Proposal title for joint access to NHR@GÖTTINGEN and NHR@ZIB

Towards QCD+QED Simulations with C* Boundary Conditions at physical QED coupling

Requested start date

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Type of proposal

"follow-up proposal" for project ID *bep00102*

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309-01 Nuclear and Elementary Particle Physics, Quantum Mechanics, Relativity, Fields

Short abstract

*This project is part of a long-term research programme aiming at calculating isospin-breaking and electromagnetic corrections in hadronic quantities from first principles in lattice QCD+QED. Building upon the first phase of this project, we propose the generation of three QCD+QED gauge ensembles with lattice spacing $a \simeq 0.05$ fm, with different values of the fine-structure constant and different lattice volumes. On these ensembles we will calculate a variety of observables, including meson and baryon masses. We will work mostly at the U-symmetric point i.e. $m_d = m_s$, but a first exploration of the effect of the splitting between down and strange quarks is also proposed. We apply for a total of **45.23Mcore-h** on Lise.*

Contents

1 Scientific part (follow-up proposal)

1.1 Report of the past project period

With our previous allocation of the **bep00102** project we have fully or partially achieved a number of goals, which are discussed separately in the following subsections.

Gauge ensembles at $\alpha = 1/137$: achieved

Planned resources: 5.78 Mcore-hours, corresponding to the runs `Q*D-32-3-TUN`, `Q*D-32-3-GEN`, `Q*D-32-4-TUN`, `Q*D-32-4-GEN` outlined in table 1 of the initial proposal.
Used resources: 10.1 Mcore-hours.

We have tuned the quark masses to the chosen line of constant physics for the QCD+QED ensemble with $\alpha = 1/137$, and we generated 2000 thermalized configurations at the tuned point.
The tuning was more difficult than expected. In particular, the strategy based on calculations of partially quenched meson masses detailed in our initial proposal systematically overshoots the tuned point. While this was already observed in ensembles with larger values of α, in that case the effect was not large enough to invalidate the strategy. At $\alpha = 1/137$ the relative error due to the partially quenched approximation on the splitting of the kaons (and ultimately on ϕ_2) becomes too large simply because the splitting becomes smaller, rendering the partially quenched strategy unusable.
To solve this problem we have developed an improved strategy based on the use of mass reweighting:

1. Generate some ensembles with smaller statistics ($\sim$200 thermalized configurations), and get a rough estimate $\hat{m}^{(0)} = (m_u^{(0)}, m_{ds}^{(0)}, m_c^{(0)})$ for the quark masses.
2. Generate an ensemble with full statistics (at least 1000 thermalized configurations) with quark masses equal to $\hat{m}^{(0)}$. Calculate the values of the $\phi^{(0)} = (\phi_1^{(0)}, \phi_2^{(0)}, \phi_3^{(0)})$ observables on these configurations.
3. Choose three new sets of quark masses $\hat{m}^{(i)}$ with $i = 1, 2, 3$ fairly close to $\hat{m}^{(0)}$, and calculate the values of the $\phi^{(i)}$ observables corresponding to these quark masses, by means of mass reweighting. Find the tuned values of the quark masses $\hat{m}^{(t)}$ by linear interpolation, i.e. by assuming that the ϕ observables depend on the masses $\hat{m}$ as in $\phi = A\hat{m} + b$, where A is a 3×3 matrix and b is a 3-vector. A few attempts may be necessary in order to find values for $\hat{m}^{(i)}$ for which the reweighting does not have an overlap problem, and for which the tuned value is found either by interpolation or by a mild extrapolation.
4. Generate an ensemble with full statistics (2000 thermalized configurations) with quark masses equal to $\hat{m}^{(t)}$. Calculate the values of the $\phi^{(t)}$ observables on these configurations.
5. If the extrapolation in point 3 is too long, then one does not get the target value for the ϕ observables, and one needs to repeat everything from step 3 with $\hat{m}^{(0)} \leftarrow \hat{m}^{(t)}$. On the other hand, some residual small mistuning due to the linear approximation is corrected by mass reweighting to the corrected tuned value, without generating new configurations.

In the case of $\alpha = 1/137$ we needed to repeat this cycle only once (after one cycle with the partially quenched strategy). We have obtained two thermalized ensembles: `A450a07b324` with reduced statistics (1000 configurations) and the final tuned ensemble `A380a07b324` with full statistics (2000 configurations), see table 1. Overall, the cost of the tuning turned out to be a factor of 3 larger than expected.

Measurement of observables: achieved

Planned resources: 4.88 Mcore-hours, corresponding to the runs `Q*D-32-4-OBS`, `Q*D-48-1-OBS` outlined in table 1 of the initial proposal.
Used resources: 4.3 Mcore-hours.

As originally planned in our initial proposal, we have measured a number of observables on all generated ensembles:

1. mass reweighting factors to correct for small mistunings when relevant (in fact only for the `A380a07b324` ensemble);
2. reweighting factor to correct the error introduced by the rational approximation of the fermionic pfaffian;
3. sign of the fermionic pfaffian, included as reweighting factor in all observables;
4. Wilson flow scale t_0, used to calculate the lattice spacing a in our ensembles (see table 2);
5. renormalized electromagnetic coupling α_R, defined by means of the gradient flow (see table 2);
6. $\pi^\pm = K^\pm$, K_0, $D^\pm = D_s^\pm$, D_0 meson masses, and mass differences (see table 3);
7. tuning observables ϕ_1, ϕ_2, ϕ_3 defined in the initial proposal (see table 4).

Gauge ensemble at $\alpha = 0.02$ and measurement of baryon masses: partially achieved

Planned resources: 7.16 Mcore-hours, corresponding to the runs `Q*D-32-5-TUN`, `Q*D-32-5-GEN`, `Q*D-32-6-TUN`, `Q*D-32-6-GEN`, `Q*D-32-6-OBS` outlined in table 1 of the initial proposal.
Used resources: 7.12 Mcore-hours.

At the beginning of the second quarter two important factors prompted us to re-assess our goals:

1. It was clear at that point that we had underestimated the time needed for tuning. In particular it was not clear that we could complete the tuning, generation and measurements of the QCD+QED ensemble with $\alpha = 0.02$ within the previous allocation.
2. As already pointed out in the initial proposal, one of our major long-term goals is to calculate baryon masses on the generated ensembles. However we did not include the calculation of baryon masses as a goal in our previous proposal, mostly because the measurement and analysis codes were not ready, and the time scale was not clear at the time of submission. Nevertheless, at the beginning of the second quarter, the `openQ*D` module for measuring baryon masses was ready and tested.

Measuring the baryon masses (as opposed to having a non-fully tuned ensemble) would put us in the position to have a more substantial publication at the end of the allocation period. Therefore we decided to postpone the tuning and generation of the gauge configurations at $\alpha = 0.02$, and to proceed with the measurement of a number of baryon masses (proton= Σ^+, neutron= Ξ^0, $\Xi^- = \Sigma^-$, Λ^0, Ω^-) and mass differences. This call proved to be justified as two publications on the results of the previous allocation are almost ready and will be submitted for publication within the next two weeks. A summary of results can be found in tables 5 and 6. For the moment we have measured baryon masses only on our small volumes.

Large volume at $\alpha = 0.05$: partially achieved

Planned resources: 13.6 Mcore-hours, corresponding to the run `Q*D-48-1-GEN` outlined in table 1 of the initial proposal.
Used resources: 9.9 Mcore-hours.

The generation of the 96×48^3 QCD+QED configurations with $\alpha = 0.05$, and the measurement of observables (reweighting factors, meson masses, sign of the pfaffian, Wilson flow observables) proceeded with no surprises (runs `Q*D-48-1-GEN` and `Q*D-48-1-OBS` in the initial proposal). We have decided to generate only 600 thermalized configurations out of the planned 1000 (+500 configurations of thermalization), in order to complete the measurement of baryon masses.

Scientific output

- J. Lücke, An update on QCD+QED simulations with C* boundary conditions, talk at the *39th International Symposium on Lattice Field Theory* scheduled for Aug 12, 2022. An associated proceedings will be published.
- R. Gruber, A first look at the HVP from QCD and QCD+QED with C* boundary conditions, talk at the *39th International Symposium on Lattice Field Theory* scheduled for Aug 11, 2022. An associated proceedings will be published.
- A. Altherr, A first look at the HVP from QCD and QCD+QED with C* boundary conditions II, talk at the *39th International Symposium on Lattice Field Theory* scheduled for Aug 11, 2022. An associated proceedings will be published.
- A. Cotellucci, Tuning of QCD+QED simulations with C* boundary conditions, poster presentation at the *39th International Symposium on Lattice Field Theory* scheduled for Aug 9, 2022. An associated proceedings will be published.
- P. Tavella, Strange and charm contribution to the HVP from C* boundary conditions, poster presentation at the *39th International Symposium on Lattice Field Theory* scheduled for Aug 9, 2022.
- J. Lücke, A. Patella, Reweighting rational approximations of $(D^\dagger D)^\alpha$, paper in preparation.
- L. Bushnaq, I. Campos, M. Catillo, A. Cotellucci, M. Dale, P. Fritzsch, J. Lücke, M. K. Marinković, A. Patella, N. Tantalo, First results on QCD+QED with C* boundary conditions, paper in preparation.

1.2 Project objectives and justification for a follow-up project

Gauge ensemble and observables at $\alpha = 0.02$

This goal remains mostly unchanged with respect to the initial proposal. In addition to the initial proposal, we plan to calculate baryon masses on the generated ensemble as well.

Large volume at $\alpha = 0.05$

Our goal is to extend the thermalized ensemble (96×48^3 with $\alpha = 0.05$) to a total of 1000 configurations, as originally planned, and to calculate all observables (except baryon masses) on the new configurations.

ensemble	n. cnfg	acc. rate	$\langle e^{-\Delta H}\rangle$	$\tau_{\rm int}(t_0)$	$\tau_{\rm int}(Q^2)$	$\tau_{\rm int}(\alpha_R)$
A400a00b324	2000	95%	0.9979(55)	51(18)	6.4(2.3)	—
B400a00b324	1082	98%	0.9950(25)	31(10)	8.0(2.8)	—
A450a07b324	1000	94%	0.9978(46)	44(19)	6.5(3.0)	2.3(1.6)
A380a07b324	2000	92%	1.0017(46)	46(15)	10.3(3.5)	2.7(1.5)
A500a50b324	1993	97%	0.9961(21)	21.4(5.5)	11.6(2.6)	1.40(55)
A360a50b324	2001	95%	0.9956(45)	47(16)	8.5(2.6)	1.1(1.0)
C380a50b324	600	98%	1.004(12)	12.5(3.9)	10.6(4.1)	3.0(1.2)

Table 1: **(Preliminary data)** For each ensemble: the number of configurations which corresponds to the number of MD trajectories, the acceptance rate, the diagnostic observable $\langle e^{-\Delta H}\rangle = 1$, the integrated autocorrelation times (in units of MD trajectories) for the scale t_0/a^2, the squared topological charge Q^2, and the renormalized fine-structure constant α_R. In our simulations, one MD trajectory is equal to $\tau = 2$ MD units. The yellow rows are results achieved within the project bep00102 whereas the white ones were already computed within project bep00085.

ensemble(+rw)	t_0/a^2	a [fm]	α_R	$\pi\sqrt{3}L^{-1}$ [MeV]
A400a00b324	7.402(66)	0.05393(24)	0	—
B400a00b324	7.383(40)	0.05400(14)	0	—
A450a07b324	7.198(84)	0.05469(32)	0.007076(24)	613.5(3.6)
A380a07b324	7.599(79)	0.05323(28)	0.007081(19)	630.4(3.3)
A380a07b324+RW1	7.525(77)	0.05349(27)	0.007080(22)	627.3(3.2)
A500a50b324	7.789(42)	0.05257(14)	0.040772(85)	638.2(1.7)
A360a50b324	8.427(89)	0.05054(27)	0.040633(80)	663.9(3.5)
A360a50b324+RW1	8.285(79)	0.05098(24)	0.04069(26)	658.2(3.2)
C380a50b324	8.400(26)	0.050625(79)	0.04073(11)	441.86(69)

Table 2: **(Preliminary data)** For each ensemble (with or without mass reweighting): reference observable t_0/a^2, lattice spacing a calculated from the measured value of t_0/a^2 and the reference value $(8t_0)^{1/2} = 0.415$ fm, the renormalized fine-structure constant α_R, the tree-level energy gap of the photon $\pi\sqrt{3}L^{-1}$. Values in MeV are obtained by using the reference value $(8t_0)^{1/2} = 0.415$ fm. The yellow rows are results achieved within the project bep00102 whereas the white ones were already computed within project bep00085.

ensemble(+rw)	$M_{\pi^\pm} = M_{K^\pm}$ [MeV]	M_{K^0} [MeV]	ΔM_K [MeV]	$M_{D^\pm} = M_{D_s^\pm}$ [MeV]	M_{D^0} [MeV]	ΔM_D [MeV]
A400a00b324	398.5(4.7)	398.5(4.7)	0	1912.7(5.7)	1912.7(5.7)	0
B400a00b324	401.9(1.4)	401.9(1.4)	0	1908.5(4.5)	1908.5(4.5)	0
A450a07b324	451.2(4.3)	451.6(4.7)	0.8(1.1)	1919.8(7.3)	1916.0(8.0)	3.6(1.2)
A380a07b324	383.6(4.4)	390.7(3.7)	7.01(26)	1926.4(7.8)	1921.1(7.6)	5.03(46)
A380a07b324+RW1	398.8(3.7)	403.1(3.8)	4.26(31)	1925.2(7.1)	1919.3(7.6)	5.8(1.1)
A500a50b324	495.0(2.8)	519.1(2.5)	24.0(1.0)	1901.1(4.1)	1870.1(4.4)	31.6(1.6)
A360a50b324	358.6(3.7)	388.8(3.5)	29.5(2.4)	1937.8(6.8)	1912.0(7.7)	26.0(2.8)
A360a50b324+RW1	398.9(3.4)	425.1(4.1)	26.1(1.3)	1926(10)	1898.8(5.8)	26.9(2.2)
C380a50b324	386.5(2.4)	414.5(2.0)	26.89(49)	1932.0(3.9)	1894.3(6.9)	34.5(5.6)

Table 3: **(Preliminary data)** For each ensemble (with or without mass reweighting): meson masses, and charged-neutral meson mass differences. Here $\Delta M_K = M_{K^0} - M_{K^\pm}$ and $\Delta M_D = M_{D^\pm} - M_{D^0}$. Values in MeV are obtained by using the reference value $(8t_0)^{1/2} = 0.415$ fm. Notice that some mesons are degenerate because in our simulations $m_d = m_s$. The yellow rows are results achieved within the project bep00102 whereas the white ones were already computed within project bep00085.

ensemble(+rw)	ϕ_1	ϕ_2	ϕ_3
A400a00b324	2.107(50)	—	12.068(36)
B400a00b324	2.143(15)	—	12.042(28)
A450a07b324	2.703(53)	4.4(6.0)	12.097(51)
A380a07b324	1.977(37)	3.39(14)	12.132(48)
A380a07b324+RW1	2.126(39)	2.13(17)	12.122(47)
A500a50b324	3.357(37)	2.60(11)	11.864(28)
A360a50b324	1.806(35)	2.41(19)	12.114(41)
A360a50b324+RW1	2.208(38)	2.348(97)	12.040(58)
C380a50b324	2.088(22)	2.350(44)	12.020(29)
target	2.13	2.37	12.1

Table 4: **(Preliminary data)** ϕ parameters for each ensemble (with or without mass reweighting), together with the target value used to define the lines of constant physics. The yellow rows are results achieved within the project bep00102 whereas the white ones were already computed within project bep00085.

ensemble(+rw)	$M_p = M_{\Sigma^+}$	$M_n = M_{\Xi^0}$	$M_{\Xi^-} = M_{\Sigma^-}$	M_{Λ^0}	$M_{\Omega^-} = M_{\Delta^-}$
A450a07b324	1214(14)	1215(15)	1216(16)	1215(15)	1473(35)
A380a07b324	1147(19)	1151(19)	1157(18)	1151(19)	1458(26)
A380a07b324+RW1	1164(15)	1167(13)	1175(14)	1167(13)	1448(20)
A500a50b324	1280(15)	1288(13)	1339(11)	1296(13)	1614(23)
A360a50b324+RW1	1212(20)	1226(22)	1268(32)	1227(24)	1584(59)

Table 5: **(Preliminary data)** Baryon masses measured on the different ensembles. The yellow rows highlight, that these masses were computed within project bep00102.

ensemble(+rw)	$M_n - M_p$	$M_{\Xi^0} - M_{\Xi^-}$	$M_{\Sigma^+} - M_{\Sigma^-}$
`A450a07b324`	-0.89(0.38)	-2.44(0.49)	-1.77(0.89)
`A380a07b324`	1.80(0.52)	-8.37(0.75)	-9.96(0.79)
`A380a07b324+RW1`	0.90(0.37)	-5.97(0.63)	-6.81(0.68)
`A500a50b324`	9.2(1.5)	-38.2(2.4)	-46.7(2.7)
`A360a50b324+RW1`	10.5(6.0)	-30.2(4.7)	-52(11)

Table 6: **(Preliminary data)** Baryon mass differences measured on the different ensembles. The yellow rows highlight, that these mass differences were computed within project bep00102.

Large volume at $\alpha = 1/137$

Our goal is to generate 1000 thermalized configurations on a 96×48^3 lattice at $\alpha = 1/137$ at the tuned point, i.e. at the same values of the parameters of our gauge ensemble `A380a07b324+RW1`. As expected, finite volume effects are generally large in QCD+QED simulations, and large volumes are essential in order to get reliable estimates of physical observables. As an outcome of the previous allocation, we have found that at the values of pion masses and lattice spacing used in our simulations, finite volume corrections are not larger than the statistical errors in mesonic observables when a 96×48^3 lattice is used.

Splitting by reweighting

So far we have generated only configurations with degenerate down and strange quarks. In order to approach physical quark masses, we need to make the down and up quarks lighter and the strange quark heavier. Our goal is to investigate how the ϕ observables defined in the initial proposal (and in particular ϕ_0) change under a small splitting of the down and strange quark by means of mass reweighting. We want to carry out this analysis on 64×32^3 gauge configurations with $\alpha = 1/137$, $\alpha = 0.02$ and $\alpha = 0.05$. This study is technical in nature, but it is essential to inform future simulations closer to physical quark masses.

1.3 Work schedule

There is a one-to-one correspondence between work packages and objectives.

Work package	2022 Q4			2023 Q1			2023 Q2			2023 Q3		
	10	11	12	1	2	3	4	5	6	7	8	9
WP1 Gauge ensemble $\alpha = 0.02$												
WP2 Large volume $\alpha = 0.05$												
WP3 Large volume at $\alpha = 1/137$												
WP4 Splitting												

Work-package 1

This work package is split in the following sequential tasks:

1. Using a first guess for quark masses obtained by interpolating between the already existing ensembles at $\alpha = 1/137$ and $\alpha = 0.05$, generate 1300 configurations (approx. 1000 thermalized configurations) on a 64×32^3 lattice with $\alpha = 0.02$.

2. Calculate the meson masses, and estimate the needed shift in the quark masses to reach the tuned point by rescaling from previously-generated ensembles. The tuned point is defined by the target value of the ϕ observables discussed in the initial proposal.
3. Calculate the mass reweighting factors and meson masses, needed to implement one cycle of the improved tuning strategy described in section 1.1. Find the tuned point by linear interpolation of the ϕ observables.
4. Generate 1300 configurations (approx. 1000 thermalized configurations) with the new parameters.
5. Repeat steps 2,3,4 once.
6. Calculate all observables (reweighting factors, sign of the pfaffian, meson masses, baryon masses) at the tuned point.

Work-package 2

This work package is split in the following sequential tasks:

1. Extend the run `Q*D-48-1-GEN` described in the initial proposal by generating extra 400 gauge configurations.
2. Calculate observables (reweighting factors, sign of the pfaffian, meson masses) on the generated configurations.

Work-package 3

This work package is split in the following sequential tasks:

1. Generate 1500 gauge configurations (approx. 1000 thermalized configurations) on a 96×48^3 lattice with $\alpha = 1/137$, and quark masses at the tuned point corresponding to the ones used for the ensemble `A380a07b324+RW1` in tables 2 and 3.
2. Calculate observables (reweighting factors, sign of the pfaffian, meson masses) on the thermalized configurations.

Work-package 4

This work package is split in the following sequential tasks:

1. On each of the following gauge ensembles: `A380a07b324`, `A360a50b324` (see tables) and the thermalized ensemble generated with WP1, measure 3 mass reweighting factors generating a splitting between the $\pi^{\pm}$ and $K^{\pm}$ mesons of about 50MeV, 100MeV and 150MeV. In splitting the down and strange quark masses symmetrically around the degenerate point, at first order in chiral perturbation theory one expects that ϕ_1 will not change, while ϕ_2 and ϕ_3 in general will change. Therefore also the up and charm quark masses will need to be changed in order to keep constant values for the ϕ_2 and ϕ_3 observables.
2. For each splitting, calculate mesons that are obtained *(1)* by changing the masses of all quarks, *(2)* by changing the masses of all quarks but the up, *(3)* by changing the masses of all quarks but the charm. Use these three set of mesons to find the values of the up and charm quark masses that keep the ϕ_2 and ϕ_3 observables fixed by means of a linear interpolation.

1.4 Change of model, and/or its numerical methodology and implementation

N/A

2 Technical part

2.1 *Software description

See the previous proposal.

2.2 *Software performance and HPC suitability

See the previous proposal.

2.3 *The necessity to use an HPC system

See the previous proposal.

2.4 Requested compute resources

We request a total of **45.23Mcore-h** on CPUs. As done in the previous allocation, we plan to run exclusively on Lise. A breakdown for the various types of runs can be found in table 7. All values in the column *Wall time/step* have been measured on Lise. In the column *problem size* we report the lattice size. The number of cores has been chosen in a region in which the scaling properties of our code are still excellent (see figure 2 in initial proposal with: 2112 cores = 22 nodes, 3072 cores = 32 nodes, 4128 core = 43 nodes on Lise). In all cases, the number of *steps per run* is chosen in such a way that the total wall-clock time of each run is close to 12h. All other values are completely determined by the goals described in the scientific section and by the size of the problem.
We briefly describe the different types of runs:

- Type *cnfg (prod).* These runs are used to generate gauge configurations. At each *step* (as used in the table) one gauge configuration is generated and saved on disk. Several runs of this type are typically sequential.
- Type *meson (post).* These runs are used to calculate meson correlators on gauge configurations generated with the corresponding production runs. Only thermalized configurations are used in these runs. At each *step* (as used in the table) one gauge configuration is processed and a set of meson correlators is calculated and saved on disk. Several runs of this type can be run concurrently. Notice that in several cases (expecially during tuning) meson correlators with different sets of parameters need to be calculated on the same gauge configuration.
- Type *mass-rw (post).* These runs are used to calculate mass reweighting factors on gauge configurations generated with the corresponding production runs. Only thermalized configurations are used in these runs. At each *step* (as used in the table) one gauge configuration is processed and a set of mass reweighting factors is calculated and saved on disk. Several runs of this type can be run concurrently. Notice that in several cases (expecially during tuning) mass reweighting factors with different sets of parameters need to be calculated on the same gauge configuration.
- Type *rw-rat (post).* These runs are used to calculate the reweighting factor used to correct for the rational approximation of the fermionic determinant, on gauge configurations generated with the corresponding production runs. Only thermalized configurations at the tuned values of the parameters are used in these runs. At each *step* (as used in the table) one gauge configuration is processed and the reweighting factor is calculated and saved on disk. Several runs of this type can be run concurrently.
- Type *sign (post).* These runs are used to calculate the sign of the fermion pfaffian on gauge configurations generated with the corresponding production runs. Only thermalized configurations at the

tuned values of the parameters are used in these runs. At each *step* (as used in the table) one gauge configuration is processed and the sign of the pfaffian is calculated and saved on disk. Several runs of this type can be run concurrently.

- Type *baryon (post).* These runs are used to calculate the baryon correlators on gauge configurations generated with the corresponding production runs. Only thermalized configurations at the tuned values of the parameters are used in these runs. At each *step* (as used in the table) one gauge configuration is processed and the baryon correlators are calculated and saved on disk. Several runs of this type can be run concurrently.

Every gauge configuration generated with the proposed project is saved on disk. The size of the gauge configuration depends only on the lattice size: each 64×32^3 gauge configuration takes about 1.19GiB, and each 96×48^3 gauge configuration takes about 6.01GiB. Any other file generated in this project is negligible with respect to the gauge configurations. We are already using about 15TiB on Lise, and we will generate additional 18TiB. The disk quota on temporary storage that we have at the moment is sufficient for these needs.

Table 7: *The following CPU-system resources are requested*

Work-package	Type of run	Problem size	# runs	# steps/ run	Wall time/ step [hours]	# cores/ run	Total [core-h]
WP1	cnfg (prod)	64×32^3	170	30	0.36	4128	7.58M
	mesons (post)	64×32^3	80	400	0.03	2112	2.03M
	rw-rat (post)	64×32^3	12	170	0.07	2112	0.31M
	sign (post)	64×32^3	13	160	0.07	4128	0.61M
	mass-rw (post)	64×32^3	61	133	0.09	4128	3.02M
	baryons (post)	64×32^3	25	80	0.14	4128	1.16M
WP2	cnfg (prod)	96×48^3	80	5	2.20	4128	3.64M
	mesons (post)	96×48^3	4	100	.09	3072	0.11M
	rw-rat (post)	96×48^3	8	50	.21	3072	0.26M
	sign (post)	96×48^3	16	25	.42	3072	0.52M
WP3	cnfg (prod)	96×48^3	300	5	2.20	4128	13.63M
	mesons (post)	96×48^3	10	100	.09	3072	0.28M
	rw-rat (post)	96×48^3	20	50	.21	3072	0.65M
	sign (post)	96×48^3	40	25	.42	3072	1.29M
WP4	mesons (post)	64×32^3	135	400	0.03	2112	3.42M
	mass-rw (post)	64×32^3	136	133	0.09	4128	6.72M
TOTAL							45.23M

2.4.1 Usage schedule

The resources are distributed by taking into account the dependences among tasks within the same work package, and among different work packages. An even distribution across the year has been preferred.

Core-h usage schedule	2022 Q4	2023 Q1	2023 Q2	2023 Q3
WP1 Gauge ensemble $\alpha = 0.02$	3.19M	3.19M	6.56M	1.77M
WP2 Large volume $\alpha = 0.05$	4.16M	0.37M		
WP3 Large volume at $\alpha = 1/137$	3.96M	3.96M	3.96M	3.97M
WP4 Splitting		3.79M	0.79M	5.56M
Total core-h demand per quarter	11.31M	11.31M	11.31M	11.30M