Adaptive Surrogate Model for Failure Probability Estimation

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ABSTRACT

Estimating failure probability becomes a fundamental task in many complex engineering designs and optimizations. Yet, evaluation of failure probability via direct sampling from a given system can be computationally expensive and sometimes impossible. Although the construction of a response surface/surrogate could reduce such computational cost, reliance on its sampling alone may still yield an erroneous estimate of the failure probability. In this paper, we employ generalized polynomial chaos and develop an adaptive method whose surrogate model evolves with the additional data sampled from the underlying system as the iteration proceeds. It is more flexible by not requiring an accurate surrogate model in priori. Via three distinct numerical examples and one practical problem on a spintronic device, we demonstrate that our novel scheme provides an efficient tool to estimate system failure probability.

CCS CONCEPTS

• **Mathematics of computing** → **Probabilistic algorithms**; • **Applied computing** → **Mathematics and statistics**; • **Computing methodologies** → **Simulation evaluation**.

KEYWORDS

Generalized polynomial chaos, adaptive refinement, surrogate modeling, failure probability, Landu-Liftshitz-Gilbert equations, STT-MRAM

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1 INTRODUCTION

Estimating system reliability is a fundamental task in many fields, ranging from integrated circuit design to financial risk assessment. In essence, it involves the evaluation of multivariate integrals in domains defined by failure modes. As systems become ever more sophisticated with increasing complexity and a number of components/parameters, computing system failure probability becomes an ever more daunting task.

Over the past years, many efforts have been devoted to designing efficient algorithms to estimate failure probability and can be generalized into three categories, namely, sampling, non-sampling, and response surface methods. The former includes the widely popular Monte Carlo sampling (MCS) and its improvements, such as directional sampling [4, 10, 31, 34], (adaptive) importance sampling [1], line sampling [26] and subset simulation [2]. In general, they approximate system failure probability by counting the number of samples within the failure domain. Despite its easy implementation, such a direct approach may incur prohibitively high computational cost due to: 1) low convergence rate for a reliable system defined by small failure probability, 2) high simulation cost of each realization for complex systems. Yet, this approach becomes ineffective when the data is limited, which is common for many practical applications.

To circumvent this data-poor scenario, researchers have developed non-sampling approaches, among which First Order Reliability Method (FORM) and the Second Order Reliability Method (SORM) are two popular frameworks [6, 13, 17–19, 23, 24, 27, 49]. In those methods, the objective is to find the limit state function that separates "failure" and "safe" regions. By first identifying the most probable points (MPP), e.g., the closest geometrical points on the limit state function to the origin of the standard Gaussian space, the limit state function can be approximated as a linear function (in FORM) or a quadratic function (in SORM) close to the MPP. The resultant integral can be further simplified using asymptotic methods. Since approximations are made in many stages, FORM and SORM are effective for linear and weakly nonlinear systems, especially in their asymptotic regimes [38, 40, 41].

Response surface method (RSM) [5, 12, 45] is an alternative approach that combines the merits of both sampling and non-sampling methods. Its main objective is to build an approximation (the response surface) of the limit state function using a reduced number of data from the original system. Failure probability can be then estimated by directly sampling the response surface instead, usually in the analytical form of a multivariate polynomial. It is widely acknowledged that successful construction of the response surface is crucial to the method's accuracy and has been the focus of many recent studies, including methods based on experiment design [16], regression[22], statistical approach [14] and the generalized polynomial chaos (gPC)[36, 37]. However, one must note here that the overall accuracy may not necessarily depend on the accuracy of the response surface. As shown in an earlier study [28], the abovementioned direct RSM approach can still lead to considerable error in estimating the failure probability, "no matter how accurate the surrogate model is".

To improve the robustness of the RSM, the hybrid approach [28] has since been proposed and widely used [7, 21]. It divides the overall parameter (probability) space into two regions: one "away" from the limit state function where the response surface (surrogate) can be employed; the other "close" to the limit state function in which the original system is simulated to ensure global accuracy. Since by definition, most of the samples would be in the "away" region, the hybrid method considerably reduces the computational cost rather than sampling the system in the entire probability space. Although the convergence of the estimated failure probability does not require the convergence of the response surface, a sufficiently accurate surrogate would improve the overall efficiency. Recently, a hierarchical neural hybrid (HNH) method was proposed in [30] which employed neural network as a surrogate model to reduce computational cost based on the hybrid method without losing the accuracy. However, in practice, such model may not be readily available and the main focus of this paper is to develop an alternative approach without such priori but of acceptable cost. To be specific, we employ generalized polynomial chaos (gPC) expansion [15, 48] to build a low-accuracy surrogate model as an initial guess and then improve its accuracy in the estimation of failure probability by adding more samples of the underlying system. Along the iteration process, the order of the model is expected to increase till a pre-defined error threshold is met.

The remainder of this paper is organized as below: in subsequent sections, we propose a novel numerical method that modified the hybrid approach with an adaptively-evolving gPC surrogate (updated iteratively). In Section 2, we formulate the failure probability problem and then briefly review three components that would be used, namely, MCS, RSM, and the hybrid method (Section 3). Our new framework and its numerical algorithm are presented in Section 4. Its numerical efficiency is tested by three distinct numerical experiments and one practical problem in a microelectronic device (Section 5). Finally, our conclusion is drawn in Section 6.

2 PROBLEM FORMULATION

System reliability can often be represented by a scalar limit state function $g(Z)$ of design parameters, i.e., $Z = (Z_1, Z_2, \cdots, Z_{n_z}) : \Omega \rightarrow \mathbb{R}^{n_z}$, whose uncertainty can be collectively treated as a n_z-dimensional random vector with known distribution function $F_Z(z) = \text{Prob}(Z \leq z)$. Here Ω is the probability space and $z \in \mathbb{R}^{n_z}$.

The hyper-surface $g(Z) = 0$ defines the limit state surface that separates the failure domain $g(Z) < 0$ and safe domain $g(Z) \geq 0$:

$$\Omega_f \triangleq \{Z : g(Z) < 0\}. \tag{1}$$

The probability of failure P_f can be computed as

$$P_f = \text{Prob}(Z \in \Omega_f) = \int_{\Omega_f} dF_Z(z) = \int \chi_{\Omega_f}(z) dF_Z(z), \tag{2}$$

where χ is the characteristic function satisfying

$$\chi_{\Omega_f}(z) = \begin{cases} 1 & \text{if} \quad z \in \Omega_f, \\ closet0 & \text{if} \quad z \notin \Omega_f. \end{cases} \tag{3}$$

In essence, the limit state function $g(Z)$ describes the relationship between the inputs Z and the failure modes Ω_f via the solution of the system. However, in practice, most underlying systems are complex/nonlinear with a large number of input parameters and thus computationally expensive to simulate. Consequently, an explicit form of $g(Z)$ is often unavailable and can only be evaluated by measurement data or direct simulation of the entire system, either of which may incur significant costs.

3 PRELIMINARIES

In this section, we shall briefly review three important methods, which will be incorporated into our adaptive scheme.

3.1 Monte Carlo simulation

The most straightforward method for evaluating failure probability is Monte Carlo sampling (MCS). In MCS, one generates realizations of random inputs based on the given probability distribution, i.e.,$\{z^{(i)}, i = 1, ...M\} \sim F_Z$, where M is the total number of samples. For each realization, the data is fixed and the problem becomes deterministic. According to the limit state g, the system output could be examined and one can determine whether a sample is "safe" or "failure". The MCS estimate of P_f is then computed as follows:

$$P_f^{mc} = \frac{1}{M} \sum_{i=1}^{M} \chi_{\{g(Z)<0\}}(z^{(i)}). \tag{4}$$

Obviously, when $M \rightarrow \infty$, this estimate converges to the true probability of failure P_f. Although MCS is straightforward to apply as it only requires repetitive executions of deterministic simulations, the solution statistics converge relatively slowly. When M is large,

this can incur exceedingly large effort. Unfortunately, for P_f^{mc} to be an accurate estimate, a large number of samples $M \gg 1$ are usually required, thus increasing the computational cost even for a relatively small probability of failure.

3.2 Response surface method

One of the alternatives to circumvent the difficulty of MCS is response surface method (RSM). In RSM, one constructs a response surface (RS) for the limit state function and assume its availability, i.e., we seek $\tilde{g}(Z) \approx g(Z)$ in a proper norm/metric. Then the failure probability could be estimated as:

$$P_f^{RSM} = \frac{1}{M} \sum_{i=1}^{M} \chi_{\{\tilde{g}(Z)<0\}}(z^{(i)}). \tag{5}$$

The most important feature of this approach is that it eliminates the need to sample the true underlying system since the sampling process is conducted on the surrogate model. Hence, sampling the surrogate could reduce computational efforts significantly and allow us to conduct an arbitrarily large number of sampling. However, the accuracy of the RSM depends critically on the accuracy of the surrogate model $\tilde{g}$. In many practical problems, one usually possesses a fixed surrogate model with limited accuracy. The accuracy of the RSM estimate of P_f is thus difficult to acquire. Moreover, even if $\tilde{g}$ is highly accurate with $O(\epsilon)$ error, there still exists pathological cases where the RSM estimate of P_f can have $O(1)$ error [28].

3.3 Hybrid method

A hybrid method using samples from both the original system (in a "small" portion) and the surrogate model (in a "large" portion) was proposed in [28]. It improves the accuracy of RSM by employing a few number of original state samples from g to "correct" the numerical error in $\tilde{g}$. When the absolute value $|\tilde{g}|$ is "small", the algorithm replaces the samples of the surrogate $\tilde{g}$ by the original state samples, as in this case the error in the surrogate $\tilde{g}$ may incorrectly predict safe or failure. For a small real parameter $\gamma > 0$, an approximate failure domain could be effectively defined as,

$$\tilde{\Omega}_f \triangleq \{Z : \tilde{g}(Z) < -\gamma\} \cup \{\{Z : |\tilde{g}(Z)| \leq \gamma\} \cap \{Z : g(Z) < 0\}\}. \tag{6}$$

Following this failure domain, the sampling of the original state g is only conducted in a subdomain of $\{\{Z : |\tilde{g}(Z)| \leq \gamma\} \cap \{Z : g(Z) < 0\}\}$. Obviously, the more accurate the surrogate $\tilde{g}$ is, the smaller the parameter γ can be, and the required number of samples of g becomes smaller correspondingly. A practical iterative algorithm presented in [28] demonstrates that one does not need to specify the parameter γ. Instead, the algorithm iteratively replaces a small number of samples of $\tilde{g}$ by g, progressively away from $|\tilde{g}| \approx 0$ till convergence is reached. It was shown that the method is able to produce a highly accurate result for failure probability even when the surrogate model is of modest accuracy, while using a very small number of original state samples. Error bound and convergence of the method were also presented in [28]. More formal mathematical analysis and extension of problems with multiple failure conditions can be found in [29].

4 NUMERICAL SCHEME

Motivated by the above developments, we now present a novel numerical scheme to compute the system failure probability. Similar to the previous hybrid approach [28], the design parameter domain would be separated into two regions: one "close" to the limit state $g(Z) = 0$, where samples of the original system are taken, and elsewhere in the domain using samples from the surrogate model. However, in contrast to previous works, the new scheme does not require the availability of a priori surrogate model of the underlying system. Instead, it builds a low-order one using gPC expansion initially and refines iteratively by applying the hybrid method.

Unless specified, we denote $S = \{z^{(i)}\}_{i=1}^{M}$ as the "candidate set", a sample set generated from the probability distribution F_Z and M is the total number of samples. Let k be the iteration count and ΔM be "step size", i.e., an integer value much smaller than M during the iteration. ΔM^0 is the upper bound of sample increment during each iteration. We will use $S^{(k)} \subset S$ to denote the subset at iteration step k, where the values of the true limit state g are known. Correspondingly, $\tilde{S}^{(k)} = S \backslash S^{(k)}$ is its complement, where the original state g are not known but the surrogate state $\tilde{g}$ are known.

The main algorithm of our adaptive method consists of the following major steps summarized in Algorithm. 1.

Algorithm 1 Overall scheme for failure probability estimation

At time step $k = 0$**:**

- *Construct a low-degree gPC surrogate model* $\tilde{g}^{(0)}$ *using non-intrusive stochastic collocation approach.*

At time step $k \geq 1$**:**

- *Adaptively refine the surrogate model* $\tilde{g}^{(k)}$ *with increasing number of original state samples.*
- *Evaluate the failure probability using the updated model.*
- *Check the stopping criterion.*

Repeat iteration step till convergence.

In the subsequent section, we will review how to construct our surrogate model using the gPC expansion (Section 4.1) and then details of the adaptive scheme in Section 4.2.

4.1 Construction of surrogate model

In our method, the construction of the surrogate model is a critical step that affects the overall accuracy. To meet such demand, we adopt the mathematically rigorous gPC approach [47] with established convergence rate and error analysis.

In a nutshell, the limit state function can be approximated by a n_gth-degree gPC expansion

$$g(Z) \approx \tilde{g}(Z) = \sum_{|\mathbf{i}|=0}^{n_g} c_{\mathbf{i}} \Phi_{\mathbf{i}}(Z), \tag{7}$$

where $\mathbf{i} = (i_1, i_2, \cdots, i_{n_z}) \in \mathbb{N}_0^{n_z}$ is a multi-index with $|\mathbf{i}| = i_1 + i_2 + \cdots + i_{n_z}$, n_g denotes a non-negative integer and $\{c_{\mathbf{i}}\}$ are the expansion coefficients. $\{\Phi_{\mathbf{i}}(Z)\}$ are the n_z-variate orthogonal polynomials

of degree up to n_g, satisfying the orthogonal relation:

$$\mathbb{E}[\Phi_i(z)\Phi_j(z)] = \int_\Omega \Phi_i(z)\Phi_j(z)dF_Z(z) = \delta_{i,j}, \tag{8}$$

where $\delta_{i,j}$ represents the multivariate Kronecker delta function

$$\delta_{i,j} = \prod_{d=1}^{n_z} \delta_{i_d,j_d} = \begin{cases} 1 & \text{if} \quad i_d = j_d, \\ 0 & \text{if} \quad i_d \neq j_d. \end{cases} \tag{9}$$

For a given distribution of the random parameter Z, one can readily find the type of orthogonal polynomial basis $\{\Phi_i(Z)\}$ using the orthogonality relationship (8). For instance, Gaussian random variable corresponds to Hermite orthogonal polynomials, while uniform distribution leads to Legendre polynomials. A detailed discussion of hypergeometric polynomials and the Askey scheme can be found in [25, 39, 48]. The cardinality of the polynomial space is:

$$N_g = \binom{n_z + n_g}{n_z} = \frac{(n_g + n_z)!}{n_z! n_g!}. \tag{10}$$

By using a single index, a linear ordering of multi-index can be employed to express the gPC expansion (7).

$$\tilde{g}(Z) = \sum_{j=1}^{N_g} c_j \Phi_j(Z). \tag{11}$$

The accuracy of the gPC method can be measured in the popular ℓ^2 norm:

$$\|g(Z) - \tilde{g}(Z)\|^2_{\ell^2_\Omega} := \int_\Omega |g(z) - \tilde{g}(z)|^2 dF_Z(z) \to 0, \qquad n_g \to \infty, \tag{12}$$

whose convergence rate is in tandem with the smoothness of the limit state function g.

Given a set of N_p ($N_p \leq M$) random parameters samples $S_z = \left\{z^{(i)}\right\}_{i=1}^{N_p}$ and their corresponding system outputs $g(S_z)$, the expansion coefficients $\{c_j\}$ are the only unknowns left to complete our surrogate model (11). Depending on the number of samples N_p, different numerical methods can be employed to compute $\{c_j\}$. Detailed discussion of those methods can be found in [46, 47]. In this paper, we employ the least squares type stochastic collocation method [3, 11, 20, 44] to construct the gPC expansion. Let $z^{(1)}, \ldots, z^{(N_p)}$ be a set of sample points, $\mathbf{g} = (g(z^{(1)}), \ldots, g(z^{(N_p)})^T$ be the data vector of the true limit state function. Then by solving the following minimization problem, the least squares gPC expansion could be constructed:

$$\min_{\mathbf{c}} \|\mathbf{Ac} - \mathbf{g}\|_2, \qquad \mathbf{A} = (a_{ij})_{1\leq i\leq N_p,\, 1\leq j\leq N_g}, \qquad a_{ij} = \Phi_j(z^{(i)}). \tag{13}$$

where $\mathbf{c} = (c_1, ..., c_{N_g})^T$ is the coefficient vector. By applying pseudo inverse $\mathbf{A}^\dagger$ of $\mathbf{A}$, the solution $\mathbf{c} = \mathbf{A}^\dagger \mathbf{g}$ could be obtained with various standard numerical solvers.

At the initialization step ($k = 0$), one may construct a low-order gPC surrogate model, typically we set $n_g^{(0)} = 1$, 2 or 3. Following its distribution F_Z, a number of N_p samples for the limit state g are randomly chosen by applying uniform probability from the total sample set. When applying the least squares method, the number of samples at each iteration k should be larger than the number of gPC expansion terms, i.e., $N_p^{(k)} > N_g^{(k)}$. Empirically, we set the oversampling ratio $\alpha = 1.5 \sim 3$ for $N_p^{(k)} = \alpha N_g^{(k)}$. However, in order to obtain asymptotically stable polynomial least squares approximation [9, 32, 33], one needs the oversampling ratio to scale as, at least, $\alpha \sim \log(N_g^{(k)})$. This is now a nonlinear oversampling ratio instead of a fixed number. Both methods shall be used in our numerical tests. Upon evaluating the true limit state g at the chosen points, we have the subset $S^{(0)}$ and the newly constructed initial gPC surrogate using least squares approach, thus obtaining $\tilde{g}^{(0)}(Z)$ with degree $n_g^{(0)}$.

4.2 Adaptive Surrogate Model

After the construction of the initial low-order gPC surrogate model $\tilde{g}^{(0)}(Z)$, our adaptive method starts an iterative procedure. At each iteration step k, a gPC surrogate model $\tilde{g}^{(k-1)}(Z)$ of degree $n_g^{(k-1)} \geq 1$ is available. Let $M^{(k-1)} = \#S^{(k-1)}$ be the number of samples where the values of the true limit state g are known at the $(k-1)$-th iteration. Based on $\tilde{g}^{(k-1)}(Z)$, we shall adaptively enrich the current set $S^{(k-1)}$ by adding additional sample set $\Delta S^{(k)}$ of size ΔM (when $\Delta M > 0$) from the complement set $\tilde{S}^{(k-1)}$. With the new sample set $S^{(k)} = S^{(k-1)} \cup \Delta S^{(k)}$, the gPC model will be refined via the least square approach and increase the gPC order when possible. Finally, to ensure the convergence, we shall propose the following two-step check: (1) if the the difference of the failure probability at successive iterations $|P_f^{(k)} - P_f^{(k-1)}|$ is smaller than the tolerance ϵ. (2) if it satisfies (1), we further add a "safety check" step: we recalculate the failure probability $\tilde{P}_f^{(k)}$ by adding an additional sample set of size ΔT to see if the resulted difference $|P_f^{(k)} - \tilde{P}_f^{(k)}|$ is smaller than the tolerance ϵ. We shall repeat the above steps until the two-step stopping criterions are satisfied.

The adaptive algorithm consists of successive application of the hybrid method and gPC surrogate refinement. Specifically, it has the following major steps:

- **Adaptive Refinement**: At the k-th ($k \geq 1$) iteration,
  (1) Calculate the oversampling condition for the next-order gPC refinement
    - *Let $M^{(k-1)} = \#S^{(k-1)}$, the number of samples where the values of the true limit state g are known at the $(k-1)$-th iteration.*
    - Set

$$N_b = \binom{n_z + (n_g^{(k-1)} + 1)}{n_z} = \frac{\left((n_g^{(k-1)} + 1) + n_z\right)!}{n_z!(n_g^{(k-1)} + 1)!}, \tag{14}$$

      which is the number of terms in the gPC surrogate of one degree higher than the current order $n_g^{(k-1)}$.
    - Set $R^{(k)} = \alpha \cdot N_b$ is the required number of samples at the degree of $n_g^{(k-1)} + 1$.
  (2) Check whether the number of original state g samples satisfies the oversampling condition for the next-order gPC refinement and set the adaptive sample increment ΔM:
    - *If $R^{(k)} < M^{(k-1)}$, increase the gPC order: $n_g^{(k)} = n_g^{(k-1)} + 1$ and set $\Delta M = 0$.*

- *If $R^{(k)} > M^{(k-1)} + \Delta M^0$, keep the current gPC order: $n_g^{(k)} = n_g^{(k-1)}$ and set $\Delta M = \Delta M^0$.*
- *If $M^{(k-1)} \le R^{(k)} \le M^{(k-1)} + \Delta M^0$, increase gPC order: $n_g^{(k)} = n_g^{(k-1)} + 1$ and set $\Delta M = R^{(k)} - M^{(k-1)}$.*

We refer more detailed discussion about this step in Remark. 1.

(3) If $\Delta M > 0$, enrich set $S^{(k-1)}$ with the additional samples of size ΔM.
- *Evaluate the surrogate model $\tilde{g}^{(k-1)}$ at the complement set $\tilde{S}^{(k-1)}$, and sort $\{|\tilde{g}^{(k-1)}(\tilde{S}^{(k-1)})|\}$ in ascending order.*
- *Choose the first ΔM elements in the sorted sequence of $|\tilde{g}^{(k-1)}(\tilde{S}^{(k-1)})|$ and identify their corresponding sample locations z in $\tilde{S}^{(k-1)}$. Denote the collection of these samples as set $\Delta S^{(k)}$.*
- *Evaluate the true limit state g at the samples in $\Delta S^{(k)}$ and obtain $g(\Delta S^{(k)})$.*
- *Update the sets $S^{(k)} = S^{(k-1)} \cup \Delta S^{(k)}$, $\tilde{S}^{(k)} = S \backslash S(k)$.*

(4) *Updated the gPC model. Construct $\tilde{g}^{(k)}(Z)$ using the sample set $S^{(k)}$ and $n_g^{(k)}$ via least squares method* (13).

(5) *Estimate the failure probability*

$$P_f^{(k)} = \frac{1}{M}\left[\sum_{z^{(i)}\in\tilde{S}^{(k)}} \chi_{\{\tilde{g}^{(k)}<0\}}(z^{(i)}) + \sum_{z^{(i)}\in S^{(k)}} \chi_{\{g<0\}}(z^{(i)})\right]. \tag{15}$$

(6) *If stopping criteria is met: $|P_f^{(k)} - P_f^{(k-1)}| < \epsilon$, then continue the following steps. Otherwise, set $k \leftarrow k+1$ and return to Step 1.*

- **Check the accuracy of the surrogate model**:
  - *Evaluate the updated surrogate model $\tilde{g}^{(k)}$ at the complement set $\tilde{S}^{(k)}$, and sort $\{|\tilde{g}^{(k)}(\tilde{S}^{(k)})|\}$ in ascending order.*
  - *Choose the first ΔT elements in the sorted sequence of $|\tilde{g}^{(k)}(\tilde{S}^{(k)})|$ and identify their corresponding sample locations z in $\tilde{S}^{(k)}$. Denote the collection of these samples as set $\Delta\tilde{S}^{(k)}$.*
  - *Evaluate the true limit state g at the samples in $\Delta\tilde{S}^{(k)}$ and obtain $g(\Delta\tilde{S}^{(k)})$.*
  - *Update the sets $S^{(k)} = S^{(k)} \cup \Delta\tilde{S}^{(k)}$, $\tilde{S}^{(k)} = S \backslash S^{(k)}$.*
  - *Estimate the failure probability*

$$\tilde{P}_f^{(k)} = \frac{1}{M}\left[\sum_{z^{(i)}\in\tilde{S}^{(k)}} \chi_{\{\tilde{g}^{(k)}<0\}}(z^{(i)}) + \sum_{z^{(i)}\in S^{(k)}} \chi_{\{g<0\}}(z^{(i)})\right]. \tag{16}$$

  - *Check if stopping criteria is met: $|P_f^{(k)} - \tilde{P}_f^{(k)}| < \epsilon$, then exit. Otherwise, $P_f^{(k)} = \tilde{P}_f^{(k)}$.*
- **Set $k \leftarrow k+1$ and return to the refinement step.**

Remark 1. *Our overall goal is to build a failure model with samples as few as possible. To achieve this, we employ adaptive schemes for both model refinement and sample enrichment strategy. To be specific, the sample increment ΔM in step 2 of the* **Adaptive** *Refinement Module is determined as:*

- *When $R^{(k)} < M^{(k-1)}$), i.e., there is sufficient data in the current data set $S^{(k-1)}$ to allow higher-order gPC model, then we increase the gPC order by one but retain the same data set with ΔM =0.*
- *When $R^{(k)} \ge M^{(k-1)}$,i.e., there is insufficient data in the current set to allow next-order gPC model:*
  - *if $R^{(k)} > M^{(k-1)} + \Delta M^0$, the gPC order is retained but we enrich the current sample set $S^{(k-1)}$ with additional $\Delta M = \Delta M^0$ samples. Here, ΔM^0 serves as the upper bound of sample increment to prevent rapid sample enlargement, and thus costs, at one iteration.*
  - *if $R^{(k)} \le M^{(k-1)} + \Delta M^0$, the gPC order is increased by one but we enrich the current sample set $S^{(k-1)}$ with additional ΔM samples. Note here $\Delta M = R^{(k)} - M^{(k-1)}$ instead of ΔM^0.*

5 NUMERICAL EXAMPLES

In this section, we evaluate the performance of our adaptive surrogate scheme through four numerical examples. Three simple examples are taken from previous works [28]. Our primary goal is to examine the new adaptive algorithm and compare it to the hybrid method from [28]. We shall see that the new algorithm produces equally accurate numerical results as the original hybrid method. However, the present adaptive method does not require the availability of a surrogate model. More importantly, the new adaptive algorithm is, in fact, more efficient, in terms of the required number of samples of the true limit state, than the original hybrid method.

To measure the performance of the proposed methods, the absolute errors between the computed failure probability (by our proposed method) and the reference solutions (by MCS) will be used. We evaluate the values on the total candidate set S by applying the updated surrogate model at the k-th iteration. Besides, we also measure the following two kinds of classification errors to understand the proposed method further:

- "total" classification errors: the percentage of the number of samples (over total samples) whose signs for the limit state are incorrectly predicted during each iteration step.
- "neg-pos" classification errors: the percentage of the number of samples whose true values of g belong to the "failure" region but are classified to the "safe " region by the current surrogate model.

We remark that we conduct MCS with $M = 10^6$ random samples for the first three examples to obtain reference solutions, and we set $M = 10^7$ for the last practical problem due to the sufficiently rare failure probability. For consistency, the same sequences of M samples are utilized in our adaptive scheme for each numerical test.

5.1 Ordinary Differential Equation

We first consider a simple example of ordinary differential equation subject to an initial condition u_0:

$$\frac{du}{dt} = -Zu, \qquad u(0) = u_0, \tag{17}$$

where the decay coefficient Z is a Gaussian random variable $Z \sim \mathcal{N}(\mu, \sigma^2)$ with mean μ and variance σ^2. The corresponding exact solution of (17) is:

$$u(t, Z) = u_0 e^{-Zt}. \tag{18}$$

We define the failure probability of the linear system (17) as

$$P_f = \text{Prob}\left[g\left(u(t, Z)\right) < 0\right], \tag{19}$$

with the limit state function g

$$g(u(t,Z)) = u(t,Z) - u_{\mathrm{d}}, \tag{20}$$

where u_{d} is a given value.

Upon setting $\mu = -2$, $\sigma = 1$, $u_0 = 1$, $t = 1$ and $u_{\mathrm{d}} = 0.5$, the exact failure probability can be computed as $P_f = 0.003539$ and the reference solution by MCS is $P_f^{mc} = 0.003558$. We shall use the MCS reference solution to compute the errors in our algorithm.

For this simple univariate case, we start with a linear gPC approximation ($n_{\mathrm{g}}^{(0)} = 1$) as the initial gPC surrogate model with $\#S^{(0)} = 10$. Hermite polynomials are employed in the gPC surrogate since the random variable is Gaussian. At each iteration step, the error tolerance ϵ is set to be 10^{-6} and $\Delta T = 100$.

The final results at the convergence with respect to the upper bounds of sample increment ΔM^0 are summarized in Table 1. The convergence history for $\Delta M^0 = 20$ is plotted in Figure 1. We observed that nearly all cases result in zero numerical errors, with only a fraction (< 200) of data in the true limit state is used, compared to the MCS reference solution using 10^6 samples and hybrid method reference solution using 6000 samples at the degree of 7 [28]. This represents a substantial computational gain, whenever the evaluation of the underlying system is non-trivial. The current adaptive method is thus not only eliminating the need for a pre-constructed surrogate model, but it is also more efficient than the original hybrid method.

To further demonstrate the benefits by using adaptive gPC model, we plot the convergence history of classification errors (based on $\tilde{g}$ with $\Delta M^0 = 20$) in Figure 2. We observed that the surrogate model is becoming more capable of predicting the sign of the limit state correctly, suggesting the effectiveness of the adaptivity.

Remark 2. *For this example, based on the results of ΔM^0 summarized in Table 1, we observed that once the upper bound of sample increment ΔM^0 is large enough, the total samples are the same, due to the adaptive sample increment ΔM at each iteration. This can be further confirmed by the history of the sample increment at each iteration shown in Figure 3.*

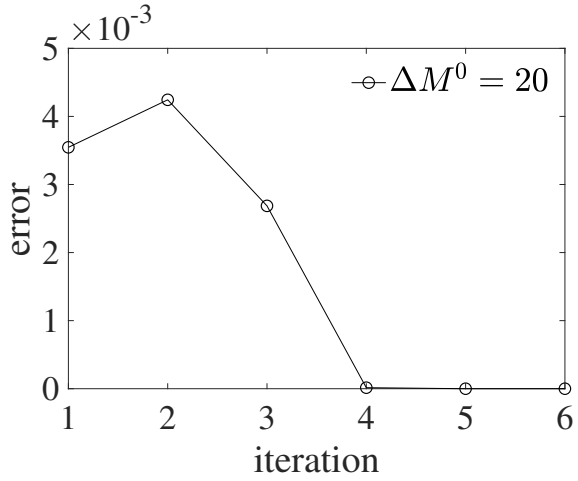

Figure 1: Error convergence versus iteration count of the adaptive algorithm when $\Delta M^0 = 20$ in the ODE Example.

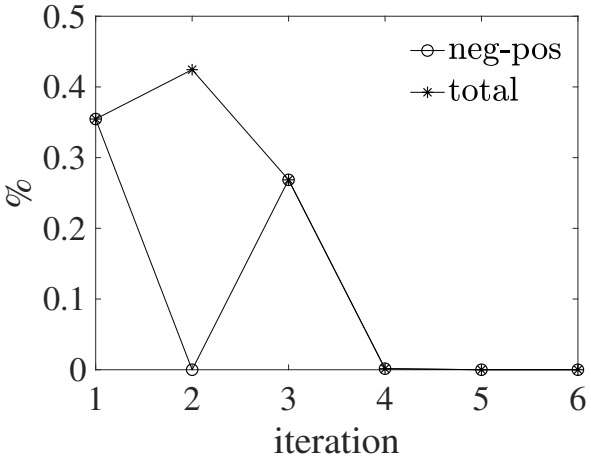

Figure 2: The classification errors versus iteration count for $\Delta M^0 = 20$ in the ODE Example.

5.2 Multivariate Benchmark

Now we consider a multivariate benchmark problem from [28]. Its failure function is defined as:

$$g(X) = X_1 + 2X_2 + 2X_3 + X_4 - 5X_5 - 5X_6, \tag{21}$$

where $X_i \sim LN(\mu_i, \sigma_i)$, for $i = 1, 2, \cdots, 6$, represents 6 independent random variables of log-normal distributions. Let $\{Z_i\}_{i=1}^6$ be i.i.d Gaussian random variables with $\mathcal{N}(0,1)$. We employ Hermite polynomials to approximate $\{X_i\}_{i=1}^6$ as

$$X_i = \sum_{k=0}^{n_{\mathrm{g}}} c_{i,k} H_k(Z_i). \tag{22}$$

We adopt the definition of failure probability $P_f = \mathrm{Prob}\,(g(Z) < 0)$ and set the means and variances of the six random parameters as:

$$\mu_1 = 0.12, \sigma_1 = 1; \quad \mu_2 = 0.12, \sigma_2 = 1; \quad \mu_3 = 0.12, \sigma_3 = 1;$$
$$\mu_4 = 0.12, \sigma_4 = 0.5; \quad \mu_5 = 0.05, \sigma_5 = 1; \quad \mu_6 = 0.04, \sigma_6 = 1,$$

The reference (MCS) solution is $P_f^{mc} = 0.653964$ with 10^6 samples.

The degree of the initial gPC model is set to be $n_{\mathrm{g}}^{(0)} = 1$ using $\#S^{(0)} = 30$ samples. We set the tolerance to be $\epsilon = 10^{-6}$ for each iteration step and $\Delta T = 100$ in this test. Since this is a $n_{\mathrm{z}} = 6$ dimensional expansion, the number of expansion terms N_{g} grows faster at higher degree n_{g}. We therefore employ a linear oversampling rate of $\alpha = 2$, instead of the nonlinear one. We emphasize that the linear oversampling rate did not induce any numerical instability in the solution, as we did not reach a very high degree in the gPC model.

The results at the final convergence with different upper bounds of sample increment ΔM^0 of the true limit state are summarized in Table 2. The convergence history with respect to the iteration counts is shown in Figure 4. It can be seen that except in the case with a small upper bound of sample increment $\Delta M^0 = 10$, the adaptive algorithm in this example generally converges to a gPC

Table 1: Results of the ODE Example($\#S^{(0)} = 10$, $\epsilon = 1e-6$ and $\Delta T = 100$)

ΔM^0	Total iteration	Errors	Final gPC degree	Total number of g samples
10	2	0.003546	2	127
20	6	0	7	184
40	6	0	7	184
80	6	0	7	184
100	6	0	7	184

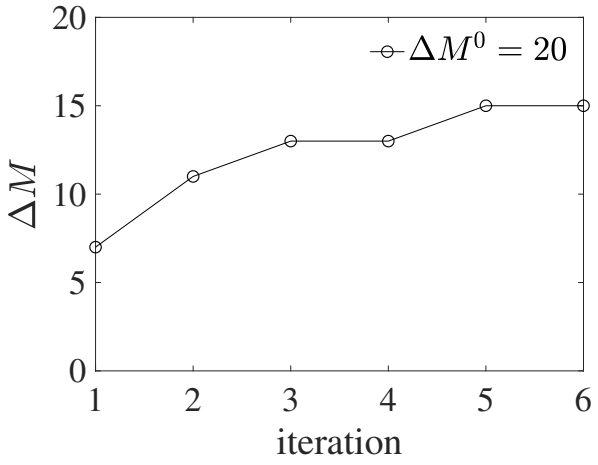

Figure 3: The sample increment ΔM versus iteration count when $\Delta M^0 = 20$ in the ODE Example.

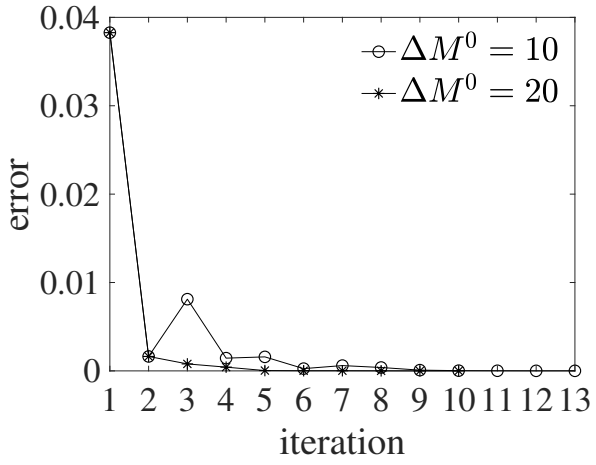

Figure 4: Error convergence versus iteration count of the adaptive algorithm when $\Delta M^0 = 10$ and $\Delta M^0 = 20$ in the 6-dimensional Example.

model at a degree of 11 with the same number of samples, and all the cases induce negligible numerical errors. Compared with the MCS solution using 10^6 samples, the adaptive method uses a much lower number of samples (234), which is superior to the performance of the hybrid method using 300 samples at the degree of 11 [28].

Again, the corresponding classification errors based on $\tilde{g}$ with respect to the iteration count for $\Delta M^0 = 20$ are plotted in Figure 5. It clearly shows that the classification performance on the failure samples is further enhanced as the iteration increases with the improvement of the gPC surrogate model during the iteration.

5.3 Partial Differential Equation.

We next consider the following 1D viscous Burgers' equation:

$$\begin{aligned} &u_t + uu_x = \nu u_{xx}, \quad x \in [-1, 1], \\ &u(-1) = 1 + \delta, \qquad u(1) = -1. \end{aligned} \tag{23}$$

Here $\nu > 0$ is the viscosity and $\delta \in (0, 0.01)$ is a small perturbation characterized as a uniformly distributed random variable.

In this example, the solution profile exhibits a transition layer, whose location x_f is the zero of the solution profile at steady state $u(x_f) = 0$. It can be computed from the equations below:

$$A \tanh\left[\frac{A}{2\nu}(1 + x_f)\right] = 1 + \delta, \qquad A \tanh\left[\frac{A}{2\nu}(1 - x_f)\right] = 1. \tag{24}$$

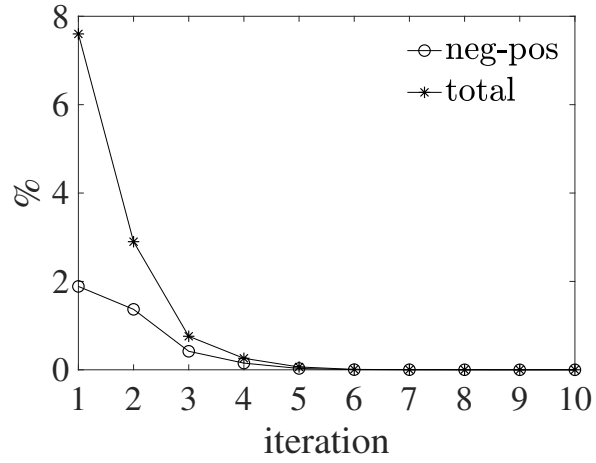

Figure 5: The classification errors versus iteration count for $\Delta M^0 = 20$ in the 6-dimensional Example.

The perturbation δ at the left boundary condition $x = -1$ may significantly affect the value of x_f. Hence the Burgers' equation (23) serves as a good numerical example for our adaptive scheme.

Table 2: Results of the 6-dimensional Example($\#S^{(0)} = 30$, $\epsilon = 1e-6$ and $\Delta T = 100$)

ΔM^0	Total iteration	Errors	Final gPC degree	Total number of g samples
10	13	3.0×10^{-6}	8	208
20	10	0	11	234
40	10	0	11	234
80	10	0	11	234
100	10	0	11	234

We adopts the same definition of the limit state function used in [28]:

$$g(x_f(\delta)) = -x_f(\delta) + 0.75, \tag{25}$$

and compute the failure probability $P_f^{mc} = 0.872768$ using MCS with 10^6 samples. We set the initial degree $n_g^{(0)} = 2$ and $\#S^{(0)} = 20$ for constructing our surrogate model. The oversampling ratio is set to $\alpha = 5\log(N_g^{(k)})$ in this case. We set an error control $\epsilon = 10^{-6}$ and $\Delta T = 100$ here.

The results with different upper bounds of sample increment ΔM^0 are shown in Table 3, along with the convergence history with respect to iteration count in Figure 6. We observe that the new adaptive method achieves remarkable accuracy (zero numerical errors) in all cases while incurring minimal computational cost (less than 600 samples of the true limit state g). Not only is this a significant computational gain compared to the brute force MCS (which uses 10^6 samples), it also outperforms the hybrid sampling method (using around 4000 samples) from [28] by a noticeable margin due to the adaptive refinement of the underlying gPC surrogate model. As the accuracy of the gPC surrogate improves, it further enhances the classification performance of the hybrid method. This can be further confirmed by the convergence history of the classification errors with respect to the iteration counts for $\Delta M^0 = 20$ in Figure 7.

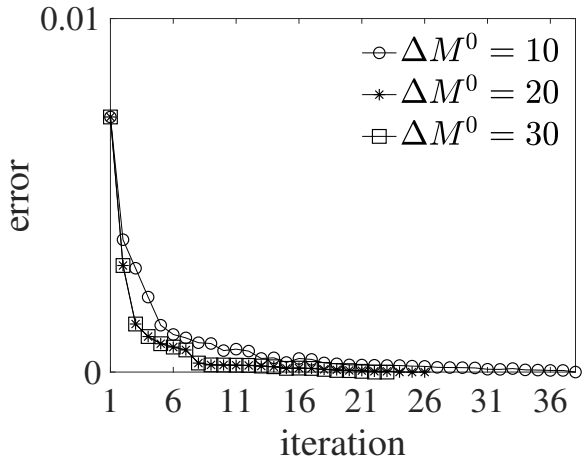

Figure 6: Error convergence versus iteration count of the adaptive algorithm when $\Delta M^0 = 10, 20, 30$ respectively in the PDE Example.

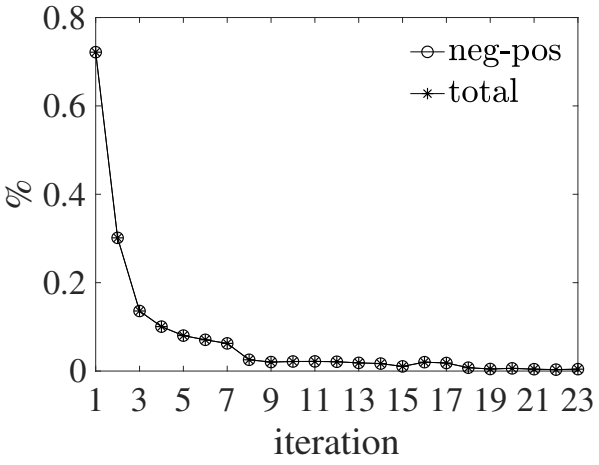

Figure 7: The classification errors versus iteration count for $\Delta M^0 = 30$ in the PDE Example.

5.4 A Microelectronics benchmark

Finally, we evaluate the performance of our adaptive scheme via a practical problem in microelectronics. Specifically, we study the failure probability of spin-transfer torque magnetic random access memory (STT-MRAM), a fast-growing technology for stand-alone and embedded memory applications [8, 42]. Since it involves a high-frequent spin-transfer for the writing process, its failure probability, or more precisely, the Write Error Rate (WER) is a key design parameter for both device and large-array yield improvement [35].

The dynamics of instantaneous magnetization ($\vec{m}$) of a magnet subject to external perturbation such as magnetic fields or spin currents is often described by the classical Landau-Liftshitz-Gilbert (LLG) equation [43] in normalized spherical coordinate:

$$(1+\lambda^2)\frac{\mathrm{d}\vec{m}}{\mathrm{d}t} = -|\Gamma|(\vec{m}\times\vec{H}) - \lambda|\Gamma|(\vec{m}\times\vec{m}\times\vec{H}) + \vec{\tau} + \lambda(\vec{m}\times\vec{\tau}). \tag{26}$$

The magnet of interest is assumed mono-domain and the orientation of normalized $\vec{m}$ is:

$$\vec{m} = \begin{bmatrix} m_x & m_y & m_z \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix}, \tag{27}$$

whose initiation starts at the x-z plane, i.e. $\vec{m}_0 = [\sin\theta_0\ 0\ \cos\theta_0]$.

We note that cross product operator ($\times$) is employed in eqn (26): $\vec{v}_1 \times \vec{v}_2 = |\vec{v}_1||\vec{v}_2|\sin(\omega)\vec{n}$, with ω as the angle between $\vec{v}_1$ and $\vec{v}_2$, and $\vec{n}$ as the unit vector perpendicular to both $\vec{v}_1$ and $\vec{v}_2$. The spin torque is denoted as $\vec{\tau} = (\vec{m}\times\vec{I}_s\times\vec{m})/(qN_s)$, with $\vec{I}_s = [0\ 0\ I_s]$ as

Table 3: Results of the PDE Example($\#S^{(0)} = 20, \epsilon = 1e-6$ and $\Delta T = 100$)

ΔM^0	Total iteration	Errors	Final gPC degree	Total number of g samples
10	38	0	21	540
20	26	0	24	523
30	23	0	25	524
40	23	0	25	524
80	23	0	25	524
100	23	0	25	524

Table 4: Results of the Microelectronics Example ($\#S^{(0)} = 60, \epsilon = 1e-7$, $\Delta T = 100$ and $\alpha = 3\mathbf{log}(N_g^{(k)})$)

ΔM^0	Total iteration	Errors	Final gPC degree	Total number of g samples
10	34	0	4	580
20	22	0	4	694
50	11	0	4	624
80	11	0	5	937
100	11	0	5	977

Table 5: Results of the Microelectronics Example ($\#S^{(0)} = 60, \epsilon = 1e-7$, $\Delta T = 100$ and $\alpha = 5\mathbf{log}(N_g^{(k)})$)

ΔM^0	Total iteration	Errors	Final gPC degree	Total number of g samples
10	29	0	3	640
20	19	1.0×10^{-7}	3	640
50	17	0	4	923
80	11	0	4	883
100	10	1.0×10^{-7}	4	1023

electrical current and q as the charge of an electron. N_s is the total number of spins in the nano-magnet and defined as: $N_s = M_s V/\mu_B$, where M_s is saturation magnetization, V refers to the volume and μ_B is the Bohr magneton. The gyromagnetic ratio is represented by Γ, and the Gilbert damping parameter λ is magnet-specific which is often determined from experiment. Finally, the internal fields on the magnet is assumed as $\vec{H} = [0 \ -h_d m_y \ m_z]$, where h_d is the dimensionless demagnetizing field while no heat is applied here.

In this study, all quantities are taken as dimensionless by using the constant $M_s/(2k_u\Gamma)$ with saturation magnetization $M_s = 780$, the unidirectional anisotropy constant $k_u = 3.14e^4$ and $\Gamma = 1.76e^7$. Other parameters are set as $h_d = 0$, $\lambda = 0.007$, $V = 2.72e^{-17}$ and $\mu_B = 9.274e^{-21}$. The LLG equation (26) is numerically computed by a variable order Adams-Bashforth-Moulton PECE solver [43].

Three random parameters, initial azimuth angle θ_0, current magnitude I_s, and period of interest (final time) T are considered and each is prescribed with the Beta distribution of $\beta(3, 1)$. Consequently, our gPC surrogate model consists of Jacobi polynomials of three dimensions ($N_z = 3$). The failure domain is set as $\theta(t = T) = \theta_T < \pi/2$ while $\theta_T \geq \pi/2$ is considered "safe". The reference MCS solution is computed as $P_f^{mc} = 0.0000892$ with 10^7 samples. In the adaptive scheme, we set the initial gPC order as $n_g^{(0)} = 3$ with $\#S^{(0)} = 60$ samples. An error control is set to be $\epsilon = 10^{-7}$ and $\Delta T = 100$ here. We test two oversampling ratios: $\alpha = 3\log(N_g^{(k)})$ and $\alpha = 5\log(N_g^{(k)})$. Results at convergence are shown in Table 4 and Table 5 using different ΔM^0. And the convergence history with respect to iteration count for $\Delta M^0 = 20, 80, 100$ when $\alpha = 3\log(N_g^{(k)})$ is plotted in Figure 8. In all cases, our adaptive scheme ends up with a gPC model with degree ≤ 5 and converges quickly to (nearly) zero numerical errors with a much less number of samples, which is roughly 0.01% of those via the traditional MCS method (10^7 samples).

We conclude that the new adaptive method achieves remarkable accuracy in all cases, while incurring a minimal computational cost. We emphasize again that the current method does not require a pre-defined surrogate model. Therefore, our adaptive method offers much more flexibility for practical applications.

6 SUMMARY

In this paper, we propose an efficient adaptive numerical scheme to estimate the probability of system failure. The method combines the idea of surrogate-based hybrid method in [28] and generalized polynomial chaos (gPC) expansion. We start by constructing a low-degree gPC expansion as an initial surrogate model for the failure probability computation. During the iteration process, our scheme adaptively updates the underlying gPC surrogate model with new samples and increases the polynomial order when possible. This results in a highly efficient method for failure probability

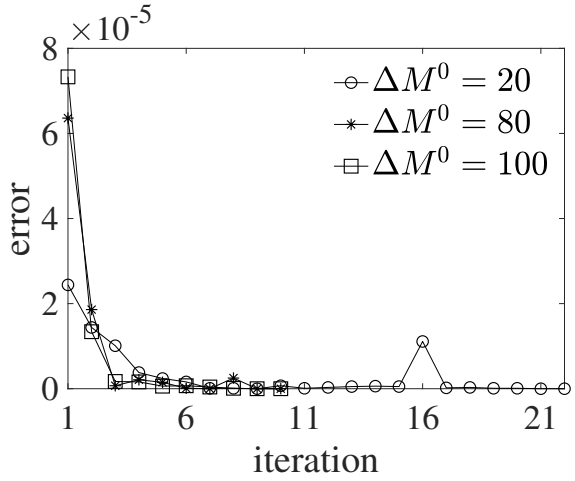

Figure 8: Error convergence versus iteration count of the adaptive algorithm when $\Delta M^0 = 20$, 80 and 100 respectively in the Microelectronics Example with $\alpha = 3\log(N_g^{(k)})$.

computation. It not only eliminates the need for a priori surrogate model, which is usually not readily available for many practical problems, but also improves the overall performance with fewer samples from the true limit state than those of the original hybrid method.

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