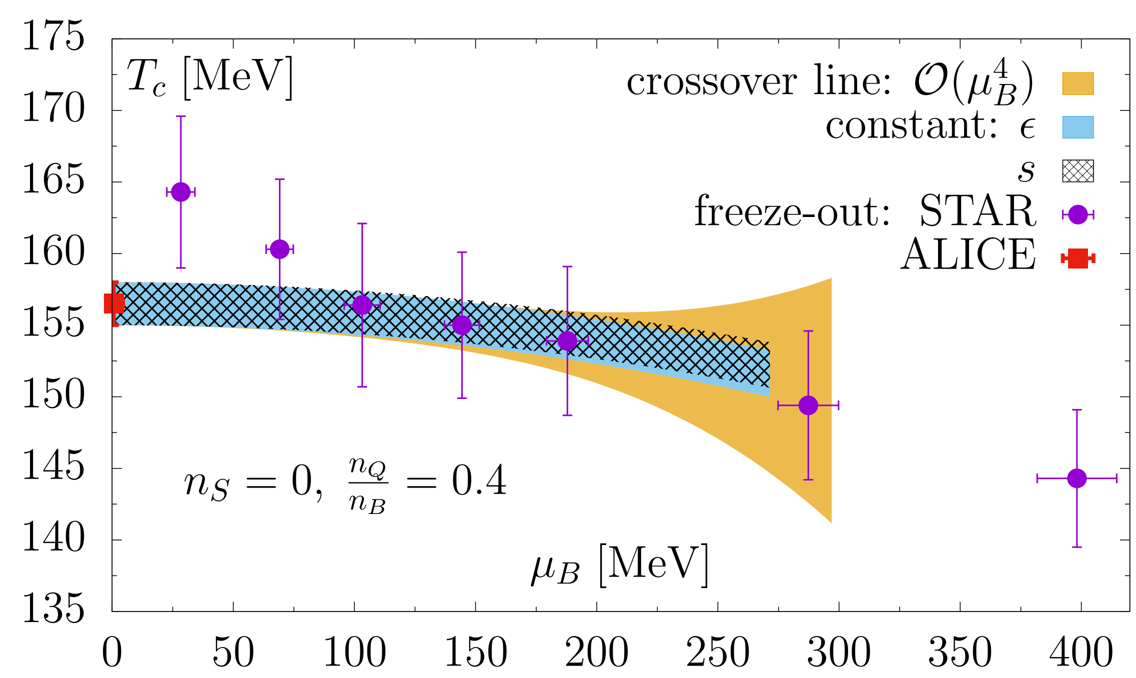


$$T_{pc}(\mu_B) = T_{pc}(0)[1 - \kappa_2^B(\mu_B/T_{pc}(O))^2]$$



HotQCD, PRL 123 (2019)

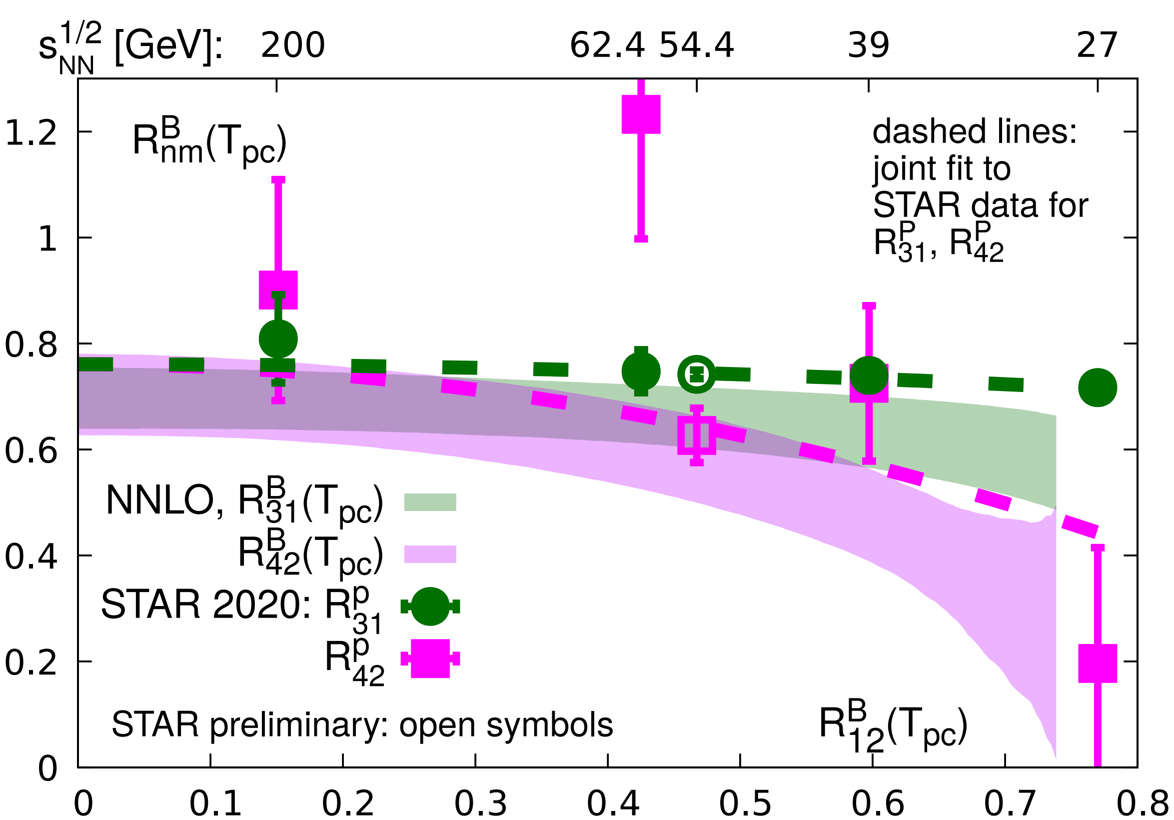
Highlighting some results

- **The pressure expansion up to $\mathcal{O}(\mu_B^8)$**
  - ➡ NNLO calculation of Skewness and Kurtosis
  - ➡ NLO calculation of Hyper-skewness and Hyper-kurtosis

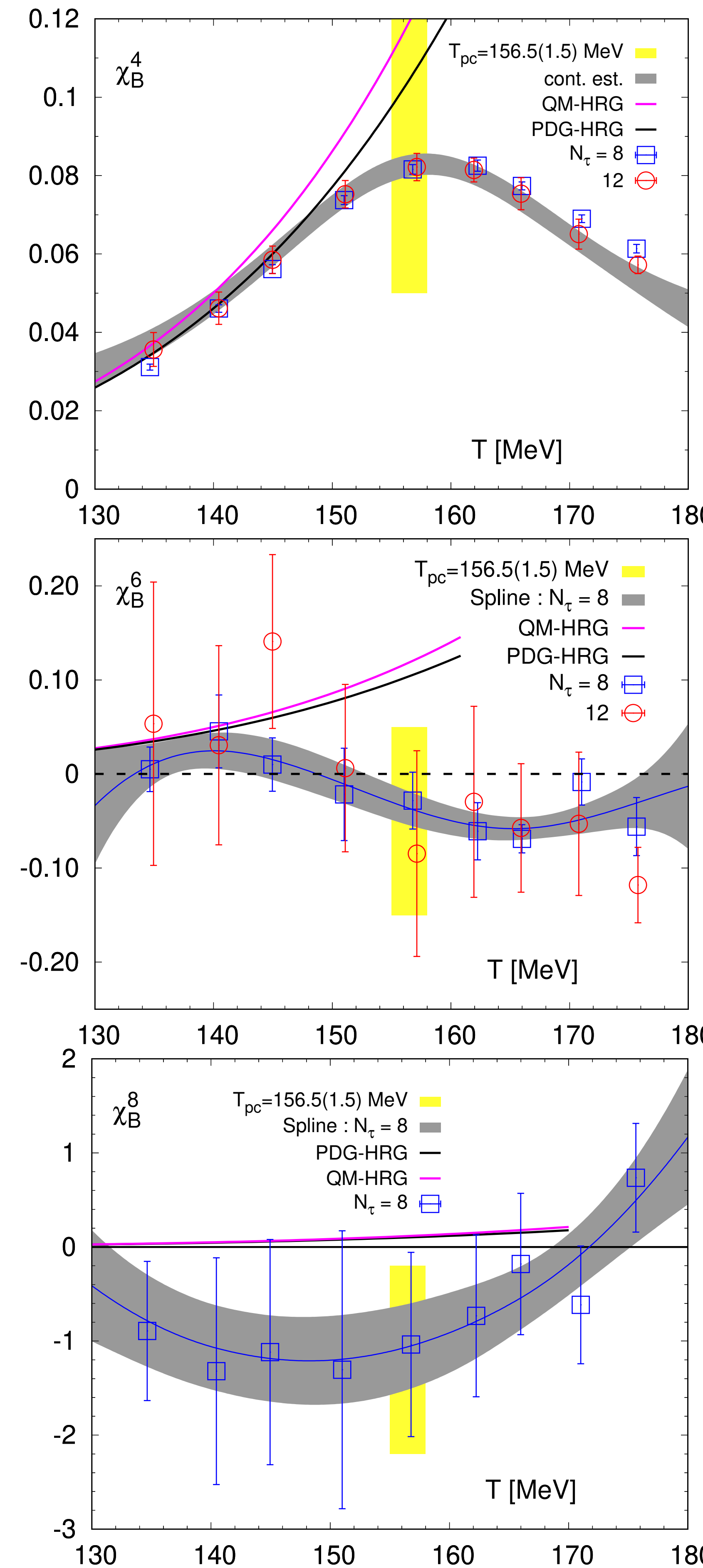
$$R^B_{nm} = \frac{\chi^B_n}{\chi^B_m}$$

$$\chi^B_n = \frac{\partial^n}{\partial \hat{\mu}^n_B} \frac{\ln Z}{T^3 V} = \frac{\partial^n}{\partial \hat{\mu}^n_B} \frac{p}{T}$$

$$\hat{\mu}_B = \mu_B / T$$



HotQCD, arXiv:2001.08530



HotQCD, arXiv:2001.08530

Lattice methods

- **Generation of gauge ensembles with dynamical HISQ fermions**
  - ➡ Rational HMC
  - ➡ Multi-scale Omelyan integrator
  - ➡ Hasenbusch mass preconditioning
  - ➡ Multiple pseudo-fermion fields
  - ➡ Et cetera …

- **Measurements (not necessary with HISQ, could be Domain Wall, …)**
  - ➡ Susceptibilities and cumulants: statistical noise method with deflation
  - ➡ Eigenvalue spectrum: Lanczos/ Kalkreuter-Simma
  - ➡ Hadronic correlation functions

Typical volumes

Physical mass:

$48^3 \times 12$

$64^3 \times 16$

Lighter than physical:

$56^3 \times 8$

$80^3 \times 8$

Typical statistics

High order cumulants:

$\mathcal{O}(10^6)$ per ensemble

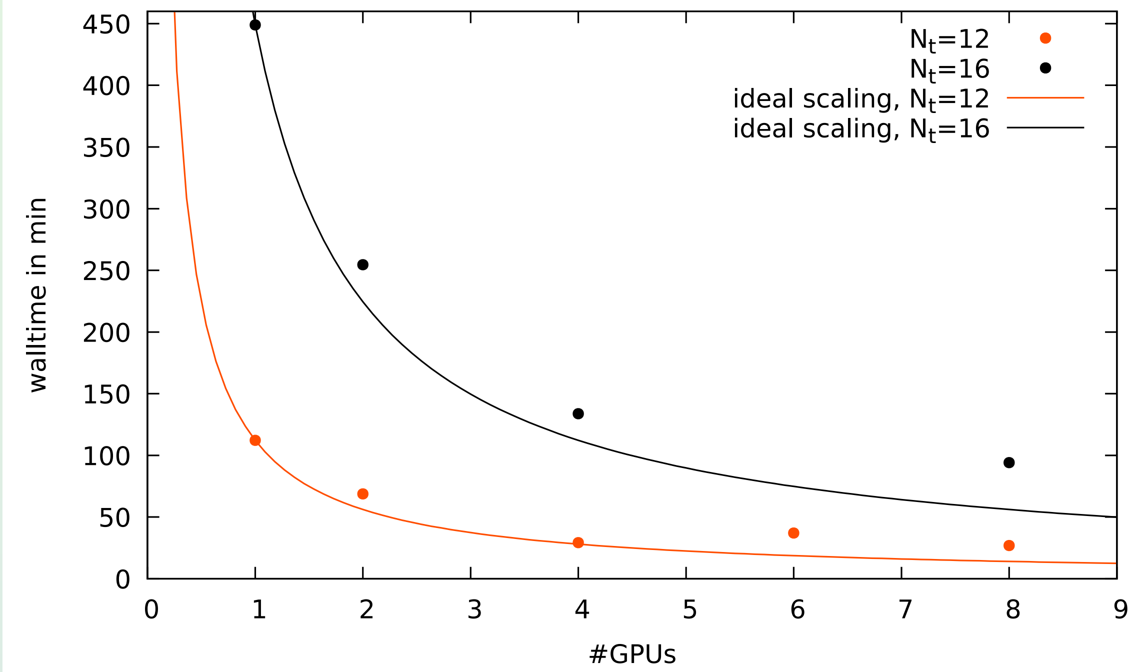
Chiral susceptibiliy:

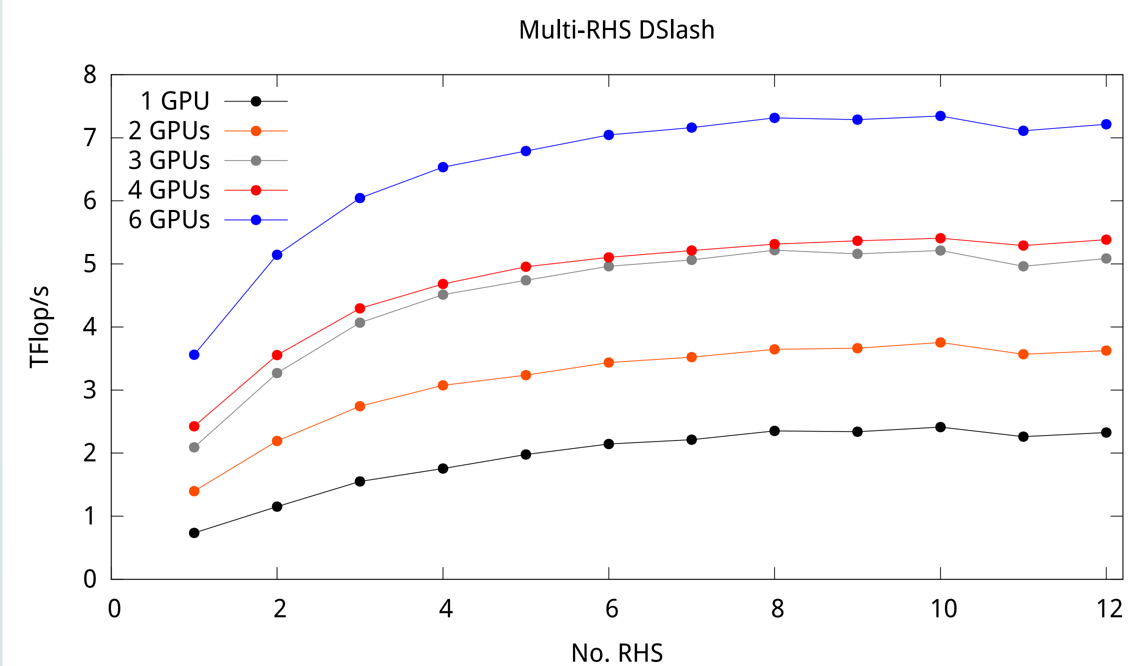
$\mathcal{O}(10^4)$ per ensamble

Hardware and performance

- **Developed massively parallel CPU (including KNL) and GPU code**
  - ➡ For generation and measurements
  - ➡ Use C++/CUDA
  - ➡ Scales good on few GPUs/nodes
  - ➡ Gain performance with appropriate memory fetching, multi-rhs solver, vectorization on CPUs, …

- **Use existing libraries for some measurements**
  - ➡ QUDA for the calculation of high order cumulants
  - ➡ Grid for Domain Wall on HISQ





Computing time in the past

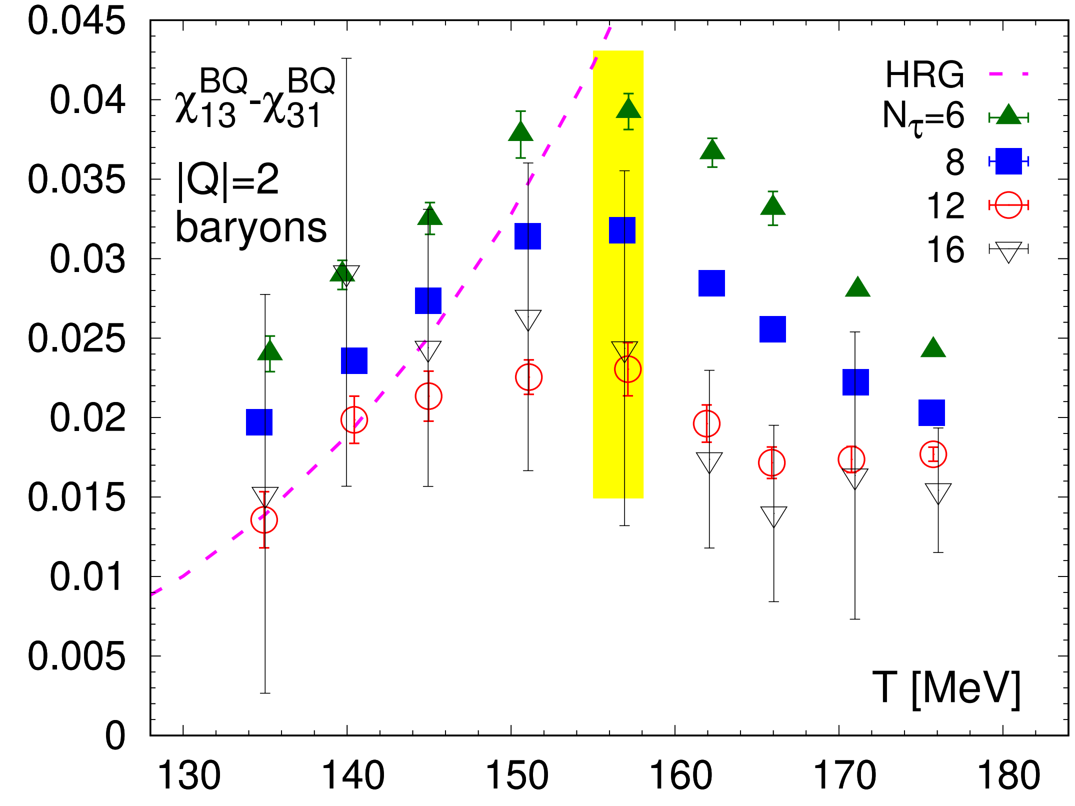
- **Computing time on own Hardware**
  - ➡ Bielefeld:
    - ➡ 2006-2011 APEnext (5TFlops)
    - ➡ 2011-2019 GPU-Cluster 500 TFlops,
    - ➡ Since 2019 GPU-Cluster 3PFlops
  - ➡ CCNU:
    - ➡ Since 2018 GPU-Cluster 6PFlops
- **Computing time in the US**
  - ➡ Applications via INCITE, ALCC and USQCD on Titan, Summit, Cori, JLab-Cluster
- **Computing time in the EU**
  - ➡ Applications via PRACE, Gauss-Alliance and NIC on JUWELS, Pitz Daint, Marconi

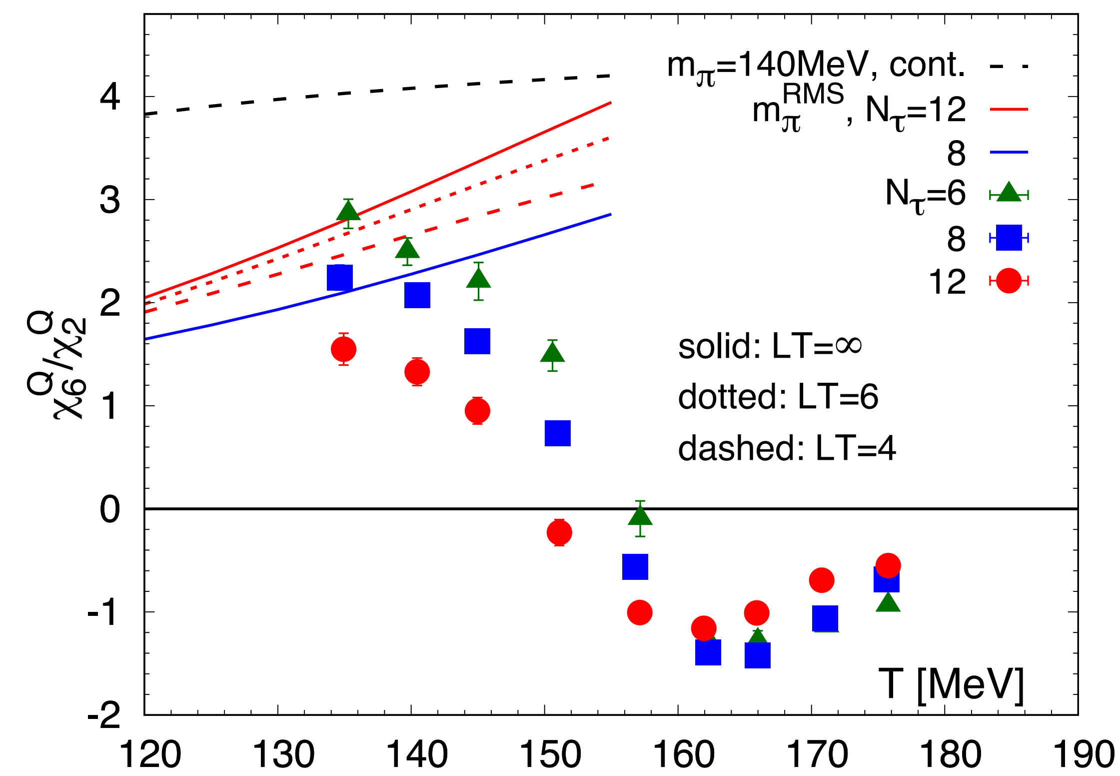
Typical resource mixture in the EU

TIER 3 (local): 46%
TIER 1 (national): 18%
TIER 0 (PRACE): 36%

Future directions

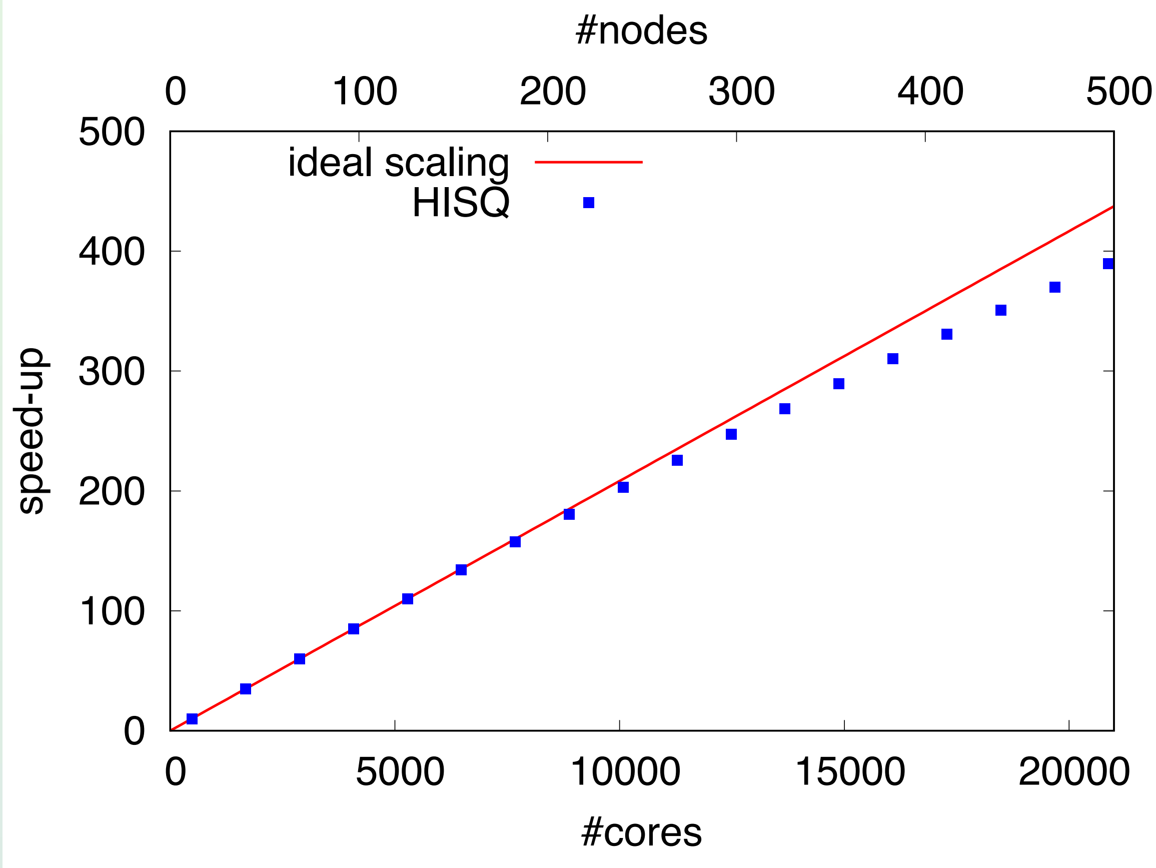
- **High order cumulants need a factor 10 more statistics**
- **Electric charge fluctuations are very sensitive to the light pion spectrum**
  - ➡ Need finer lattices
  - ➡ Need larger volume
    4th order: $96^3 \times 16$
    6th order: $48^3 \times 8$
    $72^3 \times 12$
  - ➡ More chiral actions
- **Scaling studies require smaller quark masses and larger spacial volumes**
  m_l/m_s=1/320: $80^3 \times 8$
  $120^3 \times 12$





Exascale readiness

- **The number of ensembles is huge**
  - ➡ Set of parameters is large
  - ➡ Large statistics enables splitting the run in $\mathcal{O}(1000)$ streams
  - ➡ Combine many runs into big jobs



Conclusion

- **A factor 10 increase in computing time can be very well justified**