Status of Lattice QCD Use Case(s) : From Heavy Quarks to Chiral Condensates

UNIVERSITÄT BONN

RHEINISCHE FRIEDRICH-WILHELMS-UNIVERSITÄT BONN

Simran Singh

(University of Bonn)

UseCase I : Learning chiral condensates with machine learning

with Frithjof Karsch (Bielefeld), Marius Neumann (Deutscher Wetterdienst) and Christian Schmidt (Bielefeld)

UseCase II : Heavy quark diffusion coefficient

with Olaf Kaczmarek (Bielefeld) , Ding-Ze Hu (DESY, Hamburg)

PUNCH4NFDI Annual Meeting 2024

PUNCH 4NFDI

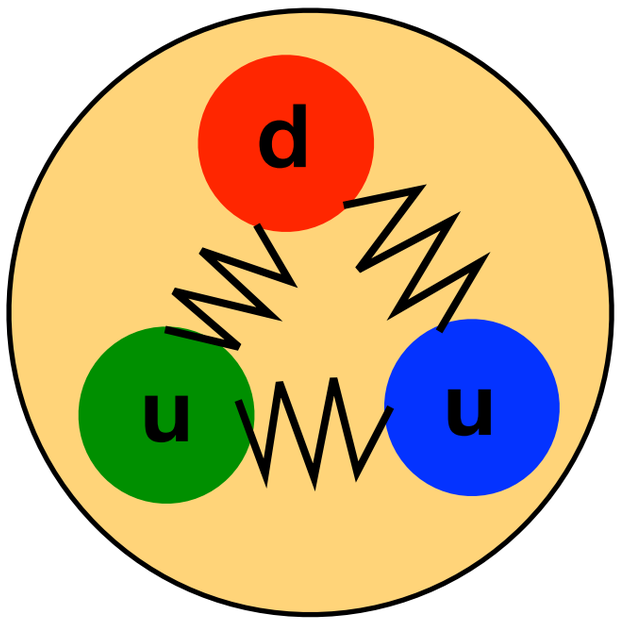
UNIVERSITÄT BIELEFELD

Faculty of Physics

28.11, Bonn

Lightning introduction : Lattice Quantum Chromodynamics

QCD is strongly interacting at low energy scales - **demanding** a **non-perturbative** approach



Lattice QCD

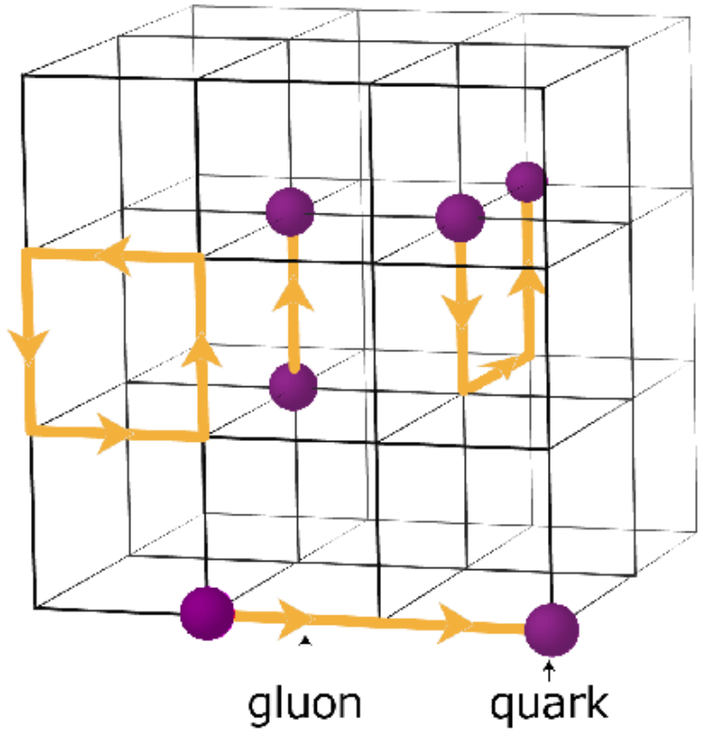
1. Generate configurations using MCMC from $p(\phi) \sim e^{-S^E_{QCD}}$

   ! Typical #real numbers to be updated each step $\sim 10^7 - 10^{10}$

2. Compute observables on statistically independent configurations

$$\langle O \rangle = \frac{1}{N} \sum_{n=1}^{N} O(U^{(n)}) \det M(U^{(n)}) e^{-S_G[U^{(n)}]}$$

3. Repeat [2,3] by varying lattice spacing and perform continuum extrapolation ~ lattice spacing to 0



https://doi.org/10.1051/epjconf/202024509008

I : Learning densities with Masked Autoregressive Flows

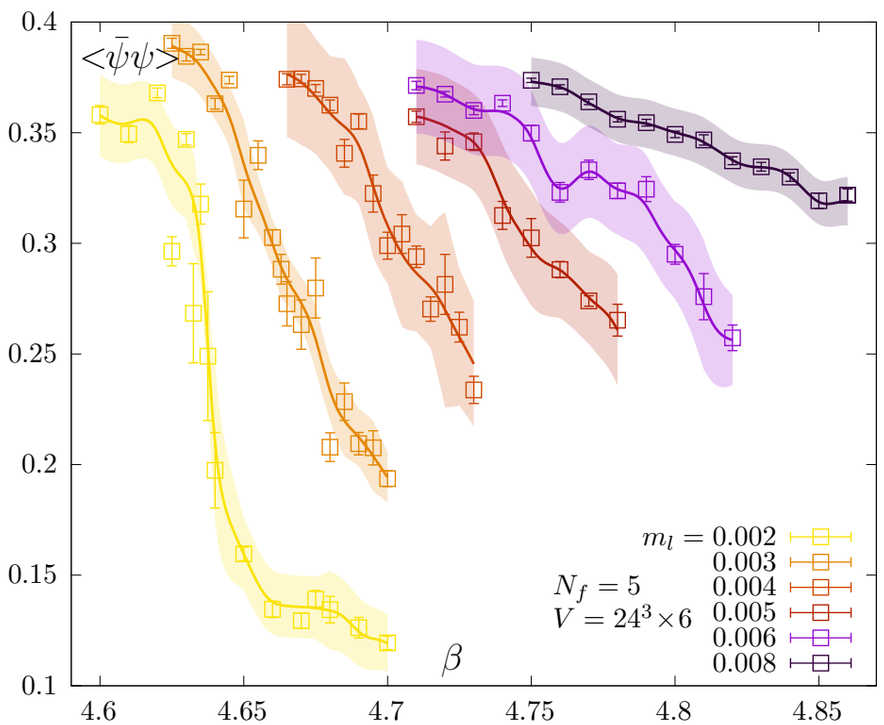
– Marius Neumann, Frithjof Karsch, Christian Schmidt, **Simran Singh**

- **Theory** : Consider a modification of QCD with 5 degenerate light quarks

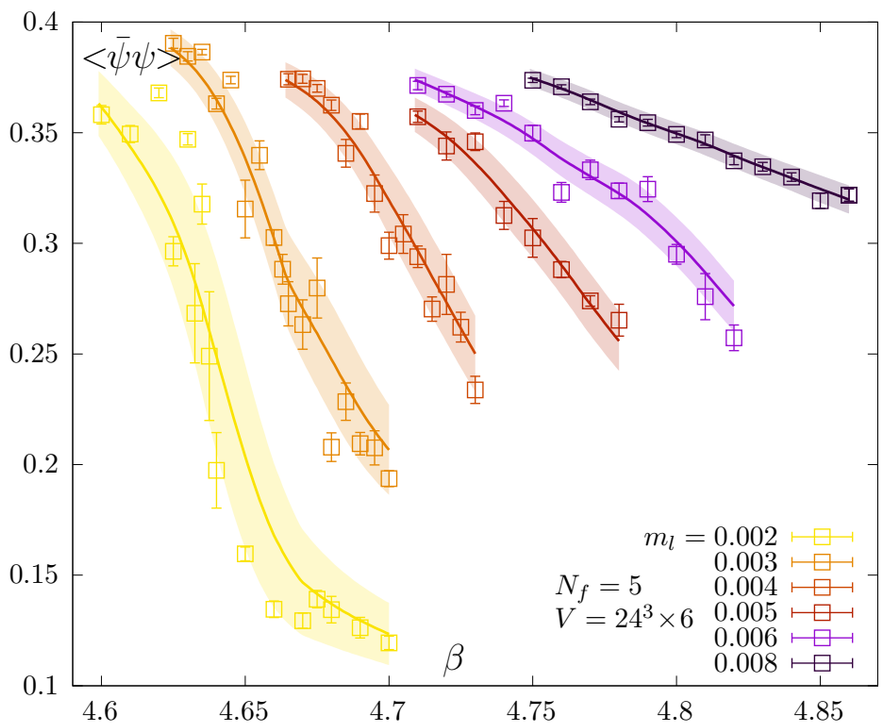
- **Goal** : Find the phase boundary for the Chiral phase transition using **Machine Learning** techniques

- **How** : Using actual lattice simulations → generate MC samples for different → $N_s, N_t, \beta, m_l \rightarrow$ to learn $p\left(\bar{\psi}\psi, S \,|\, N_\sigma, m_l, \beta\right)$

Classical β - re-weighting



Neumann M (2023) PhD Thesis Universität Bielefeld

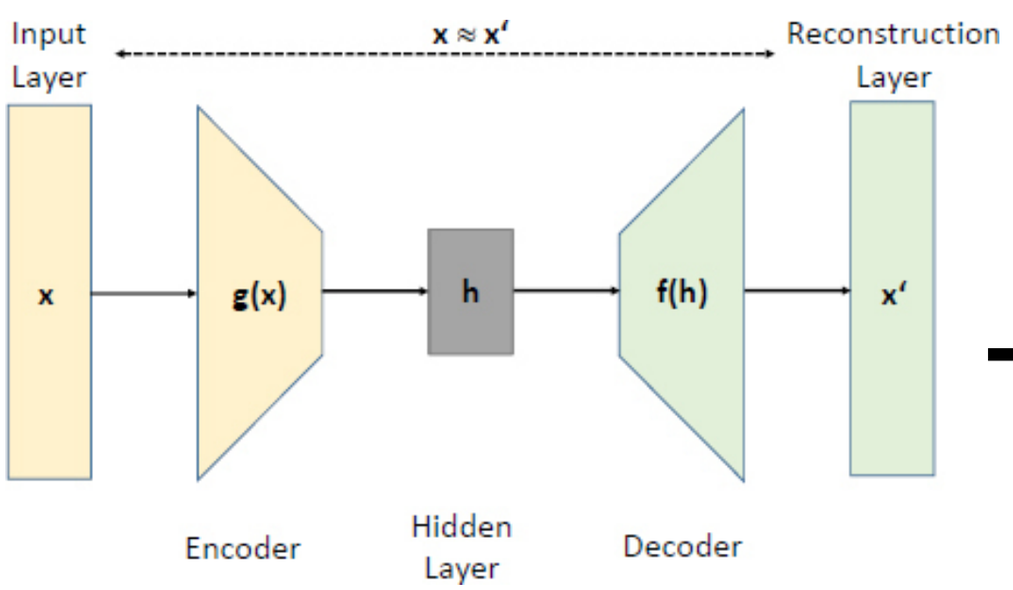


M. Neumann et.al., *PoS* LATTICE2022 (2023)

ML based β - interpolation

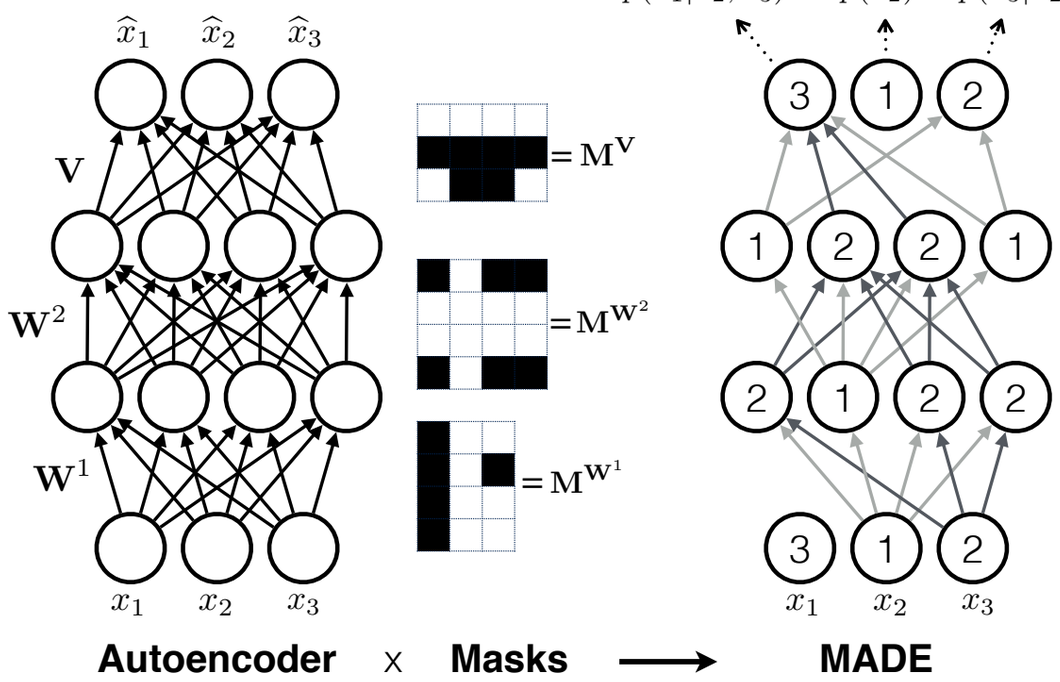
I : Learning densities with Masked Autoregressive Flows

- **ML Goal** : Learn a probability density from examples of data $\left(\vec{x}, \vec{y}\right) \rightarrow p\left(\vec{x} \,|\, \vec{y}\right)$
- **Why** : $p(x_1, x_2 \ldots x_D) = p\left(x_N | x_1, \ldots x_{N-1}\right) p\left(x_{N-1} | x_1, \ldots x_{N-2}\right) \ldots p\left(x_1\right)$
- Use **masking** to implement the **autoregressive property**



Martin Erdmann et al., Deep Learning for Physics Research, [World Scientific, 2021]

Masking



MADE : M. Germain et.al., arXiv : 1502.03539

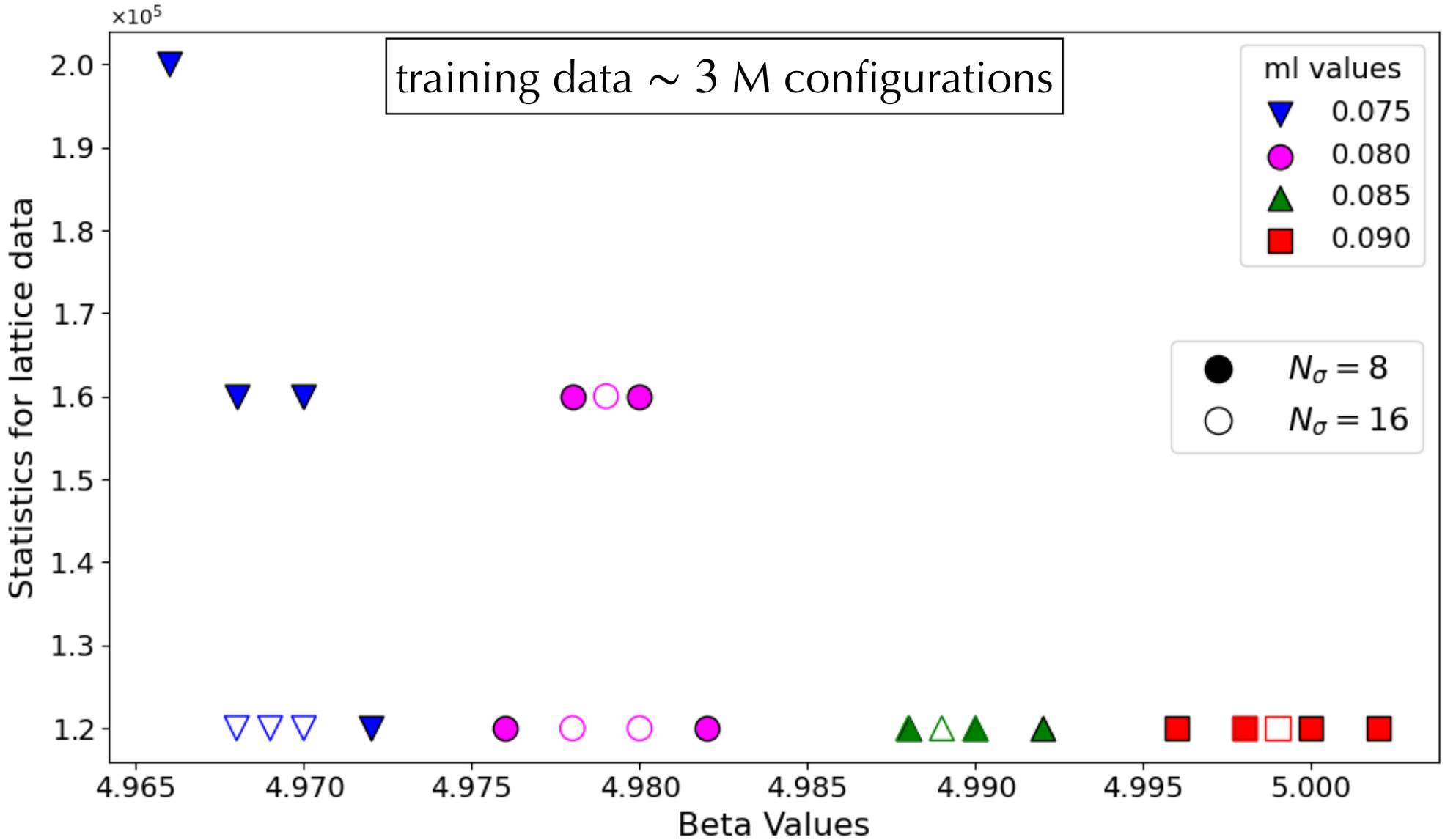
MAF : G. Papamakarios et.al., arXiv : 1705.07057

I : Learning densities with Masked Autoregressive Flows

Q. How does one test the performance of ML analysis?

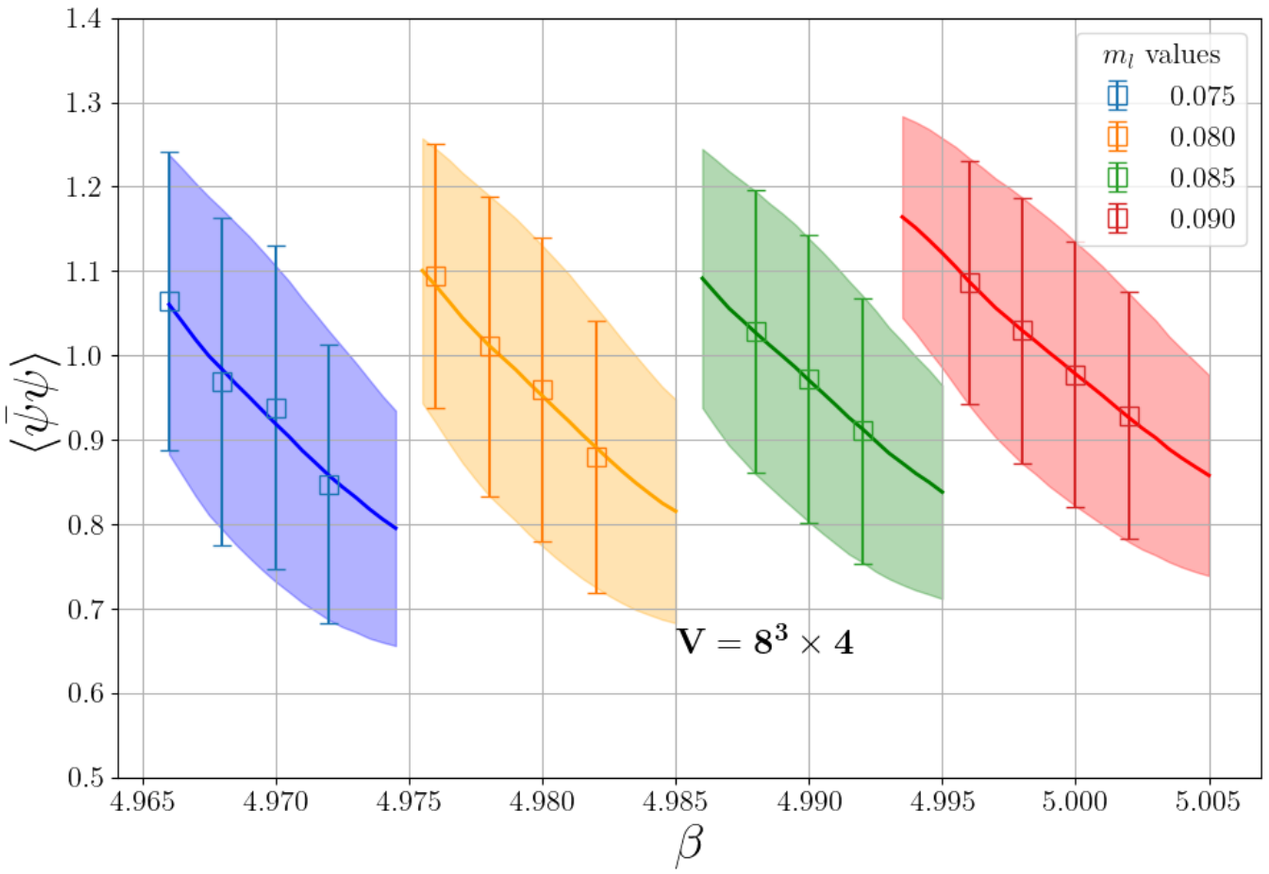
A. We test the MAF analysis on other data - F. Cuteri, O. Philipsen et.al., *JHEP* 11 (2021)

- *Different* lattice fermion action
- *Same* $N_f = 5$, $N_\tau = 4$ at $N_\sigma = \{\mathbf{8}, 12, \mathbf{16}\}$
- Time histories available for a range of m_l and β



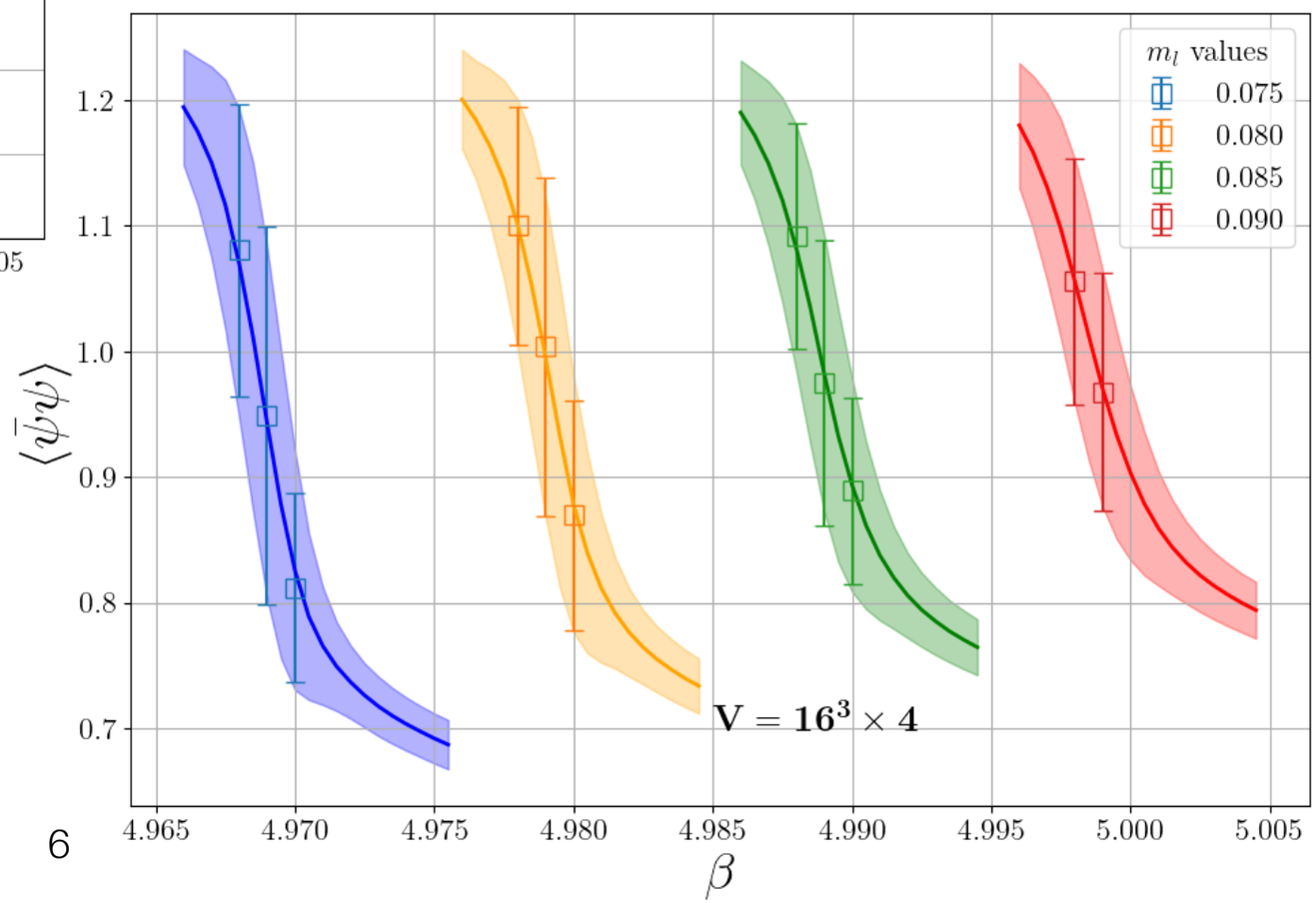
I : Learning densities with Masked Autoregressive Flows

- **Training done by removing all $N_\sigma = 12$ data** - training time ~ 4hr 30 minutes
- Evaluations ~ 0.5 sec per 1M samples at fixed N_σ, m_l, β



- $\bar{\psi}\psi \sim p(\bar{\psi}\psi) : p(\bar{\psi}\psi, S)$
- 100K model evaluations

- Solid lines + band: ML output
- Squares : Lattice Data



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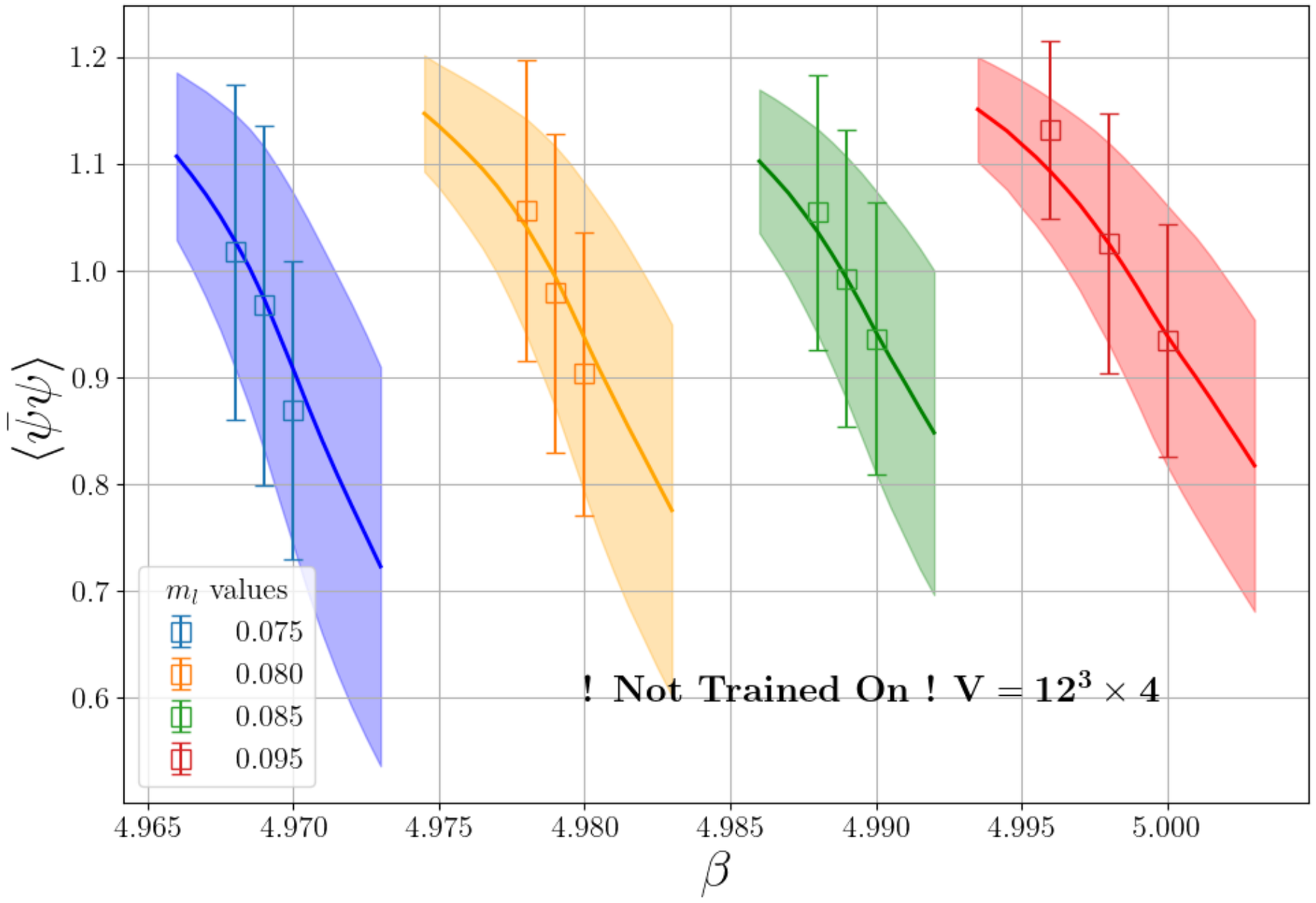

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I : Learning densities with Masked Autoregressive Flows

Why is this a good candidate for a PUNCH Use Case ?

✓ **Transparent** : Time histories* of observables from Lattice QCD simulations *directly* available!

✓ **Novel** : *Masked Autoregressive Flows* applied for the first time to learn LQCD observables !

✓ **Reusable**, **Reproducible** and **easily Modifiable** !

Steps taken to make it a user-friendly Use Case

✓ (Many) Scripts and useful files available at **https://gitlab-p4n.aip.de/punch/ta4/wp3/LatticeMLUseCase**

✓ A detailed README on the code logic and list of codes

✓ Dockerfile and instructions to build and run containers available

✓ Example trained models and data available !

README.md

Critical Mass with ML

Overview:

The final goal is to find the critical mass for a given number of flavors that marks the change of "order" from first to crossover. This is done by splitting the analysis in two parts:

1. ***Re-weighting***: Using the concept of Masked Auto-regressive Flows (MAFs) which are made up of Masked Autoencoder for Distribution Estimation (MADE) blocks to compute the 2D histograms conditioned on the volume N_σ, mass m_l and coupling β. The goal to learn the conditional probability distribution $p\left(\bar{\psi}\psi\,,\, S|N_\sigma, m_l, \beta\right)$.

punch / TA4 / WP3 / **LatticeMLUseCase**

.gitlab-ci.yml	Update .gitlab-ci.yml file
2DDensityPlots.py	Make 2D density plots
DockerSteps.txt	DockerSteps for building image and ...
Dockerfile	DockerFile
Nf5_2022_09_18_NFlow.csv	Main CSV file with time history data
README.md	Upload New File
eval_MAF_cumulants.py	Update eval_MAF_cumulants.py
eval_Maf_density.py	Make density plots from ML model
extract_unique_to_dat.py	Upload New File
filter_csv_by_pair.py	Upload New File
input_eval.txt	Update input_eval.txt
input_train.txt	Update input_train.txt for train_MAF.py
model_Flow_v13_ckpt.data...	Trained model ancillary file
model_Flow_v13_ckpt.index	Trained model on full data
plot_ml_output.py	Upload New File
ppsi1DDensityPlots.py	Make 1D projections of 2D density pl...
requirements.txt	Software Stack for Dockerfile
train_MAF.py	Update train_MAF.py

II : Heavy-Quark diffusion coefficient from lattice simulations

- Luis Altenkort, Olaf Kaczmarek et. al., Phys. Rev. Lett. 2023, **PUNCH related work** : Olaf Kaczmarek, Ding-Ze Hu, **Simran Singh**

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/`

To be made available via ILDG

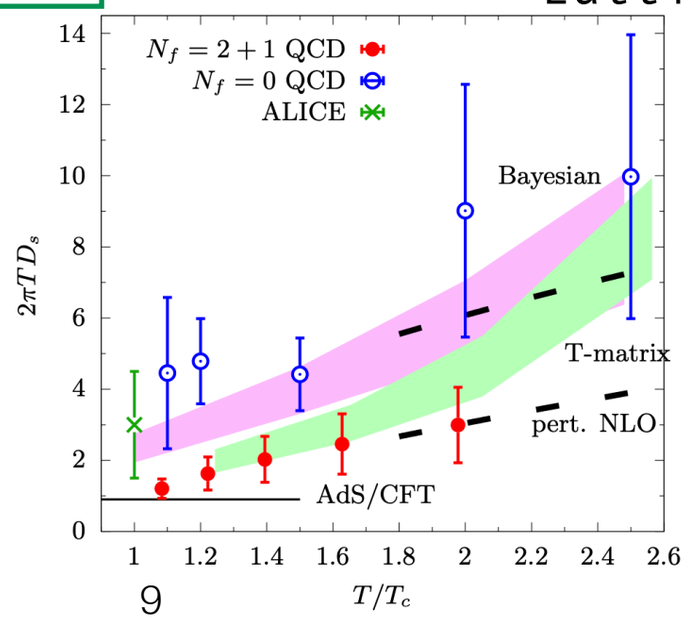
Computing resources used :

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

PUNCH output

Raw Gauge configurations used to calculate Observable of interest : chromoelectric correlator (G_E) for various Temperatures

Analysis Toolbox : Collection of Python tools developed at Bielefeld (Public): `https://github.com/LatticeQCD/AnalysisToolbox`



*Original full workflow and related data (except gauge configuration which will eventually be made available via ILDG) can be found @ https://doi.org/10.4119/unibi/2979080

Status on running the workflow on REANA : Results of workflow

- Results from some successful runs - with different environments
- Further tested using the Jupyter Interface of REANA
- Final plot of the paper successfully generated
- Documentation available on PUNCH GitLab

Your workflows Refreshed at 13:25:20 UTC

Search...

Status | Show deleted runs | Latest first

LatTestComenImage49072f8a #1 — **finished** in 1h 53m 37s
6.77 GiB — Finished 20 hours ago — step 5/5

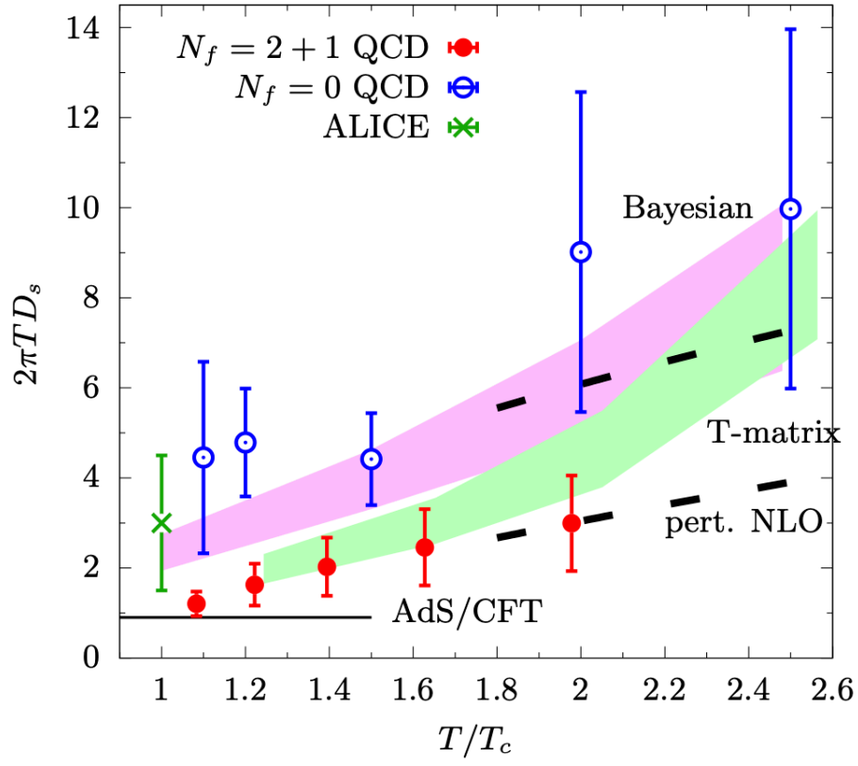
LatTestComenImagebf4b15f7 #1 — **finished** in 3h 4m 33s
6.96 GiB — Finished a day ago — step 5/5

LatTestComentOut #1 — **finished** in 1h 51m 13s
6.76 GiB — Finished a day ago — step 5/5

testBeginEx2 #2 — **finished** in 13 seconds
50 KiB — Finished a day ago — step 1/1

testdockNewDock #1 — **finished** in 7 min 26 sec

Some successfully generated figure from paper



Work on Lattice UseCase by Ding-Ze Hu

Metadata Schema

- Designed metadata schema from DataCite - applied to use-case. ✓
- *Type A for DOI minting*: Only contains the necessary information that helps us to find and identify the information. ✓
- *Type B for users* : contains information like size, format of the data, related information (software/article/...) and description of the data (methods/ technical info/...) ✓
- All the XML metadata records are tested to ensure that they are valid against the schema from DataCite using xmllint tool ✓

Docker Container tested run on Compute4Punch

- Created a Docker container specifically for the Lattice use case. ✓
- The container includes all necessary data and programs for running LQCD analysis and generating result charts. ✓
- Registered within the Compute4PUNCH platform, enabling the execution of the entire LQCD analysis workflow. ✓

Summary

UseCase I : ML for Lattice Observables

- **New Use Case** showing a novel application of ML to interpolate Lattice QCD observables
- Also a TA 3.2 contribution from Bielefeld lattice group
- Available as a repository on PUNCH GitLab ✓
- Yet to be tested on REANA and C4P 

UseCase II : Heavy Quark diffusion coefficient

- **Use Case** showing computation of transport coefficient using dynamical quark simulations (from a PRL publication)
- Showcases **AnalysisToolbox** and **SIMULATeQCD code** by Bielefeld lattice group
- Available as a repository on PUNCH GitLab ✓
- Tested on REANA ✓
- Available as a container in the PUNCH container stacks and tested on C4P ✓
- Metadata records generated and validated against the DataCite schema ✓

Thank You For Your Attention