Study of Preconditioners based on Markov Chain Monte Carlo Methods

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Abstract*-Nowadays, analysis and design of novel scalable methods and algorithms for fundamental linear algebra problems such as solving Systems of Linear Algebraic Equations with focus on large scale systems is a subject of study. This research focuses on the study of novel mathematical methods and scalable algorithms for computationally intensive problems such as Monte Carlo and Hybrid Methods and Algorithms.*

I. INTRODUCTION

Solving systems of linear algebraic equations (SLAE) or inverting a real matrix are well-known problems. Iterative or direct methods to solve these systems are costly approach. One option of reducing the effort of solving these systems is to apply preconditioners before using an iterative method. Standard deterministic preconditioners computed by the optimized parallel variant- Modified SParse Approximate Inverse Preconditioner (MSPAI) have been changed by a Monte Carlo preconditioner that relies on the use of Markov Chain Monte Carlo (MCMC) methods [1]. The study of this methods and their parallel implementation is subject of current extreme scale computing research.

Preconditioning refers to transform a complex problem into another whose solution can be tractable; preconditioner is the operator that is responsible for such transformation. A way to increase the robustness and the computational efficiency of iterative methods is based on preconditioning.

Several physical problems imply to solve SLAE as result of discretization of partial differential equations. Iterative solvers are often the method of choice due to their predictability and reliability when considering accuracy and speed. They are, however, prohibitive for large-scale problems as they can be very time consuming to compute. These methods are dependent on the size of the matrix and so the computational effort grows with the problem size [2]. On the other hand, Monte Carlo (MC) methods performing random sampling of a certain variable whose mathematical expectation is the desired solution, for some problems an estimate is sufficient or even favourable, due to the accuracy of the underlying data. MC methods can quickly yield a rough estimate of the solution.

Iterative Methods are dependent on the size of the matrix

and so the computational effort grows with the problem size. The complexity of these methods is $O(kn^2)$for dense matrices in the iterative case and $O(n^3)$ for direct methods with dense matrices while solving SLAE if common elimination are employed [3] in contrast MC methods for matrix inversion (MI) only require $O(NL)$ steps to find a single element or a row of the inverse matrix. Here N is the number of Markov chains and L is an estimate of the chain length in the stochastic process. These computations are independent of the matrix size n and also inherently parallel. Note that in order to find the inverse matrix or the full solution vector in the serial case, $O(nNL)$steps are required.

II. RELATED WORK

Research efforts in the past have been directed towards optimizing the approach of sparse approximate inverse preconditioners (SPAI) [4]. In the past there have been differing approaches and advances towards a parallelisation of the SPAI preconditioner. The method that is used to compute the preconditioner provides the opportunity to be implemented in a parallel fashion. In recent years the class of Frobenius norm minimizations that has been used in the original SPAI implementation [5] was modified and is provided in a parallel SPAI software package. One implementation of it, by the original authors of SPAI, is the Modified SParse Approximate Inverse (MSPAI) [6].

The proposed Monte Carlo algorithm has been developed and enhanced upon in the last decades, and several key advances in serial and parallel Monte Carlo methods for solving such problems have been made. There is an increased research interest in parallel Monte Carlo methods for Linear Algebra in the past year [7], [8].

III. MONTE CARLO APPROACH

Monte Carlo methods are probabilistic methods, which use random numbers to either simulate a stochastic behaviour or to estimate the solution of a problem. They are good candidates for parallelisation because of the fact that many independent samples are used to estimate the solution. These samples can be calculated in parallel, thereby speeding up the solution finding process. We design and develop parallel Monte Carlo methods with the following main generic properties:

- efficient distribution of the compute data
- minimum communication during the computation
- increased precision achieved by adding extra refinement computations

Consideration of all these properties naturally leads to scalable algorithms. The Procedure to get Monte Carlo algorithm has been presented in [9] and allows extending Monte Carlo algorithm for processing diagonally dominant matrices.

IV. MONTE CARLO APPROACH

We compared matrices from different sets that have been obtained from two collections - The Matrix Market and The University of Florida Sparse Matrix Collection. These

matrices are used as inputs to both the MSPAI and our Monte Carlo based application to compute preconditioners. The results from those calculations are two intermediate matrices MSPAI and MCSPAI, one for each type of preconditioner. In the last step these preconditioners are used as an input to the BiCGSTAB (biconjugate gradient stabilized method) solver that is provided by the SPAI application. Numerical experiments have been executed on the MareNostrum supercomputer, located at the Barcelona Supercomputing Center (BSC). It currently consists of 3056 compute nodes that are each equipped with 2 Intel Xeon 8-core processors, 64GB RAM and are connected via an InfiniBand FDR-10 communication network. The experiments have been run multiple times to account for possible external influences on the results. The computation times for both the preconditioner calculated by MSPAI, as well as our Monte Carlo based result, have been noted. While conducting the experiments, we configured the parameters for probable errors in both programs to produce preconditioners with similar properties and therefore producing residuals within similar ranges when used as preconditioners for BiCGSTAB. A random starting pattern has been chosen in MSPAI for best analogy to the stochastic nature of the Monte Carlo approach. A basic experiment was carried out on various classes of matrices from the matrix market, for example, on real non-symmetric matrix as **bcsstm13** (fig. 1)

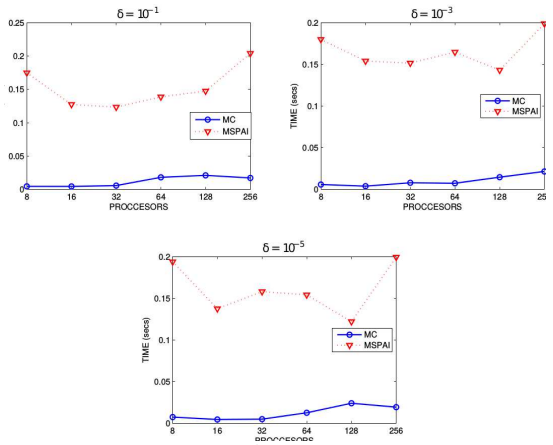

Fig. 1. Matrix bcsstm13. Run times for MC preconditioner and MSPAI.

The number of compute cores used to calculate the preconditioners has been selected to match the problem size and provide meaningful comparisons between the two differing approaches. For the small test set experiments have been run on 6 to 30 cores of the computer system. The larger examples were calculated starting from 32 or 256 cores and scaling up to 2048 cores to investigate the differing scaling behavior of the deterministic method and our stochastic algorithm.

V. SOME CONCLUSIONS AND FUTURE WORK

A Monte Carlo based preconditioner for general matrices has been proposed as an alternative to the MSPAI algorithm and its applicability demonstrated. It has been shown that the stochastic Monte Carlo approach is able to produce preconditioners of comparable quality to the deterministic approach used in MSPAI. The proposed approach enabled us to generate preconditioners efficiently (faster) and with good scaling properties outperforming the deterministic approach, especially for larger problem sizes.

Monte Carlo Method approach is a promising tool to solve the steady state heat transfer equation $-k\Delta T = 0$ in order to obtain effective homogenized heat conductivity coefficient for the porous Siliconized Silicon Carbide material, Margenov [10] propose to use MPI parallelized preconditioned conjugate gradient method with a preconditioner.

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REFERENCES

[1] J. Strassburg and V. Alexandrov, “Enhancing Monte Carlo Preconditioning Methods for Matrix Computations”, *Procedia Computer Science*, Vol. 29, pages 1580-1589, 2014.

[2] G.H. Golub, C. Loan, “Matrix computations”, *Johns Hopkins University Press*, ISBN 9780801854149, 1996 .

[3] M. Ferronato, E.Chow, K.Phoon, “Preconditioning Techniques for Sparse Linear Systems”, *Journal of Applied Mathematics*, Hindawi Publishing Corporation, Vol. 2012, article-id:518165, 2012.

[4] G. Allon, M. Benzi, and L. Giraud, “Sparse approximate inverse preconditioning for dense linear systems arising in computational electromagnetics”, *Numerical Algorithms*, vol. 16, num. 1, pages 115, 1997.

[5] M. Benzi, C. Meyer, and M. Tuma, “A Sparse Approximate Inversepreconditioner for the Conjugate Gradient Method”, *SIAM Journal on Scientific Computing*, Vol.5, pages 11351149, 1996.

[6] T. Huckle, A. Kallischko, A. Roy, M. Sedlacek, and T. Weinzierl, “Anefficient parallel implementation of the MSPAI preconditioner, Parallel Computing”, *Parallel Matrix Algorithms and Applications*, vol.36, num. 56, pages 273284, 2010.

[7] V. Alexandrov, E. Atanassov, I. Dimov, S. Branford, A. Thandavan and C. Weihrauch, “Parallel Hybrid Monte Carlo Algorithms for Matrix Computations”, In V. Sunderam, G. Albada, P. Sloot, and J. Dongarra, editors, *Computational Science* ICCS 2005, vol. 3516 of Lecture Notes in Computer Science, pages 752759. Springer Berlin / Heidelberg, 2005.

[8] V. Alexandrov and A. Karaivanova, “Parallel Monte Carlo algorithms for sparse SLAE using MPI”, in *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, pages 283290, Springer, 1999.

[9] S. Branford, “Hybrid Monte Carlo Methods for Linear Algebra Problems”, PhD thesis, *School of Systems Engineering*, The University of Reading, April 2009.

[10] S. Margenov, “Robust multilevel methods for strongly heterogeneous problems and supercomputing applications in porous media”, plenary talk, *5th International Conference on Porous Media*, Prague, Czech Republic, May 21-24, 2013.