

On Advanced Monte Carlo Methods for Linear Algebra on Advanced Accelerator Architectures

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Abstract—In this paper we present computational experiments with the Markov Chain Monte Carlo Matrix Inversion ((MC)²MI) on several accelerator architectures and investigate their impact on performance and scalability of the method. The method is used as a preconditioner and for solving the corresponding system of linear equations iterative methods, such as generalized minimal residuals (GMRES) or bi-conjugate gradient (stabilized) (BICGstab), are used.

Numerical experiments are carried out to highlight the benefits and deficiencies of both approaches and to assess their overall usefulness in light of scalability of the method.

Index Terms—Monte Carlo Matrix Inversion, Scalable Hybrid Algorithms for Linear Algebra, accelerators

I. INTRODUCTION

Solving systems of linear algebraic equations (SLAE) in the form of $Bx = b$ or inverting a matrix B is of unquestionable importance in many scientific fields. Iterative solvers are used widely to compute the solutions of these systems and such approaches are often the method of choice due to their predictability and reliability when considering accuracy and speed. They, however, may become prohibitive for large-scale problems as they can be very time consuming to compute. The complexity of these methods, in the serial case, is $O(kn^2)$ for dense matrices in the iterative methods case and $O(n^3)$ for direct methods with dense matrices while solving SLAE if common elimination or annihilation schemes (e.g. Gaussian elimination, Gauss-Jordan methods) are employed [1]. Therefore, these algorithms often rely on preconditioners to speed up the computations and/or to ensure faster convergence.

Monte Carlo (MC) methods complexity is linear in matrix size [2], [3] and can quickly yield a rough estimate of the solution by sampling a random 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. Therefore, it should be pointed out, that Monte Carlo methods may be efficiently used as preconditioners.

Depending on the method used to compute the preconditioner, the savings and end-results vary. A very sparse preconditioner may be computed quickly, but it is unlikely to greatly reduce the run time to solution. On the other hand, computing a rather dense preconditioner is computationally

expensive and might be time or cost prohibitive. Therefore, finding a good preconditioner that is computationally efficient, while still providing substantial improvement to the iterative solution process, is a worthwhile research topic.

A variety of parallel Monte Carlo methods have been developed within the past 20 years. A comprehensive compendium of the Monte Carlo functions and strategies of parallelization can be found in [2]–[6].

In this work we present an enhanced version of a SPAI (SParse Approximate Inverse) preconditioner that is based on parallel Monte Carlo methods presented in [2] and [3]. This new optimized version is compared against the previous one, taken as a baseline, as well as against MSPAI, which is the main accepted deterministic algorithm for SPAI preconditioning. Our results show that the Monte Carlo-based algorithm can be used instead of MSPAI to reduce the computation time and resource usage while producing results with similar or better quality.

Also a scalability analysis is carried out, showing that the random patterns in the memory access have a strong influence on the performance of the algorithm. Further research, to solve this issues, is proposed within the context of quasi-Monte Carlo Methods.

The next section gives an overview of related work. Monte Carlo methods, and the specific matrix inversion algorithm that is discussed as a SPAI preconditioner, are presented in section III. Section IV presents parallel approach of the Monte Carlo and the hybrid algorithm. Section IV shows the approach and methodology applied in the enhancement of the parallel implementations. Sections V and VI present corresponding results and analysis of the implementations. The conclusion VII summarises the results and outlines the future work.

II. RELATED WORK

Research efforts in the past have been directed towards optimizing the approach of sparse approximate inverse preconditioners. Improvements to the computation of the Frobenius norm have been proposed for example by concentrating on sparse pattern selection strategies [7], or building a symmetric preconditioner by averaging off-diagonal entries [8]. Further, it has been shown that the sparse approximate inverse

preconditioning approach is also a viable course of action on large-scale dense linear systems [9]. This is of special interest to us, as the Monte Carlo method we are proposing in this paper is part of a bigger family. It includes serial and parallel Monte Carlo algorithms for the inversion of sparse, as well as dense matrices, and the solution of systems of linear algebraic equations. The proposed Monte Carlo algorithm has been developed and enhanced in the last decades, and several key advances in serial and parallel Monte Carlo methods for solving such problems have been made [10]–[12]. There has been an increased research interest in parallel Monte Carlo methods for linear algebra in the past few years, and recent example is the Monte Carlo Synthetic Acceleration (MCSA) developed through MCREX project at ORNL [13]. Future work that deals with a parallel implementation of the presented algorithm is being considered further in this section and in section III.

In the past there have been differing approaches and advances towards a parallelisation of the SPAI preconditioner. In recent years the class of Frobenius norm minimizations that has been used in the original SPAI implementation [14] 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 [15]).

This version provides a class of modified preconditioners such as MILU (modified ILU), interface probing techniques and probing constraints to the original SPAI, apart from a more efficient, parallel Frobenius norm minimization. Further, this package also provides two novel optimization techniques. One option is using a dictionary in order to avoid redundant calculations, and to serve as a lookup table. The second option is an option to switch to a less computationally intensive, sparse QR decomposition whenever possible. This optimized code runs in parallel, together with a dynamic load balancing.

A. Using SParse Approximate Inverse as Preconditioner (SPAI)

The SPAI algorithm [16] is used to compute a sparse approximate inverse matrix M for a given sparse input matrix B . This is done by minimizing $\|BM - I\|_F$. The algorithm explicitly computes the approximate inverse, which is intended to be applied as a preconditioner of an iterative method. The SPAI application provides the option to fix the sparsity pattern of the approximate inverse a priori or capture it automatically. Since the introduction of the original SPAI in 1996, several advances, building upon the initial implementation, have been made. Two newer implementations are provided by the original authors, the aforementioned MSPAI, and the highly scalable Factorized SParse Approximate Inverse (FSPAI [17]). The intended use of both differs depending on the problem at hand. Whereas MSPAI is used as a preconditioner for large sparse and ill-conditioned systems of linear equations, FSPAI is applicable only to symmetric positive definite systems of this kind. FSPAI is based around an inherently parallel implementation, generating the approximate inverse of the Cholesky factorization for the input matrix. MSPAI on the

other hand is using an extension of the well-known Frobenius norm minimization that has been introduced in the original SPAI.

The algorithm attempts to solve a system of linear equations of the form $Bx = b$. Its input is a sparse, square coefficient matrix B . The right hand side vector b can either be provided by the user, or is arbitrarily defined by the software implementation. In the case of the SPAI application suite, if no right hand side vector is handed to the algorithm, it constructs one by multiplying matrix B with a vector consisting of all ones. In a general case, an input matrix B is passed to SPAI as a file. The program then computes a preconditioner using the Frobenius norm, afterwards it uses this intermediate result as an input to an appropriate solver.

III. MONTE CARLO APPROACH

Monte Carlo methods are probabilistic methods that use random numbers to either simulate a stochastic behaviour or to estimate the solution of a problem. They are good candidates for parallelisation due to the fact that, in principle, many independent samples are used to estimate the solution. These samples can be calculated in parallel, thereby speeding up the solution finding process. The so designed and developed parallel Monte Carlo methods possess the following main generic properties [2], [3]: efficient distribution of the compute data, minimum communication during the computation and increased precision being achieved by adding extra refinement computations. Consideration of all these properties naturally leads to scalable algorithms. It has to be noted that the quality of the solutions obtained using a Monte Carlo method is dependent upon the availability of independent (pseudo) random numbers, which is a concern in parallel environments.

A. Algorithm

The following procedure has been presented in [6] and allows to extend the Monte Carlo algorithm for processing diagonally dominant matrices, that is used as the foundation for this work (c.f. [18]), to the case of general matrices [2] [3].

Let us recall for simplicity the key details from [2], [3], [18]. We assume the general case where $\|B\| > 1$, with $\|\cdot\|$ being an arbitrary matrix norm, and consider the splitting

$$B = \hat{B} - C, \quad (1)$$

where the off-diagonal elements of \hat{B} are the same as those of B , and the diagonal elements of \hat{B} are defined as $\hat{b}_{ii} = b_{ii} + \alpha_i \|B\|$, choosing in most cases $\alpha_i > 1$ for $i = 1, 2, \dots, n$. For the simplicity of the algorithm it is often easier to fix single α . In the general case, $\|B\| > 1$, make the initial split $B = \hat{B} - C$. From this compute $A = B_1^{-1} B_2$, $B_1 = \text{diag}(\hat{B})$ which satisfies $\|A\| < 1$. Then the inverse of \hat{B} is generated by

$$[\hat{B}^{-1}]_{rr'} \approx \frac{1}{N} \sum_{s=1}^N \left[\sum_{(j|s_j=r')} W_j \right], \quad (2)$$

where $(j|s_j = r')$ means that only

$$W_j = \frac{a_{rs_1} a_{s_1 s_2} \cdots a_{s_{j-1} s_j}}{p_{rs_1} p_{s_1 s_2} \cdots p_{s_{j-1} s_j}},$$

for which $s_j = r'$ are included in the sum (2). Calculating $\|B\|$ can be an expensive operation, so any *a-priori* information allowing for a reasonable estimate here is useful but not strictly necessary. From this it is then necessary to work back and recover B^{-1} from \hat{B}^{-1} . To do this an iterative process ($k = n - 1, n - 2, \dots, 0$) is used on \hat{B}^{-1} :

$$B_k^{-1} = B_{k+1}^{-1} + \frac{B_{k+1}^{-1} S_{k+1} B_{k+1}^{-1}}{1 - \text{Tr}(B_{k+1}^{-1} S_{k+1})}, \quad (3)$$

where $B_n^{-1} = \hat{B}^{-1}$ and S_i is all zero except for the $\{ii\}^{th}$ component, which is from the matrix $S = \hat{B} - B$. Then $B^{-1} = B_0^{-1}$.

The make up of matrix S means that while (3) looks complicated it is, in fact simply an update of the matrix by a scaled outer product of the $(k + 1)^{th}$ column with the $(k + 1)^{th}$ row. There are obvious simplifications possible to ensure that many multiplications by zero are not performed. This method of splitting and recovery leads to Algorithm 1 [2], which details a MC algorithm for inverting general matrices and is given below for completeness. Further details on the recovery of the original inverse can be found in [19].

Algorithm 1: Monte Carlo Algorithm for Inverting General Matrices

- 1) Read in matrix B
 - a) Input matrix B , parameters ε and δ
- 2) Remove a set percentage of the smallest (in magnitude) entries of the matrix.
- 3) Calculate intermediate matrices (\hat{B}, B_1)
 - a) Split $B = \hat{B} - (\hat{B} - B)$, where \hat{B} is a diagonally dominant matrix
- 4) Apply the algorithm for inverting diagonally dominant matrices from [18] with $B = \hat{B}$ to obtain \hat{B}^{-1}
- 5) Recovery of B^{-1} from \hat{B}^{-1}
 - a) Compute $S = \hat{B} - B$
 - i) Let S_i for $i = 1, 2, \dots, n$ where each S_i has just one of the n non-zero elements of the matrix S
 - ii) Set $B_n^{-1} = \hat{B}^{-1}$
 - iii) Apply $B_{i-1}^{-1} = B_i^{-1} + \frac{B_i^{-1} S_i B_i^{-1}}{1 - \text{Tr}(B_i^{-1} S_i)}$ for $i = n, n - 1, \dots, 1$
 - b) Then $B^{-1} = B_0^{-1}$

Note that the second step is optional and is relevant only when a reduction in the amount of data being communicated is desired. Its influence has been investigated and the results are presented in sec. VI-B.

The above algorithm was modified to develop an MPI version of the algorithm. Several enhancements of the algorithm, as well as modifications concerning GPU implementation, are listed in the next section and were able to substantially

improve its performance in generating rough inverses of the input matrices. The result can then be used directly as a preconditioner for solving a system of linear algebraic equations or further improved. We propose the use of an iterative refinement process, a parallel filter, or a combination of the two to further enhance the quality of the preconditioner. The decision whether those additional steps are taken is based upon the required accuracy and can be freely selected, depending on user requirements.

IV. PARALLELIZATION DETAILS AND ISSUES

The previous algorithm can be split into the following 5 phases (Notice that phases 1 and 5 are only necessary when the initial matrix is not a *diagonally dominant matrix (ddm)*): 1) Initial matrix is transformed into a ddm, 2) Transformation of ddm for suitable *Neumann series expansion*, 3) Monte Carlo method is applied to calculate sparse approximation of the inverse matrix, 4) Given 2, calculate the inverse of the ddm from 3, 5) Recovery process is applied to calculate the inverse of the original matrix due to the transformation in 1. It must be noted that the last phase requires in general $\mathcal{O}(n^3)$ operations and hence is generally neglected. Prior numerical experiments have demonstrated that it is not compulsory to obtain an effective preconditioner.

This algorithm was originally designed for a HPC cluster composed of single-core compute nodes. It is written in C and uses the MPI library. It also makes use of the BeBOP sparse matrix converter [20] to translate the input matrix format into a CSR format.

A. MPI implementation

Matrices A , B_1 and P (the transition probability matrix) are calculated during the phases mentioned above. Note that $A = (I - C)$, $C = B_1^{-1} \hat{B}$ and $B_1 = \text{diag}(\hat{B})$. Then a procedure is called by all the processes in which the partitioning of the matrix A is carried out. The distribution of the work is done evenly when the number of rows is divisible by the number of processes. In the opposite case, the remaining rows are distributed among the smaller MPI processes (without including the Master process). After that, matrices A , B_1 and P are *broadcast* using `MPI_Broadcast()`. Then the Monte Carlo process (phase 3) is started in parallel by all MPI processes. During the Monte Carlo phase, each MPI process will calculate a piece of the inverse matrix of C (C^{-1}), using matrix A ; remember that $C = (I - A)$. Column-scaling by B_1^{-1} will then be applied to each row, to get the respective part of \hat{B}^{-1} (phase 4). After finishing the Monte Carlo process and phase 4, each process will send its part of the matrix (\hat{B}^{-1}) to the master process by calling `MPI_Send()`. The master process will perform a corresponding `MPI_Receive()` and will merge the received parts with its own. Given a concatenation issue due to the CSR format, the Send-Receive process has to be ordered, having to receive first the data from process 1, then process 2 and so on. Finally the last phase (5) is optionally executed by the master processes on matrix (\hat{B}^{-1}) to calculate B^{-1} . This step is optional and must

be enabled explicitly. This process is difficult to parallelize due to its iterative nature. On the other hand, using an approach in which each iteration is executed in parallel, would imply a high increment in the communications given, that a synchronization would be required at each iteration.

B. GPU implementaion

Regarding the GPU implementation it must be noted, that due to the irregular data access and comparatively short computation kernels the method appears to be ill-suited for a GPU. Nevertheless a GPU can be used to accelerate the computation of the preconditioner using (MC)²MI if care is taken to keep the GPU sufficiently busy.

If the requirement for a sparse inverse is abandoned the algorithm, with or without recovery, yields itself well to an implementation for GPUs. This restricts the dimensionality of the matrices the algorithm is applicable to those that fit entirely into the main memory of the accelerator device. If a preconditioner is to be computed using (MC)²MI on one or more GPUs for large, sparse, matrices a non-negligible amount of overhead is introduced in order to ensure that only the most relevant entries of the inverse are retained for each row. In a first implementation for NVIDIA GPUs the entire sparse inverse was stored on the device, along with the necessary (preprocessed) matrix. Since the number of different entries visited by a chain is not known a-priori the entire set of Markov Chains is simulated at once and used to fill a contiguous array corresponding to one row of the approximate inverse. Afterwards only a prescribed number of entries largest in magnitude are retained for the sparse approximate inverse. The rationale behind this is that if the inverse is itself considered as a Markov Chain only the entries largest in magnitude will contribute significantly to its inverse (the original matrix). As was the case with the previous implementation an extension to multiple GPUs is comparatively simple and has therefore been implemented.

V. ALGORITHMIC MODIFICATIONS

The original code, provided by Diego Dávila, was corrected to adhere to the MPI 3.0 standard and therefore be portable. This was crucial for performance analysis on the testing system c.f. sec. VI. Furthermore a parallelizable pseudo-random number generator (PRNG) was used to replace the original generator, which was not suited for parallel environments.

A. Matrix Reduction

The computation of an approximate inverse using Markov Chain Monte Carlo (MCMC) requires the knowledge of the whole state space - hence of the entire matrix A . The distribution of A among the parallel workers becomes increasingly expensive with growing matrix size.

An obvious way to accelerate the method is to reduce the amount of data being transferred, i.e., to reduce the number of non-zero entries of the matrix. Since the magnitude of the entries of A signifies its importance in the MCMC simulation we decided to drop a set percentage of the smallest entries

of the matrix. This modifies the linear system and hence the correctness of the approach had to be verified.

B. Implementation Specifics - MPI

As a first step the pseudo-random number generator used in the original version of the program was replaced by TRNG¹. This was necessary since the original code used the standard C PRNG, which does not possess a sufficiently long period to guarantee statistic independence of the Markov chains for large matrices. Additionally it is not designed for parallel environments. Both flaws are rectified by using TRNG.

The amount of communications has already been reduced to an almost-minimum in the previous implementation of (MC)²MI. In one iteration of the improvement of the code the broadcast of the transition probabilities (necessary for the MCMC simulation) was eliminated. Instead these probabilities were computed by every worker from its knowledge of A .

Furthermore a minor non-conformity to the MPI standard was eliminated, which made the code reliant upon a specific implementation of MPI, thus preventing the use of the preferred compiler and optimized MPI implementation on MareNostrum 4.

C. Implementation Specifics - GPU

Compared to the host machine the GPU has a very limited amount of memory and requires a more elaborate approach to memory handling. Due to memory constraints storage of a dense block of an inverse on the device is not feasible, and neither is on-the-fly transfer of computed entries to the host - due to latency constraints. We have opted to allocate and fill a block of the sparse inverse on the device and transfer it to the host matrix at the end of the computation. This differs from the MPI implementation in so far as the computation of each row requires additional memory management overhead but the final reduction of the separate blocks of the inverse is cheaper since the necessary storage and data layout is known beforehand. The downside being that for some matrices entries of the inverse may be lost for some rows, whilst others contain unused entries ($= 0$). This deficiency will be addressed in future versions of the GPU implementation. A further difference from the MPI implementation is the usage of $\alpha \cdot \|B\| \cdot \text{sgn}(B_{i,i})$ as entries of the matrix B_2 , as opposed to $\alpha \cdot \|B\|$. This ensures that even if the signs of the diagonal elements are non-uniform the augmentation will yield a diagonally-dominant matrix. This approach also reduces the perturbation of the original matrix caused by the augmentation procedure. Usage of multiple GPUs was implemented by letting each device be controlled by a dedicated OpenMP process.

VI. NUMERICAL EXPERIMENTS

A. Execution Environment

The set of matrices chosen for the assessment of the proposed modifications is listed in tbl. I. The set contains symmetric and non-symmetric matrices of varying sizes and filling fractions. Matrices `nonsym_r3_a11` and `sym_r6_a11`

¹<https://www.numbercrunch.de/trng>

TABLE I
MATRIX SET.

Matrix	Dimension	Non-zeros	Sparsity
ID1_2_P3_7_stiffness	514,369 × 514,369	8,702,911	0.003%
nonsym_r3_a11	20,930 × 20,930	638,733	0.15%
rd2048_noL	2,048 × 2,048	12,032	0.29%
sym_r6_a11	1,314,306 × 1,314,306	36,951,316	0.02%

have been provided by our collaborators and are representative of systems occurring in climate simulations. The matrix `rd2048` has been taken from the Florida University’s matrix collection and `ID1_2_P3_7_stiffness` is a discretized Laplacian using cubic finite elements on a fine mesh.

Almost all numerical experiments were carried out on the MareNostrum 4 (MN4) cluster at the Barcelona Supercomputing Centre in Spain. The machine consists of 3456 nodes with 2 Intel Xeon Platinum 8160@2.1 GHz per node. The nodes are connected via Intel Omni-Path HFI Silicon 100 (100 GBit/s) adapters. The evaluation of the preconditioners was performed using 3 nodes of MareNostrum 4. The number was chosen arbitrary but kept constant, thereby ensuring that the execution times of the preconditioned iterative solvers would be comparable for preconditioners computed using CPUs and GPUs.

Earlier experiments evaluating the performance of Tesla K80 GPUs were performed on a GPU workstation and on the institutional cluster set up by AL at the Institute for Theoretical Physics. Said cluster consists of 12 Nodes connected by a common 10Gbit ethernet network and each containing two Intel Xeon E5-2640v4 CPUs.

On MN4 both, $(MC)^2MI$ and MSPAI, were compiled using the INTEL compiler (v 17.0.4) and MPI implementation (build 20170405). Execution was carried out in exclusive mode with CPU clock speeds fixed to the second-highest speed-step using batch script options to SLURM.

The computed preconditioners were validated using the GMRES implementation provided by Trilinos(v. 12.10.1).

For most experiments a precision of $\epsilon, \delta = 2^{-4}$ was chosen for MSPAI and MCMCMI. Additionally, for MCMCMI the scaling of the diagonal was performed using $\alpha = 5$.

To ensure that the GPUs are well-utilized a precision of $\epsilon, \delta \in \{0.01, 0.005\}$ has been chosen in the numerical experiments comparing GPUs and CPUs. This choice provides a first limit on the range of parameters for which the use of $(MC)^2MI$ on accelerators could be considered.

B. Fitness of purpose

All of the numerical experiments in this section have been carried out with a fixed execution configuration of 48 processes spread evenly over two nodes of MN4.

The total execution time (preconditioner computation and GMRES execution) is provided in fig. 1 and 2 for two different matrices. Henceforth `none` refers to the method without preconditioner and the preconditioner (computed using MSPAI or MCMCMI) is designated *P*. MSPAI is more effective in the case of the larger of the two matrices but only in the case

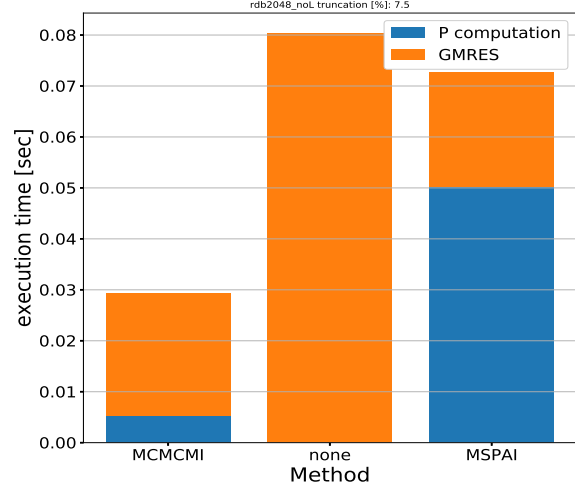


Fig. 1. Total execution time for `rd2048_noL` with 7.5% of the value range of the entries removed.

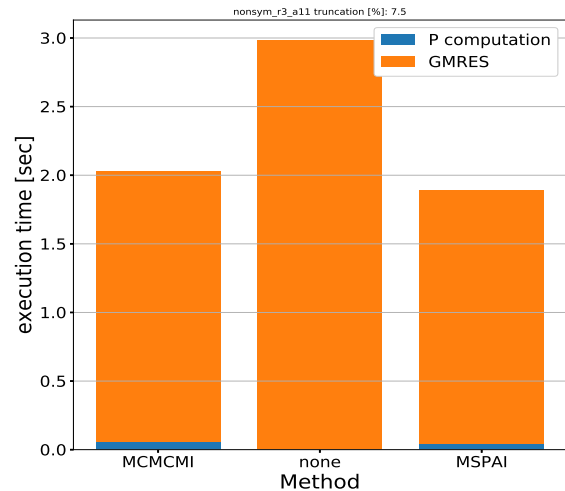


Fig. 2. Total execution time for `nonsym_r3_a11` with 7.5% of the value range of the entries removed.

when $> 7\%$ of the value range of the elements of the matrix have been dropped. If less elements are removed (c.f. fig. 4) $(MC)^2MI$ will require less computation time.

In fig. 3 one can see, that the idea of removing a set amount of small elements may well accelerate the computation of the preconditioner. The outcome depends on the matrix and there will, in general, be an optimal amount of negligible entries for each matrix. In the case of `nonsym_r3_a11` that amount is between 2% and 6%. If more entries are removed the amount of information contained in the matrix becomes insufficient to create a good preconditioner.

As can be seen in fig. 4 the reduction of the amount of

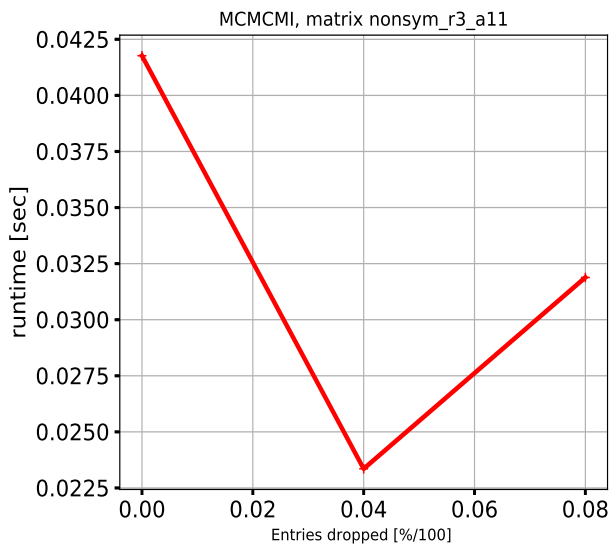


Fig. 3. Execution time of the preconditioner computation.

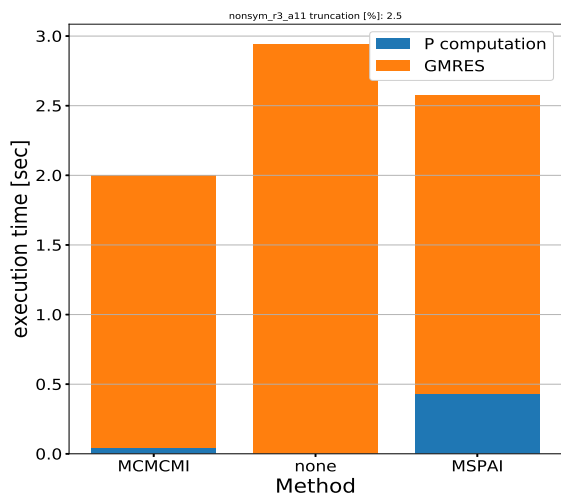


Fig. 4. Total execution time for `nonsym_r3_a11`. When using GMRES with a termination condition $\frac{\|r\|_2}{\|b\|_2} \leq 10^{-6}$ and a precision of $\epsilon = 0.0625$ for the computation of the preconditioner and removing 2.5% of the entries smallest in magnitude.

information required to be broadcast, coupled with a moderate precision requirements for the approximate inverse will result in a shorter overall execution time when a preconditioner is computed using $(MC)^2MI$. This demonstrates that the method may be used in cases where the preconditioner has to be recomputed every time prior to its usage (i.e., in iterative methods where the matrix changes in every step).

Finally we attempted to use the Monte Carlo method to compute a preconditioner for the `bcsstk38` matrix of the sparse matrix collection, whose condition number surpasses $5 \cdot 10^{16}$ and which has a non-trivial nullity. Accordingly the

iterative solver used to test the preconditioner for this case (BiCGstab) fails to converge if no preconditioner is used, reaching the defined upper bound of 30000 iterations for a desired precision of $\frac{\|r\|_2}{\|b\|_2} \leq 0.45$. Using the preconditioner computed with $(MC)^2MI$ for $\epsilon = 0.01$ enables BiCGstab to converge, reducing the number of steps required to achieve the desired bound to 3852 and the total execution time (preconditioner + BiCGstab) from 9.7[sec] to 1.3[sec] - in this case using 96 instead of 48 processes.

C. Scaling to Moderate Number of Cores/Processors

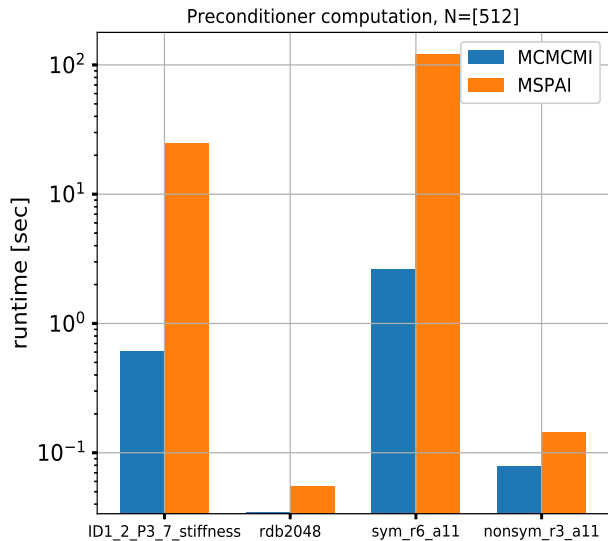


Fig. 5. Execution time of the preconditioner computation for different matrices. Transition probabilities were computed by the master process and broadcast to the workers.

In fig. 5 the execution time of the preconditioner computation using 512 processes is shown for all matrices of tbl. I. It is obvious that $(MC)^2MI$ is superior to MSPAI in every case, with the largest savings being achieved for rather dense or very large matrices. Note that this is purely a comparison of the time required to compute a preconditioner using the appropriate method.

D. $(MC)^2MI$ on Accelerators

In a final set of numerical experiments we investigated the feasibility of using accelerators, specifically NVIDIA GPUs to speed up the computation of the preconditioners using $(MC)^2MI$. To this end the algorithm delineated in sec. III-A was implemented in CUDA and evaluated for matrices of tbl. I. Here we have to note that unlike for the pure MPI implementation a sufficiently small ϵ, δ (i.e., a high precision) is necessary to fully utilise the GPU as such a precision of $\epsilon = 0.01$ was chosen for the experiments. The latter were performed on Tesla K80 as well as Volta V100 devices using a variable number of GPUs.

Fig. 6 shows the typical behaviour of the Markov Chain Monte-Carlo method when implemented on GPUs using

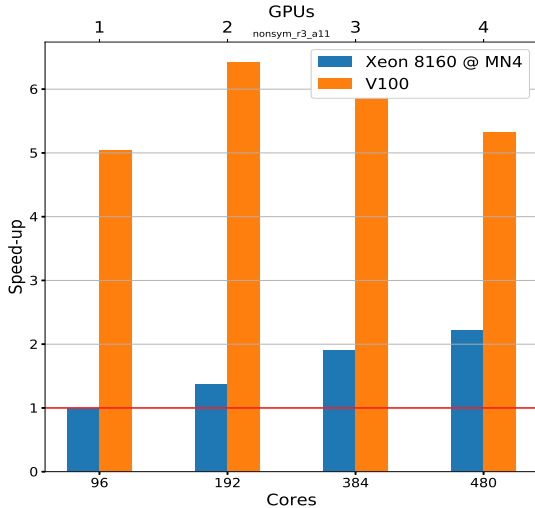


Fig. 6. Speed-up of the calculation performed on a NVIDIA V100 in comparison to CPU cores for the nonsym_r3_a11 matrix and a precision of $\epsilon = 0.01$. The red line represents $1\times$.

nonsym_r3_a11 as an example. The execution time of the pure MPI implementation on two nodes of MareNostrum 4 serves as a reference. It is immediately obvious that a GPU is significantly faster by up to a factor of ~ 6.5 . The speed-up decreases when using 3 or more GPUs, which is to be attributed to the overhead introduced by the memory management. Profiling results indicate that in this case the time required to sort the entries of the inverse row matches the time required to compute them using $(MC)^2MI$. An additional factor limiting the performance, which has not yet been eliminated, is the necessity to compact the pre-processed matrix on the host before the MC iteration may be performed. In the present case this reduces the achievable speed-up by a factor of ~ 2 . Note that for this comparison the α parameter was chosen to be 4.0 instead of 5.0. This change results in a 20% longer execution time. The effect of an increased amount of work can be seen in fig. 7, where the speed-up achieved in comparison to an older CPU architecture is shown. The comparison is provided due to the given CPU and GPU resources being an easily accessible resource maintained by AL at the Institute for Theoretical Physics in Tübingen as well as to their availability to common users (in comparison to multiple V100). The speed-up provided by the older Teslas is limited for the given case due to the sparsity of the matrix. Further numerical experiments indicate that utilisation of the GPU may be improved by increasing the desired precision.

Finally fig. 8 shows the speed-up achieved by two generations of NVIDIA GPUs for the nonsym_r3_a11 matrix compared to the small institutional cluster in Tübingen. As has been demonstrated in fig. 6 the amount of work provided by this matrix is insufficient to mask the overhead of data management and the CPU portion of the preprocessing stage. Both are currently being adressed in development. The striking

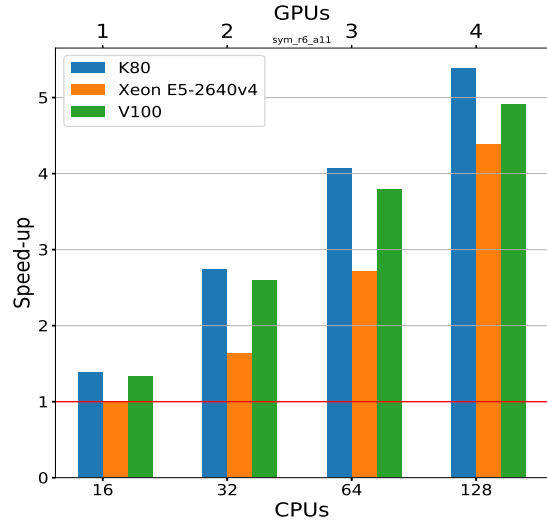


Fig. 7. Speed-up of the calculation performed on a NVIDIA V100 in comparison to CPU cores of a Broadwell cluster and to NVIDIA K80 GPUs for the sym_r6_a11 matrix. The red line represents $1\times$.

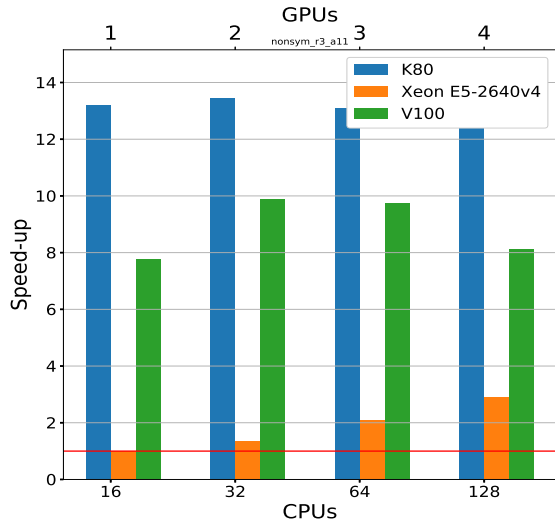


Fig. 8. Speed-up of the calculation performed on a NVIDIA V100 in comparison to CPU cores of a Broadwell cluster and to NVIDIA K80 GPUs for the nonsym_r3_a11 matrix. The red line represents $1\times$.

feature is that the newer architecture appears to perform worse than the older one. We believe this to be an artefact due to an insufficient optimization of the GPU code for the NVIDIA Volta architecture, since it has been originally developed and optimized for the Kepler architecture.

VII. CONCLUSIONS AND FUTURE WORK

In summary we have shown that the computation of a preconditioner using $(MC)^2MI$ method can be accelerated by ballancing the precision with which the preconditioner is calculated as well as dropping entries of the original matrix

depending on the precision. The quality of the resulting preconditioner does not deteriorate as fast as is the case if the same approach is applied to MSPAI. The approach shows that in most cases the number of iterations required by GMRES or BiCGstab to solve the resulting system of Linear Algebraic Equations can be substantially reduced. If only a rough estimate of the inverse is required the combination of (MC)²MI and an appropriate (for the matrix type) iterative method can result in a lower total execution time, when compared to a non-preconditioned method.

The numerical experiments indicate that for $\epsilon, \delta < 0.01$ (at high precisions) the usage of GPUs should be considered. It has been demonstrated, that despite the apparent bad suitability for a GPU the (MC)²MI method may still be successfully used with it. Future work will focus on a merging of the CPU and GPU implementations using the tasking constructs of OpenMP 4.5. This approach promises to reduce the overhead of memory management on the GPU whilst simultaneously utilising the host to its full extend. Preliminary profiling suggests a potential increase in performance by a factor of $\gtrsim 2$. Furthermore an integrated application test for the Markov Chain Monte Carlo preconditioners is planned, to observe the performance on a wider set of matrices than the set used so far, as well as an investigation of the potential for a MPI+CUDA parallelisation of the method. On the host side the pure MPI implementation will be rewritten to utilise hybrid parallelism using MPI+OpenMP and implement a better load balancing.

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APPENDIX A

ARTIFACT DESCRIPTION APPENDIX: ON ADVANCED MONTE CARLO METHODS FOR LINEAR ALGEBRA ON ADVANCED ACCELERATOR ARCHITECTURES

A. Abstract

We present observations on the performance of the implementation of the Markov Chain Matrix Inversion method for different versions of the x86 CPU architecture (Broadwell, Skylake) and NVIDIA GPUs of the Kepler and Volta architectures. The performance and correctness of the method as a means of obtaining preconditioners for iterative systems is evaluated using Trilinos and compared to MSPAI.

The CPU (MPI) and GPU implementations of the Markov Chain method are compared to each other to determine the feasibility and limitations of a GPU implementation of the method.

B. Description

1) Check-list (artifact meta information):

- **Algorithm:** Markov Chain Monte Carlo Matrix Inversion, pre-allocated row storage on CPU, stream compaction and sorting on GPU
- **Compilation:** *MareNostrum 4*: INTEL toolchain v 2017.4, with `-xHost -O3` optimization flags. *ITP Tübingen*: GCC v. 6.3.1 (20170216) with `-march=native -O3 -mfma -malign-data=cacheline` optimization flags.
- **Run-time environment:** *MareNostrum 4*: SLES 12-SP2, Kernel: 4.4.120-92.70. *ITP Tübingen*: CentOS 7, Kernel: 3.10.0-514.26.2 (no KPTI mitigation). *CTE Power* RHEL 7.4, Kernel: 4.11.0-44
- **Hardware:** *MareNostrum 4* Nodes with 2 Xeon Platinum 8160 CPUs each. 96GB RAM per node. Connected via 100Gbit Intel Omni-Path HFI Silicon 100 in a fat tree network topology. *CTE Power* (V100 machine) Nodes with 2 x IBM Power9 8335-GTG 3.00GHz each. 512GB RAM and 4 V100 GPUs with 16GB HBM2 VRAM. *ITP Tübingen* Nodes with 2 Intel Xeon E5-2640v4 CPUs each. 128GB RAM per node. Connected via 10Gbit Ethernet, star network topology. Network parameters not optimized.
- **Execution:** Via SLURM scheduler.
- **Output:** Execution times (in milliseconds) are printed to standard output and processed from there.
- **Experiment workflow:** Automated filling of SLURM script templates and automated enqueueing of the jobs by a generator script written in Python. An index of numerical experiments is stored in the top-level directory where the generator script was called. This index is used to collect and pre-process the results using an evaluation script written in Python. Graphical analysis of the data is performed using a Jupyter notebook.
- **Experiment customization:** Execution configuration of the job scripts customized to stay within storage quota. K80 experiments driven by a separate script.
- **Publicly available?:** Currently not publicly available. Access to the authors repository can be granted upon request.

2) *How software can be obtained:* The GPU implementation can be obtained through the authors private Bitbucket repository upon request. The CPU implementation will be publicly available from said repository by the end of November.

3) *Hardware dependencies:* The optimal block and grid size of the GPU implementation are dependent on the used GPU and have hence to be adapted accordingly. A rough

search for minimal execution time using the `sym_r6_a11` matrix suggested a block size of 96 threads (3 warps) and a grid size of 170 for the Volta GPUs.

4) Software dependencies:

CPU: The CPU implementation uses version 4.15 of Tina's Random Number Generator library. The library implements parallel pseudorandom number generators and is therefore key to the correctness of the presented method. It is available from www.numbercrunch.de/trng. It also relies on the BeBOP sparse matrix library to handle CRS matrices.

GPU: The GPU version has been implemented in C++ and CUDA. Of the CUDA libraries it utilises cuRAND in the core routines and cuBLAS in some auxiliary routines and for testing purposes. The V100 compilation was performed using CUDA Toolkit v9.1, the K80 compilation was performed using CUDA Toolkit v8.0. Parsing of execution parameters is done using BOOST program options library (tested with BOOST 1.{56, 64, 66}) and the Eigen linear algebra template library (<http://http://eigen.tuxfamily.org/>) to handle sparse matrices with a minor correction in the unsupported `saveMarket` routine.

Testing: Correctness checks of the preconditioners are carried out using a parallel implementation of CG/CGS/BiCG(stab)/GMRES. The code performing these checks has been written in C++ and uses Trilinos (v 12.10.1 on MN4, 12.13 on the ITP cluster).

On *MareNostrum 4* both the CPU implementation and the preconditioner testing code rely on the MPI implementation provided by INTEL. On the ITP cluster the MPI library is MPICH 3.2.1.

C. Installation

1) *MareNostrum 4:* The MPI implementation is compiled using a simple Makefile and utilising the INTEL compiler `mpiicc` to compile all but the TRNG files, which are compiled using `mpiicpc`. Compiler options are `-O3 -xHost -DPRECISION=1 -DP_UMMAO=0 -DVER=3.0` and linked to BeBOP libraries via `-Wl, -rpath=$(USRLIB) -lbebop_util -lsparse_matrix_converter` and statically linked to the TRNG library `libtrng4.a`

D. CTE-POWER

The GPU code is compiled using `nvcc` v9.1.85 with the following compiler flags

```
-std=c++11 -m64 -Wno-deprecated-declarations
-D EIGEN_NO_CUDA -arch=compute_70 -rdc=true
-DNDEBUG -O3
```

 using a simple makefile which constitutes just a collection of source files to be compiled and linked.

1) *ITP Tübingen:* The process is the same as for the other two, except for the optimization flags: `-O3 -march=broadwell -ftree-vectorize -funroll-loops -ffunction-sections -malign-data=cacheline`

E. Experiment workflow

The numerical experiments carried out on the MareNostrum 4 and CTE-Power clusters at the Barcelona Supercomputing Centre were executed in two stages:

1) **Stage:** Generate a set of preconditioners

The numerical experiments were executed using the SLURM scheduler. A generator script was written in Python. Said script accepts a set of template files for the preconditioner computation and testing parameters as well as job scripts for generation and testing of preconditioners. The execution parameters are collected in a separate parameter file and indexed by matrix in dictionaries. The user may provide a desired number of repetitions the experiments will be run (10 as a default) - each repetition will generate a preconditioner which will be stored with a file name containing the repetition number. The generator script generates a directory structure and an index file for the desired numerical experiments. All of the jobs to generate preconditioners are launched using a simple launcher script and the generated index file.

2) **Stage:** Test the preconditioners.

The tests of the generated preconditioners must be enqueued manually by the user since no guarantee can be made, that storage quota will not be reached during the generation phase. The `--dependency=singleton` option for SLURM has been used to ensure that the tests of generated preconditioners are started only after all repetitions of the generation script have been run. The testing stage produces, for each parameter set (experiment) and each repetition a unique text file containing the results of the execution of the chosen iterative method.

Execution on the K80s differs in so far as the second stage is omitted and the first one is executed sequentially by a dedicated Python script into which all the required parameters are hard-coded.

F. Evaluation and expected result

Evaluation of the numerical experiments is carried out by first consolidating the results into a single Pandas data frame. This is done automatically by a preprocessing script which utilises the index of experiments generated in the first stage of the experiments. The collected data is stored in CSV format. It is then imported into a Jupyter notebook and further evaluation and visualization is performed in accordance with the requirements documented therein.

Raw results include plain-text output files from the SLURM scheduler and the code used to test the preconditioners. Intermediate results are consolidated into CSV files and final results consist of a collection of plots showing the speed-up and execution time of different parameter configurations for different matrices. The images are stored in EPS format.

G. Notes

The MSPAI preconditioner may be obtained at <https://www5.in.tum.de/wiki/index.php/MSPAI> and is compiled with the provided Makefiles, which require the ATLAS library.