

# Speeding up lattice QCD simulation on Arm architectures with multigrid algorithm



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## Introduction

Lattice quantum chromodynamics (lattice QCD) is the non-perturbative definition of the QCD theory from first principle and can be systematically improved, meanwhile, it is one of the most important high performance computing application in high energy physics. The physics research of lattice QCD benefited enormously from the development of computer hardware and algorithm, and particle physicist can now study strong interaction at physical pion mass, smaller lattice spacing and larger volume. On the other hand, with the emerging of supercomputers and clusters based on Arm architectures, it is necessary to implement the algorithm and conduct the simulation on these machines to maximize the utilization of the limited computing resources. In this paper, we implemented and ported the multigrid (MG) algorithm, the state of the art algorithm to solve the sparse linear Dirac equation  $Dx = b$  on the lattice, on a cluster with Arm based processors for clover fermion.

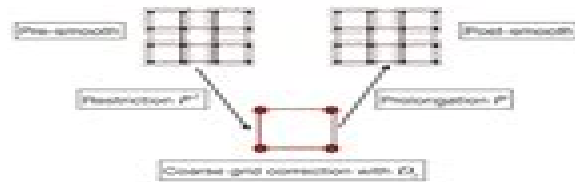
## Arm architecture



- Kunpeng 920 @ 2.6 GHz
- 7nm, Arm v8.2
- 96 cores / CPU

## Multigrid algorithm

- multigrid V-cycle



- generate near null vector with  $Dv_1 = 0$
- construct prolongator  $P$  and restrictor  $R$  from  $v_1$
- create coarse operator with Galerkin projection  $D_c = RDP$ , usually choose  $R = P^T$
- use MG as preconditioner of Krylov solver (e.g., FGMRES)
- ported eg\_proto<sup>2</sup> library on KNL and Intel Xeon to Arm with NEON vectorization

<sup>2</sup>[https://github.com/jeffersonlab/mg\\_proto](https://github.com/jeffersonlab/mg_proto)

## Distillation method

A quark field smearing scheme, factorizing operator construction and propagator computation and large operator set can be used to do GEVP analysis.

- generate Laplace eigenvectors  $V$
- compute perambulators  $\tau_{\alpha\beta}(t', t) = V^T(t') D_{\alpha\beta}^{-1}(t', t) V(t)$
- compute elementals  $\Phi_{\alpha\beta}(t) = V^T(t) [\Gamma(t)]_{\alpha\beta} V(t)$
- construct two point functions with  $\tau$  and  $\Phi$ s.

Large amount of  $Dx = b$  solve

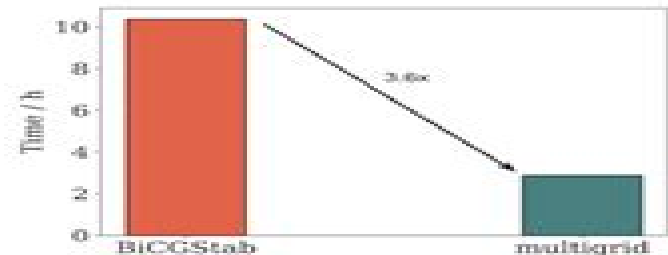
- on every configuration,  $N_c \times N_{\text{spin}} \times N_{\text{vec}}$
- very suitable for multigrid especially at light quark
- reuse multigrid setup for every source  $b$

## Results

Test on  $16^3 \times 128$  lattice with  $m_\pi = 350$  MeV

$L^3 \times T$	$\beta$	$a_t(\text{fm})$	$\xi$	$N_{\text{vec}}$	$m_\pi(\text{MeV})$
$16^3 \times 128$	2.0	0.1517	5	70	350

BiCGStab vs. multigrid on distillation



- on single time source
- on single Kunpeng 920 node
- solve  $Dx = b$  ( $N_{\text{vec}} \times N_{\text{spin}} = 280$  times)
- convergence residual  $1e-7$
- multigrid is 3.6x faster than biCGstab

## Summary

- The state of art multigrid algorithm is ported to Kunpeng 920 CPU, a Arm based processor
- We then use the multigrid algorithm in the distillation method to compute the perambulators and gain 3.6x speed up compared to the conventional BiCGStab algorithm, on a gauge ensemble with lattice volume  $16^3 \times 128$  and pion mass  $m_\pi = 350$  MeV.
- We can now use the Arm cluster more efficiently and we expect further speed up when approaching to the near physical pion mass.

# Contributions To Multigrid

**Todor Boyanov**



## Contributions To Multigrid:

**Contributions to Multigrid** P. W. Hemker, Pieter Wesseling (Dr. Ir.), 1994      Contributions to Multigrid P. W. Hemker, 1994      Contributions to Multigrid P. W. Hemker, Pieter Wesseling (Dr. Ir.), 1994      *Multigrid Methods VI* Erik Dick, Kris Riemsdijk, Jan Vierendeels, 2012-12-06 This volume contains 39 of the papers presented at the Sixth European Multigrid Conference held in Gent Belgium September 27 30 1999 The topics treated at the conference cover all aspects of Multigrid Methods theory analysis computer implementation applications in the fields of physics chemistry fluid mechanics structural mechanics and magnetism      Numerical Treatment of Coupled Systems Wolfgang Hackbusch, 2013-04-17 The GAMM Committee for Efficient Numerical Methods for Partial Differential Equations organizes seminars and workshops on subjects concerning the algorithmic treatment of partial differential equations The topics are discretisation methods like the finite element and the boundary element method for various type of applications in structural and fluid mechanics Particular attention is devoted to the advanced solution methods The series of such seminars was continued in 1995 January 20 22 with the 11th Kiel Seminar on the special topic Numerical Treatment of Coupled Systems at the Christian Albrechts University of Kiel The seminar was attended by 100 scientist from 9 countries 23 lectures were given including two survey lectures Different kinds of couplings are considered in this volume The coupling of different components may occur in the physical model On the other hand a coupling of subsystems can be generated by the numerical solution technique General examples of the latter kind are the domain decomposition see p 128 or subspace decomposition p 117 The local defect correction method couples different discretizations of the same problem in order to improve the results although the basic linear system to be solved remains unchanged p 47 In general the aim of the numerical coupling is to make use of efficient subsystem solvers p 1 The combination of different discretization techniques is mentioned on page 59      *Domain Decomposition Methods in Scientific and Engineering Computing* David E. Keyes, Jinchao Xu, 1994 This book contains proceedings from the Seventh International Conference on Domain Decomposition Methods held at Pennsylvania State University in October 1993 The term domain decomposition has for nearly a decade been associated with the partly iterative partly direct algorithms explored in the proceedings of this conference Noteworthy trends in the current volume include progress in dealing with so called bad parameters in elliptic partial differential equation problems as well as developments in partial differential equations outside of the elliptically dominated framework Also described here are convergence and complexity results for novel discretizations which bring with them new challenges in the derivation of appropriate operators for coarsened spaces Implementations and architectural considerations are discussed as well as partitioning tools and environments In addition the book describes a wide array of applications from semiconductor device simulation to structural mechanics to aerodynamics Presenting many of the latest results in the field this book offers readers an up to date guide to the many facets of the theory and practice of domain decomposition      Multigrid Methods W. Hackbusch, U. Trottenberg, 2006-11-15

Development of the Discontinuous Galerkin Method for High-resolution, Large Scale CFD and Acoustics in Industrial Geometries Koen Hillewaert, 2013-02-10 The main objective of this work is the practical development of the discontinuous Galerkin method arguably the most mature high order discretisation for the scale resolving simulations of turbomachinery flows

**Computational Optimization of Systems Governed by Partial Differential Equations** Alfio Borzi, Volker Schulz, 2012-01-26 This book provides a bridge between continuous optimization and PDE modelling and focuses on the numerical solution of the corresponding problems Intended for graduate students in PDE constrained optimization it is also suitable as an introduction for researchers in scientific computing or optimization

Numerical Methods and Applications Todor Boyanov, 2007-02-20 This book constitutes the thoroughly refereed post proceedings of the 6th International Conference on Numerical Methods and Applications NMA 2006 held in Borovets Bulgaria in August 2006 The 84 revised full papers presented together with 3 invited papers were carefully reviewed and selected from 111 submissions The papers are organized in topical sections on numerical methods for hyperbolic problems robust preconditioning solution methods Monte Carlo and quasi Monte Carlo for diverse applications metaheuristics for optimization problems uncertain control systems and reliable numerics interpolation and quadrature processes large scale computations in environmental modelling and contributed talks

Multigrid Methods IV P.W. Hemker, P. Wesseling, 2012-12-06 This volume contains a selection from the papers presented at the Fourth European Multigrid Conference held in Amsterdam July 6 9 1993 There were 78 registered participants from 14 different countries and 56 presentations were given The preceding conferences in this series were held in Cologne 1981 1985 and in Bonn 1990 Also at the other side of the Atlantic special multigrid conferences are held regularly at intervals of two years always in Copper Mountain Colorado US The Sixth Copper Mountain Conference on Multigrid Methods took place in April 1993 Circumstances prevented us from putting a larger time interval between the Copper and Amsterdam meetings The next European meeting is planned in 1996 a year later than the next Copper Meeting When the first multigrid conference was held in 1981 there was no doubt about the usefulness of a conference dedicated specially to multigrid because multigrid was a new and relatively unexplored subject still in a pioneering stage and pursued by specialists The past twenty years have shown a rapid growth in theoretical understanding useful applications and widespread acceptance of multi grid in the applied disciplines Hence one might ask whether there is still a need today for conferences specially dedicated to multigrid The general consensus is that the answer is affirmative New issues have arisen that are best addressed or need also be addressed from a special multigrid point of view

**Multigrid Methods for Process Simulation** Wolfgang Joppich, Slobodan Mijalkovic, 2012-12-06 It was about 1985 when both of the authors started their work using multigrid methods for process simulation problems This happened in dependent from each other with a completely different background and different intentions in mind At this time some important monographs appeared or have been in preparation There are the three classical ones from our point of view the so called 1984 Guide 12J by Brandt the

Multi Grid Methods and Applications 49J by Hackbusch and the so called Fundamentals 132J by Stiiben and Trottenberg Stiiben and Trottenberg in 132J state a delayed acceptance resent ments with respect to multigrid algorithms They complain Nevertheless even today s situation is still unsatisfactory in several respects If this is true for the development of standard methods it applies all the more to the area of really difficult complex applications In spite of all the above mentioned publications and without ignoring important theoretical and practical improvements of multigrid this situa tion has not yet changed dramatically This statement is made under the condition that a numerical principle like multigrid is accepted if there exist professional programs for research and production purposes Professional in this context stands for solving complex technical prob lems in an industrial environment by a large community of users Such a use demands not only for fast solution methods but also requires a high robustness with respect to the physical parameters of the problem

**Numerical Methods for Structured Matrices and Applications** Dario Andrea Bini,Volker Mehrmann,Vadim Olshevsky,Eugene Tyrtsyhnikov,Marc van Barel,2011-02-09 This cross disciplinary volume brings together theoretical mathematicians engineers and numerical analysts and publishes surveys and research articles related to topics such as fast algorithms in which the late Georg Heinig made outstanding achievements

**Mathematical Reviews** ,1994 [Domain Decomposition Methods in Science and Engineering XXII](#) Thomas Dickopf,Martin J. Gander,Laurence Halpern,Rolf Krause,Luca F. Pavarino,2016-03-11 These are the proceedings of the 22nd International Conference on Domain Decomposition Methods which was held in Lugano Switzerland With 172 participants from over 24 countries this conference continued a long standing tradition of internationally oriented meetings on Domain Decomposition Methods The book features a well balanced mix of established and new topics such as the manifold theory of Schwarz Methods Isogeometric Analysis Discontinuous Galerkin Methods exploitation of modern HPC architectures and industrial applications As the conference program reflects the growing capabilities in terms of theory and available hardware allow increasingly complex non linear and multi physics simulations confirming the tremendous potential and flexibility of the domain decomposition concept

*Numerical Methods in Laminar and Turbulent Flow* ,1995 , *Algebraic Multilevel Iteration Methods with Applications* ,1996

**Radial Basis Function Methods For Large-Scale Wave Propagation** Jun-Pu Li,2021-12-24 This book details the development of techniques and ideas from the radial basis function It begins with a mathematical description of the basic concept of radial function method with chapters progressively delving into the derivation and construction of radial basis functions for large scale wave propagation problems including singularity problems high frequency wave problems and large scale computation problems This reference written by experts in numerical analysis demonstrates how the functions arise naturally in mathematical analyses of structures responding to external loads Readers are also equipped with mathematical knowledge about the radial basis function for understanding key algorithms required for practical solutions Key features Introduces basic concepts of radial basis function methods Provides detailed derivations of several radial basis functions Explains

complex problems using simple language Contains a wide range of numerical examples to demonstrate applications of relevant functions Combines the radial basis function with other known numerical methods boundary element methods and differential equations Includes references and appropriate chapter appendices Includes MATLAB codes for origin intensity factors and nearly singular factors for radial basis calculations The book is designed to make information about radial basis function methods more accessible to research scientists professional engineers and postgraduate students with a specific focus on large scale wave propagation problems

High Performance Computing in Science and Engineering ' 08 Wolfgang E. Nagel, 2009-01-10 The discussions and plans on all scientific advisory and political levels to realize an even larger European Supercomputer in Germany where the hardware costs alone will be hundreds of millions Euro much more than in the past are getting closer to realization As part of the strategy the three national supercomputing centres HLRS Stuttgart NIC JSC Jülich and LRZ Munich have formed the Gauss Centre for Supercomputing GCS as a new virtual organization enabled by an agreement between the Federal Ministry of Education and Research BMBF and the state ministries for research of Baden Württemberg Bayern and Nordrhein Westfalen Already today the GCS provides the most powerful high performance computing infrastructure in Europe Through GCS HLRS participates in the European project PRACE Partnership for Advances Computing in Europe and tends its reach to all European member countries These activities align well with the activities of HLRS in the European HPC infrastructure project DEISA Distributed European Infrastructure for Supercomputing Applications and in the European HPC support project HPC Europa Beyond that HLRS and its partners in the GCS have agreed on a common strategy for the installation of the next generation of leading edge HPC hardware over the next few years The University of Stuttgart and the University of Karlsruhe have furthermore agreed to bundle their competences and resources

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