

# An Interval Multi-level Monte Carlo Method for Reliability Analysis of Imprecise Probabilistic Systems

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## Abstract

In the reliability analysis of systems, we will in general encounter both aleatoric and epistemic uncertainty. To account for epistemic uncertainty, we need to consider an imprecise probabilistic framework in the calculation of quantities of interest. In this work, we present a method for accurate estimation of interval-valued probabilities by applying an implementation of the multi-level Monte Carlo (MC) algorithm with an iterative optimization strategy. We postulate this to be a more mathematically rigorous alternative to the use of probability boxes to estimate the unknown CDF for the system being analyzed. We present several numerical examples to demonstrate the superior efficiency of the multi-level MC approach over the more traditional MC approach for estimating failure probabilities.

*Keywords:* Reliability analysis, Uncertainty quantification, Imprecise probability, Failure probability, Multi-level Monte Carlo, Optimization

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## 1. Introduction

Physical systems are often subject to uncertainty. The study of such systems requires uncertainty quantification (UQ), a process concerned with the characterization and propagation of uncertainty in the system. Most UQ methodologies are set in a probabilistic framework; see e.g. [22, 1, 8, 26, 6, 7, 13]. All these approaches assume that the uncertainty in the system is precisely known and can be described by precise probability density functions (PDFs). They may therefore be suitable for treating aleatoric (or random) uncertainty that arises from inherent randomness/variability in a system. Many physical systems may however exhibit a mixture of aleatoric and epistemic uncertainty, referred to as hybrid uncertainty, due to limited and/or in-

accurate information. For instance, the available data may be insufficient, or the mathematical model describing a system may be inaccurate. Such types of hybrid uncertainty may not be accurately represented by precise PDFs. Rather, one may need to consider an imprecise probabilistic framework; see e.g. [21, 23, 25, 24, 5]. One approach in this framework is to synthesize interval analysis and probability theory and build up interval-valued probability distributions [25]. This approach constructs a probability-box (or a *p-box*) consisting of a family of cumulative distribution functions (CDFs). The left and right envelopes of the family will form a *box* and bound the “unknown” distribution of the uncertain parameter from above and below.

In the present work we are concerned with the reliability analysis of systems that are subject to hybrid aleatoric-epistemic uncertainty. We particularly consider physical systems that are described by differential equations. Hence, the underlying mathematical models that we consider include sets of ordinary or partial differential equations with uncertain parameters represented by interval-valued probability distributions. An important quantity of interest (QoI) in reliability analysis is the *probability of failure*, measuring the likelihood that the system will fail at a given time or over a period of time. Examples include the probability that the maximum stress in a structure reaches a critical stress and the probability that the energy in a system exceeds a critical level. In an interval-valued probabilistic framework, as considered here, this quantity is an interval rather than a crisp real number. Our main goal is then the efficient computation of interval-valued failure probabilities in physical systems.

The computation of interval-valued failure probabilities requires interval arithmetic [12, 15], a numerical global optimization method; see e.g. [14, 20], and an algorithm for computing statistical moments; see e.g. [6, 4, 11, 10, 17, 8, 2, 27, 18]. Current computational methods are based on classical MC and quasi-MC techniques coupled with a numerical global optimization method, referred to as interval MC and interval quasi-MC, respectively; see e.g. [28]. Although quasi-MC sampling may improve the slow convergence rate of classical MC sampling in some cases, for QoIs with low regularity, such as failure probabilities, the advantage of quasi-MC over classical MC sampling is not significant and cannot be guaranteed; see e.g. [3, 16]. Hence, a major problem with both methods is that they feature a slow convergence rate. In the context of differential equations, among the available MC sampling techniques [6, 4, 11, 10, 17], two algorithms are particularly advantageous in terms of improving the convergence of classical MC sampling in the absence

of stochastic regularity: 1) multi-level MC sampling [4], and 2) multi-order MC sampling [17]. Here, we consider and explore the former and present an interval multi-level MC sampling strategy for computing interval-valued failure probabilities. In particular, we combine multi-level MC sampling with an implementation of Nelder-Mead algorithm [19] and apply the method to the reliability analysis of imprecise probabilistic systems.

The rest of the paper is organized as follows. Section 2 provides the mathematical formulation of the problem, including the representation of interval-valued probability distributions and the probability of failure. In Section 3 we discuss and analyze an interval MC sampling approach for computing failure probability. We next present our interval multi-level MC sampling strategy in Section 4. Finally, in Section 5 we provide two numerical examples and demonstrate the performance of the proposed multi-level MC sampling technique.

## 2. Problem Formulation

In this section, we first provide the mathematical foundations of interval-valued probability. We next present the formulation of the problem in an interval-valued probabilistic framework and the ultimate goal of computations. We then address the numerical treatment of the problem. Throughout the present paper, we denote by  $\mathbb{R}$  and  $\mathbb{R}_+$  the set of all real numbers and the set of all strictly positive real numbers, respectively.

### 2.1. Interval-valued probability

An interval-valued random variable is a generalization of a random variable. A random variable  $y : \Omega \rightarrow \mathbb{R}$  is a real-valued measurable function defined on a probability space  $(\Omega, \Sigma, P)$ , where  $\Omega$  is a sample space,  $\Sigma$  is a non-empty *sigma*-field on  $\Omega$ , and  $P$  is a probability measure assigned to each measurable subset of  $\Omega$  satisfying Kolmogorov's axioms [9]. Every realization of a random variable  $y(\omega)$ , for some  $\omega \in \Omega$ , is a real number. If  $P$  is an absolutely continuous measure [9], it can be described by a single CDF denoted by  $F$ , or alternatively by a single PDF denoted by  $\pi$  through the following relations

$$F(y_0) = P(y \leq y_0) = \int_{-\infty}^{y_0} \pi(\tau) d\tau, \quad y_0 \in \mathbb{R}.$$

72 The CDF and PDF are usually presented as functions of  $y_0 \in \mathbb{R}$  and a set of  
 73  $n$  crisp parameters  $\mathbf{z} = (z_1, \dots, z_n) \in \mathbb{R}^n$ :

$$F(y_0; \mathbf{z}) = \int_{-\infty}^{y_0} \pi(\tau; \mathbf{z}) d\tau, \quad y_0 \in \mathbb{R}, \quad \mathbf{z} \in \mathbb{R}^n. \quad (1)$$

This specifies a “parameterized CDF” for a random variable. For instance, for a normal random variable  $y \sim \mathcal{N}(z_1, z_2^2)$  with two parameters being the mean  $z_1 \in \mathbb{R}$  and standard deviation  $z_2 \in \mathbb{R}_+$ , the parameterized CDF reads:

$$F(y_0; \mathbf{z}) = \frac{1}{\sqrt{2\pi}z_2} \int_{-\infty}^{y_0} e^{\frac{-(\tau-z_1)^2}{2z_2^2}} d\tau, \quad y_0 \in \mathbb{R}, \quad \mathbf{z} = (z_1, z_2) \in \mathbb{R} \times \mathbb{R}_+.$$

74 This concept can be generalized to define interval-valued random variables.

75 **Definition 1.** Let  $\mathcal{I}(\mathbb{R})$  be the set of all closed intervals on the real line. An  
 76 interval-valued random variable  $\tilde{y} : \Omega \rightarrow \mathcal{I}(\mathbb{R})$  is an interval-valued measur-  
 77 able function on the sample space  $\Omega$ . Every realization of an interval-valued  
 78 variable  $\tilde{y}(\omega)$ , for some  $\omega \in \Omega$ , is a closed interval rather than a real number.

79 Throughout the present paper, we denote an interval-valued random vari-  
 80 able by the superimposition of a tilde over a letter. Hence by  $y$  and  $\tilde{y}$  we mean  
 81 a random variable and an interval-valued random variable, respectively.

82 One type of interval-valued random variables that we consider is a random  
 83 variable with interval-valued parameters. For example, a normal random  
 84 variable with mean  $Z_1 \in \mathcal{I}(\mathbb{R})$  and standard deviation  $Z_2 \in \mathcal{I}(\mathbb{R}_+)$  being  
 85 two closed intervals is a normal interval-valued random variable, denoted by  
 86  $\tilde{y} \sim \mathcal{N}(Z_1, Z_2^2)$ . It can be written in terms of a standard normal random  
 87 variable  $y \sim \mathcal{N}(0, 1)$  and the intervals  $Z_1$  and  $Z_2$  as  $\tilde{y} = Z_1 + y Z_2$ .

88 For this type of interval-valued random variables the *interval-valued CDF*,  
 89 denoted by  $\tilde{F}$ , can be defined by generalizing the parameterized representa-  
 90 tion (1) of the CDF for random variables as follows.

91 **Definition 2.** Let  $Z_i \in \mathcal{I}(\mathbb{R})$ ,  $i = 1, \dots, n$ , be  $n$  closed, bounded inter-  
 92 vals. Consider an interval-valued random variable  $\tilde{y}$ , consisting of a random  
 93 variable with  $n$  interval-valued parameters  $Z_1, \dots, Z_n$ . For any fixed point  
 94  $\mathbf{z} = (z_1, \dots, z_n)$  in  $\mathbf{Z} = (Z_1, \dots, Z_n)$ , the CDF of  $\tilde{y}$  is a parameterized CDF  
 95  $F(y_0; \mathbf{z})$  given as a function of  $y_0 \in \mathbb{R}$  and  $\mathbf{z}$  by (1). Let  $F_L$  and  $F_R$  be the  
 96 extrema of the family of all parameterized CDFs over  $\mathbf{Z}$ :

$$F_L(y_0) = \max_{\mathbf{z} \in \mathbf{Z}} F(y_0; \mathbf{z}), \quad F_R(y_0) = \min_{\mathbf{z} \in \mathbf{Z}} F(y_0; \mathbf{z}). \quad (2)$$

97 Then the interval-valued CDF of  $\tilde{y}$ , evaluated at  $y_0 \in \mathbb{R}$ , is the interval:

$$\tilde{F}(y_0) = [F_L(y_0), F_R(y_0)]. \quad (3)$$

98 The sets  $\{F_L(y_0), y_0 \in \mathbb{R}\}$  and  $\{F_R(y_0), y_0 \in \mathbb{R}\}$  form two left (upper) and  
 99 right (lower) envelopes encapsulating the family of all parameterized CDFs  
 100 from above and below and form a  $p$ -box.

101 We next define interval-valued random functions by generalizing the no-  
 102 tion of random functions.

103 **Definition 3.** Let  $\mathbf{y} = (y_1, \dots, y_m) \in \Gamma \subset \mathbb{R}^m$  be a vector of  $m$  random vari-  
 104 ables with a bounded joint PDF  $\pi = \pi(\mathbf{y}) : \Gamma \rightarrow \mathbb{R}_+$ . Let  $\mathbf{Z} = (Z_1, \dots, Z_n)$  be  
 105 a vector of  $n$  closed, bounded intervals  $Z_i \in \mathcal{I}(\mathbb{R})$ ,  $i = 1, \dots, n$ . An interval-  
 106 valued random function is a crisp map with arguments  $\mathbf{y}$  and  $\mathbf{Z}$ , generating  
 107 an output interval-valued random variable, written as  $\tilde{u} = u(\mathbf{y}, \mathbf{Z})$ .

We notice that an interval-valued random function can also be interpreted pointwise in  $\mathbf{y} \in \Gamma$ : at every realization, say  $\mathbf{y}_0 \in \Gamma$ , if the mapping  $u$  is continuous, the output  $u(\mathbf{y}_0, \mathbf{Z})$  is an interval given by

$$u(\mathbf{y}_0, \mathbf{Z}) = [\min_{\mathbf{z} \in \mathbf{Z}} u(\mathbf{y}_0, \mathbf{z}), \max_{\mathbf{z} \in \mathbf{Z}} u(\mathbf{y}_0, \mathbf{z})], \quad \forall \mathbf{y}_0 \in \Gamma.$$

If the mapping  $u$  is not continuous but is defined for all points  $\mathbf{z} \in \mathbf{Z}$ , we have:

$$\min_{\mathbf{z} \in \mathbf{Z}} u(\mathbf{y}_0, \mathbf{z}) \leq u(\mathbf{y}_0, \mathbf{Z}) \leq \max_{\mathbf{z} \in \mathbf{Z}} u(\mathbf{y}_0, \mathbf{z}), \quad \forall \mathbf{y}_0 \in \Gamma.$$

108 Similarly, we can define interval-valued spatio-temporal random processes  
 109 by generalizing the notion of spatio-temporal random processes.

**Definition 4.** Let  $D \subset \mathbb{R}^d$  be a compact spatial domain, with  $d = 1, 2, 3$ . Let further  $[0, T]$  be a time interval between zero and a final time  $T > 0$ . Consider a spatial variable  $\mathbf{x} = (x_1, \dots, x_d) \in D$ , a temporal variable  $t \in [0, T]$ , and let  $\mathbf{y}$  and  $\mathbf{Z}$  be as in Definition 3. An interval-valued spatio-temporal random processes, written as  $\tilde{u}(\mathbf{x}, t) = u(\mathbf{x}, t, \mathbf{y}, \mathbf{Z})$ , is an infinite collection of interval-valued random variables corresponding to all  $t \in [0, T]$  and all  $\mathbf{x} \in D$ :

$$\tilde{u} = \{u(\mathbf{x}, t, \mathbf{y}, \mathbf{Z}), \mathbf{x} \in D, t \in [0, T]\}.$$

110 Two particular types of interval-valued spatio-temporal random processes  
 111 include interval-valued temporal random processes (in the absence of  $\mathbf{x}$ ) and  
 112 interval-valued spatial random processes (in the absence of  $t$ ).

## 113 2.2. Problem statement

114 We are interested in computing the interval-valued failure probability of  
 115 physical systems described by a set of ODEs or PDEs within an interval-  
 116 valued probabilistic framework. In what follows, we consider the more gen-  
 117 eral case of time-dependent PDEs with uncertain parameters described by  
 118 interval-valued spatio-temporal random processes. Time-independent PDEs  
 119 and ODEs will then be particular cases of this general case.

120 Let  $u(\mathbf{x}, t, \mathbf{y}, \mathbf{Z})$  be the solution to a time-dependent PDE problem with  
 121 uncertain parameters described by interval-valued spatio-temporal random  
 122 processes. For example, we may consider the acoustic wave equation

$$u_{tt}(\mathbf{x}, t, \mathbf{y}, \mathbf{Z}) - \nabla \cdot (a^2(\mathbf{x}, \mathbf{y}, \mathbf{Z}) \nabla u(\mathbf{x}, t, \mathbf{y}, \mathbf{Z})) = f(\mathbf{x}, t, \mathbf{y}, \mathbf{Z}), \quad (4)$$

123 augmented with some initial-boundary conditions. Here,  $\mathbf{x} = (x_1, \dots, x_d) \in$   
 124  $D \subset \mathbb{R}^d$  and  $t \in [0, T]$  denote the  $d$ -dimensional spatial variables and time,  
 125 respectively,  $\mathbf{y} = (y_1, \dots, y_m) \in \Gamma \subset \mathbb{R}^m$  is a vector of  $m$  random variables  
 126 with a bounded joint PDF  $\pi$ , and  $\mathbf{Z} = (Z_1, \dots, Z_n)$  is a vector of  $n$  closed,  
 127 bounded intervals  $Z_i \in \mathcal{I}(\mathbb{R})$ ,  $i = 1, \dots, n$ . In this example the PDE solution  
 128  $u$  represents acoustic pressure, and the hybrid uncertainty may be in the  
 129 sound speed  $a$  and/or in the sound source  $f$ .

130 Let  $g(\mathbf{y}, \mathbf{Z})$  be an interval-valued random function related to  $u$ , referred  
 131 to as the *limit state function* [28]. The state function may be obtained by  
 132 applying an algebraic, differential, or integral operator on  $u$ . Suppose that  
 133 failure occurs when  $g(\mathbf{y}, \mathbf{Z}) \leq 0$ . For example, a mode of damage in a system  
 134 may initiate when the PDE solution at a fixed point  $(\mathbf{x}_0, t_0)$  in space and  
 135 time reaches a critical value  $u_{cr}$ , that is,  $g(\mathbf{y}, \mathbf{Z}) = u_{cr} - u(\mathbf{x}_0, t_0, \mathbf{y}, \mathbf{Z})$ .

136 The main goal is to compute the probability of failure, denoted by  $P_f$   
 137 and given by

$$P_f(\mathbf{Z}) := \int_{[g(\mathbf{y}, \mathbf{Z}) \leq 0]} \pi(\mathbf{y}) d\mathbf{y} = \mathbb{E}[\mathbb{I}_{[g(\mathbf{y}, \mathbf{Z}) \leq 0]}]. \quad (5)$$

138 Here,  $\mathbb{I}_{[.]}$  is the indicator function, taking the value 1 or 0 if the event  $[.]$  is  
 139 “true” or “false”, respectively. Introducing the QoI

$$Q(\mathbf{y}, \mathbf{Z}) = \mathbb{I}_{[g(\mathbf{y}, \mathbf{Z}) \leq 0]}, \quad (6)$$

140 we can express the failure probability (5) as the expected value of  $Q$  in (6):

$$P_f(\mathbf{Z}) = \mathbb{E}[Q(\mathbf{y}, \mathbf{Z})]. \quad (7)$$

141 We note that the failure probability, given by either (5) or (6)-(7), takes a  
 142 range of values rather than being a crisp number. However, since  $Q$  in (6)  
 143 may be discontinuous, the failure probability may not be a closed interval.  
 144 Hence, we are interested in computing its lower and upper bounds, denoted  
 145 by  $\underline{P}_f$  and  $\overline{P}_f$ , respectively:

$$\underline{P}_f := \min_{\mathbf{z} \in \mathbf{Z}} \mathbb{E}[Q(\mathbf{y}, \mathbf{z})] \leq P_f(\mathbf{Z}) \leq \max_{\mathbf{z} \in \mathbf{Z}} \mathbb{E}[Q(\mathbf{y}, \mathbf{z})] =: \overline{P}_f. \quad (8)$$

### 146 2.3. Numerical approach

147 A general method to numerically compute the minimum and maximum  
 148 failure probabilities in (8) consists of two parts: 1) a numerical global op-  
 149 timization procedure for computing global extrema, and 2) a sample-based  
 150 numerical algorithm for computing the expectation of a QoI given by solu-  
 151 tions to systems of differential equations. More precisely, we need to take  
 152 the following two steps:

- 153 1. We first need to utilize a numerical optimization procedure which can  
 154 find the global extrema of  $P_f(\mathbf{z})$  for  $\mathbf{z} \in \mathbf{Z}$ . This can be done, for  
 155 instance, by an iterative method; see e.g. [14, 20]. The choice of the  
 156 method would depend on the dimension of  $\mathbf{Z}$ . In general, an iterative  
 157 optimization algorithm requires  $M_o$  function evaluations  $P_f(\mathbf{z}^{(k)})$  at  
 158 some fixed points  $\{\mathbf{z}^{(k)}\}_{k=1}^{M_o} \in \mathbf{Z}$ , to be determined by the algorithm.
- 159 2. Each function evaluation  $P_f(\mathbf{z}^{(k)})$  amounts to computing the expecta-  
 160 tion  $\mathbb{E}[Q(\mathbf{y}, \mathbf{z}^{(k)})]$ , which may be done by a MC sampling strategy; see  
 161 e.g. [6, 4, 11, 10, 17]. Using  $M_s$  samples, the sampling algorithm needs  
 162  $M_s$  realizations of  $Q(\mathbf{y}^{(m)}, \mathbf{z}^{(k)})$ , with  $m = 1, \dots, M_s$ , for each fixed  $k$ .  
 163 The approximation of each realization  $Q(\mathbf{y}^{(m)}, \mathbf{z}^{(k)})$  can be done by a  
 164 deterministic discretization method to compute the numerical solution  
 165 to the underlying set of differential equations and thereby to obtain  
 166 an approximation  $Q_h(\mathbf{y}^{(m)}, \mathbf{z}^{(k)})$ , where  $h$  denotes the time step or the  
 167 mesh/grid size in the discretization.

168 We notice that one may think that in step 2 a spectral stochastic method (see  
 169 e.g. [8, 2, 27, 18]) would be a better alternative to a MC sampling approach.  
 170 However, since  $Q$  is the indicator function and hence irregular with respect  
 171 to  $\mathbf{y}$ , spectral stochastic methods that rely on the high regularity of QoIs will  
 172 not work.

Now let  $\underline{\mathcal{P}}_f$  and  $\overline{\mathcal{P}}_f$  be the approximations to  $\underline{P}_f = \min_{\mathbf{z} \in \mathbf{Z}} P_f(\mathbf{z})$  and  $\overline{P}_f = \max_{\mathbf{z} \in \mathbf{Z}} P_f(\mathbf{z})$ , respectively, obtained by the above two steps. In these approximations two major errors are incurred. The first error is due to the sample-based algorithm for estimating the expectation

$$P_f(\mathbf{z}) = \mathbb{E}[Q(\mathbf{y}, \mathbf{z})] \approx \mathcal{P}_f(\mathbf{z}), \quad \forall \mathbf{z} \in \mathbf{Z},$$

at any given point  $\mathbf{z} \in \mathbf{Z}$ . The second error is due to imperfect minimization or maximization

$$\min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) \approx \underline{\mathcal{P}}_f, \quad \max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) \approx \overline{\mathcal{P}}_f.$$

Correspondingly, we may split the total error in the approximation into two parts, as follows. We write

$$\begin{aligned} \underline{\varepsilon} &:= |\underline{P}_f - \underline{\mathcal{P}}_f| \leq \left| \min_{\mathbf{z} \in \mathbf{Z}} P_f(\mathbf{z}) - \min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) \right| + \left| \min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \underline{\mathcal{P}}_f \right| \\ &\leq \max_{\mathbf{z} \in \mathbf{Z}} |P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})| + \left| \min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \underline{\mathcal{P}}_f \right|, \end{aligned}$$

$$\begin{aligned} \overline{\varepsilon} &:= |\overline{P}_f - \overline{\mathcal{P}}_f| \leq \left| \max_{\mathbf{z} \in \mathbf{Z}} P_f(\mathbf{z}) - \max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) \right| + \left| \max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \overline{\mathcal{P}}_f \right| \\ &\leq \max_{\mathbf{z} \in \mathbf{Z}} |P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})| + \left| \max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \overline{\mathcal{P}}_f \right|, \end{aligned}$$

173 where  $\underline{\varepsilon}$  and  $\overline{\varepsilon}$  are the error in the approximate lower and upper bounds,  
174 respectively. We now set

$$\varepsilon_s := \max_{\mathbf{z} \in \mathbf{Z}} |P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})|, \quad \varepsilon_o := \max(|\min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \underline{\mathcal{P}}_f|, |\max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z}) - \overline{\mathcal{P}}_f|), \quad (9)$$

175 where  $\varepsilon_s$  is the error in the sample-based algorithm, and  $\varepsilon_o$  is the error in  
176 the numerical optimization procedure. We then have

$$\varepsilon_{\text{TOTAL}} := \max(\underline{\varepsilon}, \overline{\varepsilon}) \leq \varepsilon_s + \varepsilon_o. \quad (10)$$

177 In practical applications, we usually need to numerically compute the  
178 minimum and maximum failure probabilities in (8) to within a desired tol-  
179 erance  $\varepsilon_{\text{TOL}}$ , that is, we need to have  $\varepsilon_{\text{TOTAL}} \leq \varepsilon_{\text{TOL}}$ . Moreover, it is often  
180 desired to achieve this tolerance with minimum computational cost. This  
181 suggests that we may select the numerical optimization method and the  
182 numerical parameters in the sampling method, including  $M_s$  and  $h$ , by mini-  
183 mizing the computational cost subject to the error constraint  $\varepsilon_s + \varepsilon_o = \varepsilon_{\text{TOL}}$ .



### 184 3. Interval Monte Carlo sampling

185 In this section, we discuss and analyze an interval MC sampling approach  
186 for computing interval-valued failure probabilities.

#### 187 3.1. General strategy

The goal is to compute both  $\underline{P}_f$  and  $\overline{P}_f$  to within a given tolerance  $\varepsilon_{\text{TOL}}$ , that is, we want

$$\underline{\varepsilon} = |\underline{P}_f - \underline{\mathcal{P}}_f| \leq \varepsilon_{\text{TOL}} \quad \text{and} \quad \overline{\varepsilon} = |\overline{P}_f - \overline{\mathcal{P}}_f| \leq \varepsilon_{\text{TOL}}.$$

188 For this purpose, we use (10) and require

$$\varepsilon_o + \varepsilon_s \leq \alpha \varepsilon_{\text{TOL}} + (1 - \alpha) \varepsilon_{\text{TOL}} = \varepsilon_{\text{TOL}}, \quad \alpha \in (0, 1), \quad (11)$$

189 where  $\alpha$  is a splitting parameter. As an example we may set  $\alpha = 0.5$ .

190 We consider an implementation of the Nelder-Mead direct simplex search  
191 algorithm [19] to numerically find both the minimum and maximum of  $\mathcal{P}_f(\mathbf{z})$ .  
192 The algorithm takes initial guesses for  $\arg \min_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z})$  and  $\arg \max_{\mathbf{z} \in \mathbf{Z}} \mathcal{P}_f(\mathbf{z})$   
193 and iteratively finds a sequence of test points in  $\mathbf{Z} \subset \mathbb{R}^n$  arranged as the  
194 vertices of a set of  $(n + 1)$ -dimensional simplexes, until the following two  
195 conditions are satisfied:

- 196 • The maximum Euclidean distance between any pair of the last  $n + 1$   
197 test points in the final simplex is within  $\alpha \varepsilon_{\text{TOL}}$ .
- 198 • The maximum distance between  $\mathcal{P}_f(\mathbf{z})$  evaluated at any pair of the last  
199  $n + 1$  test points in the final simplex is within  $\alpha \varepsilon_{\text{TOL}}$ .

200 We use the above two stopping criteria as indications of the convergence of  
201 the optimiaztion algorithm satisfying the requirement  $\varepsilon_o \leq \alpha \varepsilon_{\text{TOL}}$  in (11).  
202 Assuming this can be achieved with  $M_o$  iterations, we need  $M_o$  evaluations of  
203  $\mathcal{P}_f(\mathbf{z})$  at the points  $\mathbf{z}^{(k)}$ ,  $k = 1, \dots, M_o$ . At any such fixed point, the Monte  
204 Carlo estimator reads

$$\mathcal{P}_f(\mathbf{z}^{(k)}) = \frac{1}{M_s} \sum_{m=1}^{M_s} \mathbb{I}_{[g_h(\mathbf{y}^{(m)}, \mathbf{z}^{(k)}) \leq 0]}, \quad k = 1, \dots, M_o. \quad (12)$$

205 Here,  $g_h(\mathbf{y}^{(m)}, \mathbf{z}^{(k)})$  is the approximate value of the *limit state function* at the  
206 point  $(\mathbf{y}^{(m)}, \mathbf{z}^{(k)})$  computed by a discretization method with a time step or a  
207 mesh/grid size  $h$ . The parameter  $h$  and the number of MC samples  $M_s$  are  
208 selected so that  $|\underline{P}_f(\mathbf{z}^{(k)}) - \mathcal{P}_f(\mathbf{z}^{(k)})| \leq (1 - \alpha) \varepsilon_{\text{TOL}}$  for all  $k = 1, \dots, M_o$ .  
209 This will guarantee that  $\varepsilon_s \leq (1 - \alpha) \varepsilon_{\text{TOL}}$  in (11) is achieved.

210 **Remark 1.** Another MC formulation for minimum and maximum failure  
 211 probability estimates is suggested in [28], given by

$$\underline{P}_f = \frac{1}{M_s} \sum_{m=1}^{M_s} \mathbb{I}_{[\max_{\mathbf{z} \in \mathbf{Z}} g_h(\mathbf{y}^{(m)}, \mathbf{z}) \leq 0]}, \quad \bar{P}_f = \frac{1}{M_s} \sum_{m=1}^{M_s} \mathbb{I}_{[\min_{\mathbf{z} \in \mathbf{Z}} g_h(\mathbf{y}^{(m)}, \mathbf{z}) \leq 0]}. \quad (13)$$

212 Obviously, compared to our formulation, these estimates are conservative.  
 213 In addition, the estimators  $\underline{P}_f$  and  $\bar{P}_f$  in (13) do not necessarily converge  
 214 to  $\underline{P}_f$  and  $\bar{P}_f$ , respectively, as  $M_s \rightarrow \infty$  and  $h \rightarrow 0$ . This latter issue is  
 215 demonstrated for the two numerical examples in Section 5.

216 In the remainder of this section, we discuss a general strategy for the  
 217 optimal selection of the numerical parameters,  $h$  and  $M_s$ , and apply the  
 218 strategy to ODEs and time-dependent PDEs.

### 219 3.2. Cost-error analysis

220 We propose to optimally select the numerical parameters  $h$  and  $M_s$  in the  
 221 MC estimator (12) by minimizing the computational cost subject to the error  
 222 constraint  $\varepsilon_s \leq (1 - \alpha) \varepsilon_{TOL}$ . We use the method of Lagrange multipliers as  
 223 follows.

224 We first note that  $\varepsilon_s \geq |P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})|$ ,  $\forall \mathbf{z} \in \mathbf{Z}$ ; see (9). We then split  
 225 the error due to the sample-based algorithm into two parts:

$$|P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})| \leq \underbrace{|\mathbb{E}[Q(\mathbf{y}, \mathbf{z})] - \mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})]|}_{\varepsilon_I} + \underbrace{|\mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})] - \mathcal{P}_f(\mathbf{z})|}_{\varepsilon_{II}} \leq (1 - \alpha) \varepsilon_{TOL}. \quad (14)$$

226 The first term  $\varepsilon_I$  in (14) is the discretization error of the deterministic solver  
 227 that satisfies

$$\varepsilon_I \leq c_1 h^q, \quad \forall \mathbf{y} \in \Gamma, \quad (15)$$

228 where  $c_1$  is a positive constant, and  $q$  is the order of the deterministic dis-  
 229 cretization solver in computing  $\mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})]$ . Note that we cannot actually  
 230 calculate  $\mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})]$  and therefore must choose a reasonably large number  
 231 of random samples and use the same set of random samples for a set of dif-  
 232 ferent step sizes in order to estimate  $c_1$  and  $q$ . Note also that for different  
 233 parameters  $\mathbf{z}$ , there will be different values of  $c_1$  and  $q$ . As the optimal step  
 234 size  $h$  and sample size  $M_s$  will each depend on  $c_1$  and  $q$ , we want to settle  
 235 on one value of  $q$  and one value of  $c_1$  which will work for any input  $\mathbf{z} \in \mathbf{Z}$ .  
 236 This is done by estimating values of  $c_1$  and  $q$  using least squares for a set

of step sizes for each of a set of values of  $\mathbf{z}$ . The maximum least squares estimator  $\hat{c}_1(\mathbf{z})$  is taken to be  $c_1$ , and the minimum least squares estimator  $\hat{q}(\mathbf{z})$  is taken to be  $q$ . This is to be conservative because, as shown later in this section, the optimal step size decreases for larger  $c_1$  and smaller  $q$ . The optimal sample size  $M_s$  also increases for smaller  $q$ .

The second error term,  $\varepsilon_{II}$  is the statistical error. First, we know that the variance,  $\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  of our QoI is bounded (since the expected value is bounded; see proof in Section 4). Then the Central Limit Theorem gives

$$\varepsilon_{II} = |\mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})] - \frac{1}{M_s} \sum_{i=1}^{M_s} \mathbb{I}_{[g_h(\mathbf{y}_i, \mathbf{z}) \leq 0]}| \leq c_2 \frac{\sqrt{\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]}}{\sqrt{M_s}} \quad (16)$$

with the notation  $\leq$  understood to mean that

$$P\left(\varepsilon_{II} \leq c_2 \frac{\sqrt{\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]}}{\sqrt{M_s}}\right) = 2\phi(c_2) - 1, \quad \text{as } M_s \rightarrow \infty \quad (17)$$

where  $P$  denotes a probability measure, and  $\phi(c_2) = \int_{-\infty}^{c_2} \frac{1}{\sqrt{2\pi}} e^{-\tau^2/2} d\tau$  is the CDF for the standard normal random variable  $c_2$ . The computational cost, or work, of computing the Monte Carlo estimator for each input vector  $\mathbf{z}$  is denoted by  $W_{MC}$ . The expression of computational cost will be different depending on whether we are working with an ODE or a PDE, and it is appropriate to break into two subsections at this point.

### 3.3. ODEs

For ODEs, because we are dealing with one independent variable, the work is given by  $W_{MC} \propto M_s q h^{-1}$ . To choose optimal  $h$  and  $M_s$ , we solve the following minimization problem, with  $c_3 = c_2 \sqrt{\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]}$ .

$$\min_{h, M_s} M_s q h^{-1} \quad \text{s.t.} \quad c_1 h^q + c_3 M_s^{-1/2} = (1 - \alpha) \varepsilon_{TOL} \quad (18)$$

The Lagrangian is given by

$$L(h, M_s, \lambda) = M_s q h^{-1} + \lambda(c_1 h^q + c_3 M_s^{-1/2} - (1 - \alpha) \varepsilon_{TOL}) \quad (19)$$

We enforce  $\partial_h L = \partial_{M_s} L = \partial_\lambda L = 0$ . After some algebraic manipulations, the optimal step size and optimal sample size are found to be

$$\begin{aligned} h &= \left( \frac{(1 - \alpha) \varepsilon_{TOL}}{c_1 (1 + 2q)} \right)^{1/q} \\ M_s &= c_2^2 \mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})] \left( \frac{1 + 2q}{2q} \right) ((1 - \alpha) \varepsilon_{TOL})^{-2} \end{aligned} \quad (20)$$

259 Finally, with the expressions given in (20), the optimal work is

$$W_{OPT} \propto \mathcal{O}(((1 - \alpha)\varepsilon_{TOL})^{-(2+1/q)}) \quad (21)$$

### 260 3.4. Time-Dependent PDEs

261 For time-dependent PDEs, we consider the Method of Lines in which  
 262 the PDE is discretized in space with the time variable considered contin-  
 263 uous. This changes the PDE into an initial value ODE problem. Finite  
 264 differencing is used for both spatial and temporal discretization. Assuming  
 265 that the temporal step size may be computed from the grid size (e.g. the  
 266 CFL condition for hyperbolic PDEs), the computational cost is estimated  
 267 by  $W_{MC} \propto M_s h^{-(1+d)}$ , for  $d$  spatial dimensions where  $h$  is the characteristic  
 268 grid size for the spatial discretization. For ODEs,  $d = 0$ . The optimization  
 269 problem is given by

$$\min_{h, M_s} M_s h^{-(1+d)} \quad \text{s.t.} \quad c_1 h^q + c_3 M_s^{-1/2} = (1 - \alpha)\varepsilon_{TOL} \quad (22)$$

270 The Lagrangian is given by

$$L(h, M_s, \lambda) = M_s h^{-(1+d)} + \lambda(c_1 h^q + c_3 M_s^{-1/2} - (1 - \alpha)\varepsilon_{TOL}) \quad (23)$$

271 Enforcing  $\partial_h L = \partial_{M_s} L = \partial_\lambda L = 0$  and performing the necessary algebraic  
 272 manipulations, the optimal grid size  $h$  and sample size  $M_s$  are given by

$$\begin{aligned} h &= \left( \frac{\varepsilon_s}{c_1(1 + 2q/(1 + d))} \right)^{1/q} \\ M_s &= c_2^2 \mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})] \left( \frac{1 + d + 2q}{2q} \right) ((1 - \alpha)\varepsilon_{TOL})^{-2} \end{aligned} \quad (24)$$

273 Using (24), the optimal work is

$$W_{OPT} \propto \mathcal{O}(((1 - \alpha)\varepsilon_{TOL})^{-(2+1/q+d/q)}) \quad (25)$$

274 As expected, the cost for the Interval Monte Carlo sampling where the QoI  
 275 depends on the solution to a PDE will be increase exponentially as the di-  
 276 mension of the problem increases.

## 277 4. Interval Multi-Level Monte Carlo Sampling

278 In this section, we discuss and analyze an interval multi-level Monte Carlo  
 279 sampling approach for computing failure probability. The optimization ap-  
 280 proach is the same as in Section 3, We consider the problem of computing  
 281  $\mathcal{P}_f(\mathbf{z})$  such that  $|P_f(\mathbf{z}) - \mathcal{P}_f(\mathbf{z})| \leq (1 - \alpha)\varepsilon_{TOL}$ , but this time with the esti-  
 282 mator  $\mathcal{P}_f$  defined as

$$\mathcal{P}_f(\mathbf{z}) = \mathcal{A}_{MLMC}(\mathbf{z}), \quad (26)$$

283 where  $\mathcal{A}_{MLMC}$  is the multi-level Monte Carlo (MLMC) estimator of  $\mathbb{E}[Q(\mathbf{y}, \mathbf{z})]$ .  
 284 In this section, the goal is to achieve the same error condition (14).

### 285 4.1. General method for multi-level Monte Carlo sampling

286 To build up the MLMC estimator, we start with a decreasing sequence  
 287 of mesh sizes  $h_0 > h_1 > \dots > h_L$  defined by

$$h_l = h_0 \beta^{-l}, \quad l = 0, 1, \dots, L \quad \beta \geq 2 \quad (27)$$

With a telescoping sum,

$$\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z})] = \mathbb{E}[Q_0(\mathbf{y}, \mathbf{z})] + \sum_{i=1}^L \mathbb{E}[Q_i(\mathbf{y}_i, \mathbf{z}) - Q_{i-1}(\mathbf{y}_i, \mathbf{z})],$$

288 where  $\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z})] = \mathbb{E}[Q_h(\mathbf{y}, \mathbf{z})]$  with  $h = h_0 \beta^{-L}$ . The MLMC estimator is  
 289 an approximation of  $\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z})]$  computed by taking sample averages.

$$\mathcal{A}_{MLMC}(\mathbf{z}) = \frac{1}{M_0} \sum_{m_0=1}^{M_0} Q_0(\mathbf{y}^{m_0}, \mathbf{z}) + \sum_{l=1}^L \frac{1}{M_l} \sum_{m_l=1}^{M_l} [Q_l(\mathbf{y}^{m_l}, \mathbf{z}) - Q_{l-1}(\mathbf{y}^{m_l}, \mathbf{z})] \quad (28)$$

290 The term  $\varepsilon_I$  in (14) is the discretization error, and follows the relationship

$$\varepsilon_I \leq c_1 h_L^q \quad \forall \mathbf{y} \in \Gamma \quad (29)$$

291 where  $c_1 > 0$  and  $q$  is the order of accuracy of the DE solver in comput-  
 292 ing  $\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L+1}(\mathbf{y}, \mathbf{z})]$ . For this implementation of MLMC, it is only  
 293 necessary to have a good estimate of  $q$ . This estimate of  $q$  is obtained by  
 294 estimating  $\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L+1}(\mathbf{y}, \mathbf{z})]$  with a common, large sample set and  
 295 small set of step sizes for a set of vlues of  $\mathbf{z}$  and performing least squares  
 296 on the data for each input  $\mathbf{z}$ . Again, to be conservative, the minimum of

the estimators  $\hat{q}(\mathbf{z})$  is taken to be  $q$ . From the Central Limit Theorem, the statistical error,  $\varepsilon_{II}$  can be written as

$$\begin{aligned} \varepsilon_{II} &= |\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z})] - \mathcal{A}_{MLMC}(\mathbf{z})| \\ &\leq c_2 \sqrt{\frac{\mathbb{V}[Q_0(\mathbf{y}, \mathbf{z})]}{M_0} + \sum_{l=1}^L \frac{\mathbb{V}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})]}{M_l}} =: c_2 \sqrt{\sum_{l=0}^L \frac{V_l}{M_l}} \end{aligned} \quad (30)$$

with the shorthand notation defined by  $V_0 = \mathbb{V}[Q_0(\mathbf{y}, \mathbf{z})]$  and  $V_l = \mathbb{V}[Q_l(\mathbf{y}, \mathbf{z})]$  for  $l = 1, 2, \dots, L$ . As with Monte Carlo, the relation in (30) is interpreted by

$$P(\varepsilon_{II} \leq c_2 \sqrt{\sum_{l=0}^L \frac{V_l}{M_l}}) = 2\phi(c_2) - 1, \quad \text{as } M_l \rightarrow \infty \quad (31)$$

where  $P$  denotes a probability measure, and  $\phi(c_2) = \int_{-\infty}^{c_2} \frac{1}{\sqrt{2\pi}} e^{-\tau^2/2} d\tau$  is the CDF for the standard normal random variable  $c_2$ . In what follows, we also need to define the *strong error* given by

$$|\mathbb{V}[Q(\mathbf{y}, \mathbf{z}) - Q_l(\mathbf{y}, \mathbf{z})]| \leq |\mathbb{E}[(Q(\mathbf{y}, \mathbf{z}) - Q_l(\mathbf{y}, \mathbf{z}))^2]| \leq c_1' h_l^{q'} \quad \forall \mathbf{y} \in \Gamma \quad (32)$$

where  $c_2 > 0$  and  $q'$  is related to the order of accuracy of the DE solver. For the numerical examples in Section 5, the value of  $q'$  is estimated using least squares in the same way as was done in estimating  $q$  - taking the minimum least squares estimate of a power-law fit to the quantity  $|\mathbb{E}[(Q(\mathbf{y}, \mathbf{z}) - Q_l(\mathbf{y}, \mathbf{z}))^2]|$  for a large common set of random samples, a set of grid sizes, and a set of  $\mathbf{z}$ -values. As a remark, it is typical for  $q' \approx 2q$  [\[CITE\]](#). However, this is not the case for estimating failure probabilities. This is important to point out because for the numerical examples in Section 5, it is seen that  $q' \approx q$ , and this has theoretical justification. For the QoI defined in (6),  $q' \approx q$ .

*Proof.* Begin by writing the QoI as

$$\mu(\mathbf{z}) := \mathbb{E}[Q(\mathbf{y}, \mathbf{z})] = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N Q(\mathbf{y}_i, \mathbf{z}) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \mathbb{I}_{[g(\mathbf{y}_i, \mathbf{z}) \leq 0]}.$$

Then, the variance,  $\mathbb{V}[Q(\mathbf{y}, \mathbf{z})] = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N [\mathbb{I}_{[g(\mathbf{y}_i, \mathbf{z}) \leq 0]} - \mu(\mathbf{z})]^2$

$$\begin{aligned} &= \lim_{N \rightarrow \infty} \frac{1}{N} [\sum_{i=1}^N \mathbb{I}_{[g(\mathbf{y}_i, \mathbf{z}) \leq 0]}^2 - 2\mu(\mathbf{z}) \sum_{i=1}^N \mathbb{I}_{[g(\mathbf{y}_i, \mathbf{z}) \leq 0]} + \sum_{i=1}^N \mu(\mathbf{z})^2] \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} [N\mu(\mathbf{z}) - 2\mu(\mathbf{z}) \sum_{i=1}^N \mathbb{I}_{[g(\mathbf{y}_i, \mathbf{z}) \leq 0]} + N\mu(\mathbf{z})^2] \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} [N\mu(\mathbf{z}) - N\mu(\mathbf{z})^2] \\ &= \mu(\mathbf{z})(1 - \mu(\mathbf{z})) \end{aligned}$$

Thus, if  $\mu(\mathbf{z}) = \mathbb{E}[Q_l(\mathbf{y}, \mathbf{z})] + \mathcal{O}(h_l^q)$ , then  $\mu(\mathbf{z})(1 - \mu(\mathbf{z})) = \mathbb{E}[Q_l(\mathbf{y}, \mathbf{z})] +$

322  $\mathcal{O}(h_l^{q'})$  as well. Noting that  $\mathbb{V}[Q(\mathbf{y}, \mathbf{z})] = \mathbb{V}[Q_l(\mathbf{y}, \mathbf{z})] + \mathcal{O}(h_l^{q'})$ , it is clear that  
 323  $q' \approx q$ .  $\square$

324 In order to optimally select the number of samples  $M_l$  at each level and  
 325 the final level  $L$  required to achieve  $\varepsilon_s$ , we introduce a splitting parameter,  
 326  $\theta \in (0, 1)$  and split the tolerance as follows:

$$\varepsilon_{MLMC} \leq \varepsilon_I + \varepsilon_{II} \leq (1 - \theta)(1 - \alpha)\varepsilon_{TOL} + \theta(1 - \alpha)\varepsilon_{TOL} = (1 - \alpha)\varepsilon_{TOL} \quad (33)$$

327 That is, we require  $\varepsilon_I \leq (1 - \theta)(1 - \alpha)\varepsilon_{TOL}$  and  $\varepsilon_{II} \leq \theta(1 - \alpha)\varepsilon_{TOL}$ . Note  
 328 that the cost of computing  $Q_l(\mathbf{y}^{m_l}, \mathbf{z}) - Q_{l-1}(\mathbf{y}^{m_l}, \mathbf{z})$  is dominated by the cost  
 329 of computing  $Q_l(\mathbf{y}^{m_l}, \mathbf{z})$ . Hence, the cost of computing the MLMC estimator  
 330 (28) is given by

$$W_{MLMC} \propto \sum_{l=0}^L M_l W_l \quad (34)$$

331 Recall from Section 3 that for ODEs,  $W_l \propto qh_l^{-1}$ , and for time-dependent  
 332 PDEs solved numerically via the Method of Lines,  $W_l \propto h_l^{-(1+d)}$ .

333 The MLMC algorithm implemented in this paper is iterative and consists  
 334 of two main steps.

### 335 1. Optimal Sample Size for Each Level

336 We minimize  $W_{MLMC}$  subject to the accuracy constraint  $\varepsilon_{II} \leq \theta\varepsilon_s$ . The  
 337 Lagrangian is given by

$$L(M_l, \lambda) = \sum_{l=0}^L M_l W_l + \lambda \left( \sum_{l=0}^L \frac{V_l}{M_l} - \left( \frac{\theta(1 - \alpha)\varepsilon_{TOL}}{c_2} \right)^2 \right) \quad (35)$$

339 By requiring  $\partial_{M_l} L = 0$  and  $\partial_\lambda L = 0$ , the optimal choice for  $M_l$  is given by

$$M_l = \left\lceil \left( \frac{\theta(1 - \alpha)\varepsilon_{TOL}}{c_2} \right)^2 \sqrt{\frac{V_l}{W_l}} \sum_{l=0}^L \sqrt{V_l W_l} \right\rceil \quad (36)$$

### 340 2. Stopping Criterion

341 We begin with  $L = 2$  and iteratively add levels until  $\varepsilon_I \leq (1 - \theta)(1 - \alpha)\varepsilon_{TOL}$   
 342 is achieved. For a practical stopping criterion, write

$$\begin{aligned} \mathbb{E}[Q(\mathbf{y}, \mathbf{z}) - Q_L(\mathbf{y}, \mathbf{z})] &= \sum_{l=L+1}^{\infty} \mathbb{E}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})] \\ &= \mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L-1}(\mathbf{y}, \mathbf{z})] \sum_{l=L+1}^{\infty} \frac{\mathbb{E}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})]}{\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L-1}(\mathbf{y}, \mathbf{z})]} \end{aligned} \quad (37)$$

343 With the assumption that  $\mathbb{E}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})] \approx ch_l^q$ , we have that

$$\frac{\mathbb{E}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})]}{\mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L-1}(\mathbf{y}, \mathbf{z})]} \approx \frac{h_l^q}{h_L^q} = \beta^{(l-L)q} \quad (38)$$

344 Thus,

$$\varepsilon_{II} \leq \mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L-1}(\mathbf{y}, \mathbf{z})] \sum_{k=1}^{\infty} \beta^{-kq} = \frac{1}{\beta^q - 1} \mathbb{E}[Q_L(\mathbf{y}, \mathbf{z}) - Q_{L-1}(\mathbf{y}, \mathbf{z})] \quad (39)$$

345 From this, the condition we use for adding levels is

$$\max_{j \in \{0,1,2\}} \frac{\beta^{-jq}}{\beta^q - 1} \mathbb{E}[Q_{L-j}(\mathbf{y}, \mathbf{z}) - Q_{L-j-1}(\mathbf{y}, \mathbf{z})] \leq (1 - \theta)(1 - \alpha)\varepsilon_{TOL} \quad (40)$$

346 Now, assuming that we have made the assignment  $L \leftarrow L + 1$ , in order to  
 347 compute the new sample size  $M_l$  by (36), we must compute the variances  
 348  $\{V_l\}_{l=0}^L$ . Setting  $Q_{-1}(\mathbf{y}, \mathbf{z}) = 0$ , the variances are approximated according to

$$\begin{aligned} V_l &\approx \frac{1}{M_l} \sum_{m_l=1}^{M_l} \left( (Q_l(\mathbf{y}^{m_l}, \mathbf{z}) - Q_{l-1}(\mathbf{y}^{m_l}, \mathbf{z}))^2 - \mu_l(\mathbf{z})^2 \right) \\ \mu_l(\mathbf{z}) &= \frac{1}{M_l} \sum_{m_l=1}^{M_l} (Q_l(\mathbf{y}^{m_l}, \mathbf{z}) - Q_{l-1}(\mathbf{y}^{m_l}, \mathbf{z})) \end{aligned} \quad (41)$$

349 When a new level is added, the variance at the new level,  $V_L$ , cannot be  
 350 calculated with (41). However, we can estimate the variance  $V_L$  by utilizing  
 351 the strong error estimate (32) and assuming that  $\mathbb{V}[Q_l(\mathbf{y}, \mathbf{z}) - Q_{l-1}(\mathbf{y}, \mathbf{z})] \approx$   
 352  $ch_l^{q'}$ . The variance at level  $L$  is thus approximated by

$$V_L \approx \beta^{-q'} V_{L-1} \quad (42)$$

353 Then, the number of samples  $\{V_l\}_{l=0}^L$ , including the newest level are updated  
 354 with (36). The MLMC algorithm is outlined in



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**Algorithm 1** MLMC Algorithm

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Start with  $L = 2$  and generate a mesh hierarchy  $\{h_l\}_{l=0}^L$  according to (27).

Choose an initial set  $\{M_l\}_{l=0}^L$  of samples.

**loop**

Approximate  $\{V_l\}_{l=0}^L$  by (41).

Update the optimal number of samples  $\{M_l\}_{l=0}^L$  by (36).

**if** (40) is satisfied

Compute  $\mathcal{A}_{MLMC}$  by (28) and terminate the loop.

**else**

Set  $L := L + 1$  and  $h_L = h_0\beta^{-L}$ .

Approximate  $V_L$  by (42) and compute  $\{M_l\}_{l=0}^L$  by (36).

**end if**

**end loop**

---

355 In [17], it is shown that the optimal cost of this implementation of multi-  
356 level Monte Carlo sampling is given by

$$W_{OPT} \propto \mathcal{O}(((1 - \alpha)\varepsilon_{TOL})^{-2}) \quad (43)$$

## 357 5. Numerical Examples

358 In this section, we consider two examples. The first example involves an  
359 ODE, and the second example involves a second-order hyperbolic PDE.

360 For both examples, we compute optimal parameters for both Monte Carlo  
361 sampling and multi-level Monte Carlo sampling in accordance with Sections  
362 3 and 4, run the sampling algorithms for a set of values of  $\mathbf{z}$ , which is a  
363 scalar in the first example, and a two-element vector in the second example,  
364 we verify that both methods are able to achieve specified tolerances, and  
365 compare the costs of the two methods for different tolerances. For both  
366 examples, we also show how minimum and maximum failure probabilities  
367 can be computed to within a specified tolerance by utilizing MLMC coupled  
368 with an implementation of the Nelder-Mead direct simplex search method  
369 [19]. Finally, we show approximate failure probability plots for both examples  
370 to confirm that the optimization method has found appropriate estimates for  
371 minimum and maximum failure probabilities.

### 372 5.1. An ODE with interval-valued random coefficient

373 Consider the following second-order linear ordinary differential equation  
374 with constant coefficients, which describes a free harmonic oscillator. The

375 initial position is 1, and the initial velocity is 0.

$$\begin{aligned}
u''(t, \mathbf{y}, \mathbf{z}) + 100a^2(\mathbf{y}, \mathbf{z})u(t, \mathbf{y}, \mathbf{z}) &= 0 \text{ on } [0, 1] \times [1 - \mathbf{z}, 1 + \mathbf{z}] \\
u(0, \mathbf{y}, \mathbf{z}) &= 1 \text{ on } \{0\} \times [1 - \mathbf{z}, 1 + \mathbf{z}] \\
u'(0, \mathbf{y}, \mathbf{z}) &= 0 \text{ on } \{0\} \times [1 - \mathbf{z}, 1 + \mathbf{z}]
\end{aligned} \tag{44}$$

376 Here,  $\mathbf{y}$  is a uniform random variable between 0 and 1, and  $\mathbf{z}$  is a fixed, de-  
377 terministic parameter defining the distribution of the interval-valued random  
378 variable  $a$ , which is given by  $a(\mathbf{y}, \mathbf{z}) = 1 + \mathbf{z}(2\mathbf{y} - 1)$ . Thus,  $a$  is a uniform  
379 random variable between  $1 - \mathbf{z}$  and  $1 + \mathbf{z}$ . Let the probability box for this  
380 example to be the set of all CDFs for which  $\mathbf{z} \in [0.3, 1]$ . The quantities  
381 of interest are the lower and upper bounds of the failure probability of the  
382 system. Define the limit state function to be  $g(\mathbf{y}, \mathbf{z}) = u(t = 1, \mathbf{y}, \mathbf{z}) + 0.9$   
383 with  $g \leq 0$  denoting failure.

384 The exact interval-valued solution of (44) is given by

$$\tilde{u}(t, \mathbf{y}, \mathbf{Z}) = \cos(10\tilde{a}(\mathbf{y}, \mathbf{Z})t) \tag{45}$$

385 For solving numerically each realization of (44), we use the 4<sup>th</sup>-order  
386 Runge-Kutta method with parameter  $h$  denoting the time step size.

387 In order to estimate failure probabilities with the Monte Carlo sampling  
388 approach, we must first obtain accurate estimates of the parameters  $c_1$  and  
389  $q$  shown in (15) as well as  $\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$ , which is the variance computed using  
390 the optimal step size. We estimate these values by taking 11 linearly-spaced  
391 values of  $\mathbf{z}$  between 0.3 and 1, and for each value of  $\mathbf{z}$ , using the same set  
392 of time step sizes  $\{h\}_{i=1}^5 = [\frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}]$  and the same set of  $20 \times 10^6$   
393 random samples  $\mathbf{y}$ , compute the errors given by  $|\mathbb{E}[Q_{h_i}(\mathbf{y}, \mathbf{z}) - Q(\mathbf{y}, \mathbf{z})]|$  for  
394  $i = 1, 2, 3, 4, 5$ . For each value of  $\mathbf{z}$ , linear regression is used to estimate  
395  $c_1$  and  $q$ . To be conservative, the largest value of  $c_1$  is taken to be  $c_1$ ,  
396 and the smallest value of  $q$  is taken to be  $q$ . We take  $\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  to be  
397 the value of  $\max_{\mathbf{z}, \mathbf{h}} \mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  over these 11 values of  $\mathbf{z}$  and over the step  
398 sizes  $\{h\}_{i=1}^5 = [\frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}]$  rounded up to the ceiling of the second  
399 decimal place. Finally, we must decide on the parameter  $c_2$ , given in (17),  
400 which defines the confidence for the error given in (16). The parameters  
401 for implementing Monte Carlo Sampling for this example are summarized in  
402 Table 1. The value of  $c_2 = 1.96$  in Table 1 corresponds to a 95% confidence  
403 level.

404 To apply the interval multi-level Monte Carlo method, we must estimate  
405 the quantities  $q$  and  $q'$  in (29) and (32), respectively. We estimate the value

Table 1: Parameters for Monte Carlo sampling.

Quantity	Value
$c_1$	$2.2 \times 10^4$
$q$	3.9
$c_2$	1.96
$\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$	0.15

406 of  $q$  by taking 11 linearly-spaced values of  $\mathbf{z}$  between 0.3 and 1, and for each  
 407 value of  $\mathbf{z}$ , using the same set of time step sizes  $\{h\}_{i=1}^5 = [\frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}]$   
 408 and the same set of  $10^6$  random samples  $\{\mathbf{y}\}$ , compute the errors given by  
 409  $|\mathbb{E}[Q_{h_i}(\mathbf{y}, \mathbf{z}) - Q_{h_{i+1}}(\mathbf{y}, \mathbf{z})]|$  for  $i = 1, 2, 3, 4$ . Similar computations are done  
 410 in order to estimate  $q'$ , except that the errors are given by  $|\mathbb{V}[Q_{h_i}(\mathbf{y}, \mathbf{z}) -$   
 411  $Q_{h_{i+1}}(\mathbf{y}, \mathbf{z})]|$  for  $i = 1, 2, 3, 4$ . For each value of  $\mathbf{z}$ , linear regression is used to  
 412 estimate  $q$  and  $q'$ . Again, to be conservative, we take the smallest value of  $q$   
 413 to be the value of  $q$ , and the smallest value of  $q'$  to be  $q'$ . The error-splitting  
 414 parameter,  $\theta$  is chosen to be 0.9, which means that most of the error will be  
 415 absorbed by the statistical error,  $\epsilon_{II}$ . Shown below in Table 2 is a summary  
 416 of the parameters used for the multi-level Monte Carlo computations for this  
 example.

Quantity	Value
$q$	3.9
$q'$	3.7
$c_2$	1.96
$\beta$	2
$\theta$	0.9
$h_0$	0.1
$M_0$	1000

Table 2: Parameters for multi-level Monte Carlo sampling.

417 We compute failure probabilities using a set of tolerances  $(1 - \alpha)\epsilon_{TOL}$ .  
 418 To verify that failure probabilities are calculated within these tolerances, we  
 419 compute reference failure probabilities for the same set of 11 input parameters  
 420  $\mathbf{z}$ . The reference failure probabilities are computed using the exact solution  
 421 of one realization (45) with tolerance of  $5 \times 10^{-5}$  via Monte Carlo sampling.  
 422 In computing these reference values, the same parameters in Table 1 are  
 423 used.  
 424

425 Using 11 linearly-spaced values of  $\mathbf{z}$  between 0.3 and 1, failure probabili-  
 426 ties are computed for each of the tolerances using both Monte Carlo sampling  
 427 and multi-level Monte Carlo sampling. For each tolerance, the maximum dif-  
 428 ference over the 11 values of  $\mathbf{z}$  between the reference failure probability and  
 429 that calculated using either the Monte Carlo sampling or the multi-level  
 430 Monte Carlo sampling is recorded. Because we are using reference values,  
 431 each with tolerance  $\delta = 5 \times 10^{-4}$ , in order to verify that the true errors  
 432 are less than  $(1 - \alpha)\varepsilon_{TOL}$ , we must verify that the absolute difference be-  
 433 tween the test failure probabilities and the references values are less than  
 434  $(1 - \alpha)\varepsilon_{TOL} - \delta$ . This is indeed the case, as shown in Figure 1. This plot  
 shows how for both methods, the desired tolerances are achieved.

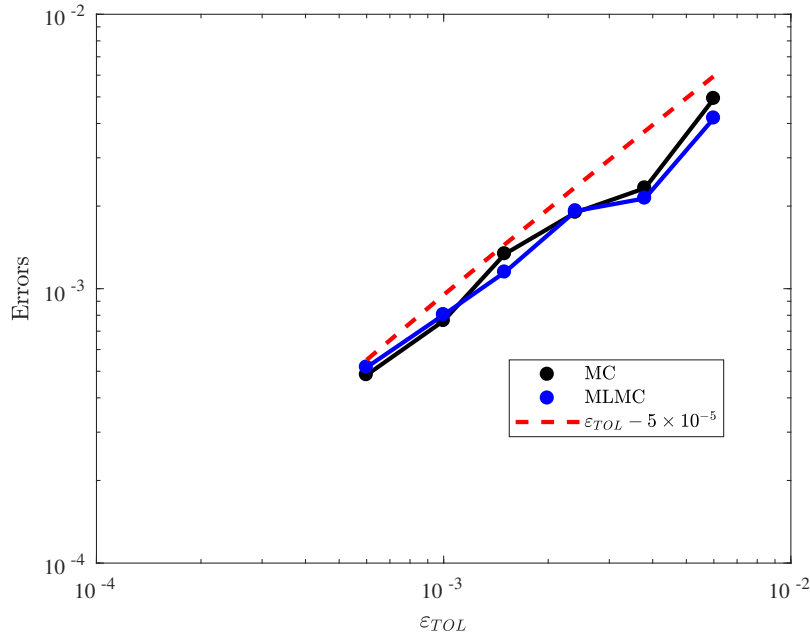


Figure 1: Verification that desired tolerances are achieved using both Monte Carlo and multi-level Monte Carlo sampling methods.

435 Figure 2 compares the costs of Monte Carlo sampling with multi-level  
 436 Monte Carlo sampling. The numerical experiments are seen to agree with  
 437 what is expected from the numerical analysis.

439 If we can have a reasonably nice failure probability function which we  
 440 can roughly estimate and thus have some knowledge of the function and  
 441 where its extrema are located, we can consider using a smart optimization

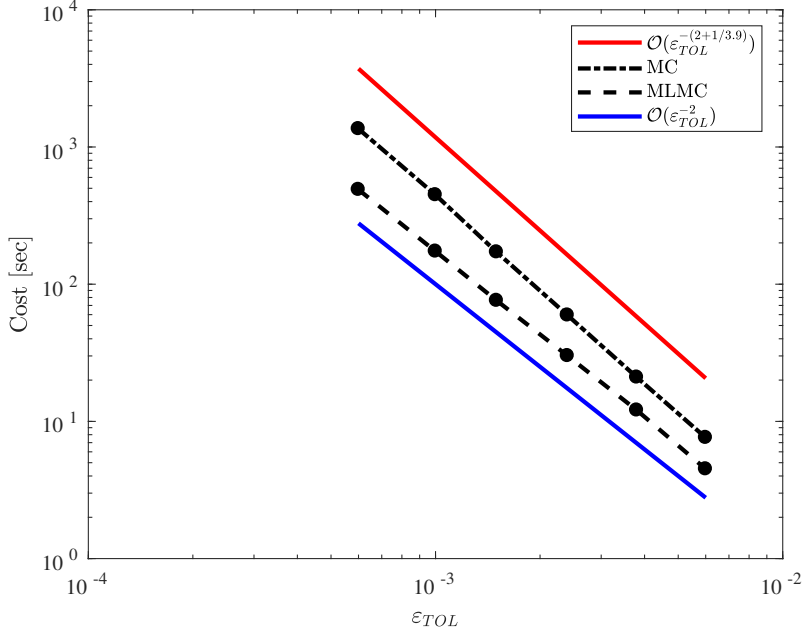


Figure 2: Computational cost is seen to be in agreement with what is predicted from numerical analysis.

442 strategy instead of a grid search over a large set of  $\mathbf{z}$ -values, which would  
 443 be highly expensive. We use an implementation of the Nelder-Mead direct  
 444 simplex search for both examples in this paper. To compute minimum and  
 445 maximum failure probabilities, we use the initial guess  $\mathbf{z}_0 = 0.4$  for the  
 446 minimum and  $\mathbf{z}_0 = 0.8$  for the maximum. The Nelder-Mead optimization  
 447 is terminated when both (1) the maximum Euclidean distance between two  
 448 points in the final simplex is within  $4 \times 10^{-4}$  and (2) the maximum difference  
 449 in absolute value between failure probability results in the final simplex is  
 450 within  $4 \times 10^{-4}$ . The chosen minimum is taken to be the point  $\mathbf{z}$  in the  
 451 final simplex which minimizes the failure probability. The maximization  
 452 problem is handled by minimizing the negative of the failure probability  
 453 function and changing the sign of the result found. For the one-dimensional  
 454 optimization in this example, the simplexes are line segments. In general, for  
 455 an optimization over  $n$ -dimensional space, the simplexes will each contain  $n +$   
 456 1 points. Figure 3 shows the failure probability plot with 1001 linearly-spaced  
 457 values of  $\mathbf{z}$ , where, for each value of  $\mathbf{z}$ , the failure probability is computed with  
 458 tolerance of  $10^{-3}$ . Shown on the plot are the minimum and maximum failure

459 probability results computed using the MLMC-Nelder-Mead optimization  
 460 approach with  $\varepsilon_I + \varepsilon_{II} \leq 6 \times 10^{-4} = (1 - \alpha)\varepsilon_{TOL}$  and  $\alpha\varepsilon_{TOL}4 \times 10^{-4}$ , so  
 461 that the minimum and maximum failure probabilities are calculated within  
 a tolerance of  $(1 - \alpha)\varepsilon_{TOL} + \alpha\varepsilon_{TOL} = 10^{-3}$ . For this example then,  $\alpha = 0.4$ .

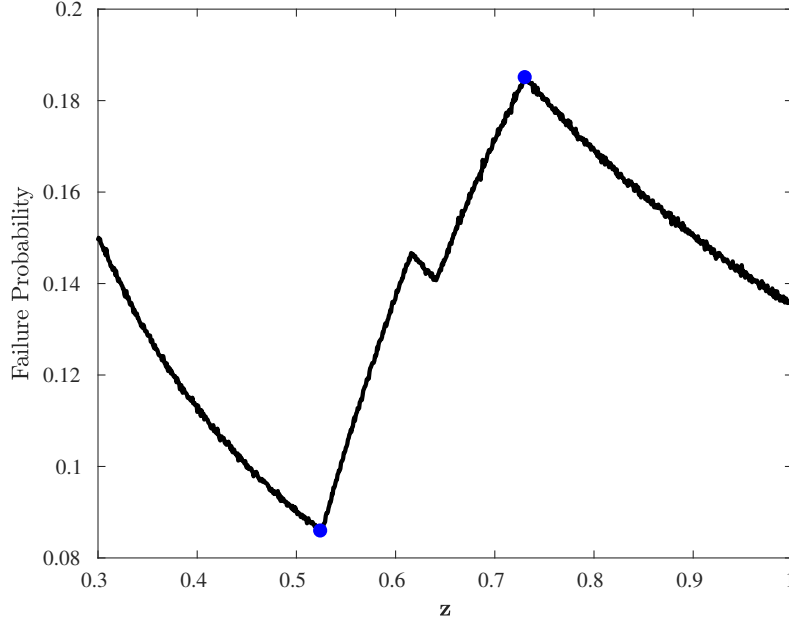


Figure 3: The MLMC strategy coupled with the Nelder-Mead direct simplex search produces the estimates shown in blue for which  $\epsilon_{TOL} = 10^{-3}$ .

462  
 463 For this example, we can easily contrast the results for upper and lower  
 464 failure probability bounds for a given tolerance using the estimators in either  
 465 (12) or (26) with the results obtained using the excessively conservative es-  
 466 timators (13). We choose a tolerance of  $\epsilon_{TOL} = 6 \times 10^{-4}$  and use the same  
 467 optimal time step size and sample size for computing (13) as were used for  
 468 computing (12). In computing the estimators (13), a grid search is done over  
 469 11 linearly-spaced value of  $\mathbf{z}$  between 0.3 and 1 for each random input sample  
 470  $\mathbf{y}$ . In computing the estimators according to (12) and (26), a grid search is  
 471 done over the same values of  $\mathbf{z}$  for each expected value estimate. The results  
 472 are summarized in Table 3.

473 As seen in Table 3, the failure probability bounds computed from (13)  
 474 are much less accurate than those computed using the other methods. The  
 475 upper bound is highly overestimated, and the lower bound is underestimated.

$p_f$	Estimator	$\underline{\mathcal{P}}_f \times 10^2$	$\overline{\mathcal{P}}_f$
	(12)	8.8	0.180
	(26)	8.8	0.180
	(13)	5.1	0.581

Table 3: Comparison of failure probability estimates using three different approaches.

476 Having demonstrated the superior performance of the multi-level Monte  
 477 Carlo sampling for computing accurate failure probability bounds for this  
 478 example, we now apply a similar analysis to a time-dependent PDE problem.

### 479 5.2. A Time-Dependent PDE with interval-valued random variables

480 Consider the following partial differential equation with constant coeffi-  
 481 cients.

$$u_{tt}(\mathbf{x}, t, \mathbf{y}, \mathbf{z}) - \nabla^2 u(\mathbf{x}, t, \mathbf{y}, \mathbf{z}) = f(\mathbf{x}, t, \mathbf{y}, \mathbf{z}) \text{ in } [0, 1] \times D \times \Gamma, \quad (46)$$

482 with  $t \in [0, 1]$ ,  $D = \mathbf{x} = [x_1, x_2]^T \in [-\frac{1}{2}, \frac{1}{2}]^2$ , and  $\mathbf{y} \in \Gamma \subset \mathbb{R}^2$ . Here,  $\mathbf{y} =$   
 483  $[y_1, y_2]^T$ , where  $y_1$  and  $y_2$  are standard uniform random variables. For each  
 484 realization, the vector  $\mathbf{z} = [z_1, z_2]^T$  is a fixed, deterministic vector defining the  
 485 uniform distribution of the vector  $\mathbf{b} = [b_1, b_2]^T$  defined by  $b_1 = z_1 + 0.5(2y_1 - 1)$   
 486 and  $b_2 = z_2 + 0.5(2y_2 - 1)$ . That is,  $b_1$  varies uniformly between  $z_1 - 0.5$  and  
 487  $z_1 + 0.5$ , and  $b_2$  varies uniformly between  $z_2 - 0.5$  and  $z_2 + 0.5$ . The probability  
 488 box for this example is the set of all CDFs for which  $z_1, z_2 \in [1, 1.8]$ . The  
 489 forcing function,  $f$ , is given by

$$f(\mathbf{x}, t, b_1, b_2) = -50b_1b_2 \cos(5b_1(t + x_1)) \sin(5b_2(t + x_2)) \quad (47)$$

490 Finally, define the limit state function to be  $g(\mathbf{y}, \mathbf{z}) = u(t = 1, \mathbf{y}, \mathbf{z}) + 0.5$   
 491 with  $g \leq 0$  denoting failure.

492 The exact interval-valued solution of (46) is given by

$$\tilde{u}(\mathbf{x}, t, \mathbf{y}, \mathbf{Z}) = u(\mathbf{x}, t, \tilde{b}_1, \tilde{b}_2) = \sin(5\tilde{b}_1(t + x_1)) \cos(5\tilde{b}_2(t + x_2)) \quad (48)$$

493 For solving numerically each realization of (46), we use 2<sup>nd</sup>-order finite  
 494 differencing with parameter  $h$ , denoting the grid size. For example, using a  
 495 grid size of  $\frac{1}{12}$  equates to setting the number of grid points in both  $x_1$  and  
 496  $x_2$ -directions to be 13.

497 As for the previous example, we must obtain accurate estimates of the  
 498 parameters  $c_1$  and  $q$  shown in (15) as well as  $\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  in order to estimate

499 failure probabilities with the Monte Carlo sampling approach. We estimate  
 500 these values by taking 7 linearly-spaced values of both  $z_1$  and  $z_2$ , each between  
 501 1 and 1.8, thereby forming a grid of 49 sample vectors  $\mathbf{z}$ . For each value of  $\mathbf{z}$ ,  
 502 using the same set of grid step sizes  $\{h\}_{i=1}^5 = [\frac{1}{6}, \frac{1}{12}, \frac{1}{24}, \frac{1}{48}]$  and the same set  
 503 of  $20 \times 10^4$  random sample vectors  $\mathbf{y}$ , we compute the error estimates given by  
 504  $|\mathbb{E}[Q_{h_i}(\mathbf{y}, \mathbf{z}) - Q(\mathbf{y}, \mathbf{z})]|$  for  $i = 1, 2, 3, 4$ . For each value of  $\mathbf{z}$ , linear regression  
 505 is used to estimate  $c_1$  and  $q$ . The largest regression estimate of  $c_1$  is taken  
 506 to be  $c_1$ , and the smallest regression estimate of  $q$  is taken to be  $q$ . We take  
 507  $\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  to be the value of  $\max_{\mathbf{z}, \mathbf{h}} \mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$  over these 49 values of  $\mathbf{z}$   
 508 and over the step sizes  $\{h\}_{i=1}^4 = [\frac{1}{6}, \frac{1}{12}, \frac{1}{24}, \frac{1}{48}]$  rounded up to the ceiling of the  
 509 second decimal place. We use the same value of the confidence parameter,  
 510  $c_2$ , as was used in the previous example. The parameters for implementing  
 Monte Carlo sampling for this example are summarized in Table 4.

Table 4: Parameters for Monte Carlo sampling.

Quantity	Value
$c_1$	4.2
$q$	1.6
$c_2$	1.96
$\mathbb{V}[Q_h(\mathbf{y}, \mathbf{z})]$	0.21

511  
 512 To apply the interval multi-level Monte Carlo method, we must estimate  
 513 the quantities  $q$  and  $q'$  in (??) and (32), respectively. We estimate the value  
 514 of  $q$  by taking the same set of 49 values of the vector  $\mathbf{z}$ , and for each value of  $\mathbf{z}$ ,  
 515 using the same set of grid sizes  $\{h\}_{i=1}^5 = [\frac{1}{6}, \frac{1}{12}, \frac{1}{24}, \frac{1}{48}, \frac{1}{96}]$  and the same set of  
 516  $2 \times 10^4$  random sample vectors  $\mathbf{y}$ , compute the errors given by  $|\mathbb{E}[Q_{h_i}(\mathbf{y}, \mathbf{z}) -$   
 517  $Q_{h_{i+1}}(\mathbf{y}, \mathbf{z})]|$  for  $i = 1, 2, 3, 4$ . Similar computations are done in order to  
 518 estimate  $q'$ , except that the errors are given by  $|\mathbb{V}[Q_{h_i}(\mathbf{y}, \mathbf{z}) - Q_{h_{i+1}}(\mathbf{y}, \mathbf{z})]|$   
 519 for  $i = 1, 2, 3, 4$ . For each value of  $\mathbf{z}$ , linear regression is used to estimate  $q$  and  
 520  $q'$ . Again, to be conservative, we take the smallest value of  $q$  to be the value  
 521 of  $q$ , and the smallest value of  $q'$  to be  $q'$ . As for the first example, we choose  
 522 the error-splitting parameter,  $\theta$  to be 0.9. Shown in Table 5 is a summary of  
 523 the parameters used for the Multi-Level Monte Carlo computations for this  
 524 example.

525 We compute failure probabilities using different sets of tolerances for  
 526 Monte Carlo sampling than for multi-level Monte Carlo sampling. To verify  
 527 that failure probabilities are calculated within these tolerances, we compute



Quantity	Value
$q$	1.3
$q'$	1.6
$c_2$	1.96
$\beta$	2
$\theta$	0.9
$h_0$	$\frac{1}{12}$
$M_0$	100

Table 5: Parameters for Multi-Level Monte Carlo sampling.

reference failure probabilities for the same set of 49 input parameter vectors  $\mathbf{z}$ . The reference failure probabilities are computed using the exact solution of one realization (48) with tolerance of  $5 \times 10^{-5}$  via Monte Carlo sampling with the same parameters that appear in Table 4. Using the 49 values of  $\mathbf{z}$  with both  $\mathbf{z}_1$  and  $\mathbf{z}_2$  between 1 and 1.8, failure probabilities are computed using both Monte Carlo sampling and multi-level Monte Carlo sampling. For each tolerance, the maximum difference over the 49 values of  $\mathbf{z}$  between the reference failure probability and that calculated using either the Monte Carlo sampling or the multi-level Monte Carlo sampling is recorded. As for the previous example, we subtract the reference tolerance  $\delta = 5 \times 10^{-4}$  from the test tolerances and plot the results in Figure 4. This plot shows how for both methods, the desired tolerances are achieved.

Figure 5 compares the costs of Monte Carlo sampling with multi-level Monte Carlo sampling. The numerical experiments are seen to agree with what is expected from the numerical analysis.

To compute minimum and maximum failure probabilities with the Nelder-Mead direct simplex search, we use the initial guess  $\mathbf{z}_0 = [1.55, 1.4]$  for the minimum and the initial guess  $\mathbf{z}_0 = [1.25, 1.4]$  for the maximum. The Nelder-Mead optimization is terminated with both (1) the maximum Euclidean distance between two points in the final simplex is within  $4 \times 10^{-3}$  and (2) the maximum difference in absolute value between failure probability results in the final simplex is within  $4 \times 10^{-3}$ . For this example, the simplexes are triangles. Figure 6 shows the failure probability plot with  $51 \times 51 = 2601$  values of  $\mathbf{z}$ , where, for each value of  $\mathbf{z}$ , the failure probability is computed with tolerance of  $10^{-2}$ . Shown on the plot are the minimum and maximum failure probability results computed using the MLMC-Nelder-Mead optimization approach with  $\varepsilon_I + \varepsilon_{II} \leq 6 \times 10^{-3} = (1 - \alpha)\varepsilon_{TOL}$  and  $\alpha\varepsilon_{TOL} = 4 \times 10^{-3}$ , so

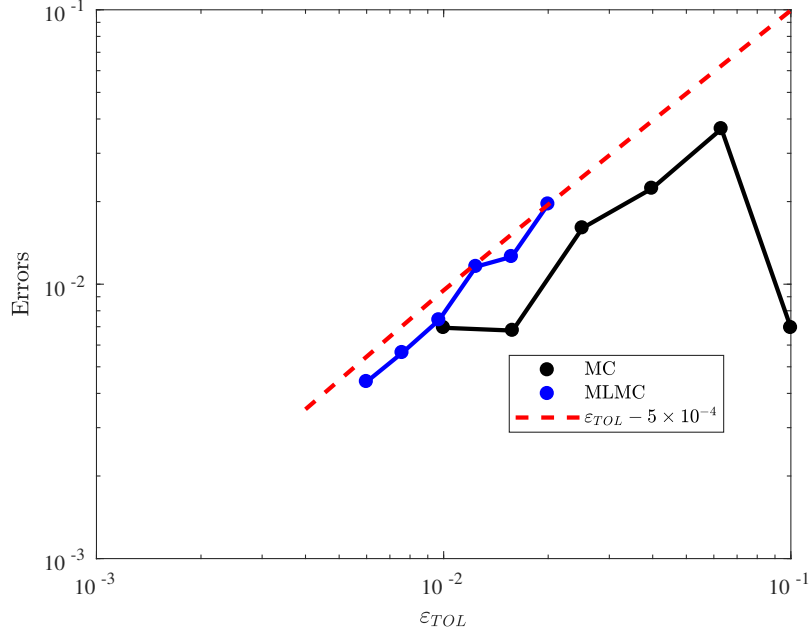


Figure 4: Verification that desired tolerances are achieved using both Monte Carlo and multi-level Monte Carlo sampling methods.

555 that the minimum and maximum failure probabilities are calculated within  
556 a tolerance of  $\varepsilon_{TOL} = (1 - \alpha)\varepsilon_{TOL} + \alpha\varepsilon_{TOL} = 10^{-2}$ . For this example as well,  
557 we chose  $\alpha = 0.4$ .

558 We can again contrast the results for upper and lower failure probability  
559 bounds for a given tolerance using the estimators in either (12) or (26) with  
560 the results obtained using the excessively conservative estimators (13). We  
561 choose a tolerance of  $6 \times 10^{-3}$  and use the same optimal time step size  
562 and sample size for computing (13) as were used for computing (12). In  
563 computing the estimators (13), a grid search is done over the same 49 values  
564 of  $\mathbf{z}$  for each random input sample  $\mathbf{y}$ . In computing (12) and (26), a grid  
565 search is done over the same values of  $\mathbf{z}$  for each expected value estimate.  
566 The results are summarized in Table 6.

567 As seen in Table 6, although the tolerance of  $10^{-2}$  is reasonably small,  
568 the failure probability bounds computed from (13) are as wide as possible  
569 and provide essentially no information about the true failure probabilities.

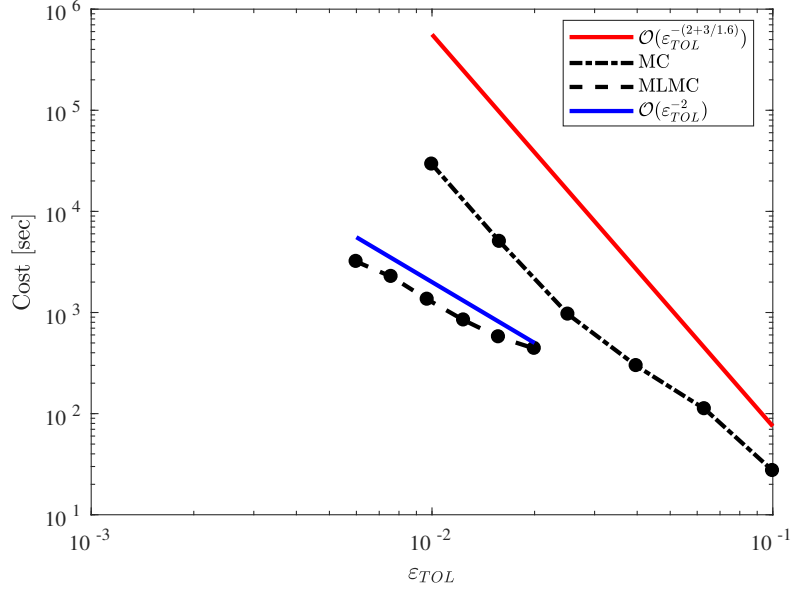


Figure 5: Computational cost is seen to be in agreement with what is predicted from numerical analysis.

$P_f$ Estimator	$\underline{\mathcal{P}}_f \times 10^2$	$\overline{\mathcal{P}}_f$
(12)	8	0.26
(26)	9	0.27
(13)	0	1

Table 6: Comparison of failure probability estimates using three different approaches.

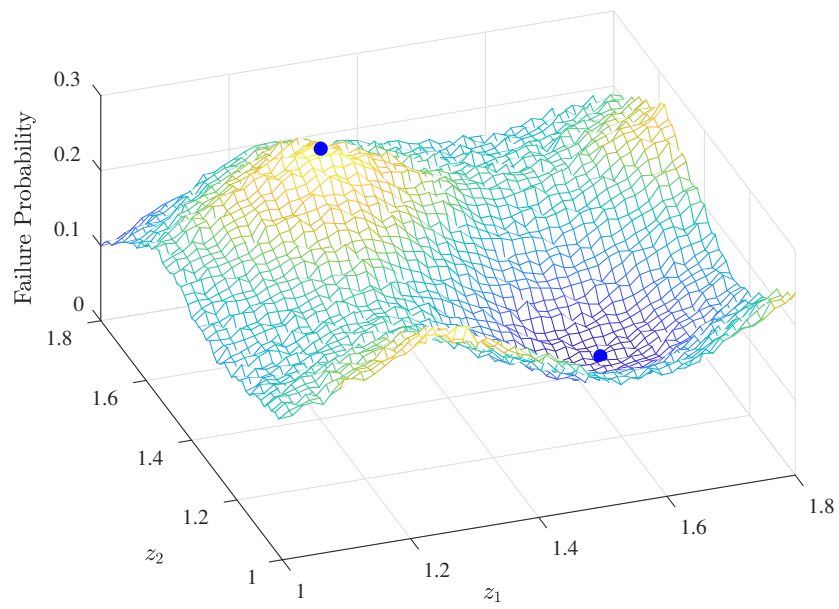


Figure 6: The MLMC strategy coupled with the Nelder-Mead direct simplex search produces the estimates shown in blue for which  $\epsilon_{TOL} = 10^{-2}$ .

## 570 6. Conclusions

571 We have presented the problem of computing interval-valued probab-  
572 ities, with one application being the calculation of failure probabilities for  
573 physical systems. Two methods were discussed in detail; the use of either  
574 standard MC sampling or multi-level MC sampling, coupled with a global  
575 optimization method. These two methods were analyzed for their computa-  
576 tional cost in estimating interval valued probabilities to within a specified  
577 tolerance. Several numerical examples were presented in order to verify  
578 the theoretical cost estimates. We have demonstrated that the use of the  
579 multi-level MC allows for much more efficient computation of interval-valued  
580 probabilities, with the improvement in efficiency over MC increasing with  
581 decreasing error tolerance.

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