Comparison of Non-Standard Simulation Methods for Performing Extremely Low Probability Assessments

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Abstract: The probabilistic analysis of possible piping rupture or significant loss of coolant accident (LOCA) is a complex problem as it involves many mechanisms and generates low to extremely low probabilities of events. This topic is of particular interest in the nuclear industry and a conjoint effort between the US NRC and EPRI over the last 10 years has led to the development of the Extremely Low Probability of Rupture (xLPR) code to assess probability of rupture in nuclear piping systems. The current codes for determining the probability of rupture for events occurring at these very low values can take days, or even weeks, to run. In this paper we provide the technical basis for the an adaptive sampling scheme that can reduce the computational time needed for the standard Monte Carlo sampling methods to propagate uncertainty by a factor of 50 to 1,000. A theoretical problem is first presented to explain the method. Afterward the adaptive method is applied to the precursor analysis for time to first leakage.

Keywords: Probabilistic fracture mechanics**,** Monte Carlo, DPD, Adaptive Sampling

1 INTRODUCTION

As structures age in the United States and throughout the world we know that the probability of failure increases. This is by definition since if the failure probability does not change then the structure is not aging. During the design phase, especially several decades ago, aging problems were not specifically addressed. Yet if the risk of failure is part of the design or assessment to license then as the structure ages this risk increases. For structures in which the consequence of failure is relatively low, e.g. inconvenience or low costs to replace, aging can be addressed in a relatively simple cost-benefit analysis. However for those structures in which there are very high consequences, e.g. loss of life, or they are extremely expensive to replace, e.g. a new bridge, it is critical to be able to assess the probability of failure, *and its associated uncertainty*, accurately and in a timely manner.

While there are many industries in which aging is a significant and growing problem, e.g. aircraft both in DoD and commercially, shipping, gas transmission pipelines, and offshore oil structures, this paper will focus on the primary water piping failures in nuclear power plants as the primary example of assessing this risk issue. This is not meant to imply that nuclear power plants have any more issues with aging than any other but to demonstrate how risk assessments can be more efficient when realistic physical models are used in an industry which has performed risk and uncertainty analyses for decades.

The focus of this paper is to discuss the development of a new method of sampling that focuses on areas of interest automatically, not to perform a review of simulation and uncertainty analysis techniques. In fact a good review of uncertainty analysis methods has been previously published [1]. This paper instead focuses on three methods that have been previously used for nuclear power plant analyses: (1) Monte Carlo; (2) Latin Hypercube Sampling (LHS); and (3) Discrete Probability Distribution (DPD). This paper assumes the reader is familiar with Monte Carlo and a companion paper discusses this sampling method, as well as importance sampling by the variance reduction technique. LHS and DPD methods are discussed since they are less widely used than Monte Carlo so that the reader has a basis

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for understanding the new methodology. After these discussions the methods are applied to an analytic problem for which Monte Carlo is efficient and detailed comparisons to all methods can be made.

While there are a variety of simulation methods for performing risk analysis we focus on four:

(1) Monte Carlo
(2) Latin Hypercube Sampling (LHS)
(3) Discrete Probability Distributions (DPD)
(4) Adaptive Sampling Method Using Golden Rule Clustering (GRC)

The next section describes the theory followed by a discussion of the application to an analytic problem.

2 SIMULATION METHODS STUDIED

2.1. Monte Carlo Analysis

The basic principles of Monte Carlo analysis are have been well known for some time, e.g. [2]. Given a set of inputs $\{x_1, x_2, \ldots, x_N\}$ that are uncertain and described by a Probability Density Function (PDF) denoted as $f(x_i)$ we construct the Cumulative distribution function by integrating $f(x_i)$

$$F(x) = \int_{-\infty}^{x} f(z)dz$$

To perform a Monte Carlo analysis we select a random number, denoted R, between 0 and 1 and invert the CDF to obtain a value for each x_i.

$$x_i = F_i^{-1}(R)$$

Figure 1 shows one such sampling for both the normal and lognormal distributions. In this example R = 0.5. Note that the value which would be selected for the normal case is 19.824 while for the lognormal case it is 18.421. These values for the x_i are input to the physics model or equation and a response is calculated, denoted Y_1. The entire process is repeated to generate a set of responses Y_K. These responses are then representative of the distribution of the responses that would be generated if an infinite number of samples were taken. How representative they are depends upon the value of K. The larger the value the more accurate the representation.

Monte Carlo is almost always the method of choice for simulation studies when the response calculation is fast. However, when there are limitations on the number of samples that can be generated then alternative methods need to be examined.

2.2. Latin Hypercube Sampling

The issue of sampling for low probability events has been a topic of intense scrutiny over the years. Many strategies have been employed but it is not the purpose of this discussion to provide a survey of these methods but rather it is the purpose to focus on one of these methods that has been used extensively in Probabilistic Risk Assessment (PRA): Latin Hypercube Sampling (LHS).

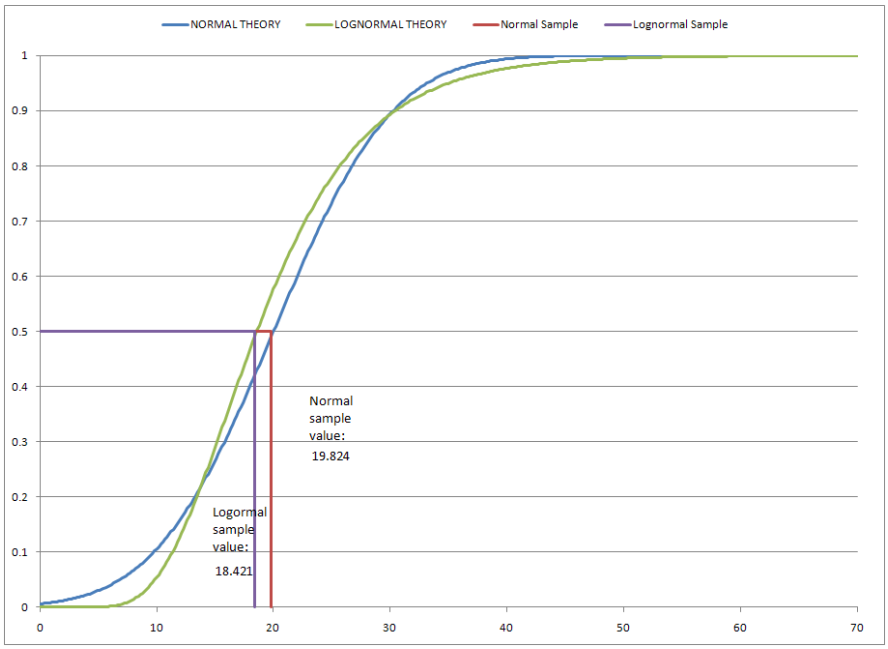


Figure 1 Monte Carlo Sampling Illustration

The purpose of LHS is to provide a "dense" sampling of the random inputs or processes to a physical model. The definition of dense is only applicable to the input space and in fact can be quite sparse when viewed from the response space as we shall see in the following discussion.

The LHS is constructed by dividing the input response distribution into N equal probability intervals. This is done for each of the inputs. The first interval for the first variable is then randomly paired with an interval from the second variable, leading to a couplet of (x_1, x_I) where I is the selected random interval for variable 2. If there is a third interval then this couplet is randomly paired with an interval from the third variable leading to a triplet, (x_1, x_I, x_J) where J is the random interval selected for the third variable. If there are M random variables then this process is repeated M-1 times leading to an M-tuplet (x_1, x_I, x_J, …, x_K). To obtain the actual value of x_L we would generate a random value according to the PDF of the variable selected from interval L. This M-tuplet then is the input that generates a single response. To obtain the next set of inputs the same process is repeated except that if a value has been previously selected it cannot be selected again. Thus a *sampling without replacement* scheme is used. This implies that there will be exactly N response generated. Thus for M variables there are N^M possible combinations of the inputs. There the LHS design will sample N^{1-M} fraction of the response space.

2.3. Discrete Space Sampling

In the LHS sampling when an interval is selected it is sampled within the interval of the sample. An alternative method for generating the response CDF is to limit our calculations to points in the discrete space. In this case we define a Discrete Probability Density (DPD) function for each of the inputs [3]. Thus, if the PDF is divided into N_{bin} intervals

$$\Phi_1 = \left[\left(x_{1,1}, p_{1,1}\right), \left(x_{1,2}, p_{1,2}\right), \cdots, \left(x_{1,N}, p_{1,N_{BIN}}\right)\right]$$

$$\Phi_2 = \left[\left(x_{2,1}, p_{2,1}\right), \left(x_{2,2}, p_{2,2}\right), \cdots, \left(x_{2,N}, p_{2,N_{BIN}}\right)\right]$$

The response DPD is constructed by taking all possible combinations of the input DPD's. Thus, for two random variables:

$$R_1 = \mathrm{x}_{1,1} \otimes \mathrm{x}_{2,1}(1), p_{1,1} * p_{2,1}$$
$$R_2 = \mathrm{x}_{1,1} \otimes \mathrm{x}_{2,2}(1), p_{1,1} * p_{2,2}$$
$$\vdots$$
$$R_{N_{bin}} = \mathrm{x}_{1,1} \otimes \mathrm{x}_{2,N_{bin}}, p_{1,1} * p_{2,N_{bin}}$$

$$R_{N_{bin}} = \mathrm{x}_{1,1} \otimes \mathrm{x}_{2,N_{bin}}, p_{1,1} * p_{1,N_{bin}}$$
$$R_{N_{bin}+1} = \mathrm{x}_{1,2} \otimes \mathrm{x}_{2,1}, p_{1,2} * p_{2,1}$$
$$R_{N_{bin}+2} = \mathrm{x}_{1,2} \otimes \mathrm{x}_{2,2}, p_{1,2} * p_{2,2}$$
$$\vdots$$
$$R_{N_{bin}^2} = \mathrm{x}_{1,N_{bin}} \otimes \mathrm{x}_{2,N_{bin}}, p_{1,N_{bin}} * p_{2,N_{bin}}$$

We know the resulting DPD is a Probability Density Function since

$$p_I p_J \leq 1 \forall I, J$$
$$\int_{-\infty}^{\infty} PdP = \sum_{I=1}^{N_{BIN}} \sum_{J=1}^{N_{BIN}} p_I p_J = \sum_{I=1}^{N_{BIN}} p_I \sum_{J=1}^{N_{BIN}} p_J = \sum_{I=1}^{N_{BIN}} p_I = 1$$

are the two conditions which must be satisfied in order for a function to be a PDF. A simple example of a three point discretization of the normal distribution is used to illustrate.

In general, to obtain the full response DPD ${N_{bin}}^{N_V}$, where N_V is the number of random variables, evaluations of the function $\otimes$ must be performed. For most engineering applications there are dozens, or even hundreds of random variables. Thus, if we have 10 bins and 20 random variables we would need to perform 10^{20} evaluations to obtain the full PDF. If if a single function evaluation only took a microsecond to generate a full PDF would require over 3,000,000 years. However, 10^{20} discrete points can be treated via Monte Carlo sampling as described in [4]. In Figure 3 we a DPD sample compared to a LHS sample when only 3 intervals, or bins, are used. It is important to note that the DPD will never change while the LHS points will change each time a new design is generated. The real benefit of DPD is when we wish to sample portions of the distribution more frequently. Because LHS uses the same sampling strategy as Monte Carlo there are no known a priori frequencies, or weights, with the LHS scheme. When the DPD method is used we know exactly how frequently these points occur and can generate responses that are not of equal probability. This method is discussed next.

2.4. Adaptive Sampling in the DPD Space

Of course it is not always (and in fact may rarely be) the case that the area of most interest is in the tails of a distribution. For example, in probabilistic fracture mechanics analysis, low values of the initial crack length are not the most likely situation to lead to pipe rupture. On the other hand low values of yield and ultimate strength can lead to pipe rupture. And in many important studies, mid-range values of the weld residual stress at the inner diameter of the pipe are most important. Therefore, when one is faced with an analysis in which we are unsure of which combinations may lead to a failure of consequence the question becomes: how does one approach this analysis?

Figure 2. Three Point DPD Calculations

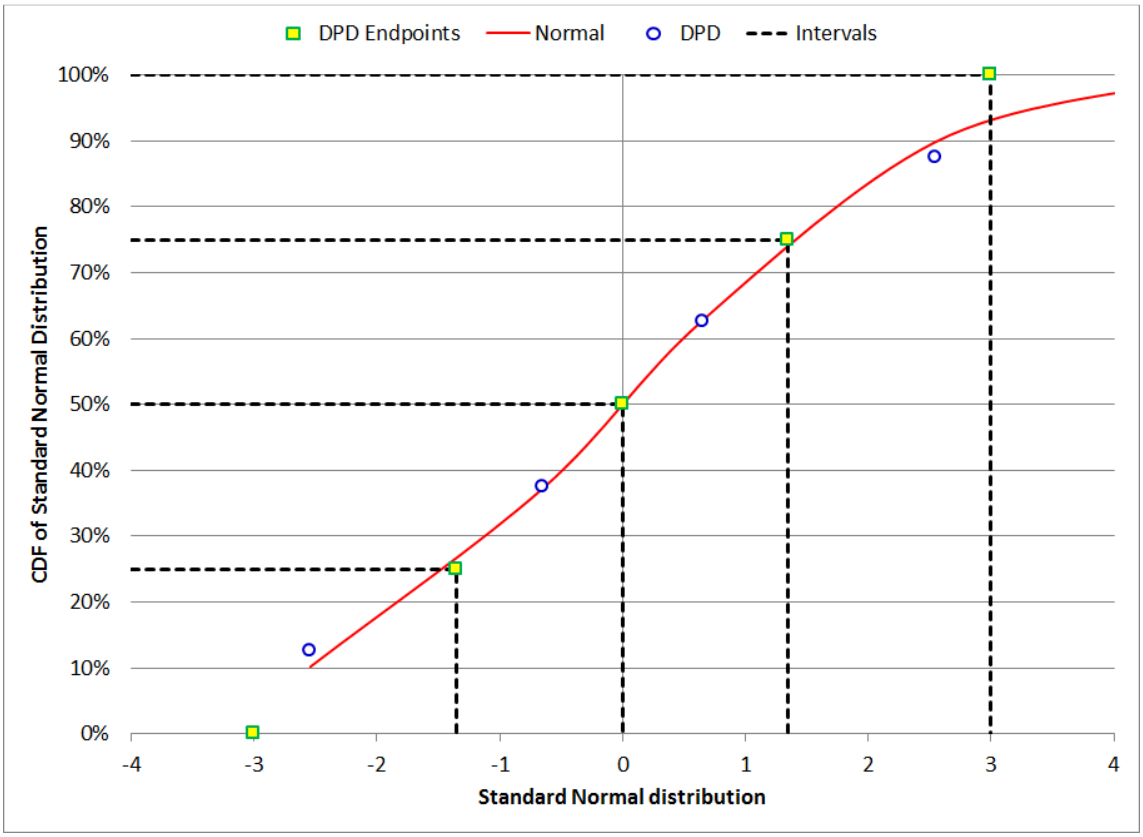
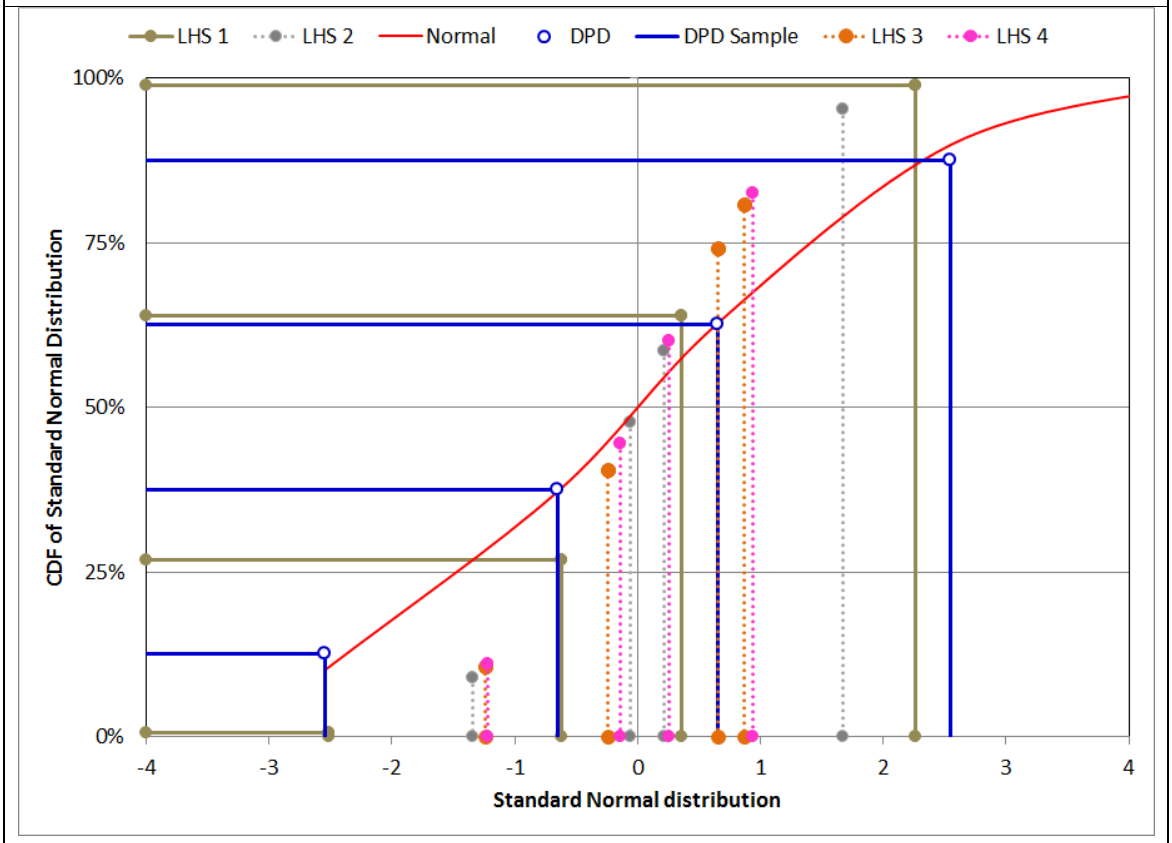


Figure 3 DPD Sampling Compared to LHS



To discuss this topic we introduce a theoretical fractured response surface. Figure 5 shows this is a case in which the response can assume several different peak values depending upon the combination of input values. Sampling from this input space to identify those regions in which there is a large response can be problematic. While LHS will cover a significant portion of the input space it covers a relatively small portion of the response space. The DPD method will cover the same portion of the response space but at the cost of requiring 5-10 times the number of evaluations. However, since the DPD method does not require equal probability intervals it is possible to rearrange the input PDF so that is sampled in areas of greatest interest. The question is: how does one know where the areas of greatest interest are a priori?

One method is to specify a value of the response above which we are interested.[*] In this case we save the input values and return to the DPD definition. Now we focus the PDF on the saved value for each input. Around this value we contract the DPD and expand it farther away from the current input value. We illustrate one method for these calculations although there many other methods could be used.

2.5. Golden Rule Clustering

We employ Fibonacci series for no reason other than its relationship to the golden rectangle and a desire to be mathematically elegant. We know that the golden rectangle ratio is $\varphi = \frac{1+\sqrt{5}}{2}$ and that the Nth Fibonacci number is given by

[*] For example, the crack depth is greater than 50% of the wall thickness.

$$F_N = \frac{\varphi^N - (1-\varphi)^N}{\sqrt{5}}$$

We now define the clustering exponent as γ. We now define intervals which are spaced according to the Golden Rule Clustering (GRC) concept. For the individual inputs we define z_0 as $x_{I,K}$ for the I[th] variable and the K[th] simulation. Then the total interval to the left and tight of z_0 is

$$\Delta_{LEFT} = \frac{2(z_0 - z_{left})}{N_{BIN}} \qquad \Delta_{RIGHT} = \frac{2(z_{Right} - z_0)}{N_{BIN}} \qquad \textbf{Equation 1}$$

We now calculate two normalization factors S_{Left} and S_{Right}. These are given by

$$S_{Left} = \sum_{I=1}^{\frac{N_{BIN}}{2}} \frac{F_I^{\gamma}}{F_{\frac{N_{Bin}}{2}}} \qquad S_{Right} = \sum_{I=\frac{N_{BIN}}{2}}^{N_{BIN}} \frac{F_I^{-\gamma}}{F_{\frac{N_{Bin}}{2}}} \qquad \textbf{Equation 2}$$

The variable γ controls the concentration at the pivot point. The new intervals for the clustering about the point z_0 are

$$x_1 \equiv x_{I,1}$$

$$x_L \equiv x_{I,L-1} + \Delta_{Left} \frac{F_L^{\gamma}}{F_{\frac{N_{BIN}}{2}}} \quad L \le \frac{N_{BIN}}{2}$$

$$x_L \equiv x_{I,L-1} + \Delta_{Right} \frac{F_L^{-\gamma}}{F_{\frac{N_{BIN}}{2}}} \quad L > \frac{N_{BIN}}{2}$$

For a value of γ equal to 1.0 this will lead to significant clustering about the input point z_0. This is because the Fibanocci series grows in magnitude very quickly. However by changing the value of γ away from zero we obtain more control of how tightly the PDF is clustered about the input (design) point.

2.6. Gamma Modification to Golden Rule Clustering

We first begin by examining the response space shown in Figure 4. In this response space the peaks of the three different points are roughly equal. We first show in Figure 5 the result of a 1,000 Monte Carlo simulation. Because it is difficult to see all of the points with the peaks and valleys we show a top down view, i.e. a projection of the results onto the X-Y plane, in Figure 6. As we see in these figures the 5,000 simulation does not find the "red" peak values. This is not unexpected since this is an area where the probability of the result if less than 1 in 1,000.

We now examine the impact of the GRC-γ methodology. One of the critical parameters for this method is the value of γ since this will define the amount of concentration of the PDF around the point of interest. To illustrate the adaptive approach a value of 1.0 is selected for γ. These results are shown in Figure 7. Because the response must be above a "trigger" value before the GRC method is employed[*] there are still some sample points in areas that are not

[*] If a trigger values is not used then the method will focus the sampling about the initial random sample which would actually make the GRC method less efficient for low probability calculations

of interest but once an area of interest is found the method becomes very efficient at sampling near the peak values.

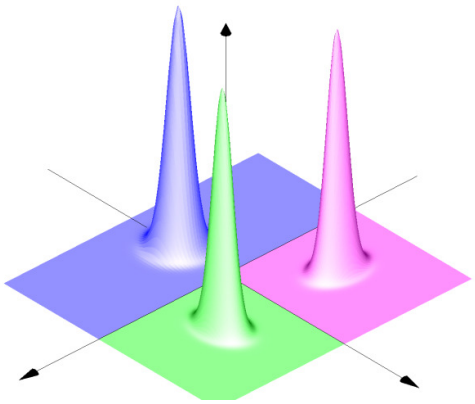


Figure 4

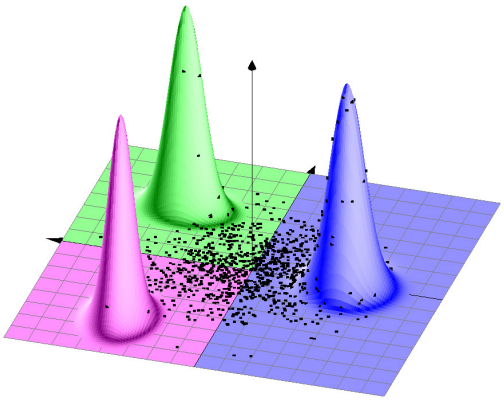


Figure 5 Monte Carlo 1,000 Simulations

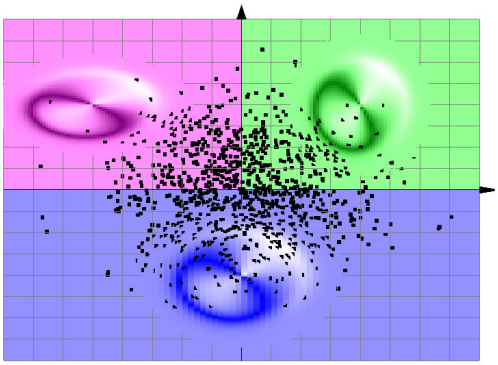


Figure 6 Projection of Monte Carlo 1,000 Simulations

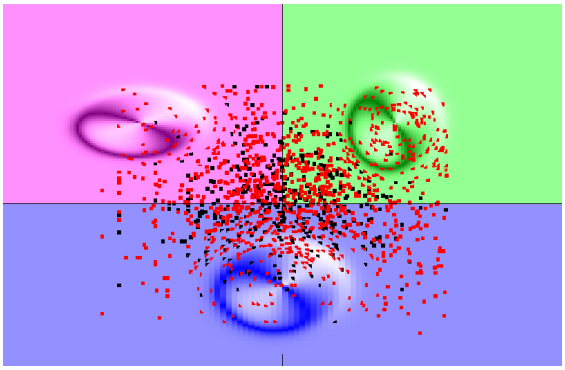


Figure 7 GRC 1,000 simulations in red compared to Monte Carlo 1,000 simulations in black

Of course if we wish to not spend as much time in areas of little interest we can set γ to a negative number. In Figure 8 we show the DPD after the GRC $+1.0\gamma$ application which we call the attractor method. In Figure 9 we show the GRC -1.0γ application, labelled the repulsar method.

In Figure 8 and Figure 9 the point indicated by the red circle, filled with yellow, is the pivot point, i.e. the point at which the contraction, or expansion, is made using Equation 1 and Equation 2.

While theoretical, hypothetical problems are useful in demonstrating the advantages and disadvantages of various methods it is also useful to assess how the methods work for actual engineering problems. This is done in the following section.

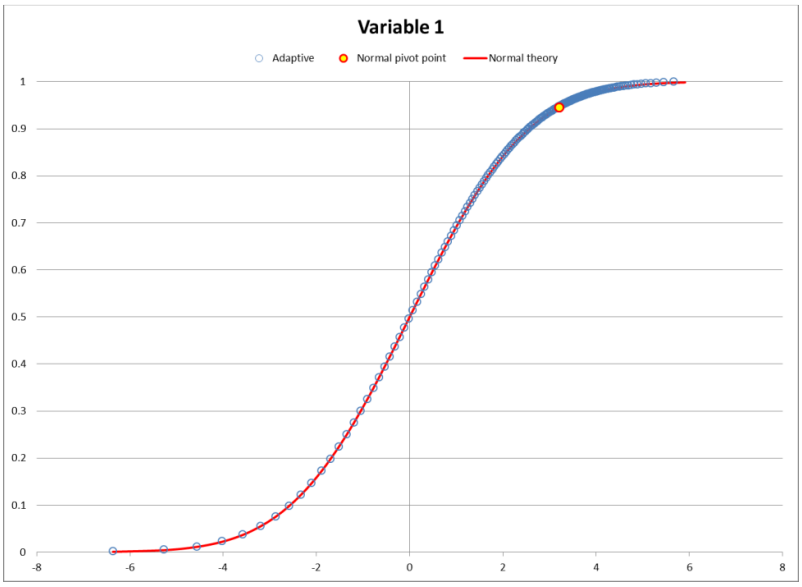


Figure 8 Variable DPD when γ is +1.0: Attractor case

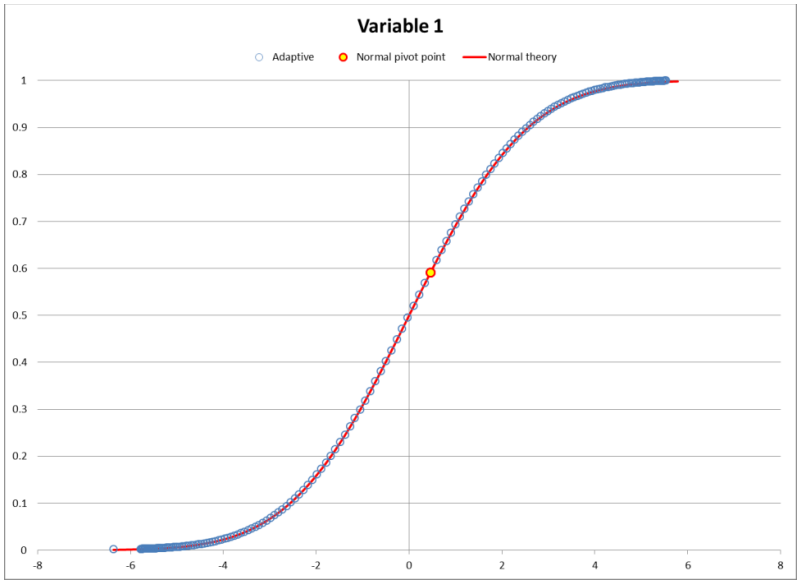


Figure 9 Variable DPD when γ is -1.0: Repulsor case

3 EXTREMELY LOW PROBABILITY OF RUPTURE (XLPR) PROGRAM DESCRIPTION

The xLPR program description is excerpted from reference [5].

> *"The Nuclear Regulatory Commission (NRC) Standard Review Plan (SRP) 3.6.3 describes Leak-Before-Break (LBB) assessment procedures that can be used to demonstrate compliance with the 10CFR50 Appendix A, GDC-4 requirement that primary system pressure piping exhibit an extremely low probability of rupture. SRP 3.6.3 does not allow for assessment of piping systems with active degradation mechanisms, such as Primary Water Stress Corrosion Cracking (PWSCC) which is currently occurring in systems that have been granted LBB exemptions.*
>
> ⋮

A multi-year project has begun that will first focus on the development of a viable method and approach to address the effects of PWSCC as well as define the requirements necessary for a modular-based assessment tool. A prototype xLPR model and pilot study case is first being conducted leveraging existing fracture mechanics models and software coupled to both a commercial and open source code framework to determine the framework and architecture requirements appropriate for building a modular-based code with this complexity. The pilot study phase is focusing on PWSCC in pressurizer surge nozzles. Later development phases will broaden the scope of xLPR to all primary piping systems in pressurized and boiling water reactors (PWR and BWR), using an incremental approach that incorporates the design requirements and lessons learned from previous iterations."

This program was used to calculate the time at which a crack growing in a nuclear pipe first becomes a through wall crack (TWC), or the time to first leakage.[*] In Figure 10 the results of a 1,000,000 Monte Carlo simulation is shown in red, while a 1,000 GRC simulation is shown in green. As this figure shows with 1,000 times less simulations the GRC method is giving a good estimate of the probability of the time to first leakage.

We compare the results of a 1,000,000 simulation standard Monte Carlo analysis and a 1,000 simulation GRC analysis in Figure 10 where the probability of the time to first leakage is calculated. With a *three order of magnitude* reduction in the number of simulations we are within 20% of the Monte Carlo analysis. In fact we obtain this reasonably accurate result in a number of simulations that is less than the number needed by the standard method to find the first instance of a TWC.

We can continue to perform GRC calculations to determine when the method reaches within the error bands of the standard Monte Carlo simulation. What we find is that a 100 bin 2,500 simulation GRC analysis obtains the 1,000,000 simulation Monte Carlo accuracy for a reduction of *400* in the computational time. These results are shown in Figure 11.

4 SUMMARY

This paper has presented an analysis methodology that can focus a complex computer simulation on areas of interest in order to calculate very low probability events and thus assess the risk. The method is fully automated so that the user does not have to do preliminary analysis to determine areas of focus for the sampling. However, as with any sampling method that focuses on specific, limited areas of interest in the input space not all variables can be included in the adaptive method. Sensitivity analyses and studies are used to identify those inputs which control the response variance. Such analyses are discussed in reference [6]. For a specific real world application of calculating the time to first leakage in a piping system it was found that the method can reduce the run times by a factor of 400 to 1,000. Because an individual simulation when the full stability analysis and leak rate codes are running take from 0.05 second to 2.5 seconds this allows a user to assess events whose probability of occurrence are 1 in 1,000,000 to reduce the rune time of the code from 14 hours (0.05 second runs) to 2 *minutes* (400 reduction in run times) or from 29 *days* (2.5 second run times) to 1.7 *hours*. This allows an analyst, designer, or regulator to quickly and accurately assess engineered systems and their uncertainty.

[*] For this discussion the probability of the first TWC is always take at 60 years of plant life.

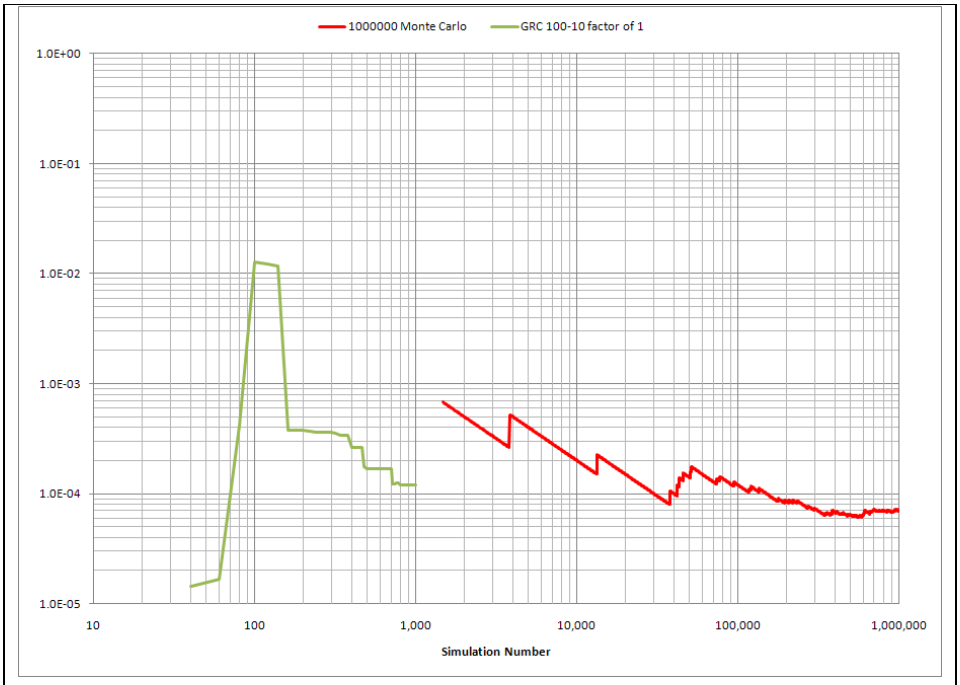


Figure 10. Comparison of 1,000,000 Monte Carlo to GRC TWC Calculations

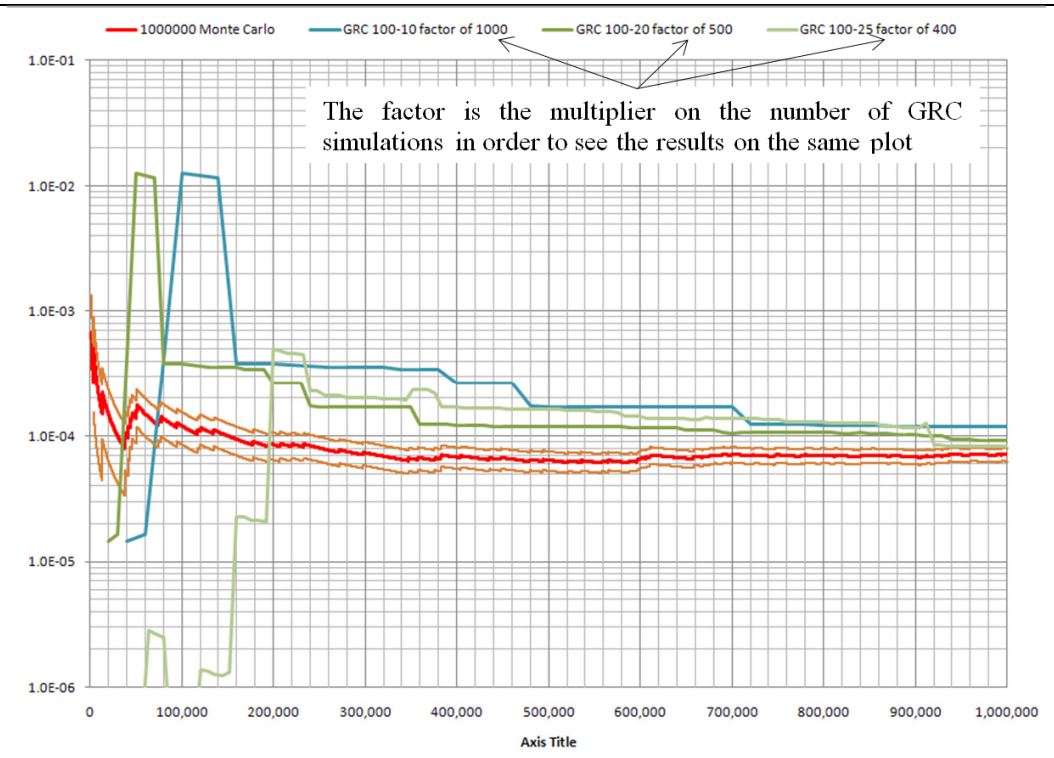


Figure 11 Number of GRC TWC Calculations Needed to Obtain Monte Carlo Accuracy

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