2023 INCITE Proposal Submission
Proposal

Title: QCD under extreme conditions
Principal Investigator: Volodymyr Vovchenko
Organization: University of Houston
Date/Time Generated: 6/17/2022 4:58:46 AM

Section 1: PI and Co-PI Information

Question #1

Principal Investigator: *The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

Principal Investigator

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Question #2

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Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Physics: Nuclear Physics

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

The goal of our project is to achieve a detailed understanding of the creation of visible matter microseconds after the big bang. We infer the properties of strongly interacting matter under extreme conditions from numerical simulations of the theory of strong interactions applied to experimental heavy ion measurements and compact stars, as well as axionic dark matter.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an Early Career Track in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

Who Can Apply*: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*
- *What review criteria will be used for the Early Career Track?*
  - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

Yes

If 'yes', what year was your PhD? If 'no' enter N/A

2018

If 'yes', how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

The proposal is crucial for my research plan, which is centered around investigating the properties of strongly interacting matter under extreme conditions. In particular, the allocation award will offer a prospect of making fundamental discoveries and research that combines various aspects of nuclear physics as well as numerical quantum field theory. The opportunity to lead a large team of established scientists will greatly enhance my leadership skills and will also allow me to establish fruitful new collaborations.

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

675500

Storage (TB)

100

Off-Line Storage (TB)

500

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Node Hours

675000

Storage (TB)

100

Off-Line Storage (TB)

1000

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Node Hours

675000

Storage (TB)

100

Off-Line Storage (TB)

1500

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel X^e) Resource Request – 2023

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Funding Source

U.S. Department of Energy

Grant Number

DE-FG02-07ER41521

Funding Source

National Science Foundation

Grant Number

PHY1654219

Funding Source

U.S. Department of Energy

Grant Number

DE-AC52-06NA25396

Funding Source

U.S. Department of Energy

Grant Number

SciDAC project NUCLEI

Funding Source

Laboratory Directed Research and Development program of Los Alamos National Laboratory

Grant Number

20220541ECR

Funding Source

Hungarian National Research, Development and Innovation Office (NKFIH)

Grant Number

KKP126769

Funding Source

Federal Ministry of Education and Research

Grant Number

05P21PXFCA

Funding Source

Deutsche Forschungsgemeinschaft

Grant Number

496127839

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Resource

HAWK, HLRS, Stuttgart, Germany

Allocation Agency

Gauss Centre of Supercomputing, Germany

Allocation

380 million core hours

Allocation Year

2022

Resource

Juwels/Booster, Juelich, Germany

Allocation Agency

Gauss Centre of Supercomputing, Germany

Allocation

167 000 node hours

Allocation Year

2022

Section 5: Project Narrative and Supplemental Materials

Question #1

Using the templates provided here, please follow the [INCITE Proposal Preparation Instructions]to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project

Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

DOE-INCITE-2023.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: QCD under extreme conditions

PI and Co-PI(s): Volodymyr Vovchenko (University of Houston), Rene Bellwied (University of Houston), Szabolcs Borsanyi (University of Wuppertal), Sandor Katz (University of Budapest), Zoltan Fodor (Penn State University), Claudia Ratti (University of Houston), Ingo Tews (Los Alamos National Laboratory)

Applying Institution/Organization: University of Houston, Texas (USA)

Number of Processor Hours Requested: 675500, 675000, 675000 Node Hours on Frontier in yrs 1, 2, 3

Amount of Storage Requested: 100, 100, 100 TB online, 500, 1000, 1500 TB offline in years 1, 2, 3

Executive Summary:
The goal of our project is to significantly advance our knowledge of the phase diagram and equation of state of strong interactions, by means of first principle simulations. We plan to achieve this goal through five major sets of observables.

Ordinary hadronic matter undergoes a transition to a deconfined phase, the Quark-Gluon Plasma (QGP), at extremely high temperature or density. In the Universe, the reverse transition took place a few microseconds after the Big Bang: the basic building blocks of nature, the hadrons, were formed at this time. The RHIC program, which ran in 2019-2021 explores the finite-density region of the phase diagram in which the balance between matter and anti-matter is broken, the main goal being the search for a critical point in the QCD phase diagram. Recent astrophysical observations of neutron stars and their mergers extend the range of density to larger values. The LHC Heavy Ion program, after its DOE-funded detector upgrade, will enable us to improve the precision in the data and thus search for new phenomena such as experimental evidence for the chiral phase transition. The experiments searching for axions, with DOE support, need theoretical guidance on the mass range for this elusive particle. This is currently affected by large uncertainty. All these programs need the specific theoretical and computational effort provided by this proposal, in order to interpret the data and reach unambiguous conclusions.

The starting point of the project is the simulation of relevant quantities for heavy-ion data: net-electric charge fluctuations, yielding information on the chemical freeze-out, and the equation of state (EoS) of QCD at finite density. Results will be obtained in an unexplored setting, namely finite baryonic and strangeness density. There is a great need for this EoS in the community, as the hydrodynamic simulations that describe the evolution of the fireball reveal large local fluctuations of the strangeness density around its vanishing equilibrium value. Our realistic EoS will be used as an input in future hydrodynamic simulations, to be compared to the experimental data from RHIC and the LHC in search e.g. of critical phenomena. Towards the end of the project, we will extend the EoS to lower temperature and higher density, in an isospin-asymmetric scenario, to reach the neutron star merger regime from first principles for the first time. We will also set more stringent constraints on the location of the critical point. At the same time, we will calculate the sub-leading terms to the axion potential, to reduce the theoretical uncertainty on its mass.

As part of our past INCITE projects, we already made fundamental contributions to the field by extracting, from first principles, the temperature at which hadrons are formed at zero and small density, and by simulating several observables, which can be directly compared to the experimental measurements from the LHC and the higher energy RHIC collisions. In this proposal we push our investigations to specific scenarios, required by the heavy-ion community to explain their forthcoming data. We also connect with the astrophysical community for the first time. A three-year budget of **2,025,500** Node Hours is requested on **Frontier**. The project is ideally complemented by an online storage of **100,100,100 TB** and an offline one of **500,1000,1500 TB** in years 1, 2, 3. The project is very timely since the high-density program at RHIC ran in 2019-2021 and high luminosity runs with improved detector capabilities at the LHC started again in 2022. Besides, LIGO will start its fourth observation run in December 2022, possibly detecting the ringdown signals from neutron star mergers for the first time.

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

1.1 Motivation

The purpose of this project is to significantly advance our knowledge of the phase diagram and equation of state of strong interactions, by means of first principle simulations. We will achieve this through five efforts:

1. We calculate the axion potential and study axion production beyond the misalignment scenario.
2. We compute electric charge/strangeness fluctuations as a thermometer for LHC heavy ion collisions.
3. We provide the QCD equation of state in the energy range of the RHIC beam energy scan.
4. We simulate at real chemical potentials to explore the dense regions of the QCD phase diagram, constraining the location of the critical end point (CEP).
5. We extend the range of the low temperature simulations in density and generalize to an isospin asymmetric scenario to reach the neutron star merger regime from first principles for the first time.

The purpose of heavy-ion collisions (HICs) is to test QCD under extreme conditions. It is expected that a transition occurred, right after the Big Bang, in which matter converted from a state of quarks and gluons to color-neutral particles, the hadrons, which populate the Universe today. The deconfined phase of QCD can be created in relativistic HICs currently taking place at the LHC (CERN) and RHIC (BNL), soon to be followed by FAIR (GSI). On the theory side, simulations on a lattice are the main tool to investigate QCD non-perturbatively. It was shown that the transition from hadrons to quarks at zero chemical potential μ_B is a broad cross-over [1]. The main open question in our field is whether this transition becomes first order at large μ_B. This might finally be answered through the Second Beam Energy Scan (BESII) at RHIC, with the help of theoretical calculations. BESII focuses on low collision energies at increased luminosity, enabling us to reach higher precision and turn trends into final answers. The LHC HICs program, after its DOE-funded detector upgrade, will achieve more precise data and search for new phenomena.

The exploration of the QCD phase diagram has gained a crucial component: astrophysical observations of compact stellar objects and their mergers. The first observation of gravitational waves and electromagnetic signals from a neutron-star merger in 2017, GW170817, by the LIGO and Virgo Collaborations (LVC) and telescopes all over the world, has opened a new field of research. Gravitational-wave data from inspiralling neutron-star mergers has already been used to study the QCD phase diagram [2–5] but uncertainties remain sizable at the moment. This might change in 2022, when LIGO will resume operations after its upgrade. Neutron-star merger simulations showed that the temperature achieved in these events can be as large as 80 MeV, suggesting that they generate conditions similar to the ones produced in low-energy HICs [3, 6–8]. Besides, densities reach the highest values in the Cosmos. Current gravitational-wave observations are only sensitive to the inspiral phase of mergers, but future next-generation detectors will be able to detect signals from the remnants of the mergers, probing matter under the most extreme conditions realized in Nature.

There is general consensus that the system formed in HICs is close to thermal equilibrium. This endorses lattice QCD as the tool to study the underlying thermodynamics [9]. Thus, a prerequisite for a successful experimental program is the knowledge of the EoS at finite μ_B. The description of the hydrodynamical evolution of the quark gluon plasma has been a key ingredient in the quantitative study of this phase (see Fig. 1). Our project aims at providing theoretical support for HICs by calculating the EoS. First, we improve on the precision of the EoS at $\mu_B = 0$, and extend this not only to non-vanishing μ_B, but also μ_S. Our earlier work already satisfies the condition $\langle n_S \rangle = 0$ [10]. However, even if strangeness is globally conserved, there can be local violations which need to be taken into account for a realistic description.

We also aim at extracting the EoS for QCD at unprecedentedly high densities and low temperatures, at chemical potentials corresponding to a fraction of protons-per-baryon $\langle n_p \rangle = (0.05 \div 0.1)\langle n_B \rangle$. We will thus reach the neutron star merger regime for the first time, building a bridge between HICs and astrophysics.

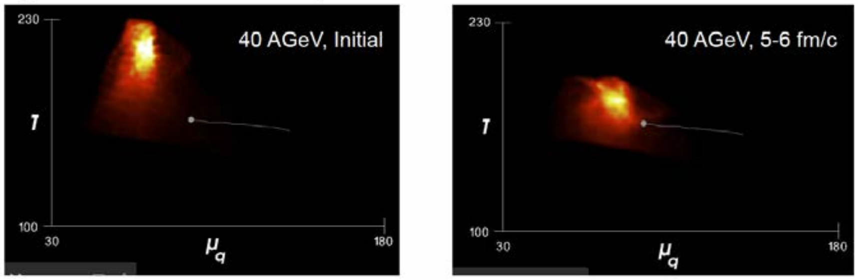

Figure 1. Distribution of the produced plasma on the QCD phase diagram in an event simulation. Each fluid cell is associated with a temperature and chemical potential, which is plotted here at an initial and later time. Knowledge of the EoS is essential in the complete $T - \mu_q$ range [11].

This project will help us to answer the following questions

- What is the QCD prediction for the self-coupling of axions?
- Can we provide an EoS from first principles, that covers the BESII range and goes beyond $\langle n_s \rangle = 0$?
- Does local strangeness neutrality violation have an effect on the measured observables in HICs?
- What realistic constraints can we set from first principles on the location of the critical point?
- Can we reach the neutron star merger regime in first principle, lattice QCD simulations?

This proposal represents the fifth installment of our long-term INCITE effort to quantitatively describe the physics of hot and dense QCD. In 2014, we focused on the flavor-dependent aspects of freeze-out [12, 13]. In 2015, we pursued a campaign to map thermodynamics with imaginary chemical potentials. In addition, we published our results for the Euclidean correlators of the stress tensor in pure gauge theory at finite T, and used them to estimate the shear viscosity of the gluon plasma [14]. We also calculated diagonal and non-diagonal fluctuations of conserved charges up to sixth-order, for a system of 2+1+1 dynamical quarks. We then studied the ratio of the cumulants of the net-baryon number distribution as functions of T and μ_B, and discussed their qualitative comparison with the RHIC experimental results [15]. In our 2020 INCITE project, we calculated the fugacity expansion coefficients of the Grand Canonical free energy, receiving contributions from processes like kaon-kaon or baryon-baryon scattering [16]. Finally, we laid the ground for the equation of state beyond strangeness neutrality by first introducing a new expansion scheme at $\mu_S = \mu_Q = 0$ [17] and then generalizing it to zero or small strangeness densities [10].

1.2 State of the art and relevant efforts from other lattice QCD collaborations

Simulations at $\mu_B = 0$ describe the physics of our Universe at an age of a few microseconds. Features of the QCD matter at these temperatures might have an observable impact on our current Universe [18], through the axion contribution to dark matter. Axions are also the most attractive solution to the strong CP problem.

Experiments scan various narrow mass ranges to find this hypothetical particle. Fig. 2 shows the current situation of exclusion regions on the axion mass vs normalized coupling plane [19]. The blue dots are theoretical predictions with their uncertainties. The largest mass range (preferred by the post-inflation scenario) is studied by the Haystac experiment. It consists of needle-like exclusion regions, reflecting the narrow range an experiment can search at once. This experimentally unavoidable condition is unfortunately in strong contrast with the large theoretical errors. The goal of subproject 1 is to reduce these uncertainties.

This task will be carried out through a multi-year complex approach. (a) Our group obtained a lower bound on the QCD axion mass by calculating the leading term of the axion potential, through the topological susceptibility of QCD at high temperatures [20]. The limit comes from the observed abundance of dark matter in the Universe. In the first year we will determine the subleading terms to the axion potential at cosmologically high temperatures (in later years we will determine contributions beyond the misalignment

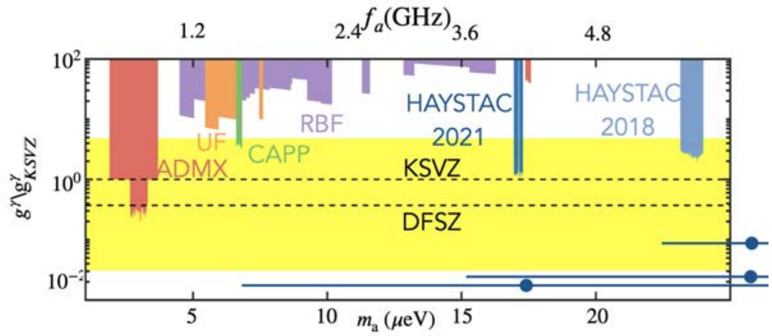

Figure 2. Summary of the present-day experimental efforts to discover the axion particle.

mechanism). (b) We are collaborating with Reina Maruyama (Yale University, member of the Haystac Collaboration and the Rydberg-Atom-Cavity Axion Search). She is also a member of this CPU-time application. This collaboration will help the experimental side to get first-hand information on our most recent investigations. At the same time we can adjust our strategy to the experimental suggestions, thus facilitating the axion search. Higher order terms in the potential demand large statistics. In particular, the kurtosis of the distribution of the topological charge has to be computed. This is possible with high statistics simulations at $\mu_B = 0$ and a subsequent evaluation of the quark eigenstates (SP1).

The EoS of QCD at $\mu_B = 0$ has been known from first principles to a few percent for a few years: in 2014 the HotQCD collaboration confirmed [21] the continuum results for thermodynamic quantities as functions of the temperature previously obtained by our collaboration [22, 23]. Both results are for a system of 2+1 flavors with physical masses in the continuum limit. Extracting the EoS (and other properties) of QCD at finite μ_B from regular Monte Carlo simulations is a difficult undertaking due to the fermion sign problem.

Over the last few years, several indirect methods have been proposed to study QCD matter at small μ_B. A conceptually straightforward method is Taylor expansion, where high statistics simulations at $\mu_B = 0$ are used to extract μ_B-derivatives [24–26]. An alternative extrapolation method uses analytic continuation from imaginary μ_B [15, 27–32]. Reweighting of the configurations to finite μ_B was often discussed in the literature [33–36], in combination with density of state methods [37, 38] or canonical ensembles [39–41]. A very promising simulation strategy is emerging, based on stochastic quantization [42]. This defines a complex Langevin equation [43] that was improved and applied to lattice QCD in the past decade [44–48].

We will apply the most recent developments of these methods to finite-μ_B QCD. A full study of the phase diagram can only be pursued using different techniques, each one in the region where it is more suitable. Overlapping regions allow for cross-checks, which are crucial in the case of emerging high-μ_B simulations.

In our past INCITE allocations, we made precise statements on the μ_B dependence of the EoS. In fact, the dominant error on the energy density at the top and intermediate RHIC energies comes not from the extrapolation to finite μ_B, but from the statistical uncertainty of the $\mu_B = 0$ EoS. We will update this “baseline” equation of state in SP3. Our new $\mu_B = 0$ simulations will, thus, improve the precision of the QCD EoS used for heavy ion phenomenology. We use the analytical continuation technique also at imaginary μ_S, thus improving our knowledge on the EoS at non-vanishing strangeness. We previously simulated at imaginary strangeness to isolate the contribution of strange resonances to the full pressure [49]. Evaluating also the fluctuations of electric charge and baryon number, a complete prediction for the statistics of conserved charges will emerge, opening new ways to extract freeze-out physics (SP2).

A recently introduced [50] and tested [51] reweighting scheme shifts the starting point of the extrapolation to an ensemble much closer to the finite-μ_B system than those used at $\mu_B = 0$ in the original works. This significantly reduces the overlap problem and mitigates the sign problem. In Ref. [51] we showed that the strength of the sign problem is predictable. This allows us to set up a realistic compute budget at finite μ_B.

With INCITE support, we can cope with the remaining sign problem, that prohibited such simulations for a long time. Depending on simulation volume, the full BESII range can be studied this way (SP4).

Direct methods, such as the complex Langevin equation, promise access to high densities at a lower cost. Gauge cooling [52] allowed the generalization to dynamical QCD [45], and the EoS was addressed [53]. Recently, a more effective dynamical stabilization method was suggested [47] that enabled low-T, high μ_B simulations [48], pointing to the maturity of this technique to be used at physical conditions in near future. With INCITE support, we can benchmark this method with the optimized reweighting and explore the region relevant for neutron star mergers in the QCD phase diagram that could not be reached before (SP5).

Our 2015 INCITE project focused on thermodynamics with imaginary chemical potentials. A key point was to maintain strangeness neutrality in each simulation. In Ref. [54] we calculated the curvature of the QCD transition line through analytical continuation, recently improved in Ref. [55]. The resulting phase diagram is shown in Fig. 3 (left). We concluded that there is no sign of criticality for $\mu_B < 300$ MeV, and we obtained the most precise values for the transition temperature, curvature and fourth-order coefficient in the literature. The only other result for the latter, with larger uncertainty, is from [56].

The same ensembles were re-analyzed for the EoS: we published the analytical continuation of the pressure and entropy in Ref. [57]. This was the first time that a continuum extrapolation was performed for the μ_B^4 and μ_B^6 orders. This would not have been possible without the INCITE allocation. Our continuum results were later followed by results at finite lattice spacing from the BNL-Bielefeld group [25]. These studies did not yet cover the whole BESII range for two reasons: i) the precision on the μ_B^6 order was not enough to extrapolate beyond $\mu_B/T > 2$, and ii) neglecting higher order terms introduces thermodynamic instabilities. Thus, in Ref. [17] we moved beyond the Taylor ansatz, as part of our 2020 INCITE allocation. Our new scheme allowed us to improve both issues: we were able to reach $\mu_B \leq 3.5T$, using just a NLO expansion in $(\mu_B/T)^2$, with a monotonic baryonic density for all values of μ_B (see Fig. 3 (center)).

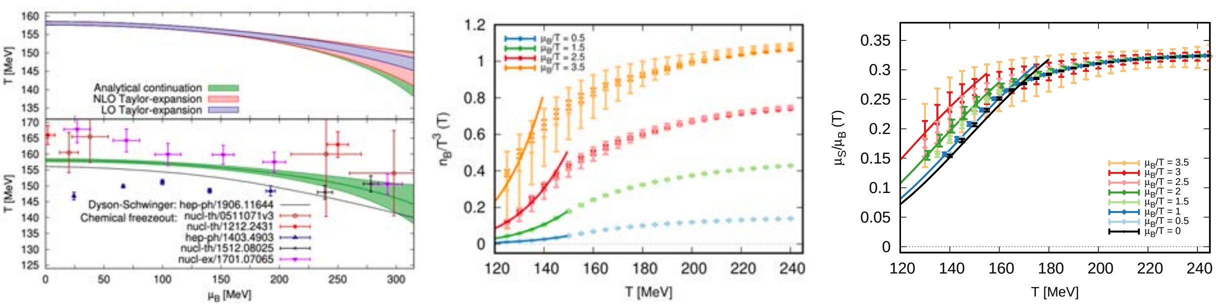

Figure 3. Left: Phase diagram from imaginary μ_B [55]. Center: baryon density vs. temperature at various μ_B/T [17]. Right: μ_S/μ_B ratio to fulfill the strangeness neutrality condition [10].

Together with our $\mu_B = 0$ EoS from 2013 [23] the result in Fig. 3 (center) gives all bulk thermodynamic variables at $\mu_S = 0$. To match the experimental setting, where the strangeness density n_S vanishes on average, we extended these simulations with multiple ensembles at various triplets of T and imaginary μ_B and μ_S. These were tuned such that $n_S = 0$ (the phase diagram in Fig. 3 (left) used such simulations too). In Fig. 3 (right) we show the strangeness neutral μ_S/μ_B ratio, extrapolated from imaginary parameters.

While strangeness is globally conserved in heavy-ion collisions, the values of μ_S in each fluid cell can fluctuate away from those yielding $\langle n_S \rangle = 0$. Small deviations can be accounted for by extrapolating the strangeness susceptibility. To address larger deviations, a full map in the (μ_B, μ_S) plane is required. We have already undertaken this as part of our 2020 INCITE project, where we calculated corrections to the HRG model [16]. Extending the temperature range, we will establish a first-principles EoS for $n_s \neq 0$ (SP3).

In SP2, we address one of the most difficult observables: χ_4^Q/χ_2^Q. In our 2016 INCITE we obtained its continuum value at one temperature, using the finest lattices ever used in QCD thermodynamics ($N_t = 32$).

This is needed because of the severe taste violation that affects χ_4^Q/χ_2^Q at finite lattice spacing. Here we will calculate it in a temperature range around the phase transition. We have the following two-fold objective:

a) define a model-independent thermometer for the chemical freeze-out. The most generic thermometer, available both at RHIC and LHC, is the ratio of cumulants of charge fluctuations, $\kappa\sigma^2 \sim \chi_4^Q/\chi_2^Q$, which is defined at $\mu_B = 0$ and $\mu_B \neq 0$. It is also sensitive to pion interactions and will help the modeling of pion condensation in the early Universe at large lepton asymmetries [58].
b) obtain the baryon number-electric charge correlator with the same simulation effort. This quantity is sensitive to the hadronic interactions, e.g. it was shown that the thermal effects of the pion-nucleon scattering improve the agreement between the thermal fits and the ALICE yields [59, 60]. We will evaluate the thermodynamic observables, so that lattice data can be used to constrain the scattering effects.

In SP4 and 5 we build on the work of our team members and extend the range of accessible densities. Ref. [51] demonstrated that, with a subtle improvement in the reweighting approach, a μ_B ~380 MeV could be reached at $T = 140$ MeV with a modest effort. Chiral condensate and n_B/μ_B were computed with reweighted simulations and analytical continuation (Fig. 4). The simulation strategy consists of two major steps: - simulations are performed where the fluctuating sign of the quark contribution is removed; - the sign is added in a second step via reweighting. Thus, μ_B is taken into account in both steps. This is unlike reweighting from $\mu_B = 0$, which would be hit by a severe overlap probem in addition to the sign problem.

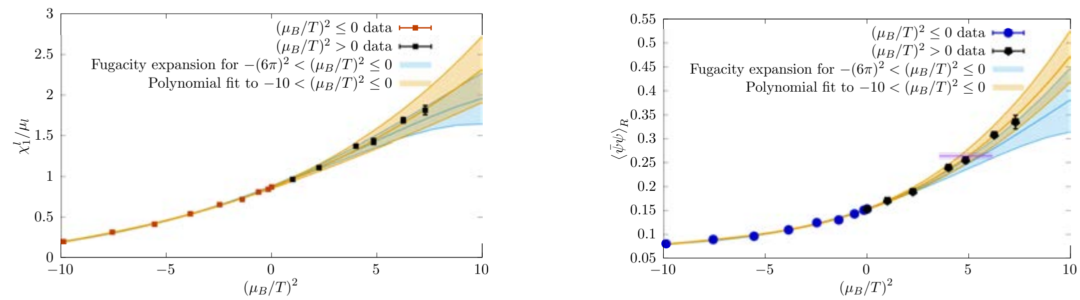

Figure 4. Normalized baryon density (left) and chiral condensate (right) as functions of μ_B^2. The bands are the result of two extrapolations from $\mu_B^2 \leq 0$. The data at $\mu_B^2 > 0$ are direct results at finite μ_B.

The use of the complex Langevin equation (CLE) in SP5 has the potential to save a significant amount of machine time, due to its favorable scaling with volume. Members of our team made significant advances in the field (see e.g. [45]), including calculating the EoS at real $\mu_B > 0$ (with unphysical pion masses) [53].

We are in the position to make a large density scan and cross-check the results of the CLE with optimized reweighting. If both approaches agree within error, we can use the cheaper method further on. Should the comparison reveal some weakness in the dynamical stabilization of CLE, we will continue with the more expensive reweighting method. In the latter case, continuum extrapolation will be postponed to future.

1.3 Relevance to the DOE mission

The proposed activities align with several components of the mission of INCITE and the US DOE:

- Better axion mass estimates will increase the chance to discover it. Partners affiliated with DOE-funded axion search experiments will be given priority access to our data.
- A first principles equation of state is calculated for large parts of the QCD phase diagram, which is crucial for the description of matter created in HICs at RHIC and at the LHC, but also for nuclear astrophysics. Its determination would not be possible without this INCITE allocation.
- Mapping the phase diagram and searching for the critical point are the main goals of RHIC's BESII.
- The students and postdocs involved in the project will learn to run simulations on High Performance Computers (HPC). Co-PIs Ratti and Bellwied will train minority undergraduate students through the DoE-funded NuSTEAM program. They will be exposed to concepts and results from this proposal.

2 RESEARCH OBJECTIVES AND MILESTONES

This project will improve our knowledge of the QCD phase diagram using lattice simulations. In particular,

A We calculate first correction to the dilute instanton gas approximation and calculate the corresponding next-order term in the axion potential at the temperature of axion decoupling (SP1).

B We calculate net-electric charge fluctuations at chemical freeze-out, in particular the fourth cumulant of the electric charge as a function of the temperature in the continuum limit for the first time (SP2).

C We use our novel EoS expansion from Ref. [17] and our fugacity expansion from Ref. [16] to derive a generic one at $\langle n_B \rangle \neq 0$ and $\langle n_S \rangle \neq 0$ (SP3).

D We improve the precision of the $\mu_B = 0$ equation of state (SP3).

E We perform direct simulations at $\mu_B \neq 0$ to describe the chiral transition at physical masses (SP4).

F We use finite size scaling to set up exclusion ranges in μ_B for the critical end-point location (SP4).

G We use the complex Langevin equation to extend the μ_B range to neutron star mergers (SP5).

H We perform first simulations combining isospin and baryo-chemical potentials. (SP5)

2.1 Methodology for the five sub-projects

2.1.1 Axion potential

The axion field θ couples to QCD through the $\sim \theta F\tilde{F}$ term. The axion potential is given by the θ-dependent effective potential. The leading term (curvature of the potential) is given by the variance of $\int F\tilde{F}dx$. The latter is an integer for periodic boundary conditions and is the topological charge of the configuration. The axion mass is determined by the variance of the topological charge and of the pre-factor in the axion term.

Higher order terms in the potential demand large statistics. In particular, the kurtosis of the distribution of the topological charge determines the next-to-leading order term of the axion potential. This is possible with the INCITE resources via simulations at $\mu_B = 0$ and a subsequent evaluation of the quark eigenstates.

2.1.2 Phenomenology of the chemical freeze-out

The features of matter produced in heavy ion collisions can be studied at the chemical freeze-out, namely the "instant" of last inelastic scatterings. The detected statistical distributions of conserved charges are connected to the susceptibilities [61, 62]. Thus, by simulating a Grand Canonical ensemble on the lattice we can identify a temperature and various chemical potentials at which the measured statistics is realized.

Particularly interesting candidates for such a study are electric charge Q correlators, e.g. $\kappa\sigma^2$ where σ^2 is the variance and κ the kurtosis of the net-Q distribution. Previous lattice results are inconclusive on such observables, mainly because of the large discretization errors. We illustrate the slow convergence of the continuum limit in Fig. 5 (left). The taste breaking artifact makes pions and other light mesons fluctuate less, except on very fine lattices. In Ref. [12] we used up to $N_t = 32$ to facilitate a continuum extrapolation. While this would be enough for a successful simulation, it reduces the efficiency of the algorithm.

Here we follow a more elegant and cheaper solution by improving the action. We consider $N_t = 10$, 12, 16. In the right panel of Fig. 5 the taste breaking of our standard staggered action (4stout) and the new 4HEX one are shown. The 4HEX name refers to four levels of hyper-cubic exponential smearing that we proposed in Ref. [63]. It is designed to suppress the UV gauge fluctuations better than the same number of stout smearing steps. In addition, we use an over-improvement in the gauge sector to suppress dislocations [64]. Dislocations, or would-be instantons at or below the scale of the lattice spacing, enhance the undesired splitting of the eigenvalue spectrum of the staggered Dirac operator. This over-improvement increases the auto-correlation times, but this is out-weighed by the larger allowed lattice spacings.

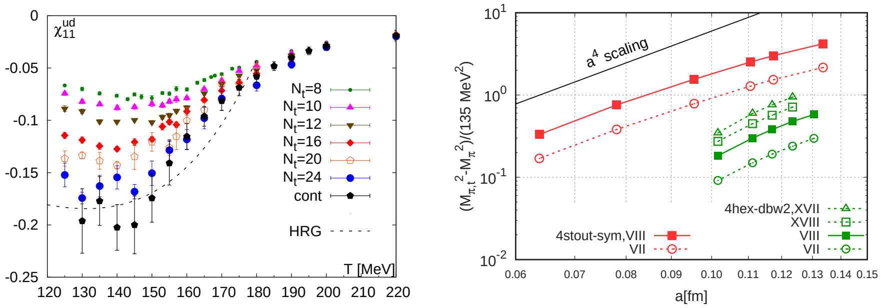

Figure 5. The large cut-off effects in the left panel (up-down correlator, $\chi_{11}^{ud}(T)$) can be understood from the spectrum of pion tastes. The right panel shows the multiplet of staggered pions as a function of lattice spacing, for the `4stout` and `4HEX` actions. The root-mean-square pion mass corresponds approximately to the operator VIII (solid line). At 150 MeV the lattice spacing range is 0.13 – 0.08 fm.

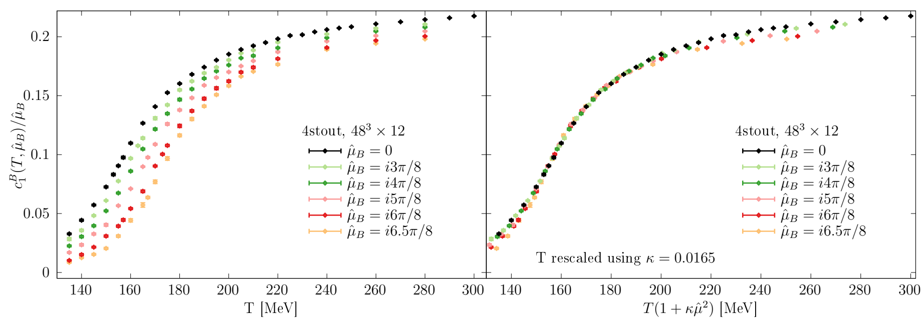

Figure 6. Normalized baryon density vs temperature at various imaginary μ_B values. In the right panel we rescaled the temperature by a factor corresponding to the shift in the transition temperature.

In this sub-project we work at $\mu_B = 0$ first. In the past we extended the range of results towards the μ_B found at RHIC, by employing imaginary values of μ_B. This extension is scheduled for the second year.

2.1.3 Equation of state for RHIC energies

Our priority is to improve the precision of the $\mu_B = 0$ EoS. To this end we double the precision on our $\mu_B = 0$ ensembles. We use the 4stout action and lattices with $N_t = 8, 10$ and 12 in the range $(130 < T < 300)$ MeV. For the subtraction of the zero-temperature divergences of the trace anomaly we generate large ($(6\text{ fm})^4$) configurations with the same bare parameters and evaluate the gauge action on the chiral condensate.

We calculate the EoS at finite μ_B by an analytical continuation from imaginary μ_B. Since this can be ambiguous, we devised a novel scheme that extrapolates in the temperature of constant physics [10, 17]. In 2022 we calculated the EoS under the constraint of $\langle n_S \rangle = 0$. In the simulation domain, μ_B was imaginary, and so was μ_S. Once extrapolated, both chemical potentials are real, yet $n_S \equiv 0$.

The leading order expansion implies a μ_B-independent $n_B/\hat{\mu}_B \equiv c_1^B/\hat{\mu}_B$, which is only a function of T. There is a sub-leading μ_B−dependence, clearly visible in the left panel of Fig. 6. This can almost entirely be accounted for by a temperature rescaling by the curvature parameter of the transition: $T^* = T(1 + \kappa_2 \hat{\mu}_B^2)$.

In Ref. [17], we worked out a novel expansion scheme for the EoS that exploits this behavior. Dropping the strangeness chemical potential for simplicity, we re-define the $\hat{\mu}_B$-expansion ($\hat{\mu}_B = \mu_B/T$) as

$$\frac{n_B(\hat{\mu}_B, T)}{\hat{\mu}_B} = \chi_2^B \left(T(1 + \kappa_2(T)\hat{\mu}_B^2 + \kappa_4(T)\hat{\mu}_B^4 + \ldots) \right) . \tag{1}$$

The expansion of the equation of state is realized by the temperature dependent coefficients $\kappa_2(T)$ and $\kappa_4(T)$. The Taylor coefficients $c_2^B(T)$ and $c_4^B(T)$ for the same quantity

$$\frac{n_B(\hat{\mu}_B, T)}{\hat{\mu}_B} = c_2^B(T) + \frac{\hat{\mu}_B^2}{6} c_4^B(T) + \frac{\hat{\mu}_B^4}{120} c_6^B(T) + \dots \quad (2)$$

can be easily related to the new parameters κ_2 and κ_4 as

$$c_4^B \;=\; 6\kappa_2 T \frac{dc_2^B}{dT} \;, \qquad c_6^B = 60T^2 \frac{d^2 c_2^B}{dT^2} \kappa_2^2 + 120T \frac{dc_2^B}{dT} \kappa_4 \;. \quad (3)$$

Once $\kappa_2(T)$ and $\kappa_4(T)$ were calculated, we used Eq. (1), thus avoiding the instabilities coming from the Taylor expansion in $\hat{\mu}_B$. This strategy turned out to be more feasible than simulating the highly noisy $\chi_B^6(T)$ (see [26] for the statistics requirement), while delivering improved results.

$\kappa_2(T)$ and $\kappa_4(T)$ were calculated for the $\langle n_S \rangle = 0$ case in the continuum limit in Ref. [10]. In this project we repeat this scheme for various strangeness values to map the entire EoS as a function of strangeness.

For this, we will have to enlarge the current set of imaginary chemical potentials. Following our strategy in Ref. [16] we simulate in a 3D mesh of T and imaginary μ_B, μ_S. For every T and μ_B we can set n_S in a broad range. We will then define an n_S/n_B-dependent $\kappa_2(T)$ and, thus, extrapolate the EoS at fixed n_S/n_B.

2.1.4 Constraints on the critical end-point

In Ref. [34] two of the co-PIs located the CEP from lattice simulations. The continuum limit was not reached ever since, because of the high costs due to the sign problem at increasing volume and resolution.

There have been several algorithmic improvements since Ref. [34]. The main ingredient, reweighting, is still the core of our method. Configurations are generated using a real action, while the quark contribution to the probability density of the gauge configurations is complex at real μ_B. However, how far the starting real action is from the complex target action plays a crucial role. Refs. [37, 65] use the isospin chemical potential parameter space, which is then reweighted to μ_B. To prevent pion condensation, the Density of States method was used, reducing the overlap problem significantly. Ref. [50] uses a variant of this method, where the intermediate real action is based on the magnitude of the real part of the quark determinant. The explicit calculation of the determinant drives the simulation cost higher, but it does not exceed the cost of calculating the reweighting factors. An investigation of the WB collaboration was conducted on $N_t = 6$ lattices to show the feasibility of the approach [51]. An extension to $N_t = 8$ in the QGP phase is in progress.

The order of the chiral transition at finite μ_B cannot be reliably determined without finite volume scaling. Yet, lattices of size $16^3 \times 8$, $20^3 \times 8$ and $24^3 \times 8$ are already feasible at $\mu_B/T = 1.5$. In the INCITE project, higher μ_B will be addressed, first with the reweighting method, then with the complex Langevin equation.

2.1.5 Towards the neutron star equation of state

QCD predicts the baryon, isospin and energy densities as functions of the Grand Canonical parameters: μ_B, μ_I and T. This prediction, however, is increasingly difficult at high μ_B from lattice simulations. The reason is that the sign problem becomes more severe with an exponential function of both the volume and μ_B. To estimate the strength of the sign problem, we consider one fluctuation of the phase of quark determinant

$$\langle \theta^2 \rangle = \frac{1}{9} \mu_B^2 L^3 T N_f^2 \left| \chi_{11}^{ud} \right| \,, \quad (4)$$

where L is the size of the simulation box, $N_f = 2$ for the two relevant flavors and χ_{11}^{ud} is the correlator already shown on the left panel of Fig. 5. The full analysis shows that this leading estimate is accurate [66]. The required statistics scales with $N \sim \langle e^{i\theta} \rangle^{-2}$, or $N \sim e^{\langle \theta^2 \rangle}$. With realistic parameters, this is still out of reach. At this point we should turn the already mentioned taste breaking to our advantage: the fact that pions fluctuate less on a coarse lattice leads to a weaker sign problem: $\chi_{11}^{ud} \approx -0.07$. A sufficiently small volume, e.g. $12^3 \times 8$, allows for an explorable range of $\mu_B < 540$ MeV if we collect 100 times the statistics that we would do at $\mu_B = 0$. A statistics of 10^5 configurations on such a small lattice is definitely feasible.

The introduction of the isospin chemical potential μ_I does not contribute to the sign problem. However, to simulate at finite μ_I an infrared regulator (λ) has to be introduced into the two-flavor Dirac operator, and later removed through a $\lambda \to 0$ limit, or a further reweighting step. In Ref. [51] we used a metropolis step to simulate at $\lambda = 0$ directly. To this end, we introduced an extra Metropolis step in the hybrid Monte Carlo algorithm where we calculated the quark determinant using dense linear algebra. This is an expensive computation, and we will limit this project to small lattices. In an exploratory run we obtain the EoS at high densities in a small volume to keep the sign problem under control. We obtain the pressure by integrating the density with respect to μ_B. Energy density and entropy are obtained as $T-$derivatives of the pressure.

We will scan the same μ_B range using the CLE with dynamical stabilization. The latter modifies the drift force to disfavor long-tailed distributions in the complex plane. Previously observed convergence to false solutions were linked to broad distributions of the dynamical variables. We will test this at large densities and low T. Depending on the success of these tests we will either pursue a continuum extrapolation in the third year, or stick to the reweighting method and increase the statistics within that framework.

2.2 Data sets and workflow

Preparatory work

Currently, we are completing a high-statistics large-volume run to determine the scale setting and renormalization parameters for the 4STOUT staggered action. With this action we can access temperatures up to 350 MeV at $N_t = 12$, including the renormalization of the trace anomaly. This large volume simulation is running at HLRS Stuttgart, Germany, and will complete by the end of 2022. The remaining renormalization runs are planned for the first year of this project.

In the past year we determined the line of constant physics for the 4HEX staggered action up to a lattice spacing of 0.072 fm. This means that we are ready to simulate with this new action for $T < 230$ MeV at $N_t = 12$ or up to $T < 170$ MeV at $N_t = 16$. An extension of this range to $T = 200$ MeV is in progress. This effort consists of simulating QCD near $T \approx 0$ and determining the pion and kaon decay constants as functions of the quark mass and gauge coupling. This action and its line of constant physics will be used in SP1 and SP2. The observables in these sub-projects are sensitive to lattice artefacts. For such simulations we use the 4HEX action that benefits from the stronger suppression of the taste breaking. In sub-projects where a broader T range is required, we use the 4STOUT action.

We have simulated fluctuations of conserved charges (SP2) on $N_t \leq 12$ lattices for temperatures relevant for chemical freeze-out ($T \leq 160$ MeV). Further analysis (e.g. scale setting dependence) is in progress.

We will further optimize the reweighting code and algorithm. We will publish (Q3/2023) an EoS using the reweighting approach of SP4 in the range $T \geq 145$ MeV, $\mu_B/T \leq 3$ at a finite lattice spacing ($N_t = 8$) in a modest volume. Thus, we demonstrate the maturity of this approach, and provide a phenomenologically relevant result at the same time. Experience with these simulations is crucial to the success of this project.

Year 2023

SP1 We generate ensembles on $64^3 \times 16$ lattices for $135 < T < 200$ MeV with a resolution of 5 MeV. This is a shared effort between SP1 and SP2. We generate 20.000 configurations/ensemble and determine the topological moments on this statistics.

SP2 The ensembles in SP1 will be analyzed for electric charge (and strangeness) fluctuations. We will be able to calculate final, continuum results on ratios of fluctuations involving electric charge, such as χ_4^Q/χ_2^Q as a function of T. These simulations are currently restricted to $\mu_B = 0$. An extension is planned for year 2.

SP3 We enhance the statistics of our $48^3 \times 12$ and $40^3 \times 10$ data sets (4STOUT action) so that an accurate result on the trace anomaly can be calculated. The gauge action and chiral condensate will be subtracted from the zero temperature simulations.

We will generate ensembles at imaginary μ_B and μ_S. In the first year we will simulate on $24^3 \times 8$ and $32^3 \times 10$ lattices in a 3D mesh of parameters at HLRS, Stuttgart. For a continuum limit, $36^3 \times 12$ lattices are also needed: these will be added in the second year. We plan for a mesh of 144 ensembles per temperature. At low temperature this has allowed us to extract the leading coefficients of the fugacity expansion. In fact, the thermodynamic potential is periodic in both Im μ_B and Im μ_S with a period of $2\pi T$. The fugacity expansion coefficients are equal to the Fourier coefficients in the 2D plane of Im μ_B and Im μ_S. Working in a large dimensional parameter space, autocorrelation times can be problematic. For this we found a solution in the use of parallel tempering [67–69]. We used this technique in our recent publication in the context of a first order phase transition [70]. This algorithm efficiently reduces the autocorrelation times allowing the use of relatively short Markov chains in a large parameter space. In this algorithm each of the 144 streams are running on a separate GPU card, exchanging the configuration (or related control information) at regular intervals (e.g. after every fifth hybrid Monte Carlo update). For this, a parallel architecture is required. Non-parallel versions of the algorithm also exist, but these have lower swap-acceptance rate than the version we use.

SP4. In the first year we make a broad scan in chemical potential and temperature with a modest lattice size to explore the QCD phase diagram at high density. Simulations require the calculation of the fermion determinant up to a sign factor. We can do this with Gaussian elimination. We determine the sign factor using the eigenvalues of the fermion matrix, which we calculate in a second step. These eigenvalues also reveal the quark density, the mass dependence of the fermion determinant gives the chiral condensate.

At the moment, we are performing a scan in T and μ_B on a $16^3 \times 8$ lattice in the range $\mu_B/T < 3$. In the first year of the INCITE project we plan to reach $\mu_B/T < 4$, and map the transition line. We will will make four more temperature scans in addition to those five performed in 2022. We will observe if the width of the transition is narrower, indicating criticality. This chemical potential range will be analyzed thoroughly with larger volumes in the final year.

SP5. Our first priority is to cut the simulation costs in presence of the sign problem. We will reproduce the results of SP4 at the lowest temperatures, with complex Langevin equation with dynamical stabilization. We perform further tuning of this novel scheme and determine its range of validity. In the first year we make deep scans for $\mu_B/T < 4$ at three temperatures, $T = 140$ MeV and below, and obtain the finite density equation of state.

Code Development We successfully ported our existing GPU codes from NVIDIA to AMD systems (the gauge force and the staggered Dirac operator account for 95% of the run-time). This was executed at a one-week porting workshop organized by AMD and Forschungszentrum Jülich. Our codes use the HIP framework. Most of the porting consisted in a trivial rewriting of the CUDA statements. The NVSHMEM backend could not be easily ported. Thus, we rely on MPI-based communication between GPUs or nodes. Our main effort for the remainder of 2022 is to port this part to ROCSHMEM or an analogous library.

Year 2024

We continue the calculation of the higher order terms of the axion potential beyond 200 MeV temperature.
We extend the fluctuation analysis of SP2 to imaginary μ_B.
We perform a multidimensional scan in μ_B, μ_S on a $36^3 \times 12$ lattice, to allow for a continuum extrapolation.
This completes our low μ_B equation of state computation.
We perform high statistics simulations using the cheapest method between reweighting and CLE.
We study the order of the chiral transition at the highest available μ_B.

Year 2025

The misalignment mechanism predicts the abundance of the axions today. However, the corrections to this mechanism can be calculated by solving the classical field theory equations of the axion fields. We plan to simulate this in the final year.

We use complex Langevin simulations to map the so-far unreachable parts of the QCD phase diagram, approaching the region relevant for neutron star mergers. Should the range accessible with the complex Langevin not reach these densities, we will use smaller lattices and continue with the reweighting strategy. Depending on the performance of these algorithms we attempt a finite size scaling near the pseudo-critical temperature at finite μ_B.

We foresee the following tasks and milestones during the first allocation year on Frontier:

1. (SP2) All $\mu_B = 0$ 4HEX simulations on $64^3 \times 16$ at $T \leq 160$ MeV are ready (Q1/2023)
2. (SP2) 4HEX simulations are analyzed for fluctuations (Q2/2023)
3. (SP3) Improved 4STOUT statistics at $\mu_B = 0$, $48^3 \times 12$ is complete (Q2/2023)
4. (SP4) Temperature scans $\mu_B/T < 3.5$ with reweighting completed (Q2/2023)
5. (SP5) First results using Complex Langevin equation near T_c (Q2/2023)
6. (SP3 4STOUT renormalization runs on $48^3 \times 64$ are complete (Q3/2023)
7. (SP1) All $\mu_B = 0$ 4HEX simulations on $64^3 \times 16$ at $T > 160$ MeV are ready and analyzed for topology (Q3/2023)
8. (SP4) Deep scan in μ_B with reweighting completed (Q3/2023)
9. (SP5) Complex Langevin equation simulated and validated up to $\mu_B/T < 3$ and $T \approx 100$ MeV (Q4/2023)
10. (SP4) Transition line from optimized reweighting (Q4/2023)

We will publish the following sequence of results over the project lifetime:

1. Electric charge fluctuations at $\mu_B = 0$ (Q2/2023)
2. Precision results on the $\mu_B = 0$ equation of state (Q3/2023)
3. Axion potential at non-zero temperature (Q4/2023)
4. Transition line on the $T - \mu_B$ diagram from direct simulations (Q4/2023)
5. Electric charge fluctuations extrapolated to RHIC energies (Q2/2024)
6. Continuum extrapolated equation of state at non-zero strangeness (Q3/2024)
7. First result on the high-density, low-T EoS, at finite lattice spacing, with $\mu_I = 0$ (Q4/2024)
8. Refined axion mass prediction from field theory simulations (Q3/2025)
9. Exclusion regions for the CEP at $T > 0$ (Q3/2025)
10. First result on the high-density, low-T EoS, at finite lattice spacing, with $\mu_I \neq 0$ (Q4/2025)

3 COMPUTATIONAL READINESS

3.1 Use of resources requested

The following table shows a summary of our node hour request on Frontier for the next three years:

	Q1/2023	Q2/2023	Q3/2023	Q4/2023	FULL YEAR	2024	2025
SP1			122849		122849	120000	200000
SP2	174283				174283	175000	0
SP3		55713	50500		106213	105000	0
SP4		25125		65750	90875	90000	200000
SP5		20833	39583	120833	181250	185000	275000
TOTAL	174283	101672	212933	186583	**675471**	675000	675000

In SP1, we generate and analyze configurations with the 4HEX action above T_c. We aim at a statistics of 20000 configurations, separated by 10 trajectories, so that higher (fourth) order moments can be calculated. The technical details are given in Ref. [20]. We extend that work by calculating the b_2 coefficient of the topological charge distribution. We will, thus, calculate the low end of the eigenvalue spectrum (Krylov-Shur algorithm) and the topological charge (gradient flow) [71] for each ensemble.

SP2 uses the same action as SP1, but at lower temperatures. Thus, both subprojects benefit from the small taste-breaking artifact of the 4HEX action, yielding near-continuum results on a $64^3 \times 16$ lattice. The coarser lattices ($48^3 \times 12$ and $40^3 \times 10$) have already been produced an analyzed. These runs confirmed that 20000 configurations will allow for less than 5% error on fourth order electric charge or strangeness fluctuations in the final continuum limit. The technical details for measurements are given in Ref. [12]

We summarize the budget of SP1 and SP2 in the table below:

Temperature [MeV]	Lattice	update [s] / stream [Summit node]	update [s] / stream	Measurement of one config, on one node [summit]	Measurement of one config, on one node	Number of parallel streams	job size with all streams together [nodes]	wall-clock [h] for the full statistics	Node hours
140	64x16	437	328	3439	2579	8	8	4158	33266
145	64x16	475	356	3738	2804	8	8	4520	36158
150	64x16	475	356.25	3738	2803.5	8	8	4520	36158
155	64x16	451	338	3551	2663	8	8	4294	34350
160	64x16	451	338	3551	2663	8	8	4294	34350
165	64x16	428	321	3364	2523	8	8	4068	32543
170	64x16	412	309	3100	2325	8	8	3846	30770
180	64x16	400	300	3052	2289	8	8	3756	30050
200	64x16	392	294	3000	2250	8	8	3686	29487
Total in SP1	T<=160 MeV								**122849**
Total in SP2	T>160 MeV								**174283**

In SP3 we calculate the equation of state at $\mu_B = 0$ with boosted statistics (×10 in comparison to Ref. [23]) using the 4stout action. To this end, we focus on the finest lattice in this study ($48^3 \times 12$) and generate configurations. The measurements will be done on the fly. Roughly the same amount of resources are necessary to calculate the renormalization (mostly on $48^3 \times 64$ lattices, except for finer lattices, some of which are ready by now).

Our approach to save idle CPU hours

Our GPU code offloads all relevant computations to the device, while the CPU cores are mostly idle. One needs only 8 cores to control the eight logical GPUs in a Frontier node. The remaining 48 cores are idle. In a compute time proposal like ours, 32 million core hours are wasted this way every year. We pledge to save these resources (or at least 70%) as follows: we organize the GPU runs in 64-node units. The GPU code communicates within one node, leaving the communication infrastructure available for a CPU job. Thus, running on 48 cores/node, a communicating job will allow to use all Frontier resources at once. This strategy was implemented successfully in our previous Summit runs. The CPU jobs will be simulations on $64^3 \times 96$ lattices, to calculate the renormalization constants for the finer lattice spacings in SP3. We list these runs below. They do not appear in the summary table, since they do not require additional resources.

beta	to renormalize T [MeV]	job size [nodes]	update [s]	statistics	wallclock [h]	core hours
3.8716	190	64	1800	5000	2500	7680000
3.8942	200	64	1800	5000	2500	7680000
3.9051	205	64	1800	5000	2500	7680000
Total						23040000

The following table shows the GPU runs:

	T>0, 48³x12 lattices																			
	110	120	126	130	135	140	143	147	152	155	160	165	170	177	190	200	205	212	240	260
beta	3.6438	3.6790	3.7000	3.7115	3.7270	3.7420	3.7500	3.7622	3.7750	3.7844	3.7978	3.8108	3.8236	3.8400	3.8716	3.8942	3.9051	3.9200	3.9759	4.0126
update [s]	114.0	115.1	116.3	117.4	119.6	121.8	124.0	124.0	124.0	116.9	117.4	110.7	95.2	80.8	76.4	67.5	69.8	68.6	65.3	60.9
job size [nodes]	4																			
total # updates	200000																			
Costs T>0 [node hours]	3167.7	3198.4	3229.2	3259.9	3321.4	3382.9	3444.4	3444.4	3444.4	3247.0	3259.9	3075.4	2644.8	2245.0	2122.0	1876.0	1937.5	1906.7	1814.5	1691.5
Renormalization	48³x64													64³x96				80³x96		96³x128
total # updates	5000														5000					
update [s]	303.0													ready	1800	1800	1800	ready	running	ready
Costs, renorm. [node hours]	4208.3	4208.3	4208.3	4208.3	4208.3	4208.3	ready	4208.3	4208.3	4208.3	4208.3	4208.3	4208.3	ready	CPU	CPU	CPU	ready	0.0	ready
Total T>0			55713.3																	
Total renormalization			50500.0																	

In SP4 we explore finite densities by simulating phase-quenched ensembles which are, in turn, reweighted to use the full complex fermion determinant. We choose $\mu_S = 0$ in this case. Our code uses MAGMA library, which worked perfectly on Nvidia GPUs. In the first two years we fix the lattice size to $16^3 \times 8$. This allows the exploration of $\mu_B/T<4$. The runs with chemical potentials $\mu_B/T<3$ will complete in 2022. From these ongoing runs, we derived an empirical formula for the strength of the sign problem. Thus, we were able to get a realistic estimate of the statistics needed to reach these previously unfeasible baryon densities.

muB/T	Sign problem <cos theta>	# configurations	Update [s] (one MI250x)	Measurements [s] (one MI250x)	# temperatures in the scan	cost [node hour]
3	0.2089	22000	25	500	6	8250
3.25	0.1490	45000	25	500	6	16875
3.5	0.1012	97000	25	500	6	36375
3.75	0.0651	235000	25	500	2	29375
Total						90875

In SP5 we solve the complex Langevin equation with small steps ($\epsilon \sim 10^{-4}$) and control its stability using i) an adaptive step size update algorithm, ii) gauge cooling and iii) dynamical stabilization. The latter changes the underlying theory in the ultraviolet, but this will not impact the continuum extrapolation.
We perform three deep scans for $\mu_B/T<4$ near T_c, below T_c and deep in the hadronic phase, close to the temperatures of neutron star mergers. We will calculate the baryon density as a function of μ_B and, at the same time, we will test and optimize the method, and compare its results to the reweighting method in SP4.

mu scan at	# chemical potentials	statistics (range in tau)	step size in tau	update [s] on 1 logical GPU	cost [node hours]
T=140 MeV	12	1000	0.0003	15	20833
T=120 MeV	12	1000	0.0002	19	39583
T=100 MeV	12	1000	0.0001	29	120833
Total					181250

These subprojects add up for the first year to **675.500 Frontier node hours.**
Year 2024 and 2025:
SP1: We proceed to high T to calculate the axion potential. In 2025 we supplement our work with numerical field theoretical simulations, to study axion production beyond the misalignment mechanism.
SP2: We repeat the analysis of electric charge fluctuations at two imaginary chemical potential values, with half of the μ_B=0 statistics. The costs match those of year 1. As a result, we will be able to extrapolate to μ_B>0.
SP3: We do a scan in T, μ_B and μ_S and extrapolate the EoS for arbitrary strangeness, in RHIC BESII range.
SP4: We extend our CEP search beyond $\mu_B/T \approx 4$. Depending on the success of the Complex Langevin simulations we will use that or continue with the more solid but also more expensive reweighting approach. For the final year a finite size scaling is planned ($20^3 \times 8$ and $24^3 \times 8$ lattices).
SP5 We reduce the temperature and continue the scans towards high densities. Depending on the cost at realistic temperatures, and the performance of the Complex Langevin equation in years 1 and 2, we will

attempt a continuum extrapolation in the final year. In year 3, we will also perform our finite μ_I and μ_B run.

3.2 Computational approach

3.2.1 Algorithms

Lattice QCD works on a discretization of the four dimensional Euclidean space-time. Gauge fields (related to links) are simulated directly, fermion fields (defined on sites) are integrated out on any given classical gauge background. The resulting non-local effective action is solved through numerical simulations, e.g. using a variant of the Rational Hybrid Monte Carlo algorithm. Our implementation benefits from the force gradient integrator on multiple time scales. We use two variants of staggered fermions at physical light, strange and charm quark masses. The difference sits in the four levels of stout vs hex smearing used.

Dirac equation is solved in double vs mixed precision in simulations vs measurements, respectively. Dirac operator and the smearing steps need nearest neighbor communication; we do two steps of nearest neighbor interaction for the Symanzik-improved gauge force/action, and optimize the number of link multiplications.

For SP1-2: The gauge configurations are generated using the 4HEX action. We use an EIG-CG algorithm to determine the generalized quark number susceptibilities for each configuration. This consists of finding the ~ 200 lowest lying eigenvectors of the lattice Dirac operator. For this we use a variant of the Lanczos algorithm with sparse linear algebra. In the full solver space, the CG algorithm is ill-conditioned. Thus, we separate the low-mode eigenspace and solve this part analytically. We thus achieve a factor 5 improvement in speed. The set-up time is less than 5% of the analysis. Storing the eigenspace needs significant memory. This is not problematic, due to the 128GB GPU memory in each of the four AMD cards in a Frontier node.

In *SP1* we use the eigenvalue spectrum to calculate a reweighting factor (see Ref. [20]) that improves the continuum limit considerably. This corrects the staggered artifacts on the would-be zero-modes of Dirac's operator. The weight of these zero modes determines the instanton density, and, thus, the axion potential.

For SP3: The algorithmic details for the calculation of the equation of state at $\mu_B = 0$ follow our previous work [23]. The high statistics shown in the budget tables is necessary to cancel a quartic divergence in the trace anomaly. The trace anomaly emerges as a renormalization factor times the difference of the finite temperature contribution subtracted from a zero temperature contribution with the same bare parameters.

For SP4: The reweighted simulations work in two steps. First, configurations are generated with the HMC algorithm followed by an extra Metropolis step, depending on the extra μ_B-dependent contribution. In our test runs we always maintained an acceptance above 50%. Step 2 is the calculation of all eigenvalues of the reduced fermion matrix (in a complex vector space of $6N_x^3$ dimensions). Both steps depend on established dense linear algebra algorithms. We have integrated the MAGMA (dense linear algebra) package with our simulation code. We can thus do multi-GPU computations (e.g. zgeev). The largest considered size is a 82944×82944 generic complex matrix. The required 110 GB memory is available in Frontier's dual AMD cards. MAGMA has recently extended to support to the HIP backend, and, thus, work with AMD cards.

For SP5: Apart from the reweighted simulations, we will use the complex Langevin equation with dynamical stabilization. While the principal algorithm is based on Ito calculus, the computational intensive part is again a conjugate gradient solver (sparse linear algebra) that calculates the fermionic drift term in each time step. The time step is controlled with a plaquette variable.

3.2.2 Implementation

The production code "Janko" was developed in Wuppertal (in C), and ported to many architectures, including the Blue Gene/Q systems using the low level communication backend, Cray XC40 (with the DMAPP backend), as well as to KNL-based clusters and GPU clusters (cuda and HIP backends).

3.2.3 Libraries and dependencies

The code requires a working MAGMA installation. Because of the large matrices, it has to be compiled to support 64-bit integers. Future versions of the program will probably depend on ROCSHMEM. can usually be compiled and linked by users.

3.2.4 Parallel I/O

Our code implements parallel writes: it translates data to disk format via point-to-point communicators, then disjoint blocks are written by a set of nodes. Configuration storage is < 1% of the run time: in SP2, configurations are read in 2s, a computation without I/O follows for ~4900s (measured on Summit). Saving checkpoints yields the main I/O load. This is set such that one configuration is written (5s) per hour.

3.2.5 Post-production and analysis

The post-production will occur on our off-site workstations. The data to be downloaded is <100 GB. The analysis is executed on two tracks, all steps are cross-checked. The analysis consists of fitting the data to several models and weighting them by fit quality. The fit codes are in C (1st track) and Python (2nd track).

3.3 Parallel Performance

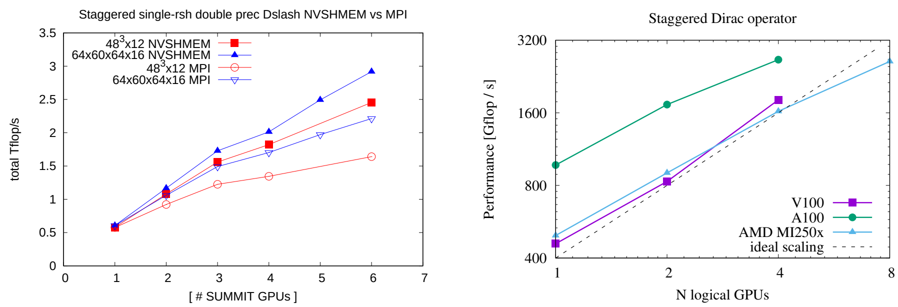

Figure 7. Strong scaling of our code on GPUs. Both panels show the performance of the staggered Dirac operator, that accounts for 95% of the run time of standard simulations and measurements. Left: Scaling within one Summit node in absolute units (Tflop/s). Right: Scaling within one AMD test node, nearly identical to Frontier nodes. The performance is normalized to one NVIDIA V100 card.

In Fig. 7 left, we show the improvement achieved by replacing MPI by NVSHMEM. For AMD cards we have the MPI backend working at the moment. Each logical GPU of AMD MI250 brings about 50% of the NVIDIA A100 and about 100% of the NVIDIA V100 performances. Since Frontier nodes combine four MI250 cards, we see the equivalent of 1.33 Summit node hours in 1 Frontier node hour. We had most of our test runs on A100 or V100 cards (e.g. on Summit). We use this factor to calculate our budget on Frontier.

Since we did not have a chance to test the inter-node scaling of the MPI code on an AMD hardware, we show it on an A100 cluster (Fig. 8). This data was taken on Juwels/Booster (FZ-Juelich, Germany) where we compare our code (open symbols) with the QUDA library (full symbols). Fig. 8 right shows the strong scaling of our code on CPUs. We will run a $64^3 \times 96$ lattice on the CPU while a GPU job is in progress. On Summit we did not experience any drop of performance of the GPU code while using the CPUs.

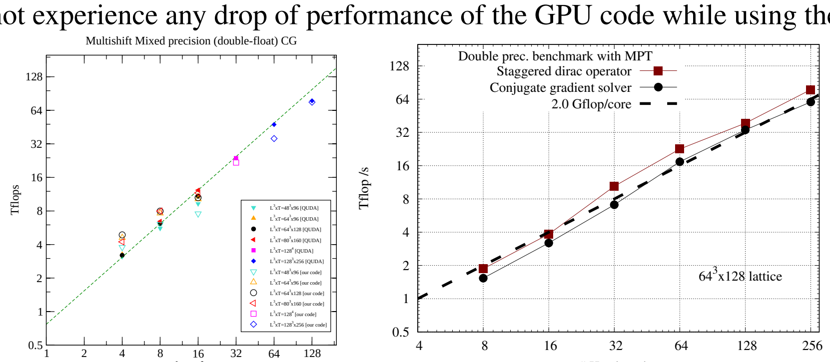

Figure 8. Left: Strong scaling of the MPI-based inter-node communication. Performance is shown in units of Teraflops/seconds, measured on Juwels/Booster (FZ-Juelich, Germany). Right: Strong scaling of our CPU-code. Data was taken on an AMD/EPYC cluster (HAWK, HRLS, Germany).

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PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

This year, Prof. Vovchenko (University of Houston) joins our team as PI, bringing his crucial expertise on fluctuations of conserved charges and QCD Equation of State at large densities. He is an early career scientist, starting his tenure-track assistant professor position at UH in September 2022. This reflects the commitment by UH to lead the computational part of the project and support its experimental one. Also a new member of the application is Prof. Reina Maruyama (Yale University, member of the DOE-funded Haystac Collaboration and the DOE-funded Rydberg-Atom-Cavity Axion Search). She will collaborate with us and provide relevant information on the experimental axion search. The rest of the personnel breakdown for this proposal is similar to the one that we submitted for our previous INCITE project on Summit. This work breakdown has already proven to be very successful. This is well documented by the fact that, over the four years in which we received computer time allocations on Mira, we have completed several publications and have been invited to give plenary talks at the most prestigious conferences in our field (Lattice 2015, Quark Matter 2015, Strong and Electroweak Matter 2016, Strangeness in Quark Matter 2016, 2017 and 2019, Lattice 2018 and 2021). Profs. Borsanyi and Fodor joined our team in 2020, bringing the additional expertise needed to run on a new machine (Summit) which went very smoothly. Dr. Tews (Los Alamos National Laboratory) joined in 2022, to guide us towards an equation of state for neutron star mergers. The theory group at the University of Houston (Vovchenko, Ratti, Portillo, Grefa) will provide the project management as well as the infrastructure and resources to conduct the analysis necessary for this project. One of the students who participated previously, Paolo Parotto, graduated in 2019 and is now a post-doc at Penn State University, from where he will continue to work on the project. The Co-PI groups at the University of Budapest in Hungary (Katz, Pasztor), the University of Wuppertal (Borsanyi, Sexty, Kara, Vig) and Penn State University (Fodor, Parotto, Godzieba) will configure and manage the submission and prioritization of all runs at ORNL, and provide analysis resources for certain configuration runs. The Co-PI experimental group at UH (Bellwied, Gangadharan, Timmins) will continue to provide the link to the experimental program and be part of the analysis team. The LANL Co-PI (Tews) will provide guidance and facilitate the connection to the neutron star merger community. All personnel is experienced in running parallelized large scale evolution code. The UH theory group will contribute significant parts of the analysis, as in previous campaigns. The two groups in Houston have experience with analyzing the datasets from the large evolution runs. All required personnel are or will be in place at the start of the project.

MANAGEMENT PLAN

The overall project leadership lies with the principal investigator (Prof. Vovchenko), who will make the final decisions about the order and the priority of the anticipated runs. Profs. Katz and Borsanyi are the code development and operations leaders and will be in charge of the code maintenance and data storage. Profs. Bellwied, Ratti and Fodor are coordinating the experimental and theoretical analysis teams, and Dr. Tews is coordinating the link to astrophysics. Prof. Maruyama will coordinate the link to the experimental axion search. They will prioritize the order in which the produced datasets are analyzed, to match them to the ongoing experimental programs. All PI's will decide the publication policy for any results. All required updates and reports will be provided by the PI, after consultation with the Co-PI's. The personnel of each team reports to its group leader, who then reports to the PI. The whole project is a collaborative effort with the purpose to map out fundamental properties of the deconfined system in the QCD phase diagram. Our previous efforts at zero and finite chemical potential allowed us to constrain the basic properties of QCD matter just above the phase transition. The link to the experimental program is provided by the UH Bellwied group. We plan to immediately distribute the results of our runs to the experimental and phenomenological communities, who will need them to interpret the results from RHIC-BES II after 2021. The significant reputation of the PI and Co-Pi's is documented in their respective bio sketches. The unique mix of experimental and theoretical expertise is expected to lead to compelling advances in the field.

Proposal Title (exactly as it appears on submission): QCD under extreme conditions

Year-1		
Milestone	**Details**	**Date and Status**
All T<=160 MeV, μ_B=0, 4HEX simulations ready	**Resource:** Frontier **Node-hours:** 174283 **Filesystem storage (TB and dates):** 80 **Archival storage (TB and dates):** 160 **Software Application:** Janko **Tasks:** Generate configurations at 5 temperatures and run the fluctuation analysis on the resulting 100000 configurations **Dependencies:** none	03.31.2023
4HEX simulations analyzed for fluctuations	**Resource: Wuppertal** **Node-hours:** 0 **Filesystem storage (TB and dates):** 0 **Archival storage (TB and dates):** 0 **Software Application:** C + Python analysis programs **Tasks:** Calculate the continuum limit for the fluctuations **Dependencies:** Configuration generation and measurements are completed (Q1/2023)	06.30.2023
Publication	Electric charge fluctuations at $\mu_B = 0$	06.30.2023
Improved 4STOUT statistics at μ_B=0, on $48^3 \times 12$ lattices completed	**Resource:** Frontier **Node-hours:** 55713 **Filesystem storage (TB and dates):** 100 **Archival storage (TB and dates):** 200 **Software Application:** Janko **Tasks:** generate $48^3 \times 12$ lattices at $\mu_B = 0$	06.30.2023

Temperature scans at $\mu_B/T<3.5$ with reweighting completed	**Resource:** Frontier **Node-hours:** 25125 **Filesystem storage (TB and dates):** 1 **Archival storage (TB and dates):** 5 **Software Application:** Janko **Tasks:** generate configurations and analyze the eigenvalue spectrum **Dependencies:** none	06.30.2023
First results using the Complex Langevin equation near Tc	**Resource:** Frontier **Node-hours:** 20833 **Filesystem storage (TB and dates):** 1 **Archival storage (TB and dates):** 5 **Software Application:** Janko **Tasks:** Complex Langeving in the range $\mu_B/T<3$ **Dependencies:** none	06.30.2023
All μB = 0 4HEX simulations on $64^3\times16$ ready and analyzed for axion potential	**Resource:** Frontier **Node-hours:** 122849 **Filesystem storage (TB and dates):** 64 **Archival storage (TB and dates):** 128 **Software Application:** Janko **Tasks:** Generate on $64^3\times16$ configurations for four higher temperatures (T>160 MeV) and extract the axion potential **Dependencies:** configurations T<=160 MeV (Q1/2023)	09.30.2023
Renormalization runs for the EoS ready	**Resource:** Frontier **Node-hours:** 50500 **Filesystem storage (TB and dates):** 32 **Archival storage (TB and dates):** 0 **Software Application:** Janko **Tasks:** Run 48^3x64 lattices (T=0) **Dependencies: none**	09.30.2023

EoS using Complex Langevin equation below T_c	**Resource:** Frontier **Node-hours:** 39583 **Filesystem storage (TB and dates):** 1 **Archival storage (TB and dates):** 1 **Software Application:** Janko **Tasks:** Extension of Complex Langeving to lower temperatures, in the range $\mu_B/T<3$ **Dependencies:** Complex Langevin results (Q2/2023)	09.30.2023
Publication	Precision results on the $\mu_B = 0$ equation of state	09.30.2023
Deep scan in chemical potential ($\mu_B/T<4$) with reweighting method completed	**Resource:** Frontier **Node-hours:** 65750 **Filesystem storage (TB and dates):** 1 **Archival storage (TB and dates):** 5 **Software Application:** Janko **Tasks:** generate configurations at $\mu_B/T<4$	12.31.2023
Transition line from optimized reweighting	**Resource:** Wuppertal **Node-hours:** 0 **Filesystem storage (TB and dates):** 0 **Archival storage (TB and dates): 0** **Software Application:** C + Python programs **Tasks:** Analysis of the chiral condensate at $\mu_B/T<4$ **Dependencies:** Reweighted Results (Q2+Q4/2023)	12.31.2023
EoS using Complex Langevin equation deeply in the hadronic phase	**Resource:** Frontier **Node-hours:** 120883 **Filesystem storage (TB and dates):** 1 **Archival storage (TB and dates):** 1 **Software Application:** Janko **Tasks:** Extension of Complex Langeving to the hadronic phase **Dependencies:** Complex Langevin results (Q3/2023)	12.31.2023

Validation of results: Complex Langevin equation vs reweighting	**Resource:** Wuppertal **Node-hours:** 0 **Filesystem storage (TB and dates):** 0 **Archival storage (TB and dates):** 0 **Software Application:** Janko **Tasks:** Analysis and comparison between results of the chiral condensate and the equation of state **Dependencies:** Complex Langevin results (Q3/2023), Reweighted simulations (Q1+Q3/2023)	12.31.2023
Publication	Axion potential at non-zero temperature	12.31.2023
Publication	Transition line on T-μ_B phase diagram with reweighting	12.31.2023
Year 2		
Publication	Electric charge fluctuations extrapolated to RHIC energies	06.30.2024
Publication	Continuum extrapolated equation of state at non-zero strangeness	09.30.2024
Publication	First result on the high-density, low-T EoS, at finite lattice spacing, with $\mu_I = 0$	12.31.2024
Year 3		
Publication	Refined axion mass prediction from field theory simulations	09.30.2025
Publication	Exclusion regions for the CEP at $T > 0$	09.30.2025

Publication	First result on the high-density, low-*T* EoS, at finite lattice spacing, with $\mu_I \neq 0$	12.31.2025

PUBLICATIONS RESULTING FROM INCITE AWARDS

2014 INCITE Project "Thermodynamics of quark flavors from lattice QCD"

S. Borsanyi, Z. Fodor, S. D. Katz, S. Krieg, C. Ratti, K. K. Szabo, Phys. Rev. Lett. 113 (2014) 052301: Freeze-out parameters from electric charge and baryon number fluctuations: is there consistency?

C. Ratti et al., Nucl. Phys. A931 (2014) 802: Freeze-out conditions from fluctuations of conserved charges.

M. Bluhm et al., Nucl. Phys. A931 (2014) 814: Determination of freeze-out conditions from fluctuation observables measured at RHIC.

S. Borsanyi et al., J. Phys. Conf. Ser. 535 (2014) 012030: Fluctuations of conserved charges on the lattice and in heavy ion collisions.

M. Bluhm et al., J. Phys. Conf. Ser. 509 (2014) 012050: Flavor-specific behavior of conserved charge fluctuations at the QCD confinement transition.

M. Bluhm et al., J. Phys. Conf. Ser. 612 (2015) 012041: Parametrization for chemical freeze-out conditions from net-charge fluctuations measured at RHIC.

2015 INCITE Project "Quark flavors and conserved charges at finite density in the QCD phase diagram"

R. Bellwied, S. Borsányi, Z. Fodor, S.D. Katz, A. Pásztor, C. Ratti, and K.K. Szabó, Phys. Rev. D. 92 (2015) 114: Fluctuations and correlations in high temperature QCD.

R. Bellwied, S. Borsanyi, Z. Fodor, J. Günther, S.D. Katz, C. Ratti, K.K. Szabo, Physics Letters B. 751 (2015) 559: The QCD phase diagram from analytic continuation.

C. Ratti, Nuclear Physics A. 956 (2016) 51: Lattice QCD: bulk and transport properties of QCD matter.

J. Gunther, R. Bellwied, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor, C. Ratti, EPJ Web Conf. 137 (2017) 07008: The QCD equation of state at finite density from analytical continuation.

J. Gunther, R. Bellwied, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor, C. Ratti, Nucl. Phys. A967 (2017) 720: The QCD equation of state at finite density from analytical continuation.

R. Bellwied, S. Borsanyi, Z. Fodor, J. Guenther, S. Katz, K. Szabo, C. Ratti, PoS ICHEP2016 (2016) 369: Fluctuations and correlations in finite temperature QCD.

C. Ratti, J.Phys.Conf.Ser. 736 no.1, (2016) 012001: Recent results on lattice QCD thermodynamics.

2016-2017 INCITE Project "Fundamental properties of QCD matter produced at RHIC and the LHC"

P. Alba *et al.*, Phys. Rev. D96 (2017) no.3, 034517: Constraining the hadronic spectrum through QCD thermodynamics on the lattice.

R. Bellwied, S. Borsanyi, Z. Fodor, J. Guenther, S.D. Katz, A. Pasztor, C. Ratti, K.K. Szabo, Nuclear Physics A. 956 (2016) 797: Towards the QCD phase diagram from analytical continuation.

M. Amaryan, E. Chudakov, K. Rajagopal, C. Ratti, J. Ritman, I. Strakovsky, Workshop on Excited Hyperons in QCD Thermodynamics at Freeze-Out (YSTAR2016) Mini-Proceedings.

C. Ratti, J.Phys.Conf.Ser. 779 (2017) 012016: Bulk properties of QCD matter from lattice simulations.

Jacquelyn Noronha-Hostler, Rene Bellwied, Jana Gunther, Paolo Parotto, Attila Pasztor, Israel Portillo Vazquez, Claudia Ratti, J. Phys. Conf. Ser. 779 no.1 (2017) 012050: Strangeness at finite temperature from Lattice QCD.

P. Parotto, J. Phys. Conf. Ser. 832 no.1 (2017) 012062: Testing the hadronic spectrum in the strange sector.

Szabolcs Borsányi *et al.*, PoS LATTICE2016 (2016) 073: Viscosity of the pure SU(3) gauge theory revisited.

R. Bellwied *et al.*, Nucl. Phys. A967 (2017) 732: Lattice QCD thermodynamics up to the perturbative regime.

V. Vovchenko, A. Pasztor, Z. Fodor, S. D. Katz, H. Stoecker, Phys. Lett. B775 (2017) 71: Repulsive baryonic interactions and lattice QCD observables at imaginary chemical potential.

J. N. Guenther, R. Bellwied, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor, C. Ratti, K. Szabo, PoS CPOD2017 (2018) 032: Recent lattice QCD results at non-zero baryon densities.

A. Pasztor, Z. Fodor, M. Giordano, S. D. Katz, C. Ratti, A. Schaefer, K. Szabo, B. Toth, Phys. Rev. D98 (2018) 014512: High statistics lattice study of stress tensor correlators in pure SU(3) gauge theory.

A. Pasztor *et al.*, EPJ Web Conf. 175 (2018) 07046: Hadron Thermodynamics from imaginary chemical potentials.

J. N. Guenther, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor, C. Ratti, EPJ Web Conf. 175 (2018) 07036:

Fluctuations of conserved charges from imaginary chemical potential.

C. Ratti, Report on Progress in Physics 81 (2018) 084301: Lattice QCD and heavy ion collisions: a review of recent progress.

S. Borsanyi, Z. Fodor, J. N. Guenther, S. Katz, K. Szabo, A. Pasztor, I. Portillo, C. Ratti, JHEP1810 (2018) 205: Higher order fluctuations and correlations of conserved charges from lattice QCD.

2020 INCITE Project "Characterization of strongly interacting matter through fluctuations"

C. Ratti, R. Bellwied, S. Borsanyi, Z. Fodor, J. N. Guenther, R. Kara, S. Katz, P. Parotto, A. Pasztor, K. Szabo, J. Phys. Conf. Ser. 1602 (2020) 012011: The QCD transition line from lattice simulations.

S. Borsanyi, Z. Fodor, J. N. Guenther, R. Kara, S. Katz, P. Parotto, A. Pasztor, C. Ratti, K. Szabo, Phys. Rev. Lett. 126 (2021) 232001: Lattice QCD equation of state at finite chemical potential from an alternative expansion scheme.

C. Ratti, R. Bellwied, S. Borsanyi, Z. Fodor, J. N. Guenther, R. Kara, S. Katz, J. Noronha-Hostler, P. Parotto, A. Pasztor, J. Stafford, K. Szabo, Acta Phys. Pol. B Proc. Suppl. 14, 281 (2021): QCD transition line and correlators of conserved charges from lattice QCD.

R. Bellwied, S. Borsanyi, Z. Fodor, J. N. Guenther, S. D. Katz, P. Parotto, A. Pasztor, D. Pesznyak, C. Ratti, K. K. Szabo, Phys. Rev. D104, 9, 094508 (2021): Corrections to the hadron resonance gas from lattice QCD and their effect on fluctuation-ratios at finite density.

Curriculum Vitae

Volodymyr Vovchenko
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Personal information

Nationality: Ukrainian
Birthplace: Kyiv, Ukraine

Education and Training

2020–2022: Feodor Lynen Research Fellow, Lawrence Berkeley National Laboratory (USA)
2018–2020: Postdoctoral Research Associate, Goethe University Frankfurt (Germany)
PhD: Physics Department, Goethe University Frankfurt, Germany, 2018
MS: Physics Department, Taras Shevchenko National University of Kyiv, Ukraine, 2013

Research and Professional Experience

From Sept. 2022: Assistant Professor, University of Houston, Texas (USA)
Apr. 2022–Aug. 2022: Research Assistant Professor, University of Washington, Seattle (USA)

Five Publications Most Relevant to This Proposal

1. *Constraining the hadronic spectrum and repulsive interactions in a hadron resonance gas via fluctuations of conserved charges*, J.M. Karthein, V. Koch, C. Ratti, V. Vovchenko, Phys. Rev. D104 (2021) 094009.
2. *Connecting fluctuation measurements in heavy-ion collisions with the grand-canonical susceptibilities*, V. Vovchenko, O. Savchuk, R.V. Poberezhnyuk, M.I. Gorenstein, V. Koch, Phys. Lett. B811 (2020) 135868.
3. *Cluster Expansion Model for QCD Baryon Number Fluctuations: No Phase Transition at* $\mu_B/T < \pi$, V. Vovchenko, J. Steinheimer, O. Philipsen, H. Stoecker, Phys. Rev. D97 (2018) 114030.
4. *Repulsive baryonic interactions and lattice QCD observables at imaginary chemical potential*, V. Vovchenko, A. Pasztor, Z. Fodor, S.D. Katz, H. Stoecker, Phys. Lett. B775 (2017) 71.
5. *van der Waals Interactions in Hadron Resonance Gas: From Nuclear Matter to Lattice QCD*, V. Vovchenko, M.I. Gorenstein, H. Stoecker, Phys. Rev. Lett. 118 (2017) 182301.

Research Interests and Expertise

Heavy-Ion Collisions: I have worked on multiple topics concerning the phenomenology of heavy-ion collisions with applications to all major heavy-ion experiments worldwide. This includes:
- freeze-out of hadron yields and fluctuations;
- effects of exact conservation laws and connections to lattice QCD;
- dynamical modeling of event-by-event fluctuations;
- production of light (anti-)(hyper-)nuclei.
In particular, I have developed an open source HRG model code called Thermal-FIST, which is in use by both theorists and experimentalists alike.
QCD Equation of State: This part of my research is devoted to the development of the QCD Equation of State construction based on effective QCD theories constrained to lattice QCD and

empirical observations. In particular, I worked on the first study to include the nuclear liquid-gas transition into the hadron resonance gas model, by means of the van der Waals interaction. I have also worked on lattice QCD constrains on baryon excluded volume parameter, as well as on the search for the QCD critical point based on the cluster expansion in fugacities, the coefficients of which are accessible in lattice simulations at imaginary chemical potentials. I am the first author in most of the relevant publications.

Synergistic Activities

1. Service to the scientific community: Referee for: Nature Comm., Phys. Rev. Lett., Phys. Rev. C, D, Journal of Physics G, Nucl. Phys. A, Eur. Phys. J. A, Phys. Lett. B; Grant proposal reviewer for National Science Centre Poland
2. Community code development: Community code development: developed open-source programs used worldwide for (non-)ideal hadron resonance gas model applications and molecular dynamics simulations of fluctuations near the critical point.
3. Activities to promote physics education: Developed several Android apps for real-time simulation and visualization of various physical systems.

Collaborators (excluding co-PIs and team members on this proposal)

M. Bleicher, A. Motornenko, O. Savchuk, J. Steinheimer, H. Stoecker, K. Zhou (FIAS, Germany), B. Dönigus, F. Cuteri, C. Greiner, K. Gallmeister, M. Hanauske, B. Kardan, M. Lorenz, O. Philipsen, T. Neidig, J. Schaffner-Bielich, R. Stock (Goethe University Frankfurt, Germany), B.B. Brandt, G. Endrodi (Bielefeld University, Germany), V.V. Begun (TH Ingolstadt, Germany), L.P. Csernai (Bergen University, Norway), F. Hajkarim (Padua University, Italy), Iu. Karpenko (Prague Technical University, Czech Republic), J.M. Karthein (MIT), V.A. Kuznietsov, O.S. Stashko (Taras Shevchenko University, Ukraine), D. Anchishkin, M.I. Gorenstein, R.V. Poberezhnyuk (BITP, Ukraine), V. Koch, J. Randrup (LBNL), S. Reddy (INT Seattle), C. Shen (Wayne State University).

Curriculum Vitae

Rene Bellwied
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Professional Preparation

PhD: Johannes Gutenberg University, Mainz, Germany, 1989
MS: Johannes Gutenberg University, Mainz, Germany, 1984
BS: Johannes Gutenberg University, Mainz, Germany, 1982

Appointments

2014-now: MD Anderson Distinguished Professor of Physics, University of Houston, TX
2010–2014: Professor of Physics, University of Houston, Houston, TX
2002–2010: Professor of Physics, Wayne State University, Detroit, MI
1996–2002: Associate Professor of Physics, Wayne State University, Detroit, MI
1992-2006: Assistant Professor of Physics, Wayne State University, Detroit, MI
1989-1992: Postdoctoral Research Associate, Stony Brook University, New York, NY

Five Publications Most Relevant to This Proposal

1. *Nonmonotonic Energy Dependence of Net-Proton Number Fluctuations*, STAR Collaboration (J. Adam, R. Bellwied et al.), Phys. Rev. Lett. 126 (2021) 9, 092301
2. *Beam energy dependence of net-Λ fluctuations measured by the STAR experiment at the BNL Relativistic Heavy Ion Collider*,STAR Collaboration (J. Adam, R. Bellwied et al.), Phys.Rev. C102 (2020) 2, 024903
3. *Enhanced production of multi-strange hadrons in high-multiplicity proton-proton collisions*, ALICE Collaboration (J.Adam, R. Bellwied et al.), Nature Physics 13 (2017) 535
4. *Freeze-out conditions from net-proton and net-charge fluctuations at RHIC*, P. Alba, W. Alberico, R. Bellwied, M. Bluhm, V. Mantovani, M. Nahrgang, C. Ratti, Phys. Lett. B738 (2014) 305
5. *Is there a flavor hierarchy in the deconfinement transition of QCD?*, R. Bellwied, S. Borsanyi, Z. Fodor, S.D. Katz, C. Ratti, Phys. Rev. Lett. 111 (2013) 202302

Research Interests and Expertise

Expertise: I am an experimental nuclear physicist working on relativistic heavy ion physics for more than 30 years. From 1989 until 1994 I was a member of four different heavy ion experiments at the AGS accelerator at Brookhaven National Laboratory (BNL). In 1991 I became one of the founding members of the STAR experiment at RHIC at BNL. I served as project leader for one of the detectors (SVT) from 1991 until the start of the heavy ion beam at RHIC in 2000. From 2001-2002 I served as the STAR deputy spokesperson before becoming one of the Physics Coordinators for STAR from 2002-2007. In 2008 I joined the ALICE collaboration at the LHC at CERN and served in several collaboration leadership roles since then. Since 2011 I am the experimental liaison to several European lattice QCD groups. From 2015-2018 I served as the coordinator of ALICE-USA. I am the author of more than 800 published and refereed papers with more than 94,000 citations. My h-index according to Google Scholar is 150.

Research Interest: My primary research interest is a deeper understanding of the formation of matter in the universe shortly after the Big Bang. Our primary tool to access the necessary temperatures and densities are relativistic heavy ion collisions. In 2005, the RHIC experiments announced the discovery of a new state of matter (Quark Gluon Plasma), a transitional state of strongly coupled degrees of freedom, which behaved like a liquid, in the crossover region of the QCD phase transition from partons to hadrons. Simultaneously lattice QCD calculations had mapped out the crossover transition and determined a critical temperature. Since then we are challenged to determine a complete of picture of the formation of hadrons from the deconfined phase of quarks and gluons. With the onset of the experimental program at the LHC in 2010, we are now able to map out specific fluctuations of the particle production on an event by event basis and compare to sophisticated, continuum extrapolated lattice calculations of fluctuations of related order parameters in order to map out the phase diagram of matter for all relevant temperature and density ranges. This will enable us to determine the formation process of nuclear matter in the universe based on first principles. A specific interest of mine in this context is the flavor dependence of the formation process and its potential implications on the existence of strange and heavy quark matter states.

Synergistic Activities

1. PI for 2014/2015 INCITE projects, Co-PI since 2016: Over the past eight years our team was awarded more than 600 Million Core Hours on the MIRA machine at ALCF and TITAN at OLCF in order to perform detailed studies of flavor dependent effects in the QCD phase diagram using lattice QCD for LHC and RHIC collision energies .
2. Experimental coordinator for ’lattice meets experiment’ effort with lattice collaboration: A targeted attempt to bring the latest experimental discoveries at RHIC and LHC together with the most state of the art lattice QCD calculations at finite densities and temperatures, in order to answer very targeted questions of the matter evolution in the universe.
3. Deputy Spokesperson and Physics Convener of the STAR collaboration (2001-2010): In my role as deputy spokesperson and physics working group (strangeness) convenor I was able to shape the physics program of the STAR collaboration in its first eight years. During this time I co-authored 125 papers.
4. U.S. coordinator and Editorial Board member for ALICE (2015-2018): In ALICE, as U.S. coordinator I significantly shaped the physics program of the U.S. in ALICE. As editorial board member I supervised and coordinated the publication of more than 200 refereed publications in the past five years.
5. National activities to promote Physics Research: I was the Associate Chair of the Physics Department at UH from 2012-2018. From 2010-2012 I served on the Physics Policy Committee of the American Physical Society, and I am presently the Chair of the Texas Section of the APS. From 2008-2012 I was the Chair of the National User Facility Organization (NUFO), which represents its 30,000+ users in Washington.

Collaborators

ALICE collaboration, CERN, (1315 collaborators)
STAR collaboration, BNL, (535 collaborators)
Claudia Ratti, Paolo Parotto, Israel Portillo, Jamie Stafford, University of Houston
Szabolcs Borsanyi and Zoltan Fodor, University of Wuppertal, Germany
Sandor Katz, University of Budapest, Hungary

Curriculum Vitae

Szabolcs Borsanyi
Theoretical Physics, University of Wuppertal, Wuppertal 42119, Germany
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Education and Training

2000–2003: PhD School in Theoretical Particle Physics, Budapest Hungary
2003–2006: Postdoctoral Research Associate, Heidelberg Univesity (Germany)
2006–2008: Postdoctoral Research Associate, Univesity of Sussex (UK)
2009–2013: Postdoctoral Research Associate, University of Wuppertal (Germany)

Research and Professional Experience

2013–2019: Faculty member, University of Wuppertal (Germany)
2019–: Full professor, University of Wuppertal (Germany),

Five Publications Most Relevant to This Proposal

1. S. Borsanyi, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg, C. Ratti and K. K. Szabo, "Is there still any T_c mystery in lattice QCD? Results with physical masses in the continuum limit III," JHEP **09** (2010), 073 doi:10.1007/JHEP09(2010)073
2. S. Borsanyi, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg and K. K. Szabo, "Full result for the QCD equation of state with 2+1 flavors," Phys. Lett. B **730** (2014), 99-104 doi:10.1016/j.physletb.2014.01.007
3. S. Borsanyi, Z. Fodor, S. D. Katz, S. Krieg, C. Ratti and K. K. Szabo, "Freeze-out parameters from electric charge and baryon number fluctuations: is there consistency?," Phys. Rev. Lett. **113** (2014), 052301 doi:10.1103/PhysRevLett.113.052301
4. R. Bellwied, S. Borsanyi, Z. Fodor, J. Günther, S. D. Katz, C. Ratti and K. K. Szabo, "The QCD phase diagram from analytic continuation," Phys. Lett. B **751** (2015), 559-564 doi:10.1016/j.physletb.2015.11.011
5. S. Borsanyi, Z. Fodor, J. Guenther, K. H. Kampert, S. D. Katz, T. Kawanai, T. G. Kovacs, S. W. Mages, A. Pasztor and F. Pittler, *et al.* "Calculation of the axion mass based on high-temperature lattice quantum chromodynamics," Nature **539** (2016) no.7627, 69-71 doi:10.1038/nature20115

Research Interests and Expertise

Thermodynamics of QCD on the lattice: Since 2008 I am a member of the Wuppertal-Budapest lattice QCD collaboration. I initiated and supervised the second generation thermodynamics program of the collaboration, which resulted the chemical potential dependence of the transition temperature, equation of state and fluctuations of conserved charges.
Lattice algorithms and code development: I wrote one of the collaboration's simulation code and I am supervising its maintenance team. Modern algorithmic ingredients (most recently the parallel tempering) are regularly added to the code and ported to GPU and other accelerator architectures.
Reweighting-based methods: in collaboration with our colleagues in Budapest we work out new methods to define and simulate lattice QCD at finite baryo-chemical potential.

Synergistic Activities

1. Teaching: Introduced the lecture "Quantum Computing" at the University of Wuppetral. I organize Journal clubs for the Master students.

2. Funding: Co-PI of the Project, "Phenomenology of the QCD transition" in the Collaborative Research Center Regensburg–Wuppertal (SFB-TRR55), 2016 – 2020
   Co-PI of the Project, "Compressed baryonic matter research at GSI/FAIR" (Funded by the German Federal Government 2021-2024)
   PI of the Project, "Phase diagram and phenomenology of the QCD transition" (Funded by the DFG, Germany 2022-2024)
3. Supervise Student Research: I supervise at the moment a PhD Student and regularly supervise Master students. I work with a team of postdoctoral researchers on computational high energy physics projects.
4. PI of computing projects: I received substantial resources as the PI of two PRACE projects in 2013, 2014. I was recently awarded with resources at the GPU cluster (JUWELS/Booster, FZJ-Jülich, Germany) e.g. to investigate the sign problem in lattice QCD. One of my GPU cluster projects received an excellence award in 2021.

Collaborators (excluding co-PIs and team members on this proposal)

S. Dürr. C. Hölbling, B. Tóth, K. K. Szabó (University of Wuppertal, Germany)
S. Krieg, (Bonn Univ., Germany)
J. Noronha-Hostler (University of Illinois, Urbana),
M. Giordano, D. Nógradi (Eotvos U, Budapest)
J. Guenther, L. Lellouch (CPT Marseille)
A. Ringwald (DESY, Hamburg)

Curriculum Vitae
Zoltan Fodor

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Professional Preparation

PhD: Eotvos Lorand University, Budapest, 1990
MS: Eotvos Lorand University, Budapest, 1987

Appointments

2021 Professor of Physics, Pennsylvania State University, University Park, USA
2003 Professor of Physics (professor ordinarius), Bergische Universitaet Wuppertal, Germany, head of Theoretical Particle Physics
1999 Professor of Physics, Eotvos University, Budapest, Hungary
1998 Associate Professor of Physics, Eotvos University, Budapest, Hungary
1997-1998 Invitation Fellowship for Long Term Research, JSPS, KEK, Tsubuka, Japan
1995-1996 Research Fellow, CERN , Geneva, Switzerland
1992-1994 Humboldt Fellow and Post-Doc, DESY, Hamburg, Germany
1990-1991 CERN, SNF Fellow, Geneva, Switzerland

Five Publications Most Relevant to This Proposal

1. *QCD Crossover at Finite Chemical Potential from Lattice Simulations*, Sz. Borsanyi, Z. Fodor, J. N. Guenther, R. Kara, S. D. Katz, P. Parotto, A. Pasztor, C. Ratti, K. K. Szabo Phys.Rev.Lett. **125** (2020) 052001.
2. *Calculation of the axion mass based on high-temperature lattice quantum chromodynamics*, Sz. Borsanyi, Z. Fodor, K. H. Kampert, S. D. Katz, T. Kawanai, T. G. Kovacs, S. W. Mages, A. Pasztor, F. Pittler, J. Redondo, A. Ringwald, K. K. Szabo, Nature **539** (2016) 69.
3. *Constraining the hadronic spectrum through QCD thermodynamics on the lattice,* P. Alba *et. al.*, Phys.Rev. D96 (2017) no.3, 034517.
4. *Fluctuations and correlations in high temperature QCD*, R. Bellwied, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor, C. Ratti and K. K. Szabo, Phys. Rev. D **92**, no. 11, (2015) 114505.
5. *Freeze-out parameters from electric charge and baryon number fluctuations: is there consistency?*, S. Borsanyi, Z. Fodor, S.D. Katz, S. Krieg, C. Ratti, K.K. Szabo, Phys.Rev.Lett. 113 (2014) 052301.

Research Interests and Expertise

Expertise: I have been working on lattice QCD for two decades. I have been involved in both $T > 0$ and $T = 0$ lattice simulations. I contributed to several areas of QCD thermodynamics. We were the first to determine important properties, such as the order and temperature of the QCD phase transition in the continuum limit. A recently developed new technique for studying non-vanishing chemical potentials gave a boost to the entire field. I have a long standing experience with HPC computing. This includes both the algorithmic issues of lattice calculations as well as the optimization for different architectures and management of highly scalable computing resources. I was awarded several CPU time allocations in Juelich, Germany, as well as via PRACE. I have over 200 publications with more than 26,000 citations and a h index of 72 according to the Google-Scholar database.

Research Interest: My primary research interest is lattice simulations of QCD, especially at non-vanishing temperatures and chemical potentials. Various properties of the QCD transition have been determined recently with high precision using lattice calculations. I am mostly interested in providing final, continuum extrapolated results. We have determined the temperature dependence of several observables, such as the chiral condensate or second order fluctuations of conserved charges in the continuum limit. There are a few exceptions of equilibrium quantities for which there is yet no continuum result. The equation of state (including the charm quark) or higher order moments of the electric charge are two important examples. Studying QCD at non-vanishing chemical potentials is significantly more difficult than at zero density. I am very much interested in developing new methods to reach large chemical potentials.

It is challenging to connect the above mentioned equilibrium quantites (such as the transition temperature or equation of state) with experiments and observations. The experimentally detected distributions of conserved quantities such as baryon number or electric charge carry information from the hot plasma that is studied via lattice simulations. I am interested in the most complete understanding of this connection. Furthermore, dense QCD is relevant for neutron star physics. High temperature QCD is also necessary to understand the cosmological generation of axions.

Further research interests are $T = 0$ lattice QCD simulations, in particular hadron masses, isospin splittings, nuclear physics, g-2 of the muon.

Synergistic Activities

1. Co-Spokesperson and PI of several projects of the Lattice-Hadron SFB Large grant (about $3 million/year) provided by the German science agency DFG to the Wuppertal University and Regensburg University.
2. Spokesperson for the Budapest-Marseille-Wuppertal collaboration.

Collaborators (*past 5 years including name and current institution*)

Daniel Godzieba, Penn State University, State Colleg, PA, USA
Rene Bellwied, Claudia Ratti, Volodymyr Vovchenko, University of Houston, TX, USA
Szabolcs Borsanyi, Stephan Durr, Jana Guenther, Christian Holbling, Karl-Heinz Kampert, Kalman Szabo, University of Wuppertal, Germany
Gergely Endrodi, University of Bielefeld, Germany
Julius Kuti, University of California San Diego, USA
Kieran Holland, University of Pacific, USA
Andreas Schafer, Regensburg University, Germany
Laurent Lellouch, CNRS, Marseille, France
Andreas Ringwald, DESY, Hamburg, Germany
Sandor Katz, Tamas Kovacs, Daniel Nogradi, Eotvos University, Budapest, Hungary
Javier Redondo, Zaragoza University, Spain

Curriculum Vitae

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Education and Training

2003-2005: Postdoctoral Fellow, Bergische Universität, Wuppertal, Germany
2001-2003: Postdoctoral Fellow, DESY, Hamburg, Germany
Habilitation: Eotvos Lorand University, Budapest, 2010
DSc: Hungarian Academy of Sciences, Budapest, 2008
PhD: Eotvos Lorand University, Budapest, 2001
MS: Eotvos Lorand University, Budapest, 1998

Research and Professional Experience

Since 2021: Director of the Institute of Physics, Eotvos University
Since 2013: Professor of Physics, Eotvos Lorand University, Budapest, Hungary
2007–2013: Assistant Professor of Physics, Eotvos Lorand University, Budapest, Hungary
2001-2007: Teaching Assistant, Eotvos Lorand University, Budapest, Hungary
2007-2008: Akademischer Rat, Bergische Universität, Wuppertal, Germany

Five Publications Most Relevant to This Proposal

1. *Lattice simulations of the QCD chiral transition at real baryon density,* S. Borsanyi *et.al.*, Phys.Rev.D 105 (2022) 5, L051506.
2. *Lattice QCD equation of state at finite chemical potential from an alternative expansion scheme,* S. Borsanyi *et.al.*, Phys.Rev.Lett. 126 (2021) 23, 232001.
3. *QCD Crossover at Finite Chemical Potential from Lattice Simulations,* S. Borsanyi *et.al.*, Phys.Rev.Lett. 125 (2020) 5, 052001.
4. *The QCD phase diagram from analytic continuation,* R. Bellwied *et.al.*, Phys.Lett. B751 (2015) 559-564.
5. *QCD equation of state at nonzero chemical potential: continuum results with physical quark masses at order* μ^2, S. Borsanyi *et.al.*, JHEP 08 (2012) 053.

Research Interests and Expertise

Expertise: I have been working on lattice QCD for about two decades. I have been involved in both $T > 0$ and $T = 0$ lattice simulations. Between 2008 and 2014 I was the PI of the ERC grant QCDTHERMO dealing with the thermodynamics of strongly interacting matter. As a continuation in 2013 and 2018 I was awarded two large Hungarian grants of order 1 million EUR each. As a member of the Wuppertal-Budapest collaboration I contributed to several areas of QCD thermodynamics. We were the first to determine important properties, such as the order and temperature of the QCD phase transition in the continuum limit. A recently developed new technique for studying non-vanishing chemical potentials gave a boost to the entire field. I have a long standing experience with HPC computing. This includes both the algorithmic issues of lattice calculations as well as the optimization for different architectures and management of highly scalable computing resources. I was awarded several CPU time allocations in JÃijlich, Germany, as well as via PRACE. I have over 190 publications with more than 17000 citations and a h index of 56 according to the INSPIRE database.

Research Interest: My primary research interest is lattice simulations of QCD, especially at non-vanishing temperatures and chemical potentials. Various properties of the QCD transition have been determined recently with high precision using lattice calculations. I am mostly interested in providing final, continuum extrapolated results. We have determined the temperature dependence of several observables, such as the chiral condensate or second order fluctuations of conserved charges in the continuum limit. Studying QCD at non-vanishing chemical potentials is significantly more difficult than at zero density. I am very much interested in developing new methods to reach large chemical potentials.

Synergistic Activities

1. PI of the ERC grant QCDTHERMO & two large Hungarian grants. In the past twelve years I have been leading a lattice group which studied QCD thermodynamics on the lattice in close collaboration with our colleagues in Debrecen and Wuppertal.
2. PI of two PRACE (Partnership for Advanced Computing in Europe) grants. I was awarded two large CPU allocations, both of them were amongst the largest in the given call. One of them was devoted to study the QCD transition with Wilson fermions, the other to locating the $N_f = 3$ critical point with overlap quarks.
3. coPI of four INCITE projects. In 2014, 2015, 2016-2017 and 2020 together with R. Belllwied and C. Ratti we were awarded CPU time from INCITE for studying conserved charge fluctuations and transport coefficients.
4. Hungarian coordinator for the Wuppertal-Budapest collaboration. I am the senior member of the lattice group in Budapest involved in all projects.

Collaborators (excluding co-PIs and team members on this proposal)

Rene Bellwied, Claudia Ratti, University of Houston, TX, USA
Szabolcs Borsanyi, Kalman Szabo and Zoltan Fodor, University of Wuppertal, Germany
Gergely Endrodi, University of Bielefeld, Germany
Tamas Kovacs, Institute for Nuclear Research, Debrecen, Hungary & Eotvos University, Budapest
Laurent Lellouch, CNRS, Marseille, France
Daniel Nogradi, Eotvos University, Budapest, Hungary

Curriculum Vitae

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Education and Training

2009–2010: Postdoctoral Research Associate, Wuppertal University (Germany)
2007–2009: Postdoctoral Research Associate, Stony Brook University, New York (USA)
2005–2007: Postdoctoral Research Associate, ECT* Trento (Italy)
2003–2005: Postdoctoral Research Associate, Technical University of Munich (Germany)
PhD: Physics Department, Torino University, Italy, 2003
MS: Physics Department, Torino University, Italy, 1999

Research and Professional Experience

Since Sept. 2017: Associate Professor, University of Houston, Texas (USA)
2014–2017: Assistant Professor, University of Houston, Texas (USA)
2010–2014: Research Assistant Professor and FIRB Grant Co-PI, Torino University

Five Publications Most Relevant to This Proposal

1. *Lattice QCD equation of state at finite chemical potential from an alternative expansion scheme*, S. Borsanyi, Z. Fodor, J. N. Guenther, R. Kara, S.D. Katz, P. Parotto, A. Pasztor, C. Ratti, K.K. Szabo, Phys. Rev. Lett. 126 (2021) 23, 232001.
2. *Lattice-based equation of state at finite baryon number, electric charge and strangeness chemical potentials*, J. Noronha-Hostler, P. Parotto, C. Ratti, J. M. Stafford, Phys. Rev. C100 (2019) 064910
3. *Higher order fluctuations and correlations of conserved charges from lattice QCD*, S. Borsanyi *et al.*, JHEP1810 (2018) 205.
4. *The QCD equation of state at finite density from analytical continuation*, J. Günther, R. Bellwied, S. Borsanyi, Z. Fodor, S.D. Katz, A. Pasztor, C. Ratti, K.K. Szabo, Nucl. Phys. A967 (2017) 720
5. *The QCD equation of state with dynamical quarks*, S. Borsanyi, G. Endrodi, Z. Fodor, A. Jakovac, S.D. Katz, S. Krieg, C. Ratti, K.K. Szabo, JHEP 08 (2010) 077.

Research Interests and Expertise

Thermodynamics of QCD on the lattice: Since 2009 I am a member of the Wuppertal-Budapest lattice QCD collaboration. We have published several fundamental results on Quark-Gluon Plasma (QGP) physics, such as the equation of state of QCD for 2+1 dynamical quark flavors at zero and small chemical potential, the transition temperature for the deconfinement phase transition, second and fourth order fluctuations of conserved charges.

Phenomenology of the QGP: I have developed several phenomenological models for QGP physics for three purposes:
- provide an interpretation of the lattice data in terms of effective degrees of freedom;
- access regions of the phase diagram which cannot be studied on the lattice;
- compute dynamical quantities in real time, such as QGP viscosity.

They include the PNJL model (I am first author of one of the pioneering works on the subject, which has 900 citations), the quasi-particle model, the Hadron Resonance Gas model.

QCD Equation of State with a critical point: this part of my research activity is based on the idea of combining the QCD equation of state from the lattice, to an Ising-model-based approach which correctly reproduces the scaling behavior of the equation of state of strongly interacting matter in the vicinity of the critical point.

Synergistic Activities

1. Funding: PI of DoE-funded Pilot Diversity Program "NuSTEAM: Nuclear Science in Texas for the Enhancement and the Advancement of Minorities", 2021-2023; PI of NSF CAREER award "Properties of Strongly interacting matter from lattice QCD", 2017-2022, to study the properties of the QGP at RHIC and LHC experiments. Co-PI of DoE-funded Beam Energy Scan Topical (BEST) Collaboration, 2016-2021.
2. PI and Co-PI for INCITE machine time proposal: We received machine time through INCITE on Mira at Argonne in 2014, 2015 and 2016-17 and on Summit at ORNL in 2020. In 2014 we determined the freeze-out conditions of heavy-ion collisions from first principles, as well as its flavor dependence. In 2015 we proposed to calculate fluctuations of conserved charges at finite density. The 2016-17 project was geared towards the electric charge fluctuations and the QGP shear viscosity. The project on SUMMIT was focused on fluctuations and cross correlators of conserved charges at finite density. All years led to successful publications and several invited talks at international conferences.
3. Service to the scientific community: Reviewer for: DoE, Deutsche Forschungsgemeinschaft (DFG), NSF (Panelist), ISCRA (Italian SuperComputing Resource Allocation), Czech Science Foundation, Austrian Science Fund; Referee for: Phys. Rev. C, D, Journal of Physics G, Nucl. Phys. A, Eur. Phys. J. C, JHEP, Phys. Lett. B, Phys. Rev. Lett.
4. Activities to promote physics to groups underrepresented in STEM: Instructor in the STEP program (STEM Teaching Equity Project) for high school teachers from disadvantaged areas. Physics representative at the UH booth for the Houston Energy day. Talks at Youth Career Development Fairs. Internships for high school students. Judge at Middle and High School science fair. Coordinator of the "Women in physics" activities at UH.
5. Meetings to promote knowledge and interaction between young scientists: Co-founder and organizer of the International Conference series "Fairness" for young scientists working on the Physics of FAIR; Since 2016: Member of the International Advisory Committee of "Quark Matter". Co-Chair of the Hard Probes 2020 conference.

Collaborators (excluding co-PIs and team members on this proposal)

V. Dexheimer (Kent State University), K. Szabo, J. Guenther (Wuppertal Univ., Germany), J. Grefa, A. Nava Acuna, A. Timmins (University of Houston, Texas), J. Harris (Yale University), T. Dore, D. Mroczek, J. Noronha, J. Noronha-Hostler, N. Yunes (UIUC), E. McLaughlin (Columbia University), J. Rose (Astronomical Institute, Bamberg), V. Mantovani Sarti (Technical University Munich, Germany), W. Alberico, A. Beraudo (University of Torino, Italy), M. Bluhm, M. Nahrgang (University of Nantes, France), R. Rougemont (Rio de Janeiro State University), M. Stephanov (Illinois University, Chicago), T. Schaefer (North Carolina State University), K. Rajagopal (MIT), I. Vitev, C. da Silva (LANL), S.Mioduszewski (Texas A&M University), I. Sarcevic (Arizona University), M. Schlegel (New Mexico State University).

Curriculum Vitae

Ingo Tews
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
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Education and Training

2018–2019: Postdoctoral Research Associate, Los Alamos National Laboratory, New Mexico (USA)
2015–2018: Postdoctoral Research Associate, Institute for Nuclear Theory, University of Washington, Washington State (USA)
PhD: Physics Department, Technical University of Darmstadt, Germany, 2015
MS: Physics Department, Technical University of Darmstadt, Germany, 2012
BS: Physics Department, Technical University of Darmstadt, Germany, 2010

Research and Professional Experience

Since Dec. 2019: Staff Scientist, Los Alamos National Laboratory, New Mexico (USA)

Five Publications Most Relevant to This Proposal

1. *Multimessenger constraints on the neutron-star equation of state and the Hubble constant*, T. Dietrich, M. W. Coughlin, P. T. H. Pang, M. Bulla, J. Heinzel, L. Issa, I. Tews, S. Antier, Science 370, 1450 (2020)
2. *Stringent constraints on neutron-star radii from multimessenger observations and nuclear theory*, C. D. Capano, I. Tews, S. M. Brown, B. Margalit, S. De, S. Kumar, D. A. Brown, B. Krishnan, S. Reddy, Nature Astron. 4, 625 (2020)
3. *Constraining the speed of sound inside neutron stars with chiral effective field theory interactions and observations*, I. Tews, J. Carlson, S. Gandolfi, S. Reddy, Astrophys. J. 860, 149 (2018)
4. *Chiral Three-Nucleon Interactions in Light Nuclei, Neutron-α Scattering, and Neutron Matter*, J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, Phys. Rev. Lett. 116, 062501 (2016)
5. *Quantum Monte Carlo calculations with chiral effective field theory Interactions*, A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. 111, 032501 (2013)

Research Interests and Expertise

Low-density nuclear theory: I have combined Quantum Monte Carlo methods to solve the nuclear many-body problem with interactions from chiral effective field theory. Our approach allowed us to calculate properties of atomic nuclei and the equation of state of dense matter probed in the core of neutron stars with theoretical uncertainty estimates. We also construct improved nuclear Hamiltonians suitable for quantum Monte Carlo methods.

Analysis of astrophysical observations: We have used Bayesian inference frameworks to constrain the neutron star equation of state with electromagnetic observations of neutron stars, e.g., by the Neutron Star Interior Composition Explorer (NICER), gravitational-wave detections by the LIGO-Virgo interferometers, and also experimental information, e.g., from the PREX experiment or heavy-ion collisions. The equations of state were constructed using nuclear-theory calculations at low densities.

Synergistic Activities

1. External Advisory Board: I am member of the External Advisory Board for the NSF Research Traineeship "Data Science in Multimessenger Astrophysics" at the University of Minnesota since 2022. I evaluate and advise the leadership team.
2. Workshop Organization: Organized a virtual Program "Nuclear Forces for Precision Nuclear Physics" at the INT Seattle in 2021.
3. Supervision of Student Research: I have supervised and am supervising three Bachelor's research projects and mentored two graduate student research projects. These projects addressed the neutron-star equation of state or nuclear interactions from chiral effective field theory.
4. Service to the Scientific Community: I have served as Reviewer for the US Department of Energy Office of Science (NP and ASCR) and the Laboratory Directed Research and Development Office at Los Alamos National Laboratory. I am serving as Referee for: The Astrophysical Journal, Physical Review Letters, C, D, Frontiers in Physics, the European Physics Journal A, Physics Letters B, and Monthly Notices of the Royal Astronomical Society.
5. Leadership: I am Astrophysics and Cosmology Focus Area Leader at the Center for Space and Earth Science at Los Alamos National Laboratory (LANL) since 2022, and responsible for awarding small grants for student or postdoctoral research at LANL.

Collaborators (excluding co-PIs and team members on this proposal)

M. Alford (Washington University in St. Louis), M. Al-Mamun, Mohammad (University of Tennessee), S. Antier (University of Amsterdam), D. Brown (Syracuse University), S. M. Brown (Max Planck Institute for Gravitational Physics Hannover), M. Bulla (Stockholm University), C. Capano (Max Planck Institute for Gravitational Physics Hannover), J. Carlson (Los Alamos National Laboratory), M. W. Coughlin (University of Minnesota), Z. Davoudi (University of Maryland), S. De (Los Alamos National Laboratory), T. Dietrich (University of Potsdam), J. C. Dolence (Los Alamos National Laboratory), C. Drischler (Michigan State University), X. Du (University of Tennessee), A. Ekström (Chalmers University), R. Essick (Perimeter Institute), C. Fryer (Los Alamos National Laboratory), S. Gandolfi (Los Alamos National Laboratory),] A. Haber (Washington University in St. Louis), S. Han (University of Washington), S. Huth (TU Darmstadt), K. Hebeler (TU Darmstadt), C. Heinke (University of Alberta), J. Heinzel (Carleton College), J. D. Holt (TRIUMF), D. E. Holz (Chicago University) L. Issa (Stockholm University) O. Korobkin (Los Alamos National Laboratory), B. Krishnan (Max Planck Institute for Gravitational Physics Hannover), S. Kumar (Max Planck Institute for Gravitational Physics Hannover), N. Kunert (University of Potsdam), P. Landry (California State University Fullerton), J. Lange H. Lim (Los Alamos National Laboratory), J. Lippuner (Los Alamos National Laboratory), D. Lonardoni (Michigan State University), A. Lovato (Argonne National Laboratory), J. E. Lynn (TU Darmstadt), B. Margalit (University of California Berkeley), J. Margueron (IP2I Lyon), J. Nättilä (Columbia University), R. O'Shaughnessy (Rochester Institute of Technology), P. T. H. Pang (NIKHEF), M. Piarulli (Washington University St. Louis), S. Reddy (University of Washington), I. Sagert (Los Alamos National Laboratory), A. Schwenk (TU Darmstadt), R. Somasundaram (IP2I Lyon), A. Steiner (University of Tennessee), C. Van Den Broeck (NIKHEF)

Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

Janko

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

Yes

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to

acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Colleagues and email notices

Question #2

Suggested Reviewers

Suggest names of individuals who would be particularly suited to assess the proposed research.

Ion-Olimpiu Stamatescu (I.O.Stamatescu@thphys.uniheidelberg.de)

Gernot Muenster (munsteg@uni-muenster.de)

Scott Pratt (prattsc@msu.edu)

Laura Tolos (tolos@ice.csic.es)

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

Testbed.pdf
The attachment is on the following page.

TESTBED RESOURCES

This proposal does not request test bed resources