Analysis of Population Control Techniques for Time-Dependent and Eigenvalue Monte Carlo Neutron Transport Calculations

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Abstract — An extensive study of population control techniques (PCTs) for time-dependent and eigenvalue Monte Carlo (MC) neutron transport calculations is presented. We define PCT as a technique that takes a censused population and returns a controlled, unbiased population. A new perspective based on an abstraction of particle census and population control is explored, paving the way to improved understanding and application of the concepts. Five distinct PCTs identified from the literature are reviewed: simple sampling, splitting-roulette (SR), combing (CO), modified combing, and duplicate-discard (DD). A theoretical analysis of how much uncertainty is introduced to a population by each PCT is presented. Parallel algorithms for the PCTs, applicable for both time-dependent and eigenvalue MC simulations, are proposed. The relative performance of the PCTs based on run time and tally mean error or standard deviation is assessed by solving time-dependent and eigenvalue test problems. It is found that SR and CO are equally the most performing techniques, closely followed by DD.

Keywords — Monte Carlo, particle transport, population control, parallel algorithm.

Note — Some figures may be in color only in the electronic version.

I. INTRODUCTION

The Monte Carlo (MC) method is indispensable in neutron transport calculations due to its ability to perform high-fidelity, continuous-energy transport simulations with minimal approximation. However, MC suffers from stochastic uncertainties requiring an expensive computation of a large number of neutron source samples or histories. Nevertheless, thanks to the advancement of high-performance parallel computing, the inherently parallel features of MC can be effectively exploited to a very large extent, which can significantly reduce run time to solution, particularly for computationally expensive time-dependent neutron transport simulations.1–10

During a time-dependent MC simulation, particle population size can monotonically grow or decay depending on the criticality of the system. This monotonic evolution of population makes time-dependent MC simulations particularly challenging in two different ways. First, in a supercritical system, particle population size can quickly grow beyond the limited computational resources. Additionally, some MC implementations and variance reduction techniques (VRTs), such as the precursor forced decay technique in Ref. 2 and the time-dependent adaptation of the hybrid source iteration methods,11,12 may promote monotonic population growth, which raises the same issue on the limited computational memory. Second, in a subcritical system without a significant persisting external source, such as in pulsed-reactor and shutdown experiments, particle population size can quickly decay to zero, which leads to a lack of samples and yields statistically noisy tally results at later times of the simulation.

One typically uses a population control technique (PCT) to address the monotonic population growth and collapse issues discussed previously. PCT essentially controls the size of a particle population to be near a desired value while preserving certain statistical expectations to achieve unbiased MC simulation. In the implementation

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of PCT, time census is employed to limit the population growth/collapse. The census introduces a time boundary that stops particles whenever they are about to cross it. When all particles have already hit the time boundary, the time census is completed, and PCT can be performed on the censored particles. More recent applications of PCT include the use of random particle duplication or discard in Serpent 2 (Ref. 13), the splitting and Russian-roulette technique in MCATK (Ref. 14), the combing technique in TRIPOLI-4 (Refs. 16 and 17) and GUARDYAN (Ref. 8), and a modified combing technique which was most recently introduced in Ref. 10.

An innovative approach to performing time-dependent MC is proposed by Ref. 9. The central idea is to repurpose the generally available k-eigenvalue MC simulation infrastructure to perform time-dependent simulations. This approach works because there is a built-in population control in k-eigenvalue MC simulations. Besides the introduction of the 1/k factor on the fission operator, which is essential in achieving a steady-state configuration, simple sampling is typically performed to ensure that a certain number of particles are sampled from the fission bank and then used as the particle source for the simulation of the next fission generation. Observing the significance of that connection between the k-eigenvalue and time-dependent MC simulations offers an improved understanding of PCT. Such a study has been done to an extent by Cullen et al. Nevertheless, one can take advantage of this connection further by exploring potential benefits from and for both of the simulation modes.

Despite the multiple distinct PCTs proposed in the literature, documented studies characterizing and assessing the relative performances of all the identified PCTs are still very limited. A more recent effort, found in Ref. 4, specifically compares the splitting and Russian-roulette technique to the particle combing technique, hereafter referred to as splitting-roulette (SR) and combing (CO), respectively. Sweezy et al. propose a normalized SR as an alternative to CO that may suffer from unwanted behavior due to possible correlations in the particle order. On the other hand, Faucher et al. and Legrady et al. prefer the use of CO instead of SR due to the inherent bias in the normalized SR (Ref. 4) and suggest that the unwanted behavior of CO is unlikely to occur in practice. This support for CO, or if you will, eutrophilia, is strengthened by an assertion stating that the SR technique described in Ref. 4 is at least two to three times less efficient than CO. This assertion is based on a comparative study of CO and a “Russian roulette and splitting” technique reported in Ref. 20. However, the Russian-roulette and splitting technique in Ref. 20 seems to be different from the SR technique described in Ref. 4; and for the record, the study does not claim that the technique compared refers to Ref. 4. Consistent implementation and fair comparison of the two techniques, SR (Ref. 4) and CO (Ref. 15), would shed light on their actual relative performance.

In this paper, we present an extensive study on PCT. In Sec. II, we start by making an abstraction of related concepts, i.e., particle census and population control, followed by reviewing PCTs identified from the literature. In Sec. III, we perform an analysis to reveal the theoretical uncertainty introduced by each of the PCTs that directly affects the performance of the technique. These theoretical uncertainties are then verified numerically. Section IV presents a parallel PCT algorithm that exploits the abstraction established in Sec. II and adapts the nearest-neighbor parallel fission bank algorithm proposed in Ref. 21. In Secs. V and VI, we implement and test the PCTs on time-dependent and eigenvalue MC neutron transport problems, respectively. Finally, Sec. VII summarizes the takeaways of the study. It is worth mentioning that while this paper is focused on PCT application for MC neutron transport, discussions and analyses presented in this paper are also applicable to PCT application in other transport simulations, such as the implicit MC thermal radiative transfer.

II. POPULATION CONTROL TECHNIQUE

Population control can be loosely defined as any MC technique that involves altering the number of particles being simulated. This includes many VRTs (e.g., cell importance and weight window) and even the introduction of the 1/k factor in eigenvalue simulations. However, in this paper we specifically define population control as a technique that controls populations of censored particles. In this section, we present an abstraction of particle census and population control (their definitions and how they are characterized) and then discuss distinct techniques identified from the literature.

II.A. Particle Census

Census is a process where we (1) stop particles, (2) remove them from the current simulation, and then (3) store them into a census bank. Census can be performed at arbitrary steps during simulation; however, there are
several triggering events that physically make sense to perform the census.

Perhaps the most obvious one is time-grid crossing. In this time census, we stop particles whenever they are about to cross a predetermined time grid. The censused particles are then removed from the current simulation and stored into a time bank (the census bank).

Another useful triggering event is fission emission. In this fission census, neutrons emitted from fission reactions are removed from the current simulation and stored into a fission bank. One can see that this is actually a standard practice that has been long used in $k$-eigenvalue MC transport simulations. We can take it a step further and census not only the fission neutrons but also the scattering neutrons. This results in collision census, which is typically used in $c$-eigenvalue MC calculations.

There are several reasons to perform particle census. One is to limit particle population growth so that population control (discussed in more detail next) can be performed. Another reason is to allow the system (the MC model) to change, which can be geometry, composition, or parameter changes due to multiphysics feedback. Additionally, one can also see census as a manifestation of an iterative scheme performed to solve an equation, e.g., power iteration in $k$-eigenvalue problem.

It is worth noting that the census time grid for population control does not necessarily need to be identical to other time grids possibly used in MC simulations. These other time grids include the one for tally scoring [also known as tally filters in some MC codes, such as OpenMC (Ref. 24)], the time grid for VRTs (e.g., weight window and forced precursor decay), and the census time grid for model change or multiphysics feedback.

II.B. Population Control

Given an initial population of size $N$, the objective of population control is to return a controlled final population with a size around, or exactly at, a predetermined value $M$, as illustrated in Fig. 1. In a supercritical system, typically $N > M$, while in a subcritical one, $N < M$. The final population is then used as the source bank for the successive census-enabled transport simulation during which a census bank is populated by a certain census mechanism (e.g., time census or fission census, as discussed in Sec. II.A). Once the transport is completed (i.e., both source and secondary particle banks are exhausted), the census bank becomes the initial population to be controlled by a PCT of choice. It is evident that population control does not care about what kind of transport simulation is being performed, whether it is a time-dependent fixed-source or an eigenvalue one. This also implies that any PCT can be used in any kind of transport simulation; as a particular example, one can use the particle combing technique in a $k$-eigenvalue simulation.

The final population basically consists of copies of the initial particles, but how many times a particle gets copied will differ between particles and some particles may not get copied at all. The procedure for determining how many times each initial particle gets copied to the final population is the essence of PCT and has to be done in such a way that the MC simulation is not biased; i.e., the expectations of the population actions, and thus the expectations of simulation tally results, are preserved.

The only requirement for a PCT to be unbiased is to preserve the expected weight of each particle in the initial population. That is, for initial particle $i$ having weight $w_i$:

$$E[C_i] = w_i, \quad i = 1, 2, ..., N$$

(1)

and

$$C_i = d_i w_i,$$

(2)

where

$E[\cdot]$ = expectation of a random variable argument

$\quad d_i =$ number of copies of particle $i$ in the final population

$\quad w_i =$ controlled weight assigned to the copies of particle $i$

$\quad C_i =$ total weight represented by the copies of particle $i$ in the final population.

Now that we have described the minimum requirements, i.e., controlling population size from $N$ to around $M$ while ensuring that Eq. (1) holds, we next point out two desirable characteristics of PCT.
The first is that we wish to have a low uncertainty in $C_i$. In particular, we want its standard deviation $\sigma[C_i]$ to be as low as possible. In the absence of PCT, each initial particle $i$ is copied once to the final population and we will have $C_i = w_i$ and $\sigma[C_i] = 0$; however, if a PCT is being used, $\sigma[C_i] \geq 0$. The value of $\sigma[C_i]$ affects the variance of the actions of particle $i$ in the MC simulation, and later we numerically demonstrate that it ultimately affects the simulation tally results.

The second desirable characteristic is that we would like our PCT to preserve the initial population total weight $W$ as much as possible; in other words, if $W'$ is the final population total weight:

$$W = \sum_{i=1}^{N} w_i$$

and

$$W' = \sum_{i=1}^{N} C_i,$$

and we would like $W'$ to be close or equal to $W$. Booth\textsuperscript{15} suggests that such strict equality of $W' = W$ is generally unimportant for neutron and photon transport, but it may be very important in charged particle transport. Therefore, we consider it a desirable characteristic, not a requirement of PCT.

As a remark, PCT is a technique that takes an initial population of size $N$ and total weight $W$ and returns a controlled final population that

1. has a size equal or close to $M$,
2. preserves the expected total weight of each particle [i.e., satisfies Eq. (1), $E[C_i] = w_i$],
3. has a low $\sigma[C_i]$, and
4. has a total weight equal or close to $W$.

We note that point 1 is the objective of PCT, point 2 is the requirement for an unbiased PCT, and points 3 and 4 are desirable characteristics.

II.C. Five Identified PCTs

Per our literature study, we identify five distinct PCTs: (1) Simple Sampling (SS), (2) Duplicate-Discard\textsuperscript{3} (DD), (3) Splitting-Roulette (SR) (Ref. 4), (4) Combing (CO) (Ref. 15), and (5) Modified Combing (COX) (Ref. 10). Additionally, there are three different sampling bases with which each of the PCTs can be implemented: uniform, weight-based, and importance-based sampling.

II.C.1. Combing (CO)

Perhaps the most standardized\textsuperscript{8} PCT is CO. Per our classification, the “Simple Comb” proposed by Booth (see Sec. II in Ref. 15) is a weight-based CO. Combing techniques are best explained with graphical illustrations. Let us consider a population control problem with $N = 6$ and $M = 4$. The weight-based CO combs the population as shown in Fig. 2, where $\xi$ is a random number (from 0 to 1) used to determine the offset of the initial tooth of the comb. Once the initial tooth location is set, the remaining teeth are spaced $W/M$ apart. Per Fig. 2, particles 1 and 5 are copied once, particle 3 is copied twice, and particles 2, 4, and 6 are not copied at all. To ensure an unbiased MC simulation [see Eq. (1)], the copies of particle $i$ are assigned with weight $w'_i = W/M$.

Booth also proposes the “Importance-Weighted Comb” (see Sec. III in Ref. 15), which per our classification is the importance-based CO. The importance-based CO is similar to the weight-based CO shown in Fig. 2, but instead of using $w_i$ for the particle axis, $W/M$ for the distance between teeth, $\xi W/M$ for the offset of the comb, and the final weight $w'_i = W/M$, we respectively use $u_i$, $U/M$, $\xi U/M$, and $w'_i = U/(MI)$, where $u_i = I_i w_i$ is the product of importance $I_i$ and weight of particle $i$, and $U = \sum u_i$ is the total of the product.

Now we discuss the other variant of CO: uniform CO. The uniform CO treats particles equally, regardless of their

\textsuperscript{8}CO is the only technique that has a single, well-known origin,\textsuperscript{15} a proper name, and a clear, unambiguous procedure.
weight or importance, and combs the initial particles as shown in Fig. 3. Per Fig. 3, each of the particles 1, 3, 4, and 6 is copied once, while particles 2 and 5 are not copied at all. To ensure an unbiased MC simulation [Eq. (1)], copies of particle 1 are assigned with weight \( w'_i = (N/M)w_i \). We believe that this uniform variant of CO (as well as those of other PCTs) has never been articulated in the literature. A discussion on the significance of the PCT sampling bases (uniform, weight based, or importance based) is given later in Sec. II.D.1.

**II.C.2. Modified Combing (COX)**

A modification of CO was recently proposed by Ajami et al.\(^{10}\) Different from the weight-based CO shown in Fig. 2, the weight-based COX combs the initial particle as shown in Fig. 4. In COX, instead of having uniformly spaced teeth and sampling the offset of the whole comb, we allow the teeth to be nonuniformly spaced by offsetting each tooth with a different random number. The controlled weight \( w'_i \) assigned to the particle copies to ensure an unbiased MC simulation [Eq. (1)] is identical to that of CO.

Ajami et al.\(^{10}\) provide a limited discussion and demonstration of how COX compares to CO. In Sec. II.D.2, we discuss how COX may actually avoid a particular drawback of CO, and then in Sec. III, we discuss how that remedy comes at a significant expense.

**II.C.3. Splitting-Roulette (SR)**

Sweezy et al.\(^4\) proposes the weight-based SR. In SR, we assign each initial particle \( i \) with splitting number \( s_i \). For uniform, weight-based, and importance-based SR, the values for \( s_i \) are, respectively, \( M/N, w_i/(W/M) \), and \( u_i/(U/M) \). We split each particle \( i \) into \( \lfloor s_i \rfloor + 1 \) copies, and then Russian-roulette the last copy with surviving probability \( s_i - \lfloor s_i \rfloor \). The function \( \lfloor \cdot \rfloor \) denotes the floor function, which produces the greatest integer not greater than the variable argument. Finally, to ensure unbiased MC simulation, the surviving particle copies are assigned controlled weight \( w'_i \), which happens to be identical to that of the CO techniques.

The SR techniques neither exactly produce a final population of size \( M \) nor exactly preserve the initial total weight \( W \); however, they preserve the expectations. To exactly preserve the population’s total weight \( W \), Sweezy et al. suggest performing a weight normalization at the end of SR. This weight normalization can be applied to other PCTs that do not exactly preserve the population’s total weight as well (e.g., uniform and importance-based CO). The significance of this PCT weight normalization is further discussed later in Sec. II.D.3.

**II.C.4. Simple Sampling (SS)**

SS is the typical PCT employed in \( k \)-eigenvalue MC simulations.\(^{24}\) In SS, we simply sample \( M \) particles from the initial population to be the final population. For uniform SS, all particles have a uniform probability to be sampled at each draw, while for weight-based and importance-based SS, the probability for a particle to be sampled at each draw is proportional to its weight \( w_i \) and the product of its weight and importance \( u_i \), respectively. Finally, to ensure an unbiased MC simulation, the

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**Fig. 3.** Uniform CO with initial and final population size \( N = 6 \) and \( M = 4 \).

**Fig. 4.** Weight-based COX with initial and final population size \( N = 6 \) and \( M = 4 \).
sampled particles are assigned controlled weight \( w'_i \), the value of which happens to be identical to that of the other PCTs.

**II.C.5. Duplicate-Discard (DD)**

We identify the PCT proposed by Leppänen in Ref. 3 as the uniform DD technique due to its mechanism of randomly duplicating or discarding particles to achieve the desired population size. In particle duplication (for \( N < M \)), we first copy each initial particle once to the final population, and then, on top of that randomly sample \( M - N \) particles from the initial population to be copied to the final population. In particle discard (for \( N > M \)), we randomly sample \( N - M \) particles from the initial population; the sampled particles do not get copied to the final population, while the rest are copied once. Finally, the controlled weight \( w'_i \) that satisfies the unbiased MC simulation requirement is identical to that of the other uniform PCTs: \( (N/M)w_i \).

One can improve the particle duplication of the uniform DD. Instead of keeping a copy of the initial population and then sampling \( M - N \) additional particles, we keep \( [M/N] \) copies and sample only \( (M \text{ mod } N) \) particles (we note that “mod” denotes the remainder operator, such that \( (M \text{ mod } N) = M - [M/N]N \)). This improvement reduces both the number of samplings performed and the uncertainty introduced by the PCT.

**II.D. Additional Notes on PCTs**

**II.D.1. PCT Sampling Basis**

As mentioned earlier, each of the five distinct PCTs (CO, COX, SR, SS, and DD) can be implemented with three different sampling bases: uniform, weight-based, and importance-based sampling.

The computational procedures of the uniform sampling PCTs are the simplest, followed by their respective weight-based and then importance-based counterparts. As an example, uniform CO (Fig. 3) is simpler than the weight-based CO (Fig. 2) as it does not require some binary search to determine where exactly each tooth falls.

If the initial population has a uniform weight, the weight-based sampling is identical to the uniform sampling since \( W = Nw_i \). However, if the initial particles have varying weights, the weight-based sampling simultaneously functions as a VRT as well. Particles having relatively large weights tend to be split into multiple copies, which leads to variance reduction, while on the other hand, particles with relatively low weights tend to be Russian-roulette, which may lead to more efficient computation by not spending time tracking small-weight particles. Nevertheless, particle weight does not necessarily indicate particle importance. If the initial particles are assigned with some importance values, the importance-based sampling offers more effective variance reduction than the weight based.

One may argue that uniform sampling is the least optimal as it assigns all particles an identical splitting number or surviving probability regardless of their weights and importance. However, uniform sampling can be the most optimum choice in two cases. The first is when the population has a uniform weight and unknown importance, which is the case in a fixed-source problem without any VRT and in a typical \( k \)-eigenvalue simulation where all the fission neutrons are emitted with uniform weight. The second case is when the MC simulation is already equipped with some VRTs, such as the weight-window or the uniform fission site method, because the particle distribution and weight profile of the population would be optimized already, such that particles can be treated equally by the PCT; in other words, redundancy is avoided in the variance reduction effort. In particular, in the application of an effective weight-window or uniform fission site method, the use of weight-based sampling may actually ruin the already optimized particle distribution.

The interplay between PCT and VRT briefly described previously is outside the scope of this study. Furthermore, while the theoretical analysis performed in Sec. III is applicable to all sampling bases, only the uniform PCTs are implemented and tested in Secs. IV, V, and VI.

**II.D.2. Correlation Issue in CO**

In Sec. II.C, it is interesting to observe that CO techniques only require one random number to perform the population control (as a comparison, SS and SR respectively require \( M \) and \( N \) random numbers); in other words, a single random number determines the fate of all particles in the population. This unfortunately yields correlation in the particle sampling. As an example, particles 1 and 2 in Fig. 2 will never be sampled together. This correlation may produce unwanted behavior depending on how the initial particles are ordered.

Sweezy et al.\(^4\) provide an illustrative demonstration of such possible unwanted behavior in CO, which is shown in the upper part of Fig. 5. In this postulated PCT problem, we wish to select two particles from an ordered initial population of size four. The initial population consists of alternating 1- and 2-MeV particles, all of which have uniform weight. If we apply CO, we will have a final population
with either all 1-MeV or all 2-MeV particles. However, this behavior does not necessarily make the MC simulation biased because each initial particle is still treated fairly individually; i.e., Eq. (1) is still satisfied. If one were to run the simulation in multiple batches, which is necessary to get a measure of result uncertainty in a census-enabled MC simulation, we would be running half of the batches with all 1-MeV particles and the other half with all 2-MeV particles. While such behavior may result in a larger tally variance, the expectation is still preserved. Outside this postulated PCT problem, some extent of physics is naturally embedded in the particle population order (e.g., adjacent particles may originate from the same emission event). However, there has never been any observable effect of this correlation issue in the practical application of CO (Refs. 2, 8, 17, 19, and 20).

If one wishes to eliminate this possible correlation issue, the initial population order must be randomized before CO is applied. However, in a massively parallel computation with a reproducibility requirement, this prerandomization process will require a large number of communications, which may ruin the parallel scalability of the simulation.

The COX proposed by Ajami et al.\textsuperscript{16} to some extent remedies this correlation issue as demonstrated in the lower part of Fig. 5. Nevertheless, this remedy comes at the expense of increasing \( \sigma[C_i] \), which is discussed later in Sec. III.

II.D.3. PCT Weight Normalization

Some PCTs i.e., uniform and importance-based PCTs, and all SR techniques do not exactly preserve the population total weight \( W \). However, the expectation of the total weight is still preserved because

\[
E[W] = \sum_{i=1}^{N} E[C_i] = W,
\]

where the first and the second equalities respectively use Eqs. (4) and (3).

To exactly preserve \( W \), Sweezy et al.\textsuperscript{4} suggest performing weight normalization after population control is performed. This is done by multiplying all of the final particles with the factor \( W/W' \) so that \( C_i^{\text{(norm.)}} = (W/W') C_i \). Unfortunately, this PCT weight normalization introduces bias as Eq. (1) is now violated:

\[
E[C_i^{\text{(norm.)}}] = E\left[ \frac{W}{W'} C_i \right] = E\left[ \frac{W}{W'} \right] w_i \geq w_i, \tag{6}
\]

where the inequality comes from Jensen’s inequality\textsuperscript{4,26} suggesting \( E[W/W'] \geq 1 \). Nevertheless, it can be seen that by using a large number of particles, the bias in the normalized PCTs can be minimized; however, it is also the case for the lack of exact total weight preservation in the nonnormalized PCTs. In other words, the PCT weight normalization suggested in Ref. 4 is only recommended if preserved total weight is more important than an unbiased MC simulation.

II.D.4. More Advanced PCTs

The techniques considered in this work are those of basic PCTs. More advanced PCTs include the one proposed by Booth in Sec. IV of Ref. 15, which introduces the idea of partial population weight adjustment, an unbiased alternative to the weight normalization proposed by Sweezy et al.\textsuperscript{4} (see Sec. II.D.3), to exactly preserve the population’s total weight \( W \). This partial adjustment is technically more advanced than the weight normalization technique; it introduces tunable parameters (i.e., the adjusted partial population size and the number of recursive partial adjustments) and additional challenges for parallel computing implementation. While the proposed partial population weight adjustment is applied to the importance-based CO in Ref. 15, it basically can be applied to other PCTs that do not exactly

Fig. 5. Illustration of the correlation issue in CO and how it is remedied in COX; \( E \) indicates particle’s energy in mega electron-volts.
preserve $W$ as well. Other developments of advanced PCTs include the more recent study by Legrady et al.,\textsuperscript{19} which introduces several advanced CO techniques specifically improved for extensive variance reduction.

### III. UNCERTAINTY INTRODUCED BY PCT

#### III.A. Theoretical Analysis

By determining the first and second moments of $C_i$ (the total weight of the copies of initial particle $i$ in the final population), we can determine the variance introduced by a PCT:

$$\text{Var}[C_i] = E[C_i^2] - E[C_i]^2. \quad (7)$$

Another and perhaps more illustrative quantity is the relative uncertainty (standard deviation) introduced by the PCT to each particle $i$ in the initial population:

$$\sigma_r[C_i] = \frac{\sigma[C_i]}{w_i} = \frac{1}{w_i} \sqrt{\text{Var}[C_i]}. \quad (8)$$

Unless normalized (as discussed in Sec. II.D.3), all of the identified PCTs (SS, SR, CO, COX, and DD) are unbiased, which means $E[C_i] = w_i$. However, the second moments $E[C_i^2]$ of the PCTs may be different and thus become the key to determining the relative performance on how large uncertainty $\sigma_r[C_i]$ is introduced by the techniques.

In SR (described in Sec. II.C.3), each initial particle $i$ is either copied $[s_i] + 1$ times with a probability of $s_i - [s_i]$, or otherwise copied $[s_i]$ times. This suggests

$$E[C_i^2]_{\text{SR}} = ([s_i] + 1)w_i + [1 - (s_i - [s_i])][s_i]w_i^2, \quad (9)$$

and

$$\sigma_r[C_i]_{\text{SR}} = \frac{1}{s_i} \sqrt{-s_i^2 + 2[s_i]s_i + ([s_i] + 1)s_i^2 - ([s_i] + 1)[s_i]^2}, \quad (10)$$

where we note that $w_i' = w_i / s_i$.

In CO (described in Sec. II.C.1), each initial particle $i$ is either copied $[s_i] - 1$ times with a probability of $[s_i] - s_i$, or otherwise copied $[s_i]$ times. The quantity $s_i$ (splitting number) used in this context happens to be identical to that of SR, and the function $[\cdot]$ denotes the ceiling function, which produces the smallest integer not smaller than the variable argument. Following a similar process to that of SR in the previous paragraph, we obtain

$$\sigma_r[C_i]_{\text{CO}} = \frac{1}{s_i} \sqrt{-s_i^2 + 2[s_i]s_i - ([s_i] - 1)s_i - ([s_i] - 1)[s_i]^2}. \quad (11)$$

In SS (described in Sec. II.C.4), each particle $i$ can be copied multiple times up to $M$, which means

$$E[C_i^2]_{\text{SS}} = \sum_{j=0}^{M} \left( \frac{M}{j} \right) \left( \frac{1}{M} \right)^{j-i} M^j (jw_i')^2, \quad (12)$$

where we use the same definition of $s_i$ used in the other PCTs. Per binomial theorem, we can find that

$$\text{Var}[C_i]_{\text{SS}} = s_i (1 - \frac{s_i}{M})w_i'^2, \quad (13)$$

and thus,

$$\sigma_r[C_i]_{\text{SS}} = \frac{1}{s_i} \sqrt{\frac{1}{s_i} - \frac{1}{M}} \approx \frac{1}{\sqrt{s_i}}, \quad (14)$$

where the approximation is due to the fact that typically $s_i \ll M$ (or equivalently $N \gg 1$ for uniform PCTs).

In uniform DD (described in Sec. II.C.5), we have two different cases. In the case of $N > M$, we uniformly discard $N - M$ particles from the initial population. Therefore, particle $i$ has to survive all of the discard draws to get copied once, otherwise it will not get copied at all. This means that for $N > M$ we have

$$E[C_i^2]_{\text{DD}} = \left( \frac{N - 1}{N} \times \frac{N - 2}{N - 1} \times \ldots \times \frac{M}{M + 1} \right) w_i^2 = \frac{M - M^2}{M + 1} w_i^2, \quad (15)$$

and

$$\sigma_r[C_i]_{\text{DD}} = \sqrt{\frac{1}{s_i} - 1}, \quad (16)$$

where again we use the same definition of $s_i$ used in the other PCTs. On the other hand, in the case of $N < M$ DD keeps $[M/N]$ copies of the initial population, and then uniformly draws a particle duplicate $(M \mod N)$ times out of it. This process is similar to that of SS, except that we
sample \((M \mod N)\) particles instead of \(M\) particles and we prekeep \([M/N]\) copies of each initial particle. This gives

\[
\sigma_r[C]_{\text{DD}} \approx \sqrt{\left(1 - \frac{1}{s_i} \right) \frac{1}{s_i}},
\]

(17)

where the approximation is again due to \(N \gg 1\).

In COX (described in Sec. II.C.2), things are more involved in that deriving the relative uncertainty \(\sigma_r[C_i]\) is not as straightforward. First, let us observe how Fig. 4 of COX differs from Fig. 2 of CO. We can see that particle 1 suffers from the same uncertainty in both methods; in this case, both CO and COX introduce identical uncertainty to particle 1. However, it is not the case for the other particles. For example, in CO particle 2 has only two possibilities, get copied once or not at all, but in COX, particle 2 has an additional possibility, which is to get copied twice. Due to this additional possibility, COX introduces higher uncertainty to particle 2 than CO does. Similar findings can be observed for particle 3. These observations indicate that \(\sigma_r[C]_{\text{COX}} \geq \sigma_r[C]_{\text{CO}}\), depending on how the particle \(i\) is located relative to the comb grid (the broken line in Fig. 4).

Figures 6 and 7 illustrate different situations of how particles can be located relative to the COX comb grid. The particle 2 and particle 3 cases discussed in the previous paragraph are illustrated in the lower parts of Figs. 6 and 7, respectively. We note that we use a unit-spaced comb grid and the same definition of \(s_i\) used in other PCTs; this makes the analysis applicable for COX with any sampling basis. Symbols in the figures, i.e., \(\zeta_i = 1 - \delta_i\) and \(\theta_i = s_i + \delta_i - [s_i]\), serve as key quantities to derive \(E[C_i^2]_{\text{COX}}\) as a function of the comb offset \(\delta_i\). By observing the figures, we found that \(E[C_i^2]_{\text{COX}}\) (and thus \(\sigma_r[C]_{\text{COX}}\)) is dependent on \(\delta_i\), and the dependency is periodic with a unit period in \(\delta_i\).

On the upper part of Fig. 6, we have \(s_i \leq 1\) and \(0 \leq \delta_i \leq 1 - s_i\); in this case, COX and CO are identical. On the lower part of Fig. 6, we have \(s_i \leq 1\) and \(1 - s_i < \delta_i \leq 1\); in this case, we have

\[
E[C_i^2]_{\text{COX}} = \zeta_i \theta_i (2w'_i)^2 + (\zeta_i + \theta_i - 2\zeta_i \theta_i)(w'_i)^2.
\]

(18)

On the upper part of Fig. 7, we have \(s_i \geq 1\) and \(0 < \delta_i \leq [s_i] - s_i\); in this case, we have

\[
E[C_i^2]_{\text{COX}} = \zeta_i \theta_i ([s_i] - 1)w'_i)^2 + (1 - \zeta_i)(1 - \theta_i)[([s_i] - 2)w'_i]^2.
\]

Finally, on the lower part of Fig. 7, we have \(s_i \geq 1\) and \([s_i] - s_i < \delta_i \leq 1\); in this case, we have

\[
E[C_i^2]_{\text{COX}} = \zeta_i \theta_i ([s_i] + 1)w'_i)^2 + (\zeta_i + \theta_i - 2\zeta_i \theta_i)([s_i]w'_i)^2 + (1 - \zeta_i)(1 - \theta_i)[([s_i] - 1)w'_i]^2.
\]

(20)

Figure 8 shows the resulting \(\sigma_r[C_i]\) of COX as a function of \(\delta_i\) at different values of \(s_i\).

The derived theoretical relative uncertainty \(\sigma_r[C_i]\) of the PCTs, i.e., Eq. (10) for SR, Eq. (11) for CO, Eq. (14) for SS, and Eqs. (16) and (17) for DD, are plotted in Fig. 9. Different from those of the other PCTs, the \(\sigma_r[C_i]\)
of COX is dependent on $\delta_i$ as shown in Fig. 8; thus, in Fig. 9 we plot its average value and shade the region (min to max) of its possible values. The $x$-axis is chosen to be $1/s_i$, which is equivalent to the ratio $w'_i/w_i$ or $N/M$ for the uniform PCTs. This $x$-axis effectively represents a measure of the system’s population growth, which is dependent on the system criticality and the census frequency. Roughly speaking, one can say that $N/M$ increases with the criticality of the system as illustrated with the arrows in Fig. 9.

The larger the $\sigma_i[C_i]$, the larger the uncertainty introduced by the PCTs, which may lead to less precise (more statistical noise) results. From Fig. 9, it is evident that in a growing population regime (“Super”), the larger the ratio $N/M$, the larger the uncertainty introduced by the PCTs. This trend generally extends to the decaying population regime (“Sub”). However, some methods (SR, CO, and DD) take advantage of the pure-splitting scenario in which $M$ is a multiple of $N$, such that $\sigma_i[C_i]$ drops to zero. We note that given a reasonably accurate prediction of the population decay rate, one can take advantage of this behavior to minimize the uncertainty introduced by the PCTs in systems with decaying population. In terms of $\sigma_i[C_i]$, SS is the worst PCT, followed by COX. Particularly, unlike the other PCTs, SS and COX introduce significant uncertainties even when $N \approx M$ (which is the case throughout the active cycles of an eigenvalue simulation, see Sec. VI). On the other hand, SR and CO are identically the best.

### III.B. Numerical Verification

To numerically verify the theoretical $\sigma_i[C_i]$ derived in the previous subsection, we implement the PCTs into a Python-based research MC code and devise a PCT test problem. Per the discussion in Sec. II.D.1, only uniform PCTs are discussed here. Nevertheless, a similar setup can be used to verify PCTs with the other sampling bases.

In the test problem, we perform population control to an initial population with a cosine statistical weight distribution:

$$w_i = \cos\left(\frac{i - 1}{N - 1} \pi\right) + 1, \quad i = 1, 2, \ldots, N. \quad (21)$$

Each initial particle $i$ is associated with tally bin $i$. All copies of particle $i$ in the final population will score their controlled weight $w'_i$ to the tally bin $i$; in other words, we are tallying $C_i$.

Figures 10 and 11 show the resulting $C_i$ of different PCTs for $N/M = 1.25$ and $N/M = 0.75$, respectively. In each subplot, the red line indicates the analog result, where no PCT is performed and no uncertainty is introduced to the population ($C_i = w_i$). We note that there are $N$ discrete values of analog $C_i$, but we present it as a line to distinguish it from the values calculated using PCT, which are marked by the blue circles. As discussed earlier in this section, PCTs introduce some uncertainties to the population, and the magnitudes of the uncertainties are illustrated by how far the blue circles deviate from the red line; the more spread away the blue circles are from the red line, the more uncertainties are introduced by the respective techniques. We note that the results shown in Figs. 10 and 11 are in agreement with the theoretical uncertainty shown in Fig. 9, i.e., SS introduces the most uncertainty, followed by COX (and DD for $N/M < 1$), while CO and SR introduce the least.
Next, we would like to use the PCT test problem to verify the theoretical PCT uncertainties $\sigma_r[C_i]$ derived in this section. We set the target size $M$ to be 1000 and consider multiple values of $N$ such that $N/M$ ranges from 0.75 to 1.25. In each case, the population control is repeated 100 times so that we can determine the relative standard deviation $\sigma_r[C_i]$ based on the accumulation of $C_i$ and $C_i^2$. Furthermore, we randomize the particle order in the population “stack” at each repetition. In uniform PCTs, $\sigma_r[C_i]$ is independent of $i$ as it only depends on the value of $N/M$, as shown in Fig. 9. Therefore, in each case of $N/M$, we take the average of $\sigma_r[C_i]$ over all $i$ as the final result. Finally,
these numerical results from all cases of $N/M$ are compared to the theoretical values, as shown in Fig. 12. The numerical results are denoted by the markers, and the lines are the theoretical values identical to those in Fig. 9. Excellent agreement is observed, even for COX with its ranging theoretical $\sigma_i [C_i]$ (the shaded area). This verifies not only the theoretical $\sigma_i [C_i]$ derived in Sec. III.A, but also the PCT implementations.
mechanism, which can be a time census for time-dependent simulation or fission census for an eigenvalue one. Once the particle census is completed, population control is performed to the census bank using one of the PCTs (SS, SR, CO, COX, or DD). Finally, the resulting final population (sampled bank) is evenly redistributed to the processors via the nearest-neighbor bank-passing algorithm, where each processor only needs to communicate (send or receive) with its adjacent neighbors as needed, without any global particle bank formation nor typical master-slave communication.21

Two exclusive scans need to be performed in the proposed parallel algorithm. An exclusive scan to the census bank is required to determine the total size \( N \) and the position of the processor’s local bank relative to the “global” bank so that reproducible population control, regardless of the number of processors, can be achieved by consistently following the same random number sequence. The other scan is performed to the sampled bank so that we can determine the local bank offsets required to perform the nearest-neighbor bank passing.

Algorithms 1 and 2 respectively show the pseudo-codes for the bank-scanning and bank-passing processes that are used in all of the PCT algorithms (Algorithms 3 through 7). The PCT algorithms only take the minimum information required to perform the population control—the census bank (which can be either fission or time bank) and the target size \( M \)—and return the controlled, evenly distributed across processors, final bank. Therefore, the proposed parallel PCT algorithms are applicable for both time-dependent fixed-source and eigenvalue MC simulation modes. We also note that the algorithms are designed to start and return with the same random number seed across all processors, which is important for maintaining reproducibility.

The parallel algorithms are implemented to the Python-based MC research code by using the Python Abstract Base Class feature to allow streamlined implementation of the different PCTs: SS, SR, CO, COX, and DD. The distributed-memory parallel communication is facilitated by using MPI4Py (Ref. 27). We use the verification test problem in Sec. III.B to verify that the PCTs are properly implemented and their results (distribution of \( C_i \)) are reproducible; i.e., the same results are produced regardless of the number of processors.

Next, we perform a weak scaling test to assess the relative parallel scalabilities of the different PCTs. The test is similar to the verification test problem in Sec. III.B, except that \( M \) is set to be \( 10^5 \) times the number of processors, \( N \in [0.5 \, M, \, 1.5 \, M] \) is randomly picked in 50 repetitions, and the initial particles are randomly distributed to the processors. We note that there is no particle transport performed. We specifically measure the run time required to perform population control and manage the particle bank, which includes

### Algorithm 1

**Scanning “global” bank to get local position and bank sizes**

1: function BANKSCANNING(bank)
2:   N_local = size(bank)
3:   idx_start = MPI_ExclusiveScan(N_local)
4:   N_global = MPI_BROADCAST(idx_start+N_local, from=last_rank)
5: return idx_start, N_local, N_global
Algorithm 2 Nearest-neighbor bank passing

1: function BANKPASSING(bank)
   -> % Get current bank indices %
2:   idx_start, N_local, N = BANKSCANNING(bank)
3:   idx_end = idx_start + N_local
   -> % Get target indices based on N %
4:   target_start, target_end = target_idx(N)
   -> % Need more or less on each side? %
5:   more_left = idx_start < target_start
6:   less_left = idx_start > target_start
7:   more_right = idx_end > target_end
8:   less_right = idx_end < target_end
   -> % Offside? %
9:   offside_left = idx_end ≤ target_start
10:  offside_right = idx_end ≥ target_end
   -> % If offside, need to receive first %
11:  if offside_left then
12:     Receive from right
13:     less_right = False
14:  if offside_right then
15:     Receive from left
16:     less_left = False
   -> % Non-blocking send %
17:  if more_left then
18:     Isend first (work_start-idx_start) particles to left
19:  if more_right then
20:     Isend last (work_start-idx_start) particles to right
   -> % Receive (and wait if Isent) %
21:  if less_left then
22:     Receive from left
23:  if less_right then
24:     Receive from right
25: return bank_final

Communicating attributes and members of the bank throughout the processors.

The weak scaling result is shown in Fig. 14. The marked lines and the shaded areas respectively show the average and the standard deviation of the run times in the 50 repetitions. It is found that SR, CO, and COX identically scale the best, followed by DD and then SS. The sampling mechanisms of SR, CO, and COX are embarrassingly parallel, which make the techniques scale very well. On the other hand, SS, which scales the worst, needs to serially sample all of the \( M \) particles. The sampling mechanism of DD is also done in serial, but it only needs to sample as many as the difference between \( N \) and \( M \); this makes DD scale better than SS and also explains why the DD run time has a relatively larger standard deviation. Finally, it is worth mentioning that we purposely picked a modest number of particles per processor \( 10^5 \) to get a balanced demonstration on the significance of work (population control sampling) and communication. Should we significantly increase the number of particles per processor, such that the amount of work far outweighs the amount of communication, the parallel scalabilities of SR, CO, and COX will improve, approaching the perfect scaling (horizontal line).

V. TIME-DEPENDENT PROBLEMS

In this section, we devise time-dependent MC test problems and then solve them with the PCTs to assess

Algorithm 3 Uniform Simple Sampling (SS)

1: function PCT_SS(bank_census, M)
2:   idx_start, N_local, N = BANKSCANNING(bank_census)
   -> % Count how many times particle is sampled %
3:   count = \{0\} * N_local
4:   for \( i = 0: (M-1) \) do
5:     idx = \geq \) random(\)*N \ j - idx_start
6:   if \( 0 \leq \) idx \ \ N_local then
7:     count[idx] += 1
   -> % Set up the Sample Bank %
8:   bank_sample = \{\}
9:   for \( i = 0: (N_{local-1}) \) do
10:  \( \text{for } j = 1: \) count < 1 \ do
11:    \( \text{particle = bank_census[i]} \)
12:    \( \text{particle.w *= N/M} \)
13:    \( \text{bank_sample.append(particle)} \)
14:  \( \text{bank_final = BANKPASSING(bank_sample)} \)
15: return bank_final
Algorithm 4 Uniform Splitting-Roulette (SR)

1: function PCT_SR(bank_census, M)
2:   idx_start, N_local, N = BANKSCANNING(bank_census)
3:   skip random number state by idx_start
4:   n_split = ⌊ M/N ⌋
5:   p_survive = M - n_split
6:   bank_sample = {}
7: for i = 0:(N_local-1) do
8:       particle = bank_census[i]
9:       particle.w *= N/M
10:      for j = 1:n_split do
11:          bank_sample.append(particle)
12:      end
13:   end
14:   skip random number state by (N_i_start)
15:   bank_final = BANKPASSING(bank_sample)
16: return bank_final

Algorithm 5 Uniform Particle Combing (CO)

1: function PCT_CO(bank_census, M)
2:   idx_start, N_local, N = BANKSCANNING(bank_census)
3:   idx_end = idx_start + N_local
4:   tooth_distance = N/M
5:   tooth_offset = random()*tooth_distance
6:   tooth_start = ⌊ (idx_start-tooth_offset)/tooth_distance ⌋
7:   tooth_end = ⌊ (idx_end-tooth_offset)/tooth_distance ⌋
8:   bank_sample = {}
9: for i = tooth_start:(tooth_end+1) do
10:     idx = ⌊ (random() + i)*tooth_distance ⌋
11:     if 0 ≤ idx ≤ N_local then
12:        particle = bank_census[idx]
13:        particle.w *= tooth_distance
14:     end
15:     bank_sample.append(particle)
16: end
17: return bank_final

Algorithm 6 Uniform New Particle Combing (COX)

1: function PCT_COX(bank_census, M)
2:   idx_start, N_local, N = BANKSCANNING(bank_census)
3:   idx_end = idx_start + N_local
4:   tooth_distance = N/M
5:   p_survive = M - n_split
6:   bank_sample = {}
7: for i = tooth_start:(tooth_end+1) do
8:       idx = ⌊ (random()+i)*tooth_distance ⌋
9:       if 0 ≤ idx ≤ N_local then
10:          particle = bank_census[idx]
11:          particle.w *= tooth_distance
12:       end
13:      bank_sample.append(particle)
14: end
15: return bank_final

Note that particle position and time are respectively measured in mean free path \((\Sigma_t)^{-1}\) and mean free time \([\nu \Sigma_t]^{-1}\), where \(v\) is particle speed. We also have the typical scattering parameter \(c = (\Sigma_s + v\Sigma_t)/\Sigma_t\). The scalar flux solution \(\phi(x,t) = \int_{-1}^{1} \psi(x,\mu,t) d\mu\) of this time-dependent problem is
Algorithm 7 Uniform Duplicate-Discard (DD)

1: function PCT_DD(bank_census, M)
2:   idx_start, N_local, N = BANKSCANNING(bank_census)
3:   * % Duplicate %
4:   if M > N then
5:     count = \{ > M/N \} * N_local
6:     N_sample = M - \lfloor M/N \rfloor * N
7:   for i = 0:(N_sample-1) do
8:     idx = \lfloor \text{random()} * N \rfloor - idx_start
9:     if 0 <= idx < N_local do
10:        count[idx] += 1
11:   end

12:   * % Set up the Sample Bank %
13:   for i = 0:(N_local-1) do
14:      for j = 1:count[i] do
15:         particle = bank_census[i]
16:         particle.w *= N/M
17:         bank_sample.append(particle)
18:      end
19:   end

20:   * % Discard %
21:   else
22:      N_discard = N - M
23:      discard_flag = \{False\} * N
24:      for i = 0:(N_discard-1) do
25:         while True do
26:            idx = \lfloor \text{random()} * N \rfloor
27:            if discard_flag[idx] = False then
28:               discard_flag[idx] = True
29:            break
30:         end
31:      end
32:   end
33:   end
34:   return bank_final

\[ \phi(x,t) = \frac{c}{2\pi} \left\{ 1 + \frac{t}{2\pi} (1 - \eta^2) \right\} \text{Re} \left[ \xi e^{i(1-\eta^2)j} \right] du \] \[ H(1-\eta^2). \] (24)

where

\[ \eta = \frac{x}{t}, \quad q = \frac{1+\eta}{1-\eta}, \]

\[ \xi(u) = \frac{\ln(q) + iu}{\eta + i\tan(\frac{\pi}{2})}, \] (25)

and \( H(\cdot) \) denotes the Heaviside function.

For our test problems, we consider the \( c \) values of 1.1 and 0.9, respectively representing supercritical and subcritical systems. The analytical solution of the total flux would be a simple exponential function of \( \phi(t) = \exp[(c - 1)t] \); however, the spatial solutions [Eq. (24)] offer some more interesting features, particularly for the supercritical case, as shown in Fig. 15 (note that the solutions \( t \leq 1 \) and \( |x| \in [10, 20] \) are not shown to better show the prominent spatial features).

The test problems are initiated by an isotropic neutron pulse at \( x = t = 0 \) [see Eq. (22)]. In both cases, the scalar flux solution gradually diffuses throughout the medium. The difference is that the significant neutron absorption promotes population decay in the subcritical case. On the other hand, while the solution of the supercritical case initially behaves similarly to that of the subcritical, it eventually raises up due to the significant fission multiplication; at \( t = 20 \), the population size reaches \( \exp(2) = 7.39 \) times the initial value.

V.A. Verifying Time-Dependent Features of the MC Code

To the authors’ knowledge, there are three different time-dependent scalar flux quantities that can be calculated via MC simulation: (1) spatial-average time-average \( \phi_{jk} \), (2) spatial-average time-edge \( \phi_{j}(t) \), and (3) spatial-edge time-average \( \phi_{k}(x) \), where \( j \) and \( k \) respectively denote spatial and time mesh indices. The first tally uses the typical track-length estimator averaged over time mesh. The second uses a time-edge estimator, which accumulates the product of neutron speed and weight whenever a time grid is crossed, averaged over spatial mesh. The third uses the typical spatial-mesh-crossing estimator, which scores particle weight divided by the absolute of the normal product of the particle direction and the surface, averaged over time mesh. The use of the track-length estimator (spatial-average time-
average $\phi_{j,k}$) is typically desired because it generally gets more samples compared to “event-triggered” estimators like time-edge crossing ($\phi_j(t)$) and spatial-mesh crossing ($\phi_k(x)$). Nevertheless, it is worth mentioning that in some applications, time-edge quantities $\phi_j(t)$ may be more desired than the time-average one $\phi_{j,k}$.

To simulate the supercritical ($c = 1.1$) and subcritical ($c = 0.9$) cases, we consider purely fission media with $v = c$. The test problems are simulated using the research MC code, and we record the scalar flux using the three tally estimators that are subject to $J = 202$ uniform spatial meshes spanning $x \in [-20.5, 20.5]$ and time grid $t = 0, 1, 2, \ldots, 20$. To limit particle population growth in the supercritical case, we set a time boundary at the final time $t = 20$; particles crossing this time boundary will be killed (analogous to spatially crossing a convex vacuum boundary). Note that we have not introduced any PCT yet; the MC simulation is still run in analog. Simulations are performed with an increasing number of histories $N_h$. The resulting 2-norms of normalized error [against the reference formula Eq. (24), normalized at each time index] of the supercritical problem are shown in Fig. 16. It is found that all of the error 2-norms converge at the expected rate of $O(1/\sqrt{N_h})$ (shown in black solid line); and the track length estimator result $\phi_{j,k}$ shows the lowest error, which is in line with the discussion in the previous paragraph. A similar convergence rate is observed in the subcritical case as well. This verifies the time-dependent features of the MC code that we are going to use in the next subsection to assess the relative performances of the PCTs. Additionally, this also suggests that this set of test problems, the AZURV1 benchmark, serve as a good verification tool to test the time-dependent features of MC codes.

**V.B. Performances of the PCTs in Solving the Time-Dependent Test Problems**

The supercritical and subcritical problems are solved using the five PCTs (SS, SR, CO, COX, and DD). Each simulation is run with $10^5$ source particles on 36 distributed-memory processors. We consider uniformly spaced population control time censuses within $t \in [0, 20]$. With increasing frequency, we consider eight numbers of censuses: 1, 2, 4, 8, 16, 32, 64, and 128. In 1 census, the census is performed at $t = 10$; while in two censuses, it is performed at $t = 20/3$ and...
Finally, each simulation is repeated 100 times with different random number seeds.

Table 1 shows the census period and the expected ratio $N/M$ associated with the simulated cases. By referring to Fig. 9, we can estimate the expected uncertainty $\sigma_{e}[C_i]$ introduced by a PCT at a given value of $N/M$. For convenience, plots showing the expected $\sigma_{e}[C_i]$ associated with the simulated cases are provided in Fig. 17. Note that this expected uncertainty is introduced every time the population control is performed; e.g., with four numbers of censuses, we perform census and population control and introduce the associated uncertainty once every four mean free times. This means a smaller $\sigma_{e}[C_i]$ due to larger census frequency does not necessarily lead to smaller uncertainty in the simulation result because the more frequently we perform population control, the more frequently we introduce the uncertainty $\sigma_{e}[C_i]$ (even though small) to the population.

Two performance metrics are considered: (1) total run time $T$ and (2) the averaged sample standard deviation of the scalar flux at the end of simulation time $\phi_0(t = 20)$ or simply $\phi_j$. The sample standard deviation $\sigma_{j}$ (not the mean standard deviation) is calculated over the $N_r = 100$ repetitions:

$$\overline{\phi}_j = \frac{1}{N_r} \sum_{i=1}^{N_r} \phi_j^{(i)}$$  \hspace{1cm} (26)

and

$$\sigma[\phi_j]^2 = \frac{1}{N_r - 1} \left[ \sum_{i=1}^{N_r} \phi_j^{(i)} - N_r \overline{\phi}_j^2 \right]$$  \hspace{1cm} (27)

where the superscript $(i)$ denotes the repetition index. We note that a repetition (or a realization) can be seen as a batch of source particles that makes a single, independent history. Finally, the averaged sample standard deviation of the scalar flux is calculated as follows:

$$\overline{\sigma}[\phi] = \frac{1}{J} \sum_{j=1}^{J} \sigma[\phi_j]$$  \hspace{1cm} (28)

The resulting performance metrics are shown in Fig. 18. A figure of merit (FOM) based on the two performance metrics,

$$\text{FOM} = \frac{1}{T \overline{\sigma}[\phi]^2}$$  \hspace{1cm} (29)
is also shown in the figure. Finally, the analog (without PCT) solution, also run in 100 repetitions, is shown in the figure as well as a reference point. Figure 18 not only compares the relative performance of the PCTs but also shows the trends of the related metrics as functions of census frequency. The figure also illustrates how PCT functions differently in supercritical and subcritical problems.

V.B.1. Supercritical Problem

The main motivation of population control in a supercritical problem is to limit the number of neutrons tracked during the simulation so that it does not exceed the allocated computational memory. In the test problem, population size exceeds seven times that of the initial value if population control is not performed. However, this comes at the expense of a less precise (more noisy) solution due to the significant uncertainty introduced by the PCT used.

Figure 18a shows that applying PCT in a supercritical problem potentially reduces the overall run time. However, too frequent census may result to a net increase in run time (relative to analog) due to the significant cost of performing too many population controls, which may involve considerable parallel communications. The figure also shows that SR, CO, and COX have the lowest run time, followed by DD and then SS, which is in agreement with the discussion in Sec. IV.

Figure 18b shows the averaged scalar flux standard deviations $\overline{\sigma}[\phi]$ of the different PCTs as functions of number of censuses performed. The averaged scalar flux standard deviation is a measure of how noisy the simulation is; the larger the $\overline{\sigma}[\phi]$, the lower the simulation precision and the larger the noise in the result. The figure demonstrates the significance of the uncertainty introduced by the PCTs (note the lower $\overline{\sigma}[\phi]$ value of the analog result). Generally, the more frequently we perform population control, the more uncertainty is introduced to the population and the larger $\overline{\sigma}[\phi]$. While $N/M$ (as well as $\overline{\sigma}[C_i]$ per Figs. 9 and 17) reduces as we increase the census frequency, the number of population controls performed and thus how often the uncertainty is introduced also increase. It is shown that all PCTs

### TABLE I

Census Configurations for the Time-Dependent Test Problems

| Number of censuses in $t \in [0, 20]$ | 1  | 2  | 4  | 8  | 16 | 32 | 64 | 128 |
|-------------------------------------|----|----|----|----|----|----|----|-----|
| Census period (mean free time)      | 10.0 | 6.67 | 4.00 | 2.22 | 1.18 | 0.61 | 0.31 | 0.16 |
| Expected $N/M$                      | Supercritical | 2.72 | 1.95 | 1.49 | 1.25 | 1.12 | 1.06 | 1.03 | 1.02 |
| Subcritical                        | 0.37 | 0.51 | 0.67 | 0.8 | 0.89 | 0.94 | 0.97 | 0.98 |

Fig. 17. Expected $\sigma/[C_i]$ of the simulated cases (see Table I and Fig. 9).
seem to yield similar averaged scalar flux standard deviations in the lower census frequency. However, as we increase the census frequency, SR, CO, and DD seem to limit their standard deviations. This demonstrates their superiority over COX and SS as the three techniques theoretically introduce the least uncertainty in supercritical problems, as shown in Figs. 9 and 17.

Finally, Fig. 18c shows that the FOMs of all PCTs are always lower than that of the analog simulation, and they monotonically decrease as we increase the census frequency (c).
As the population size increases, it becomes prohibitively expensive to perform the MC simulation. The main motivation of population control in a subcritical problem is to maintain population size so that we have enough samples to yield a more precise (less noisy) solution. However, this comes at the expense of increasing overall run time as more neutrons need to be tracked.

**Fig. 18a** shows that applying PCT in a subcritical problem increases overall run time, and it increases further as we perform the population control more frequently. It is also worth mentioning that DD has a similar run time to those of SR, CO, and DD in higher numbers of censuses. This is because DD only needs to sample as many as \(|N - M|\), which gets closer to zero as we increase census frequency.

**Figure 18b** shows that population control improves the solution precision. One may think that the solution would improve further as the population control is performed more frequently; however, we should be aware that population control introduces uncertainty in a subcritical problem, too (see Figs. 9 and 17). The effect of this uncertainty is evident in Fig. 18b. At around eight censuses, the solution improvement starts to deplete and even reverses (\(\bar{\sigma}[\phi]\) increases) for SS and COX.

Finally, **Fig. 18c** shows that the PCTs offer improved FOMs relative to the analog. The FOM is improved further as we perform population control more frequently. However, it starts to consistently degrade as the effects of the increasing run time and of the significant uncertainty introduced by the PCT start to dominate. Note that this is similar to the typical trend of a VRT: it helps to improve the FOM, but will degrade the FOM if it is used too much. Another important takeaway from **Fig. 18c** is that, similar to the supercritical case, SR, CO, and DD are in the same ballpark as the best PCT, followed by COX and then SS.

**VI. k-Eigenvalue Problem**

In a MC calculation, the \(k\)-eigenvalue transport problem is typically solved via the method of successive generations. The MC simulation involves the accumulation of fission neutrons in a fission bank. At the end of each generation (i.e., when the fission census is completed), the eigenvalue \(k\) is updated, and the generated fission bank is normalized such that its total weight is identical to the target population size \(M\), which is the number of histories per generation. Finally, the normalized fission bank is set to be the source bank for the subsequent generation.

The procedure described previously is considered to be the analog approach where there is no PCT being used. The eigenvalue update and weight normalization are useful for the MC simulation because they direct the neu-tronics system into the steady-state configuration, which helps maintain the number of source particles simulated at each generation around the user-specified value \(M\). However, in the earlier generations, when the steady-state configuration, i.e. “convergence” of the eigenvalue \(k\), has not been achieved yet, this analog technique may suffer from a highly fluctuating number of source particles, particularly if the initial guesses for the eigenvalue \(k\) and the eigenvector neutron distribution are poorly chosen. This possible issue can be avoided by performing population control (applying one of the identified PCTs) to the normalized fission bank so that the resulting source bank is well controlled regardless of the convergence of the eigenvalue \(k\).

It is worth mentioning that the eigenfunction normalization described in the previous paragraphs and the PCT normalization discussed in Sec. II.D.3 serve different purposes. The eigenfunction normalization is a necessary step to ensure that scores accumulated into simulation tallies are not arbitrary in magnitude. On the other hand, PCT normalization is an optional step to preserve the total weight of the initial population passed to the PCT (at the expense of introducing bias, as discussed in Sec. II.D.3). As another clear distinction, the eigenfunction normalization is performed before we apply the PCT, whereas the optional PCT normalization is performed after.

Similar to the PCT application in a time-dependent MC simulation, PCT application in a \(k\)-eigenvalue simulation would also introduce the uncertainty \(\sigma_0[C]\) to the population. However, it should be emphasized that this uncertainty introduced by the PCT is not a bias. There is a well-known bias associated with the method of successive generations (which can be mitigated given a sufficiently large number of
histories per generation). This bias is introduced when the fission bank is normalized, which is in effect regardless of whether population control is applied. The PCT neither enhances nor eliminates this bias; it merely introduces the additional uncertainty $\sigma_C[C_i]$ to the already biased simulation.

In an eigenvalue simulation, how many times population control is performed is determined by the total number of generations, which is typically a very large number (on the order of $10^3$ to $10^9$). This means the uncertainty $\sigma_C[C_i]$ would be introduced by the PCT to the population so many times, which, according to the findings in the previous section, may lead to highly noisy solutions. However, the effect of the uncertainty introduced by the PCT on an eigenvalue simulation is expected to be much less pronounced than that in a time-dependent one. This is because once the eigenvalue convergence is achieved, we essentially simulate a steady-state system where the ratio $N/M$ is expected to be around and close to unity, in which most PCTs introduce minimum uncertainties, as shown in Fig. 9. Nevertheless, some PCTs (SS and COX) still introduce considerably high uncertainties even with $N/M \approx 1$. In this section we would like to investigate the relative performances of the identified PCTs in a $k$-eigenvalue transport calculation. In particular, we would like to see whether there is any discernible effect due to the different magnitudes of uncertainty $\sigma_C[C_i]$ introduced by the techniques.

We consider the $k$-eigenvalue transport problem of the mono-energetic two-region slab medium from Ref. 30:

$$\left[\mu \frac{\partial}{\partial x} + \Sigma_r(x)\right] \psi(x, \mu) = \frac{1}{2} \left[ \Sigma_v(x) + \frac{1}{k} \nu \Sigma_r(x) \right] \phi(x),$$

Similar to Sec. V, all physical quantities will be presented in the unit of mean free path. The first and the second regions respectively occupy $x \in [0, 1.5]$ and $x \in [1.5, 2.5]$. The cross sections of the two regions are $\nu \Sigma_{r1} = 0.6$, $\Sigma_v = 0.9$, $\nu \Sigma_{r2} = 0.3$, and $\Sigma_v = 0.2$. Finally, the two-region slab is subject to vacuum boundaries. By using a deterministic transport method, Kornreich and Parsons 30 provide reference values for the fundamental $k$-eigenvalue, $k = 1.28657$, and the associated scalar fluxes at certain points (shown in Fig. 19).

The $k$-eigenvalue problem is solved using the analog (without population control) weight normalization technique and the five identified PCTs (SS, SR, CO, COX, and DD). The numbers of inactive and active generations are set to be 100 and 200, respectively, with $10^5$ neutron histories per generation. We tally the spatial-average neutron flux $\phi_j$ with $J = 50$ uniform meshes spanning $x \in [0, 2.5]$. Uniform isotropic flux distribution and $k = 1$ are used as the initial guess. Finally, each simulation is repeated 50 times with different random number seeds and run on 36 distributed-memory processors. The solution of each run is verified by comparing it with the reference solution shown in Fig. 19.

Three performance metrics are considered: (1) averaged sample standard deviation of the scalar flux $\bar{\sigma}[\phi]$ [see Eq. (28)], (2) sample standard deviation of the eigenvalue $\sigma[k]$, and (3) total run time. The resulting performance metrics of the different PCTs are compared in jittered box plots shown in Fig. 20.

The analog weight normalization technique is expected to have the least noisy solution. This is because, unlike the PCTs, the analog technique does not introduce any additional uncertainty to the population. The comparison presented in Fig. 20 helps in identifying the cost of performing population control (via one of the PCTs) instead of the analog weight normalization technique.

Figure 20a compares the scalar flux–averaged sample standard deviations $\bar{\sigma}[\phi]$ and the eigenvalue sample standard deviations $\sigma[k]$. The values are relative to the medians of the analog technique. Comparing $\bar{\sigma}[\phi]$, the image on the left implies that SS yields considerably larger noise to the simulation, which makes $\bar{\sigma}[\phi]$ about 8.5% larger than the analog case. A discernible increase in $\bar{\sigma}[\phi]$ is also found in COX, but only about 2%. The other PCTs (DD, SR, and CO), however, do not really suffer from an increase in $\bar{\sigma}[\phi]$. These findings are in agreement with the theoretical uncertainty introduced by the PCTs shown in Fig. 9. A similar trend can be observed in the image on the right that compares $\sigma[k]$, but it is not as pronounced since the data are
widely fluctuating. This high fluctuation in $\sigma[k]$ can be reduced by increasing the number of active generations or the number of particle histories per generation. We note that given the current configuration (200 generations, $10^5$ particles/generation), the median of $\sigma[k]$ of the analog technique is 400.3 pcm, where the associated standard deviation of the expected mean is 28.3 pcm.

From the left image in Fig. 20b, it is shown that SS runs much slower than the other PCTs as it suffers from its serial particle sampling. DD also suffers from a serial sampling; but different from SS, the serial sampling of DD only needs to be done $|N - M|$ times, which is close to zero throughout the active generations of the simulation. This makes DD significantly faster than SS. On the other hand, SR, CO, and COX benefit from their embarrassingly parallel sampling procedures, which make them the fastest among the PCTs. Although not performing any population control, the analog case still spends an amount of time as it still needs to perform the bank passing procedure (Algorithm 2). Finally, the image on the right of Fig. 20b demonstrates that fission bank handling and population control take a considerable portion of the total simulation run time (about 9% for SS and 3% for the other PCTs), which is enough to make SS about 10% slower than the analog case, while the other PCTs are just about 1.5% to 3% slower.

Finally, Figure 20c compares the resulting FOMs of the PCTs. The FOM follows the definition in Eq. (29). It is found that SS, the simplest yet the most well-known technique for $k$-eigenvalue simulation, is the least performing PCT having a FOM about 24% lower than the analog technique. On the other hand, SR, CO, and DD are the best PCTs with FOMs about 2% to 4% lower. However, it is worth mentioning that the discernible decrease in the FOMs of SR, CO, and DD is due to their higher run times (right image of Fig. 20b) since their sample standard deviations (Fig. 20a) are about the same as the one with the analog technique. The higher run times of the PCTs can be hidden should we run the simulations with a sufficiently large number of particles per processor. In such a situation, SR, CO, and DD would be as performant as the analog technique.

VII. CONCLUSION

An extensive study of PCT for time-dependent and eigenvalue MC neutron transport calculations is presented. We define PCT as a technique that takes a censused population and returns a controlled, unbiased one. A new perspective based on an abstraction of particle census and population control is explored, paving the way for improved understanding and application of the concepts. We discuss how different kinds of census, e.g., time, fission, and collision censuses, are performed in time-dependent and eigenvalue problems. We also discuss the requirements and desirable characteristics of a PCT.

Identified from the literature, five distinct PCTs are reviewed: SS, SR (Ref. 4), CO (Ref. 15), COX (Ref. 10), and DD (Ref. 3). While SS has been the typical procedure of choice for handling fission bank in MC eigenvalue simulations, the other four techniques have been almost exclusively applied for time-dependent simulations. The review encompasses the basic procedures of the techniques, the significance of their sampling bases (uniform, weight based, and importance based), the bias in PCT weight normalization, the possible correlation issue in CO, the thorough characterization of the recently introduced COX, and the relation to the more advanced PCTs (Refs. 15 and 19). Short remarks about the five PCTs, highlighting their respective caveats, are summarized in Table II.

A theoretical analysis of the uncertainty introduced to the population by each of the PCTs is presented. The resulting theoretical uncertainties (shown in Fig. 9) are useful not only for theoretically assessing the relative performance of the PCTs, but also for numerically verifying whether the techniques are appropriately implemented. It is found that CO and SR are equally the most performing techniques based on this metric (smallest uncertainty introduced), followed by DD and then COX, while SS introduces the largest uncertainty. We hypothesized that this uncertainty would proportionally affect the simulation tally results, which was later confirmed when we ran the test problems using the different PCTs.

Parallel algorithms for the five PCTs are proposed. The algorithms are based on a generalized version of the parallel fission bank algorithm and designed to be applicable for both eigenvalue and time-dependent simulations. The use of abstract base class for streamlined implementations of the five PCTs is also suggested. Weak scaling results of the PCTs are performed to demonstrate the parallel scalability of the techniques. It is found that SS and DD have limited scalabilities due to their respective significant serial sampling procedures.

Supercritical and subcritical time-dependent test problems based on the analytical benchmark AZURV1 (Ref. 28) were devised. We found that these test problems serve as a good benchmark suite for verifying the time-dependent features of a MC code. With the test problems we not only compared the relative performances of the PCTs, but also demonstrated typical behaviors of the PCTs in supercritical and subcritical problems as a function of
(a) (Left) averaged sample standard deviation of the scalar flux and (Right) sample standard deviation of the eigenvalue. The values are relative to the median of the analog technique.

(b) (Left) Runtime spent in population control and managing particle fission bank and (Right) total runtime.

(c) Figure of merit. The values are relative to the median of the analog technique.

Fig. 20. Performance metrics of different PCTs for the $k$-eigenvalue test problem. Magenta line indicates median; box indicates lower $Q_1$ and upper $Q_3$ quartiles; lower and upper whiskers indicate minimum and maximum values that are not outliers (within the range $[Q_1 - 1.5IQR, Q_3 + 1.5IQR]$, where $IQR = Q_3 - Q_1$).
census frequency. Two performance metrics were considered, total run time and averaged sample standard deviation of the scalar flux, which are aggregated into FOMs. Similar analysis was performed for a \( k \)-eigenvalue test problem. We found that SR and CO are equally the most performing PCTs, closely followed by DD and then COX.

The results of the time-dependent and \( k \)-eigenvalue test problems demonstrated the superiority of SR and CO. However, that does not mean that everyone should be confident in using one of these techniques in all of their MC simulations. This is particularly true since there is a caveat for each of the PCTs, as summarized in Table II. The proposed generalized and streamlined PCT algorithm offers MC code developers a minimally invasive way to implement all of the PCTs into their code and allows the code users to pick the technique themselves. Finally, it is worth mentioning that the proposed PCT parallel algorithm can be generally applied to other MC eigenvalue simulations, such as \( c \)-eigenvalues\(^{23} \) and \( \alpha \)-eigenvalues.\(^{31} \)

Future work includes implementing the generalized parallel PCT algorithm into a production MC code and assessing the relative performances of the PCTs in simulating more practical, multidimensional, continuous-energy problems. Additionally, investigating the interplay between the PCT and VRT, which is briefly discussed in Sec. II.D.1, can be a potential future work. Finally, a recent analysis of neutron clustering in \( k \)-eigenvalue transport calculation demonstrates that sampling source sites without replacement (which is a variation of DD) versus with replacement (which is SS) can greatly reduce the degree of clustering.\(^{32} \) Studying how the different PCTs (particularly those that are not included in Ref. 32, i.e., SR, CO, and COX) affect the clustering phenomenon can be a potential future work as well.

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