# Heavy Quark Diffusion ResearchProduct in PUNCH4NFDI

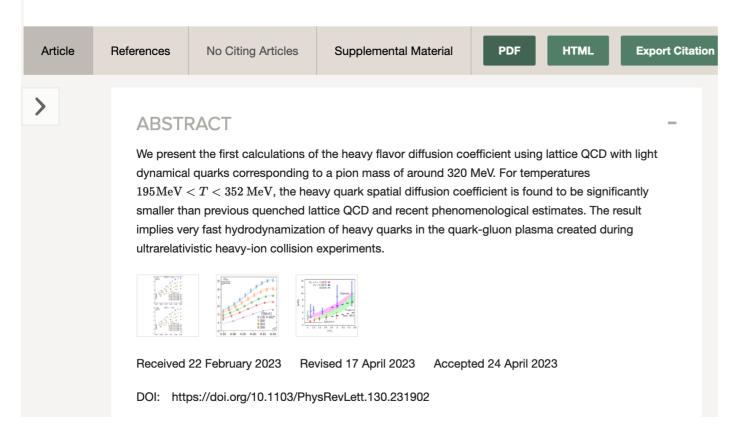
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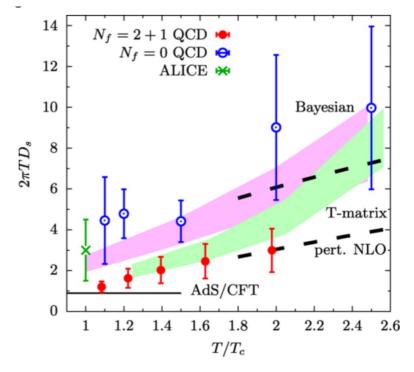
https://doi.org/10.1103/PhysRevLett.130.231902

# Heavy Quark Diffusion from $\mathbf{2} + \mathbf{1}$ Flavor Lattice QCD with 320 MeV Pion Mass

Luis Altenkort, Olaf Kaczmarek, Rasmus Larsen, Swagato Mukherjee, Peter Petreczky, Hai-Tao Shu, and Simon Stendebach (HotQCD Collaboration)

Phys. Rev. Lett. 130, 231902 - Published 6 June 2023



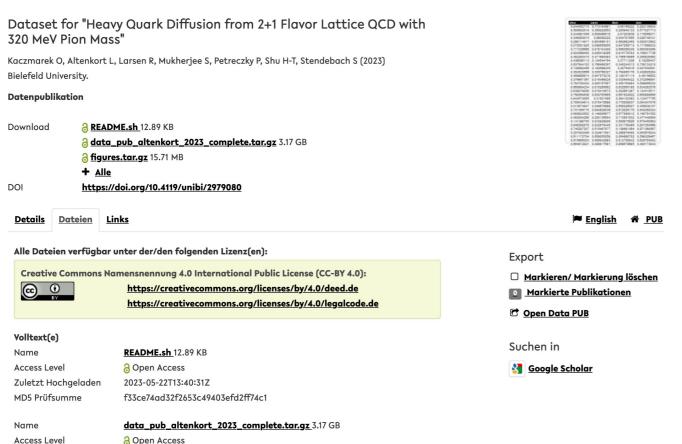


## Heavy Quark Diffusion ResearchProduct in PUNCH4NFDI

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

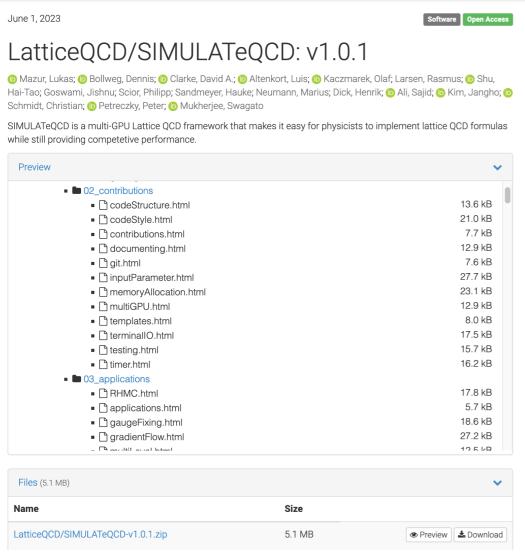
All analysis performed on Bielefeld PUNCH compute server (not yet in Compute4Punch)

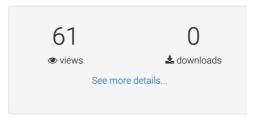
All data and lattice and analysis software as well as a workflow (bash/python) of the project published as open access

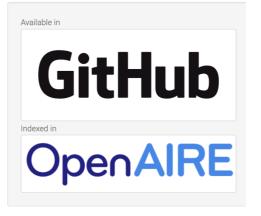


https://doi.org/10.4119/unibi/2979080

# Heavy Quark Diffusion - SIMULATeQCD code development









### TA3 ongoing work

Lattice and Analysis Software development

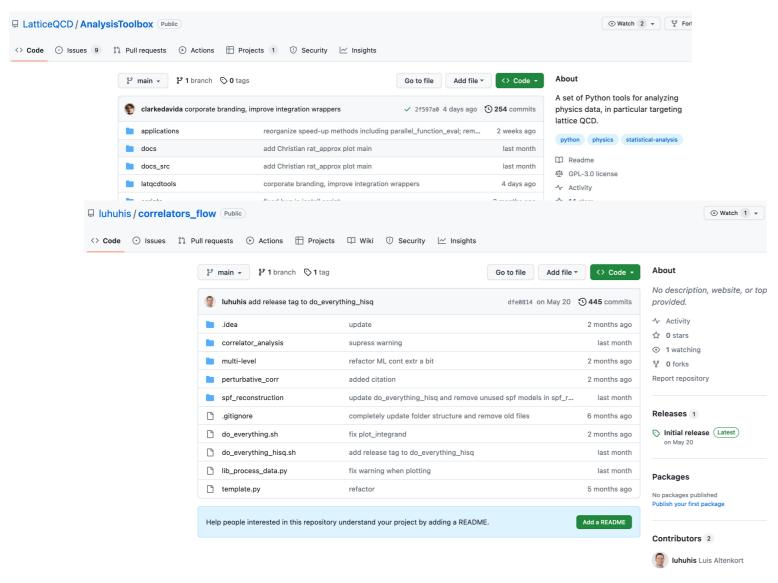
Optimization for supercomputing resources

Frontier, LUMI-G, JUWELS, Leonardo

https://doi.org/10.5281/zenodo.7994982 https://arxiv.org/abs/2306.01098

### Already "FAIR" Research Software

# **Heavy Quark Diffusion – Analysis Software**



### TA3 ongoing work

Analysis Toolbox Software development

https://github.com/LatticeQCD/AnalysisToolbox

Heavy quark diffusion analysis based on this

https://github.com/luhuhis/correlators\_flow

### Already "FAIR" Research Software

## **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 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 SDP

# LDG MDC/FC for non-lattice (gaugefield) data

### Open for any use case and any metadata scheme

- Astro (Jörn Künsemöller) and Heavy quark diffusion project planned

### Some work is still needed in the LDG development

- change of database server to postgres
- authentification : certificate → token based
- interface for Open Archives Initiative Protocol for Metadata Harvesting (OAI-PHM API)