

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.

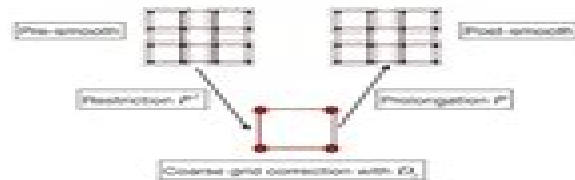
Arm architecture



- 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_proto² library on KNL and Intel Xeon to Arm with NEON vectorization

²https://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 τ and Φ s.

Large amount of $Dx = b$ solve

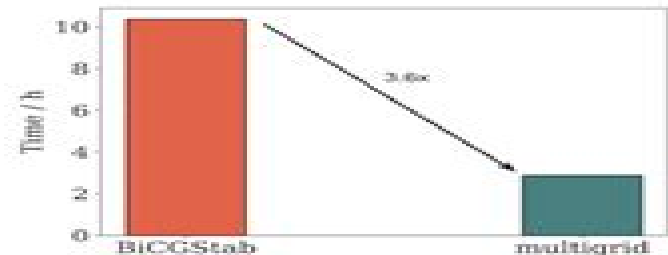
- on every configuration, $N_c \times N_{\text{spin}} \times N_{\text{vec}}$
- very suitable for multigrid especially at light quark
- reuse multigrid setup for every source b

Results

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

$L^3 \times T$	β	$a_t(\text{fm})$	ξ	N_{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

W. Hackbusch



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Contributions to Multigrid P. W. Hemker, 1994 *Contributions to Multigrid* P. W. Hemker, Pieter Wesseling (Dr. Ir.), 1994 **Contributions to Multigrid** P. W. Hemker, Pieter Wesseling (Dr. Ir.), 1994 Multigrid Methods VI Erik Dick, Kris Riemsdagh, 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 Multigrid Methods W. Hackbusch, U. Trottenberg, 2006-11-15 **Inside Finite Elements** Martin Weiser, 2016-05-10 All relevant implementation aspects of finite element methods are discussed in this book The focus is on algorithms and data structures as well as on their concrete implementation Theory is covered only as far as it gives insight into the construction of algorithms In the exercises a complete FE solver for stationary 2D problems is implemented in Matlab Octave Contents Finite Element Fundamentals Grids and Finite Elements Assembly Solvers Error Estimation Mesh Refinement Multigrid Elastomechanics Fluid Mechanics Grid Data Structure Function Reference

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 Mathematical Reviews , 1994

Algebraic Multilevel Iteration Methods with Applications , 1996 **Numerical Treatment of Coupled Systems** Wolfgang Hackbusch, Gabriel Wittum, 1995 The coupling considered in this volume may be of physical or numerical nature Examples of the first kind are the solid fluid interactions microelectronic systems and the coupled modelling in groundwater flow Examples of the latter kind are the domain or subspace decomposition the local defect correction method and the very important FEM BEM coupling *Facing the Multicore-Challenge II* Rainer Keller, David Kramer, Jan-Philipp Weiss, 2012-05-13 This state of the art survey features topics related to the impact of multicore manycore and coprocessor technologies in science and for large scale applications in an interdisciplinary environment The papers cover issues of current research in mathematical modeling design of parallel algorithms aspects of microprocessor architecture parallel programming languages hardware aware computing heterogeneous platforms manycore technologies performance tuning

and requirements for large scale applications The contributions presented in this volume offer a survey on the state of the art the concepts and perspectives for future developments They are an outcome of an inspiring conference conceived and organized by the editors at the Karlsruhe Institute Technology KIT in September 2011 The twelve revised full papers presented together with two contributed papers focus on combination of new aspects of microprocessor technologies parallel applications numerical simulation and software development thus they clearly show the potential of emerging technologies in the area of multicore and manycore processors that are paving the way towards personal supercomputing and very likely towards exascale computing

Multigrid Methods for Integral and Differential Equations D. J. Paddon, Horst Holstein, 1985 Levels and scales Multigrid methods of the second kind Some implementations of multigrid linear system solvers Multigrid and conjugate gradient methods as convergence acceleration techniques Efficient solution of finite difference and finite element equations Algebraic formalisation of the multigrid method in the symmetric and positive definite case a convergence estimation for the V Cycle A variational theory for Multi level adaptive techniques Spectral multigrid methods for dirichlet problems MG techniques for staggered differences Multigrid analysis of linear elastic stress problems Multigrid methods for oil reservoir simulation in three dimensions A multigrid algorithm using a hierarchical finite element basis

Fast Solvers for Flow Problems Wolfgang Hackbusch, Gabriel Wittum, 1995 The GAMM Committee for Efficient Numerical Methods for Partial Differential Equations organises seminars 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 types of applications in structural and fluid mechanics Particular attention is devoted to the advanced solution methods The series of such seminars was continued in 1994 January 14 16 with the 10th Kiel Seminar on the special topic Fast Solvers for Flow Problems at the Christian Albrechts University of Kiel The seminar was attended by 100 scientist from 9 countries 23 lectures were given including two invited survey lectures The central topic of most of the contributions are the Navier Stokes equations The authors discuss robust methods parallel implementations defect correction techniques adaptive methods including error estimators domain decompositions and FEM BEM coupling The invited lectures concern the hierarchical multigrid method for unstructured grids and structured adaptive finite volume multigrid for compressible flows

Journal of analysis and its applications ,1982 **Multigrid Methods** ,1982 Applied Mechanics Reviews ,1986 *Multigrid Methods II* W. Hackbusch, U. Trottenberg, 1986 **Multigrid Techniques for Unstructured Meshes** D. J. Mavriplis, 1995 **Robust Multi-Grid Methods** W. Hackbusch, 1989 In full multigrid methods for elliptic difference equations one works on a sequence of meshes where a number of pre and or postsmoothing steps are performed on each level As is well known these methods can converge very fast on problems with a smooth solution and a regular mesh but the rate of convergence can be severely degraded for problems with anisotropy or discontinuous coefficients unless some form of robust smoother is used Also problems can arise with the increasingly coarser meshes

because for some types of discretization methods coercivity may be lost on coarse meshes and on massively parallel computers the computation cost of transporting information between computer processors devoted to work on various levels of the mesh can dominate the whole computing time For discussions about some of these problems see 11 Here we propose a method that uses only two levels of meshes the fine and the coarse level respectively and where the corrector on the coarse level is equal to a new type of preconditioner which uses an algebraic substructuring of the stiffness matrix It is based on the block matrix tridiagonal structure one gets when the domain is subdivided into strips This block tridiagonal form is used to compute an approximate factorization whereby the Schur complements which arise in the recursive factorization are approximated in an indirect way i e

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