The 39th International Symposium on Lattice Field Theory

Gauge Ensembles of the HotQCD Collaboration

Christian Schmidt for HotQCD

UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC-TR 211

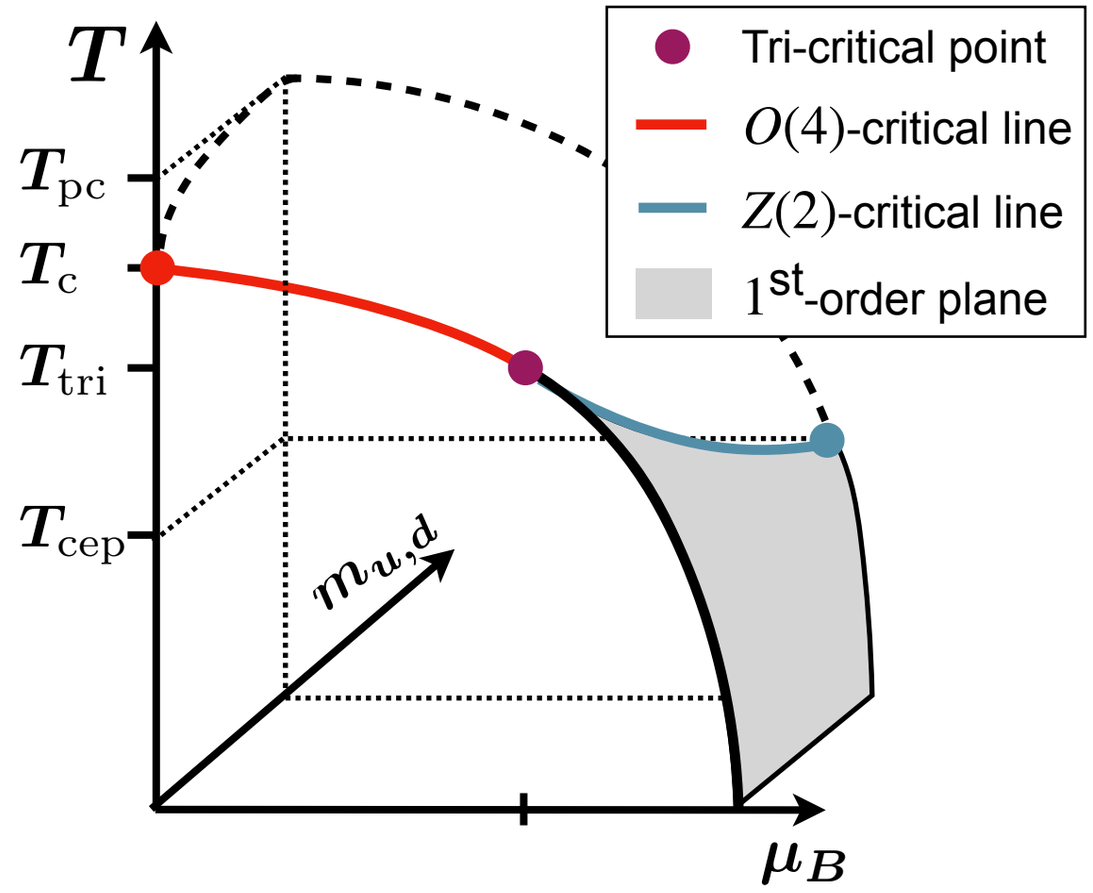
PUNCH 4NFDI

August 8-13, Bonn, Germany

HotQCD Collaboration:
S. Ali, L. Altenkort, D. Bala, A. Bazavov, D. Bollweg, D. Clarke, H.-T. Ding, J. Goswami, P. Hegde, O. Kaczmarek, F. Karsch, A. Lahiri, R. Larsen, S.-T. Li, S. Mukherjee, M. Neumann, H. Ohno, P. Petreczky, M. Sarkar, CS, S. Sharma, H.-T. Shu

What are the properties of matter under extreme conditions?

- Critical behaviour in QCD and the exploration of the QCD phase digram
- The equation of state and nonzero temperature and density
- Fluctuations of conserved charges and effective degrees of freedom
- In-medium properties of Hadrons and melting of bound states



Action

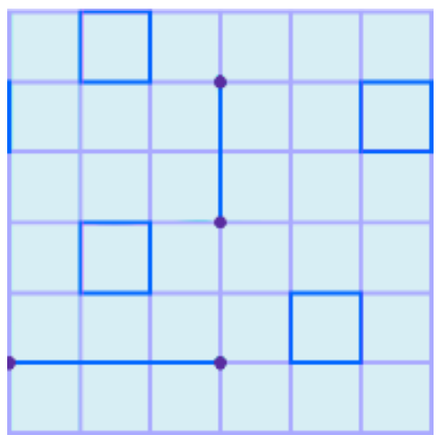
- We are using (2+1), 3, and 5-flavor of Highly Improved Staggered Quarks (HISQ/tree).

Algorithm

- Rational Hybrid Monte Carlo (RHMC) with a 3-level leap-frog or Omelyan Integrator.
- Step sizes of light, strange and gauge force integrators are tuned to a meet an acceptance of ~70%.
- Trajectory length is 0.5-1.0 time units

Code

- SIMULATeQCD, a SImple MUlti-GPU LATtice code for QCD calculations
- Available on GitHub: https://github.com/LatticeQCD/SIMULATeQCD



[L. Altenkort, D.Bollweg, D. A. Clarke, O. Kaczmarek, L. Mazur, C. Schmidt, P. Scior, H.-T. Shu, HotQCD on Multi-GPU Systems, PoS LATTICE2021, Bielefeld University (2021), https://arxiv.org/abs/2111.10354]

→ see also the poster by O. Kaczmarek

Ensembles:

- (2+1)-flavor with physical quark masses: $m_l/m_s = 1/27$, aspect ratio $N_\sigma/N_\tau = 4$

$32^3 \times 8$				$48^3 \times 12$				$64^3 \times 16$			
$N_\tau = 8$				$N_\tau = 12$				$N_\tau = 16$			
β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.
6.175	0.003307	125.28	1,471,861								
6.245	0.00307	134.84	1,275,380	6.640	0.00196	135.24	330,447	6.935	0.00145	135.80	17671
6.285	0.00293	140.62	1,598,555	6.680	0.00187	140.80	441,115	6.973	0.00139	140.86	23855
6.315	0.00281	145.11	1,559,003	6.712	0.00181	145.40	416,703	7.010	0.00132	145.95	26122
6.354	0.00270	151.14	1,286,603	6.754	0.00173	151.62	323,738	7.054	0.00129	152.19	26965
6.390	0.00257	156.92	1,602,684	6.794	0.00167	157.75	299,029	7.095	0.00124	158.21	21656
6.423	0.00248	162.39	1,437,436	6.825	0.00161	162.65	214,671	7.130	0.00119	163.50	18173
6.445	0.00241	166.14	1,186,523	6.850	0.00157	166.69	156,111	7.156	0.00116	167.53	19926
6.474	0.00234	171.19	373,644	6.880	0.00153	171.65	144,633	7.188	0.00113	172.60	17163
6.500	0.00228	175.84	294,311	6.910	0.00148	176.73	131,248	7.220	0.00110	177.80	3282

~ 912 TB (uncompressed, fp32)

~ 938 TB (uncompressed, fp32)

~ 210 TB (uncompressed, fp32)

[Phys.Rev.D 104 (2021) 7, 074512, Table I]

- (2+1)-flavor, below physical mass runs ($N_\tau = 8$)

$40^3 \times 8$, $H = 1/40$

β	m_l	T[MeV]	#conf
6.260	0.002025	136.98	71824
6.285	0.001975	140.62	71547
6.300	0.001930	142.85	71514
6.315	0.001900	145.11	71571
6.330	0.001865	147.40	70212
6.354	0.001820	151.14	51135
6.365	0.001790	152.88	49879
6.390	0.001735	156.92	51707
6.423	0.001675	162.39	52051
6.445	0.001630	166.14	50689
6.474	0.001580	171.19	28080
6.500	0.001535	175.84	29505

~ 98 TB
(uncompressed, fp32)

$56^3 \times 8$, $H = 1/80$

β	m_l	T[MeV]	#conf
6.285	0.0009875	140.62	23423
6.300	0.0009650	142.85	23184
6.315	0.0009500	145.11	23135
6.330	0.0009325	147.40	23132
6.354	0.0009100	151.14	22942
6.372	0.0008891	154.00	17242
6.390	0.0008675	156.92	17814
6.423	0.0008375	162.39	10937
6.445	0.0008150	166.14	10883

~ 70 TB
(uncompressed, fp32)

$56^3 \times 8$, $H = 1/160$

β	m_l	T[MeV]	#conf
6.285	0.00049375	140.62	9954
6.300	0.00048250	142.85	9999
6.315	0.00047500	145.11	6333
6.330	0.00046625	147.40	6314
6.354	0.00045500	151.14	6360
6.372	0.00044456	154.00	4551
6.390	0.00043375	156.92	6929
6.423	0.00041875	162.39	4544
6.445	0.00040750	166.14	4879

~ 24 TB
(uncompressed, fp32)

$\rightarrow$ plan for generation of corresponding $N_\tau = 12$ ensembles ($72^3 \times 12$)

- Gauge files are stored binary fp32 format with a small header in ASCII (formats are Bielefeld or NERSC) some are currently compressed (two columns of the SU(3) matrixes).
  → tools for the conversion to ILDG are ready to use
- For all configurations we have a checksum and plaquette value for validation.
- Log-files are also stored which contain some provenance information.

Example:

```
# [2022-05-12 09:23:24] INFO: Initializing MPI with (1 proc)
# [2022-05-12 09:23:24] INFO: Reading parameters from file :: ./rhmc.param
# [2022-05-12 09:23:24] INFO: # PARAM :: Lattice = 36 36 36 6
# [2022-05-12 09:23:24] INFO: # PARAM :: Nodes = 1 1 1 1
# [2022-05-12 09:23:24] INFO: # PARAM :: Topology = 0 0 0 0  (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: beta = 6.325
# [2022-05-12 09:23:24] INFO: # PARAM :: endianness = auto (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: conf_nr = 1820
# [2022-05-12 09:23:24] INFO: # PARAM :: prec_out = 0 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: measurements_dir = ./ (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: use_unit_conf = 0 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: no_pf = 1
# [2022-05-12 09:23:24] INFO: # PARAM :: no_md = 50
# [2022-05-12 09:23:24] INFO: # PARAM :: no_step_sf = 8
# [2022-05-12 09:23:24] INFO: # PARAM :: no_sw = 15
# [2022-05-12 09:23:24] INFO: # PARAM :: step_size = 0.02
# [2022-05-12 09:23:24] INFO: # PARAM :: mu0 = 0
# [2022-05-12 09:23:24] INFO: # PARAM :: integrator = 0 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: residue = 1e-12 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: residue_force = 1e-07 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: cgMax = 6500
# [2022-05-12 09:23:24] INFO: # PARAM :: residue_meas = 1e-12 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: cgMax_meas = 20000 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: always_acc = 0
# [2022-05-12 09:23:24] INFO: # PARAM :: cgMixedPrec = 0 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: cgMixedPrec_delta = 0.1 (default)
# [2022-05-12 09:23:24] INFO: # PARAM :: no_updates = 100
# [2022-05-12 09:23:24] INFO: # PARAM :: write_every = 10
# [2022-05-12 09:23:24] INFO: # PARAM :: rat_file = ../param/in.rational_l366f21b6325m00277m0748
# [2022-05-12 09:23:24] INFO: # PARAM :: mass_ud = 0.00277267
# [2022-05-12 09:23:24] INFO: # PARAM :: mass_s = 0.0748622
# [2022-05-12 09:23:24] INFO: # PARAM :: rand_file = rand
# [2022-05-12 09:23:24] INFO: # PARAM :: gauge_file = l366f21b6325m00277m0748_s0.
# [2022-05-12 09:23:24] INFO: # PARAM :: seed = 6170000
# [2022-05-12 09:23:24] INFO: # PARAM :: rand_flag = 1
# [2022-05-12 09:23:24] INFO: # PARAM :: load_conf = 2
# [2022-05-12 09:23:24] INFO: Reading parameters from file :: ../param/in.rational_l366f21b6325m00277m0748
```

Data Management

- Our Data Management Plan requires separate data publications (with DOI) for all derived data used in figures of publications (publisher: Bielefeld University).
  Example: *https://doi.org/10.4119/unibi/2962427*

- Our Data Management Plan does currently not cover gauge configurations, however, we want to preserve that data as long as possible.

- Gauge configurations are stored in Data Projects at NERSC, ORNL, JLAB and Jülich.

- We Plan to **make all HISQ ensembles available through ILDG (LDG)**.
  → this is subject to the available storage within LDG.

- We contribute to ILDG (partly funded through PUNCH4NFDI), current activities include development of format conversion tools and meta data collection.