Heavy Quark Diffusion ResearchProduct in PUNCH4NFDI

https://doi.org/10.1103/PhysRevLett.130.231902

PHYSICAL REVIEW LETTERS **130,** 231902 (2023)

Heavy Quark Diffusion from 2 + 1 Flavor Lattice QCD with 320 MeV Pion Mass

Luis Altenkort,[1,*] Olaf Kaczmarek,[1] Rasmus Larsen,[2] Swagato Mukherjee,[3] Peter Petreczky,[3] Hai-Tao Shu,[4,†] and Simon Stendebach[5]

(HotQCD Collaboration)

[1]*Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany*
[2]*Department of Mathematics and Physics, University of Stavanger, Stavanger, Norway*
[3]*Physics Department, Brookhaven National Laboratory, Upton, New York 11973, USA*
[4]*Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany*
[5]*Insitut für Kernphysik, Technische Universität Darmstadt, Schlossgartenstraße 2, D-64289 Darmstadt, Germany*

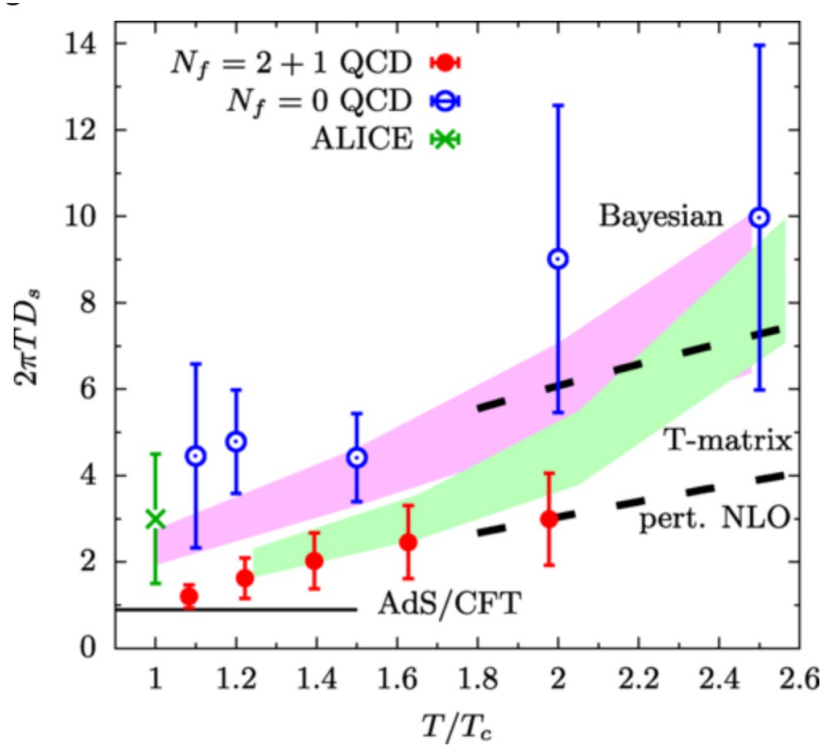
(Received 22 February 2023; revised 17 April 2023; accepted 24 April 2023; published 6 June 2023)

We present the first calculations of the heavy flavor diffusion coefficient using lattice QCD with light dynamical quarks corresponding to a pion mass of around 320 MeV. For temperatures 195 MeV $< T <$ 352 MeV, the heavy quark spatial diffusion coefficient is found to be significantly smaller than previous quenched lattice QCD and recent phenomenological estimates. The result implies very fast hydrodynamization of heavy quarks in the quark-gluon plasma created during ultrarelativistic heavy-ion collision experiments.

DOI: 10.1103/PhysRevLett.130.231902

Ongoing studies towards physical pion masses

Diffusion coefficient for heavy quarks in the Quark Gluon Plasma:



- Important input for hydro and transport models for the study of heavy quarks in the QGP

- Provides information on the thermalization or hydrodynamization of heavy quarks

Heavy Quark Diffusion - SIMULATeQCD code development

https://github.com/LatticeQCD/SIMULATeQCD
https://doi.org/10.5281/zenodo.7994982
https://arxiv.org/abs/2306.01098

SIMULATeQCD: A simple multi-GPU lattice code for QCD calculations

Lukas Mazur[a,*], Dennis Bollweg[b,*], David A. Clarke[c,*], Luis Altenkort[d], Olaf Kaczmarek[d,*], Rasmus Larsen[e], Hai-Tao Shu[f], Jishnu Goswami[g], Philipp Scior[b], Hauke Sandmeyer[d], Marius Neumann[d], Henrik Dick[d], Sajid Ali[d,h], Jangho Kim[i], Christian Schmidt[d], Peter Petreczky[b], Swagato Mukherjee[b,*],

(HotQCD collaboration)

[a] Paderborn Center for Parallel Computing, Paderborn University, Paderborn, Germany
[b] Physics Department, Brookhaven National Laboratory, Upton, New York, United States
[c] Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah, United States
[d] Fakultät für Physik, Universität Bielefeld, Bielefeld, Germany
[e] Department of Mathematics and Physics, University of Stavanger, Stavanger, Norway
[f] Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany
[g] RIKEN Center for Computational Science, Kobe 650-0047, Japan
[h] Government College University Lahore, Department of Physics, Lahore 54000, Pakistan
[i] Institute for Advanced Simulation (IAS-4), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Abstract

The rise of exascale supercomputers has fueled competition among GPU vendors, driving lattice QCD developers to write code that supports multiple APIs. Moreover, new developments in algorithms and physics research require frequent updates to existing software. These challenges have to be balanced against constantly changing personnel. At the same time, there is a wide range of applications for HISQ fermions in QCD studies. This situation encourages the development of software featuring a HISQ action that is flexible, high-performing, open source, easy to use, and easy to adapt. In this technical paper, we explain the design strategy, provide implementation details, list available algorithms and modules, and show key performance indicators for `SIMULATeQCD`, a simple multi-GPU lattice code for large-scale QCD calculations, mainly developed and used by the HotQCD collaboration. The code is publicly available on GitHub.

Keywords: lattice QCD, CUDA, HIP, GPU

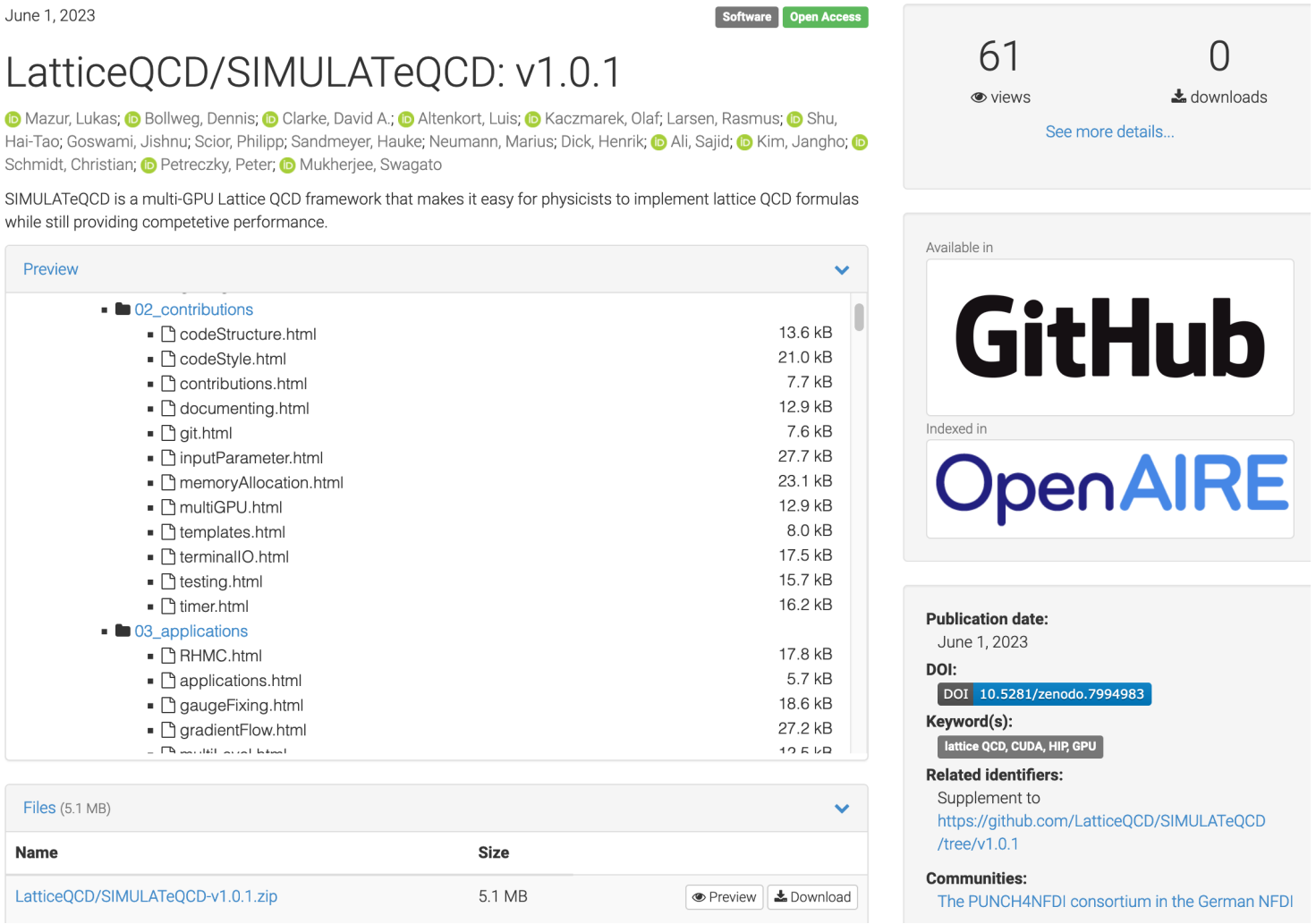
- Developed by HotQCD collaboration (Bielefeld, Brookhaven,…)
- Lattice and Analysis Software development
- Highly optimized lattice QCD code for multi-GPU
- Optimization for supercomputing resources Frontier, LUMI-G, JUWELS, Leonardo
- SIMULATeQCD selected for EuroHPC JU extraordinary support program (ESP) (with AMD and HPE for LUMI-G)
- Section Metadata WG research software metadata (Christian Schmidt & OK)
- Plan to add code metadata, e.g. CodeMeta schema

ongoing work partly done in TA3

All software is already openly available

Heavy Quark Diffusion - SIMULATeQCD code development

https://github.com/LatticeQCD/SIMULATeQCD
https://doi.org/10.5281/zenodo.7994982
https://arxiv.org/abs/2306.01098



- Developed by HotQCD collaboration (Bielefeld, Brookhaven,…)
- Lattice and Analysis Software development
- Highly optimized lattice QCD code for multi-GPU
- Optimization for supercomputing resources Frontier, LUMI-G, JUWELS, Leonardo
- SIMULATeQCD selected for EuroHPC JU extraordinary support program (ESP) (with AMD and HPE for LUMI-G)
- Section Metadata WG research software metadata (Christian Schmidt & OK)
- Plan to add code metadata, e.g. CodeMeta schema

ongoing work partly done in TA3

All software is already openly available

Gauge Field Generation with Rational Hybrid Monte Carlo using SIMULAeQCD

Previous project: 81 TB gauge field configurations

$96^3 \times N_\tau$ lattice

N_τ	36	32	28	24	20
T [MeV]	195	220	251	293	352
# conf.	2256	912	1680	688	2488

~55.000 gauge field configurations with m_π= 320 *MeV*

$64^3 \times N_\tau$ lattices

T [MeV]	β	am_s	am_l	N_τ	# conf.
195	7.570	0.01973	0.003946	20	5899
	7.777	0.01601	0.003202	24	3435
220	7.704	0.01723	0.003446	20	7923
	7.913	0.01400	0.002800	24	2715
251	7.857	0.01479	0.002958	20	6786
	8.068	0.01204	0.002408	24	5325
293	8.036	0.01241	0.002482	20	6534
	8.147	0.01115	0.002230	22	9101

Generated on supercomputing resources Perlmutter, JUWELS, Marconi

Current project: ~200 TB gauge field configurations

$128^3 \times N_\tau$ and $96^3 \times N_\tau$ lattices with physical pion masses
compute projects on Frontier and LUMI-G

All gauge field configurations will be stored in the ILDG

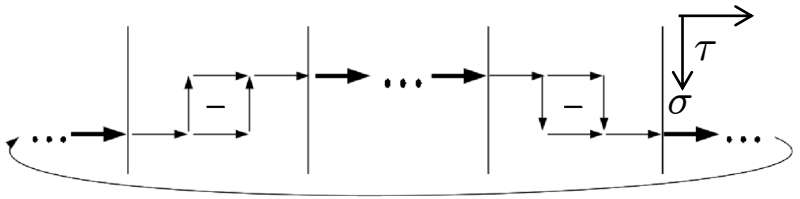
Measurements of operators and correlation functions

Operators and correlation functions
need to be calculated on each gauge field configuration

Needs optimized multi-GPU code
measurement routines in SIMULATeQCD

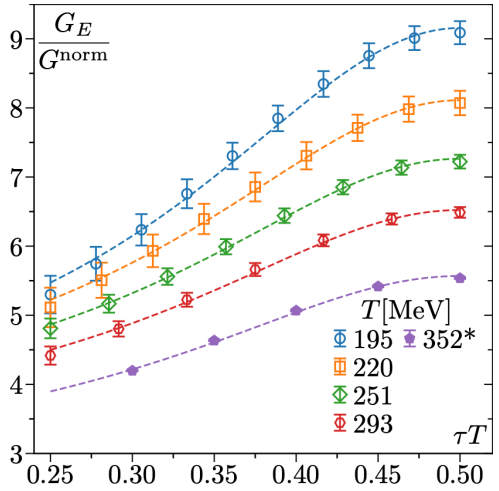
Color-electric correlator:

$$G_E(\tau) \equiv -\frac{1}{3}\sum_{i=1}^{3} \frac{\left\langle \mathrm{Re\,Tr}\left[U(\tfrac{1}{T};\tau)\, g\, E_i(\tau,\mathbf{0})\, U(\tau;0)\, g\, E_i(0,\mathbf{0})\right]\right\rangle}{\left\langle \mathrm{Re\,Tr}[U(\tfrac{1}{T};0)]\right\rangle}$$



Vector meson correlator:

$$G_{\mu\nu}(\tau,\vec{x}) = \langle J_\mu(\tau,\vec{x}) J_\nu^\dagger(0,\vec{0})\rangle$$
$$J_\mu(\tau,\vec{x}) = 2\kappa Z_V \bar{\psi}(\tau,\vec{x})\Gamma_\mu\psi(\tau,\vec{x})$$



Measurement of correlation functions on Bielefeld GPU Cluster

- Large set of correlation measurement data
- Need to be analyzed, Jackknife, Bootstrap…
- Continuum and flow time extrapolations
- Sophisticated analysis software needed

Heavy Quark Diffusion ResearchProduct in PUNCH4NFDI

Project already benefits from PUNCH developments and could profit more in the future

All analysis performed on Bielefeld PUNCH compute server (not yet in Compute4Punch)

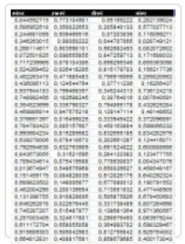
All data and lattice and analysis software as well as a workflow (bash/python) of the project published as open access

https://doi.org/10.4119/unibi/2979080

Dataset for "Heavy Quark Diffusion from 2+1 Flavor Lattice QCD with 320 MeV Pion Mass"

Kaczmarek O, Altenkort L, Larsen R, Mukherjee S, Petreczky P, Shu H-T, Stendebach S (2023)
Bielefeld University.

Datenpublikation



Download
README.sh 12.89 KB
data_pub_altenkort_2023_complete.tar.gz 3.17 GB
figures.tar.gz 15.71 MB
+ Alle

DOI https://doi.org/10.4119/unibi/2979080

Details | Dateien | Links | English | PUB

Alle Dateien verfügbar unter der/den folgenden Lizenz(en):

Creative Commons Namensnennung 4.0 International Public License (CC-BY 4.0):
https://creativecommons.org/licenses/by/4.0/deed.de
https://creativecommons.org/licenses/by/4.0/legalcode.de

Export
Markieren/ Markierung löschen
0 Markierte Publikationen
Open Data PUB

Suchen in
Google Scholar

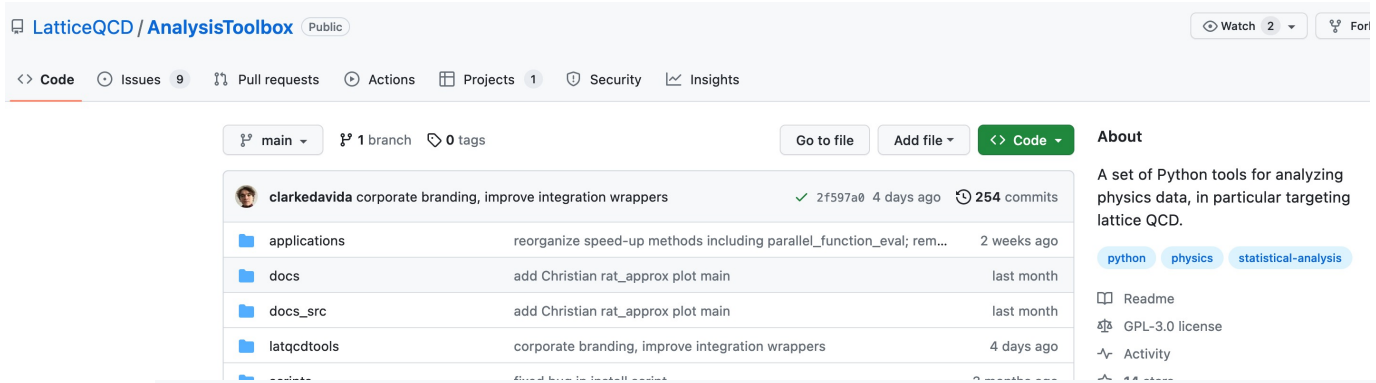
Volltext(e)

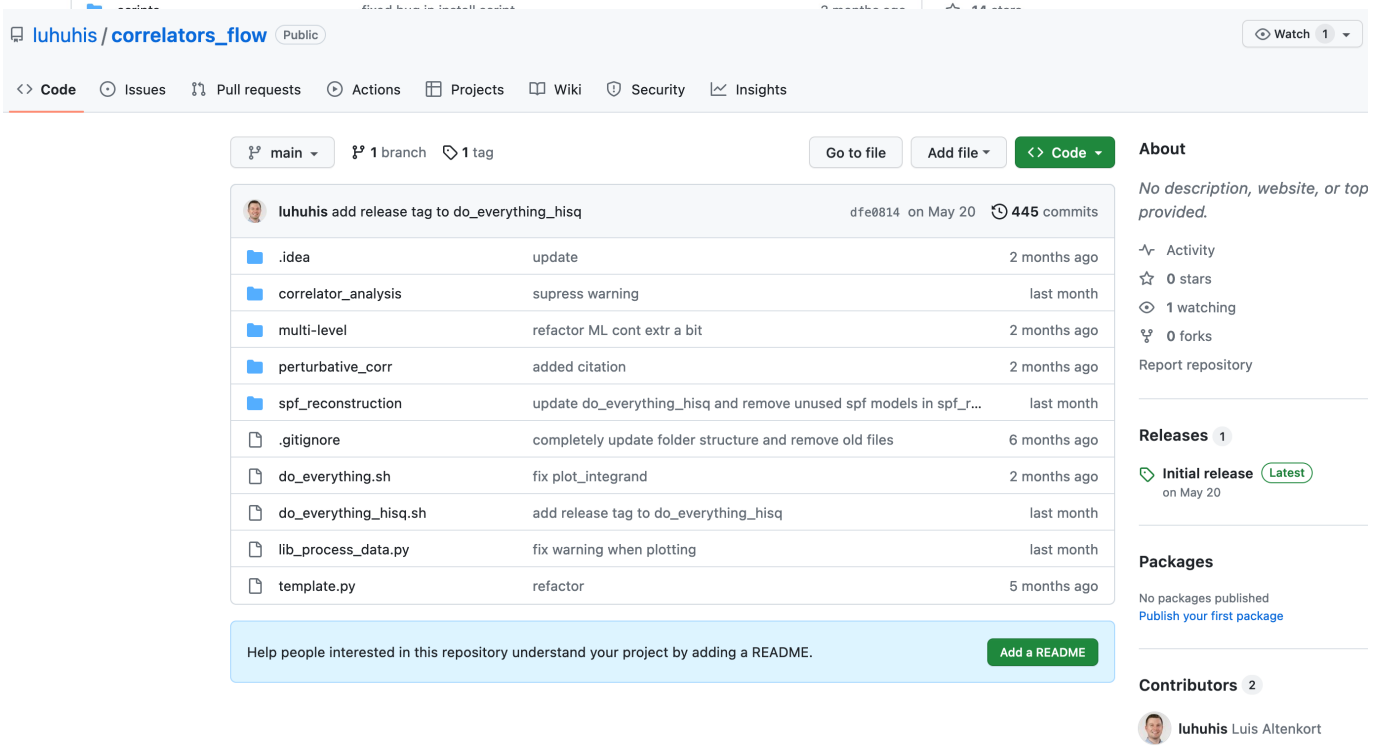
Name	README.sh 12.89 KB
Access Level	Open Access
Zuletzt Hochgeladen	2023-05-22T13:40:31Z
MD5 Prüfsumme	f33ce74ad32f2653c49403efd2ff74c1

Name	data_pub_altenkort_2023_complete.tar.gz 3.17 GB
Access Level	Open Access

All raw and derived data is already openly available (ILDG or PUNCH storage for future projects?)

Heavy Quark Diffusion – Analysis Software





Analysis Software developments

Analysis Toolbox Software development

https://github.com/LatticeQCD/AnalysisToolbox

Heavy quark diffusion analysis based on this

https://github.com/luhuhis/correlators_flow

ongoing work partly done in TA3

All analysis software is already openly available

Heavy Quark Diffusion RDP in PUNCH4NFDI

TA2

Storage of gauge field configurations in LDG

- Upload of ~ 500TB to storage elements at NERSC and JSC planned for 2023

Metadata Catalogue and Storage of data in LDG/PUNCH

- metadata server and file server in PUNCH → LDG or other MDC/FC for non-lattice data

Analysis workflow on Storage4PUNCH and Compute4PUNCH

(Lattice calculations on supercomputers outside of PUNCH)

TA3

Software development of optimized lattice code and analysis tools and workflows

TA4

metadata and file formats to be developed for all data in the analysis workflow
metadata integration of software, ILDG gauge field configurations, analysis software, raw data, analyzed data, final results
publish the whole project on the PUNCH platform

Planned and ongoing work (Simran Singh, Ding-Ze Hu and OK)

- Tests on Compute4PUNCH & Storage4PUNCH
- Docker/Singularity container of the analysis

  https://gitlab-p4n.aip.de/punch/ildg/-/tree/main/use-case/lqcd_analysis
- Jupyter Notebook of the analysis
- Data formats and Metadata in the data analysis steps
- Test of different workflow systems for the analysis
- Test of the Science Portal
- PIDs and DOI registration

Gauge configurations generated from LQCD simulations of
N_f = 2+1 at pion mass 320 MeV using SIMULATeQCD :
a multi-GPU C++ code public & published :
https://latticeqcd.github.io/SIMULATeQCD/

Computing resources used :

- *Bielefeld GPU cluster*
- *JUWELS at GCS@FZJ*
- *Marconi 100 at CINECA*

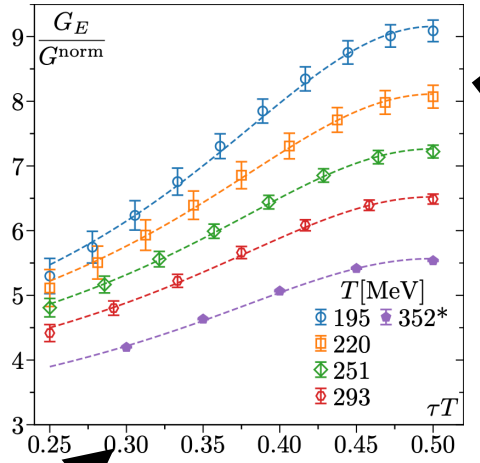
Raw Gauge configurations used to calculate Observable of interest : **chromoelectric correlator** (G_E) for various Temperatures.
All Measured data public & published:
DOI
https://doi.org/10.4119/unibi/2979080

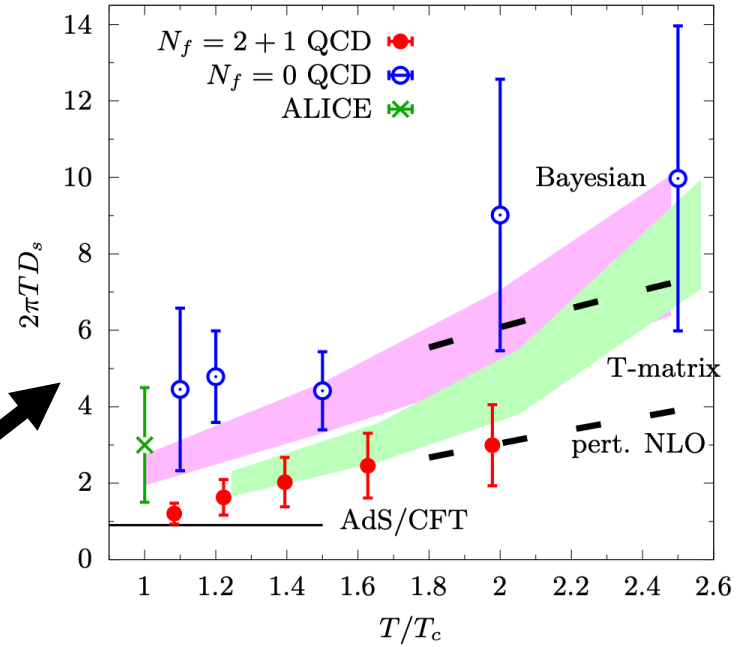
Lattice Toolbox : Collection of Python tools developed at Bielefeld (Public):
https://github.com/LatticeQCD/LatticeToolbox

Complete workflow including: sampling, bootstrapping, interpolation & continuum extrapolation is implemented as a single bash/python script that runs on : **Compute4Punch**

Also ongoing : migration of the bash script to a user friendly JupyterNotebook – with the aim of running the notebook on a cluster server

First results on heavy Quark diff coefficients Using dynamical light Quarks from lattice!!
https://doi.org/10.1103/PhysRevLett.130.231902





Planned & Ongoing **PUNCH** activities :

- *Interplay between task areas : TA2 , TA3 & TA4*
- *Compute4PUNCH provides the infrastructure for running the container that includes this entire workflow(already partially successful)*
- *Metadata of the datasets used in this workflow will be designed and extracted*
- *Ideally the datasets and the metadata will be stored in Storage4PUNCH– END GOAL : Publish the entire project on PUNCH platform*