The Tenth International Workshop on Lattice QFT and Numerical Analysis (QCDNA X)

Report of Contributions

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

Contribution ID: **1** Type: **Talk**

An Eigensolver for the Hermitian Dirac Operator with Multigrid Acceleration

Thursday, June 29, 2017 11:15 AM (30 minutes)

In this talk we present a Davidson type eigensolver combined with the DD-αAMG multigrid solver library. The basic Davidson method is adjusted to our multigrid method and the structure of the hermitian Dirac operator in a way that both methods benefit from each other.

We compare the resulting eigensolver with a Chebychev filtered Arnoldi method (PARPACK) and the multi purpose eigensolver library PRIMME based on a variety of scaling and performance studies.

Title

An Eigensolver for the Hermitian Dirac Operator with Multigrid Acceleration

Primary authors: Mr STREBEL, Artur (University of Wuppertal); Dr ROTTMANN, Matthias (University of Wuppertal); Prof. FROMMER, Andreas (University of Wuppertal); Dr KAHL, Karsten (University of Wuppertal)

Presenter: Mr STREBEL, Artur (University of Wuppertal)

Contribution ID: **2** Type: **Talk**

MILC code performance on high end CPU and GPU supercomputer clusters

Tuesday, June 27, 2017 5:30 PM (30 minutes)

With recent developments in parallel supercomputing architecture, many core, multi-core, and GPU processors are now commonplace resulting in more levels of parallelism, memory hierarchy, and programming complexity. It has been necessary to adapt the MILC code to these new processors starting with NVIDIA GPUs and more recently the Intel Xeon Phi processors. We report on our efforts to port and optimize our code for the Intel Knights Landing architecture. We consider performance of the MILC code with MPI and OpenMP, and optimizations with QOPQDP and QPhiX. For the latter approach we concentrate on the staggered conjugate gradient and gauge force. We also consider performance on recent NVIDIA GPUs using the QUDA library.

Title

MILC code performance on high end CPU and GPU supercomputer clusters

Primary authors: LI, Ruizi; Prof. DETAR, Carleton (University of Utah); Prof. GOTTLIEB, Steven (Indiana University); Prof. TOUSSAINT, Doug (University of Arizona)

Presenter: LI, Ruizi

Contribution ID: **3** Type: **Talk**

An in-depth evaluation of the Intel Omni-Path network for LQCD applications

Several parallel machines on which Lattice LQCD applications are being run utilize a new fabric, Intel Omni-Path. We present an overview of Omni-Path, comparing it to the well-known competitor InfiniBand. In the process of adding support for Omni-Path to our communication library pMR we discovered several insights which we discuss along some general usage recommendations. We substantiate our findings with benchmarks obtained on QPACE 3, which is based on Intel KNL and Omni-Path.

Title

Primary author: Mr GEORG, Peter (University of Regensburg)

Presenter: Mr GEORG, Peter (University of Regensburg)

Contribution ID: **4** Type: **Talk**

Algorithmic advances in NSPT

Wednesday, June 28, 2017 9:30 AM (45 minutes)

Numerical stochastic perturbation theory (NSPT) is a powerful tool that allows perturbation expansions in QCD and other interesting theories to be estimated to high order in the interactions. The standard algorithms on which NSPT is based on, however, suffer from several limitations which in practice restrict the potential of these techniques. In this talk I will review the recent algorithmic advances in this field and show how these significantly reduce the computational effort for precise and accurate determinations. This opens up the way to tackle challenging and interesting new problems, as will be illustrated by a highly non-trivial computation.

Title

Algorithmic advances in NSPT

Primary author: Dr DALLA BRIDA, Mattia (Universita' di Milano-Bicocca & INFN)

Presenter: Dr DALLA BRIDA, Mattia (Universita' di Milano-Bicocca & INFN)

Contribution ID: **5** Type: **Talk**

Progress and Challenge of Lattice Quantum Finite Elements (QFE) on Spheres

Tuesday, June 27, 2017 11:15 AM (1 hour)

Extending lattice field to ultraviolet complete quantum field theory on any smooth Riemann manifolds is a challenging problem. By adapting element methods (FEM) and Regge geometry one recovers classical (IR) solution in the continuum. However to correctly handle UV divergences requires new counter terms to construct a what we call a "Quantum Finite Elements" (QFE) discrete Lagrangian on the simplicial complex. These UV counters for 2d phi 4th theory and free fermions on the two sphere (S2) have been tested numerically to high precession against the exact Ising solution. Methods to generalize the QFE construction to radial quantized 3d super renormalizable theories on R x S2 and challenges for asymptotical free 4d gauge theories on R x S3 will be presented.

Title

Primary author: Dr BROWER, Richard (Boston University)

Presenter: Dr BROWER, Richard (Boston University)

Contribution ID: **6** Type: **Talk**

Deflation for Monte-Carlo estimation of the trace of a matrix inverse

Tuesday, June 27, 2017 10:15 AM (30 minutes)

In the context of computing disconnected diagrams, we investigate the efficient estimation of the trace of large-scale matrix inverses. Our approach is based on the Hutchinson method (Monte-Carlo averaging over matrix quadratures). Previous work showed that combining deflation against the lowest part of the spectrum with Hierarchical Probing can accelerate the convergence significantly. As the size of the matrix grows, however, the computation of enough singular vectors to achieve a reduction in the variance can be a bottleneck.

In this work we take advantage of the fact that the singular vectors corresponding to the lowest modes can be represented well in a sparse basis. This allows us to compute and store efficiently the first 500˜1000 lowest modes of the matrix spectrum, which is enough to obtain a good reduction in the variance. Moreover we discuss different projectors for deflating and the performance impact when the matrix is close to singular.

Title

Primary authors: Mr ROMERO ALCALDE, Eloy (College of William and Mary); Dr STATHOPOULOS, Andreas (College of William and Mary)

Presenter: Mr ROMERO ALCALDE, Eloy (College of William and Mary)

Contribution ID: **7** Type: **Talk**

An implementation of the DD-αAMG multigrid solver on Intel Knights Landing

We describe our experiences porting the Regensburg implementation of the DD-αAMG solver from the first-generation Intel Xeon Phi processor (Knights Corner) to its successor (Knights Landing). We present the performance of the code on a single processor as well as the scaling behavior on many nodes of QPACE 3, which utilizes Intel's new Omni-Path fabric.

Title

Primary author: Mr RITCHMANN, Daniel (University of Regensburg)

Presenter: Mr RITCHMANN, Daniel (University of Regensburg)

Track Classification: Poster

Contribution ID: **8** Type: **Talk**

Novel Approaches for Staggered Multigrid Algorithms

Thursday, June 29, 2017 10:15 AM (30 minutes)

Critical slowing down in the fermion sector is a leading obstacle facing the approach to the continuum in lattice gauge theory simulations. Adaptive multigrid (α-MG) methods offer a solution to the resulting superlinear growth in the cost of iterative Krylov solves. Ongoing research has suggested that previously developed α-MG methods, such as the successful formulation for Wilson-clover fermions, cannot be applied in a black-box fashion to other discretizations. In this talk I will expand on subtle issues offered by the staggered discretization. I will also discuss novel approaches that may sidestep these issues.

Title

Novel Approaches for Staggered Multigrid Algorithms

Primary author: WEINBERG, Evan

Co-authors: STRELCHENKO, Alexei (F); Dr BROWER, Richard (Boston University); Dr CLARK, Kate (NVIDIA)

Presenter: WEINBERG, Evan

Contribution ID: **9** Type: **Talk**

Scaling Multigrid to the Exascale

Thursday, June 29, 2017 9:30 AM (45 minutes)

Owing to its success in removing the critical slowing down of Dirac linear systems, adaptive multigrid is now a standard solver in the arsenal of tools that the lattice field theorist expects. In this work we report on the latest progress in improving the strong scaling of adaptive multigrid algorithms when running on GPU-accelerated architectures using the QUDA library. Techniques include Schwarz preconditioning, pipelined solvers, precision truncation and RDMA-enabled MPI. Furthermore, we report on progress on optimizing the adaptive setup process in order to increase its applicability to Hybrid Monte Carlo. Finally we discuss the challenges in scaling multigrid to the Exascale-generation of supercomputers.

Title

Scaling Multigrid to the Exascale

Primary author: Dr CLARK, Kate (NVIDIA)

Presenter: Dr CLARK, Kate (NVIDIA)

Contribution ID: **10** Type: **Talk**

Quark-antiquark excited flux tube

Tuesday, June 27, 2017 3:30 PM (30 minutes)

We present color field profiles for some of the first SU(3) gluonic excitations of the flux tube in the presence of a static quark-antiquark pair.

Title

Quark-antiquark excited flux tube

Primary author: CARDOSO, Nuno (IST)

Co-authors: CARDOSO, Marco (Instituto Superior Técnico); BICUDO, Pedro (IST Lisboa)

Presenter: CARDOSO, Nuno (IST)

Contribution ID: **11** Type: **Talk**

Local Adaptive Refinement on Lattice Gauge Fields

Thursday, June 29, 2017 11:45 AM (30 minutes)

Adaptive Mesh Refinement (AMR) has been widely used in computational fluid dynamics, shock hydrodynamics, astrophysics, turbulence modeling and combustion to improve the performance of algorithms running large, complex problems. The results are often impressive. However, for various reasons which will be discussed, traditional AMR is not directly applicable to lattice QCD. This talk proposes a new numerical method, Local Adaptive Refinement (LAR), for lattice QCD. LAR is strongly motivated by AMR, and is designed to work with the aggregation-based algebraic multigrid framework of lattice QCD. The premise behind all adaptive refinement methods is that certain numerical problems have solutions that exhibit local variations, which can be examined more fully at higher resolution (more closely spaced grid or lattice points) than the base level of resolution used for the simulation. As a result, problems that would normally require very high resolution over a large domain (which is very computationally expensive) could instead be solved at lower resolution over the large domain, with automated local refinement to higher resolution as needed. The scale and nature of the problems commonly found at the leading edge of today's lattice QCD work suggest that the field could be a benefit from adaptive refinement. Among the topics that will be discussed are the need for an algebraic variable-based approach to refinement, as opposed to a geometric grid-based approach, methods of determining the regions in which refinement should occur, and ways to implement LAR in a parallel machine environment.

Title

Local Adaptive Refinement on Lattice Gauge Fields

Primary author: Mr WHITE, JR., Edward

Presenter: Mr WHITE, JR., Edward

Contribution ID: **12** Type: **Talk**

Numerical Stochastic Perturbation Theory in φ^4 Theory

Wednesday, June 28, 2017 10:15 AM (30 minutes)

Numerical stochastic perturbation theory (NSPT) is a powerful tool for estimating high-order perturbative expansions in lattice field theory. The standard NSPT is based on the Langevin equation. In this contribution, we investigate in φ^4 theory some alternative methods. In particular, we present a study of the recently proposed Instantaneous Stochastic Perturbation Theory, as well as a formulation of numerical stochastic perturbation theory based on Generalised Hybrid Molecular Dynamics algorithms.

Title

Numerical Stochastic Perturbation Theory in φ^4 Theory

Primary authors: GAROFALO, Marco (Higgs Centre for Theoretical Physics, The University of Edinburgh); DALLA BRIDA, Mattia (DESY - Zeuthen); Prof. KENNEDY, Anthony (Higgs Centre for Theoretical Physics, The University of Edinburgh)

Presenter: GAROFALO, Marco (Higgs Centre for Theoretical Physics, The University of Edinburgh)

Contribution ID: **13** Type: **Talk**

Algebraic Multigrid: Theory and Practice

Wednesday, June 28, 2017 11:45 AM (45 minutes)

This talk gives an overview of recent progress made in the design and analysis of algebraic multigrid methods. The focus is on the setup algorithm that automatically constructs the multilevel hierarchy used in the solve phase. A sharp two-grid theory is introduced and then used to derive various quality measures of the coarse spaces constructed by the setup algorithm, based on the ideas of compatible relaxation, a related identity that assumes the use of the so-called ideal interpolation operator, and an optimal form of classical algebraic multigrid interpolation that gives the best possible two-grid convergence rate. Various numerical results are presented to illustrate these theoretical results. As a test problem, we focus on a finite volume discretization of a scalar diffusion problem with highly varying (discontinuous) diffusion coefficient.

Title

Primary author: Dr BRANNICK, James

Presenter: Dr BRANNICK, James

Contribution ID: **14** Type: **Talk**

Lattice QCD with mixed action - Borici-Creutz valence quarks on staggered sea

Tuesday, June 27, 2017 3:00 PM (30 minutes)

We used Borici-Creutz fermion to study discrete chiral symmetry breaking at strong coupling in 2-dim Gross-Neveu model and mass spectra in 2-dim field theories. Mixed action lattice QCD study with Borici-Creutz valence quarks on staggered sea quarks is carried out. The counter terms are fixed nonperturbatively to restore the broken symmetries. The effect of partial quenching and unitarity violation is investigated.

Title

Primary authors: GOSWAMI, J. (IIT Kanpur); CHAKRABARTI, D. (IIT Kanpur); BASAK, Subhasish (NISER)

Presenter: BASAK, Subhasish (NISER)

Contribution ID: **15** Type: **not specified**

HMC: Geometry and Applications

Tuesday, June 27, 2017 9:30 AM (45 minutes)

Title

Primary author: BARP, Alessandro

Presenter: BARP, Alessandro

Contribution ID: **16** Type: **not specified**

Lattice Quantum Field Theory: Numerical Integration in an Infinite Number of Dimensions

Tuesday, June 27, 2017 2:00 PM (1 hour)

Relativistic Quantum Field Theory (QFT) is the formalism upon which the Standard Model of particle physics is built, and it is remarkably successful and accurate. When the interactions are weak then the techniques of renormalized perturbation theory using Feynman diagrams works beautifully, but when the interactions are strong we have to turn to numerical evaluation of the functional integrals that define the quantum theory. The only way we know of to evaluate such infinite-dimensional integrals is to use Markov Chain Monte Carlo (MCMC) techniques. I shall attempt to give an overview of the functional integral formalism of QFT, and how MCMC integration works. If time permits I will discuss how fermions (half-integer spin) are dealt with, and maybe introduce the Hybrid (or Hamiltonian) Monte Carlo algorithm.

Title

Primary author: Prof. KENNEDY, Anthony (Higgs Centre for Theoretical Physics, The University of Edinburgh)

Presenter: Prof. KENNEDY, Anthony (Higgs Centre for Theoretical Physics, The University of Edinburgh)

Track Classification: Public Talks

Contribution ID: **20** Type: **Talk**

Nonperturbative anisotropy calibration in lattice QCD at strong coupling

Wednesday, June 28, 2017 11:15 AM (30 minutes)

We propose a simple criterion for the nonperturbative renormalization of the anisotropy coupling in lattice QCD with massless staggered fermions, in the strong coupling limit. We compute numerically and to high precision the renormalised anisotropy, and the analogue of Karsch's coefficients, using diagrammatic Monte Carlo algorithms and multi-histogram reweighting. We observe a large nonperturbative correction to the mean field anisotropy, and we analyse the implications of such a correction on the continuous time limits of the phase diagram of lattice QCD at strong coupling, and of the baryon mass.

Title

Primary authors: CALEIRO VAIRINHOS, Helvio Jose (Fisica Teorica e Met. Mat.-Inst. Nacional de Invest. Cientif.-Un); DE FORCRAND DE COISELET, Philippe (Eidgenoessische Technische Hochschule Zuerich (CH)); UNGER, Wolfgang (ETH Zuerich)

Presenter: CALEIRO VAIRINHOS, Helvio Jose (Fisica Teorica e Met. Mat.-Inst. Nacional de Invest. Cientif.-Un)

Contribution ID: **21** Type: **Talk**

GPU Computing to the Exascale and Beyond

Wednesday, June 28, 2017 2:00 PM (1 hour)

With the demise of Denard scaling, it is well known that we cannot go faster for greater throughput, rather we have to go wider. However, with the imminent demise of Moore's Law, there lies continued challenges in reaching and exceeding the Exascale. We discuss how and why GPU computing provides a solution to take computational science to this next level. We consider some of the software and algorithm challenges that the Exascale will bring. Lastly, we take a dive into the newly-launched Volta GPU architecture, the architecture that will drive the next-generation CORAL Supercomputers.

Title

Primary author: Dr CLARK, Kate (NVIDIA)

Presenter: Dr CLARK, Kate (NVIDIA)

Track Classification: Public Talks

Contribution ID: **22** Type: **Talk**

DD-αAMG on QPACE 3

Tuesday, June 27, 2017 4:30 PM (1 hour)

We describe our experiences porting the Regensburg implementation of the DD-αAMG solver from QPACE 2 to QPACE 3. We first review porting from the first generation Intel Xeon Phi processor (Knights Corner) to its successor (Knights Landing). Secondly, we present an overview of Omni-Path, comparing it to the well-known competitor InfiniBand. Finally, we present the performance of the code on a single processor as well as the scaling on many nodes.

Title

Primary authors: Mr RITCHMANN, Daniel (University of Regensburg); Mr GEORG, Peter (University of Regensburg); Dr WETTIG, Tilo (University of Regensburg)

Presenters: Mr RITCHMANN, Daniel (University of Regensburg); Mr GEORG, Peter (University of Regensburg)

Contribution ID: **23** Type: **Talk**

Analyzing AMA data on 48ˆ3 × 96 lattices

Wednesday, June 28, 2017 3:45 PM (25 minutes)

As an example for analyzing data on RBC-UKQCD's 48ˆ3 x 96 ensemble with physical pions, I investigate correlations between propagator sources placed on the same configuration and discuss options for analyzing this data set to extract the Bs-meson decay constant. The data are generated taking advantage of all-mode averaging (AMA) to reduce the numerical costs.

Title

Primary author: WITSEL, Oliver

Presenter: WITSEL, Oliver

Contribution ID: **24** Type: **Talk**

HMC, high level structures and architecture support in Grid

Wednesday, June 28, 2017 3:00 PM (45 minutes)

I will present the strategies we developed in Grid for the HMC sector, in order to support a variety of behaviours without code replication. I will also discuss the current status of the architecture support in view of the upcoming machines.

Title

Primary author: COSSU, Guido (The University of Edinburgh)

Presenter: COSSU, Guido (The University of Edinburgh)