Efficient Ranking and Selection in Parallel Computing Environments

Eric C. Ni
Cornell University
Ithaca, New York 14853, USA
cn254@cornell.edu

Dragos F. Ciocan
INSEAD
Fontainebleau 77305, FRANCE
florin.ciocan@insead.edu

Shane G. Henderson
Cornell University
Ithaca, New York 14853, USA
sgh9@cornell.edu

Susan R. Hunter
Purdue University
West Lafayette, Indiana 47907, USA
susanhunter@purdue.edu

Abstract

The goal of ranking and selection (R&S) procedures is to identify the best stochastic system from among a finite set of competing alternatives. Such procedures require constructing estimates of each system’s performance, which can be obtained simultaneously by running multiple independent replications on a parallel computing platform. However, nontrivial statistical and implementation issues arise when designing R&S procedures for a parallel computing environment. Thus we propose several design principles for parallel R&S procedures that preserve statistical validity and maximize core utilization, especially when large numbers of alternatives or cores are involved. These principles are followed closely by our parallel Good Selection Procedure (GSP), which, under the assumption of normally distributed output, (i) guarantees to select a system in the indifference zone with high probability, (ii) runs efficiently on up to 1,024 parallel cores, and (iii) in an example uses smaller sample sizes compared to existing parallel procedures, particularly for large problems (over $10^6$ alternatives). In our computational study we discuss two methods for implementing GSP on parallel computers, namely the Message-Passing Interface (MPI) and Hadoop MapReduce and show that the latter provides good protection against core failures at the expense of a significant drop in utilization due to periodic unavoidable synchronization.

1 Introduction

The simulation optimization (SO) problem is a nonlinear optimization problem in which the objective function is defined implicitly through a Monte Carlo simulation, and thus can only be observed with error. Such problems are common in a variety of applications including transportation, public health, and supply chain management; for these and other examples, see SimOpt.org
We consider the case of SO on finite sets, in which the decision variables can be categorical, integer-ordered and finite, or a finite “grid” constructed from a continuous space. Formally, the SO problem on finite sets can be written as

$$\max_{i \in S} \mu_i = E[X(i;\xi)]$$ (1)

where $S = \{1, \ldots, k\}$ is a finite set of design points or “systems” indexed by $i$, and $\xi$ is a random element used to model the stochastic nature of simulation experiments. (In the remainder of the paper we assume that $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_k$, so that system $k$ is the best.) The objective function $\mu : S \to \mathbb{R}$ cannot be computed exactly, but can be estimated using output from a stochastic simulation represented by $X(\cdot;\xi)$. While the feasible space $S$ may have topology, as in the finite but integer-ordered case, we consider only methods to solve the SO problem in (1) that (i) do not exploit such topology or structural properties of the function, and that (ii) apply when the computational budget permits at least some simulation of every system. Such methods are called ranking and selection (R&S) procedures.

R&S procedures are frequently used in simulation studies because structural properties, such as convexity, are difficult to verify for simulation models and rarely hold. They can also be used in conjunction with heuristic search procedures in a variety of ways (Pichitlamken et al. 2006, Boesel et al. 2003), making them useful even if not all systems can be simulated. See Kim and Nelson (2006a) for an excellent introduction to, and overview of, R&S procedures. We remark here that while R&S problems are closely related to best-arm problems, there are several differences between these bodies of literature. Almost always, the algorithms developed in the best-arm literature assume that only one system is simulated at a time (see, e.g., Jamieson and Nowak 2014, Bubeck and Cesa-Bianchi 2012) and that simulation outputs are bounded, or that all variances have a known bound.

R&S procedures are designed to offer one of several types of probabilistic guarantees, and can be Bayesian or frequentist in nature. Bayesian procedures offer guarantees related to a loss function associated with a non-optimal choice; see Branke et al. (2007) and Chen et al. (2015, Chapter 3). Frequentist procedures typically offer one of two statistical guarantees; in defining these guarantees, let $\delta > 0$ be a known constant and let $\alpha \in (0, 1)$ be a parameter selected by the user. The Probability of Correct Selection (PCS) guarantee is a guarantee that, whenever $\mu_k - \mu_{k-1} \geq \delta$, the probability of selecting the best system $k$ when the procedure terminates is greater than $1 - \alpha$. Henceforth, the assumption that $\mu_k - \mu_{k-1} \geq \delta$ will be called the PCS assumption; if $\mu_k - \mu_{k-1} < \delta$ then a PCS guarantee does not hold. In contrast, the Probability of Good Selection (PGS) guarantee is a guarantee that the probability of selecting a system with objective value within $\delta$ of the best is greater than $1 - \alpha$. A PGS guarantee makes no assumption about the configuration of the means and is the same as the “probably approximately correct” guarantee in best-arm literature.
Traditionally, R&S procedures were limited to problems with a modest number of systems $k$, say $k \leq 100$, due to the need to assume worst-case mean configurations to construct validity proofs. The advent of screening, i.e., discarding clearly inferior alternatives early on (Nelson et al. 2001, Kim and Nelson 2006, Hong 2006), has allowed R&S to be applied to larger problems, say $k \leq 500$. Exploiting parallel computing is a natural next step as argued in, e.g., Fu (2002). By employing parallel cores, simulation output can be generated at a higher rate, and a parallel R&S procedure should complete in a smaller amount of time than its sequential equivalent, and allowing larger problems to be solved.

Heidelberger (1988), Glynn and Heidelberger (1990, 1991) explored the use of parallel computers to construct valid simulation estimators, but R&S procedures that exploit parallel computing have emerged only recently. Luo et al. (2000) and Yoo et al. (2009) employ a web-based computing environment and present a parallel procedure under the optimal computing budget allocation (OCBA) framework. (OCBA has impressive empirical performance, but does not offer PCS or PGS guarantees.) Chen (2005) tests a sequential pairwise hypothesis testing approach on a local network of computers. More recently, Luo et al. (2013) develop a parallel adaptation of a fully-sequential R&S procedure that provides an asymptotic (as $\delta \to 0$) PCS guarantee. Luo et al. (2013) is the best known existing method for parallel ranking and selection that provides a form of PCS guarantee on the returned solution.

In this paper, we (i) identify opportunities and challenges that arise from adopting a parallel computing environment to solve large-scale R&S problems, (ii) propose a Good Selection Procedure (GSP) that solves R&S problems on parallel computers, and (iii) implement our procedure in two different parallel computing frameworks. We make the following contributions.

Theoretical contributions. We propose a number of design principles that promote efficiency and validity in such an environment, and demonstrate them in a new parallel GSP. GSP showcases the power of these design principles in that it greatly extends the boundary on the size of solvable R&S problems. While the method of Luo et al. (2013) can solve on the order of $10^4$ systems, one of our implementations of GSP is capable of solving R&S problems with more than $10^6$ systems. Our computational results include such a problem, which we solve in under 6 minutes on $10^3$ cores. Another important theoretical contribution of this paper is the redesigned screening method in GSP which, unlike many fully-sequential procedures (Kim and Nelson 2001, Hong 2006), does not rely on the PCS assumption. Accordingly, many systems can lie within the indifference-zone, i.e., have an objective function value within $\delta$ of that of System $k$, as will usually be the case when the number of systems is very large. Our procedure then provides the same PGS guarantee as existing indifference-zone procedures like Nelson et al. (2001) but with far smaller sample sizes.

Practical contributions. The GSP procedure discussed in this paper is intended for any parallel, shared or non-shared memory platform where cores can communicate with each other. As long as no core fails during execution, it should deliver expected results regardless of the hardware specification. The procedure is also amenable to a range of existing parallel computing frameworks. We offer implementations of GSP based on MPI (Message-Passing Interface) and Hadoop MapRe-
duce, and show how they differ in construction and in performance. The reasons for our choice of implementation frameworks are twofold:

- Both MPI and MapReduce are among the most popular and mature platforms for deploying parallel code, on a wide range of systems ranging from high performance supercomputers to commodity clusters such as Amazon EC2.

- MPI and MapReduce provide points of comparison between two different parallel design philosophies. Broadly speaking, the former enables low level tailoring and optimization in the implementation of a parallel procedure, while the latter is more of a “one-size-fits-all” framework which delegates as much of the implementation complexity as possible to the MapReduce package itself.

As we shall see, MPI is the more efficient of the two, achieving speed and utilization gains of around a factor of magnitude over MapReduce. On the other hand, MapReduce offers acceptable performance for large scale problems, and is more robust to reliability issues that may arise in cloud-computing environments where parallel tasks may fail to complete due to unresponsive cores.

The remainder of the paper is organized as follows. §2 discusses the design principles followed in creating GSP to promote efficiency and ensure the procedure’s validity. §3 describes our multi-stage parallel R&S procedure GSP, and establishes the PGS guarantee. Computational studies in §4 support our assertions on the quality of GSP and its parallel implementations, and point to open-access repositories where the code can be obtained. An appendix contains more proof detail, and further information on the MPI and MapReduce implementations. This paper is a considerable outgrowth of the conference papers Ni et al. (2013, 2014, 2015).

2 Design Principles for Parallel R&S Procedures

R&S procedures are essentially made up of three computational tasks: (1) deciding what simulations to run next, (2) running simulations, and (3) screening (computing statistical estimators and determining which systems are inferior). On a single-core computer, these tasks are repeatedly performed in a certain order until a termination criterion is met. On a parallel platform, multiple cores can simultaneously perform one or several of these tasks.

In this section, we discuss various issues that arise when a R&S procedure is designed for and implemented on parallel platforms to solve large-scale R&S problems. We argue that failing to consider these issues may result in impractically expensive or invalid procedures. We recommend strategies by which these issues can be addressed, and illustrate how we incorporate them in our procedure presented in §3 which iteratively runs Tasks (1) through (3) in multiple stages.

For discussing the design principles for parallel R&S procedures in this section, we consider a parallel computing environment that satisfies the following properties.

Assumption 1. (Core Independence) A fixed number of processing units ("cores") are employed to execute the parallel procedure. Each core is capable of performing its own set of computations
without interfering with other cores unless instructed to do so. Each core has its own memory and does not access the memory of other cores.

Assumption 2. (Message-passing) The cores are capable of communicating through sending and receiving messages of common data types and arbitrary lengths.

Assumption 3. (Reliability) Cores do not “fail” or suddenly become unavailable. Messages are never “lost”.

Many parallel computer platforms satisfy the first two assumptions, but some are subject to the risk of core failure, which may interrupt the computation in various ways. For clarity, we work under the reliability assumption and defer the design of failure-proof procedures to §4.2.2 where we discuss Hadoop MapReduce. Similar to Luo et al. (2013) and Ni et al. (2013), we consider a master-worker framework, using a uniquely executed “master” process (typically run on a dedicated “master” core) to coordinate the parallel procedure, and letting other cores (the “workers”) work according to the master’s instructions. To the extent possible we want to avoid synchronization delays, where one core cannot continue until another core completes its task, as we will see in §4.2.

2.1 Implications of Random Completion Times

Consider the simplest case where only Task (2), running simulations, is run in parallel, and each simulation replication completes in a random amount of time. To construct estimators for a single system simulated by multiple cores, one can either collect a fixed number of replications in a random completion time, or a random number of replications in a fixed completion time (Heidelberger 1988). Heidelberger (1988) and Glynn and Heidelberger (1990, 1991) discuss unbiased estimators of each type. Because a random number of replications collected after a fixed amount of time may not be i.i.d. with the desired distribution upon which much of the screening theory depends (Heidelberger 1988, Glynn and Heidelberger 1991, Ni et al. 2013, Luo et al. 2013), we confine our attention to estimators that produce a fixed number of replications in a random completion time. (The cause of this difficulty can be traced to dependence between the estimated objective function and computational time.)

Using estimators that produce a fixed number of replications in a random completion time for parallel R&S places a restriction on the manner in which replications can validly be farmed out to and collected from the workers. Consider the case where more than one core simulates the same system, and replications generated in parallel are aggregated to produce a single estimator. A naïve way is to collect replications from any core following the order in which they are generated, but as demonstrated in Ni et al. (2013, §3.1), the estimators may be biased, making it hard to establish provable statistical guarantees. In contrast, a valid method is to place the finished replications in a predetermined order and use them as if they are generated following that order, to avoid “re-ordering” of the simulation replications caused by random completion time.

Under this principle, our GSP in §3 ensures that the simulation results generated in parallel are initiated, collected, assembled and used by the screening routine in an ordered manner. Specifically,
in Stage 2 of GSP, when the master instructs a worker to simulate system \( i \) for a batch of replications (Step 4(c)), the batch index is also received by the worker. When the batch is completed, its statistics are sent back to the master alongside the batch index (Step 4(c)), which signals its pre-determined position in the assembled batch sequence on the master. This ensures that the batch statistics sent to workers for screening (Step 4(d)) follow the exact order in which they were initiated, and constructed estimators are unbiased with the correct distribution. Luo et al. (2013) discuss a similar approach which they refer to as “vector-filling”.

2.2 Allocating Tasks to the Master and Workers

Previous work on parallel R&S procedures (Chen et al. 2000, Yoo et al. 2009, Luo and Hong 2011, Luo et al. 2013) focuses almost exclusively on pushing Task (2), running simulations, to parallel cores. In those procedures, usually the master is solely responsible for Tasks (1) and (3), deciding what simulations to run next and screening, and the workers perform Task (2) in parallel. In this setting, the benefit of using a parallel computing platform is entirely attributed to distributing simulation across parallel cores, hence reducing the total amount of time required by Task (2).

However, the master could potentially become a bottleneck in a number of ways. First, as noted by Luo and Hong (2011), the master can be overwhelmed with messages. Second, for the master to keep track of all simulation results requires a large amount of memory, especially when the number of systems is large (Luo et al. 2013). Finally, when the number of systems is large and simulation output is generated by many workers concurrently, running Tasks (1) and (3) on the master alone may become relatively slow, resulting in a waste of core hours on workers waiting for the master’s further instructions. Therefore, a truly scalable parallel R&S procedure should allow its users a simple way to control the level of communication, use the memory efficiently, and distribute as many tasks as possible across parallel cores. In addition, it should perform some form of load-balancing to minimize idling on workers.

2.2.1 Batching to Reduce Communication Load

One way to reduce the number of messages handled by the master is to control communication frequency by having the workers run simulation replications in batches and only communicate once after each batch is finished.

Since R&S procedures typically use summary statistics rather than individual observations when screening systems, it may even suffice for the worker to compute and report batch statistics instead of point observations from every single replication. Indeed, a useful property of our statistic for screening systems \( i \) and \( j \) is that it is updated using only the sample means over the entirety of the most recent batch \( r \), instead of requiring the collection of individual replication outcomes. These sample means can be independently computed on the worker(s) running the \( r \)th batch of systems \( i \) and \( j \), and the amount of communication needed in reporting them to the master is constant and does not grow with the batch size.
The distribution of batches in parallel must be handled with care. Most importantly, since using a random number of replications after a fixed run time may introduce bias (as we have shown in §2.1), a valid procedure should employ a predetermined and fixed batch size for each system, which may vary across different systems. Batches generated in parallel for the same system should be assembled according to a predetermined order, following the same argument used in §2.1. Furthermore, if the procedure requires screening upon completion of every batch, then it is necessary to perform screening steps following the assembled order.

2.2.2 Allocating Simulation Time to Systems

When multiple systems survive a round of screening, R&S procedures need to decide which system(s) to simulate next (possibly on multiple cores), and how many replications to take. While sequential procedures usually sample one replication from the chosen system(s), or multiple replications from a single system, it is natural for a parallel procedure to consider strategies that sample multiple replications from multiple systems. In doing so, the parallel procedure may adopt sampling strategies such that simulation resources are allocated to surviving systems in a most efficient manner.

The best practice in making such allocations depends on the specific screening method. For instance, in [Hong (2006)] as well as GSP, screening between systems $i$ and $j$ is based on a scaled Brownian motion $B([\sigma_i^2/n_i + \sigma_j^2/n_j]^{-1})$ where $B(\cdot)$ denotes a standard Brownian motion (with zero drift and unit volatility), $n_i$ is the sample size and $\sigma_i^2$ is the variance of system $i$. To drive this Brownian motion rapidly with the fewest samples possible, which accelerates screening, [Hong (2006)] recommended that the ratio $n_i/\sigma_i$ be kept equal across all surviving systems.

The above recommendation implicitly assumes that simulation completion time is fixed for all systems, and is suboptimal when completion time varies across systems. Suppose all workers are identical, and each replication of system $i$ takes a fixed amount of time $T_i$ to simulate on any worker. We can then formulate the problem of advancing the above Brownian motion as

$$\max \left[ \sigma_i^2/n_i + \sigma_j^2/n_j \right]^{-1}$$

subject to $n_i T_i + n_j T_j = T$

which yields the optimal computing time allocation

$$\frac{n_i T_i}{n_j T_j} = \frac{\sigma_i \sqrt{T_i}}{\sigma_j \sqrt{T_j}}.$$  \hfill (2)

This result is consistent with a conclusion in [Glynn and Whitt (1992)], that when simulation completion time $T_i$ varies, an asymptotic measure of efficiency per replication is inversely proportional to $\sigma_i^2 E[T_i]$.

In practice, $T_i$ is unknown and possibly random, so both $E[T_i]$ and $\sigma^2$ need to be estimated in a preliminary stage. Suppose they are estimated by some estimators $\bar{T}_i$ and $S_i^2$. Then we recommend
setting the batch size for each system $i$ proportional to $S_i / \sqrt{T_i}$ following $2$.

### 2.2.3 Distributed screening

In fully sequential R&S procedures, e.g., Kim and Nelson (2006b), Hong (2006), each screening step typically involves doing a fixed amount of calculation between every pair of systems to decide if one system is better than another with a certain degree of statistical confidence. The amount of work is proportional to the number of pairs of systems, which is $O(k^2)$.

In the serial R&S literature, the computational cost of screening is assumed to be negligible compared to that of simulation because the number of systems $k$ is usually quite small and each simulation replication may take orders of magnitude longer than $O(k^2)$ screening operations required in each iteration. Under this assumption, it is tempting to simply have the master handle all screening after the workers complete a simulation batch. This approach can easily be implemented and proven to be statistically valid. However, it may become computationally inefficient because all workers stay idle while the master screens, so a total amount of $O(c k^2)$ processing time is wasted, where $c$ is the number of workers. For a large problem with a million systems solved on a thousand cores, the wasted processing time per round of screening can easily amount to thousands of core hours, reducing the benefits from a parallel implementation dramatically. Moreover, if the procedure requires computing and storing in memory some quantities for each system pair (for instance, the variance of differences between systems), then the total amount of $O(k^2)$ memory may easily exceed the limit for a single core.

It is therefore worth considering strategies that distribute screening among workers. A natural strategy is to assign roughly $k/c$ systems to each worker, and let it screen among those systems
only, as illustrated in Figure 1. By doing so, each worker screens \( k/c \) systems, occupying only \( O(k^2/c^2) \) memory, and performing \( O(k^2/c^2) \) work in parallel. Hence the wall-clock time for each round of screening is reduced by a factor of \( c^2 \).

Under the distributed screening scheme, not all pairs of systems are compared, so fewer systems may get eliminated. The reduction in effectiveness of screening can be compensated by sharing some good systems across workers. In Figure 1, for example, each core shares its own (estimated) best system with other cores, and each system is screened against other systems on the same core, as well as \( O(c) \) good systems from other cores. This greatly improves the chance that each system is screened against a good one, despite the extra work to share those good systems. As illustrated in Figure 1, the additional number of pairs that need to be screened on each core is only \( O(k) \) when the best system on each core is shared. Alternatively, the procedure may also choose to share only a smaller number \( c' \ll c \) of good systems, so that the communication workload associated with this sharing does not increase as the number of workers increases.

The statistical validity of some screening-based R&S procedures (e.g., Kim and Nelson 2001, Hong 2006, Luo et al. 2013) requires screening to be performed once every replication (or batch of replications) is simulated. This implies that, when the identity of the estimated-best system(s) changes, the master has to communicate all previous replication results of the new estimated-best system(s) to the workers, so that they can perform all of the screening steps up to the current replication to ensure validity of the screening. (If screening on a strict subsequence of replications, it may be sufficient to communicate summary statistics.) Such “catch-up” screening was used, for instance, in Pichitlamken et al. (2006), in a different context. In §3, we employ a probabilistic bound that removes the need for catch-up screening in GSP.

Besides core hours, distributing screening across workers also saves memory space on the master. In our implementation of GSP, the master keeps a complete copy of batch statistics only for a small number of systems that are estimated to be the best. For a system that is not among the best, the master acts as an intermediary, keeping statistics for only the most recent batches that have not been collected by a worker. Whenever some batch statistics are sent to a worker (for screening in Steps 3(c) or 5(d) of GSP), they can be deleted on the master. This helps to even out memory usage across cores, making the procedure capable of solving larger problems without the need to use slower forms of storage.

2.3 Random Number Stream Management

The validity and performance of simulation experiments and simulation optimization procedures relies substantially on the quality and efficiency of (pseudo) random number generators. For a discussion of random number generators and their desirable properties, see L’Ecuyer (2006).

To avoid unnecessary synchronization, each core may run its own random number generator independently of other cores. Some strategies for generating independent random numbers in parallel have been proposed in the literature. Mascagni and Srinivasan (2000) consider a class of random number generators which are parametrized so that each valid parametrization is assigned
to one core. Karl et al. (2014) adopt L’Ecuyer et al. (2002)’s RngStream package, which supports streams and substreams, and demonstrated a way to distribute RngStream objects across parallel cores.

Both methods set up parallel random number generation in such a way that once initialized, each core will be able to generate a unique, statistically independent stream of pseudo random numbers, which we denote as $U_w$, for each $w = 1, 2, \ldots, c$. If a core has to switch between systems to simulate, one can partition $U_w$ into substreams $\{U^i_w : i = 1, 2, \ldots, k\}$, simulating system $i$ using $U^i_w$ only. It follows that for any system $i$, $U^i_w$ for different $w$ are independent as they are substreams of independent $U_w$’s, so simulation replicates generated in parallel with $\{U^i_w : w = 1, 2, \ldots, c\}$ are also i.i.d. Moreover, if it is desirable to separate sources of randomness in a simulation, it may help to further divide $U^i_w$ into subsubstreams, each used by a single source of randomness.

In practice, one does not need to pre-compute and store all random numbers in a (sub)stream, as long as jumping ahead to the next (sub)stream and switching between different (sub)streams are fast. Such operations are easily achievable in constant computational cost; see L’Ecuyer et al. (2002) for an example.

Although our procedure does not support the use of common random numbers (CRN), it is worth noting that the above framework easily extends to accommodate CRN as follows. Begin by having one identical stream $U_0$ set up on all cores and partitioning it into substreams $\{U_0(\ell) : 1 \leq \ell \leq L\}$ for sufficiently large $L$. Let the master keep variables $\{\ell_i : i = 1, 2, \ldots, k\}$ which count the total number of replications already generated for system $i$ over all workers. Each time the master initiates a new replication of system $i$ on a worker, it instructs the worker to simulate system $i$ using substream $\{U_0(\ell_i + 1)\}$ and adds 1 to $\ell_i$. This ensures that for any $\ell > 0$, the $\ell$th replication of every system is generated by the same substream $\{U_0(\ell)\}$.

3 The Parallel Good Selection Procedure

In this section, we provide a R&S procedure GSP that incorporates the design principles from §2 and is implementable on a wide spectrum of parallel platforms. Our procedure applies to the general case in which the system mean and variance are both unknown and need to be estimated (an earlier version of the procedure under the known variance case is discussed in Ni et al. 2014), and does not permit the use of common random numbers. We prove that the procedure offers a PGS guarantee for normally distributed observations.

3.1 The Setup

GSP consists of four broad stages. In an optional Stage 0, workers run $n_0$ simulation replications for each system in parallel to estimate completion times, which are subsequently used to try to balance the workload. As discussed in §2.2, Stage 0 samples are then dropped and not used to form estimators of $\mu_i$’s due to the potential correlation between simulation output and completion time. In Stage 1, a new sample of size $n_1$ is collected from each system to obtain variance estimates.
\[ S_i^2 = \sum_{i=1}^{n_1} (X_{i1} - \bar{X}_i(n_1))^2 / (n_1 - 1), \text{ where } \bar{X}_i(n) = \sum_{i=1}^{n} X_{il}/n. \] Prior to Stage 2, obviously inferior systems are screened. In Stage 2, the workers iteratively visit the remaining systems and run additional replications, exchange statistics and independently perform screening over a subset of systems until either all but one are eliminated, or a pre-specified limit on sample size is reached. The screening rule and the limit on sample size are jointly chosen such that inferior systems can be eliminated efficiently, while the best system \( k \) survives this stage with high probability regardless of the configuration of true means \( \mu_1, \ldots, \mu_k \). Finally, in Stage 3, all systems surviving Stage 2 enter a Rinott (1978) procedure where a maximum sample size is calculated, additional replications are simulated if necessary, and the system with the highest sample mean is selected as the best.

The sampling rules used in Stages 0, 1, and 3 are relatively straightforward, for they each require a fixed number of replications from each system. In Stage 2, where the procedure iteratively switches between simulation and screening, a sampling rule needs to be specified to fix the number of additional replications to take from each system before each round of screening. Prior to the start of the overall selection procedure we define increasing (in \( r \)) sequences \( \{n_i(r) : i = 1, 2, \ldots, k, r = 0, 1, \ldots\} \) giving the total number of replications to be collected for system \( i \) by batch \( r \), and let \( n_i(0) = n_1 \) since we include the Stage 1 sample in mean estimation. Following the discussion in §2.2.2 where we recommend that batch size for system \( i \) be proportional to \( S_i / \sqrt{T_i} \) in order to efficiently allocate simulation budget across systems, we use

\[ n_i(r) = n_1 + r \left[ \beta \left( \frac{S_i}{\sqrt{T_i}} \right) / \left( 1 + \frac{1}{k} \sum_{j=1}^{k} \frac{S_j}{\sqrt{T_j}} \right) \right] \tag{3} \]

where \( T_i \) is an estimator for simulation completion time of system \( i \) obtained in Stage 0 if available, and \( \beta \) is the average batch size and is specified by the user.

The parameters for the procedure are as follows. Before the procedure initiates, the user selects an overall confidence level \( 1 - \alpha \), type-I error rates \( \alpha_1, \alpha_2 \) such that \( \alpha = \alpha_1 + \alpha_2 \), an indifference-zone parameter \( \delta \), Stage 0 and Stage 1 sample sizes \( n_0, n_1 \geq 2 \), and average Stage 2 batch size \( \beta \). The user also chooses \( \bar{r} > 0 \) as the maximum number of iterations in Stage 2, which governs how much simulation budget to spend in iterative screening before moving to indifference-zone selection in Stage 3.

Typical choices for error rates are \( \alpha_1 = \alpha_2 = 0.025 \) for guaranteed PGS of 95%. The indifference-zone parameter \( \delta \) is usually chosen within the context of the application, and is often referred to as the smallest difference worth detecting. The sample sizes \( n_0 \) and \( n_1 \) are typically chosen to be small multiples of 10, with the view that these give at least reasonable estimates of the runtime per replication and the variance per replication.

For non-normal simulation output, we recommend setting \( \beta \geq 30 \) to ensure normally distributed batch means. The parameter \( \beta \) also helps to control communication frequency so as not to overwhelm the master with messages. Let \( T_{\text{sim}} \) be a crude estimate of the average simulation time (in seconds) per replication, perhaps obtained in a debugging phase. Then ideally the master
Hence, the fraction of time the master is busy is \( \rho = cT_{\text{comm}}/\beta T_{\text{sim}} \). We recommend setting \( \beta \) such that \( \rho \leq 0.05 \), in order to avoid significant waiting of workers.

We recommend choosing \( \bar{r} \) such that a fair amount of simulation budget (no more than 20% of the sum of Rinott sample sizes) will be spent in the iterative screening stages. Note that a small \( \bar{r} \) implies insufficient screening whereas a large \( \bar{r} \) may be too conservative.

Under these general principles, our choices of \( \beta = 100, \bar{r} = 10 \) and \( \beta = 200, \bar{r} = 5 \) in the experiments in [4] work reasonably well on our testing platform, but it is conceivable that other values could improve performance.

Finally, we define some quantities used in the iterative screening stages. Let \( \eta \) be the solution to

\[
E \left[ 2\tilde{\Phi} \left( \eta \sqrt{R} \right) \right] = 1 - (1 - \alpha_1)^{1/\bar{r}},
\]

where \( \tilde{\Phi}(\cdot) \) denotes the complementary standard normal distribution function, and \( R \) is the minimum of two i.i.d. \( \chi^2 \) random variables, each with \( n_1 - 1 \) degrees of freedom. Let the distribution function and density of such a \( \chi^2 \) random variable be denoted \( F_{\chi^2_{n_1-1}}(x) \) and \( f_{\chi^2_{n_1-1}}(x) \), respectively. Hence \( R \) has density \( f_R(x) = 2[1 - F_{\chi^2_{n_1-1}}(x)]f_{\chi^2_{n_1-1}}(x) \). Also, for any two systems \( i \neq j \), define

\[
t_{ij}(r) = \left[ \frac{\sigma_i^2}{n_i(r)} + \frac{\sigma_j^2}{n_j(r)} \right]^{-1}, \quad Z_{ij}(r) = t_{ij}(r)[\bar{X}_i(n_i(r)) - \bar{X}_j(n_j(r))],
\]

\[
\tau_{ij}(r) = \left[ \frac{S_i^2}{n_i(r)} + \frac{S_j^2}{n_j(r)} \right]^{-1}, \quad Y_{ij}(r) = \tau_{ij}(r)[\bar{X}_i(n_i(r)) - \bar{X}_j(n_j(r))],
\]

\[
a_{ij}(\bar{r}) = \eta \sqrt{(n_1 - 1)\tau_{ij}(\bar{r})}.
\]

### 3.2 Good Selection Procedure under Unknown Variances

1. **(Stage 0), optional** Master assigns systems to workers, so that each system \( i \) is simulated for \( n_0 \) replications and the average simulation completion time \( \bar{T}_i \) is reported to the master.

2. **(Stage 1)** Master assigns systems to load-balanced (using \( \bar{T}_i \) if available) simulation groups \( G^w_i \) for \( w = 1, \ldots, c \). Let \( \mathcal{I} \leftarrow \mathcal{S} \) be the set of surviving systems.

3. For \( w = 1, 2, \ldots, c \) in parallel on workers:

   (a) Sample \( X_{i\ell}, \ell = 1, 2, \ldots, n_1 \) for all \( i \in G^w_1 \).

   (b) Compute Stage 1 sample means and variances \( \bar{X}_i(n_1) \) and \( S_i^2 \) for \( i \in G^w_1 \).

   (c) Screen within group \( G^w_1 \): system \( i \) is eliminated (and removed from \( \mathcal{I} \)) if there exists a system \( j \in G^w_1 : j \neq i \) such that \( Y_{ij}(0) < -a_{ij}(\bar{r}) \).

   (d) Report survivors, together with their Stage 1 sample means \( \bar{X}_i(n_i(0)) \) and variances \( S_i^2 \), to the master.
4. **(Stage 2)** Let $G_1 \leftarrow \mathcal{I}$ be the set of systems surviving Stage 1. Master computes sampling rule \ref{eq:2} using $S_1^2$ obtained in Stage 1, and divides $G_1$ to approximately load-balanced screening groups $G_w^2$ for $w = 1, \ldots, c$. Let $s_i \leftarrow 0, i \in G_1$ be the count of the number of batches simulated in Stage 2 for system $i$.

5. For $w = 1, 2, \ldots, c$ in parallel on workers, let $r_w \leftarrow 0$ be the count of the number of batches screened on worker $w$ (which is common to all systems in the screening), and iteratively switch between simulation and screening as follows (this step entails some communication with the master, the details of which are omitted):

   (a) Check termination criteria with the master: if $|\mathcal{I}| = 1$ (only one system remains) or $r_w \geq \bar{r}$ for all $w$ (each worker has screened up to $\bar{r}$, the maximum number of batches allowed), go to Stage 3; otherwise continue to Step \ref{5b}.

   (b) Decide to either simulate more replications or perform screening based on available results: check with the master if the $(r_w + 1)$th iteration has completed for all systems $i \in G_w^2$ and $|G_w^2| > 1$, if so, go to Step \ref{5d}; otherwise go to Step \ref{5c}.

   (c) Retrieve the next system $i$ in $G_1$ (not necessarily $G_w^2$) from the master and simulate it for an additional $n_i(s_i + 1) - n_i(s_i)$ replications. Set $s_i \leftarrow s_i + 1$. Report simulation results to the master. Go to Step \ref{5a}.

   (d) Screen within $G_w^2$ as follows. Retrieve necessary statistics for systems in $G_w^2$ from the master (recall that a system in $G_w^2$ is not necessarily simulated by worker $w$). Let $r_w \leftarrow r_w + 1$. A system $i \in G_w^2$ is eliminated if $r_w \leq \bar{r}$ and there exists a system $j \in G_w^2 : j \neq i$ such that $Y_{ij}(r_w) < -a_{ij}(\bar{r})$. Also use a subset of systems from other workers, e.g., those with the highest sample mean from each worker, to eliminate systems in $G_w^2$. Remove any eliminated system from $G_w^2$ and $\mathcal{I}$. Go to Step \ref{5a}.

6. **(Stage 3)** Let $G_2 \leftarrow \mathcal{I}$ be the set of systems surviving Stage 2. If $k' := |G_2| = 1$, select the single system in $G_2$ as the best. Otherwise, set $h = h(1 - \alpha_2, n_1, k')$, where the function $h(\cdot)$ gives Rinott’s constant (see e.g. Bechhofer et al. 1995, Chapter 2.8). For each remaining system $i \in G_2$, compute $N_i = \max\{n_i(\bar{r}), [(hS_i/\delta)^2]\}$, and take an additional $\max\{N_i - n_i(\bar{r}), 0\}$ sample observations in parallel. Once a total of $N_i$ replications have been collected in Stages 1 through 3 for each $i \in G_2$, select the system $K$ with the highest $\bar{X}(N_K)$ as the best.

### 3.3 Guaranteeing Good Selection

Our probabilistic guarantee on the final solution relies on the following assumption on the distribution of simulation output, which is common to the sequential R&S literature.

**Assumption 4.** For each system $i = 1, 2, \ldots, k$, the simulation output random variables $\{X_{i\ell}, \ell = 1, 2, \ldots\}$ are i.i.d. replicates of a random variable $X_i$ having a normal distribution with finite mean $\mu_i$ and finite variance $\sigma_i^2$, and are mutually independent for different $i$. 

13
In §2.1 we gave conditions under which the simulation output generated by parallel cores satisfies the i.i.d. assumption.

We now formally state our good selection guarantee.

**Theorem 1.** Under Assumption 4, GSP selects a system $K$ that satisfies $\mu_k - \mu_K \leq \delta$ with probability at least $1 - \alpha$.

We discuss the key insights that yield the PGS guarantee here and defer the full proof of Theorem 1 to §A.1.

**Sketch of Proof.** First, we show that the best system, System $k$, survives the iterative screening in Stages 1 and 2 with probability at least $1 - \alpha_1$, irrespective of whether the best solution is unique or not. Indeed, conditioning on the Stage 1 variance estimates $\{S_i^2 : 1 = 1, 2, \ldots, k\}$, we can, for any system $i \neq k$, relate the batch statistics $Z_{ki}(r) : r = 0, 1, \ldots, \bar{r}$ to a properly scaled Brownian motion with drift $\mu_k - \mu_i \geq 0$. Then, using the reflection principle of Brownian motion, we can upper-bound the probability that the scaled Brownian motion falls below some number $-a$ before some time $t$, or equivalently, the probability that $Y_{ki}(r) \leq -a_{ki}(\bar{r})$ in some $r$th iteration where $r \leq \bar{r}$, which is the criterion used to eliminate system $k$ in the iterative screening stages. The construction of continuation region parameter $\eta$ and the fact that $(n_1 - 1)S_i^2/\sigma_i^2 \sim \chi_{n_1 - 1}^2$ for all $i$ jointly ensure that the unconditional probability of eliminating $k$ is no greater than $\alpha_1$.

Second, as Stage 3 is closely related to the Rinott (1978) procedure with confidence level $1 - \alpha_2$, it follows from Theorem 1 of Nelson and Matejcik (1995) that

$$P \left\{ \bar{X}_K(N_K) - \bar{X}_i(N_i) > -\delta, \forall i \in G_2 : i \neq K \right\} \geq 1 - \alpha_2$$

where $K$ is the system with the highest sample mean after Stage 3. Therefore we conclude that if $k \in G_2$ (the best system $k$ survives Stages 1 and 2), then $P \left\{ \bar{X}_K(N_K) - \bar{X}_i(N_i) - (\mu_K - \mu_k) > -\delta \right\} \geq 1 - \alpha_2$, that is, Stage 3 selects a good system $K$ such that $\mu_K \geq \mu_k - \delta$ with high probability.

Finally, we complete the proof by invoking a result from Nelson et al. (2001) that guarantees an overall PGS of $1 - \alpha_1 - \alpha_2$ for two-stage procedures.

The key difference between the screening methods used in GSP and the $KN$ family procedures (Kim and Nelson 2001, Hong and Nelson 2005, Hong 2006) is that the $KN$ family relies on the PCS assumption ($\mu_k - \mu_i \geq \delta > 0$ for all $i \neq k$) to guarantee PCS, whereas our approach does not. Therefore, GSP works for any indifference-zone parameter $\delta > 0$, and when there exist multiple systems $i$ such that $\mu_i \geq \mu_k - \delta$, GSP is guaranteed to select one such system with probability at least $1 - \alpha$.

### 3.4 Choice of parameter $\eta$

One way to compute $\eta$, the solution to (4), is by integrating the LHS using Gauss-Laguerre quadrature and using bisection to find the root of (4). Alternatively, we may employ a bounding technique...
to approximate $\eta$ as follows. Indeed, the LHS of (4) is

$$E\left[2\Phi(\eta\sqrt{R})\right] = \int_{y=0}^{\infty} 2\Phi(\eta\sqrt{y})2\left[1 - F_{\chi_{n_1-1}^2}(y)\right]f_{\chi_{n_1-1}^2}(y)dy$$

$$\leq \int_{y=0}^{\infty} 4\Phi(\eta\sqrt{y})f_{\chi_{n_1-1}^2}(y)dy$$

$$\leq \int_{y=0}^{\infty} \frac{e^{-\eta^2 y/2} y^{n_1-1} - e^{-y/2}}{\eta^{2n_1} \Gamma(\frac{n_1-1}{2})}dy$$

$$= \frac{4\Gamma(\frac{n_1-2}{2})\frac{\Gamma(\frac{n_1}{2}+1)}{\eta^{n_1-1} \sqrt{\pi \Gamma(\frac{n_1-1}{2})}}}{} \int_{y=0}^{\infty} \frac{y^{\frac{n_1-2}{2} - 1 - \frac{1}{2} e^{-\frac{y^2-1}{2}\eta^2}}}{\Gamma(\frac{n_1-2}{2})}dy$$

$$= \frac{2\Gamma(\frac{n_1-2}{2})}{\sqrt{\pi \Gamma(\frac{n_1-1}{2})} \eta^{n_1-1} \sqrt{\pi \Gamma(\frac{n_1-1}{2})}}$$

where (5) holds because distribution functions are non-negative and is inspired by a similar argument in Hong (2006), (6) follows from the fact that $\Phi(x) \leq e^{-x^2/2/(x\sqrt{2\pi})}$ for all $x > 0$, and the integrand in (7) is the pdf of a Gamma distribution with shape $(n_1 - 1)/2$ and scale $2/(\eta^2 + 1)$, and hence integrates to 1.

Note that (8) is an upper-bound on the left-hand side of (4). Setting (8) to $1 - (1 - \alpha_1)^{\frac{1}{k-1}}$ and solving for $\eta$ yields an overestimate $\eta'$, which is more conservative and does not reduce the PGS. Furthermore, as (8) is strictly decreasing in $\eta$, $\eta'$ can be easily determined using bisection.

The parameter $\eta$ determines the value of $a_{ij}(\bar{r})$, and hence how quickly an inferior system is eliminated in screening Steps 3(c) and 5(d). The value of $\eta$ therefore directly impacts the effectiveness of the iterative screening. Hence, it is desirable that $\eta$ does not grow dramatically as the problem gets bigger. Observe that (8) can be further bounded by

$$\frac{2\Gamma(\frac{n_1-2}{2})}{\sqrt{\pi \Gamma(\frac{n_1-1}{2})} \eta^{n_1-1} \sqrt{\pi \Gamma(\frac{n_1-1}{2})}} := C\eta^{1-n_1}.$$  

(9)

Setting (9) to $1 - (1 - \alpha_1)^{\frac{1}{k-1}}$ implies that the right-hand side of (9) must be small. After some further manipulations we have

$$\log(1 - \alpha_1) = (k-1) \log \left(1 - C\eta^{1-n_1}\right) \approx (k-1)(-C\eta^{1-n_1})$$

(10)

where the approximation holds because $\log(1 - \epsilon) \approx -\epsilon$ for small $\epsilon > 0$. It follows from (10) that for fixed $\alpha_1$, the parameter $\eta$ grows very slowly with respect to $k$, at a rate of $k^{1/(n_1-1)}$. Therefore, the continuation region defined by $\eta$ and $\bar{r}$ as well as the power of our iterative screening are not substantially weakened as the number of systems increases, especially when $n_1$ or $k$ is large. In this regime, we should expect the total cost of this R&S procedure to grow approximately linearly with respect to the number of systems.
4 Computational Study

In this section, we discuss our parallel computing environment and test problem, discuss two parallel implementations of GSP, and discuss the results of our numerical experiments.

4.1 Parallel Computing Environment and Test Problem

Our numerical experiments are conducted on Extreme Science and Engineering Discovery Environment (XSEDE)’s Stampede high-performance cluster. The Stampede cluster contains over 6,400 computer nodes, each equipped with two 8-core Intel Xeon E5 processors and 32 GB of memory and runs a Linux Centos 6.3 operating system (Texas Advanced Computing Center 2014). Parallel programs are submitted through the Simple Linux Utility for Resource Management (SLURM) batch environment which enables users to specify the number of cores to use. The high-performance processors on Stampede are highly reliable and we have never seen a core failure.

We test R&S procedures on a throughput-maximization problem taken from SimOpt.org (Henderson and Pasupathy 2014). In this problem, we solve

\[
\max_x E[g(x; \xi)]
\]

\[
\text{s.t. } r_1 + r_2 + r_3 = R
\]

\[
b_2 + b_3 = B
\]

\[
x = (r_1, r_2, r_3, b_2, b_3) \in \{1, 2, \ldots \}^5
\]

where the function \( g(x; \xi) \) represents the random throughput of a three-station flow line with finite buffer storage in front of Stations 2 and 3, denoted by \( b_2 \) and \( b_3 \) respectively, and an infinite number of jobs in front of Station 1. The processing times of each job at stations 1, 2, and 3 are independently exponentially distributed with service rates \( r_1, r_2 \) and \( r_3 \), respectively. The overall objective is to maximize expected steady-state throughput by finding an optimal (integer-valued) allocation of buffer and service rate.

For each choice of the problem parameters \( R, B \in \mathbb{Z}^+ \), the number of feasible allocations is finite and can be easily computed. We consider three problem instances with very different sizes presented in Table 1. Since the service times are all exponential, we can analytically compute the expected throughput of each feasible allocation by modeling the system as a continuous-time Markov chain. Furthermore, it can be shown that \( E[g(r_1, r_2, r_3, b_2, b_3; \xi)] = E[g(r_3, r_2, r_1, b_3, b_2; \xi)] \) for any feasible allocation \( (r_1, r_2, r_3, b_2, b_3) \), so the problem may have multiple optimal solutions. Therefore, this is a problem for which the PCS assumption \( \mu_k - \mu_{k-1} \geq \delta > 0 \) can be violated and R&S procedures that only guarantee correct selection might be viewed as heuristics.

By default, in each simulation replication, we warm up the system for 2,000 released jobs starting from an empty system, before observing the simulated throughput to release the next 50 jobs. This may not be the most efficient way to estimate steady-state throughput compared to taking batch means from a single long run, but it suits our purpose which is to obtain i.i.d. random replicates.
Table 1: Summary of three instances of the throughput maximization problem.

| $(R, B)$ | Number of systems $k$ | Highest mean $\mu_k$ | $p = 75$ | $p = 50$ | $p = 25$ | No. of systems in $[\mu_k - \delta, \mu_k]$ |
|----------|----------------------|----------------------|---------|---------|---------|----------------------------------|
| (20, 20) | 3,249                | 5.78                 | 3.52    | 2.00    | 1.00    | 6, 21, 256                      |
| (50, 50) | 57,624               | 15.70                | 8.47    | 5.00    | 3.00    | 12, 43, 552                     |
| (128, 128)| 1,016,127            | 41.66                | 21.9    | 13.2    | 6.15    | 28, 97, 866                     |

from the $g(x; \xi)$ distribution in parallel. Due to the fixed number of jobs, the wall-clock time for each simulation replication exhibits low variability.

4.2 Parallel Implementations of GSP

In this section, we discuss two implementations of GSP proposed in §3. Although we will primarily test them on Stampede, both procedures can be configured to run on a wide range of parallel platforms from multi-core personal computers to the Amazon EC2 cloud.

4.2.1 MPI

Message-Passing Interface (MPI) is a popular distributed-memory parallel programming framework with libraries available in C/C++ and Fortran and the de-facto standard for parallel programming on many high-performance parallel clusters including Stampede. Using MPI, programs operate in an environment where Assumptions 1 and 2 hold. The method by which parallel cores independently execute instructions and communicate through message-passing can be highly customized to serve different purposes.

The MPI implementation is a realization of GSP presented in §3 and is fully described in §A.2. We designate one core as the master and let it control other worker cores. We observe that communication is fast on Stampede, taking only $10^{-6}$ to $10^{-4}$ seconds each time depending on the size of the message. Therefore, with an appropriate choice of the batch-size parameter $\beta$, the master remains idle most of the time so the workers are usually able to communicate with the master without much delay.

Our MPI implementation is designed primarily for high-performance clusters like Stampede and does not detect and manage core failures. As simulation output is distributed across parallel cores without backup, the MPI implementation is vulnerable to core failures which may cause loss of data and break the program. In practice, such failures can occur for a number of reasons, including faulty hardware but also cores aborting due to being re-assigned to higher priority tasks by the system. Therefore, for cheap and less reliable parallel platforms, the MPI implementation needs to be augmented with a “fault-tolerant” mechanism in order to allow the procedure to continue even if some cores fail. This motivates us to seek alternative programming tools such as MapReduce that handle core failures automatically. Our MPI implementation uses the mvapich2 library and its source code and documentation is hosted in the open-access repository [2015].
4.2.2 Hadoop MapReduce

MapReduce (Dean and Ghemawat 2008) is a distributed computing model typically used to process large amounts of data. Conceptually, each MapReduce instance consists of a Map phase where data entries are processed by “Mapper” functions in parallel, and a Reduce phase where Mapper outputs are grouped by keys and summarized using parallel “Reducer” functions. MapReduce has become a popular choice for data intensive applications such as PageRank and TeraSort, thanks to the following advantages.

- **Simplicity.** The MapReduce programming model allows its users to solely focus on designing meaningful Mappers and Reducers that define the parallel program, without explicitly handling the complex details of the message-passing and the distribution of workload to cores, a task which is completely delegated to the MapReduce package.

- **Portability.** Hadoop is a highly popular and portable MapReduce system that can be easily deployed with minimal changes on a wide range of parallel computer platforms such as the Amazon EC2 cloud.

- **Resilience to core failures.** On less reliable hardware where there is a non-negligible probability of core failure, the Apache Hadoop system can automatically reload any failed Mapper or Reducer job on another worker to guide the parallel job towards completion.

Despite these advantages, the use of MapReduce for computationally intensive and highly iterative applications, such as simulation and simulation optimization, is less documented. Moreover, most popular MapReduce implementations such as Apache Hadoop have limitations that may potentially reduce the efficiency of highly iterative algorithms such as parallel R&S procedures.

- **Synchronization.** By design, each Reduce phase cannot start before the previous Map phase finishes and each new MapReduce iteration cannot be initiated unless the previous one shuts down completely. Hence, a R&S procedure using MapReduce has to be made fully synchronous. If load-balancing is difficult, for instance as a result of random simulation completion times, then core hours could be wasted due to frequent synchronization.

- **Absence of Cache.** In Apache Hadoop, workers are not allowed to cache any information between Map and Reduce phases. As a result, the outputs generated by Mappers and Reducers are often written to a distributed file system (which are usually located on hard drives) before they are read in the next iteration. Compared to the MPI implementation where all intermediate variables are stored in memory, the MapReduce version could be slowed down by repeated data I/O. Moreover, the lack of cache requires the simulation program, including any static data and/or random number generators, to be initialized on workers before every MapReduce iteration.

- **Nonidentical Run Times.** By default, Apache Hadoop does not dedicate each worker to a single task. It may simultaneously launch several Mappers and Reducers on a single worker,
Table 2: Major differences between GSP implementations

| Task                                         | MPI                  | Hadoop MapReduce                |
|----------------------------------------------|----------------------|---------------------------------|
| Master                                       | Explicitly coded     | Automated                       |
| Message-passing                              | Explicitly coded     | Automated                       |
| Synchronization                             | Once after each stage| More frequent: required in every iteration of Stage 2 |
| Simulation                                   | Each worker simulates one system per iteration | Each worker simulates multiple systems per iteration |
| Load-balancing                               | Via asynchronous communications between the master and a single worker | By assigning approximately equal number of systems (Mappers) to each worker in each synchronized iteration |
| Batch statistics and random number seeds     | Always stored in workers’ memory | Written to hard disk after each iteration |

run multiple MapReduce jobs that share workers on the same cluster, or even use workers that have different hardware configurations. In any of these cases, simulation completion times may be highly variable and time-varying. Therefore, Stage 0 of GSP (estimation of simulation run time) is dropped from our MapReduce implementation.

Although there are specialized MapReduce variants such as “stateful MapReduce” that attempt to address these limitations [Elgohary 2012], we do not explore them as they are less available for general parallel platforms, at least at present. However, some of these limitations (such as the lack of caching across multiple MapReduce rounds) are idiosyncratic to specific packages like Hadoop rather than the framework itself. Nevertheless, the a priori expectation is that, for a highly iterative procedure like ours, a highly optimized MPI approach will outperform a Hadoop one; thus our question is not which is fastest, but whether MapReduce can offer most of the speed of MPI along with its advantages discussed above.

We propose a variant of GSP using iterative MapReduce as follows. In each Mapper function, we treat each surviving system as a single data entry, obtain an additional batched sample, and output updated summary statistics such as sample sizes, means, and variances. Each output entry is associated with a key which represents the screening group to which it belongs. Once output entries of Mappers are grouped by their keys, each Reducer receives a group of systems, screens amongst them, and writes each surviving system as a new data entry which in turn is used as the input to the next Mapper.

To fully implement GSP, MapReduce is run for several iterations. The first iteration implements Stage 1, where both $\bar{X}_i(n_1)$ and $S^2_i$ are collected. Then, a maximum number of $r$ subsequent iterations are needed for Stage 2, with only $n_i(r)$ and $\bar{X}_i(n_i(r))$ being updated in each iteration. (Additional MapReduce iterations can be run where the best system from each group is shared for additional between-group screening.) The same Reducer can be applied in both Stages 1 and 2, as the screening logic is the same. Finally, a Stage 3 MapReduce features a Mapper that calculates the additional Rinott sample size, simulates the required replications, and a different Reducer that simply selects the system with the highest sample mean at the end. Full details of each stage are
Table 3: A comparison of procedure costs using parameters $n_0 = 20$, $n_1 = 50$, $\alpha_1 = \alpha_2 = 2.5\%$, $\beta = 100$, $\bar{r} = 10$. (Results to 2 significant figures)

| Configuration | $\delta$ | Procedure | Wall-clock time (sec) | Total number of simulation replications ($\times 10^6$) |
|---------------|---------|-----------|-----------------------|-----------------------------------------------|
| 3,249 systems on 64 cores | 0.01 | GSP | 14 | 2.3 |
|               |        | NHH | 14 | 2.5 |
|               |        | NSGS$_p$ | 120 | 13 |
| 0.1 | GSP | 3.4 | 0.57 |
|       | NHH | 2.6 | 0.44 |
|       | NSGS$_p$ | 3.4 | 0.48 |
| 57,624 systems on 64 cores | 0.01 | GSP | 720 | 130 |
|               |        | NHH | 520 | 89 |
|               |        | NSGS$_p$ | 11,000 | 1600 |
| 0.1 | GSP | 60 | 10 |
|       | NHH | 71 | 12 |
|       | NSGS$_p$ | 150 | 23 |
| 1,016,127 systems on 1,024 cores | 0.1 | GSP | 260 | 320 |
|               |        | NHH | 1,000 | 430 |
|               |        | NSGS$_p$ | 1,400 | 1900 |

Our MapReduce implementation is based on the native Java interface for MapReduce provided in Apache Hadoop 1.2.1. It is hosted in the open-access repository Ni (2015a). Table 2 summarizes some of the major differences between the MPI and Hadoop implementations.

4.3 Numerical Experiments

We now demonstrate the practical performance of GSP by using it to solve the throughput maximization test problem.

4.3.1 GSP vs Existing Parallel Procedures

GSP is motivated by an earlier computational study by Ni et al. (2014), which compares the performance of two parallel procedures, NHH (Ni et al. 2013) and NSGS$_p$ (Ni et al. 2014). NHH is a parallel procedure that adopts the fully-sequential serial procedure proposed in Hong (2006), and only provides a PCS guarantee (Hong and Nelson 2014). For problems where multiple optimal solutions exist, it is used as a heuristic because the PCS assumption does not hold. NHH can be viewed as a variant of GSP using a different screening method and without a Rinott-like Stage 3. NSGS$_p$ is a parallel implementation of the NSGS procedure (Nelson et al. 2001), and is a simplification of GSP without the iterative screening Stage 2.

We implement all three procedures using MPI and test them on different instances of the throughput maximization problem. We measure the performance of these procedures in terms of total wall-clock time and simulation replications required to find a solution, and report them
Table 4: A comparison of two implementations of GSP using parameters \( \delta = 0.1, n_0 = 50, \alpha_1 = \alpha_2 = 2.5\%, \bar{r} = 1000/\beta \). “Total time” is summed over all cores. (Results to 2 significant figures)

| Configuration | \( \beta \) | Version | Number of replications \( \times 10^6 \) | Wall-clock time (sec) | Total time Simulation \( \times 10^3 \) sec | Screening time (sec) | Utilization % |
|---------------|----------|---------|-------------------------------|------------------|-----------------|------------------|----------|
| 3,249 systems on 64 cores | 100 | HADOOP | 0.46 | 460 | 0.34 | 0.14 | 1.2 |
| | | MPI | 0.50 | 3.0 | 0.18 | 0.01 | 94 |
| | 200 | HADOOP | 0.63 | 280 | 0.41 | 0.10 | 2.3 |
| | | MPI | 0.69 | 4.1 | 0.25 | 0.01 | 95 |
| 57,624 systems on 64 cores | 100 | HADOOP | 8.8 | 550 | 5.1 | 1.9 | 15 |
| | | MPI | 9.1 | 53 | 3.3 | 0.89 | 98 |
| | 200 | HADOOP | 12 | 410 | 7.0 | 1.7 | 27 |
| | | MPI | 13 | 75 | 4.7 | 0.83 | 98 |
| 1,016,127 systems on 1,024 cores | 100 | HADOOP | 280 | 1300 | 160 | 120 | 12 |
| | | MPI | 320 | 120 | 110 | 30 | 91 |
| | 200 | HADOOP | 340 | 810 | 190 | 89 | 23 |
| | | MPI | 380 | 140 | 140 | 29 | 97 |

in Table 3. Preliminary runs on smaller test problems suggest that the variation in these two measures between multiple runs of the entire selection procedure are limited. Therefore we only present results from a single replication to save core hours.

Ni et al. (2014) argue that NHH tends to devote excessive simulation effort to systems with means that are very close to the best, whereas NSGS\(_p\) has a weaker screening mechanism but its Rinott stage can be effective when used with a large \( \delta \), which is associated with higher tolerance of an optimality gap. GSP, by design, combines iterative screening with a Rinott stage. Like NSGS\(_p\), we expect that GSP will cost less with a large \( \delta \) as the Rinott sample size is \( O(1/\delta^2) \), but its improved screening method should eliminate more systems than NSGS\(_p\) before entering the Rinott stage. Therefore, we expect GSP to work particularly well when a large number of systems exist both inside and outside the indifference zone. This intuition is supported by the outcomes of the medium and large test cases with \( \delta = 0.1 \), when GSP outperforms both NHH and NSGS\(_p\).

4.3.2 A Comparison of MPI and Hadoop Versions of GSP

We now focus on GSP and test its two implementations discussed in §4.2. Since Stage 0 is not included in the MapReduce implementation, we also remove it from the MPI version to have a fair comparison. Both procedures are tested on Stampede. While the cluster features highly optimized C++ compilers and MPI implementations, it provides relatively less support for MapReduce. Our MapReduce jobs are deployed using the myhadoop software (Lockwood 2014), which sets up an experimental Hadoop environment on Stampede.

Another difference is that we perform less screening in MPI than in Hadoop. In our initial experiments, we observed that the master could become overwhelmed by communication with the
workers in the screening stages, and we fixed this problem by screening using only the 20 best systems from other cores, versus the best systems from all other cores in Hadoop. While less screening is not a non-negligible effect, it will be apparent in our results that it is dominated by the time spent with simulation.

Before we proceed to the results, we define core utilization, an important measure of interest, as

$$\text{Utilization} = \frac{\text{total time spent on simulation}}{\text{wall-clock time} \times \text{number of cores}}.$$  

Utilization measures how efficiently the implementations use the available cores to generate simulation replications. The higher the utilization, the less overhead the procedure spends on communication and screening.

In Table 4 we report the number of simulation replications, wall-clock time, and utilization for each of the GSP implementations. The MPI implementation takes substantially less wall-clock time than MapReduce to solve every problem instance, although it requires slightly more replications due to its asynchronous and distributed screening. The gap in wall clock times narrows as the batch size $\beta$ and/or the system-to-core ratio are increased. Similarly, the MPI implementation also yields much higher utilization, spending more than 90% of the total computation time on simulation runs in all problem instances. Compared to the MPI implementation, the MapReduce version utilizes core hours less efficiently but again its utilization significantly improves as we double batch size and increase the system-to-core ratio.

To further understand the low utilization, we give the number of active Mapper and Reducer jobs over an entire MapReduce run in Figure 2. The plot reveals a number of reasons for low utilization. First, there are non-negligible gaps between Map and Reduce phases, which are due to an intermediary “Shuffle” step that collects and sorts the output of the Mappers and allocates it to the Reducers. Second, as the amount of data shuffled is likely to vary, the Reducers start and finish at different times. Third, owing to the varying amount of computing required for different
Table 5: A comparison of GSP implementations using a random number of warm-up job releases distributed like \( \min\{\exp(X), 20,000\} \), where \( X \sim N(\mu, \sigma^2) \). We use parameters \( \delta = 0.1, n_0 = 50, \alpha_1 = \alpha_2 = 2.5\%, \beta = 200, \bar{r} = 5 \). (Results to 2 significant figures)

| Configuration | \( \mu \) | \( \sigma^2 \) | Version | Wall-clock time (sec) | Utilization % |
|---------------|--------|------------|---------|----------------------|---------------|
| 3,249 systems on 64 cores | 7.4   | 0.5        | HADOOP  | 280                  | 2.3           |
|                |        |            | MPI     | 4.2                  | 94            |
|                | 6.6   | 2.0        | HADOOP  | 280                  | 2.0           |
|                |        |            | MPI     | 4.0                  | 93            |
| 57,624 systems on 64 cores | 7.4   | 0.5        | HADOOP  | 400                  | 27            |
|                |        |            | MPI     | 74                   | 98            |
|                | 6.6   | 2.0        | HADOOP  | 400                  | 26            |
|                |        |            | MPI     | 70                   | 98            |
| 1,016,127 systems on 1,024 cores | 7.4   | 0.5        | HADOOP  | 850                  | 25            |
|                |        |            | MPI     | 150                  | 97            |
|                | 6.6   | 2.0        | HADOOP  | 850                  | 22            |
|                |        |            | MPI     | 150                  | 97            |

systems, some Mappers take longer than others. In all, the strictly synchronized design of Hadoop causes some amount of core idleness that is perhaps inherent in the methodology, and therefore unavoidable. Nevertheless, the fact that utilization increases as average batch size \( \beta \) or the system-to-core ratio increases suggests that the Hadoop overhead becomes less pronounced as the amount of computation work per Mapper increases. Therefore we expect utilization to also improve and become increasingly competitive with MPI’s for problems that feature a larger solution space or longer simulation runs.

4.3.3 Robustness to Unequal and Random Run Times

The MapReduce implementation allocates approximately equal numbers of simulation replications to each Mapper and the simulation run times per replication are nearly constant for our test problem, so the computational workload in each MapReduce iteration should be fairly balanced. Indeed, in Figure 2 we observe that Mapper jobs terminate nearly simultaneously, which suggests that load-balancing works well. However, if the simulation run times exhibit enough variation that one Mapper takes much longer than the others, then we would expect synchronization delays that would greatly reduce utilization.

To verify this conjecture, we design additional computational experiments where variability in simulation run times is introduced by warming up each system for a random number \( W \) of job releases (by default, we use a fixed 2,000 job releases in the warm-up stage). We take \( W \) to be (rounded) log-normal, parameterized so that the average warm-up period is approximately 2,000, in the hope that the heavy tails of the log-normal distribution will lead to occasional large run times that might slow down the entire procedure. We also truncate the log-normal distributions from above at 20,000 job releases to avoid exceeding a built-in timeout limit in Hadoop. Parameters of the truncated log-normal distribution and the results of the experiment are given in Table 5.
We observe very similar wall-clock time and utilization in all instances compared to the base cases in Table 4 where we used fixed warm-up periods. Both implementations seem quite robust against the additional randomness in simulation times, despite our intuition that the MapReduce version might be noticeably impacted due to additional synchronization waste. A potential explanation is that as each core is allocated at least 50 systems and each system is simulated for an average of 200 replications in each step, the variation in single-replication completion times is averaged out. Rather extreme variations would be required for MapReduce to suffer a sharp performance decrease. For problems with much longer simulation times and a lower systems-to-core ratio, the averaging effect might not completely cancel the variations across simulation run times.

Acknowledgements

This work was partially supported by NSF grant CMMI-1200315, and used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575.

References

Andradóttir, S. 1998. A review of simulation optimization techniques. D. J. Medieros, E. F. Watson, J. S. Carson, M. S. Manivannan, eds., Proceedings of the 1998 Winter Simulation Conference. Institute of Electrical and Electronics Engineers: Piscataway, New Jersey, 151–158.

Bechhofer, Robert E., Thomas J. Santner, David M. Goldsman. 1995. Design and analysis of experiments for statistical selection, screening, and multiple comparisons. Wiley New York.

Boesel, J., B. L. Nelson, S.-H. Kim. 2003. Using ranking and selection to ‘clean up’ after simulation optimization. Operations Research 51(5) 814–825.

Branke, J., S. E. Chick, C. Schmidt. 2007. Selecting a selection procedure. Management Science 53(12) 1916–1932.

Bubeck, Sébastien, Nicolo Cesa-Bianchi. 2012. Regret analysis of stochastic and nonstochastic multi-armed bandit problems. Foundations and Trends in Machine Learning 5(1) 1–122.

Casella, George, Roger L. Berger. 2002. Statistical inference. Thomson Learning, Australia; Pacific Grove, CA.

Chen, C.-H., S. E. Chick, L. H. Lee. 2015. Ranking and selection: Efficient simulation budget allocation. Michael C. Fu, ed., Handbook of Simulation Optimization, International Series in Operations Research & Management Science, vol. 216, chap. 3. Springer, New York, 45–80.

Chen, C.-H., J. Lin, E. Yücesan, S. E. Chick. 2000. Simulation budget allocation for further enhancing the efficiency of ordinal optimization. Discrete Event Dynamic Systems 10(3) 251–270.

Chen, E. Jack. 2005. Using parallel and distributed computing to increase the capability of selection procedures. M. E Kuhl, N. M. Steiger, F. B. Armstrong, J. A. Joines, eds., Proceedings of the 2005 Winter Simulation Conference. 723–731.

Dean, Jeffrey, Sanjay Ghemawat. 2008. MapReduce: simplified data processing on large clusters. Communications of the ACM 51(1) 107–113.
Elgohary, Ahmed. 2012. Stateful MapReduce. Retrieved May 15, 2015, http://bbs.chinacloud.cn/attachment.aspx?attachmentid=4762.

Fu, M. 1994. Optimization via simulation: A review. *Annals of Operations Research* **53** 199–247.

Fu, M. C. 2002. Optimization for simulation: theory vs. practice. *INFORMS Journal on Computing* **14** 192–215.

Fu, M. C., F. W. Glover, J. April. 2005. Simulation optimization: a review, new developments, and applications. M. E. Kuhl, N. M. Steiger, F. B. Armstrong, J. A. Joines, eds., *Proc. of the 2005 Winter Simulation Conference*. Institute of Electrical and Electronics Engineers, Inc., Piscataway, NJ, 83–95.

Glynn, P. W., P. Heidelberger. 1990. Bias properties of budget constrained simulations. *Operations Research* **38** 801–814.

Glynn, P. W., P. Heidelberger. 1991. Analysis of parallel replicated simulations under a completion time constraint. *ACM Transactions on Modeling and Computer Simulation* **1**(1) 3–23.

Glynn, P. W., W. Whitt. 1992. The asymptotic efficiency of simulation estimators. *Operations Research* **40** 505–520.

Heidelberger, P. 1988. Discrete event simulations and parallel processing: statistical properties. *Siam J. Stat. Comput.* **9**(6) 1114–1132.

Henderson, S. G., R. Pasupathy. 2014. Simulation optimization library. URL http://www.simopt.org.

Hong, L. J., B. L. Nelson. 2005. The tradeoff between sampling and switching: new sequential procedures for indifference-zone selection. *IIE Transactions* **37** 723–734.

Hong, L. Jeff. 2006. Fully sequential indifference-zone selection procedures with variance-dependent sampling. *Naval Research Logistics (NRL)* **53**(5) 464–476.

Hong, L. Jeff, Barry L. Nelson. 2014. Personal communication.

Jamieson, K., R. Nowak. 2014. Best-arm identification algorithms for multi-armed bandits in the fixed confidence setting. *Information Sciences and Systems (CISS), 2014 48th Annual Conference on*. 1–6.

Karl, Andrew T., Randy Eubank, Jelena Milovanovic, Mark Reiser, Dennis Young. 2014. Using RngStreams for parallel random number generation in C++ and R. *Computational Statistics* 1–20.

Kim, S.-H., B. L. Nelson. 2006a. Selecting the best system. S. G. Henderson, B. L. Nelson, eds., *Simulation, Handbooks in Operations Research and Management Science*, vol. 13. North-Holland Publishing, Amsterdam, 501–534.

Kim, Seong-Hee, Barry L. Nelson. 2001. A fully sequential procedure for indifference-zone selection in simulation. *ACM Transactions on Modeling and Computer Simulation* **11**(3) 251–273.

Kim, Seong-Hee, Barry L. Nelson. 2006b. On the asymptotic validity of fully sequential selection procedures for steady-state simulation. *Operations Research* **54**(3) 475–488.

L’Ecuyer, Pierre. 2006. Uniform random number generation. S. G. Henderson, B. L. Nelson, eds., *Simulation*. Handbooks in Operations Research and Management Science, Volume 13, Elsevier, 55–81.

L’Ecuyer, Pierre, Richard Simard, E. Jack Chen, W. David Kelton. 2002. An object-oriented random-number package with many long streams and substreams. *Operations Research* **50**(6) 1073–1075.

Lockwood, G. K. 2014. myHadoop. URL https://github.com/glennlockwood/myhadoop.

Luo, Jun, Jeff L. Hong, Barry L. Nelson, Yang Wu. 2013. Fully sequential procedures for large-scale ranking-and-selection problems in parallel computing environments. *Working Paper*.
Luo, Jun, L. Jeff Hong. 2011. Large-scale ranking and selection using cloud computing. S. Jain, R.R. Creasey, J. Himmelspach, K.P. White, M. Fu, eds., Proceedings of the 2011 Winter Simulation Conference. 4051–4061.

Luo, Yuh-Chuyn, Chun-Hung Chen, E. Yucsesan, Insup Lee. 2000. Distributed web-based simulation optimization. Proceedings of the 2000 Winter Simulation Conference, vol. 2. 1785–1793.

Mascagni, Michael, Ashok Srinivasan. 2000. Algorithm 806: Sprng: A scalable library for pseudorandom number generation. ACM Trans. Math. Softw. 26(3) 436–461.

Nelson, B. L., F. J. Matejcik. 1995. Using common random numbers for indifference-zone selection and multiple comparisons in simulation. Management Science 41(12) 1935–1945.

Nelson, Barry L., Julie Swann, David Goldsman, Wheyming Song. 2001. Simple procedures for selecting the best simulated system when the number of alternatives is large. Operations Research 49(6) 950–963.

Ni, Eric C. 2015a. MapRedRns: Parallel ranking and selection using MapReduce. URL https://bitbucket.org/ericni/mapredrns

Ni, Eric C. 2015b. mpiRns: Parallel ranking and selection using MPI. URL https://bitbucket.org/ericni/mpirns

Ni, Eric C., Dragos F. Ciocan, Shane G. Henderson, Susan R. Hunter. 2015. Comparing Message Passing Interface and MapReduce for large-scale parallel ranking and selection. L. Yilmaz, W. K. V. Chan, I. Moon, T. M. K. Roeder, C. Macal, M. D. Rossetti, eds., Proceedings of the 2015 Winter Simulation Conference. Submitted.

Ni, Eric C., Shane G. Henderson, Susan R. Hunter. 2014. A comparison of two parallel ranking and selection procedures. A. Tolk, S. D. Diallo, I. O. Ryzhov, L. Yilmaz, S. Buckley, J. A. Miller, eds., Proceedings of the 2014 Winter Simulation Conference. 3761–3772.

Ni, Eric C., Susan R. Hunter, Shane G. Henderson. 2013. Ranking and selection in a high performance computing environment. R. Pasupathy, S.-H. Kim, A. Tolk, R. Hill, M. E. Kuhl, eds., Proceedings of the 2013 Winter Simulation Conference. 833–845.

Pasupathy, R., S. Ghosh. 2013. Simulation optimization: A concise overview and implementation guide. H. Topaloglu, ed., TutORials in Operations Research, chap. 7. INFORMS, 122–150. doi:10.1287/educ.2013.0118.

Pichitlamken, Juta, Barry L. Nelson, L. Jeff Hong. 2006. A sequential procedure for neighborhood selection-of-the-best in optimization via simulation. European Journal of Operational Research 173(1) 283–298.

Rinott, Yosef. 1978. On two-stage selection procedures and related probability-inequalities. Communications in Statistics - Theory and Methods 7(8) 799–811.

Tamhane, Ajit C. 1977. Multiple comparisons in model I one-way ANOVA with unequal variances. Communications in Statistics - Theory and Methods 6(1) 15–32.

Texas Advanced Computing Center. 2014. TACC stampede user guide. Retrieved May 11, 2014, https://www.tacc.utexas.edu/user-services/user-guides/stampede-user-guide

Yoo, Taejong, Hyunbo Cho, Enver Yücesan. 2009. Web Services-Based Parallel Replicated Discrete Event Simulation for Large-Scale Simulation Optimization. Simulation 85(7) 461–475.
Appendices

A.1 Proof of Theorem 1

Proving Theorem 1 requires the following lemmas, where we use $B_\Delta(\cdot)$ to denote a Brownian motion with drift $\Delta$ and volatility one.

**Lemma 1.** (Hong 2006. Theorem 1) Let $m(r)$ and $n(r)$ be arbitrary nondecreasing integer-valued functions of $r = 0, 1, \ldots$ and $i, j$ be any two systems. Define $Z(m, n) := \left[\sigma_i^2/m + \sigma_j^2/n\right]^{-1} [\tilde{X}_i(m) - \tilde{X}_j(n)]$ and $Z'(m, n) := B_{\mu_i - \mu_j}([\sigma_i^2/m + \sigma_j^2/n]^{-1})$. Then the random sequences $\{Z(m(r), n(r)) : r = 0, 1, \ldots\}$ and $\{Z'(m(r), n(r)) : r = 0, 1, \ldots\}$ have the same joint distribution.

**Lemma 2.** Let $i \neq j$ be any two systems. Define $\bar{a}_{ij}(\bar{r}) := \min\{S_i^2/\sigma_i^2, S_j^2/\sigma_j^2\}a_{ij}(\bar{r})$ and $\bar{t}_{ij}(\bar{r}) := \min\{S_i^2/\sigma_i^2, S_j^2/\sigma_j^2\}t_{ij}(\bar{r})$. It can be shown (Hong 2006) that $\min\{S_i^2/\sigma_i^2, S_j^2/\sigma_j^2\} \leq t_{ij}(r)/t_{ij}(r)$ for all $r \geq 0$ regardless of the sampling rules $n_i(\cdot)$ and $n_j(\cdot)$. Therefore $\bar{a}_{ij}(\bar{r}) \leq t_{ij}(r)a_{ij}(\bar{r})/t_{ij}(r)$ and $\bar{t}_{ij}(\bar{r}) \leq t_{ij}(r)t_{ij}(\bar{r})/t_{ij}(\bar{r})$ regardless of the sampling rules $n_i(\cdot)$ and $n_j(\cdot)$ for all $r \geq 0$.

**Lemma 3.** (Hong 2006. Lemma 4) Let $g_1(\cdot)$, $g_2(\cdot)$ be two non-negative-valued functions such that $g_2(t') \geq g_1(t')$ for all $t' \geq 0$. Define symmetric continuations $C_m := \{(t', x) : -g_m(t') \leq x \leq g_m(t')\}$ and let $T_m := \inf\{t' : B_\Delta(t') \notin C_m\}$ for $m = 1, 2$. If $\Delta \geq 0$, then $P[B_\Delta(T_1) < 0] \geq P[B_\Delta(T_2) < 0]$.

**Lemma 4.** By the reflection principle of Brownian motion, $P[\min_{0 \leq t' \leq t} B_0(t') < -a] = 2P[B_0(t) < -a] = 2\Phi(a/\sqrt{t})$ for all $a, t > 0$.

**Lemma 5.** (Tamhane 1977) Let $V_1, V_2, \ldots, V_k$ be independent random variables, and let $G^w(v_1, v_2, \ldots, v_k)$, $j = 1, 2, \ldots, p$, be non-negative, real-valued functions, each one nondecreasing in each of its arguments. Then

$$E \left[ \prod_{j=1}^{p} G^w(V_1, V_2, \ldots, V_k) \right] \geq \prod_{j=1}^{p} E[G^w(V_1, V_2, \ldots, V_k)].$$

**Lemma 6.** (After Nelson and Matejcik 1995 and Nelson et al. 2001. Lemma 1) For any $G_2 \subseteq S$, Stage 3 guarantees to select a system $K \in G_2$ such that $\Pr[\max_{i \in G_2} \mu_i - \mu_K \leq \delta] \geq 1 - \alpha_2$. If, in addition, Stages 1 and 2 jointly guarantee that $\Pr[k \in G_2] \geq 1 - \alpha_1$, then

$$\Pr[\text{The procedure selects system } K : \mu_k - \mu_K \leq \delta] \geq 1 - \alpha_1 - \alpha_2.$$
Proof. Proof of Theorem \[1\]

First, note that for any system \(i\), it is well known \cite[(Casella and Berger 2002, page 218)]{casella2002} that \(X_i(n_i)|S_i^2\) is normally distributed and \(X_{i\ell}\) is independent of \(S_i^2\) for all \(\ell > n_i\). Furthermore, \(T_i\) is obtained in Stage 0 independently of all \(X_{i\ell}\)’s. Therefore, choosing the sampling rule based on \(T_i\) and \(S_i^2\) does not affect the normality of the \(\{X_i(n_i(r)) : r = 0, 1, \ldots, \bar{r}\}\) sequence.

For any two systems \(i\) and \(j\), let \(KO_{ij}\) be the event that system \(i\) eliminates system \(j\) in Stages 1 or 2. It then follows that

\[\Pr[KO_{ik} \text{ in Stages 1 or 2}] = E[\Pr[KO_{ik} \text{ in Stages 1 or 2}|S_k^2, S_i^2]]\]

\[\leq E[\Pr[Y_{ki}(\tau_{ki}(r)) < -a_{ij}(\bar{r}) \text{ for some } r \leq \bar{r}|S_k^2, S_i^2]]\]

since system \(i\) could be eliminated by some other system before it can eliminate system \(k\)

\[= E[\Pr[Y_{ki}(\tau_{ki}(r)) < -a_{ij}(\bar{r}) \text{ and } \tau_{ki}(r) \leq \tau_{ki}(\bar{r}) \text{ for some } r|S_k^2, S_i^2]]\]

\[= E[\Pr[Z_{ki}(t_{ki}(r)) < -\frac{t_{ki}(r)}{\tau_{ki}(r)}a_{ij}(\bar{r}) \text{ and } t_{ki}(r) \leq \frac{t_{ki}(r)}{\tau_{ki}(r)}\tau_{ki}(\bar{r}) \text{ for some } r|S_k^2, S_i^2]] \text{ by Lemma } [1]\]

\[\leq E[\Pr[B_{\mu_k-\mu_i}(t_{ki}(r)) < -\bar{a}_{ij}(\bar{r}) \text{ and } t_{ki}(r) \leq \bar{t}_{ij}(\bar{r}) \text{ for some } r|S_k^2, S_i^2]] \text{ by Lemmas } [2] \text{ and } [3]\]

\[= E[\Pr[B_{0}(t) < -\bar{a}_{ij}(\bar{r}) \text{ for some } t \leq \bar{t}_{ij}(\bar{r})|S_k^2, S_i^2]] \text{ since } \mu_k \geq \mu_i\]

\[= E \left[ 2\Phi \left( \frac{-a_{ij}(\bar{r})}{\sqrt{\tau_{ij}(\bar{r})(n_i-1)}} \right) \right] \text{ by Lemma } [4]\]

\[= E \left[ 2\Phi \left( \frac{-a_{ij}(\bar{r})}{\sqrt{\tau_{ij}(\bar{r})(n_i-1)}} \sqrt{\min \left\{ \frac{(n_i-1)S_i^2}{\sigma_i^2}, \frac{(n_i-1)S_k^2}{\sigma_k^2} \right\}} \right) \right]

\[= E \left[ 2\Phi \left( \eta \sqrt{\min \left\{ \frac{(n_i-1)S_i^2}{\sigma_i^2}, \frac{(n_i-1)S_k^2}{\sigma_k^2} \right\}} \right) \right] \text{ by choice of } a_{ij}(\bar{r})\]

\[= 1 - (1 - \alpha_1)^{\frac{1}{n_i-1}} \text{ by } [4], \text{ since } (n_i-1)S_i^2/\sigma_i^2 \text{ and } (n_i-1)S_k^2/\sigma_k^2 \text{ are i.i.d. } \chi_{n_i-1}^2 \text{ random variables.} \]
Master Core Routine

Input: List of systems $S$; Average Stage 2 batch size $\beta$; Parameters $\delta, \alpha_1, \alpha_2, n_0, n_1$; $\bar{r}$ and a random number seed.

begin Preparation: Setting up random number streams
  Initialize random number generator using the seed;
  foreach worker $w = 1, 2, \ldots, c$ do
    Generate a new random number stream $U_w$;
    Send $U_w$ to $w$;
  end
end

begin Stage 0: Estimating simulation completion time
  \{ $G_{0w}$ : $w = 1, 2, \ldots, c$ $\}$ $\leftarrow$ Partition($S, 0$);
  foreach worker $w = 1, 2, \ldots, c$ do
    Send $G_{0w}$ to Worker $w$;
  end
  Collect($T_i$);
end

begin Stage 1: Estimating sample variances
  \{ $G_{1w}$ : $w = 1, 2, \ldots, c$ $\}$ $\leftarrow$ Partition($S, 1$);
  foreach worker $w = 1, 2, \ldots, c$ do
    Send $G_{1w}$ to Worker $w$;
  end
  Collect($S_2^i$ and Stat$_0$);
  \{ $S, G_{1w}$ $\}$ $\leftarrow$ RecvScreen($w$);
end

Worker Core Routine

Input: List of systems $S$; Parameters $\delta, \alpha_1, \alpha_2, n_0, n_1$.

begin Preparation: Setting up random number streams
  Receive random number stream $U_w$;
  Initialize random number generator using $U_w$;
end

begin Stage 0: Estimating simulation completion time
  Receive the set of systems to simulate, $G_{0w}$
  foreach system $i \in G_{0w}$ do
    Simulate($i, n_0, \text{simulation time } T_i$);
  end
  Return \{ $T_i$ : $i \in G_{0w}$ \} to master;
end

begin Stage 1: Estimating sample variances
  Receive the set of systems to simulate, $G_{1w}$
  foreach system $i \in G_{1w}$ do
    Simulate($i, n_1, (S_2^i, \text{Stat}_i,0)$);
  end
  Return \{ $(S_2^i, \text{Stat}_i,0) : i \in G_w$ $\}$ to master;
  $G_w$ $\leftarrow$ Screen($G_{1w}, 0, 0, \text{false}$);
  SendScreen($G_{1w}$);
end

Figure A.2.1: Stages 0 and 1, MPI Implementation: Master (left) and workers (right) routines

Then, noting that simulation results from different systems are mutually independent, we have

$$Pr[\text{system } k \in S_1] = E \left[ \prod_{i=1}^{k-1} Pr \left\{ K_i \mid X_{k1}, X_{k2}, \ldots \right\} \right]$$

$$= E \left[ \prod_{i=1}^{k-1} Pr \left\{ K_i \mid X_{k1}, X_{k2}, \ldots \right\} \right]$$

$$\geq \prod_{i=1}^{k-1} E \left[ Pr \left\{ K_i \mid X_{k1}, X_{k2}, \ldots \right\} \right] \text{ by Lemma 5}$$

$$= \prod_{i=1}^{k-1} Pr \left\{ K_i \right\} \geq \prod_{i=1}^{k-1} \left[ 1 - \left( 1 - (1 - \alpha_1)^{\frac{1}{k-1}} \right) \right] = 1 - \alpha_1.$$ 

Finally, we invoke Lemma 6 to complete the proof.

A.2 Full Description of the MPI implementation

The purpose of this section is to provide additional insight into our parallel codes. In Figures A.2.1 through A.2.3 we demonstrate in greater detail how the master core allocates and distributes
Figure A.2.2: Stage 2, MPI Implementation: Master (left) and workers (right) routines
begin Stage 3: Rinott Stage
\[ G_2 \leftarrow \text{systems that survived Stage 2}; \]
\[ \text{if } |G_2| = 1 \text{ then} \]
\[ \text{Report the single surviving system as the best;} \]
\[ \text{else} \]
\[ h \leftarrow h(1 - \alpha_2, n_1 |G_2|); \]
\[ \text{foreach system } i \in G_2 \text{ do} \]
\[ N_i \leftarrow \max\{n_i(\bar{r}), \lceil hS_i/\delta \rceil \}; \]
\[ N^\text{sent}_i \leftarrow 0; N^\text{received}_i \leftarrow 0; \]
\[ \text{end} \]
\[ \text{flag}_w \leftarrow 0 \text{ for all } w = 1, 2, \ldots, c; \]
\[ \text{while } N^\text{received}_i < N_i - n_i(\bar{r}) \text{ for some } i \in G_2 \text{ do} \]
\[ \text{while } N^\text{received}_i < N_i - n_i(\bar{r}) \text{ for some } i \in G_2 \text{ do} \]
\[ \text{Wait for the next worker } w \text{ to call } \]
\[ \text{Communicate();} \]
\[ \text{if } \text{flag}_w = 1 \text{ then} \]
\[ \text{Receive } i, b'_i \text{ and sample mean of the } \]
\[ \text{current batch;} \]
\[ \text{Merge sample mean into } \bar{X}_i; \]
\[ N^\text{received}_i \leftarrow N^\text{received}_i + b'_i; \]
\[ \text{end} \]
\[ \text{if } N^\text{sent}_i < N_i - n_i(\bar{r}) \text{ for some } i \in G_2 \text{ then} \]
\[ \text{Find an appropriate batch size } \]
\[ b'_i = \min\{b_i, N_i - n_i(\bar{r}) - N^\text{sent}_i \} \]
\[ \text{for system } i; \]
\[ \text{Send system } i \text{ and } b'_i \text{ to worker } w; \]
\[ N^\text{sent}_i \leftarrow N^\text{sent}_i + b'_i; \]
\[ \text{flag}_w \leftarrow 1; \]
\[ \text{end} \]
\[ \text{Report the system } i^* = \arg \max_{i \in G_2} \bar{X}_i(N_i) \]
\[ \text{as the best;} \]
\[ \text{end} \]
\[ \text{Send a termination instruction to all workers;} \]
\[ \text{end} \]

Figure A.2.3: Stage 3, MPI Implementation: Master (left) and workers (right) routines
systems, how random number streams are created and distributed together with the assigned systems to ensure independent sampling, and how simulation results are communicated between cores.

We use the following notation for some subroutines in Figures A.2.1 through A.2.3:

**Partition**($S$, $Stage$) The master divides the set of systems $S$ into disjoint partitions $\{G_w^{Stage} : w = 1, 2, \ldots, c\}$:

- In $Stage 0$, all systems are simulated for $n_0$ replications to estimate simulation completion time. The master randomly permutes $S$ (in case of long runtimes for some systems that are indexed closely) and assigns approximately equal numbers of systems to each $G_w^0$.
- In $Stage 1$, a fixed number $n_1$ of replications are required from each system. To balance the simulation work among workers, the master chooses $G_w^1$ such that the estimated completion time $\sum_{i \in G_w^1} n_1 \bar{T}_i/n_0$ is approximately equal for all $w$.
- In $Stage 2$, both simulation and screening are performed iteratively. Simulation of a system is no longer dedicated to a particular worker, and $G_w^2$ is the set of systems that worker $w$ needs to screen. To load-balance the screening work, the master assigns approximately equal numbers of systems to each $G_w^2$.

**Collect**($info$) The master collects $info$ from all workers for all systems, in arbitrary order.

**Simulate**($i, n, info$) Worker $w$ simulates system $i$ for $n$ replications and records $info$ using the next subsubstream in $U^i_w$.

**Stat**$_{i,r}$ The batch statistics for the $r$th batch of system $i$. This includes sample size $n_i(r)$ and sample mean $\bar{X}_i(n_i(r))$ as described in §3.

**BatchSize**($i, \beta$) The master calculates batch size $b_i$ system $i$ used in Stage 2. Following the recommendation from §2.2.2, we let

$$b_i = \left\lceil \frac{S_i \sqrt{T_i}}{\sqrt{\sum_{j \in S} S_j \sqrt{T_j}}} \beta \right\rceil$$

(12)

where $\beta$ is a pre-determined average batch size.

**Screen**($G^w, r_0, r_1, useothers$) Screen systems in $G^w$ from batches $r_0$ through $r_1$ inclusive. It can
be checked that worker $w$ has received $\text{Stat}_{i,r}$ for all $i \in S$, all $r \leq r_1$ and stored the data in its memory.

A system $i \in G^w$ is eliminated if there exists system $j \in G^w$ where $j \neq i$ and some $r' : r_0 \leq r' \leq r_1$ such that $r' \leq \bar{r}$ and $Y_{ij}(r') < -a_{ij}(\bar{r})$ where $Y_{ij}$ and $a_{ij}$ are defined in §3.

In addition, if $\text{useothers} = \text{true}$ and $W \neq \emptyset$, then for each $w' \in W$ the worker also screens the systems in $G^{w'}$ against system $i^*_w$, the best system from worker $w'$, using batch statistics $\{\text{Stat}_{i^*_w,r'} : r' \leq r_{w'}\}$ up to batch $\min\{r_{w'}, r_1\}$.

SendScreen($G^w, r_w$) and RecvScreen($w$) Worker $w$ sends $r_w$ and screening results (updated $G^w$) to the master, which then updates $G^w$ and $S$ on its own memory accordingly. The master also receives $r_w$ and lets $r_w^{\text{screened}} \leftarrow r_w$.

Communicate() Worker sends a signal to master and waits for the master to receive the signal, before proceeding.

SendSim($w, i, q_i, b_i$) and RecvSim() The master instructs worker $w$ to simulate the $q_i$th batch of system $i$, for $b_i$ replications. Worker $w$ receives $i, q_i, b_i$ from the master.

SendOutput($i, q_i, \text{Stat}_{i,q_i}$) and RecvOutput($w$) Worker $w$ sends simulation output $\text{Stat}_{i,q_i}$ for the $q_i$th batch of system $i$ to the master. The master stores $\text{Stat}_{i,q_i}$ in memory.

SendBest() and RecvBest($w$) Worker $w$ sends its estimated-best system $i^*_w$ (the one in $G^w$ with the highest batch mean) to the master, together with all batch statistics for system $i^*_w$, $\{\text{Stat}_{i^*_w,r} : r \leq r_w\}$; the master receives $r_w$ and lets $r_w^{\text{received}} \leftarrow r_w$.

CountBatch($w$) The master finds the largest $r_{\text{current}} \geq r_w$ such that $\text{Stat}_{i,r}$ for all $i \in G^w$, $r_w < r \leq r_{\text{current}}$ have been received by the master.

SendAction($w, \text{flag}_w$) and RecvAction() The master sends an indicator $\text{flag}_w$ to worker $w$, where $\text{flag}_w = 1$ indicates “simulate a batch” and $\text{flag}_w = 2$ indicates “perform screening”.

SendStats($w$) and RecvStats() The master sends $\text{Stat}_{i,r}$ for all $i \in G^w$, $r_w < r \leq r_{\text{current}}$ to worker $w$; the worker receives $r_{\text{current}}$ and lets $r_{\text{new}} \leftarrow r_{\text{current}}$; the worker should have $\text{Stat}_{i,r}$ for all $i \in G^w$, $0 < r \leq r_{\text{new}}$ upon completion.
SendBestStats($w$) andRecvBestStats() The master computes $\mathcal{W} = \{ w' \neq w : |G_{w'}| > 0 \}$ and sends $\mathcal{W}$ to worker $w$; the master then sends all available batch statistics for best systems, $\{ \text{Stat}_{w',r} : w' \in \mathcal{W}, r \leq r_{w'}^{\text{received}} \}$, to worker $w$.

### A.3 Full Description of the Hadoop implementation

We present in this section the full details of the MapReduce implementation of GSP.

Each Mapper reads a comma-separated string of varied length, denoted by [value 1, value 2, . . . , $\text{type}$], where the last component $\text{type}$ is used to indicate the specific information captured in the string. A Mapper usually runs some simulation, updates batch statistics, and generates one or more key: {value} pairs. All pairs under the same key are sent to the same Reducer, which is typically responsible for screening. A Reducer may generate one or more comma-separated strings which become the input to the Mapper in the next iteration.

Each system $i$ is coupled with $\text{stream}_i$ which is used by some random number generator and updated each time a random number is generated. The coupling of systems and streams ensures that the random numbers generated for each system in each iteration are all mutually independent. We also assume that each system $i$ is preallocated to a particular screening group, as determined by the function $\text{Group}(i)$.

The procedure begins with Steps 1-3 which implements Stage 1, then enters Stage 2 where Steps 4 and 5 are run repeatedly for a maximum of $\bar{r}$ iterations. If multiple systems survive Stage 2, the procedure runs Steps 6 and 7 to finish Stage 3.

**Step 1.**  
- **Map:** Estimate $S_i^2$

  **Input** $[i]$

  **Operation** Initialize $\text{stream}_i$ with seed $i$; Simulate system $i$ for $n_1$ replications to obtain $\bar{X}_i(n_1)$ and $S_i^2$.

  **Output** $i$: $\{\bar{X}_i(n_1), S_i^2, \text{stream}_i, \$S0\}$

- **Reduce**

  **Input** $i$: $\{\bar{X}_i(n_1), S_i^2, \text{stream}_i, \$S0\}$

  **Operation** Calculate $\sum_i S_i$. 

34
Output \([i, \bar{X}_i(n_1), S_i^2, \text{stream}_i, \$S0]\)

Step 2.  

- **Map:** Calculate batch size

  \text{Input} \([i, \bar{X}_i(n_1), S_i^2, \text{stream}_i, \$S0]\)

  \text{Operation} Calculate batch size \(b_i = \beta S_i / (\sum_i S_i / k)\).

  \text{Output} \text{Group}(i): \{i, \bar{X}_i(n_1), n_1, b_i, S_i^2, \text{stream}_i, \$Sim\}

- **Reduce:** Screen within a group

  \text{Input} \text{Group}: \{i, \bar{X}_i(n_1), n_i, b_i, S_i^2, \text{stream}_i, \$Sim\} for all \(i\) in the \text{Group}

  \text{Operation} Screen all systems in the \text{Group} and find the one \(i^*\) with the highest mean.

  \text{Output} \([i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim]\) for each surviving system \(i\), and \([i^*, \bar{X}_{i^*}(n_{i^*}), n_{i^*}, b_{i^*}, S_{i^*}^2, \$Best]\) for the best system \(i^*\)

Step 3.  

- **Map:** Share best systems between groups

  \text{Input} (1) \([i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim]\)

  \text{Operation} (1) Simply output to \text{Group}(i).

  \text{Output} (1) \text{Group}(i): \{i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim\}

  \text{Input} (2) \([i^*, \bar{X}_{i^*}(n_{i^*}), n_{i^*}, b_{i^*}, S_{i^*}^2, \$Best]\)

  \text{Operation} (2) Output to all groups.

  \text{Output} (2) \text{Group}: \{i^*, \bar{X}_{i^*}(n_{i^*}), n_{i^*}, b_{i^*}, S_{i^*}^2, \$Best\} for every \text{Group}

- **Reduce:** Screen against the best systems from other groups

  \text{Input} \text{Group}: \{i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim\} for all \(i\) in the \text{Group}, and 

  \text{Group}: \{i^*, \bar{X}_{i^*}(n_{i^*}), n_{i^*}, b_{i^*}, S_{i^*}^2, \$Best\} from every other \text{Group}

  \text{Operation} Screen all systems in \text{Group} against the best systems from other groups.

  \text{Output} \([i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim]\) for each surviving system \(i\)

Step 4.  

- **Map:** Simulation

  \text{Input} \([i, \bar{X}_i(n_i), n_i, b_i, S_i^2, \text{stream}_i, \$Sim]\)

  \text{Operation} Simulate system \(i\) for additional \(b_i\) replications, update \(n_i, \bar{X}_i(n_i)\), and \text{stream}_i.

  \text{Output} \text{Group}(i): \{i, \bar{X}_i(n_1), n_1, b_i, S_i^2, \text{stream}_i, \$Sim\}
• **Reduce**: Screen within a group.

( Same as Step 2 Reduce.)

**Step 5.** Screen against best systems from other groups.

( Same as Step 3.)

**Step 6.**

• **Map**: Determine Rinott sample sizes

\[
\text{Input } [i, \bar{X}_i(n_i), n_i, b_i, S^2_i, \text{stream}_i, $Sim$]
\]

**Operation** Output to Reducer.

**Output** \(i: \{\bar{X}_i(n_i), n_i, S^2_i, \text{stream}_i, $Sim$\}

• **Reduce**

\[
\text{Input } i: \{\bar{X}_i(n_i), n_i, S^2_i, \text{stream}_i, $Sim$\}
\]

**Operation** Calculate Rinott sample size and divide the additional sample into batches.

For each batch \(j\), generate a substream \(\text{stream}_j^i\) using \(\text{stream}_i\).

**Output** \([i, \bar{X}_i(n_i), n_i, $S2]\), and

for each batch \(j\): \([i, \text{stream}_j^i, \text{size of batch } j, $S3]\)

**Step 7.**

• **Map**: Simulate additional batches

\[
\text{Input (1) } [i, \bar{X}_i(n_i), n_i, $S2] \]

**Operation (1)** Output to Reducer, since this is the batch statistics generated in Stage 2.

**Output (1)** \(1: \{i, \bar{X}_i(n_i), n_i, $S2\}\)

\[
\text{Input (2) } [i, \text{stream}_j^i, \text{size of batch } j, $S3]\]

**Operation (2)** Simulate batch \(j\) of system \(i\) for the given batch size using \(\text{stream}_j^i\), calculate batch sample mean \(\bar{X}_j^i\).

**Output (2)** \(1: \{i, \bar{X}_j^i, \text{size of batch } j, $S3\}\)

• **Reduce**: Merge batches and find the best system

**Input** (This step has only one Reducer)

1: \(\{i, X_i(n_i), n_i, $S2\}\) and

1: \(\{i, \bar{X}_j^i, \text{size of batch } j, $S3\}\) for all system \(i\) and all batch \(j\)
Operation  For each system $i$, merge all batches (including the one from Stage 2) to form a single sample mean.

Output  Report the system $i^*$ that has the highest sample mean.