Heavy Quark Diffusion ResearchProduct in PUNCH4NFDI

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

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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.

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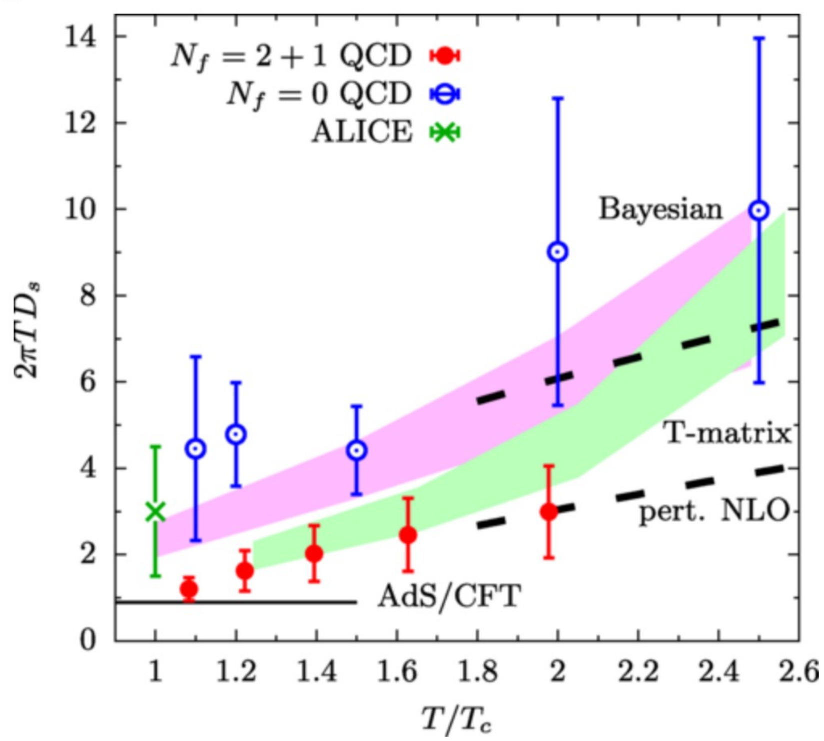
Diffusion coefficient for heavy quarks in the Quark Gluon Plasma:



- 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

Ongoing studies towards physical pion masses

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

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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 competetive performance.

Preview

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Files (5.1 MB)

Name	Size	
LatticeQCD/SIMULATeQCD-v1.0.1.zip	5.1 MB	Preview Download

Available in GitHub

Indexed in OpenAIRE

Publication date:
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DOI 10.5281/zenodo.7994983
Keyword(s):
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Supplement to
https://github.com/LatticeQCD/SIMULATeQCD/tree/v1.0.1
Communities:
The PUNCH4NFDI consortium in the German NFDI

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Gauge Field Generation with Rational Hybrid Monte Carlo using SIMULAeQCD

Previous project: 81 TB gauge field configurations

$96^3 \mathrm{x} N_\tau$ 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*

$64^3 \mathrm{x} N_\tau$ 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

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

All gauge field configurations will be stored in the ILDG

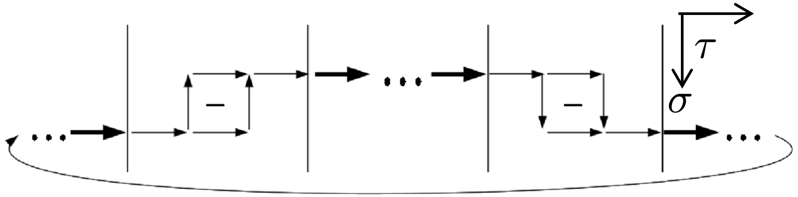
Measurements of operators and correlation functions

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:

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



Vector meson correlator:

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

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

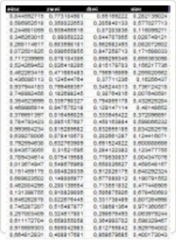
All analysis performed on Bielefeld PUNCH compute server (not yet in Compute4Punch)

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**

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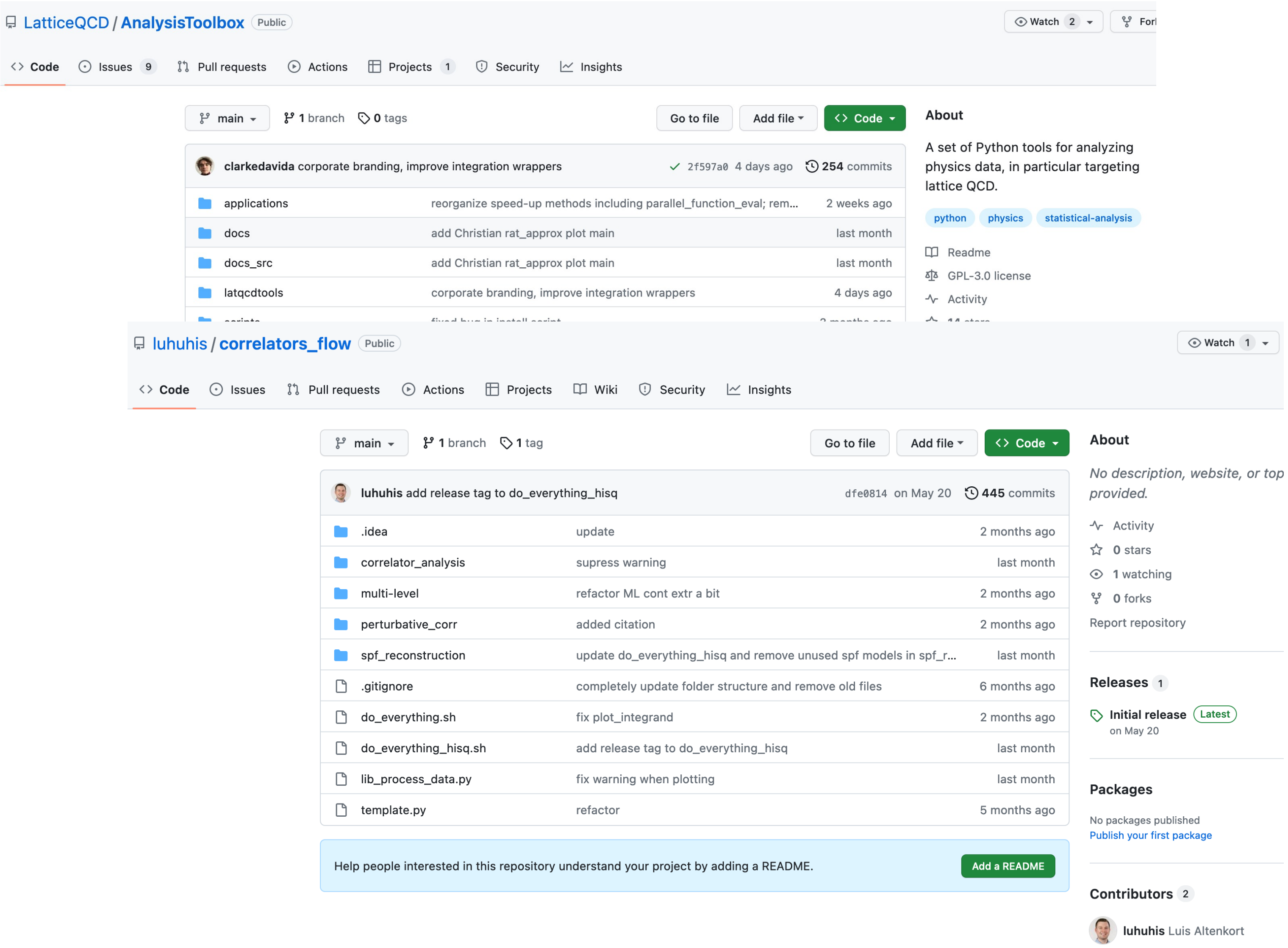
All raw and derived data is already openly available (ILDG or PUNCH storage for future projects?)

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

- Tests on Compute4PUNCH & Storage4PUNCH
- Jupyter Notebook of the analysis
- Docker container 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