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HIGH DIMENSIONAL UNCERTAINTY QUANTIFICATION USING THE DERIVATIVE APPROACH

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Abstract. In this paper a new non-intrusive method for estimation of uncertainty in computational models is presented. The method is based on a new equation, which is derived from the ANOVA-decomposition. The method decomposes a stochastic space into sub-domains, which then are separately interpolated. This leads to a dramatic reduction of necessary samples for high dimensional spaces.

The non-intrusive interpolation technique couples the Multi-dimensional Lagrange Interpolation technique with the Derivative Equation, while samples are obtained through a new sampling strategy, the non-complete tensor product, which allows arbitrary number of samples for higher dimensions. The Monte Carlo simulation is then applied on the surrogate model to obtain full statistical properties of the considered expensive function.

The proposed method is compared to the Non-intrusive Polynomial Chaos (Point collocation approach) with Smolyak Sparse Grid sampling strategy, which is used as a surrogate model and statistical properties are obtained by the MC simulation. The comparison is made on well known analytic functions used as test problems for uncertainty quantification methods. The proposed method converges faster to low level of errors and, therefore, it is expected that it could be very useful for practical applications.

1 INTRODUCTION

The non-intrusive Uncertainty Quantification (UQ) techniques try to estimate the function behavior by interpolating samples in the stochastic space. One of the biggest limitation of the high dimensional space interpolation is related to the Curse of Dimensionality (CoD), which states that the number of necessary samples grows exponentially with each

new stochastic random variable considered. This fundamental problem limits usage of non-intrusive methods to a lower number of stochastic dimensions.

Various sampling techniques were proposed to handle the CoD problem. The Latin Hyper-cube sampling (LHS) was successfully used in various problems [1] and more different approaches are available such as LaPSO [2], Uniform Design (UD) [1] or Hammersley Sampling [3]. For UQ, Smolyak Sparse grid [4] and its various modification became very popular. This sampling strategy combined with Non-intrusive Polynomial Chaos (NIPC) gives very accurate results for a low number of samples. Unfortunately, even this approach is not affordable for problems with high cardinality.

In this work a new surrogate approach is proposed, which is based on the coupling of a new equation with the Lagrange interpolation. The equation allows to sample the stochastic domain only where it is necessary, thus dramatically reducing the necessary number of samples for high dimensional spaces.

The paper is structured as follows. In the first part, the equation is derived. The second part is given to the numerical application of the new equation and its application to surrogate modeling. Third part describes necessary sampling strategy for surrogate models. Fourth part is given to applied examples of forward uncertainty quantification and lastly, the obtained results are discussed and conclusions are given.

2 THEORY

The Derivative Equation (DE), as this new equation is called, is derived from the ANOVA decomposition [5, 6]. Let us consider an integrable function, $f(x)$, which is defined on a n-dimensional unit hypercube - $[0,1]^n$ and $x \in [0,1]^n$. The representation of $f(x)$ can be

$$f(x) = f_0 + \sum_{s=1}^{n} \sum_{i_1<..<i_s}^{n} f_{i_1 \dots i_s}(x) \tag{1}$$

The explicit form of the equation (1) is

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{i,j}(x_i, x_j) + ... + f_{1,\dots,n}(x_1, ..., x_n) \tag{2}$$

and its total number of summands is 2^n. The above function is called ANOVA decomposition if

$$f_0 = \int f(x) dx \tag{3}$$

and

$$\int_0^1 f_{i_1 \dots i_s}(x) dx_{i_p} = 0 \tag{4}$$

where $1 \leq i_1 < i_2 < ... < i_s \leq n$, $1 \leq s \leq n$ and $1 \leq p \leq s$. To define all the one dimensional terms, integration over all the variables except x_i is done. The result leads

to

$$\int f(x) \prod_{p \neq i} dx_p = f_0 + f_i(x_i) \tag{5}$$

after all the one dimensional terms are defined. Then the same procedure can be extended to the two dimensional problem by integrating all variables except x_i and x_j:

$$\int f(x) \prod_{p \neq i,j} dx_p = f_0 + f_i(x_i) + f_j(x_j) + f_{i,j}(x_i, x_j) \tag{6}$$

in the same way, higher terms can be computed and the last term in equation (1) is defined. An important property of an equation (1) is orthogonality of given terms, i.e.

$$\int f_{i_1 \ldots i_s}(x) f_{k_1 \ldots k_l}(x) dx = 0 \tag{7}$$

where $(i_1 \ldots i_s) \neq (k_1 \ldots k_l)$, which is direct consequence of equation 4.

To obtain DE, consider a function, $f(x)$, which is derivable and integrable. Then all terms in equation (2) are integrable and derivable too. Let us assume that each term represents a derivation of the function according to its generic variable x_i

$$f_i(x_i) = \frac{\partial f(x)}{\partial x_i} \tag{8}$$

which for the two dimensional terms is

$$f_{i,j}(x_i, x_j) = \frac{\partial f(x)}{\partial x_i, x_j} \tag{9}$$

Higher order terms are derived accordingly. The first term in the equation (2) is a constant, i.e. $f_0 = C$, hence $df_0 = 0$. The left side term of the equation (2) is derived as $f(x) = df(x)$ and then we have

$$df(x) = \sum_i \frac{\partial f(x)}{\partial x_i} dx_i + \sum_{i<j} \frac{\partial f(x)}{\partial x_i, x_j} dx_i dx_j + \ldots + \frac{\partial f(x)}{\partial x_1, \ldots, x_n} dx_1 \ldots dx_n \tag{10}$$

The equation (10) is the basic form of DE. Note that each term is multiplied by the derivative according to its variable to be mathematically consistent. To prove validity of equation (10) and obtain its integral form, let us integrate the equation (10) in the same way as derivations were applied

$$f_i(x_i) = \int \frac{\partial f(x)}{\partial x_i} dx_i \tag{11}$$

which for the two dimensional terms is

$$f_{i,j}(x_i, x_j) = \int \int \frac{\partial f(x)}{\partial x_i, x_j} dx_i dx_j \tag{12}$$

Higher order terms are derived accordingly. The left hand side term in the equation (10) is integrated in the following way

$$\int df(x) = f(x) + C \tag{13}$$

where $C = -f_0$, i.e. it is a constant. For more useful application, let us rewrite equation (13) in the following form

$$\int_{f(^c x)}^{f(x)} df(x) = f(x) - f(^c x) \tag{14}$$

Using the equation (14) and a definite integral for each summand, the integrated form of the equation (10) reads

$$\begin{aligned} f(x) - f(^c x) = \sum_i \int_{^c x_i}^{x_i} \frac{\partial f(x)}{\partial x_i} dx_i + \\ \sum_{i<j} \int_{^c x_i}^{x_i} \int_{^c x_j}^{x_j} \frac{\partial f(x)}{\partial x_i, x_j} dx_i dx_j + ... + \int_{^c x_1}^{x_1} ... \int_{^c x_n}^{x_n} \frac{\partial f(x)}{\partial x_1, ..., x_n} dx_1 ... dx_n \end{aligned} \tag{15}$$

where ${}^c x_i$ represents a central position in the stochastic space. In this case, the central point is considered a statistical mean value of given stochastic random variable, i.e. ${}^c x_i = mean(x_i)$. The integral form of the DE is used for practical applications.

Note that if we look at the term $df(x)$ alone, that part can be understood as a change of a function along the stochastic space. One can intuitively think, that $df(x)$ is basically infinitesimal change around the central point of a given function. Let x_i be a random variable with assigned distribution, then $df(x)$ will represent an infinitesimal change in the final Probability Density Function (PDF) given by the equation (10). If we focus on the right hand side of the equation 10, it can be seen that this change is given only by its derivations. Therefore, we can say:

Definition Let $f(x)$ be a function with range $D \in [-\infty \ \infty]$ and its domain $x \in \Re$. Let x be a random variable with given PDF, then the shape of resulting PDF is given only by input distributions and derivations of given function, $f(x)$.

3 NUMERICAL APPROACH

The numerical approach is based on the equation (15) and the well know First Fundamental Theorem of Calculus [7]. The theorem can be written in the following way

$$f(b) - f(a) = \int_a^b F(x) dx \tag{16}$$

Using the Second Fundamental theorem of Calculus [7], the equation (16) can be rewritten such that

$$f(b) - f(a) = \int_a^b \frac{\partial f(x)}{\partial x} dx \tag{17}$$

This simple formula can be applied to the integral form of DE (equation (15)) for all the first order derivations.

To closely explain the numerical application, let us consider a continuous function $F(x_1, x_2, x_3)$. The first term in the integral form of DE using the equation (17) reads

$$dF_1(x_1) = \int_{c_{x_1}}^{x_1} \frac{\partial F(x_1, {}^c x_2, {}^c x_3)}{\partial x_1} dx_1 = F(x_1, {}^c x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) \tag{18}$$

where ${}^c x_i$ represents the position of the central point of the random variable x_i. The increment function, $dF(x)$, assumes only one random variable and all other random variables are hold constant at their central value. Note that an interpolation model of $dF_1(x_1)$ is created from samples on the abscissa, x_1, and it is independent of other samples. Increment functions for other variables (x_2, x_3) are created in a similar way.

Second order derivations are a bit more complex to handle. Let us consider the previous function and assume a point on a plane, e.g. $x_3 = {}^c x_3$. All integration parts of the integral DE, which are involving x_3, are zero and this assumption allows to rewrite the integral form of DE into the following form

$$\begin{aligned} F(x_1, x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) = \\ \int_{c_{x_1}}^{x_1} \int_{c_{x_2}}^{x_2} \frac{\partial F(x_1, x_2, {}^c x_3)}{\partial x_1 \partial x_2} dx_1 dx_2 \\ + \int_{c_{x_1}}^{x_1} \frac{\partial F(x_1, {}^c x_2, {}^c x_3)}{\partial x_1} dx_1 + \int_{c_{x_2}}^{x_2} \frac{\partial F({}^c x_1, x_2, {}^c x_3)}{\partial x_2} dx_2 \end{aligned} \tag{19}$$

It is obvious that one dimensional integrals of equation (19) can be replaced by equation (18) and a similar equation for x_2. This leads to the following simplification

$$\begin{aligned} F(x_1, x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) = \int_{c_{x_1}}^{x_1} \int_{c_{x_2}}^{x_2} \frac{\partial F(x_1, x_2, {}^c x_3)}{\partial x_1 \partial x_2} dx_1 dx_2 \\ + F(x_1, {}^c x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) + F({}^c x_1, x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) \end{aligned} \tag{20}$$

which can be rewritten into the following form

$$\begin{aligned} dF_{12}(x_1, x_2) = \int_{c_{x_1}}^{x_1} \int_{c_{x_2}}^{x_2} \frac{\partial F(x_1, x_2, {}^c x_3)}{\partial x_1 \partial x_2} dx_1 dx_2 = \\ F(x_1, x_2, {}^c x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) - F(x_1, {}^c x_2, {}^c x_3) \\ + F({}^c x_1, {}^c x_2, {}^c x_3) - F({}^c x_1, x_2, {}^c x_3) + F({}^c x_1, {}^c x_2, {}^c x_3) \end{aligned} \tag{21}$$

where the increment function, $dF_{12}(x_1, x_2)$, is treated as a function with only two variables and the rest is hold constant. The same approach can be applied to remaining parts of the integral form of DE. The final step is to put all increment functions into the basic shape of the integral form of DE, which reads

$$\begin{aligned} F(x_1, x_2, x_3) - F({}^c x_1, {}^c x_2, {}^c x_3) = dF_1(x_1) + dF_2(x_2) + dF_3(x_3) + dF_{12}(x_1, x_2) + \\ dF_{13}(x_1, x_3) + dF_{23}(x_2, x_3) + dF_{123}(x_1, x_2, x_3) \end{aligned} \tag{22}$$

Each increment function is then interpolated by an independent technique and the equation (22) represents a sum of independent interpolation techniques. Various techniques for interpolation of increment functions such Kriging surrogate model [1] or Stochastic collocation approach [8] can be used. In this work, the Multidimensional Lagrange Interpolation technique (MLI) [9] was used. Note that higher increment functions in equation (22) can be a zero and, therefore, they can be easily neglected. This will lead to a simplification of the sampling space and dramatic reduction of necessary samples.

4 SAMPLING STRATEGY

The Derivative Uncertainty Quantification approach (DUQ) requires a special sampling strategy. Sample points cannot be completely randomly spread around the stochastic domain. Therefore, random sampling strategies such as LHS or UD cannot be used. This problem occurs from the increment function as each increment function use samples from all involved sub-spaces.

The first step in the sampling strategy is to sample the first order increment functions, i.e. $dF_i(x_i)$. To illustrate the sampling process, consider a function with 3 random stochastic variables. The first order increment functions (function (18)) require samples only on the abscissas, i.e. x_1, x_2, x_3. The sampling strategy for the 1-D increment functions are selected: Chebyshev-Gauss nodes [10] and Clenshaw-Curtis nodes [11]. The Chebyshev-Gauss nodes are used in case of a normal distribution and Clenshaw-Curtis nodes are selected in case of other distribution. The derivative method requires a sample at the central position of the stochastic space. It is a natural choice to put the central point at the mean value for a given distribution of a random variable, i.e. $mean(x_i) = {}^c x_i$. 1-D interpolation model can be constructed for each variable using the central point and samples on the corresponding abscissa. Note that if the function does not have any interaction term, the process of sampling is over (no more samples are required) and the CoD is completely broken.

Let us now focus on the higher derivation case. From equation (21), it can be clearly seen the necessity to have samples positioned on the abscissas. It can be estimated that for each higher order increment function, all samples, belonging to the domain of given function, have to lie on the intersection of samples from all involved sub-spaces. This is later on called cross section condition. Note that if one of the integration limits is $x_i = {}^c x_i$ then the increment function is zero. Therefore, the influence of the interaction term and only the interaction term can be estimated.

4.1 Design technique of Non-complete tensor product and selection of higher order derivations

For higher order derivations, it is not necessary to have the same number of samples as in lower order derivations. We observed that higher order interactions play non-significant role. Therefore, an engineering approach for the estimation of samples in higher dimensions is used. The basic equation for establishing the number of samples used in higher dimensions reads

$$N = n_i^{-\frac{1}{K}} O^{-K} \tag{23}$$

where n_i is the number of samples in 1-D quadrature for given direction, O is the selected order of derivation and k is the coefficient of growth (COG). The COG is pre-selected by the user at the beginning of the DUQ process. The final number is halved and rounded to get an integer. We observed that tails of the final distribution are given by higher order increment functions, i.e. $df(x_1, ..., x_n)$, and require only a low number of samples. The position of samples in given stochastic domain is selected to be uniformly distributed and holding the cross section condition.

The selection of increment functions is based on cross validation. One sample is randomly sampled on the border of the stochastic domain and the value of the increment function is estimated. If the value is lower then $< 10^{-14}$, the increment function is neglected. The testing sample have to hold the cross section condition. The algorithm for the selection and sampling of higher increment functions reads

for $i = 1$ *to Number of increment functions* **do**
  Beginning;
  1. Randomly sample given domain on its border;
  if $df_i(x_i) < 10^{-14}$ **then**
    1. Delete the increment function, $df_i(x_i)$, from the final model and go to beginning;
  end
  2. Compute the equation (23) for each direction;
  3. Sample the stochastic domain in given directions;
  4. Create a surrogate model from samples in given domain;
  5. Go to beginning;
end

Algorithm 1: Sampling strategy for higher order increment functions

The example of a non-complete tensor product can be seen in Figure 1. In this work, the same COG is used for all dimensions and Figure 1 is created with $COG = 1.5$.

5 ANALYTIC CASE STUDIES

Three test cases were selected. On each test case, the Monte Carlo (MC) simulation with 100000 samples was applied and it represents the reference method. The MC simulation is applied on the surrogate technique DUQ and NIPC with Smolyak sparse grid.

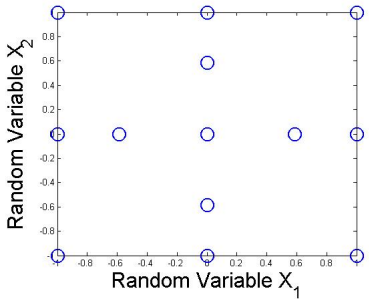

Figure 1: Non-complete tensor product for the two dimensional problem

Statistical properties are obtained by the MC simulation and compared with the reference method.

5.1 Rosenbrock function

The first test problem is the 5-D Rosenbrock function. The function can be found in [12, 9] and it reads

$$F(x) = \sum_{i_1=1}^{d-1} [100(x_{i+1} - x_i^2)^2 + (x_i + 1)^2] \tag{24}$$

The case A considers all input variables as a normal random variable with mean 0 and standard deviation 0.5. The interpolation range for each variable is set to [-2, 2]. The case B considers all inputs as uniform random variables with range [-2, 2]. Results are summarized in Tables 1, 2 and 3.

Case	Function calls	Mean	Standard deviation	Input Distribution
A	100000	180.1435	197.8647	Normal
B	100000	1.8233e+03	1.3315e+03	Uniform

Table 1: Monte Carlo simulation for the 5-D Rosenbrock function

5.2 Borehole model

Second test case is the Borehole model [1]. It represents an 8-D physical problem and the function reads

$$F(x) = \frac{2\pi T_u (H_u - H_l)}{ln\frac{r}{r_w}(1 + \frac{2LT_u}{ln\frac{r}{r_w} r_w^2 K_w} + \frac{T_u}{T_l})} \tag{25}$$

Results are summarized in Tables 4, 5 and 6.

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Max. Order	COG
1	11	329.7644	217.3431	0.7562	0.0984	1	-
2	21	179.6395	176.0975	0.0025	0.1100	1	-
3	31	179.6395	176.0975	0.0025	0.1100	1	-
4	33	180.1435	235.4845	0.7587	0.1901	2	1
5	43	180.1435	197.8647	4.3093e-16	2.8728e-16	2	1
6	53	180.1435	197.8647	1.4364e-16	2.8728e-16	2	1.5
7	11	2.6725e+03	1.1435e+03	0.6378	0.1412	1	-
8	21	1.8205e+03	1.0392e+03	0.0021	0.2196	1	-
9	31	1.8205e+03	1.0392e+03	0.0021	0.2196	1	-
10	33	2.6754e+03	1.4143e+03	0.6399	0.0622	2	1
11	43	1.8233e+03	1.3315e+03	3.4153e-16	1.7076e-16	2	1
12	53	1.8233e+03	1.3315e+03	3.4153e-16	1.7076e-16	2	1.5

Table 2: DUQ approach for the 5-D Rosenbrock function - 1-6 Case A, 7-12 Case B

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Order of PC
1	11	507.7477	1.9992	1.6557	0.9899	1
2	61	267.6256	247.2805	0.4421	0.2497	2
3	61	268.1873	249.1075	0.4450	0.2590	3
4	241	180.1435	197.8647	4.7605e-11	1.5624e-11	4
5	801	180.1435	197.8647	2.6421e-11	1.4142e-11	5
6	11	1.4615e+03	4.6179	0.2717	0.9965	1
7	61	2.6346e+03	1.2881e+03	0.6093	0.0326	2
8	61	2.6376e+03	1.4828e+03	0.6115	0.1136	3
9	241	1.8233e+03	1.3315e+03	4.2178e-14	2.5614e-15	4
10	801	1.8233e+03	1.3315e+03	1.1138e-14	1.4321e-15	5

Table 3: NIPC approach for the 5-D Rosenbrock function - 1-5 Case A, 6-10 Case B

5.3 Wing weight model

The wing weight model represents a 10-D physical model. The function can be found in [13] and it reads

$$F(x) = 0.036 S_w^{0.758} W_{fw}^{0.0035} \left(\frac{A}{\cos^2 \Lambda}\right)^{0.6} q^{0.006} \lambda^{0.04} \left(\frac{100 t_c}{\cos \Lambda}\right)^{-0.3} (N_z W_d g)^{0.49} + S_w W_p \qquad (26)$$

Results are summarized in Tables 7, 8 and 9.

Function calls	Mean	Standard deviation
100000	73.9639	28.7191

Table 4: The MC simulation for the 8-D Borehole model

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Max. Order	COG
1	17	73.9956	27.7282	0.0011	0.0345	1	-
2	33	73.9791	27.6946	5.3190e-04	0.0357	1	-
3	49	73.9792	27.6947	5.3395e-04	0.0357	1	-
4	142	73.9657	28.7214	6.4488e-05	8.1155e-05	2	1
5	147	73.9658	28.7215	6.6573e-05	8.5043e-05	2	1.5
6	575	73.9640	28.7184	4.4116e-06	2.4218e-05	3	1
7	1031	73.9640	28.7193	5.0391e-06	9.2827e-06	3	0.4

Table 5: DUQ approach for the 8-D Borehole model

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Order of PC
1	17	71.6365	27.5577	0.0810	0.0404	1
2	145	73.9715	28.3289	2.6417e-04	0.0136	2
3	849	73.9722	28.7227	2.8927e-04	1.2510e-04	3
4	849	73.9644	28.7254	1.9738e-05	2.1838e-04	4
5	3937	73.9642	28.7193	1.1930e-05	8.7870e-06	5
6	3937	73.9639	28.7192	1.1260e-06	2.7243e-06	6

Table 6: NIPC approach for the 8-D Borehole model

6 DISCUSSION

The fast convergence of DUQ in the Rosenbrock function can be explained by its low order interactions. Also, its shape is given by a polynomial function, therefore, it is easy for MLI technique to interpolate the function exactly. The higher order derivations are given by a low order polynomial and therefore, the function is fully described with high COG coefficient, i.e. a low number of samples. This emphasizes the need of different number of samples in higher dimensions. The Borehole model represents a very well known test case for sensitivity analysis. The DUQ gives very good approximation of the PDF shape with a limited number of samples (142 samples). The wing weight model represents a function with high interaction terms, which is not supposed to be predicted well with a low maximum order, but results show that the DUQ has excellent performance with a low maximum order. This is well explained in the work of Sobol [6].

The main advantage of DE is its independence of an interpolation technique. The

Function calls	Mean	Standard deviation
100000	268.1526	48.3024

Table 7: MC simulation for the 10-D Wing Weight Model

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Max. Order	COG
1	21	268.1847	48.3024	6.6445e-04	0.0014	1	-
2	41	268.1314	47.7784	4.3820e-04	0.0108	1	-
3	61	268.1318	47.7808	4.2891e-04	0.0108	1	-
4	197	268.1489	48.3177	7.6083e-05	3.1775e-04	2	1.5
5	641	268.1497	48.2955	5.8390e-05	1.4372e-04	2	0.4
6	869	268.1515	48.3223	2.2722e-05	4.1148e-04	3	1
7	1313	268.1523	48.3000	5.0292e-06	5.0147e-05	3	0.4

Table 8: DUQ approach for the 10-D Wing weight model

Test case	Function calls	Mean	Standard Deviation	Relative error of Mean	Relative error of S. D.	Order of PC
1	240	268.2225	48.6084	0.0014	0.0063	2
2	1762	268.2180	48.3253	2.6417e-04	0.0136	3
3	1762	268.1515	48.3148	2.2100e-05	1.2510e-04	4
4	9978	268.1515	48.3029	1.9738e-05	9.7195e-06	5

Table 9: NIPC approach for the 10-D Wing weight model

DE can be coupled with Kriging surrogate, MLI and many others. The only condition is that the interpolation technique must be able to handle a structured grid. This can be extended into a case, where two surrogate techniques are used for one problem, e.g. for the first order increment functions can be used MLI and for higher order Kriging interpolation. Also, if higher order derivations are neglected, a significant reduction of samples can be gained. Another part of DE is its ability to show behavior of a function in higher dimensions, but this part is not currently properly understood as more examples and research needs to be done.

7 CONCLUSION

In this paper, the Derivative Equation was presented. The equation allows to decouple the stochastic space into sub-spaces and separately interpolate each one of them. This leads to a significant reduction of necessary samples as only important volumes are interpolated. Efficiency of the proposed method was showed on practical examples. Future research will be focused on visualization of high dimensional uncertainty, a multi-fidelity

application and better mitigation of the CoD problem.

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