Numerical Challenges in Lattice QCD 2022

Report of Contributions

https://indico.cern.ch/e/1115433

Contribution ID: **25** Type: **not specified**

Properties of the η and η' mesons

Monday 15 August 2022 16:50 (40 minutes)

We summarize our results for the η and η' masses and their four independent decay constants at the physical point as well as their anomalous gluonic matrix elements $a_{\eta^{(\prime)}}$.

The computation employs twenty-one $N_f = 2 + 1$ Coordinated Lattice Simulations (CLS) ensembles with non-perturbatively improved Wilson fermions at four different lattice spacings and along two trajectories in the quark mass plane, including one ensemble very close to physical quark masses. We give details on the evaluation of the disconnected contributions to the pseudoscalar and axialvector matrix elements. The direct determination of both allows us to investigate the singlet PCAC relation and to study the QCD scale dependence of the singlet currents.

Primary authors: BALI, Gunnar (Universität Regensburg); COLLINS, Sara (University of Regensburg); SIMETH, Jakob (University of Regensburg)

Presenter: SIMETH, Jakob (University of Regensburg)

Session Classification: Stochastic Trace Estimation

Contribution ID: **26** Type: **not specified**

Interpolation as a means of shift selection in multilevel Monte Carlo with lattice displacements

Monday 15 August 2022 15:10 (40 minutes)

The calculation of disconnected diagram contributions to physical signals is a computationally expensive task in Lattice QCD. To extract the physical signal, the trace of the inverse Lattice Dirac operator, a large sparse matrix, must be stochastically estimated. Because the variance of the stochastic estimator is typically large, variance reduction techniques must be employed. Multilevel Monte Carlo (MLMC) methods reduce the variance of the trace estimator by utilizing a telescoping sequence of estimators. Frequency Splitting is one such method that uses a sequence of inverses of shifted operators to estimate the trace of the inverse lattice Dirac operator, however there is no a priori way to select the shifts that minimize the cost of the multilevel trace estimation. We present a sampling and interpolation scheme
that is able to predict the variances associated with Frequency Splitting under displacements of the underlying space time lattice. The interpolation scheme is able to predict the variances to high accuracy and therefore choose shifts that correspond to an approximate minimum of the cost for the trace estimation. We show that Frequency Splitting with the chosen shifts displays significant speedups over multigrid deflation, and that these shifts can be used for multiple configurations within the same ensemble with no penalty to performance.

Primary authors: Dr WHYTE, Travis (College of William & Mary); Dr STATHOPOULOS, Andreas (College of William & Mary); Dr ROMERO, Eloy (JLab); Dr ORGINOS, Kostas (College of William & Mary/Jlab)

Presenter: Dr WHYTE, Travis (College of William & Mary)

Session Classification: Stochastic Trace Estimation

Contribution ID: **27** Type: **not specified**

Tackling critical slowing down using global correction steps with equivariant flows within the 2D Schwinger model

Tuesday 16 August 2022 14:30 (40 minutes)

Discretisation of gauge theories are an elegant and successful way to solve them via supercomputers. To obtain results at the continuum, the discretised model is simulated via Monte Carlo simulations at fixed physics at different lattice spacings and then extrapolated to the continuum. In many cases the major systematic effect of the obtained result is given by the extrapolation error. To minimise this error, simulations at finer lattice spacing are necessary, which are often prevented by increasing autocorrelation times, caused by a freezing of extensive quantities, such as the topological charge.

We will discuss a potential method to overcome topological freezing in gauge models with fermions. The method combines flow-based generative models for local gauge field updates and hierarchical updates of the factorised fermion determinant. The flow-based generative models are restricted to proposing updates to gauge-fields within subdomains, thus keeping training times moderate while increasing the global volume. We apply our method to the 2-dimensional (2D) Schwinger model and show that sampling of topological sectors can be achieved also at fine lattices.
Moreover, we will discuss the potential of combining the correction steps with the Hybrid Monte Carlo method.

Primary author: FINKENRATH, Jacob

Presenter: FINKENRATH, Jacob

Session Classification: Machine Learning

Contribution ID: **28** Type: **not specified**

Machine learning for ensemble generation

Tuesday 16 August 2022 10:40 (40 minutes)

I will discuss the use of machine learning methods to accelerate algorithms for gauge field generation, in particular via flow models.

Primary author: SHANAHAN, Phiala

Presenter: SHANAHAN, Phiala

Session Classification: Machine Learning

Contribution ID: **29** Type: **not specified**

Continuous Normalizing Flow for Lattice QCD based on Trivializing Maps

Tuesday 16 August 2022 11:20 (40 minutes)

In this presentation we will show the connection between Continuous Normalizing Flows (CNF) and Trivializing Maps by Luescher. Based on the latter, we will construct a CNF that can be trained to simulate lattice field theories. We discuss strategies to train the CNF for 2D and 4D SU(3) pure-gauge theories.

Primary authors: BACCHIO, Simone; Dr KESSEL, Pan (TU-Berlin); SCHAEFER, Stefan; Mr VIATL, Lorenz (TU-Berlin)

Presenter: BACCHIO, Simone

Session Classification: Machine Learning

Contribution ID: **30** Type: **not specified**

Fermion loops at the physical point

Wednesday 17 August 2022 11:20 (40 minutes)

We present results obtained for disconnected fermion loops contributing to nucleon observables using simulations of twisted mass lattice QCD with physical quark masses and three lattice spacings. We focus on the methods employed, including multi-grid, hierarchical probing, low-mode deflation, and the so-called one-end trick.

Primary author: KOUTSOU, Giannis

Presenter: KOUTSOU, Giannis

Session Classification: Stochastic Trace Estimation

Contribution ID: **31** Type: **not specified**

Temporal factorization of the Wilson fermion determinant and multi-level integration

Monday 15 August 2022 09:00 (40 minutes)

When lattice QCD is formulated in sectors of fixed quark numbers, the canonical fermion determinants can be expressed explicitely in terms of transfer matrices defined at fixed time. This in turn provides a complete factorization of the fermion determinants in temporal direction. In this talk I describe this factorization for Wilson-type fermions and present explicit constructions of the transfer matrices. Possible applications of the factorization include the construction of improved estimators for generic n-point correlation functions and multi-level integration schemes. The latter is of particular interest for the calculation of disconnected correlation functions.

Primary author: WENGER, Urs (Universität Bern (CH))

Presenter: WENGER, Urs (Universität Bern (CH))

Session Classification: Multi-Level

Contribution ID: **32** Type: **not specified**

Disconnected Diagrams and High-Degree GMRES Polynomials

Monday 15 August 2022 10:40 (40 minutes)

We build upon our lattice QCD POLY and HFPOLY methods by using high-degree polynomials in the context of noisy disconnected diagram evaluations. Using a new, stable form of the GMRES polynomial, we obtained a subtracted error reduction in the Wilson-Dirac scalar operator on the order of a tenth the error of the non-subtracted measurement. The associated trace of subtracted high-degree polynomials can be evaluated stochastically through a multilevel polynomial cascade method using deflation as well as a new and efficient double-polynomial construction. For demonstration purposes, our methods were tested at kappacrit in the quenched approximation.

Primary author: WILCOX, Walter

Co-authors: Dr MORGAN, Ronald (Baylor University); Mr LASHOMB, Paul (Baylor University); Dr WHYTE, Travis (College of William and Mary)

Presenter: WILCOX, Walter

Session Classification: Numerical Solvers

Contribution ID: **33** Type: **not specified**

AMG+: Extended Multilevel Principles

Monday 15 August 2022 09:40 (40 minutes)

By employing new extended multilevel hierarchy construction principles, AMG can be applied to many new types of problems. The extended principles include general rules for choosing relaxation, constructing the coarse-level variables, the coarse-to-fine interpolation, and coarse-level equations, and a quantitative performance predictor of the multi-level cycle convergence rate, called the mock cycle. As an illustrative example, a fast solver for the highly indefinite 1D Helmholtz equation is developed.

Primary authors: Prof. BRANDT, Achi (Weizmann Institute of Science); Prof. BRANNICK, James (Penn State); KAHL, Karsten; Dr LIVNE, Oren E (Lab126)

Presenter: Prof. BRANNICK, James (Penn State)

Session Classification: Multi-Level

Contribution ID: **34** Type: **not specified**

Analysis of block GMRES using a *-algebra-based approach

Monday 15 August 2022 11:20 (40 minutes)

We discuss the challenges of extending convergence results of classical Krylov subspace methods to their block counterparts and propose a new approach to this analysis. Block KSMs such as block GMRES are generalizations of classical KSMs, and are meant to iteratively solve linear systems with multiple right-hand sides (a.k.a. a block right-hand side) all-at-once rather than individually. However, this all-at-once approach has made analysis of these methods more difficult than for classical KSMs because of the interaction of the different right-hand sides. We have proposed an approach built on interpreting the coefficient matrix and block right-hand side as being a matrix and vector over a *-algebra of square matrices. This allows us to sequester the interactions between the right-hand sides into the elements of the *−algebra and (in the case of GMRES) extend some classical GMRES convergence results to the block setting. We then discuss some challenges which remain and some ideas for how to proceed.

This is joint work with Marie Kubiínová from Czech Academy of Sciences, Institute of Geonics, Ostrava, Czech Republic (formerly)

[1] Marie Kubínová and Kirk M. Soodhalter. Admissible and attainable convergence behavior of block Arnoldi and GMRES. SIAM Journal on Matrix Analysis and Applications, 41 (2), pp. 464-486, 2020.

Primary author: SOODHALTER, Kirk (Trinity College Dublin)

Co-author: Dr KUBÍNOVÁ, Marie (Czech Academy of Sciences, Institute of Geonics, Ostrava, Czech Republic (formerly))

Presenter: SOODHALTER, Kirk (Trinity College Dublin)

Session Classification: Numerical Solvers

Contribution ID: **35** Type: **not specified**

HMC on Riemannian Manifolds

Tuesday 16 August 2022 08:45 (55 minutes)

I shall give a pedagogical introduction to the Hamiltonian/Hybrid Monte Carlo algorithm (HMC) on Riemannian manifolds. I will explain how Hamiltonian systems are most naturally formulated in terms of Hamiltonian vector fields $\hat{X}$ on symplectic manifolds: the relationship between commutators of Hamiltonian vector fields and Poisson brackets, $[\hat{X},\hat{Y}]=\widehat{\{X,Y\}}$; why a conserved shadow Hamiltonian exists; and why the natural Riemannian volume element $\sqrt{\det g}$ appears automatically. I will show that the symplectic integrator step $e^{\hat{T}\delta\tau}$ is a geodesic on a Riemannian manifold, and how this corresponds to matrix exponentiation on Lie groups. Finally, time permitting, I will explain how this leads to a practical HMC algorithm on symmetric spaces (and slightly more generally on homogeneous reductive manifolds) such as $\mathbb{C}P^n$ or $\mathbb{S}^2$ using Hamiltonian reduction.

Primary author: KENNEDY, Anthony

Presenter: KENNEDY, Anthony

Session Classification: Numerical Integration

Contribution ID: **36** Type: **not specified**

The potential of Padé approximations for molecular dynamics simulation

Tuesday 16 August 2022 09:40 (40 minutes)

Presenter: SCHAEFERS, Kevin

Session Classification: Numerical Integration

Contribution ID: **37** Type: **not specified**

New ideas and developments for solvers for distillation?

Presenter: URREA-NINO, Juan Andres

Session Classification: Numerical Solvers

Contribution ID: **38** Type: **not specified**

Opening

Monday 15 August 2022 08:45 (15 minutes)

Presenter: KNECHTLI, Francesco Giacomo (Bergische Universitaet Wuppertal (DE))

Contribution ID: **39** Type: **not specified**

Podium discussion contribution

Tuesday 16 August 2022 16:10 (10 minutes)

Some selected questions:Critical slowing down with $a \to 0$.
- Rounding issues on large volumes.
- Multiscale approaches to increase signal over noise
- Benefits of (approximate eigenvectors) and how to obtain these
- Approaches to excited state contributions: multi-state fits, GEVP, smearing.
- efficient stochastic estimation of traces, all-to-all propagators, perambulators

These are based on an analysis of challenges:
* Large lattice volumes (due to small a and M_π)
- Computational cost does not nexessarily translate into better signal/noise.
- critical slowing down (in general with small a)
- precision issues
- how to maintain good acceptance in HMC?
- algorithms that scale like V^2, e.g., number of eigenvectors in estimators/deflation, algorithms that scale like V/a^2 (smearing).
- How to beat noise of disconnected contributions on large volumes?
* n-point functions with $n > 3$:
- QED corrections to QCD, $K \to \pi\pi$ etc.
- Quasi-, Pseudo-, etc. PDFs
- transitions to scattering states/resonances
* Bigger excited state problems at small quark masses
- go to larger times? How?
- improve smearing? Examples: momentum smearing, perambulators.
- several interpolators, including multi-quark states?
* More mixing with lower dimensional operators than in the continuum if chiral symmetry is broken
- grandient flow?

Primary author: BALI, Gunnar (Universität Regensburg)

Presenter: BALI, Gunnar (Universität Regensburg)

Session Classification: Podium Discussion

Contribution ID: **42**   Type: **not specified**

Contribution to Podium Discussion

Tuesday 16 August 2022 16:30 (10 minutes)

The following questions emerged from an e-mail discussion with Gustavo Ramirez:

1) Deflation (with approximate projection) as a multigrid method seems tricky to be ported to GPU architectures in an efficient way.

2) Can one understand why ? Is that solely due to the poor scalability of the 'little Dirac operator' ?

3) Isn't that then a general problem for multigrid methods on GPU ? The same scalability issue should be present for the near-kernel Dirac operator.

4) Are there more ideal solvers for pure GPU architectures (not hybrid CPU-GPU) ?

Primary author: Prof. DELLA MORTE, Michele

Presenter: Prof. DELLA MORTE, Michele

Session Classification: Podium Discussion

Contribution ID: **44** Type: **not specified**

Nucleon axial formfactors from lattice QCD

Wednesday 17 August 2022 10:40 (40 minutes)

A precise knowledge of nucleon axial formfactors is needed for the new generation of terrestrial neutrino experiments. This is particularly challenging due to increased contamination, in this sector, from excitations, in particular from $N\pi$ scattering states. Transitions from a N to a $N\pi$, mediated by an axial current are also interesting themselves, as these can be related to neutrino induced pion production. We explain how we compute the relevant Wick contractions, combining stochastic and sequentual all-to-all propagator techniques. We then employ the generalized eigenvalue approach to extract the energy levels and matrix elements of interest.

Primary authors: BALI, Gunnar (Universität Regensburg); Mr BARCA, Lorenzo (Universität Regensburg); COLLINS, Sara

Presenter: BALI, Gunnar (Universität Regensburg)

Session Classification: Stochastic Trace Estimation

Contribution ID: **46** Type: **not specified**

Gradient estimators for normalising flows

Tuesday 16 August 2022 15:10 (40 minutes)

ecently a machine learning approach to Monte-Carlo simulations called Neural Markov Chain Monte-Carlo (NMCMC) is gaining traction. In its most popular form it uses neural networks to construct normalizing flows which are then trained to approximate the desired target distribution. The training is done using some form of gradient descent so gradient estimation is necessery. In my talk I will review several gradient estimators that can be used for this purpose and discuss their pros and cons in terms of required computational time and quality of the training.

Primary authors: Prof. BIAŁAS, Piotr (Jagiellonian University); Dr KORCYL, Piotr (Jagiellonian University); Dr STEBEL, Tomasz (Jagiellonian University)

Presenter: Prof. BIAŁAS, Piotr (Jagiellonian University)

Session Classification: Machine Learning

Contribution ID: **47** Type: **not specified**

Multilevel Monte Carlo for quantum mechanics on a lattice

Monday 15 August 2022 16:10 (40 minutes)

Monte Carlo simulations of quantum field theories on a lattice become increasingly expensive as the continuum limit is approached since the cost per independent sample grows with a high power of the inverse lattice spacing. Simulations on fine lattices suffer from critical slowdown, the rapid growth of autocorrelations in the Markov chain with decreasing lattice spacing a. This causes a strong increase in the number of lattice configurations that have to be generated to obtain statistically significant results. We discuss hierarchical sampling methods to tame this growth in autocorrelations; combined with multilevel variance reduction techniques, this significantly reduces the computational cost of simulations. We recently demonstrated the efficiency of this approach for two non-trivial model systems in quantum mechanics in https://arxiv.org/abs/2008.03090. This includes a topological oscillator, which is badly affected by critical slowdown due to freezing of the topological charge. On fine lattices our methods are several orders of magnitude faster than standard, single level sampling based on Hybrid Monte Carlo. For very high resolutions, multilevel Monte Carlo can be used to accelerate even the cluster algorithm, which is known to be highly efficient for the topological oscillator. Performance is further improved through perturbative matching. This guarantees efficient coupling of theories on the multilevel lattice hierarchy, which have a natural interpretation in terms of effective theories obtained by renormalisation group transformations.

Primary authors: MUELLER, Eike (University of Bath); JANSEN, Karl (DESY); Prof. SCHEICHL, Robert (Heidelberg University)

Presenter: MUELLER, Eike (University of Bath)

Session Classification: Multi-Level

Contribution ID: **48** Type: **not specified**

Computational strategies for nucleon matrix elements

Wednesday 17 August 2022 09:00 (40 minutes)

Nucleon matrix elements are a major lattice QCD input to the search of new physics. Their determination can be challenging, in particular at near physical quark masses. On the one hand large Euclidean time separations are necessary to determine ground state matrix elements. On the other hand the signal over noise ratio deteriorates exponentially with the time. I will detail some of the techniques our group use for the efficient calculation of quark line disconnected as well as of connected contributions to various matrix elements.

Primary authors: BALI, Gunnar (Universität Regensburg); COLLINS, Sara

Presenter: COLLINS, Sara

Session Classification: Numerical Solvers

Contribution ID: **49** Type: **not specified**

Meson distillation profiles and their applications

Wednesday 17 August 2022 09:40 (40 minutes)

An improvement to the widely used distillation technique is presented in the context of meson spectroscopy. Introducing meson profiles in distillation space and optimizing them for the different operators of interest significantly increases the overlap between the created states and the energy eigenstates at no considerable extra cost. These profiles give more versatility to the smearing technique, allowing to adapt it to the different operators and use it to reveal relevant spatial information. This improved version of distillation can also be extended to meson-glueball mixing calculations as well as to studies involving other hadronic operators where distillation is applicable. The proposed improvement is tested in two ensembles with N_f = 2 clover-improved Wilson quarks at half of the physical charm quark mass but different lattice volume and lattice spacing for the study of different quantum numbers. The resulting effective masses, together with the meson-glueball mixing, display the advantages of the improvement compared to standard distillation. Additionally, possible directions for further improvements to distillation related to the linear solver are briefly presented.

Primary authors: KNECHTLI, Francesco Giacomo (Bergische Universitaet Wuppertal (DE)); Mr URREA NINO, Juan Andres (Bergische Universität Wuppertal); PEARDON, Mike (Trinity College Dublin); KORZEC, Tomasz (Bergische Universität Wuppertal)

Presenter: Mr URREA NINO, Juan Andres (Bergische Universität Wuppertal)

Session Classification: Numerical Solvers