

Heavy Quark Diffusion from 2+1 Flavor Lattice QCD with 320 MeV Pion Mass (PUNCH4NFDI use case)

DESY.

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Goal: Perform the analysis on PUNCH platform. Combine workflow, raw data, additional metadata, simulation and analysis software to a Research Product.

Gauge configurations generated on supercomputers with $N_f = 2+1$ at pion mass 320 MeV using SIMULATeQCD, a multi-GPU C++ code public & published : $\frac{\text{https://github.com/LatticeQCD/SIMULATeQCD}}{\text{arXiv:2306.01098}}$

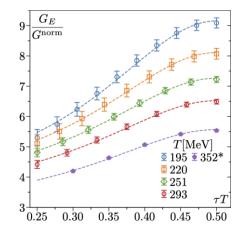
Computing resources

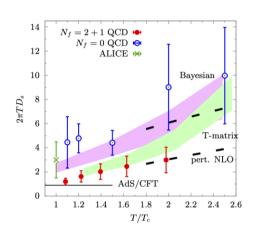
- Bielefeld GPU cluster
- JUWELS at GCS@FZJ
- used: Marconi 100 at CINECA

Raw Gauge configurations used to calculate Observable of interest:

chromo-electric correlator (G_E) for various Temperatures. All Measured data public & published: https://doi.org/10.4119/unibi/2979080

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





First results on heavy quark diffusion coefficients using dynamical light quarks from lattice!! https://doi.org/10.1103/PhysRevLett.130.231902

First success: Complete workflow including: sampling, bootstrapping, interpolation & continuum extrapolation implemented as a single bash/python script already runs as a container on:

Compute4Punch

Planned & Ongoing activities:

- Migration of the bash script to a user friendly Jupyter
 Notebook with the aim of running it on
 Compute4PUNCH
- Metadata of the datasets used in this workflow will be designed and extracted
- Use Storage4PUNCH for data and metadata catalog for storing metadata



FINAL GOAL: Publish the entire project as a Digital Research Product (DRP) on the PUNCH Science Data Platform (SDP)

