APPLICATION OF N-SPHERE MONTE CARLO TO TOY PROBLEMS IN RELIABILITY ANALYSIS

A THESIS SUBMITTED IN PARTIAL FULFILMENT OF THE

REQUIREMENTS FOR THE DEGREE OF

MASTER OF TECHNOLOGY

IN

FACULTY OF ENGINEERING

BY

PRASHANT ANIL JADHAO

M.TECH IN COMPUTATIONAL AND DATA SCIENCE

INDIAN INSTITUTE OF SCIENCE

UNDER THE SUPERVISION OF

PROF. MURUGESAN VENKATAPATHI

DEPARTMENT OF COMPUTATIONAL AND DATA SCIENCES

INDIAN INSTITUTE OF SCIENCE

Declaration of Originality

I, **Prashant Anil Jadhao**, with SR No. **06-18-01-10-51-23-1-22432** hereby declare that the material presented in the thesis titled

Application of n-Sphere Monte Carlo to Toy Problems in Reliability Analysis

represents original work carried out by me in the **Department of Computational and Data Sciences** at **Indian Institute of Science** during the years **2023-2025**.
With my signature, I certify that:

- I have not manipulated any of the data or results.
- I have not committed any plagiarism of intellectual property. I have clearly indicated and referenced the contributions of others.
- I have explicitly acknowledged all collaborative research and discussions.
- I have understood that any false claim will result in severe disciplinary action.
- I have understood that the work may be screened for any form of academic misconduct.

Date: 26.06.2025

Jadhao.
Student Signature

In my capacity as supervisor of the above-mentioned work, I certify that the above statements are true to the best of my knowledge, and I have carried out due diligence to ensure the originality of the report.

murugesan V
Advisor Signature

Advisor Name:
Prof. Murugesan Venkatapathi

DEDICATED TO

My beloved grandfather

who has always been my inspiration.

Acknowledgements

I would like to express my profound gratitude to my guide, Prof. Murugesan Venkatapathi, for his exceptional guidance, constant encouragement, and invaluable insights throughout my M.Tech journey. His expertise in computational methods and patient mentoring have been instrumental in shaping this research. I am deeply thankful for the intellectual freedom he provided, allowing me to explore diverse approaches while keeping me focused on the core research objectives. His mentorship has profoundly influenced my approach to research and problem-solving.

I extend my sincere appreciation to Prof. Manohar C.S. for his constructive feedback. His expertise helped strengthen the methodological aspects of this work.

A special acknowledgment goes to Abhijeet Jawalekar, whose collaboration and technical discussions were invaluable during the development of the algorithms presented in this thesis. His insights into N-sphere Monte Carlo methods significantly contributed to overcoming key computational challenges.

I am grateful to Dr. Rajesh Sharma for his assistance in clarifying fundamental concepts in computational methods and reliability theory, which helped solidify the theoretical foundations of this research.

I would like to thank all my friends and lab mates who made this journey memorable and enriching. The numerous discussions, both academic and casual, contributed significantly to my growth during these years.

Finally, I express my deepest gratitude to my parents for their unwavering belief and constant encouragement throughout my academic journey. Their support has been my strength. I am also thankful to my sister and brother-in-law for their invaluable support during my stay in Bengaluru, making it feel like a home away from home.

Abstract

Monte Carlo methods are widely employed for high-dimensional integration and its application to structural reliability analysis. These methods utilize random sampling to estimate integrals/volumes and failure probabilities, yet encounter significant computational challenges as the number of dimensions/parameters increases. Traditional numerical quadrature approaches suffer from slow convergence rates and exponential growth in computational cost, rendering them inefficient in high-dimensional spaces. Markov Chain Monte Carlo (MCMC) methods exhibit $O(n^5)$ scaling for smooth, convex bodies but face convergence difficulties in non-convex and non-smooth domains. Quasi-Monte Carlo methods provide enhanced convergence properties but may not be suited for geometries that are not n-orthotopes (cuboids in 3D).

The n-Sphere Monte Carlo (NSMC) method addresses these limitations through a fundamentally different approach. NSMC employs one-dimensional line integrals along random directions combined with a volume transformation. This methodology remains agnostic to domain boundary shape and surface roughness while achieving favorable $O(n^3)$ scaling with dimension n, when the distribution of extents of the domain is fixed. One can use the naive NSMC method for reliability analysis, estimating failure probabilities by uniformly sampling points within the domain's extents and evaluating the limit state function $g(x)$ at these sampled points. This method is agnostic to the domain's size and roughness, making it suitable for estimating volumes of distributed failure regions in the domain with varied geometries. This work presents two key contributions:

Adaptive offset NSMC : that changes the origin of NSMC sampling based on identification of clusters of failure samples in the domain. This clustering can be adaptively concentrate samples around the failure region and reducing variance in the failure estimation.

Random Walk-NSMC Variants : We introduce NSMC variants based on a Deterministic Walk and a Random Walk that leverage Markov chain principles enabling accurate estimation of failure probabilities with significantly fewer samples, particularly in high-dimensional spaces where traditional techniques become computationally prohibitive. Here the origin of the NSMC sampling is shifted based on selected criterion among the samples as in the Markov Chain

methods. While a walk in the origin of the NSMC sampling helps achieve a quicker convergence to a stationary probability density of sampling, the original flexibility of NSMC in estimating volumes using its simple formula i.e. of arbitrary disconnected failure regions is retained.

Acronyms

MCMC	Markov Chain Monte Carlo
NSMC	N-Sphere Monte Carlo
FEA	Finite Element Analysis
$\hat{\mathbf{s}}$	Unit vector in arbitrary direction
θ	Planar angle
$\tilde{\epsilon}$	Relative root mean squared error
$\zeta[\cdot]$	Coefficient of variation
f_R	Distribution of length of extents
$i(\hat{\mathbf{s}})$	Partial line integral in direction $\hat{\mathbf{s}}$
N	Number of extent samples
n	Number of dimensions
S^{n-1}	Surface of n-dimensional unit sphere
V_K	Volume of domain K
$R(\hat{\mathbf{s}})$	Length of extent in $\hat{\mathbf{s}}$ direction

Contents

List of Figures

List of Tables

Chapter 1

Introduction

High-dimensional integration represents a fundamental computational challenge in reliability analysis across multiple engineering domains. Traditional numerical integration methodologies face significant barriers when operating in spaces $\gtrsim 10$, a phenomenon widely recognized as the "curse of dimensionality." This computational bottleneck manifests as an exponential increase in complexity with each additional dimension, rendering conventional deterministic quadrature schemes computationally intractable for many practical engineering reliability assessments.

The reliability analysis of complex engineered systems often involves evaluation of failure probabilities in the presence of multiple interacting variables and failure modes. As engineering systems become more sophisticated, the dimensionality of these problems continues to increase, creating an urgent need for efficient computational approaches capable of handling high-dimensional spaces.

1.1 Motivation

In reliability engineering, the probability of failure is mathematically expressed as:

$$P_f = \int_{g(\mathbf{x})\leq 0} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \tag{1.1}$$

where $g(\mathbf{x})$ is the limit state function distinguishing failure from the safe domains of operation, and $f_{\mathbf{X}}(\mathbf{x})$ represents the joint probability density of random variables [8, 24]. This integration problem represents a significant computational challenge, particularly in high dimensions, as noted by Simonovits [27] in his early work on high-dimensional volume computation. Standard Monte Carlo methods [2, 20], while dimension-agnostic for cubic and spherical geometries, converge at a rate of $\mathcal{O}(N^{-1/2})$ [25], making them impractical for rare failure events with probabilities of 10^{-3} to 10^{-6} that are common in high-consequence systems.

A critical challenge in practical reliability analysis is the high computational cost associated with each sample i.e. evaluating the limit state function for the given set of parameters. This demands the even a low probability of failure is identified and estimated using as few samples in the domain as possible. In many engineering applications, each evaluation of $g(\mathbf{x})$ requires an expensive finite element analysis (FEA) [15, 28]. The computational complexity of FEA-based reliability assessment is particularly prohibitive, with a single nonlinear FEA evaluation potentially requiring hours of computation time. This complexity typically scales as $O(n_e^\alpha)$ where n_e is the number of finite elements and α ranges from 1.5 to 3 depending on the solver and problem characteristics [23]. For problems involving complex geometries, material nonlinearities, or time-dependent behavior, this computational burden becomes even more significant. Stochastic finite element methods [13] attempt to address the uncertainty propagation systematically but often introduce additional computational overhead that scales poorly with the number of random variables.

These computational demands make traditional Monte Carlo approaches with hundreds of thousands of samples computationally prohibitive for FEA-based reliability assessment. This necessitates the development of methods that can provide accurate failure probability estimates with substantially fewer limit state function evaluations. Advanced sampling techniques like importance sampling [3] and subset simulation [4, 5] attempt to improve efficiency but struggle in high dimensions due to sample sparsity. As documented by Tabandeh et al. [30] in their comprehensive review, importance sampling approaches can dramatically reduce variance, but constructing an effective importance sampling density becomes increasingly challenging as dimensionality increases. Similarly, while subset simulation methods [4] have proven effective for many reliability problems, they may face challenges with complex failure domains in very high dimensions. These limitations parallel the broader challenges in high-dimensional integration identified by researchers in computational geometry [22, 11], where even approximating volumes of simple convex bodies becomes computationally intractable beyond moderate dimensions.

Metamodeling approaches such as polynomial chaos expansions [29, 6] and Kriging surrogates [12, 9, 26] reduce computational burden by approximating expensive simulations, yet face their own dimensionality challenges in basis function growth and training data requirements. The curse of dimensionality affects these methods as well, with the number of basis functions growing exponentially with dimension in traditional polynomial chaos expansions, and the complexity of fitting accurate Kriging models increasing rapidly with dimension.

Recent computational advances in high-dimensional integration [17, 21] offer promising new approaches for reliability analysis. The n-Sphere Monte Carlo (NSMC) method introduced by Isaac et al. [17] provides a new approach to high-dimensional integration that has been shown

to scale more favorably with dimension compared to traditional MCMC methods for arbitrary geometries. Jawlekar et al. [18] further enhanced this approach through importance sampling techniques, extending its applicability to problems with varying densities. The development of efficient and reliable high-dimensional integration techniques is critical for advancing the state-of-the-art in engineering reliability assessment, particularly for complex engineered systems where failure regions may be highly non-convex and limit state function evaluations are computationally expensive.

1.2 Related Work

The field of high-dimensional integration has seen some recent methodological advances through the n-Sphere Monte Carlo (NSMC) method. Isaac et al. [17] introduced the approach, which decomposes n-dimensional volumes into integrals of weighted n-sphere volumes. Their method overcomes traditional limitations of Markov Chain Monte Carlo (MCMC) approaches [14], particularly in handling boundary roughness and non-convexity. The authors demonstrated that NSMC achieves better efficiency than MCMC for dimensions $n \lesssim 100$, with more favorable scaling properties that may make it particularly suitable for reliability analysis problems.

Abhijeet Jawlekar et al. [18] enhanced the NSMC framework by incorporating importance sampling, specifically addressing challenges in domains with varying and heavy-tailed distributions. Their two-tiered sampling approach, combining inverse f_R sampling with adaptive Metropolis-Hastings algorithms, showed notable improvements over standard NSMC. This integration of importance sampling techniques with NSMC methodology creates a powerful framework that can be adapted to reliability analysis problems.

These developments in NSMC methodology mirror broader advancements in high-dimensional integration and volume computation [27, 22, 11]. The fundamental challenge of efficiently sampling high-dimensional spaces has been addressed through various algorithmic approaches, from the polynomial-time approximation algorithms of Dyer et al. [11] to the hit-and-run mixing techniques of Lovász [21]. These theoretical advances provide a rich foundation for developing specialized methods for reliability analysis.

In the reliability analysis domain, Au and Beck [3, 4] made significant contributions with their adaptive importance sampling schemes and subset simulation approach. Their work on subset simulation [4], further developed with Wang [5], has become a cornerstone of modern reliability analysis for small failure probabilities. Tabandeh et al. [30] provide a comprehensive review of importance sampling methods for reliability analysis, categorizing them into analytical optimization approaches and surrogate-based methods.

These developments in NSMC methodology, particularly the improvements in handling non-

convex domains and the integration of importance sampling, provide a strong avenue for reliability analysis applications. Our proposed algorithmic enhancements, building on these advances, show promise for more efficient and accurate reliability assessments, especially in complex engineering systems where failure regions may have challenging geometric properties. The improved algorithm's ability to handle higher dimensions while maintaining accuracy makes it particularly suitable for modern reliability analysis challenges.

1.3 Contribution

This paper presents advancements in applying the n-Sphere Monte Carlo (NSMC) methodology to reliability analysis problems using realistic toy examples. Our primary objective is to reduce the computational complexity and sample requirements for high-dimensional reliability assessments. We began by implementing a naïve NSMC approach to reliability analysis, which demonstrated promising results but revealed opportunities for further optimization in handling complex failure domains.

Our first algorithmic innovation, Offset-NSMC with clustering, enhances performance by strategically decomposing the failure domain into distinct regions. This approach identifies natural clusters within the failure points using unsupervised learning algorithms (K-means or DB-Scan), then applies separate NSMC estimations centered at each cluster's centroid. By focusing computational resources on regions with high failure concentration, this method achieves more efficient exploration of the failure domain, particularly beneficial for problems with disconnected or irregularly shaped failure regions. The final failure probability is computed by combining results from these separate estimations, weighted appropriately by their respective domain volumes.

Building on these insights, we developed two advanced sampling strategies that further improve efficiency: Deterministic-Walk-NSMC and Random-Walk-NSMC. The Deterministic-Walk approach employs a systematic exploration strategy where the origins of the NSMC sampling shift deterministically only to failure points, thereby concentrating samples in critical regions while maintaining statistical rigor. In contrast, Random-Walk-NSMC introduces a probabilistic transition mechanism between sampling centers based on the values of the limit state functions evaluated at each sample point, creating an adaptive Markov process that naturally gravitates toward regions with higher failure probability density. Our experimental evaluation demonstrates that these algorithmic innovations lead to significant reductions in required sample size—often by orders of magnitude compared to conventional Monte Carlo methods—while maintaining or improving estimation accuracy across a range of high-dimensional reliability problems.

1.4 Outline of the Report

The report is structured as follows:

- Chapter 2. **Problem Formulation and n-Sphere Monte Carlo Methodology**
  This chapter establishes the mathematical foundations for reliability analysis and introduces the n-Sphere Monte Carlo (NSMC) methodology as our proposed solution to high-dimensional integration challenges. We define limit state functions and failure probability estimation, then explain how NSMC decomposes n-dimensional volumes into integrals of weighted n-sphere volumes. Building on work by Isaac, A., Jawlekar, A. & Venkatapathi, M. [17], we demonstrate how this approach efficiently handles non-convex failure domains and overcomes limitations of traditional Monte Carlo methods in high-dimensional reliability analysis.

- Chapter 3. **Methodology: Novel Algorithms for Reliability Assessment**
  We present our methodological contributions with three novel algorithms: Cluster-Based NSMC for handling disconnected failure regions, Deterministic-Walk-NSMC that strategically shifts sampling centers to failure points, and Random-Walk-NSMC with a probabilistic transition mechanism based on limit state function values. For each algorithm, we provide theoretical foundations and implementation strategies.

- Chapter 4. **Experimental Results**
  In this chapter, we evaluate our proposed algorithms on benchmark reliability problems with varying dimensions and failure domain geometries. We conduct a comparative analysis among the different NSMC variants we developed: Naive NSMC, Offset NSMC, Deterministic Walk NSMC, and Random Walk NSMC. Our experiments quantify the progressive improvements in accuracy, sample efficiency, and convergence behavior across different dimensional ranges. We demonstrate how each algorithmic enhancement addresses specific limitations of its predecessors, with particular focus on performance in high-dimensional spaces and the ability to detect rare failure events. The results validate our theoretical predictions regarding dimensional scaling and computational efficiency.

- Chapter 5. **Conclusion & Future Work**
  Finally, we summarize our contributions to reliability analysis through NSMC enhancements and discuss their significance. We identify limitations of current approaches and outline promising research directions, including extensions to higher dimensions, integration with meta-modeling techniques, and applications to time-dependent reliability analysis.

Chapter 2

Preliminaries

2.1 Reliability Analysis Fundamentals

Reliability analysis is fundamentally concerned with estimating the probability of failure in complex engineering systems [24]. This involves calculating the probability that a system will fail to perform its intended function under specified conditions over a defined period [8]. The failure event is typically defined through a limit state function $g(\mathbf{x})$, where $\mathbf{x}$ represents the vector of random variables characterizing the system.

2.1.1 Problem Formulation

2.1.1.1 Response Function

Let us consider a system where failure is characterized by the exceedance of a critical response variable Y over a threshold γ. The response variable is determined by:

$$Y = g(\mathbf{X}) \tag{2.1}$$

where $\mathbf{X} = [X_1, \ldots, X_n]$ represents the input random variables with joint probability density function $f(\mathbf{x})$.

2.1.1.2 Failure Probability Definition

The failure probability is formally defined as :

$$P(F) = P(Y > \gamma) = \int_F f(\mathbf{x}) d\mathbf{x} \tag{2.2}$$

where F represents the failure region:

$$F = \{\mathbf{x} : g(\mathbf{x}) > \gamma\} \tag{2.3}$$

2.1.2 Equivalent Formulations

The above formulation can be equivalently expressed in terms of a limit state function [24]. If we define a limit state function $G(\mathbf{x}) = \gamma - g(\mathbf{x})$, then failure occurs when $G(\mathbf{x}) \leq 0$. This gives us the traditional reliability analysis formulation:

$$P(F) = P(G(\mathbf{x}) \leq 0) = \int_{G(\mathbf{x})\leq 0} f(\mathbf{x})d\mathbf{x} \tag{2.4}$$

2.1.3 Computation of Failure Probability

The failure probability integral is typically analytically intractable for complex systems with non-linear response functions and correlated random variables. Therefore, various numerical methods are employed:

1. **Monte Carlo Simulation (MCS)** [25, 20]: Generates random samples from $f(\mathbf{x})$ and estimates the failure probability as:

$$P(F) \approx \frac{1}{N}\sum_{i=1}^{N} I[g(\mathbf{x}_i) > \gamma] \tag{2.5}$$

   where $I[\cdot]$ is the indicator function and N is the number of samples.

2. **FORM/SORM** [16, 7]: First/Second Order Reliability Methods approximate the failure boundary with linear or quadratic surfaces after transforming to standard normal space.

3. **Importance Sampling** [3]: Improves efficiency by sampling from a distribution that focuses on the failure region:

$$P(F) = \int_F \frac{f(\mathbf{x})}{h(\mathbf{x})}h(\mathbf{x})d\mathbf{x} \approx \frac{1}{N}\sum_{i=1}^{N} I[g(\mathbf{x}_i) > \gamma]\frac{f(\mathbf{x}_i)}{h(\mathbf{x}_i)} \tag{2.6}$$

   where $h(\mathbf{x})$ is an importance sampling density. As reviewed by Tabandeh et al. [30], the effectiveness of importance sampling depends critically on the choice of the importance sampling density.

4. **Subset Simulation** [4, 5]: Decomposes the failure probability into a product of larger conditional probabilities that can be estimated more efficiently using Markov Chain Monte Carlo sampling techniques:

$$P(F) = P(F_1) \prod_{i=1}^{m-1} P(F_{i+1}|F_i) \tag{2.7}$$

where $F_1 \supset F_2 \supset \ldots \supset F_m = F$ is a sequence of nested failure events.

2.2 Monte Carlo Integration Method

The Monte Carlo integration method provides a probabilistic approach to volume estimation and integration [2, 25]. This section presents the theoretical foundation and implementation methodology.

2.2.1 Theoretical Framework

Consider a bounded region $\Omega \subset \mathbb{R}^d$ enclosed within a hypercube of side length a. The Monte Carlo method estimates the volume through the following steps [25, 20]:

1. **Domain Bounding**: The region Ω is enclosed within a n-dimensional hypercube $[-a, a]^n$ where:

$$V_{\text{hypercube}} = (2a)^n \tag{2.8}$$

2. **Uniform Sampling**: Generate N independent random points $\{x_i\}_{i=1}^N$ distributed according to:

$$x_i \sim \text{Uniform}([-a, a]^n) \tag{2.9}$$

3. **Volume Estimation**: The volume is estimated through the ratio:

$$A = \frac{\text{Number of points in } \Omega}{\text{Total number of points}} \times a^n \tag{2.10}$$

2.3 The Curse of Dimensionality

The volume ratio between an n-dimensional unit sphere and its circumscribing unit hypercube provides crucial insight into sampling efficiency [27]:

$$\frac{V_{\text{sphere}}}{V_{\text{cube}}} = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2} + 1)} \tag{2.11}$$

For large dimensions n, this ratio approximates to [27, 11]:

$$\frac{V_{\text{sphere}}}{V_{\text{cube}}} \approx 2^{-n} \tag{2.12}$$

The implications include [27, 22]:

- Exponential growth in required sample points
- Rapidly decreasing sampling efficiency
- High proportion of wasted samples
- Computational overhead scaling with 2^n

2.4 n-Sphere Monte Carlo Integration

2.4.1 Problem Formulation

Consider a function h defined over an arbitrary domain characterized by an extent density function [17]. The objective is to estimate the integral of h over this domain, with volume estimation representing the special case where $h = 1$ throughout the domain.

2.4.2 Spherical Coordinate Integration

In spherical coordinates, with r representing the radial coordinate and $d\hat{S}$ denoting the surface element of the unit sphere, the integral takes the form [17, 18]:

$$I = \oint_{S_{n-1}} \int_0^{R(\hat{S})} r^{n-1} h(r\hat{S})\, dr\, d\hat{S} \tag{2.13}$$

For any given direction $\hat{S}$, the partial integral $i(\hat{S})$ is defined as:

$$i(\hat{S}) = \int_0^{R(\hat{S})} r^{n-1} h(r\hat{S})\, dr \tag{2.14}$$

2.4.3 Integral over Arbitrary Domain

The complete integral over the arbitrary domain can be expressed in terms of the partial integral $i(\hat{S})$ [17]:

$$I = \oint_{S_{n-1}} i(\hat{S})\, d\hat{S} = s_n \mathbb{E}[i(\hat{S})] \tag{2.15}$$

For the special case where $h(r\hat{S}) = 1$, the volume computation becomes [17, 18]:

$$V = \frac{s_n}{n} \int_{R_{min}}^{R_{max}} r^n f_R(r)\, dr = v_n \mathbb{E}[R^n] \tag{2.16}$$

where the volume coefficients v_d are given by [17]:

$$v_n = \left(2, \pi, \frac{4}{3}\pi, ..., \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}\right) \tag{2.17}$$

2.5 Comparison of Computational Methods for High-Dimensional Integration

Before examining specific algorithmic innovations, it is important to understand the computational scaling properties of various integration methods when applied to reliability analysis. The efficiency of these methods varies significantly with dimensionality, domain characteristics, and the nature of the integrand function [27, 5, 22].

Traditional analytical methods, while dimension-independent, are severely restricted to simple domains and integrands with closed-form solutions [1, 19]. Conventional numerical integration techniques face exponential computational growth with increasing dimensions—the fundamental manifestation of the curse of dimensionality [27]. Several specialized approaches have emerged to address these challenges, each with its own computational characteristics and domain applicability [22, 11, 5].

Table 2.1 summarizes the computational scaling properties of different integration methods, highlighting their domain restrictions and dimensional scaling behavior. This comparison reveals why specialized approaches like the n-Sphere Monte Carlo method are particularly promising for high-dimensional reliability analysis [17, 18].

Table 2.1: Comparison of Computational Scaling for High-Dimensional Integration Methods

Estimation Method	**Domain/Integral Applicability**	**Computational Complexity**
Analytical Integration	Closed-form expression of integral and standard domain	Dimension-independent
Numerical Quadrature [19]	Any domain with defined boundaries	Exponential with dimension
Monte Carlo Integration [25]	Any domain with probability density	$O(N)$ computation with error $O(N^{-1/2})$
Markov Chain Monte Carlo [14]	Smooth convex domains	$O(n^5)$ mixing time for convex bodies [11]
Quasi-Monte Carlo [20]	Low effective dimensionality in cubical domain	$O(N)$ computation with error $O(N^{-1})$
Adaptive n-Sphere Monte Carlo [17]	Fixed extent density domains	$O(n^3)$ with enhanced sampling strategies
Subset Simulation [5]	Rare event simulation	$O(n^4)$ with increasing complexity in high dimensions

Chapter 3

Methodology: Algorithms for Reliability Analysis

Building upon the foundation established in the introduction chapter, we know high-dimensional integration or volume estimation remains a central challenge in computational reliability analysis. The theoretical complexity of volume computation [27, 11] directly impacts failure probability estimation, particularly when combined with computationally intensive finite element simulations that scale as $O(n_e^\alpha)$ [23].

While traditional reliability methods have evolved from basic Monte Carlo sampling to more sophisticated techniques including subset simulation [4] and importance sampling [30], they continue to face efficiency challenges in high-dimensional spaces. The recently developed n-Sphere Monte Carlo (NSMC) method [17] offers improved dimensional scaling by decomposing integration into radial and angular components, providing the foundation for our proposed algorithms specifically tailored for reliability analysis.

Our work extends these approaches to address the computational challenges of high-dimensional reliability problems, particularly those involving expensive limit state function evaluations, by strategically focusing computational resources on critical regions of the probability space.

3.1 Naive NSMC for Reliability Analysis

The naive implementation of NSMC for reliability analysis provides a foundation for estimating failure probabilities in high-dimensional spaces. It leverages the fundamental principle of decomposing volume integrals into weighted spherical coordinates to enhance computational efficiency over traditional Monte Carlo methods.

The reliability analysis problem requires estimation of the failure probability P_f:

$$P_f = \int_{g(\mathbf{x}) \leq \gamma} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \tag{3.1}$$

where $g(\mathbf{x})$ is the limit state function, γ is the failure threshold, and $f_{\mathbf{X}}(\mathbf{x})$ is the joint probability density function.

3.1.1 Volume-Based Formulation

The NSMC framework reformulates this as a volume estimation problem by partitioning the reliability space into failure domains (Ω_f) and safe (Ω_s) domains:

$$\Omega_f = \{\mathbf{x} : g(\mathbf{x}) \leq \gamma\}, \quad \Omega_s = \{\mathbf{x} : g(\mathbf{x}) > \gamma\} \tag{3.2}$$

Using the spherical coordinate framework from Section 2.4, the failure volume becomes:

$$V_f = v_n \mathbb{E}[R^n \cdot I_{g(R\hat{S}) \leq \gamma}] \tag{3.3}$$

where $I_{g(R\hat{S}) \leq \gamma}$ is the indicator function for the failure domain.

The failure probability is estimated as the volume ratio:

$$\hat{P}_f = \frac{V_f}{V_f + V_s} \tag{3.4}$$

where both volumes are computed through radial sampling with the indicator function determining failure versus safe contributions.The fundamental insight is that, rather than directly sampling the failure probability, the NSMC method estimates the relative volumes of failure and safe regions, from which the failure probability naturally emerges as the ratio of these volumes.

3.1.2 Implementation Strategy

The algorithm 1 proceeds as follows :

1. Initialize the sampling center at a predefined origin $\mathbf{c}_0$ (initial center point)
2. Sample a unit random direction and extent along that direction
3. Sample a point $\mathbf{x}_i$ on this extent with uniform distribution
4. Based on the point's classification:

- If failure ($g(\mathbf{x}_i) \leq \gamma$): Add sampled extent to failure collection
- If non-failure ($g(\mathbf{x}_i) > \gamma$): Add sampled extent to non-failure collection

5. Iteratively update failure and non-failure extent collections until convergence

6. Calculate failure probability as the ratio of average volumes:

$$\hat{P}_f = \frac{\bar{V}_f}{\bar{V}_f + \bar{V}_s} \tag{3.5}$$

where $\hat{P}_f$ is the estimated failure probability, $\bar{V}_f$ is the average failure volume, $\bar{V}_s$ is the average non-failure volume .

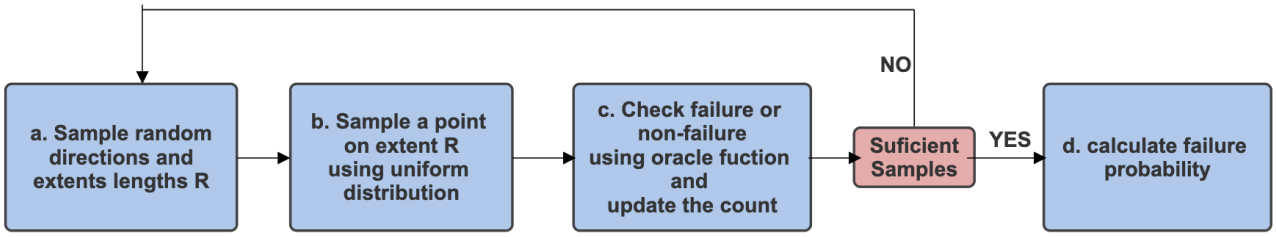


Figure 3.1: Naive-NSMC for reliability analysis

The theoretical foundation of this approach draws on the spherical decomposition of integrals explored by computational geometers [1, 19], but tailored specifically for reliability analysis applications.

3.2 Offset NSMC with Clustering

The Offset NSMC with Clustering algorithm enhances the naive approach by adaptively identifying and leveraging the geometric structure of the failure domain. By clustering failure points and performing targeted sampling within each cluster, this method significantly improves efficiency for problems with complex or disconnected failure regions. The detailed implementation of this algorithm is presented in Algorithm 2.

The Offset NSMC with Clustering algorithm introduces two key approaches:

1. **Clustering based Offsets**: Instead of sampling the entire domain from a single origin, we sample clusters centered at strategic offset points, focusing sampling efforts where failure regions are more likely to exist.

2. **Weighted clustering**: Each cluster's centroid is calculated using weights based on the limit state function g(x) values for more accurate centroid estimation, positioning centroids closer to failure boundaries for more efficient sampling.

3.2.1 Implementation Strategy

The Offset-NSMC algorithm proceeds through the following steps, as detailed in Algorithm 2:

1. Perform an initial sampling phase to identify potential failure points using naive NSMC

2. Apply clustering algorithms (here K-means) to group failure point

3. For each identified cluster:

   - Set the cluster centroid as the new sampling origin
   - Perform NSMC by sampling the extents from this origin as detailed in 6
   - Compute the local failure probability estimate

4. Combine results from all clusters, weighted by their relative volumes as detailed in 3, to obtain the global failure probability

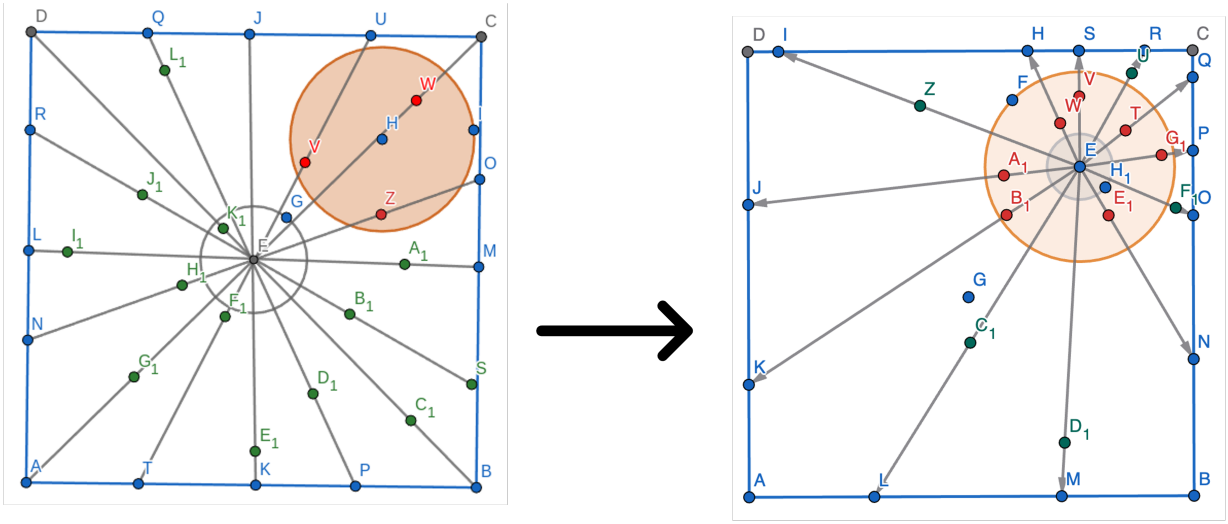


Figure 3.2: Visualization of the Cluster-Based NSMC algorithm. Left: Initial configuration with uniform cluster distribution. Right: Restructured clusters with concentrated sampling in the identified failure region, demonstrating the algorithm's adaptive clustering strategy.

Figure 3.2 shows how the Cluster-Based NSMC algorithm works. At first, clusters are spread evenly around a central point. When the algorithm finds failure regions, it moves clusters to focus sampling around these areas, making exploration of complex spaces more efficient.

The weighted centroid method improves sampling by using limit state function values within each cluster. For each cluster i, the centroid location is calculated as:

$$\text{centroid}_i = \frac{\sum_{k=1}^{N_i} w_{k,i} \cdot x_k}{\sum_{k=1}^{N_i} w_{k,i}} \tag{3.6}$$

where $w_{k,i} = h(g(x_k))$ gives more weight to points closer to the failure boundary. Specifically, we use a weighting function that increases as $|g(x_k) - \gamma|$ decreases, giving maximum weight to points precisely at the failure boundary ($g(x) = \gamma$). This ensures that the cluster centroids naturally migrate toward failure region boundaries, improving the algorithm's efficiency in locating and characterizing these critical regions.

This weighted method is better than simple averaging because it places cluster centers in better positions for sampling. Computing resources are shared equally among clusters. This approach helps the algorithm focus on the most important parts of the parameter space, especially the boundaries between failure and safe regions.

3.3 Deterministic-Walk NSMC

The Deterministic-Walk NSMC algorithm, formalized in Algorithm 4, introduces a deterministic exploration strategy that concentrates samples in the failure region. The sampling center is shifted based on the classification of sampled points:

1. If a point is classified as failure, the sampling center shifts to this point
2. If a point is classified as non-failure, the sampling center remains unchanged

This creates a deterministic walk that gravitates toward and explores the failure region.

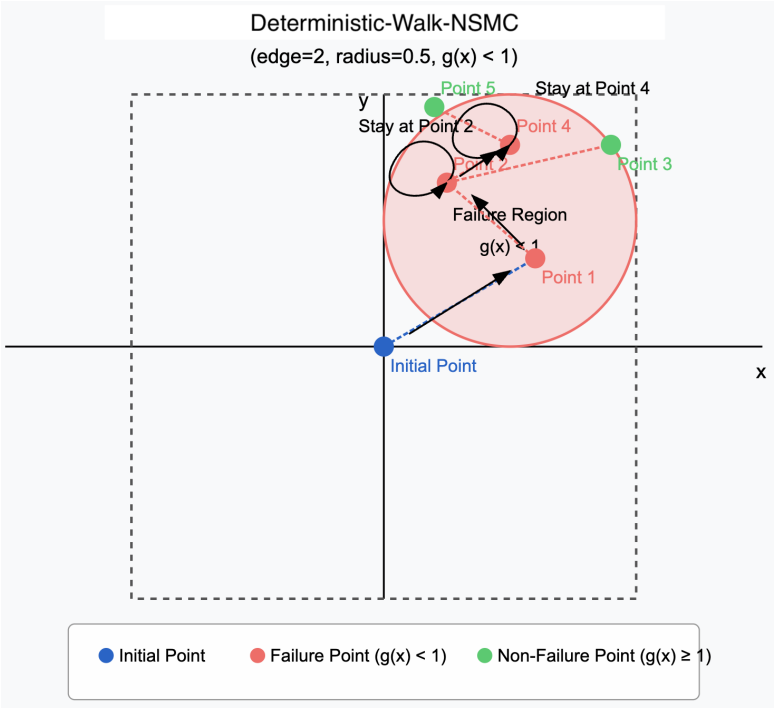


Figure 3.3: Visualization of the Deterministic-Walk-NSMC

3.3.1 Implementation Strategy

The algorithm proceeds as follows:

1. Initialize the sampling center at a predefined origin $\mathbf{c}_0$ (initial center point)
2. Sample a unit random direction and extent along that direction
3. Sample a point $\mathbf{x}_i$ on this extent with uniform distribution and evaluate the limit state function

4. Based on the point's classification:
    - If failure: Add to failure extent collection and use as new center
    - If non-failure: Add to non-failure collection and retain the current center
5. Iteratively update failure and non-failure extent collections
6. Compute the failure probability estimates the ratio of average volumes

3.4 Random-Walk NSMC

The Random-Walk NSMC algorithm, presented in Algorithm 5, incorporates a random walk in the domain based on the values of a limit state function that is assumed to be smoothly varying. This creates an adaptive Markov process that naturally gravitates toward regions with higher failure probability density.

3.4.1 Algorithm Formulation

The probability of shifting to a new sampling point depends on the comparison between the limit state function values at the current and potential new points. Let $g(x_i)$ represent a smooth limit state function value at the current center and $g(x_j)$ the value at a newly sampled point. The probability of shifting the sampling centre is governed by the following rules:

1. If $g(\mathbf{x}_j) < \gamma$: Always move to the new point $\mathbf{x}_j$ (automatically accept points in the failure region)
2. Else if $g(\mathbf{x}_j) > g(\mathbf{x}_i)$: Always stay at the current point $\mathbf{x}_i$ (reject moves to points with higher limit state function values)
3. Else if $\text{random}(0,1) > \left(1 - \frac{g(\mathbf{x}_j)}{g(\mathbf{x}_i)}\right)$: Move to the new point $\mathbf{x}_j$ (probabilistic acceptance)
4. Else: Stay at the current point $\mathbf{x}_i$ (probabilistic rejection)

This random walk ensures that the chain preferentially explores regions where $g(\mathbf{x}) < \gamma$ (the failure region) while still allowing sufficient exploration of the state space. The conditional acceptance probability in rule 3 decreases as $g(\mathbf{x}_j)$ approaches $g(\mathbf{x}_i)$, ensuring a smooth transition behavior near the failure boundary.

3.4.2 Implementation Strategy

The algorithm implementation proceeds as follows:

1. Initialize the sampling center at a predefined origin $\mathbf{c}_0$ (initial center point)
2. Sample a unit random direction and extent along that direction
3. Sample a point $\mathbf{x}_i$ on this extent with uniform distribution and evaluate the limit state function
4. Estimate the probability of shifting the sampling center to the next potential point using random walk rules formulated in 3.4.1

5. Classify and store the sampled extents based on their limit state function value

6. Iteratively update failure and non-failure extent collections until sufficient samples are collected

7. Compute the failure probability estimates the ratio of average volumes

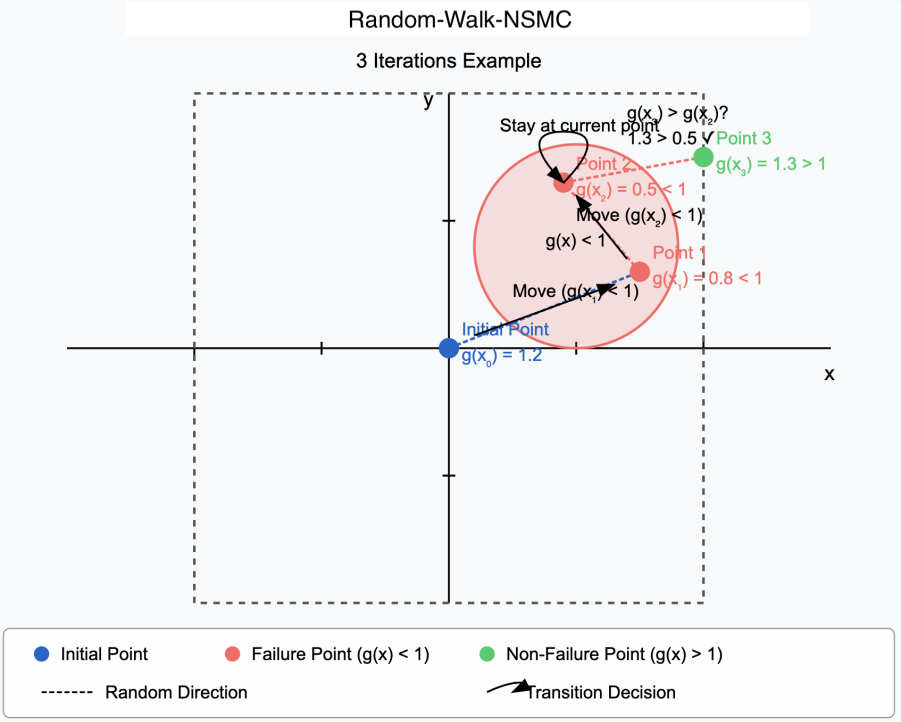


Figure 3.4: Visualization of the Random-Walk-NSMC

The probabilistic transition mechanism based on limit state function values creates an adaptive sampling strategy that outperforms both the naive NSMC and deterministic-walk approaches for many problem types. For the sampling of extent from an offset center, we developed an efficient algorithm detailed in Algorithm 6.

Chapter 4

Experimental Results

In this section, we present a comprehensive evaluation of the proposed n-Sphere Monte Carlo (NSMC) algorithms for reliability estimation. First, we describe the benchmark reliability toy problems used in our experiments. Then, we analyze the performance of each variant of our algorithm individually. Finally, we provide a comparative analysis with summarized tables and graphs highlighting key performance of algorithms

4.1 Benchmark Problems

To evaluate our algorithms, we utilized a set of benchmark problems that allow us to assess algorithm performance under different conditions systematically. Our set of toy problems consisted of:

1. **Spherical Failure Regions**: We implemented spherical failure domains with various radii and origins to test the algorithms' ability to identify and estimate the volumes of the failure regions. These problems provide a controlled setting where analytical solutions are available for validation.

2. **Single and Multiple Failure Regions**: To evaluate the algorithms' performance with varying failure domains, we tested both:

    - Single failure region cases, with a spherical failure domain centered at various offset positions
    - Multiple failure region cases, with two or more non-overlapping spherical failure domains positioned at different locations in the parameter space

3. **Exponential Limit State Function**: We employed the exponential function to represent a smoothly varying limit state function:

$$g(\mathbf{x}) = 2(1 - 2^{-\|\mathbf{x}-\mathbf{x}_c\|/r}) \tag{4.1}$$

where $\mathbf{x}_c$ is the center of the failure region and r is the radius. This function provides a smooth transition across the failure boundary, with the key properties:

- $g(\mathbf{x}) = 0$ at the center of the failure region
- $g(\mathbf{x}) = 1$ exactly at the failure boundary (at distance r from the center)
- $g(\mathbf{x}) > 1$ in the safe region (outside the failure boundary)

We varied parameters of this function to create different test cases, including adjusting the radius r and the offset position $\mathbf{x}_c$ to evaluate algorithm performance under varying conditions.

For the case of two failure regions, the limit state function becomes:

$$g(\mathbf{x}) = 2\left(1 - 2^{-\frac{\|\mathbf{x}-\mathbf{x}_{c1}\|}{r_1}} - 2^{-\frac{\|\mathbf{x}-\mathbf{x}_{c2}\|}{r_2}}\right) \tag{4.2}$$

where $\mathbf{x}_{c1}$ and $\mathbf{x}_{c2}$ are the centers of the two failure regions, and r_1, r_2 are the corresponding radii.

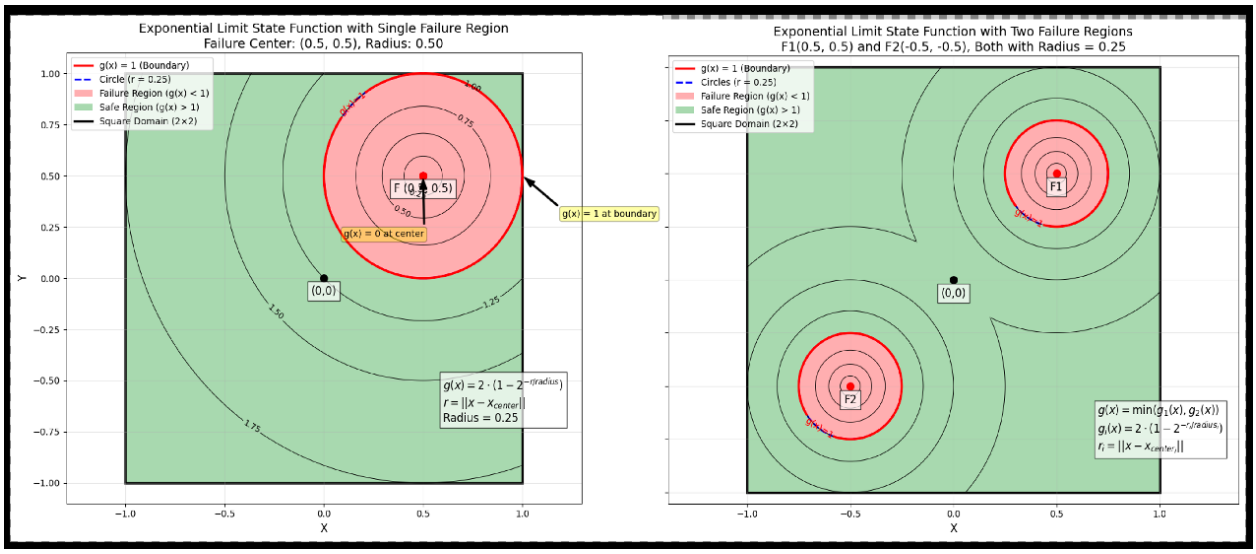


Figure 4.1: Varying Limit State Function Visualization

For each problem type, we systematically varied the dimension from $n = 2$ to $n = 20$ to assess dimensional scaling effects, with particular focus on performance in the critical range of $n = 10$ to $n = 20$ where traditional methods typically begin to deteriorate. All experiments were repeated multiple times to ensure statistical significance of the results. The use of these benchmark problems allowed us to isolate and evaluate specific aspects of our algorithms, including accuracy in failure probability estimation, computational efficiency, and robustness to different failure region configurations.

4.2 Naive n-Sphere Monte Carlo

Our first proposed algorithm is the Naive n-Sphere Monte Carlo method, which leverages the geometric properties of high-dimensional spaces. We conducted experiments with both single and multiple failure regions to evaluate the algorithm's performance across different failure domain configurations.

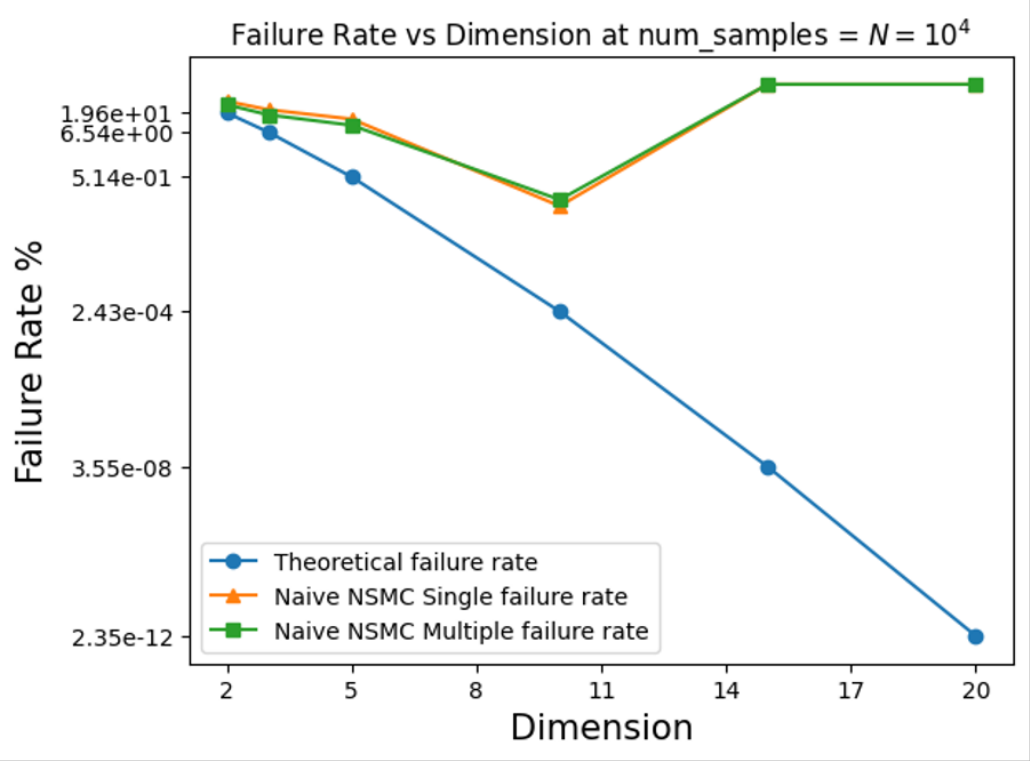


Figure 4.2: Failure rate vs. dimension for $N = 10^4$ samples for Naive n-Sphere Monte Carlo for single and multiple failure regions.

Figure 4.2 validates our Basic n-Sphere Monte Carlo implementation by showing that estimated failure rates match theoretical predictions and remain consistent across single and

multiple failure domains. The algorithm correctly follows the expected exponential decline in failure rates with increasing dimensions. However, beyond dimension 11, estimates diverge from theoretical values due to insufficient samples (10^4) for capturing rare events that reach 10^{-12} probability at dimension 20.

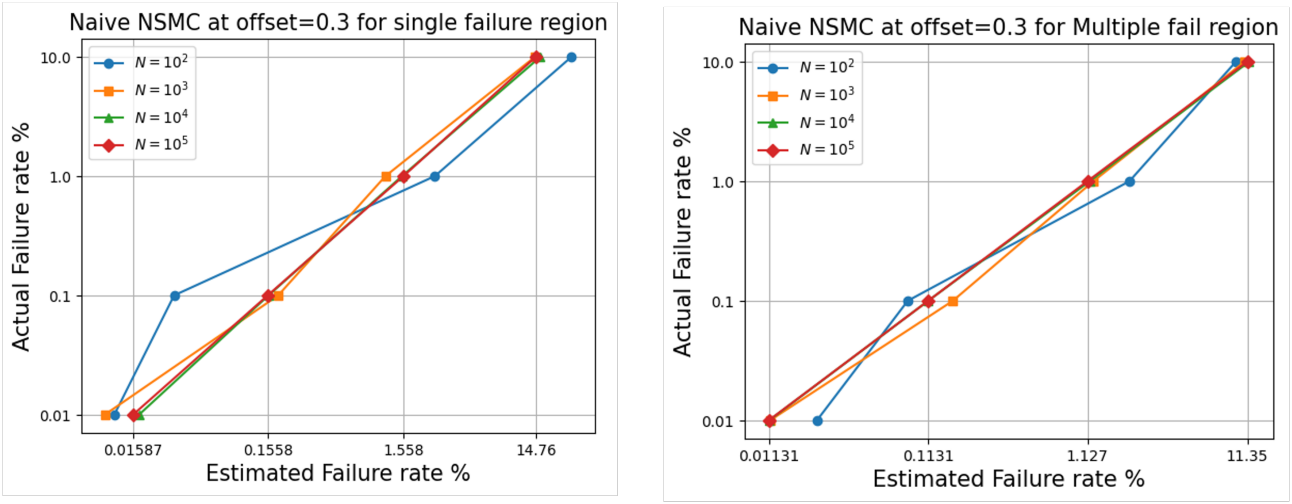


Figure 4.3: Convergence of Naive n-Sphere Monte Carlo for single failure region (left) and multiple failure regions (right) at offset = 0.3 with varying sample sizes.

Figure 4.3 demonstrates convergence behavior as sample sizes increase from $N = 10^2$ to $N = 10^5$. Both single and multiple failure region scenarios show similar convergence patterns, confirming the algorithm's robustness to failure region geometry. The diagonal alignment indicates good correlation between estimated and actual failure rates across probabilities ranging from 0.01% to 10%.

These results confirm that our implementation correctly captures high-dimensional reliability properties regardless of failure domain complexity. However, performance degrades beyond certain dimensional thresholds with fixed sample sizes, motivating our Enhanced n-Sphere Monte Carlo algorithms with clustering.

4.3 Offset n-Sphere Monte Carlo with Clustering

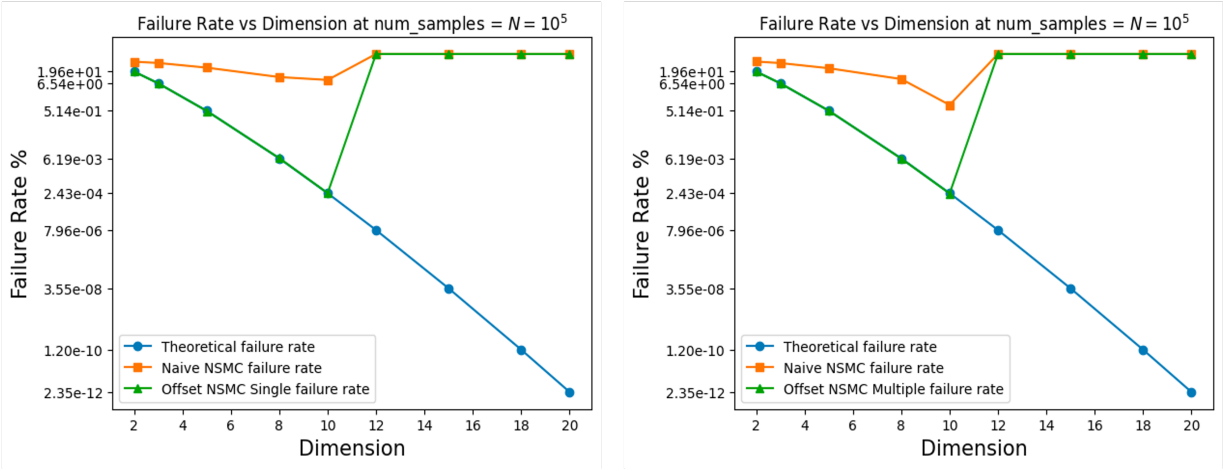


Figure 4.4: shows the performance of the Offset n-Sphere Monte Carlo algorithm compared to theoretical failure rates and the naive n-Sphere Monte Carlo method for both single and multiple failure regions.

For dimensions up to 10, the Offset n-Sphere Monte Carlo algorithm follows the theoretical failure rate closely and performs much better than the Naive n-Sphere Monte Carlo approach. However, the algorithm fails to extend our ability to estimate failure probabilities in higher dimensions at the given computational cost, facing the fundamental limitation of insufficient samples to capture extremely rare events in high-dimensional spaces. The results are consistent for both single and multiple failure regions, demonstrating the algorithm's robustness across different failure region types.

4.3.1 Variance Reduction through Weighted Clustering

A key advantage of the Offset Cluster n-Sphere Monte Carlo approach is the reduction in estimation variance through weighted clustering.

Table 4.1: Variance comparison between naive and weighted clustering for centroid estimation (n=10)

Method	**Average Variance**	**Reduction**
Naive Clustering	0.02378	–
Weighted Clustering	0.01780	25.15%

The results in Table 4.1 demonstrate that weighted clustering significantly reduces the

variance in centroid estimation by approximately 25% for problems of dimension $n = 10$. This reduction in estimation variance translates directly to more stable and accurate identification of failure region boundaries, which is critical for reliable probability estimates in high-dimensional spaces. The improvement confirms that incorporating $g(x)$ values in the weighting function for centroid calculation leads to more consistent cluster positioning around critical regions.

4.4 Deterministic Walk n-Sphere Monte Carlo

This approach incorporates a deterministic random walk in the n-Sphere Monte Carlo, resulting in improved accuracy with the same number of samples as compared to naive NSMC.

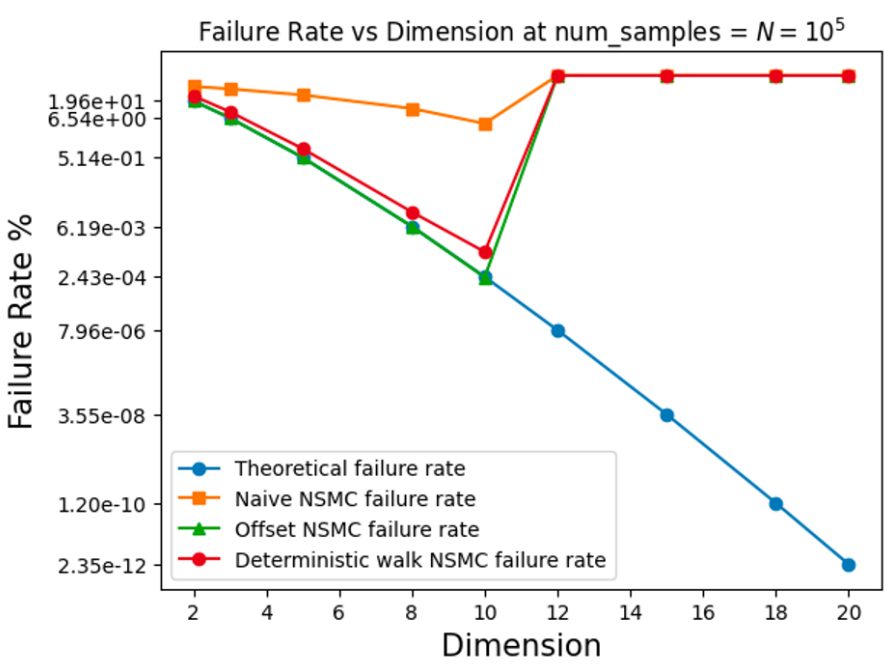


Figure 4.5: Failure rate vs. dimension for $N = 10^5$ samples for DW-NSMC failure rate (red).

Figure 4.5 presents a comparative analysis of the Deterministic Walk n-Sphere Monte Carlo algorithm against theoretical failure rates and our previous n-Sphere Monte Carlo variants. For dimensions between 2 and 10, the Deterministic Walk n-Sphere Monte Carlo algorithm consistently tracks closer to the theoretical failure rate than the Naive n-Sphere Monte Carlo. This demonstrates that the deterministic walk approach provides improved accuracy compared to the naive implementation in this dimensional range.

However, like the other variants, the Deterministic Walk n-Sphere Monte Carlo fails to estimate failure probabilities in high dimensions for the given number of samples. While the Offset and deterministic walk approach offers improved accuracy over the naive approach, it

does not extend our ability to handle high-dimensional reliability problems effectively with our computational constraints. This limitation motivates the development of our next algorithm to handle high-dimensional reliability problems effectively.

4.5 Random Walk n-Sphere Monte Carlo with Smoothly Varying $g(x)$

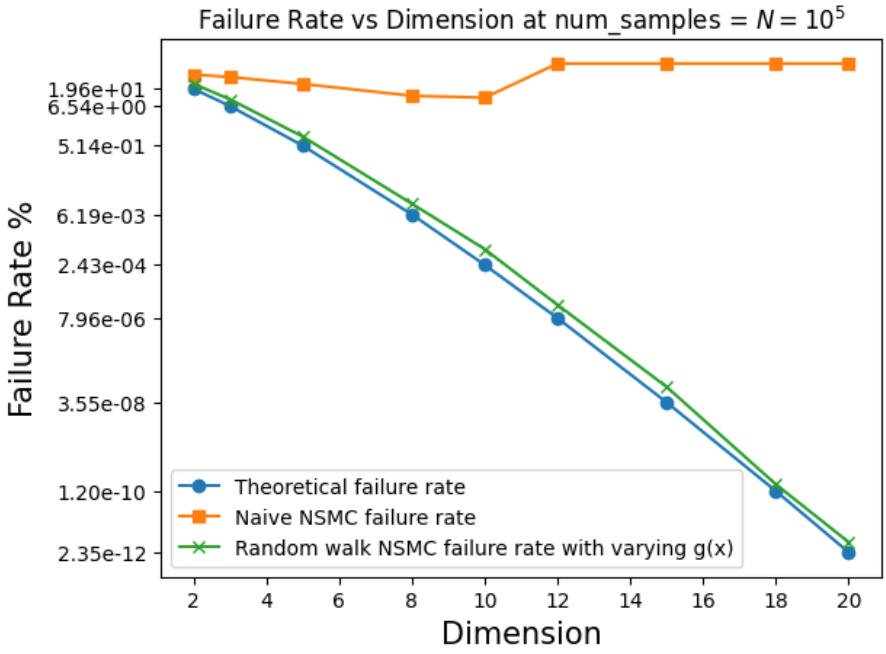


Figure 4.6: Failure rate vs. dimension for $N = 10^5$ samples for RW-NSMC failure rate with varying g(x) (green).

The Random Walk n-Sphere Monte Carlo algorithm demonstrates similar accuracy as the Deterministic Walk n-Sphere Monte Carlo in moderate dimensions while achieving a significant breakthrough in high-dimensional spaces. At dimension 20, where the theoretical failure rate approaches 2.35×10^{-12}, this algorithm maintains accuracy within the threshold while other methods completely fail due to insufficient samples.

Traditional approaches would require billions of samples to detect such rare events, making them computationally infeasible. This method reaches the same accuracy with much fewer samples, making high-dimensional reliability analysis more practical and cost-effective.

4.6 Comparative Analysis of All Algorithms

To provide a comprehensive overview of our algorithm development, we conducted a detailed comparison of all n-Sphere Monte Carlo variants across different dimensions at $N = 10^5$. This analysis quantifies the improvements achieved through our progressive enhancements to the basic algorithm.

Table 4.2 presents a quantitative comparison of the probabilities of failure estimated across different methods and dimensions. The values demonstrate how algorithmic enhancements improve the ability to detect rare events in higher dimensions.

Table 4.2: Failure probability estimates across NSMC variants

Dimension	**Theoretical**	**Naive NSMC**	**Offset-NSMC**	**DWNSMC**	**RWNSMC**
2	19.63	37.78	19.80	27.45	27.87
3	6.54	24.54	6.57	10.25	10.43
5	0.51	11.87	0.51	0.92	0.95
10	2.43×10^{-4}	2.35	2.33×10^{-4}	7.43×10^{-4}	5.15×10^{-4}
15	3.55×10^{-8}	–	–	–	11.3×10^{-8}
20	2.35×10^{-12}	–	–	–	3.28×10^{-12}

1. **Naive n-Sphere MC:** Performance rapidly deteriorates with increasing dimensions, showing exponential error growth at dimension 8 and complete failure beyond moderate dimensions due to insufficient sampling of rare events.

2. **Offset n-Sphere MC with clustering:** Achieves exceptional accuracy in low dimensions with less than 1% error in dimensions 2-5, maintaining effectiveness up to dimension 10 through targeted sampling near failure boundaries.

3. **Deterministic Walk n-Sphere MC:** Employs strategic sampling to improve performance in intermediate dimensions compared to the naive approach, though still limited by fundamental sampling constraints in high-dimensional spaces.

4. **Random Walk n-Sphere MC:** Represents a breakthrough in high-dimensional reliability analysis, extending reliable estimation capabilities to dimension 20 and enabling accurate detection of ultra-rare events with significantly improved computational efficiency.

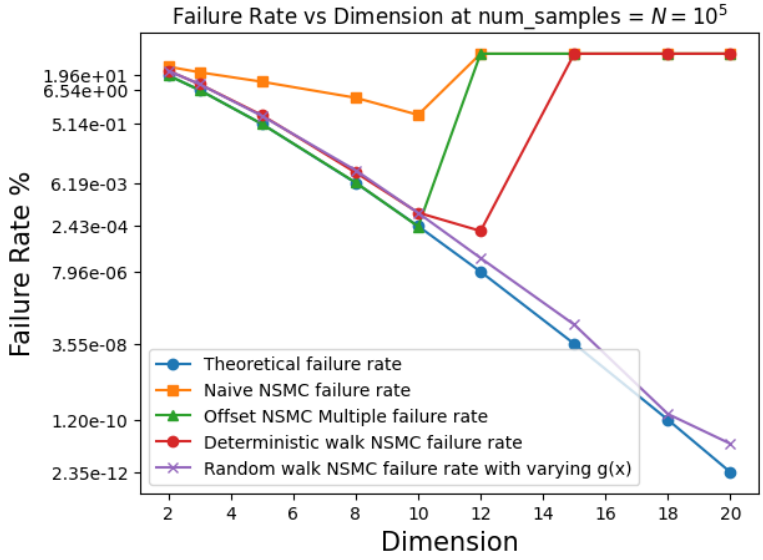
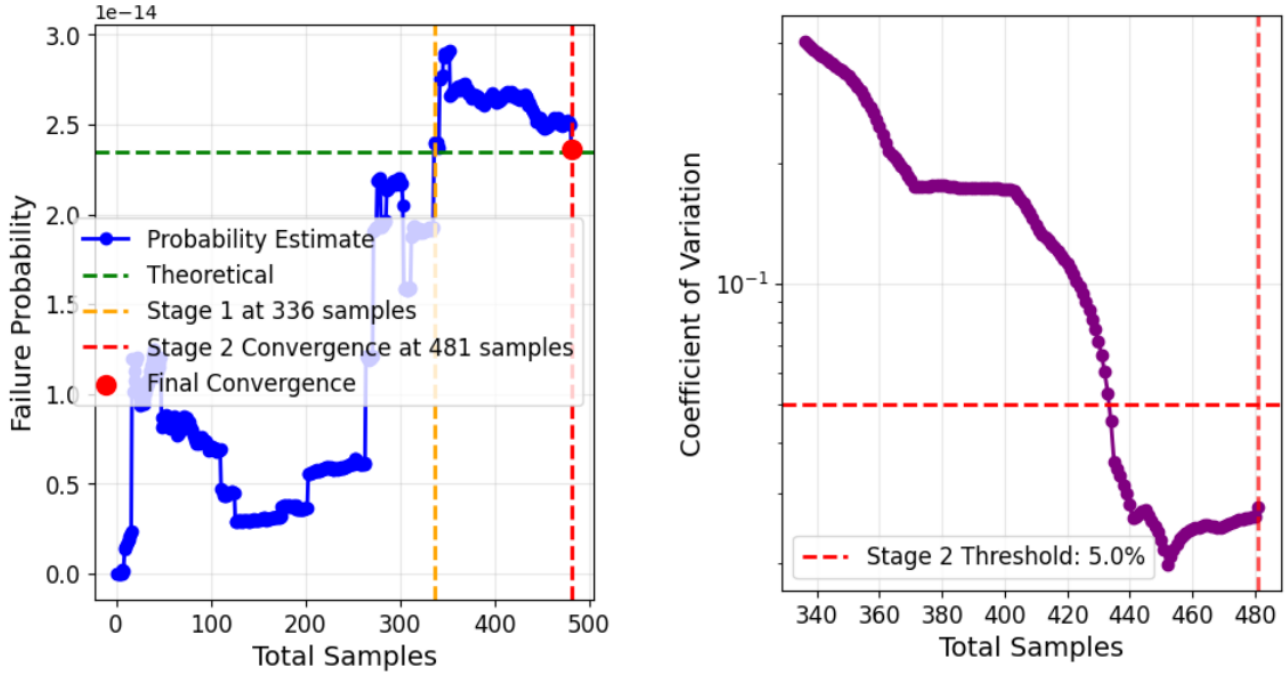


Figure 4.7: presents the failure rate estimates at $N = 10^5$ samples for all methods compared to theoretical values across dimensions 2-20.

This comparative analysis demonstrates the advancements achieved through the proposed algorithms, with each enhancement addressing specific limitations of previous approaches and extending the practical dimensional limits of reliability analysis.

4.6.1 CV Convergence Analysis

Figure 4.8 demonstrates the dual-stage stopping criterion employed in the reliability estimation algorithm. Figure 4.8(a) tracks the evolution of failure probability estimates relative to the analytical solution, while Figure 4.8(b) monitors the coefficient of variation (CV) computed over a sliding window of 100 samples.



(a) Relative Error convergence

(b) CV convergence

Figure 4.8: Dual-stage convergence analysis for reliability estimation

We conducted this analysis for $n = 20$ and observed the following convergence pattern. Stage 1 (relative error within 5% threshold) was achieved at $N = 336$ samples, while Stage 2 (stable CV below 5% threshold) required an additional 145 samples, reaching convergence at $N = 481$ samples. This sequential convergence behavior is typical for rare event problems, where statistical stability consistently requires more samples than initial accuracy, ensuring reliable termination before algorithm completion.

This sequential approach—first ensuring estimation accuracy, then confirming statistical stability—provides a robust termination mechanism for rare event simulations. The dual-stage method prevents premature termination by monitoring both estimation accuracy and result consistency, ensuring adequate failure event observation while preventing false convergence due to random variations in small sample sizes.

Chapter 5

Conclusion and Future Work

5.1 Research Highlights

This research addressed fundamental challenges in high-dimensional reliability analysis by applying n-Sphere Monte Carlo algorithm to realistic toy examples. Our experimental validation demonstrates significant advantages :

1. **Superior Dimensional Scaling and Sample Efficiency**: The proposed algorithms demonstrate substantially improved computational performance as problem dimensions increase, even for estimation of low failure probabilities, representing a significant improvement over existing methods. This translates to requiring up to 10,000 times fewer samples than conventional approaches while maintaining comparable accuracy in high dimensions. For example, methods accurately estimate failure probabilities as low as 10^{-14} in dimensions up to 20, where traditional methods completely fail. The Random Walk NSMC method maintained excellent tracking of the theoretical failure rates across the entire dimensional range, potentially enabling reliability verification for safety-critical aerospace, nuclear, and medical systems.

2. **Robust Geometric Adaptability**: The algorithms demonstrated consistent performance across diverse failure region configurations, including single and multiple failure regions, spherical and non-spherical domains, and varying geometric parameters. This addresses the reality of engineering systems with multiple simultaneous failure mechanisms.

5.2 Future Work

Application to complex engineering systems across various domains, including structural, mechanical, and safety-critical systems, would demonstrate practical value through comprehensive case studies. This would involve testing the methods on actual engineering problems and their limit state functions with corresponding geometric constraints, and input parameters such as material properties and loading conditions to validate the effectiveness of the proposed approach.

While RWNSMC demonstrates promising scalability, a formal proof of convergence to the true failure probability is currently unavailable. Future work may involve incorporating additional normalization or sample reweighting techniques to ensure theoretical convergence guarantees.

Appendix: Algorithms

Algorithm 1 n-Sphere Monte Carlo for Reliability Analysis using Volumes

Require: N - Number of samples; $g(\mathbf{x})$ - Limit state function; n - Dimension; R_{max} - Maximum sampling radius

Ensure: Failure probability estimate p_f

$V_f \leftarrow 0$ ▷ Initialize failure volume

$V_t \leftarrow 0$ ▷ Initialize total volume

for $i = 1$ to N **do**

  $\hat{\mathbf{s}}_i \leftarrow$ random unit direction vector in $\mathbb{R}^n$

  $r_i \leftarrow$ random extent in $[0, R_{max}]$ ▷ Sample extent

  $\mathbf{x}_i \leftarrow r_i \hat{\mathbf{s}}_i$ ▷ Convert to Cartesian coordinates

  $g_i \leftarrow g(\mathbf{x}_i)$ ▷ Evaluate limit state function

  if $g_i \leq 1$ **then** ▷ Check failure condition

    $V_f \leftarrow V_f + v_n(r_i)^n$ ▷ Update failure volume

  end if

  $V_t \leftarrow V_t + v_n(r_i)^n$ ▷ Update total volume

end for

$p_f \leftarrow \frac{V_f}{V_{total}}$ ▷ Compute Failure probability

return p_f

Algorithm 2 Offset n-Sphere Monte Carlo with K-means Clustering

Require: N - Number of samples; $g(\mathbf{x})$ - Limit state function; n - Dimension; k - Number of clusters; R_{max} - Maximum sampling radius

Ensure: Failure probability estimate p_f

$\mathcal{X}_f \leftarrow \emptyset$ ▷ Initialize failure points set

$V_f \leftarrow 0$ ▷ Initialize failure volume

$V_t \leftarrow 0$ ▷ Initialize total volume

for $i = 1$ to N_{initial} **do**

  $\hat{\mathbf{s}}_i \leftarrow$ random unit direction vector in $\mathbb{R}^n$

  $r_i \leftarrow$ random extent in $[0, R_{max}]$ ▷ Sample extent

  $\mathbf{x}_i \leftarrow r_i \hat{\mathbf{s}}_i$ ▷ Convert to Cartesian coordinates

  $g_i \leftarrow g(\mathbf{x}_i)$ ▷ Evaluate limit state function

  if $g_i \leq 1$ **then** ▷ Classify failure points

    $\mathcal{X}_f \leftarrow \mathcal{X}_f \cup \{\mathbf{x}_i\}$

  end if

end for

$\{\mathbf{c}_1, ..., \mathbf{c}_k\} \leftarrow \text{KMeans}(\mathcal{X}_f, k)$ ▷ K-means clustering

for each centroid $\mathbf{c}_j$ **do**

  $V_{f,j} \leftarrow \text{NSMC}(N_j, g, \mathbf{c}_j)$ ▷ Estimate failure volume at each centroid

end for

$V_f \leftarrow \sum_{j=1}^{k} V_{f,j}$ ▷ Sum all failure volumes

$V_{total} \leftarrow$ Volume of sampling domain ▷ Total domain volume

$p_f \leftarrow \frac{V_f}{V_{total}}$ ▷ Compute Failure probability

return p_f

Algorithm 3 n-Sphere Monte Carlo with g(x)-Weighted Centroid Estimation

Require: N - Number of samples; $g(\mathbf{x})$ - Limit state function; n - Dimension; k - Number of clusters; R_{max} - Maximum sampling radius
Ensure: Failure probability estimate p_f

$\mathcal{X} \leftarrow \emptyset$ ▷ Initialize sample points set
$\mathcal{G} \leftarrow \emptyset$ ▷ Initialize g-values set
for $i = 1$ to N_{initial} **do**
    $\hat{\mathbf{s}}_i \leftarrow$ random unit direction vector in $\mathbb{R}^n$
    $r_i \leftarrow$ random extent in $[0, R_{max}]$ ▷ Sample extent
    $\mathbf{x}_i \leftarrow r_i \hat{\mathbf{s}}_i$ ▷ Convert to Cartesian coordinates
    $g_i \leftarrow g(\mathbf{x}_i)$ ▷ Evaluate limit state function
    $\mathcal{X} \leftarrow \mathcal{X} \cup \{\mathbf{x}_i\}$
    $\mathcal{G} \leftarrow \mathcal{G} \cup \{g_i\}$
end for
$\mathcal{X}_f \leftarrow \{\mathbf{x}_i \in \mathcal{X} \mid g_i \leq 1\}$ ▷ Identify failure points
if $|\mathcal{X}_f| < k$ **then**
    $k \leftarrow |\mathcal{X}_f|$ ▷ Adjust cluster count if needed
end if
Partition $\mathcal{X}_f$ into k initial clusters $\{C_1, \ldots, C_k\}$
for $iter = 1$ to $max\_iterations$ **do**
    for $j = 1$ to k **do**
        $\mathcal{W}_j \leftarrow \emptyset$ ▷ Weights for points in cluster j
        for each $\mathbf{x}_i \in C_j$ with corresponding g_i **do**
            $w_i \leftarrow \exp(-|g_i - 1|)$ ▷ Weight based on proximity to boundary
            $\mathcal{W}_j \leftarrow \mathcal{W}_j \cup \{w_i\}$
        end for
        $\mathbf{c}_j \leftarrow \frac{\sum_{i \in C_j} w_i \cdot \mathbf{x}_i}{\sum_{i \in C_j} w_i}$ ▷ Weighted centroid
    end for
    Reassign points to closest centroids to form new clusters
end for
for each centroid $\mathbf{c}_j$ **do**
    $V_{f,j} \leftarrow \text{NSMC}(N_j, g, \mathbf{c}_j)$ ▷ Estimate failure volume at each centroid
end for
$V_f \leftarrow \sum_{j=1}^{k} V_{f,j}$ ▷ Sum all failure volumes
$V_{total} \leftarrow$ Volume of sampling domain ▷ Total domain volume
$p_f \leftarrow \frac{V_f}{V_{total}}$ ▷ Compute Failure probability
return p_f

Algorithm 4 Deterministic-Walk n-Sphere Monte Carlo

Require: N - Number of samples; $g(\mathbf{x})$ - Limit state function; n - Dimension; $\mathbf{x}_0$ - Initial center

Ensure: Failure probability estimate p_f

$V_f \leftarrow 0$ ▷ Initialize failure volume
$V_t \leftarrow 0$ ▷ Initialize total volume
$\mathbf{c} \leftarrow \mathbf{x}_0$ ▷ Initialize current center
$\mathcal{F} \leftarrow \emptyset$ ▷ Failure extents collection
$\mathcal{S} \leftarrow \emptyset$ ▷ Non-failure extents collection
for $i = 1$ to N **do**
    $\hat{\mathbf{s}}_i \leftarrow$ random unit direction vector in $\mathbb{R}^n$
    $r_i \leftarrow$ random extent in $[0, R_{max}]$
    $\mathbf{x}_i \leftarrow \mathbf{c} + r_i \hat{\mathbf{s}}_i$ ▷ Sample point
    $g_i \leftarrow g(\mathbf{x}_i)$ ▷ Evaluate limit state function
    if $g_i \leq 1$ **then** ▷ Classified as failure (g(x) $\leq$ 1)
        $\mathcal{F} \leftarrow \mathcal{F} \cup \{r_i\}$ ▷ Add to failure extents
        $\mathbf{c} \leftarrow \mathbf{x}_i$ ▷ Update center to current point
    else ▷ Classified as non-failure (g(x) > 1)
        $\mathcal{S} \leftarrow \mathcal{S} \cup \{r_i\}$ ▷ Add to non-failure extents
        $\mathbf{c} \leftarrow \mathbf{c}$ ▷ Retain current center
    end if
    $V_f \leftarrow V_f + v_n(r_i)^n \cdot \mathbf{1}_{g_i \leq 1}$ ▷ Update failure volume
    $V_t \leftarrow V_t + v_n(r_i)^n$ ▷ Update total volume
end for
$p_f \leftarrow V_f / V_t$ ▷ Compute failure probability
return p_f

Algorithm 5 Random-Walk n-Sphere Monte Carlo

Require: N - Number of samples; $g(\mathbf{x})$ - Limit state function; n - Dimension; $\mathbf{x}_0$ - Initial center

Ensure: Failure probability estimate p_f

$V_f \leftarrow 0$ ▷ Initialize failure volume
$V_t \leftarrow 0$ ▷ Initialize total volume
$\mathbf{c} \leftarrow \mathbf{x}_0$ ▷ Initialize current center
$g_c \leftarrow g(\mathbf{c})$ ▷ Evaluate limit state function at initial center
$\mathcal{F} \leftarrow \emptyset$ ▷ Failure extents collection
$\mathcal{S} \leftarrow \emptyset$ ▷ Non-failure extents collection
for $i = 1$ to N **do**
    $\hat{\mathbf{s}}_i \leftarrow$ random unit direction vector in $\mathbb{R}^n$
    $r_i \leftarrow$ random extent in $[0, R_{max}]$
    $\mathbf{x}_i \leftarrow \mathbf{c} + r_i \hat{\mathbf{s}}_i$ ▷ Sample point
    $g_i \leftarrow g(\mathbf{x}_i)$ ▷ Evaluate limit state function
    if $g_i \leq 1$ **then** ▷ Rule 1: Point in failure region
        $\mathbf{c} \leftarrow \mathbf{x}_i$; $g_c \leftarrow g_i$ ▷ Always move to failure points
        $\mathcal{F} \leftarrow \mathcal{F} \cup \{r_i\}$ ▷ Add to failure extents
        $V_f \leftarrow V_f + v_n r_i^n$ ▷ Update failure volume
    else if $g_i \leq g_c$ **then** ▷ Rule 2 & 3: Probabilistic decision for lower g(x)
        $p_j \leftarrow 1 - \frac{g_i}{g_c}$ ▷ Calculate transition probability
        $u_j \leftarrow$ random number from $[0, 1]$
        if $u_j < p_j$ **then** ▷ Probabilistic acceptance
            $\mathbf{c} \leftarrow \mathbf{x}_i$; $g_c \leftarrow g_i$ ▷ Move center
        end if
        $\mathcal{S} \leftarrow \mathcal{S} \cup \{r_i\}$ ▷ Add to non-failure extents
    else ▷ Rule 4: Higher g(x) value than current
        $\mathcal{S} \leftarrow \mathcal{S} \cup \{r_i\}$ ▷ Add to non-failure extents, no move
    end if
    $V_t \leftarrow V_t + v_n r_i^n$ ▷ Update total volume
end for
$p_f \leftarrow V_f / V_t$ ▷ Compute failure probability
return p_f

Algorithm 6 Extent Estimation from Offset Centre

Require: $\mathbf{x}$ - Starting point in $\mathbb{R}^n$; $\hat{\mathbf{s}}$ - Unit direction vector in $\mathbb{R}^n$; $\mathbf{L}$ - Cuboid edge lengths
Ensure: Sampled point $\mathbf{x}_s$ and extent distance r_s

if $\mathbf{L}$ is scalar **then**
    $\mathbf{L} \leftarrow \mathbf{L} \cdot \mathbf{1}_n$ ▷ Convert scalar to vector
end if
$\mathbf{h} \leftarrow \mathbf{L}/2$ ▷ Calculate half-lengths of cuboid edges
$\mathcal{D} \leftarrow \emptyset$ ▷ Initialize collection of potential intersection distances
for $i = 1$ to n **do** ▷ For each dimension
    if $\hat{\mathbf{s}}[i] = 0$ **then**
        continue ▷ Skip if ray is parallel to this dimension's faces
    end if
    $d_{neg} \leftarrow \frac{-\mathbf{h}[i]-\mathbf{x}[i]}{\hat{\mathbf{s}}[i]}$ ▷ Distance to negative boundary
    $d_{pos} \leftarrow \frac{\mathbf{h}[i]-\mathbf{x}[i]}{\hat{\mathbf{s}}[i]}$ ▷ Distance to positive boundary
    if $\hat{\mathbf{s}}[i] > 0$ **then**
        $\mathcal{D} \leftarrow \mathcal{D} \cup \{d_{pos}\}$ ▷ Add distance to positive face
    else
        $\mathcal{D} \leftarrow \mathcal{D} \cup \{d_{neg}\}$ ▷ Add distance to negative face
    end if
end for
$r_{max} \leftarrow \min\{d \in \mathcal{D} : d > 0\}$ ▷ Find first boundary intersection distance
if $\mathcal{D} = \emptyset$ or $\nexists d \in \mathcal{D} : d > 0$ **then**
    $r_{max} \leftarrow \infty$ ▷ Default if no boundary intersection
end if
$r_s \leftarrow$ random number from $[0, r_{max}]$ ▷ Sample random extent before boundary
$\mathbf{x}_s \leftarrow \mathbf{x} + r_s \cdot \hat{\mathbf{s}}$ ▷ sampled point
return $\mathbf{x}_s, r_s$

Algorithm 7 Two-Stage CV-Based Monte Carlo Convergence

Require: ΔN - Sample increment per iteration; ε_{rel} - Relative error threshold (Stage 1); ε_{CV} - CV threshold (Stage 2); N_{max} - Maximum samples; w - Window size

Ensure: Total samples N_{conv} and converged probability $\hat{p}_{f,conv}$

Compute theoretical failure probability p_{th}
$N \leftarrow 0$ ▷ Initialize total sample count
$\mathcal{W} \leftarrow \emptyset$ ▷ Initialize sliding window for probability estimates
$\mathcal{F} \leftarrow \emptyset$ ▷ Initialize cumulative failure extents
$\mathcal{S} \leftarrow \emptyset$ ▷ Initialize cumulative non-failure extents
$stage_1 \leftarrow$ false ▷ Flag for Stage 1 completion
$converged \leftarrow$ false ▷ Initialize convergence flag
while $N < N_{max}$ **and not** $converged$ **do**
    $N \leftarrow N + \Delta N$ ▷ Increment total sample count
    Generate ΔN new samples; update $\mathcal{F}$ and $\mathcal{S}$
    $\hat{p}_f \leftarrow$ calculate_failure_probability$(\mathcal{F}, \mathcal{S}, N)$
    if not $stage_1$ **then**
        $e_{rel} \leftarrow |\hat{p}_f - p_{th}|/p_{th}$ ▷ Calculate relative error
        if $e_{rel} \leq \varepsilon_{rel}$ **then**
            $stage_1 \leftarrow$ true ▷ Stage 1 achieved
            Record $N_1 \leftarrow N$ and $\hat{p}_{f,1} \leftarrow \hat{p}_f$
        end if
    else
        $\mathcal{W} \leftarrow \mathcal{W} \cup \{\hat{p}_f\}$ ▷ Add new estimate to window
        if $|\mathcal{W}| > w$ **then**
            Remove oldest estimate from $\mathcal{W}$ ▷ Maintain window size w
        end if
        if $|\mathcal{W}| = w$ **then**
            $\bar{p}_f \leftarrow \frac{1}{w}\sum_{p\in\mathcal{W}} p$ ▷ Window mean
            $s \leftarrow \sqrt{\frac{1}{w-1}\sum_{p\in\mathcal{W}}(p-\bar{p}_f)^2}$ ▷ Window standard deviation
            if $\bar{p}_f \neq 0$ **then**
                $CV \leftarrow s/\bar{p}_f$ ▷ Calculate coefficient of variation
            else
                $CV \leftarrow \infty$ ▷ Handle zero-mean case
            end if
            $e_{rel} \leftarrow |\hat{p}_f - p_{th}|/p_{th}$ ▷ Calculate relative error
            if $CV \leq \varepsilon_{CV}$ **and** $e_{rel} \leq \varepsilon_{rel}$ **then**
                $converged \leftarrow$ true ▷ Both CV and relative error thresholds met
                $N_{conv} \leftarrow N$ ▷ Store convergence sample count
                $\hat{p}_{f,conv} \leftarrow \hat{p}_f$ ▷ Store converged probability
            end if
        end if
    end if
end while
return $N_{conv}, \hat{p}_{f,conv}$

Bibliography

[1] Allgower, E.L. & Schmidt, P.H. (1986). Computing volumes of polyhedra. *Mathematics of Computation*, 46(173), 171–174. 10, 14

[2] Anderson, E.C. (1999). Monte Carlo methods and importance sampling. *Lecture Notes for Statistical Genetics*, 578. 1, 8

[3] Au, S.K. & Beck, J.L. (1999). A new adaptive importance sampling scheme for reliability calculations. *Structural Safety*, 21(2), 135–158. 2, 3, 7

[4] Au, S.K. & Beck, J.L. (2001). Estimation of small failure probabilities in high dimensions by subset simulation. *Probabilistic Engineering Mechanics*, 16(4), 263–277. 2, 3, 8, 12

[5] Au, S. & Wang, Y. (2014). *Engineering Risk Assessment with Subset Simulation*. John Wiley & Sons, Singapore. 2, 3, 8, 10, 11

[6] Blatman, G. & Sudret, B. (2011). Adaptive sparse polynomial chaos expansion based on least angle regression. *Journal of Computational Physics*, 230(6), 2345–2367. 2

[7] Der Kiureghian, A., Lin, H.Z. & Hwang, S.J. (1987). Second-order reliability approximations. *Journal of Engineering Mechanics*, 113(8), 1208–1225. 7

[8] Ditlevsen, O. & Madsen, H.O. (1996). *Structural Reliability Methods*. John Wiley & Sons, Chichester. 1, 6

[9] Dubourg, V., Sudret, B. & Deheeger, F. (2013). Metamodel-based importance sampling for structural reliability analysis. *Probabilistic Engineering Mechanics*, 33, 47–57. 2

[10] Dyer, M.E. & Frieze, A.M. (1988). On the complexity of computing the volume of a polyhedron. *SIAM Journal on Computing*, 17(5), 967–974.

[11] Dyer, M., Frieze, A., & Kannan, R. (1991). A random polynomial-time algorithm for approximating the volume of convex bodies. *Journal of the ACM (JACM)*, 38(1), 1–17. 2, 3, 9, 10, 11, 12

[12] Echard, B., Gayton, N. & Lemaire, M. (2011). AK-MCS: An active learning reliability method combining Kriging and Monte Carlo Simulation. *Structural Safety*, 33(2), 145–154. 2

[13] Ghanem, R.G. & Spanos, P.D. (1991). *Stochastic Finite Elements: A Spectral Approach*. Springer-Verlag, New York. 2

[14] Haario, H., Saksman, E., & Tamminen, J. (2001). An adaptive Metropolis algorithm. *Bernoulli*, 223–242. 3, 11

[15] Haldar, A. & Mahadevan, S. (2000). *Reliability Assessment Using Stochastic Finite Element Analysis*. John Wiley & Sons, New York. 2

[16] Hasofer, A.M. & Lind, N.C. (1974). Exact and invariant second-moment code format. *Journal of the Engineering Mechanics Division*, 100(1), 111–121. 7

[17] Isaac, A., Jawlekar, A. & Venkatapathi, M. (2023). An algorithm for estimating non-convex volumes and other integrals in n dimensions. *Computational and Applied Mathematics*, 42, 242. https://doi.org/10.1007/s40314-023-02299-6 2, 3, 5, 9, 10, 11, 12

[18] Jawlekar, A. & Venkatapathi, M. (2023). An importance sampling in N-Sphere Monte Carlo and its performance analysis for high-dimensional integration. Technical Report, Department of Computational and Data Sciences, Indian Institute of Science, Bangalore. 3, 9, 10

[19] Keshavarzzadeh, V., Kirby, R.M., & Narayan, A. (2018). Numerical integration in multiple dimensions with designed quadrature. *SIAM Journal on Scientific Computing*, 40(4), A2033–A2061. 10, 11, 14

[20] Kroese, D.P., Taimre, T. & Botev, Z.I. (2011). *Handbook of Monte Carlo Methods*. John Wiley & Sons, Hoboken. 1, 7, 8, 11

[21] Lovász, L. (1999). Hit-and-run mixes fast. *Mathematical Programming*, 86, 443–460. 2, 3

[22] Lovász, L. & Vempala, S. (2006). Simulated annealing in convex bodies and an O*(n4) volume algorithm. *Journal of Computer and System Sciences*, 72(2), 392–417. 2, 3, 9, 10

[23] Matthies, H.G., Brenner, C.E., Bucher, C.G., & Soares, C.G. (2007). Uncertainties in probabilistic numerical analysis of structures and solids—Stochastic finite elements. *Structural Safety*, 19(3), 283–366. 2, 12

[24] Melchers, R.E. & Beck, A.T. (2018). *Structural Reliability Analysis and Prediction*. John Wiley & Sons, Chichester, 3rd edition. 1, 6, 7

[25] Robert, C.P. & Casella, G. (2004). *Monte Carlo Statistical Methods*. Springer, New York, 2nd edition. 1, 7, 8, 11

[26] Schueremans, L. & Van Gemert, D. (2005). Benefit of splines and neural networks in simulation based structural reliability analysis. *Structural Safety*, 27(3), 246–261. 2

[27] Simonovits, M. (2003). How to compute the volume in high dimension? *Mathematical Programming*, 97, 337–374. 1, 3, 8, 9, 10, 12

[28] Stefanou, G. (2009). The stochastic finite element method: Past, present and future. *Computer Methods in Applied Mechanics and Engineering*, 198(9–12), 1031–1051. 2

[29] Sudret, B. (2008). Global sensitivity analysis using polynomial chaos expansions. *Reliability Engineering & System Safety*, 93(7), 964–979. 2

[30] Tabandeh, A., Jia, G., & Gardoni, P. (2022). A review and assessment of Importance Sampling Methods for reliability analysis. *Structural Safety*, 97, 102216. 2, 3, 7, 12

[31] S.-K. Au and J.L. Beck, "Estimation of small failure probabilities in high dimensions by subset simulation," *Probabilistic Engineering Mechanics*, 2001.

[32] J.L. Beck and S.-K. Au, "Subset simulation and its application to seismic risk based on dynamic analysis," *Journal of Engineering Mechanics*, 2003.

[33] G.I. Papaioannou, V. Sudret, and I. Andrianakis, "Surrogate-based subset simulation for extreme rare-event estimation," *Structural Safety*, 2015.