Using Approximate Computing for the Calculation of Inverse Matrix $p$-th Roots

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Abstract—Approximate computing has shown to provide new ways to improve performance and power consumption of error-resilient applications. While many of these applications can be found in image processing, data classification or machine learning, we demonstrate its suitability to a problem from scientific computing. Utilizing the self-correcting behavior of iterative algorithms, we show that approximate computing can be applied to the calculation of inverse matrix $p$-th roots which are required in many applications in scientific computing. Results show great opportunities to reduce the computational effort and bandwidth required for the execution of the discussed algorithm, especially when targeting special accelerator hardware.

I. INTRODUCTION

Approximate computing has gained a lot of attention over the last years as a technique to accelerate systems or applications or increase their power efficiency by allowing errors or a loss of precision. Many different techniques have been proposed, such as bit truncation, approximate adder circuits, analog computing and usage of neural networks. Typical applications for approximate computing are from the areas of image processing, data classification and machine learning where small variations in the output are barely noticeable and can be tolerated.

Chippa et al. [1] showed that additionally, iterative algorithms are often inherently resilient to approximation because errors introduced in one iteration are likely to be fixed in later iterations. Iterative algorithms can be found for many numeric problems encountered in scientific computing. Klavik et al. [2] demonstrated that the Conjugate Gradient method used to solve systems of linear equations performs well using low precision arithmetic for the computationally expensive parts. Schöll et al. [3], [4] describe the application of efficient fault-tolerance to Preconditioned Conjugate Gradient in order to execute this algorithm on approximate hardware. In this work we focus on an iterative algorithm which is used to calculate the inverse $p$-th root $A^{-1/p}$ for a given symmetric positive definite matrix $A$.

Calculating inverse $p$-th roots is important for a large variety of different applications in scientific computing such as preconditioning, Kalman filtering, non-linear optimization, solving linear least squares problems and systems of linear equations, as well as generalized eigenvalue problems, particularly solving Schrödinger and Maxwell equations, to name just a few. While for the former applications an approximation is generally sufficient, the latter ought to be solved exactly. Nevertheless, as will be demonstrated in the following, it is even possible to obtain essentially exact results using the approximate computing paradigm.

In this work, we contribute an analysis of the error resiliency of the given algorithm and discuss the potential benefits of using low-precision arithmetic and data representation in applications using this algorithm to calculate inverse $p$-th roots of large matrices.

II. CALCULATION OF INVERSE MATRIX $p$-TH ROOTS

The iterative algorithm discussed in this work was first described by Bini et al. [5]. We briefly describe the algorithm in the following. Let $C_k$, $k = 0, 1, \ldots$ be the sequence of intermediate result matrices. Starting with an initial guess $C_0$, in each iteration the result is refined by

$$C_{k+1} = \frac{1}{p} \left( (p+1)C_k - C_k^{p+1}A \right)$$  \hspace{1cm} (1)

If the initial guess $C_0$ was already close to $A^{-1/p}$ such that

$$\|I - C_0^p A\|_2 < 1$$  \hspace{1cm} (2)

$C_k$ for $k \to \infty$ converges against $A^{-1/p}$. For $p = 1$ the algorithm corresponds to the well-known Newton-Schulz method [6] used to iteratively calculate inverse matrices.

There are different possible choices for $C_0$. For our evaluation we use

$$C_0 = (\|A\|_1 \cdot \|A\|_\infty)^{-1} A^T$$  \hspace{1cm} (3)

which is proven to always fulfill constraint (2) and therefore guarantees convergence [7].

III. USE-CASES FOR APPROXIMATION

Approximate computing is applicable to the presented algorithm in different use-cases. As described, some applications benefit from having an approximation of inverse $p$-th roots if these can be calculated quickly. However, even if exact results are required, the iterative nature of the algorithm allows using imprecise arithmetic for the majority of iterations and then refining the result in few iterations using precise arithmetic. There are different scenarios that suggest using approximate
arithmetic or approximate storage which are discussed in the following.

A. Approximate Arithmetic

Approximating the arithmetic operations in the presented algorithm or using low precision can be beneficial for overall performance or the energy efficiency, depending on the underlying compute platform. Recent GPUs targeting the data center, such as the NVIDIA Tesla P100, support half-precision floating-point operations, doubling the peak performance compared to single-precision arithmetic and quadrupling it compared to double-precision arithmetic.

For custom hardware accelerators, the data width also plays an important role. Currently, FPGAs are becoming more and more common as an accelerator platform, next to CPUs and GPUs. Reduced precision can significantly lower resource requirements on FPGAs, e.g. for current Xilinx devices using less than 17 stored mantissa bits reduces the number of required DSPs by half compared to single-precision. For custom CMOS designs it has been shown that the power consumption of multipliers rises at least quadratically with the number of input bits. Because the delay increases too, this has an amplified effect on the energy consumption. Using fixed-point arithmetic with only few bits can further simplify custom designs for FPGAs or ASICs.

Lastly, more advanced approximate computing techniques such as biased voltage over-scaling, approximate arithmetic circuits or specifically targeted overclocking have the potential to improve clock speeds or lower the complexity and power consumption of custom hardware designs.

B. Approximate Storage

In applications using the examined algorithm, data sets are typically very large, i.e. calculations need to be performed on matrices containing billions of entries. This not only leads to great computational demands but also requires large memories and high memory bandwidth. Even if calculations are performed precisely, the required memory space and bandwidth can be reduced by storing intermediate results after each iteration as well as the input data itself with less precision, using fewer bits.

If the computations are to be performed on special hardware accelerators such as GPUs or FPGAs, the data needs to be transferred between the host and these devices. In this case, bandwidth quickly becomes a limiting factor, motivating the use of low precision representations for the transferred data.

In the scope of this work, we evaluate the impact of both, low precision arithmetic and low precision storage of intermediate results, on the examined algorithm.

IV. Evaluation

To assess the resiliency of the given algorithm to certain errors, we simulate simple approximation techniques. First, we use custom-precision floating-point and fixed-point arithmetic for all involved calculations in order to get an understanding of the required data ranges and precision. Second, we restrict the use of these data types to the input data and stored intermediate results, simulating approximate storage or data exchange of the involved matrices.

A. Problem and Data Set

We use the examined algorithm to efficiently compute two particularly time-consuming kernels of effective single-particle Schrödinger equations, which are to orthogonalize and solve the corresponding generalized eigenvalue problem. For that purpose, we first calculate the inverse square-root \( S^{-1/2} \) of the so-called overlap matrix \( S \), which is of dimension \( N \times N \) and whose elements read as \( S_{ij} = \langle \varphi_i | \varphi_j \rangle \), where \( \varphi_i \) are the \( N \) non-orthogonal basis functions spanning the Hilbert space, and subsequently \( S^{-1} \) to efficiently solve the resulting orthogonalized matrix eigenvalue equation.

Figure 1 shows an overlap matrix \( S \) of size \( N = 786 \) which we used for our evaluation. It is a symmetric positive definite matrix with 25% non-zero elements in the range of \([-1, 1]\), representing a system of 128 H\(_2\)O molecules. For larger matrices density decreases to 12.4% (\( N = 1572 \)), 6.2% (\( N = 3072 \)) and 3.1% (\( N = 6144 \)) non-zero elements. This is a manifestation of the nearsightedness principle of electronic matter and the foundation of linear scaling electronic algorithms.

B. Methodology

For the presented simulations we use Python along with NumPy and SciPy, which provide the required data structures and numeric operations. This allows us to define entirely custom data types, e.g. floating-point types with a custom number of bits in the exponent and mantissa, and fixed-point types with a selectable number of bits and selectable scaling factor. Implementing basic arithmetic operations like addition, subtraction and multiplication for our custom data types enables NumPy to use these data types in its own array data structures and numeric operations.
This approach allows a very flexible and fast implementation of simulators for different approximation techniques. Besides the mentioned floating-point and fixed-point data types, influences like noise or random bitflips can be easily implemented and adjusted. This flexibility comes at the cost of a performance penalty as each arithmetic operation now implies doing a function call, performing the necessary simulation steps and instantiating a return object. We deal with this performance degradation by implementing all classes in Cython [14], producing statically typed C-code which executes orders of magnitude faster than interpreted Python code, and distributing the simulations over many machines of a large compute cluster.

C. Results

1) Overall Error Resiliency: To assess the overall error resiliency of the algorithm, we chose overlap matrices of dimension $N = 768$ and set $p = 2$ to calculate the inverse square root for these matrices, which is one step of solving the generalized eigenvalue problem as described in Section IV-A. With simulation, we determine the convergence of the algorithm, depending on the given precision. The iterative algorithm shows to be rather resilient to low precision, both for storage of intermediate matrices as well as for all used arithmetic operations.

Figure 2 shows the error between the intermediate solutions obtained from the algorithm using floating-point with custom mantissa widths and a solution that was precomputed using double-precision. The error is determined by the Frobenius norm

$$
\|C_k - S^{-1/p}\|_F := \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} |\gamma_{ij} - \chi_{ij}|^2}
$$

where $C_k = (\gamma_{ij})$ and $S^{-1/p} = (\chi_{ij})$.

The observed convergence of the algorithm can be split into two phases: First the error steadily decreases, following a curve described by

$$
f(x) = 2^{-P(x)}
$$

with $P(x)$ being a polynomial function of at least second degree. In the second phase, being limited by the given precision of the data type, the algorithm does not converge further but oscillations may be observed.

This shows that the convergence in the first phase is barely influenced by the introduced errors. Only for less than 10 mantissa bits the algorithm does not converge at all. Consequently, half-precision floating-point arithmetic is sufficient to retain convergence. Approximation does however increase the lower bound for the error. Therefore the second phase of conversion start earlier for lower precision. Increasing the precision in later iterations allows the algorithm to further converge against a lower error, opening the possibility for dynamic precision scaling. Observing the changes introduced in each iteration, the necessity of increased precision can be detected at runtime.

Approximating only the storage of intermediate results allows significantly stronger approximation while achieving similar precision in the output. For example, storing only 10 mantissa bits allows a similar error as doing all calculation using 18 mantissa bits. In our use case the algorithm still converges if only two mantissa bits are used for all stored values.

Figure 3 shows similar behavior when using fixed-point arithmetic with a low number of bits. To retain convergence, 18 fractional bits are required for arithmetic operations. Again, restricting the approximation to stored intermediate results permits stronger approximation. In our evaluation, storing only four fractional bits showed to be sufficient to retain convergence.

2) Influence of the Matrix Size: Most of the results presented before apply directly to larger matrices from our problem set, in particular when only approximating the storage of intermediate results. Approximating all arithmetic operations using low-precision fixed-point arithmetic however exhibits a limitation. As shown in Figure 4 using 18 fractional bits is sufficient to retain convergence for $N = 786$ but for $N = 1536$ the error eventually increases. The reason for this behavior is that larger matrices from our set are more sparse (see Section IV-A) and therefore their inverse contain
independend of the applied approximation.

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to retain convergence of the algorithm, further precision is only
metic and storage. While a certain precision has to be provided
algorithm against errors introduced due to low precision arith-

smaller values which cannot be represented appropriately with
the given number of fractional bits.

For floating-point this effect is not relevant, as depicted in
Figure 4. The slightly larger final error for \( N = 1536 \) can be
3) Influence of \( p \): Calculating the inverse \( p \)-th root for \( p \neq 2 \) shows similar behavior as for \( p = 2 \), as shown in
Figure 5 for custom-precision fixed-point arithmetic and
storage. With increasing \( p \) the algorithm in general needs an
increasing number of iterations to converge. This effect is
independent of the applied approximation.

V. CONCLUSION

The presented results show the resiliency of the examined
algorithm against errors introduced due to low precision arith-
metic and storage. While a certain precision has to be provided
to retain convergence of the algorithm, further precision is only
required in final iterations if a precise result is desired.

It stands out that the number of iterations required to reach
a certain precision does not significantly increase with the
amount of approximation. This sets the examined algorithm
apart from other iterative methods like the preconditioned
conjugate gradient method which was modified to run on
approximate hardware by Schöll et al. [4] and showed to
require additional iterations when using approximation.

explained by the use of the Frobenius norm as error metric
since it adds up the quadratic errors of all matrix elements.

This opens up great opportunities for the acceleration of
applications in the scientific computing domain requiring the
calculation of inverse \( p \)-th roots: Using half-precision floating-
point in the first iterations can lead to a \( 2 \times \) speedup for
these iterations on suitable GPUs. Resource requirements on
FPGAs can be reduced by half and for custom CMOS designs,
power consumption of the multipliers can be reduced by \( 3/4 \).
Moreover, the overhead required for data exchange when using
GPUs or custom hardware can be significantly reduced as data
can be represented using low precision data types.

If a precise solution for \( A^{-1/p} \) is required for the application,
results obtained using approximation can be refined into a
precise solution in very few additional iterations. In a scenario
using approximate hardware accelerators, this can be done in
software while leaving the main part of the work to the external
accelerators.

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