

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

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(HotQCD Collaboration)

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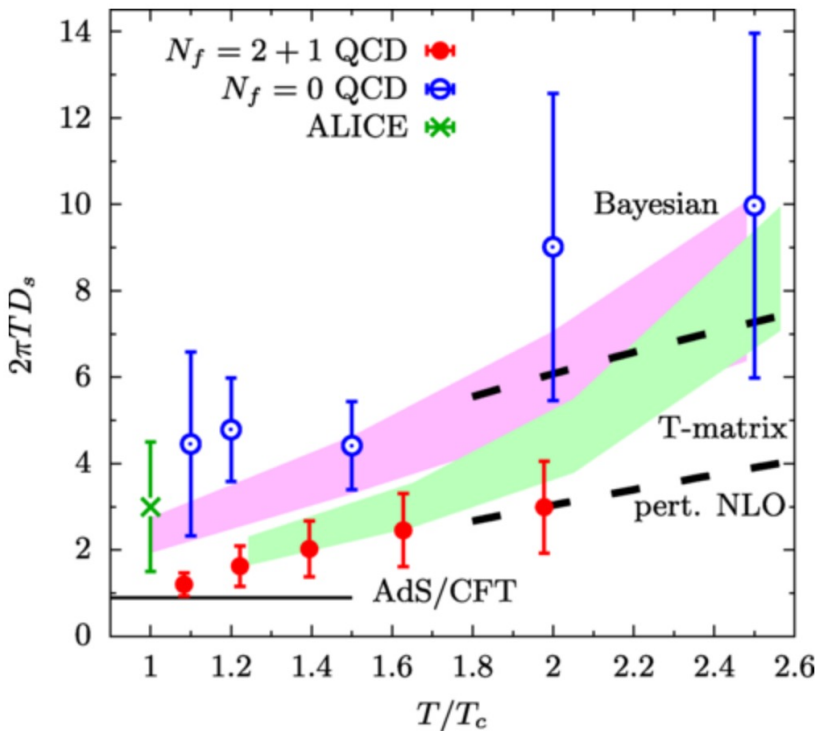
(Received 22 February 2023; revised 17 April 2023; accepted 24 April 2023; published 6 June 2023)

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 $195 \text{ MeV} < T < 352 \text{ MeV}$, 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](https://doi.org/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 Kimⁱ, Christian Schmidt^d, Peter Petreczky^b, Swagato Mukherjee^{b,*},

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ⁱInstitute 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>

June 1, 2023

Software Open Access

LatticeQCD/SIMULATeQCD: v1.0.1

Mazur, Lukas; Bollweg, Dennis; Clarke, David A.; Altenkort, Luis; Kaczmarek, Olaf; Larsen, Rasmus; Shu, Hai-Tao; Goswami, Jishnu; Scior, Philipp; Sandmeyer, Hauke; Neumann, Marius; Dick, Henrik; Ali, Sajid; Kim, Jangho; Schmidt, Christian; Petreczky, Peter; Mukherjee, Swagato

SIMULATeQCD is a multi-GPU Lattice QCD framework that makes it easy for physicists to implement lattice QCD formulas while still providing competitive performance.

Preview

02_contributions

codeStructure.html

codeStyle.html

contributions.html

documenting.html

git.html

inputParameter.html

memoryAllocation.html

multiGPU.html

templates.html

terminalIO.html

testing.html

timer.html

03_applications

RHMC.html

applications.html

gaugeFixing.html

gradientFlow.html

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Files (5.1 MB)	
Name	Size
LatticeQCD/SIMULATeQCD-v1.0.1.zip	5.1 MB

Preview

Download

61

views

0

downloads

[See more details...](#)

Available in

GitHub

Indexed in

OpenAIRE

Publication date:

June 1, 2023

DOI:

DOI 10.5281/zenodo.7994983

Keyword(s):

lattice QCD, CUDA, HIP, GPU

Related identifiers:

Supplement to
<https://github.com/LatticeQCD/SIMULATeQCD/tree/v1.0.1>

Communities:

The PUNCH4NFDI consortium in the German NFDI

- 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
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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

96³xN_τ 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

64³xN_τ lattices

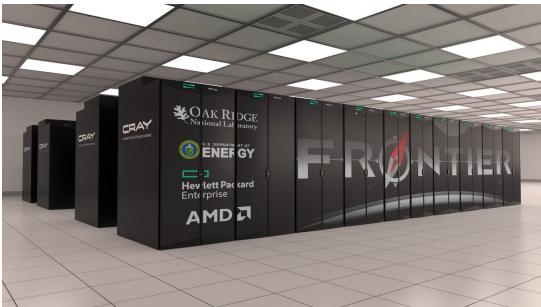
T [MeV]	β	am _s	am _l	N _τ	# conf.
195	7.570	0.01973	0.003946	20	5899
	7.777	0.01601	0.003202	24	3435
220	7.704	0.01723	0.003446	20	7923
	7.913	0.01400	0.002800	24	2715
251	7.857	0.01479	0.002958	20	6786
	8.068	0.01204	0.002408	24	5325
293	8.036	0.01241	0.002482	20	6534
	8.147	0.01115	0.002230	22	9101

Generated on supercomputing resources
Perlmutter, JUWELS, Marconi



Current project: ~200 TB gauge field configurations

128³xN_τ and 96³xN_τ lattices with physical pion masses
compute projects on Frontier and LUMI-G



All gauge field configurations will be stored in the ILDG

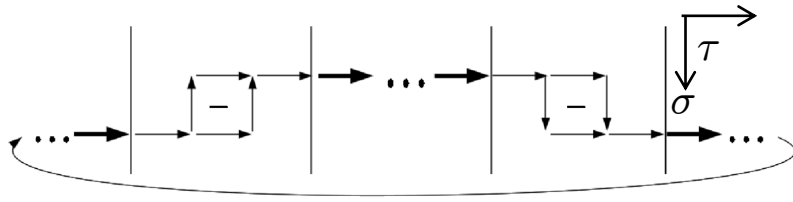
Measurements of operators and correlation functions

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

Needs optimized multi-GPU code
measurement routines in SIMULATEQCD

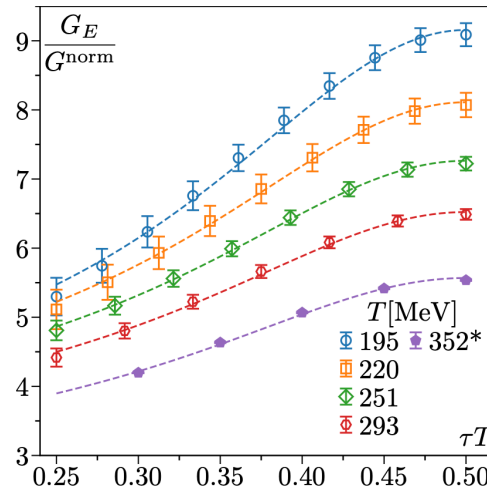
Color-electric correlator:

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



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>

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Access Level

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Suchen in

 Google Scholar

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

Heavy Quark Diffusion – Analysis Software

LatticeQCD / AnalysisToolboxPublic

<> CodeIssues9Pull requestsActionsProjects1SecurityInsights

main1 branch0 tags

Go to fileAdd fileCode

clarkedavida

corporate branding, improve integration wrappers2f597a84 days ago254 commits

applications

reorganize speed-up methods including parallel_function_eval; rem...2 weeks ago

docs

add Christian rat_approx plot mainlast month

docs_src

add Christian rat_approx plot mainlast month

latqcdtools

corporate branding, improve integration wrappers4 days ago

...

...

About

A set of Python tools for analyzing physics data, in particular targeting lattice QCD.

pythonphysicsstatistical-analysis

ReadmeGPL-3.0 licenseActivity

luhuhis / correlators_flowPublic

<> CodeIssuesPull requestsActionsProjectsWikiSecurityInsights

main1 branch1 tag

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luhuhis

add release tag to do_everything_hisqdfc0814on May 20445 commits

.idea

update2 months ago

correlator_analysis

supress warninglast month

multi-level

refactor ML cont extr a bit2 months ago

perturbative_corr

added citation2 months ago

spf_reconstruction

update do_everything_hisq and remove unused spf models in spf_r...last month

.gitignore

completely update folder structure and remove old files6 months ago

do_everything.sh

fix plot_integrand2 months ago

do_everything_hisq.sh

add release tag to do_everything_hisqlast month

lib_process_data.py

fix warning when plottinglast month

template.py

refactor5 months ago

About

No description, website, or top provided.

Activity0 stars1 watching0 forks

Report repository

Releases1

Initial releaseLateston May 20

Packages

No packages published

Publish your first package

Contributors2

luhuhisLuis Altenkort

Help people interested in this repository understand your project by adding a README.

Add a README

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 :

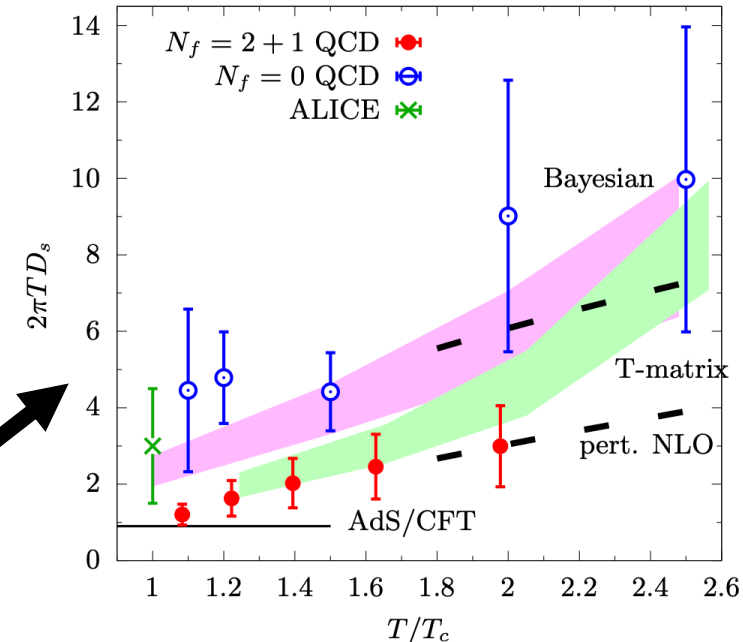
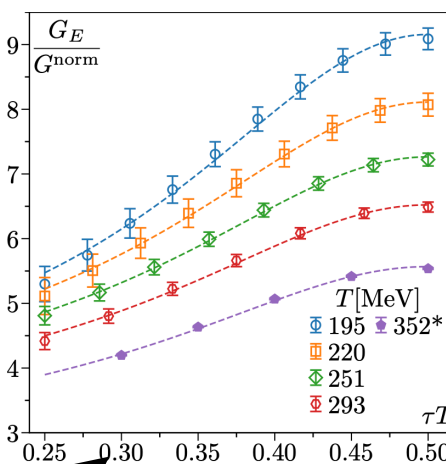
- Bielefeld GPU cluster
- JUWELS at GCS@FZJ
- Marconi 100 at CINECA

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>

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**

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

Lattice Toolbox : Collection of Python tools developed at Bielefeld (Public):

<https://github.com/LatticeQCD/LatticeToolbox>