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DAKOTA Reliability Methods applied to RAVEN/RELAP-7

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Abstract

This report summarizes the result of a NEAMS project focused on the use of reliability methods within the RAVEN and RELAP-7 software framework for assessing failure probabilities as part of probabilistic risk assessment for nuclear power plants. RAVEN is a software tool under development at the Idaho National Laboratory that acts as the control logic driver and post-processing tool for the newly developed Thermal-Hydraulic code RELAP-7. Dakota is a software tool developed at Sandia National Laboratories containing optimization, sensitivity analysis, and uncertainty quantification algorithms. Reliability methods are algorithms which transform the uncertainty problem to an optimization problem to solve for the failure probability, given uncertainty on problem inputs and a failure threshold on an output response. The goal of this work is to demonstrate the use of reliability methods in Dakota with RAVEN/RELAP-7. These capabilities are demonstrated on a demonstration of a Station Blackout analysis of a simplified Pressurized Water Reactor (PWR).

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Chapter 1

Introduction

This report summarizes the result of a NEAMS project focused on the use of reliability methods within the RAVEN/RELAP-7 software framework for assessing failure probabilities as part of probabilistic risk assessment for nuclear power plants. RAVEN [1] is a software tool under development at the Idaho National Laboratory (INL) that acts as the control logic driver and post-processing tool for the newly developed Thermal-Hydraulic code RELAP-7. Dakota is a software tool developed at Sandia National Laboratories (SNL) containing optimization, sensitivity analysis, and uncertainty quantification algorithms. [2] Reliability methods are algorithms which transform the uncertainty problem to an optimization problem to solve for the failure probability, given uncertainty on problem inputs and a failure threshold on an output response. The goal of this work is to demonstrate the use of reliability methods in Dakota with RAVEN/RELAP-7. These capabilities are demonstrated on a demonstration of a Station Blackout analysis of a simplified Pressurized Water Reactor (PWR).

RAVEN (**R**eactor **A**nalysis and **V**irtual control **EN**vironment) is a software tool that provides on-line control and post-processing for the thermal-hydraulic RELAP-7 code (**R**eactor **E**xcursion and **L**eak **A**nalysis **P**rogram.) [1] [3] RAVEN is a multi-purpose Probabilistic Risk Assessment (PRA) software framework that is designed to derive and actuate the control logic required to simulate the plant control system and operator actions (guided procedures). It also can perform both Monte-Carlo sampling of random distributed events and event tree based analysis. RAVEN has been developed in a modular way. The RAVEN control logic and calculation driver are in Python, and the RAVEN/RELAP-7 interface is in C++. Note that both RAVEN and RELAP-7 are based on the MOOSE computational framework [4] which allows for rapid development of codes involving the solution of partial differential equations using the finite element method.

RAVEN has capabilities for performing uncertainty quantification (UQ), such as Monte Carlo sampling and other sampling methods. The focus of this project is to demonstrate a complementary class of algorithms, reliability methods, available in Dakota. In some contexts, reliability methods can be very efficient at determining probability of failure, requiring much fewer samples (e.g. RELAP-7 code runs) than sampling. We investigate the use of these methods on a problem of interest to RAVEN, Station Blackout for a PWR.

The outline of this report is as follows: Section 2 outlines reliability methods. Section 3 outlines the Station Blackout problem. Section 4 discusses the software integration of Dakota with RAVEN/RELAP-7, and Section 5 presents results.

Chapter 2

Reliability Methods

Reliability methods are probabilistic algorithms for quantifying the effect of uncertainties on response metrics of interest. In particular, they perform uncertainty quantification (UQ) by computing approximate response function distribution statistics based on specified probability distributions for input random variables. These response statistics include mean, standard deviation, and cumulative or complementary cumulative distribution function (CDF/CCDF) response level, and probability/reliability level pairings. These methods are often more efficient at computing statistics in the tails of the response distributions (events with low probability) than sampling-based approaches because the number of samples required to resolve a low probability can be prohibitive. Thus, these methods, as their name implies, are often used in a reliability context for assessing the probability of failure of a system when confronted with an uncertain environment.

Local reliability methods include the Mean Value method and the family of most probable point (MPP) search methods. Each of these methods is gradient-based, employing local approximations and/or local optimization methods. Global reliability methods include EGRA, the Efficient Global Reliability Analysis method. Local reliability methods, while computationally efficient, have well-known failure mechanisms. When confronted with a limit state function that is nonsmooth, local gradient-based optimizers may stall due to gradient inaccuracy and fail to converge to an MPP. Moreover, if the limit state is multimodal (multiple MPPs), then a gradient-based local method can, at best, locate only one local MPP solution. Finally, reliability methods may fail to adequately capture the contour of a highly nonlinear limit state. EGRA, which relies on a global Gaussian process surrogate model, is designed to overcome these limitations.

The following subsections explain the reliability methods in more detail. For a thorough explanation, the reader is encouraged to read Chapter 1 in the Dakota Theory Manual [5].

2.1 Mean Value Methods

The reliability method approximations are based on a Taylor Series expansion of the response. The form of the expansions and of the degree of the approximating analytical expression has evolved over time [6]. The Mean Value method (MV, also known as MVFOSM in [6]) is the simplest, least-expensive reliability method because it estimates the response means, response standard deviations, and all CDF/CCDF response-probability-reliability levels from a single evaluation of

response functions and their gradients at the uncertain variable means. This approximation can have acceptable accuracy when the response functions are nearly linear and their distributions are approximately Gaussian, but can have poor accuracy in other situations. The expressions for approximate response mean μ_g, approximate response variance σ_g^2, response target to approximate probability/reliability level mapping ($\bar{z} \rightarrow p, \beta$), and probability/reliability target to approximate response level mapping ($\bar{p}, \bar{\beta} \rightarrow z$) are

$$\mu_g = g(\mu_{\mathbf{x}}) \tag{2.1}$$

$$\sigma_g^2 = \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}}) \tag{2.2}$$

$$\bar{z} \rightarrow \beta: \qquad \beta_{\text{CDF}} = \frac{\mu_g - \bar{z}}{\sigma_g}, \quad \beta_{\text{CCDF}} = \frac{\bar{z} - \mu_g}{\sigma_g} \tag{2.3}$$

$$\bar{\beta} \rightarrow z: \qquad z = \mu_g - \sigma_g \bar{\beta}_{\text{CDF}}, \quad z = \mu_g + \sigma_g \bar{\beta}_{\text{CCDF}} \tag{2.4}$$

respectively, where $\mathbf{x}$ are the uncertain values in the space of the original uncertain variables ("x-space"), $g(\mathbf{x})$ is the limit state function (the response function for which probability-response level pairs are needed), and β_{CDF} and β_{CCDF} are the CDF and CCDF reliability indices, respectively.

The first-order CDF probability $p(g \leq z)$, first-order CCDF probability $p(g > z)$, β_{CDF}, and β_{CCDF} are related to one another through

$$p(g \leq z) = \Phi(-\beta_{\text{CDF}}) \tag{2.5}$$

$$p(g > z) = \Phi(-\beta_{\text{CCDF}}) \tag{2.6}$$

$$\beta_{\text{CDF}} = -\Phi^{-1}(p(g \leq z)) \tag{2.7}$$

$$\beta_{\text{CCDF}} = -\Phi^{-1}(p(g > z)) \tag{2.8}$$

$$\beta_{\text{CDF}} = -\beta_{\text{CCDF}} \tag{2.9}$$

$$p(g \leq z) = 1 - p(g > z) \tag{2.10}$$

where $\Phi()$ is the standard normal cumulative distribution function. A common convention in the literature is to define g in such a way that the CDF probability for a response level z of zero (i.e., $p(g \leq 0)$) is the response metric of interest. Second-order methods can also be used to calculcate CDF probability values. The second-order methods incorporate a curvature correction based on the principle curvatures of the limit state function.

2.2 MPP Search Methods

All other local reliability methods calculate the probability of failure by changing the uncertainty problem to an optimization problem. The uncertainty problem we are trying to solve is to calculate

a failure probability which is defined by the multi-dimensional integral given below:

$$P_{fail} = \iiint_{g(\mathbf{x})<0} f(x_1, x_2, ..., x_n)\, dx_1\, dx_2 ..., dx_n \tag{2.11}$$

The MPP search methods involve the transformation of the user-specified uncertain variables, $\mathbf{x}$, with a probability density function which can be non-normal and correlated, to a space of independent Gaussian random variables, $\mathbf{u}$, possessing a mean value of zero and unit variance (i.e., standard normal variables). In standard normal space, the probability contours are circular in nature. Also, the multi-dimensional integrals can be approximated by simple functions of a single parameter, β, called the reliability index. β is the minimum Euclidean distance from the origin in the transformed space to the response surface. This point is also known as the most probable point (MPP) of failure. The reliability methods use equality-constrained, nonlinear optimization algorithms to compute a most probable point (MPP) and then integrate about this point to compute probabilities. The MPP search is performed in uncorrelated standard normal space ("u-space") since it simplifies the probability integration: the distance of the MPP from the origin has the meaning of the number of input standard deviations separating the mean response from a particular response threshold. The transformation from correlated non-normal distributions (x-space) to uncorrelated standard normal distributions (u-space) is denoted as $\mathbf{u} = T(\mathbf{x})$ with the reverse transformation denoted as $\mathbf{x} = T^{-1}(\mathbf{u})$. These transformations are nonlinear in general, and possible approaches include the Rosenblatt [7] and Nataf [8] transformations. A graphic depicting reliability formulation in standard normal space is shown in Figure 2.1.

The forward reliability analysis algorithm of computing CDF/CCDF probability/reliability levels for specified response levels is called the reliability index approach (RIA), and the inverse reliability analysis algorithm of computing response levels for specified CDF/CCDF probability/reliability levels is called the performance measure approach (PMA) [9]. The differences between the RIA and PMA formulations appear in the objective function and equality constraint formulations used in the MPP searches. For RIA, the MPP search for achieving the specified response level $\bar{z}$ is formulated as computing the minimum distance in u-space from the origin to the $\bar{z}$ contour of the limit state response function:

$$\begin{aligned} &\text{minimize} && \mathbf{u}^T\mathbf{u} \\ &\text{subject to} && G(\mathbf{u}) = \bar{z} \end{aligned} \tag{2.12}$$

where $\mathbf{u}$ is a vector centered at the origin in u-space and $g(\mathbf{x}) \equiv G(\mathbf{u})$ by definition. For PMA, the MPP search for achieving the specified reliability level $\bar{\beta}$ or first-order probability level $\bar{p}$ is formulated as computing the minimum/maximum response function value corresponding to a prescribed distance from the origin in u-space:

$$\begin{aligned} &\text{minimize} && \pm G(\mathbf{u}) \\ &\text{subject to} && \mathbf{u}^T\mathbf{u} = \bar{\beta}^2 \end{aligned} \tag{2.13}$$

where $\bar{\beta}$ is computed from $\bar{p}$ using Eq. 2.7 or 2.8.

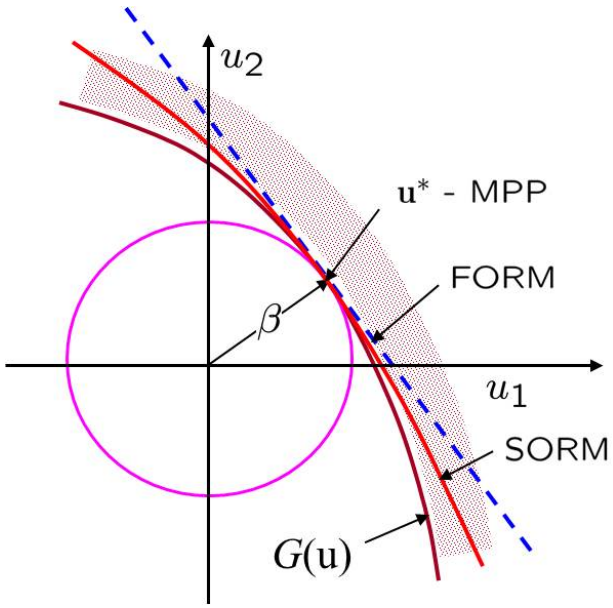

Figure 2.1. Reliability Optimization Formulation in standard normal space with two normalized inputs, u1 and u2. The failure region where $g(X) < 0$ is shown with shading: various approximations are noted. The Most Probable Point of Failure (MPP) is shown as well as the reliability index β.

In the RIA case, the optimal MPP solution $\mathbf{u}^*$ defines the reliability index from $\beta = \pm\|\mathbf{u}^*\|_2$, which in turn defines the CDF/CCDF probabilities (using Equations 2.5-2.6 in the case of first-order integration).

There are a variety of algorithmic variations that are available for use within RIA/PMA reliability analyses. First, one may select among several different limit state approximations that can be used to reduce computational expense during the MPP searches. Local, multipoint, and global approximations of the limit state are possible. For example, a commonly used approximation is a single Taylor series per response/reliability/probability level in x-space centered at the uncertain variable means. The first-order approach is commonly known as the Advanced Mean Value (AMV) method:

$$g(\mathbf{x}) \cong g(\mu_\mathbf{x}) + \nabla_x g(\mu_\mathbf{x})^T (\mathbf{x} - \mu_\mathbf{x}) \tag{2.14}$$

and the second-order approach has been named AMV^2:

$$g(\mathbf{x}) \cong g(\mu_\mathbf{x}) + \nabla_\mathbf{x} g(\mu_\mathbf{x})^T (\mathbf{x} - \mu_\mathbf{x}) + \frac{1}{2}(\mathbf{x} - \mu_\mathbf{x})^T \nabla^2_\mathbf{x} g(\mu_\mathbf{x})(\mathbf{x} - \mu_\mathbf{x}) \tag{2.15}$$

In addition, one can expand in u-space, one can use multi-point expansions, one can refine the estimate of the MPP iteratively, and one can perform the MPP search on the limit state directly without without the use of any approximations. Combining the last option with first-order and second-order integration approaches results in the methods called FORM (first-order reliability method) and SORM (second-order reliability method). Finally, there are variations on the way one calculates the Hessian matrix, one can use warm-starts if a sequence of reliability optimizations are performed, etc. These details are outlined in [5].

2.3 Global Reliability Methods

The global reliability method we use is called EGRA: Efficient Global Reliability Analysis. It is described in [10]. The idea is to construct an initial Gaussian process model of the response function and then update it strategically, by adding points that are likely to be near the region of the limit state surface, to get a better approximation of the limit state surface. In brief, EGRA begins with a Gaussian process model built from a very small number of samples, and then adaptively chooses where to generate subsequent samples to ensure that the model is accurate in the vicinity of the limit state. The resulting Gaussian process model is then sampled using multimodal adaptive importance sampling to calculate the probability of exceeding (or failing to exceed) the response level of interest.

By locating multiple points on or near the limit state, more complex and nonlinear limit states can be modeled, leading to more accurate probability integration. By concentrating the samples in the area where accuracy is important (i.e. in the vicinity of the limit state), only a small number of true function evaluations are required to build a quality surrogate model. The resulting method is computationally efficient even for expensive response functions. Note that EGRA does have some limitations: the response function needs to be well-approximated by a Gaussian process and the

Gaussian process construction is limited to at most dozens of random variables: Gaussian process models are usually built on ten variables or less. Thus, EGRA is not a method to use if one has hundreds or thousands of random inputs.

EGRA is described in [10] and in the DAKOTA Theory manual.

Chapter 3

Example Problem: Station Blackout

In order to show the capabilities of RAVEN coupled with RELAP-7/MOOSE, a simplified PWR PRA analysis has been employed.

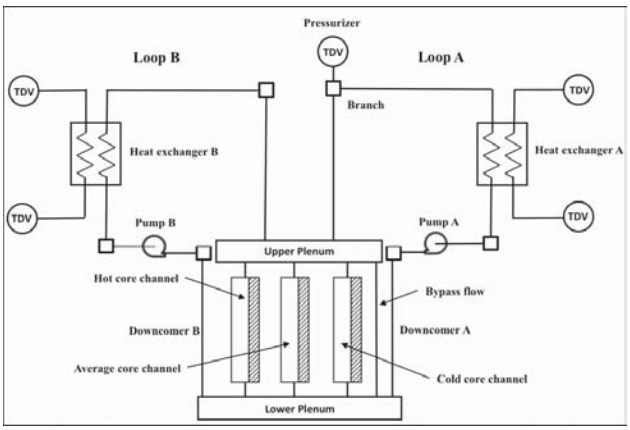

Figure 3.1. PWR model scheme.

Figure 3.1 shows the scheme of the PWR model. The reactor vessel model consists of the Down-comers, the Lower Plenum, the Reactor Core Model and the Upper Plenum. Core channels (flow channels with heat structure attached to each of them) were used to describe the reactor core. The core model consists of three parallel core channels and one bypass flow channel. There are two primary loops, i.e., loop A and loop B. Each loop consists of the Hot Leg, a Heat Exchanger and its secondary side pipes, the Cold Leg and a primary Pump. A Pressurizer is attached to the Loop A piping system to control the system pressure. A Time Dependent Volume (pressure boundary conditions) component is used to represent the Pressurizer. Since the RELAP-7 code does not have the two-phase flow capability yet, single-phase counter-current heat exchanger models are implemented to mimic the function of steam generators in order to transfer heat from the primary to the secondary.

The PRA station blackout sequence of events involves the following (starting from a steady-state operational condition of a Nuclear Power Plant [11]):

- 100.0 seconds: transient begins

- 101.0 seconds: loss of power grid and immediate shutdown of the reactor(scram):
  - Pump coast-down;
  - Decay heat power;
  - Diesel Generators and residual heat removal system (RHRS) not available.
- t_1: recovery of the diesel generators
- t_2: end of transient either for clad failure or 2500 seconds of simulation (PRA success)

A PRA analysis has been performed for a Station Black Out accident scenario by sampling the probability thresholds (i.e. branching triggers) on the CDFs of the recovery time of the diesel generators (DGs) t_1 (Normal distribution, mu = 800 s, sigma = 200 s) and the clad failure temperature TC_f (Triangular distribution, xPeak = 1477.59[1] K, xMin = 1255.37[2] K, xMax = 1699.82 K [12]).

For this problem, we defined failure to occur if the actual clad temperature in one of three channels tracked in the RAVEN/RELAP-7 simulation became greater than the clad failure temperature threshold. The implementation of the software and scripts necessary to assess the probability of failure is described in the next section.

[1] Typical PRA success criteria.
[2] 10 CFR50.46 limit.

Chapter 4

Software Framework

The software framework is one of the significant accomplishments of this effort. The framework involves coupling Dakota, RAVEN, and RELAP-7. Typically, RAVEN drives multiple simulations of RELAP-7 through its "Raven Runner" Python script. Figure 4.1 shows an example of how RAVEN drives multiple RELAP-7 runs to generate a Monte Carlo sample.

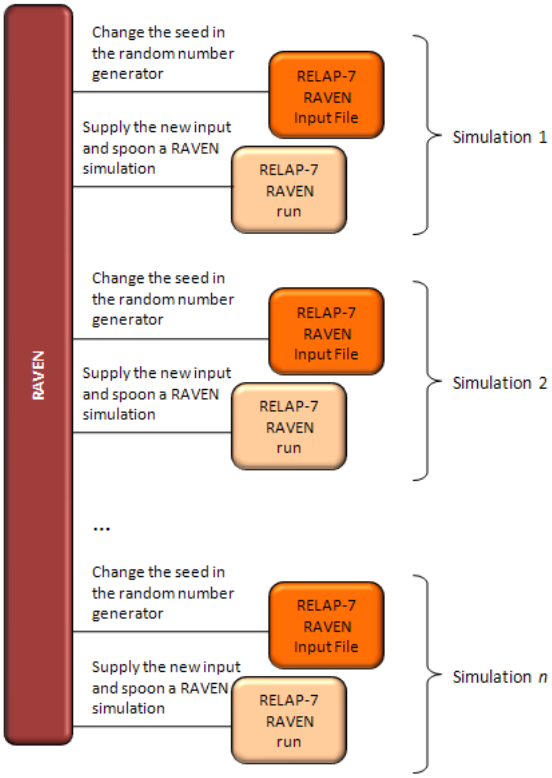

Figure 4.1. Schematic of RAVEN driving multiple RELAP-7 Runs for a Monte Carlo Sampling Study.

Dakota has a similar role as RAVEN: it iterates over simulation codes, and generates multiple simulation runs depending on the governing algorithms the user specifies (e.g. optimization, relia-

bility methods, sampling, sensitivity analysis). The generic role of Dakota governing a computational simulation is shown in Figure 4.2. Some types of analyses, such as optimization algorithms and reliability methods, involve feedback where Monte Carlo sampling does not. For example, after results are returned from a particular function evaluation, a Dakota algorithm may decide to go in a particular direction (e.g. an optimization method may want to go in the steepest descent direction), so the next set of parameters generated by Dakota for evaluation will reflect that.

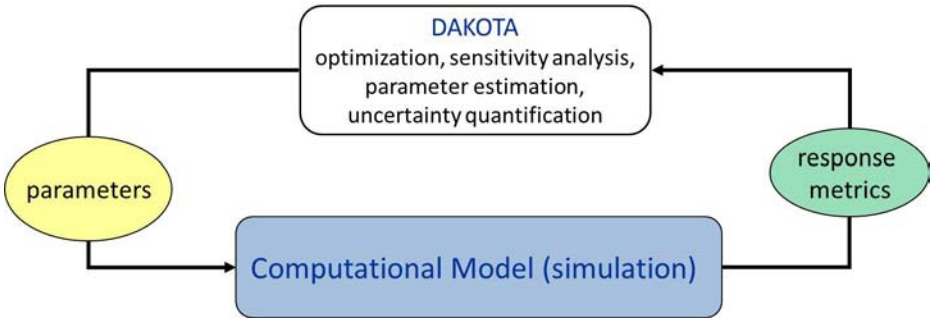

Figure 4.2. Generic Dakota Interface to Simulation

Figure 4.3 shows the particular implementation of Dakota around RAVEN/Relap-7. We have written a C-shell script (called run_raven_script) that is invoked every time Dakota requests a RAVEN/RELAP-7 function evaluation. This script substitutes the parameters for the diesel generator recovery time and clad failure temperature into the input file for RAVEN. The RAVEN controller in this particular example has been modified so that the RAVEN controller is not generating distributions as it typically does: RAVEN uses the Dakota parameters instead. RAVEN initializes and runs RELAP-7 through the RAVEN/RELAP-7 interface. More details on the tight coupling of the RAVEN/RELAP-7 interface are provided in [1].

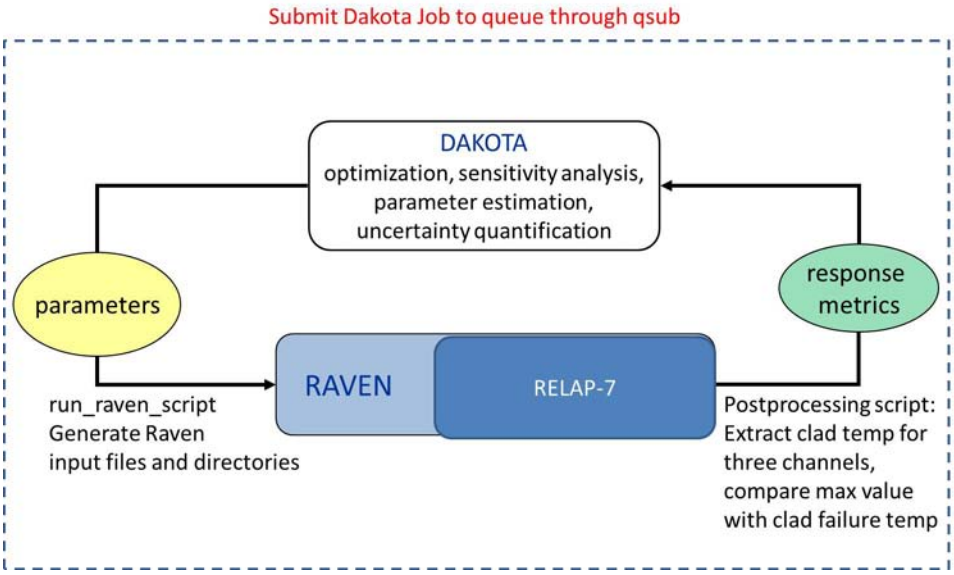

Figure 4.3. Specific Dakota interface to RAVEN/RELAP-7

Chapter 5

Results

For this problem, we ran 500 Latin Hypercube samples to determine a "baseline" probability of failure, where failure is defined as the actual clad temperature in one of three channels becoming greater than the clad failure temperature level. In the LHS run, 65 samples had a clad temperature greater then the failure threshold, resulting in a 13% failure probability. We ran two versions of local methods: the mean value method and the advanced mean value method (AMV), each with a Taylor series expansion of the limit state around the mean. These methods performed very well with a small number of function evaluations, as shown in Table 5.1. The fact that the mean value method did so well with only three function evaluations points to the fact that this is a fairly linear limit state that works well in this situation. Note that the mean value method takes a function evaluation at the mean of the input variables, and two more function evaluations (one in each direction of the two uncertain variables) to calculate the derivatives. We used a finite difference relative step size of 1.e-4. Thus the mean value method involved the following three function evaluations as shown in Table 5.2. The advanced mean value method performed the same three function evaluations, then created a Taylor series expansion which was used in an optimization step, with the fourth point being the optimal point from the optimization.

Figure 5.1 shows a graphical depiction of the limit state as a function of the two uncertain input variables. Finally, EGRA (the global reliability method, gave a good result after 27 function evaluations. EGRA first constructed six function evaluations (six is the number of points needed in two dimensions to create a second-order regression model). Then, EGRA consecutively adds points to refine the limit state until the "expected improvement criterion" converges. The expected improvement incorporates the accuracy of the limit state with the probability there may be other points which potentially could lie on the limit state.

In summary, this work shows the application of reliability methods to the SBO problem. It is

Table 5.1. Probability of Failure Estimates from Different Methods

Method	Number of Function Evaluations	Probability of Failure Estimate
Latin Hypercube Sampling (LHS)	500	0.13
Local Reliability Mean Value Method	3	0.13006
Local Reliability AMV	4	0.14023
Global Reliability (EGRA)	27	0.13211

Table 5.2. Function Evaluations performed in the Mean Value Method

Diesel Generator Recovery Time (s)	Clad Failure Threshold (K)	Maximum Clad Temperature from simulation (K)
800.0	1477.59297	1346.69
800.08	1477.59297	1346.69
800.0	1477.74073	1346.71

only a two-D problem with a fairly linear limit state function, but the results demonstrate the potential savings of using reliability methods to assess probability of failure for this class of problems. Future work may include the treatment of more uncertain variables with different distributions and more complicated limit states.

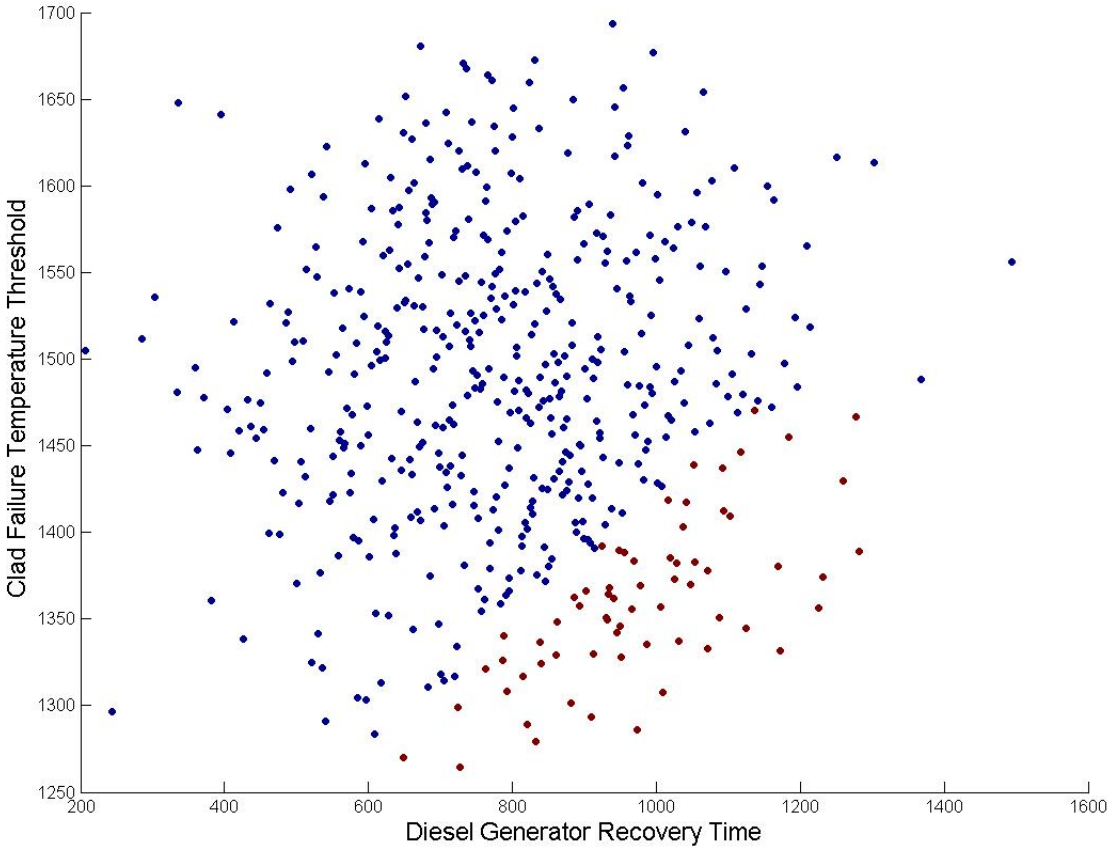

Figure 5.1. Failure (red dots) and Success (blue dots) points in the input space for the SBO problem

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