On the Need for Reproducible Numerical Accuracy through Intelligent Runtime Selection of Reduction Algorithms at the Extreme Scale

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***Abstract*—The inherent nondeterminism present in reduction operations on an exascale system, coupled with the nonassociativity of floating-point arithmetic, makes achieving reproducible results difficult or impossible. Work investigating the irreproducibility phenomenon has generally proceeded along one of two veins: (1) development of algorithms that produce reproducible numerical results irrespective of nondeterminism in the reduction tree and (2) study of the system-level factors that induce nondeterminism.**

Our work builds on the latter and unveils the power of mathematical methods to mitigate error propagation at the exascale. We focus on floating-point error accumulation over global summations where enforcing any reduction order is expensive or impossible. We model parallel summations with reduction trees and identify those parameters that can be used to estimate the reduction's sensitivity to variability in the reduction tree. We assess the impact of these parameters on the ability of different reduction methods to successfully mitigate errors. Our results illustrate the pressing need for intelligent runtime selection of reduction operators that ensure a given degree of reproducible accuracy.

***Index Terms*—Prerounded summation; Kahan's compensated summation; composite precision summation; reduction tree.**

I. Introduction

Scientific simulations are increasingly being migrated to extreme-scale platforms consisting of hundreds (or thousands) of multicore servers equipped with many-core accelerators. Because floating-point numbers have finite precision, no simulation can be completely free of error. As hardware resources grow, the scientific computation taking advantage of that hardware has become increasingly complex. A consequence of the scale of computation is that even small errors at the beginning of the simulation may eventually compound into significant accuracy problems, which may call into question the validity of hours and hours of computation.

Multithreading complicates matters by introducing nondeterminism. Not only do errors accumulate throughout a computation, but a scientist may run the same computation several times with differing results. According to a recent report from the Department of Energy [1], by the end of this decade the level of concurrency of the supercomputing platforms on which simulations are executed is expected to increase by a factor of at least 4000. The question that must be answered is: Can the scientific community trust simulations executed on next-generation exascale architectures?

In this paper, we assess the effectiveness of several mathematical techniques to pursue reproducible accuracy on exascale platforms with multithreading hardware consisting of multicore processors coupled with many-core accelerators. We refer to *reproducibility* as "closeness of agreement among repeated simulation results under the same initial conditions" and *accuracy* as "conformity of a resulting value to an accepted standard, or scientific laws" (from Van Nostrands Scientific Encyclopedia). Rather than focusing on bitwise reproducibility, we study methodologies to minimize the propagation of errors and, thereby, limit their impact on the results of a simulation, increasing both the reproducibility of the simulation and the meaningfulness of the results. The contributions of this paper are as follows:

- We evaluate and compare the reproducibility of four summation techniques applied to a simulated exascale environment.
- We demonstrate that commonly accepted practices for predicting and mitigating errors offer incomplete characterizations of the reproducibility of numerical algorithms when applied in isolation.
- We demonstrate the need for data-aware software to intelligently choose reduction algorithms to guarantee reproducibility without an unnecessary loss in performance.

The rest of this paper is structured as follows. Section II summarizes both well-known and emerging sources of numerical inaccuracy; Section III describes techniques for supporting reproducible accuracy; Section IV proves the inadequacy of conventional wisdom when dealing with this problem; Section V provides strong evidence of the need for intelligent reduction operations at the extreme scale; and Section VI concludes this paper.

II. Sources of Numerical Inaccuracy

Achieving reproducible numerical accuracy at exascale faces two fundamental roadblocks: nonassociativity of floating-point arithmetic and nondeterminism in the order by which operands are reduced. In this section, we provide an overview of the challenges that arise when nonassociativity collides with nondeterministic reduction. To that end, we discuss the primary mechanisms by which floating-point error arises and propagates. We also summarize the existing body of work addressing issues of nondeterminism at exascale.

A. Nonassociativity: A Consequence of Finite Precision

Floating-point computations suffer loss of accuracy, compared with the same expression's evaluation in exact arithmetic, through two primary mechanisms: alignment error and subtractive cancellation. Alignment error, by far the most common error modality, results from summation of values whose exponents differ. Alignment error is possible whenever two floating-point numbers that differ in magnitude by at least a factor of 2 are added [2]. The amount of information about the smaller operand lost due to alignment error is related to the disparity between the operands' magnitudes. The other mechanism is subtractive cancellation, which occurs when very small values are obtained from the addition of two values with similar magnitude and opposite sign. Subtractive cancellation, in contrast to alignment error, is not a source of error *per se*, but a means by which inaccuracy in low-order mantissa bits of operands is transferred to high-order mantissa bits of their sum.

A consequence of these inaccuracies is the well-known fact that floating-point arithmetic operations are nonassociative, so the order in which floating-point numbers are reduced via an operator (e.g., +, -, *, /) influences the result. For example, let $a = 10^9$, $b = -10^9$, and $c = 10^{-9}$. In infinite precision, the summation orders $(a+(b+c))$ and $((a+b)+c)$ are equivalent, but even in double-precision floating-point arithmetic, the two distinct summation orders yield different values.

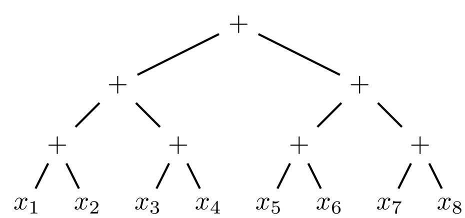
$$((a+b)+c) = ((10^9 - 10^9) + 10^{-9}) = 10^{-9}$$
$$(a+(b+c)) = (10^9 + (-10^9 + 10^{-9})) = 0$$

For a small example such as this one, the flaw is clear, namely, that the small-magnitude value c is "absorbed" by the much larger value b.

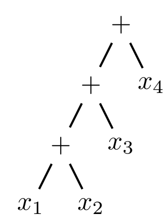
B. High Concurrency: A Consequence of Extreme Scale

Contemporary petascale platforms consist of up to millions of processor cores that must act in concert to effect large simulations. Even at these scales, the cost of achieving not only accuracy in floating-point reductions but reproducible accuracy is felt. The scientific community at large has set its sights on deployment of an exascale computing platform, and in response the HPC community has identified a canonical set of challenges to implementing an exascale machine [1]. Although emerging developments in low-power hardware, advanced systems software, and algorithm design show promise, it has become increasingly evident that achieving reproducible numerical accuracy at exascale cannot rely on deterministic reduction. Exascale computations will simply have to weather perturbations in their reduction trees through algorithmic means. In this section, we summarize key results demonstrating how variability in reduction trees induces variability in sums of floating-point numbers. Additionally, we present a set of findings, commentary, and expert recommendations supporting our claim that deterministic reduction trees at exascale will be unfeasible.

Throughout this section and the remainder of the paper, we adopt the view of a concurrent sum of floating-point numbers at the extreme scale as a *reduction tree*, which we define as a full binary tree whose N leaf nodes correspond to floating-point operands and whose internal nodes correspond to the partial reductions formed in the process of computing the final result–the root node. Reduction trees can vary in two ways: shape and assignment of operands to leaves. When we refer to the shape of a reduction tree, we mean the particular way in which nodes are linked by edges. Figure 1 shows two differently shaped reduction trees: a balanced (parallel) reduction tree and an unbalanced (serial) reduction tree. For a fixed set of operands, even two reduction trees with the same shape can yield different values for the reduction if the assignment of operands to leaves differ between the two trees.



(a) A balanced (parallel) reduction tree



(b) An unbalanced (serial) reduction tree

Fig. 1. Two reduction trees at the opposite ends of the spectrum.

The effect of varying reduction tree shape and varying operand-to-leaf assignment is explored in [3]. In their work, a set of eight identical floating-point values is summed via three differently shaped reduction trees, yielding in each case a different value for the sum. Another set of eight floating-point values, six small and two large, is summed via three reduction trees of the same shape, but with different assignments of summands to leaves. Again, all three computed sums disagreed. One key observation is that the consequences of nondeterministic reduction and floating-point nonassociativity are felt even for extremely small examples.

On exascale systems the high level of concurrency will not allow the user to enforce any specific reduction order because doing so is either too expensive or impossible. At the same time variability in floating-point error accumulation may become so great that debugging is impaired or, worse, fundamentally incorrect results are accepted. An exascale algorithm must exploit the extreme level of concurrency, minimize communication (for speed and power reduction), tolerate frequent hardware failures, and utilize resources as they become available [1], all the while providing some trust in the computation's result.

The conflict between achieving reproducible accuracy and achieving performance is primarily due to the fact that even on current HPC platforms, communication costs dominate arithmetic costs. Simply put, the most performant reduction trees are those that take into account the underlying physical topology of the system, which means reducing values in an order based on which core produced them, not necessarily their arithmetical properties. Conversely, the reduction trees that result in the least error accumulation reduce values based on their arithmetical properties, not their position in the topology of the system. Recently, Balaji and Kimpe [4] showed not only that topology-aware reduction trees for MPI collective operations outperform fixed-reduction trees but that the performance advantage of allowing the reduction tree to conform to the system topology, as opposed to a specified ordering of partial reduction, increases with the number of cores.

III. Mathematical Techniques

In response to the challenges posed by the nonassociativity of floating-point summation and the nondeterminism at the extreme scale, mathematical techniques can be applied to mitigate the degree to which computed sums exhibit sensitivity to reduction order. Lower sensitivity results in increasingly reproducible results. Techniques can range from simple fixed-reduction orders to more sophisticated prerounded algorithms. In this section we provide a general overview of the techniques; however, in the rest of the paper, we consider only the compensated summation algorithms (Kahan and composite precision) as well as the prerounded algorithms for our studies because they are the only methods that can be feasibly applied at the exascale.

A. Fixed-Reduction Order

To apply fixed-reduction order, we need to ensure that all floating-point operations are evaluated in the same order from run to run. Two major problems exist for this strategy. The obvious problem is that ensuring that the reduction proceeds according to a user-determined reduction tree incurs massive communication and synchronization costs. Additionally, determining exactly which reduction tree achieves minimal error for a given set of summands is nontrivial. Conventional wisdom suggests summing the values in ascending order if they all have the same sign, and in descending order of magnitude if they are not. The first case is rare, however, and the second case assumes that no error beyond initial representation error is present in the summands; otherwise it is far more vulnerable to catastrophic cancellation. In summary, fixing the reduction order is difficult to do correctly where it is possible, but the salient point is that it cannot be done in a cost-effective way at exascale [5].

B. Interval Arithmetic

Techniques based on interval arithmetic replace floating-point types with custom types representing finite-length intervals of real numbers. The actual value of the reduction is guaranteed to lie within the interval. The width of the interval increases with the uncertainty of the computation. While the techniques are reproducible by design, they also cause large slowdown and are not suitable for applications needing many digits of accuracy.

C. High-Precision Arithmetic

Perhaps the most obvious technique, and certainly the most popular in real applications, is to use higher-precision floating-point types. To our knowledge, the earliest work directly addressing the issue of numerical reproducibility [6] demonstrates the use of the double-double precision floating-point type in a critical section of code to curtail variability in a global sum. In that work, the goal of using multiple floating-point types was explicitly to achieve reproducible results. Parallel to that effort, significant progress has been made in the field of automated floating-point precision tuning (e.g., [7]). Precision tuning is an attempt to reduce precision where possible while maintaining a prescribed degree of accuracy. While one can achieve greater reproducibility by pursuing greater accuracy, the use of high-precision arithmetic can result in memory-demanding algorithms. By increasing the size of floating-point variables in most numerically sensitive parts of the algorithm, for example with manual changes made by an expert or by some form of analysis, we can reduce the memory requirements. Still the technique relies on either human experts or other software and thus is probably unsuitable for many of the use cases discussed in the recent DOE exascale report [1].

D. Compensated Summation Algorithms

To compute the sum of n values, we obtain $n-1$ partial sums in the process. For each of these partial sums, the magnitude of error can be estimated. Based on that estimate, an attempt can be made to compensate for that error by adding an error term to each partial sum. Compensated summation is a relatively old technique, having been introduced by Kahan in [8]; but families of more sophisticated compensated summation algorithms have been developed, such as composite precision (CP) summation [9]. In Kahan's algorithm the estimated error is added back into the sum at each step. In CP, the error summation is kept and propagated as each of the summations are performed and added back in only at the end.

E. Preround Summation Algorithms

More recently, an approach called preround summation has emerged for reproducible and accurate summation. The common strategy used by this type of algorithm is splitting the operands into "high-order" and "low-order" parts with the property that the high-order parts can be summed irrespective of summation order and the low-order parts can be neglected, or recursed upon, for higher accuracy. The algorithms proposed by Demmel and his group are integrated into the ReproBLAS library [10], which at this time is undergoing active development.

IV. Inadequacy of Conventional Wisdom

The management of reproducible numerical accuracy is closely related to the task of estimating and predicting error accumulation. Three common approaches exist, typically used in isolation, to quantify and mitigate error accumulation. Two of the approaches can be broadly classified as techniques for error estimation: using worst-case error bounds and attempting to track or avoid subtractive cancellation. The third approach is the use of summation algorithms that are believed to be inherently less sensitive to variability in the reduction tree. We emphasize that these approaches have significant value. However, we demonstrate that the use of any one approach, in isolation, will not guarantee the reproducibility desired without a potentially significant loss of performance.

A. Using Analytical Error Bounds

The analysis of the error for a single floating-point sum can be extended to produce a worst-case error bound for the reduction of multiple floating-point values. For IEEE-compliant implementations of floating-point arithmetic, we have the following bound on the roundoff error for a single operation. Let x, y be floating-point numbers, let $\texttt{fl}(x+y)$ be their rounded sum according to a given rounding rule, and let $(x+y)$ be their exact sum:

$$\texttt{fl}(x+y) = (x+y)\cdot(1+\delta)$$

where $|\delta| \leq u$ where u is the unit-roundoff and may be written $u = \frac{1}{2}\beta^{1-p}$, where β is the base and p is the number of mantissa bits of the representation of x and y. Equivalently, if we let z denote the exact sum $x+y$, we obtain a bound on the absolute error $|\texttt{fl}(x+y) - z| \leq u$. With some algebra, one can prove an upper bound on the error in a sum of n floating-point numbers. We do not include the proof here (it may be found in [11]), but we state the result. Let $x_1, \ldots, x_n$ be floating-point numbers, let z denote their exact sum, and let $\sum_{i=1}^{n} x_i$ denote their sum in floating-point arithmetic. Then we have the following upper bound on the absolute error in the sum:

$$|\sum_{i=1}^{n} x_i - z| < n \cdot u \cdot \sum_{i=1}^{n} |x_i|.$$

Using analytical or statistical worst-case error bounds causes overestimation of the errors. Figure 2 shows an empirical case study in which we measure the error magnitudes for $10,000$ values sampled in the range $(-1000, +1000)$ and summed by using $10,000$ different summation orders. The

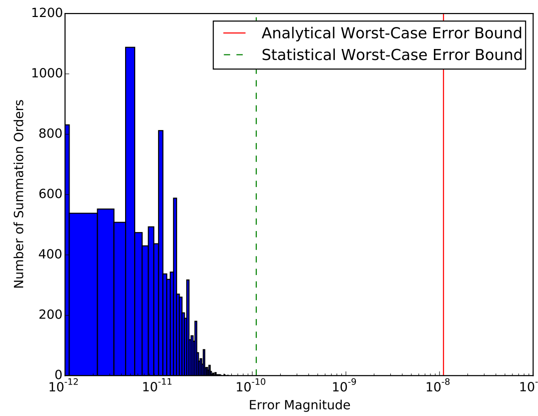


Fig. 2. Empirical study of error magnitudes and worst-case error bounds for $10,000$ summations of $10,000$ values randomly sorted.

figure also shows both the analytical and statistical worst-case error bounds. Both error bounds significantly overestimate the error magnitude. At the same time we observe the large range of measured errors obtained for the same set of values just by randomly shuffling the order in which the terms are summed.

B. Tracking Cancellations

When considering sets of summands with both positive and negative values, the potential for *catastrophic cancellation* arises in the computation of the sum. This numerical phenomenon can result in large relative errors in both the partial and final sums, leading to the intuitively appealing perspective of achieving reproducible accuracy by structuring reductions to avoid cancellation.

Cancellation in general refers to the scenario where the sum of two floating-point values has a smaller exponent than both of the summands. In order to subtract one floating-point number from another, their binary points are aligned and the mantissa of their difference is determined by subtracting the mantissas of the operands bitwise and then *renormalizing* the result. The effect of the renormalization process is that the lower-order bits of the operands determine the higher-order bits of the result. If both summands are exact in the sense that their mantissa bits are not carrying the error from previous computations—as is almost never the case—then their difference can be considered accurate. However, if the low-order bits of the operands are inaccurate due to alignment error, many or all of the mantissa bits of the difference of the operands may be inaccurate. This is the "catastrophic" case.

We emphasize, however, that cancellation does not in and of itself cause error to accumulate. Rather, it reveals error that has already accumulated in the operands. In a sense, relative error can increase because of catastrophic cancellation as uncertainty in less-significant bits of the operands' mantissas is transferred to uncertainty in the most significant bits of the result's mantissa. Nevertheless, the number of cancellations is not a reliable indicator of the overall problem.

To prove this claim, we generate a counterexample with a set of $1,000$ floating-point numbers uniformly distributed in $[-1, 1]$. We compute the sum of these numbers using 100 distinct summation orders and determine the error for each order. We assess cancellation for each order using the numerical library CADNA [12]. CADNA uses the CESTAC method to identify instances of cancellation in a sum and, for each instance, estimate the difference between the number of accurate digits in the operands and the number of accurate digits in the result. In this sense, a cancellation resulting in the loss of four digits of accuracy is more severe than a cancellation resulting in the loss of only two digits. Figure 3 shows the cancellation counts and error magnitudes for several summation orders of the set of interest for our counterexample. Each summation order is represented by five bars, four showing the number of cancellations resulting in the loss of one, two, four, and eight digits, respectively, and a fifth bar showing the error magnitude, scaled for ease of viewing. We observe that the number of cancellations, at any of the considered severities, does not consistently predict error magnitude. In particular, consider summation orders 2 and 4. Order 2 has about 5X as many digit cancellations as order 4, but only half the error. This result lends credence to the view that although it is tempting to view "keeping track of cancellations" as a valid strategy for managing error and ensuring reproducibility, there is not a simple correspondence between instances of cancellation and error magnitude. Rather, the relationship between cancellation and error depends on knowledge of how much error has already accumulated in the operands involved in the cancellation, a quantity whose estimation is impeded by the previously discussed loose error bound.

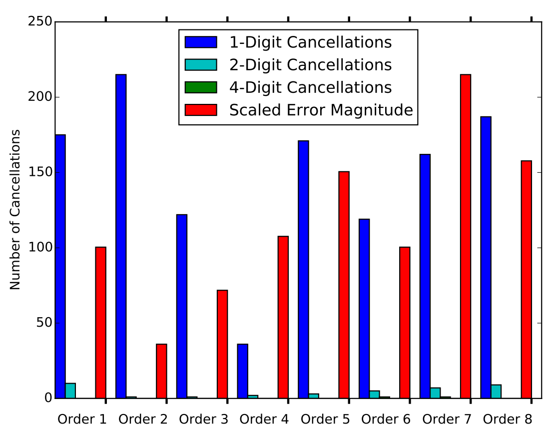


Fig. 3. Empirical study of cancellations vs. error magnitude for different summation orders.

C. *Choice of Summation Algorithm*

Apart from the standard iterative summation algorithm, we examine other summation algorithms that exhibit reduced sensitivity to variability in the reduction tree. However, each of these algorithms incurs a certain performance penalty relative to the standard summation. Standard summation is the cheapest and least complex. Kahan's compensated summation, then composite precision summation, and finally prerounded summation are expected to progressively provide more accuracy at the expense of performance. To assess this performance impact, we measure the execution times of a case study designed to emulate scenarios in scientific computing in which partial data is locally generated on multiple processes and then is globally reduced across the processes. Specifically, on each process, we generate a chunk of a vector of values of length 10^6 from a series that is known to sum to zero under exact arithmetic. We locally reduce these values using each of the four summation algorithms: in the case of Kahan and composite precision, we use the summation operators in [13] and in the case of prerounded summation, we use the dIAddd operator provided in [14]. Finally, we globally reduce the local sums by using MPI_Reduce with custom reduction operators for Kahan, composite precision, and prerounded summations. To avoid time variations due to network contention we run our tests on a single dedicated 48-core AMD node. Each tests is repeated 20 times with a warmed cache. Figure 4 shows the average execution times and Figure 5 shows the performance penalties associated with more-reproducible summation. The latter figure confirms the proposed ranking of the summation algorithms in terms of performance expense.

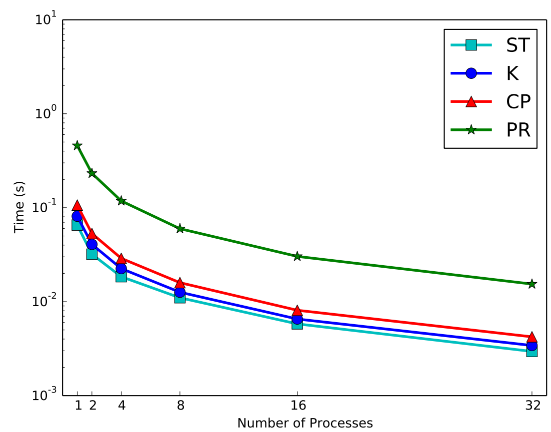


Fig. 4. Comparison of execution time to sum 10^6 terms for standard summation (ST), Kahan's compensated summation (K), composite precision summation (CP), and prerounded summation (PR).

We argue that applying a judicious mixture of these algorithms, as opposed to uniformly applying a single technique, is necessary for achieving numerical reproducibility to the degree required by an application, for a cost acceptable for that application. Figures 6(a) and 6(b) support this claim by showing the relative sensitivity of the three summation algorithms: Kahan's compensated summation (K), composite precision summation (CP), and prerounded summation (PR). For a fixed set of data we generate multiple reduction trees of the same shape but with different assignments of operands to leaves. We construct the set of summands to have mathematical properties that render its reduction especially prone to both alignment error

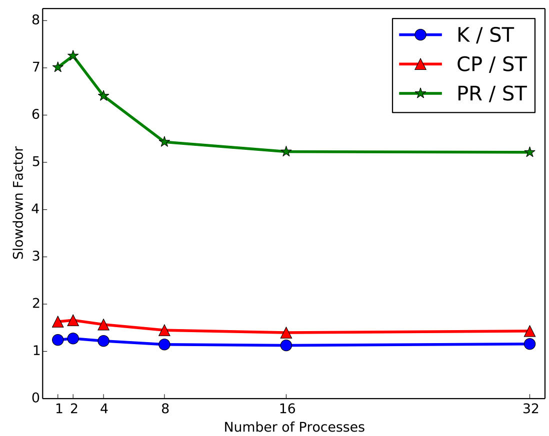
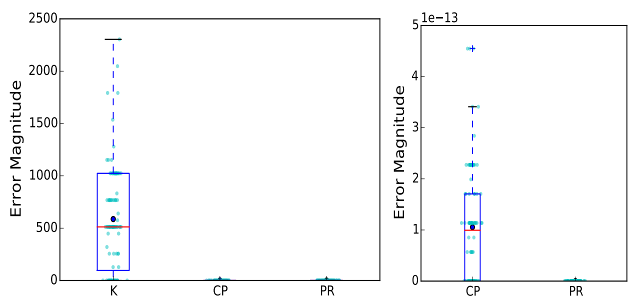


Fig. 5. Performance losses of Kahan's compensated summation (K), composite precision (CP), and prerounded (PR) summations compared to the standard summation (ST).

and loss of accuracy due to cancellation. For each reduction tree, we compute the sum using each of the four algorithms. By plotting the error magnitude, we see that as a progressively greater amount of computation is invested in compensating for roundoff error, the sum becomes less sensitive to the varying reduction tree.



(a) (b)

Fig. 6. Empirical study of relative sensitivity of three summation algorithms: Kahan's compensated summation (K), composite precision summation (CP), and prerounded summation (PR). Note that (a) zooms into (b).

V. Exploring the Reproducibility Space

Previous work [3], [4] found that reduction tree shape and assignment of operands to its leaves (or threads) can have a profound effect on the concurrent sum of n floating-point numbers, even when the operands themselves are subject to minimal alignment error and have the same sign avoiding cancellation. We build the work in this paper on this previous work by targeting a much larger reduction scale and investigating the impact of four independent parameters on the variability of a sum when the reduction order is non-deterministic. The four parameters we consider are the condition number, the dynamic range, the level of concurrency, and the reduction algorithm. We present three kinds of results. First, we examine the sensitivity to variations in the reduction tree of four summation algorithms at increasing levels of concurrency. Second, we study the impact of concurrency, condition number, and dynamic range on reproducible numerical accuracy. Third, we provide evidence of the need for selecting application-aware reduction algorithms.

A. Experimental Environment and Parameters

Building on the results of small nondeterministic reduction trees established in [3], [15], we consider reduction trees at the size expected for exascale systems consisting of floating-point operands reflective of those actually reduced in simulations. Since an exascale system is not available, we emulate the reduction process with n threads, each computing one of the n partial sums. We consider two tree shapes at opposite ends of the spectrum: a completely balanced (see Figure 1(a)) tree and a completely unbalanced (see Figure 1(b)) tree. For each tree shape, we generate distinct reduction trees by randomly assigning operands to leaves. We also focus on sets of floating-point summands whose mathematical properties are less amenable to reproducible summation. We characterize sets of floating-point values by their sum condition number and dynamic range. These are intrinsic properties of the set of values; they are independent of any imposed ordering. For a set of floating-point numbers $\{x_1, \ldots, x_n\}$, the sum condition number is defined as

$$k = \left(\sum_{i=1}^{n} |x_i| \right) / \left| \sum_{i=1}^{n} x_i \right|$$

and the dynamic range is defined as

$$dr = \texttt{exp}(\texttt{max}(|x_i|)) - \texttt{exp}(\texttt{min}(|x_i|)),$$

where $exp(x)$ is the value of the exponent in the representation of x. If the dynamic range of two numbers is larger than zero, then alignment error will occur. For this reason, we use the dynamic range of a set of values as a rough estimator of alignment error. The condition number does not correspond to a single mechanism by which error accumulates. Instead, it describes how sensitive the final sum is to small errors in the partial sums.

Table I shows small sample sets of values presenting dynamic range dr equal to 0, 8, and 16 as well as condition number k equal to 1, 1000, and ∞. Note that dr equal to 0 means "all exponents are the same" and not that the numbers are large or small; on the other hand a larger dr, for example 8 or 16, means that a larger discrepancy exists between the largest and smallest exponents. In other words, the sign on the summands makes no difference, and the sum of summands makes no difference. A condition number equal to 1 means "all values in sum have the same sign," while a condition number number infinity means "the sum of all the values is 0." In [3] the operands are well-conditioned; they have $k = 1$ (the best possible condition number) and, when varying tree shape, have $dr = 0$. We instead focus on ill-conditioned inputs with high dynamic range because reality is not so rosy. For example, N-body simulations [16] involve reductions of floating-point values that are ill-conditioned; both k and dr can frequently be very large.

TABLE I
EXAMPLE OF SAMPLE SET OF VALUES WITH SPECIFIED DYNAMIC RANGE, dr, AND CONDITION NUMBER, k.

Sample Set of Values	dr	k
{1.23e+32, 1.35e+32, 2.37e+32, 3.54e+32}	0	1
{1.23e-32, 1.35e-32, 2.37e-32, 3.54e-32}	0	1
{-1.23e+16, -1.35e+16, -2.37e+16,-3.54e+16}	0	1
{2.37e+16, 3.41e+8, 4.32e+8, 8.14e+16}	8	1
{3.14e+32, 1.59e+16, 2.65e+18, 3.58e+24}	16	1
{2.505e+2, 2.5e+2, -2.495e+2, -2.5e+2}	0	1000
{5.00e+2, 4.99999e-1, 1.0e-6, -4.995e+2}	8	1000
{5.00e+2, 4.99...99e-1, 1.0e-14, -4.995e+2}	16	1000
{3.14e+8, 1.59e+8, -3.14e+8, -1.59e+8}	0	∞
{3.14e+4, 1.59e-4, -3.14e+4, -1.59e-4}	8	∞
{3.14e+8, 1.59e-8, -3.14e+8, -1.59e-8}	16	∞

B. Sensitivity of Summation Algorithms

To examine the sensitivity of summation algorithms to variability in the reduction tree, we generate and reduce two sets of summands constructed to have the exact sum of zero and dynamic range of 32. One set has $n = 8K$ values, and the other has $n = 1M$ values. These sets of values are more prone to both alignment error and catastrophic cancellation than are those studied in [3]. They are also more reflective of the values that may arise in simulations (e.g., when the net force on a particle is close to zero).

Figures 7(a)–(h) show the distribution of error magnitudes for sums computed by using varying reduction trees for the four summation algorithms of interest in this paper: the standard iterative summation algorithm (ST); Kahan's compensated summation algorithm (K); the composite precision summation (CP), which can be considered an enhanced form of compensated summation; and the prerounded summation (PR), which offers guaranteed bitwise reproducibility at a user-specified level of accuracy. We consider two types of reduction trees: completely balanced, with results shown in Figures 7(a), (b), (c), and (d), and completely unbalanced, with results shown in Figures 7(e), (f), (g), and (h). For each tree type, we consider both smaller levels of concurrency (8K leaves in the tree) and higher levels (1M leaves in the tree). The boxplots in the figures are obtained by considering 100 distinct reduction trees with the same shape but randomly permuted assignments of the values to leaves. Note that Figures 7(b), (d), (f), and (h) provide a zoom-in into Figures 7(a), (c), (e), and (g), respectively.

The effect of nondeterminism in the reduction tree is exhibited in Figures 7. For a given summation algorithm, the distribution of data points and width of the box indicate how much the sum tends to vary when the overall shape of the reduction tree is constant but the arrangement of summands to its leaves is variable. Within the subfigures, we see that although Kahan summation tends in general to produce more reproducible sums than standard summation, only composite precision and prerounded summations offer reproducible numerical accuracy at an acceptable level. Across a row of subfigures, we see that as the level of concurrency rises, the absolute error in the sum rises as expected. However, by comparing results across a column of subfigures, for example, the ST data from Figure 7(a) and the ST data from Figure 7(e), we see that much more variation in the sum occurs when the tree is unbalanced than when it is balanced for the standard summation algorithm. To cope with intermittent faults and inconsistently available resources, we expect that the reduction trees employed by an exascale system will vary not only in terms of arrangement of data among their leaves but also in overall shape. We conclude that because of the difference in reproducibility observed for differently shaped reduction trees, exascale applications will need to maintain awareness of the degree of fluctuation in reduction tree shape and employ more robust reduction operators accordingly.

C. Effect of Concurrency, Conditioning, and Dynamic Range

For a fixed level of concurrency, the mathematical properties of the summands can have a significant impact on the sensitivity of the sum to variations in the reduction tree. In the previous section, we considered a set of values with a fixed condition number k and dynamic range dr. In this section, we examine the effects of varying k and dr at a fixed level of concurrency $n = 1M$; varying dr and n at a fixed k; and varying k and n at a fixed dr. We represent the spaces of (k, dr), (n, dr), and (n, k) as a grid of cells, where for each cell we generate a set of floating-point values with the cell parameters. The degree to which these sets of values can be summed reproducibly is tested. For all sets of summands under consideration, we measure their potential for irreproducibility by computing their sum with 1,000 distinct, balanced reduction trees obtained by permuting the assignment of summands to leaves. As in the our previous experiment we test four summation algorithms. However, we display results only for the first three because the composite precision and prerounded summations performed identically for all sets of inputs considered. Once all the sums have been computed for a cell, the error in each sum is calculated with respect to an accurate reference sum, which we compute in quad-double precision using the GNU MPFR high-precision library. To visualize the level of irreproducibility observed, we compute the standard deviation of the errors and shade the cell according to that value. Figure 8 illustrates the process in a visual (and more intuitive) way.

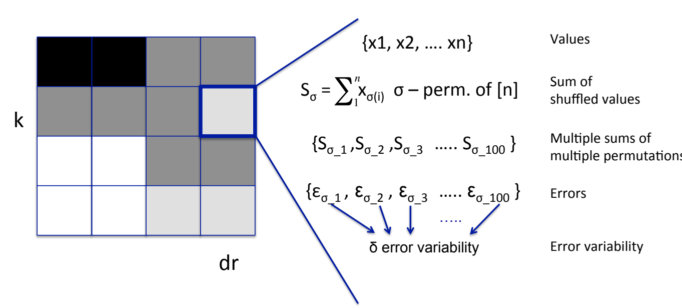
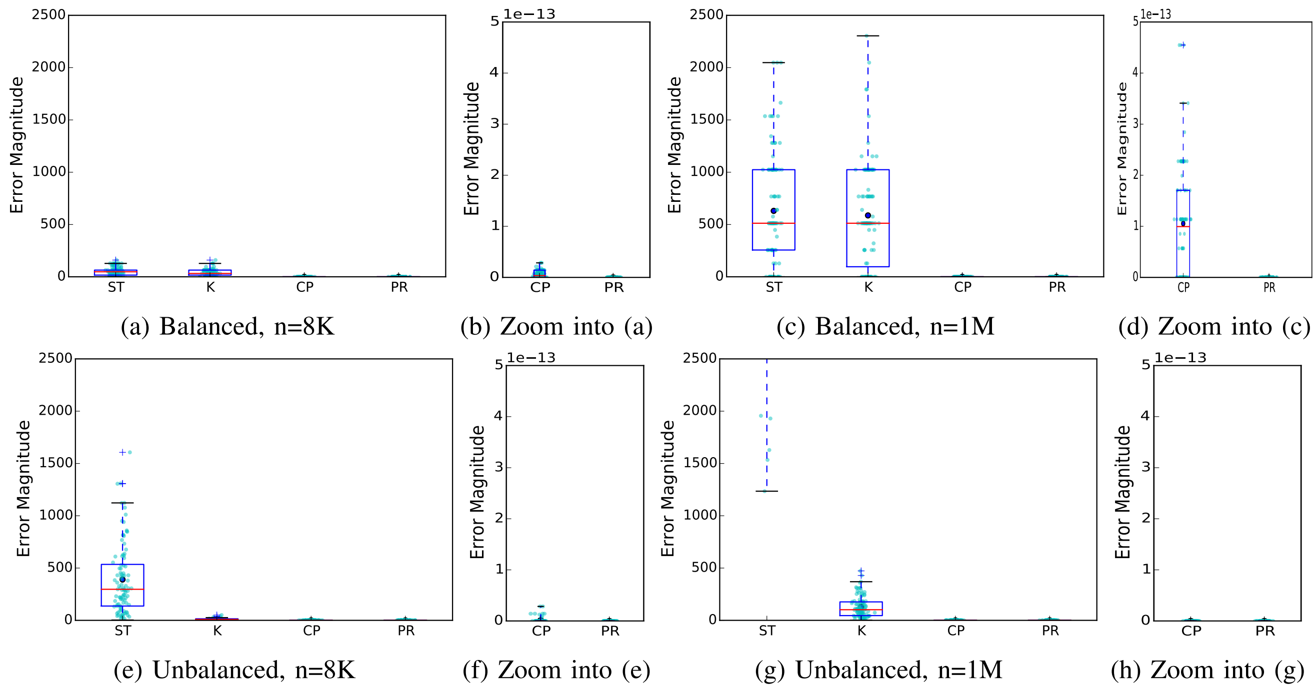


Fig. 8. Overview of the grid with its cells used to study the effect of concurrency, conditioning, and dynamic range.



(a) Balanced, n=8K (b) Zoom into (a) (c) Balanced, n=1M (d) Zoom into (c)

(e) Unbalanced, n=8K (f) Zoom into (e) (g) Unbalanced, n=1M (h) Zoom into (g)

Fig. 7. Error distributions for the four summation algorithms considered in this paper for balanced and unbalanced reductions: three at a smaller (8K leaves) and one at higher (1M leaves) levels of concurrency.

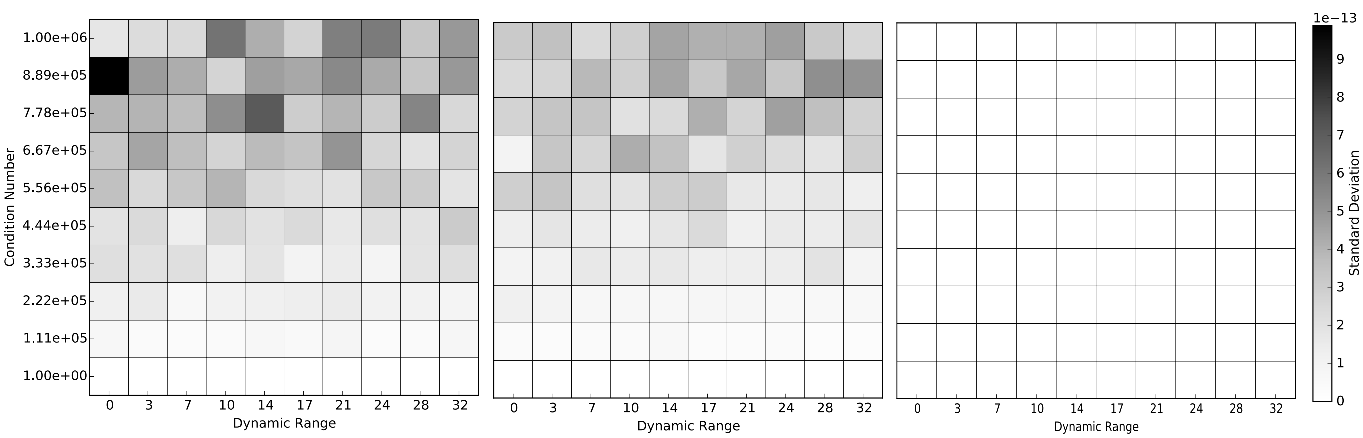


Fig. 9. Standard deviation errors for standard summation (left), Kahan summation (middle), and composite precision summation (right) for different (k, dr) values and fixed concurrency n.

Figure 9 shows how position in the space of possible (k, dr) values influences the variability of a sum at a fixed level of concurrency. The darker cells toward the top and right of the two leftmost grids indicate sets of summands whose sums varied much more than the level of variation observed for sets of summands with lower condition number. The darkest cell in the standard summation grid is anomalous but likely due to particularly severe subtractive cancellation, since its condition number is large. The rightmost grid shows that for all considered sets of summands, the result according to the composite precision summation did not vary with changes in the reduction tree.

Figure 10 presents the impact of dynamic range for a fixed condition number. For these grids, each cell's summands have condition number $k = 1$ so that the ability of dynamic range to estimate alignment error can be assessed. Note that the scale by which the cells are shaded for these grids is not the same as for the grids examining the (k, dr) or (n, k) spaces. There is a tendency for high-concurrency, high-dynamic-range cells to exhibit greater variability; but the most valuable lesson from these visualizations is that dynamic range exerts much less influence over variability of the sums than does the condition number, as seen in Figure 11. Here, we observe a strong relationship between high variability of sums and sets of summands with high condition number. These results suggest the need for applications to maintain awareness of

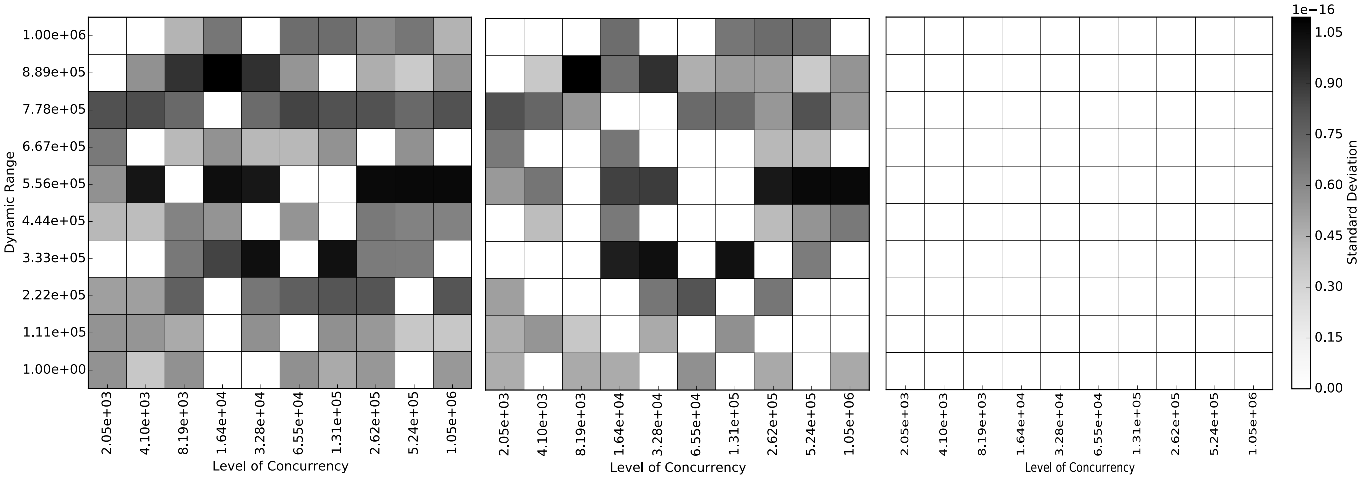


Fig. 10. Standard deviation errors for standard summation (left), Kahan summation (middle), and composite precision summation (right) for different (n, dr) values and fixed condition number k.

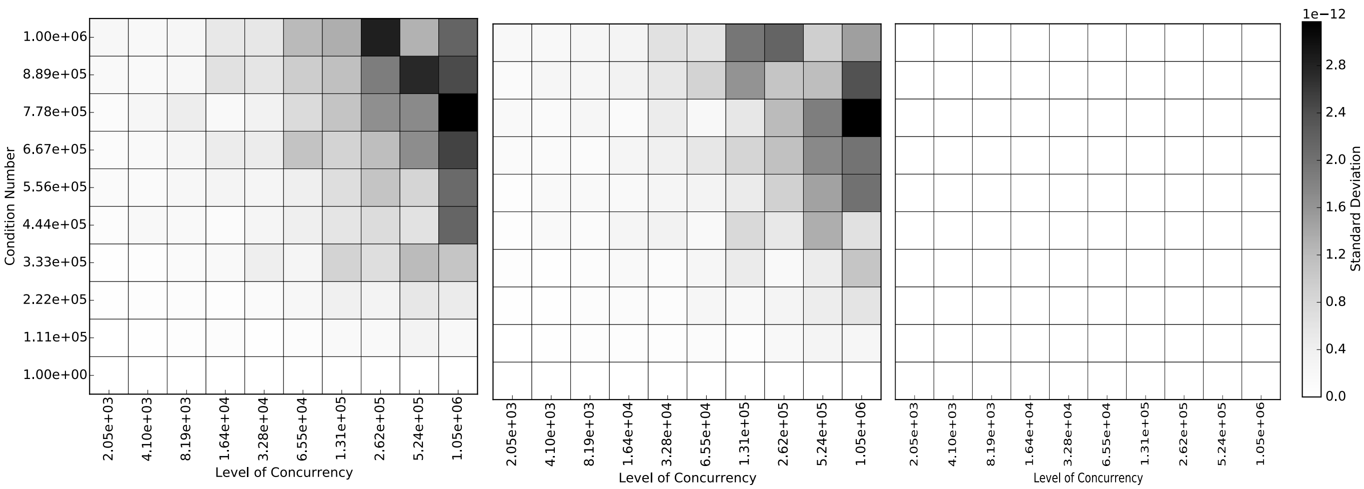


Fig. 11. Standard deviation errors for standard summation (left), Kahan summation (middle), and composite precision summation (right) for different (n, k) values and fixed dynamic range dr.

the mathematical properties of sets of floating-point values generated at runtime, and if the reduction tree is expected to change from run to run, to select reduction algorithms that take those mathematical properties into account.

D. Intelligent Selection of Reduction Algorithms

Techniques such as compensated summation can reduce the amount of variability observed in repeated summation when the summation order changes from run to run. However, application developers are faced with the challenge of selecting the summation algorithm that gives them the level of reproducibility and accuracy required by their application. At exascale, judicious selection of reduction algorithms will be vital so that application-specific reproducible numerical accuracy can be achieved at tolerable cost. In contrast to the old notion of bitwise reproducibility, application-specific reproducibility requires developers to specify an upper bound on the amount of variability in the values of floating-point reductions that can be tolerated while maintaining the trustworthiness of the application's output.

A set of floating-point values occupies a position in a complex parameter space: the number of values, reduction tree, condition number, and dynamic range all exert influence over which reduction algorithm can cost-effectively achieve a specified level of reproducibility. Our data suggests that in order to avoid exceeding a fixed level of variability, if one cannot control the reduction tree, it may be possible to use standard summation when values are uniform and well-conditioned and to adaptively switch to a more robust summation algorithm if the values to be reduced become less uniform or less well-conditioned. We argue that unlike attempting to achieve reproducible numerical accuracy by additional data movement, as would be required to fix a reduction tree, estimable quantities such as condition number and dynamic

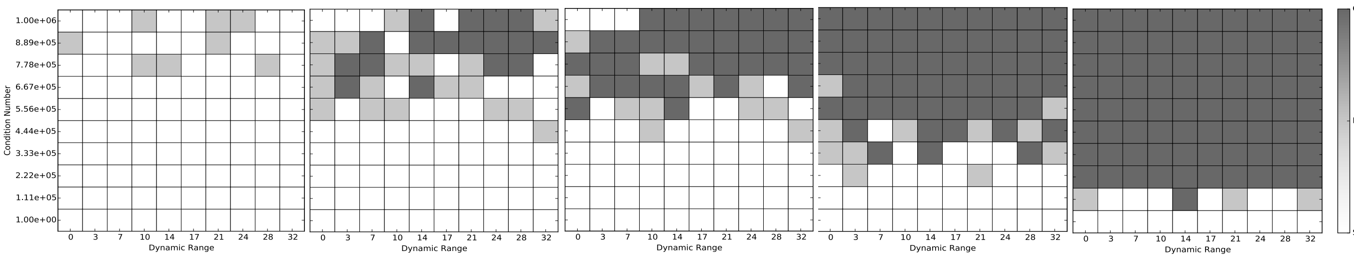


Fig. 12. Selection of the cheapest but acceptably accurate reduction algorithm among the Kahan (K), composite precision (CP), and prerounding (PR) algorithms for different error variability thresholds (left to right: $t = 5e-13, 3e-13, 2.5e-13, 1.5e-13, 5e-14$).

range can guide runtime selection of a reduction operator with the appropriate performance/reproducibility tradeoff for the application at hand. In Figure 12, we show the (k, dr) grid for several error variability thresholds. Here cells are shaded based on the cheapest summation algorithm that achieves a given degree of reproducibility at that cell. As we reduce the variability threshold, effectively stepping toward bitwise reproducibility with smaller and smaller thresholds, we see that increasingly costly summation algorithms are required for the more challenging regions in the space (i.e., those with high condition number and high dynamic range).

Achieving reproducible numerical accuracy by intelligent runtime selection of reduction algorithms depends on being able to assess the mathematical properties of the floating-point values to be reduced. We show that if this assessment can be done, one can avoid using a more expensive reduction algorithm when a cheaper one will do. These results present a strong case for further research into tools that, at exascale, profile parameters of interest (e.g., n, k, dr, and tree shape) at runtime and apply cheaper but acceptably accurate reduction algorithms to subtrees based on the profile.

VI. Conclusion

In this paper we identify relevant parameters that, when analyzed in concert, can provide insight into intelligent selection of reduction algorithms to achieve reproducible numerical accuracy on soon-to-exist exascale platforms.

Three main observations emerge from our study on reproducible numerical accuracy. First, reduction tree shape has a large impact on reproducible numerical accuracy. Second, mathematical properties of a set of summands have an impact on the reproducibility of their sum. In applications where the conditioning and dynamic range can change dramatically over the course of the runtime, this effect is especially relevant. Third, we show that if we fix a target level of reproducibility, we can classify regions of the parameter space by the cheapest algorithm that achieves the desired level of reproducibility at that point in the space. This is an important step toward implementing intelligent runtime selection of reduction operators on future exascale platforms.

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