AN EFFICIENT AND ACCURATE NUMERICAL METHOD FOR HIGH-DIMENSIONAL STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. The Analysis of Variance (ANOVA) expansion is often used to represent multivariate functions in high dimensions. Using the anchored (Dirac) ANOVA expansion results in a substantially reduced cost of evaluation of such functions. However, this approach has two significant flaws. First, the accuracy of the approximation is sensitive to the choice of the anchor point, which is hard to make *á priori*. Secondly, when the number of the parameters is large, the construction of the ANOVA expansion becomes prohibitively expansive. In this case, efforts were made to recognize which input dimensions have the largest effect upon the output, and the ANOVA expansion was built using only these important inputs and their interactions. However, we show that such a simplification can result in a loss of accuracy, since unimportant inputs often have important interactions. We propose a method for representation of multivariate functions, which does not depend on the choice of the anchor point, and tracks all the important inputs and important interactions, therefore constructing the expansion with the exact minimum of the needed terms. We also provide an example of a real life application where our method is not only computationally attractive, but it is the only approach capable of approximating the given multivariate function with the expected accuracy.

Key words. analysis of variance, important inputs, interactions, screening, multivariate functions

1. Introduction. Realistic simulations of complex systems governed by nonlinear partial differential equations must account for "noisy" features of modeled phenomena, such as material properties, coefficients, domain geometry, excitations and boundary data. "Noise" can be understood as uncertainties in the specification of the physical model. In real life applications one often knows only the statistical properties of the problem's parameters, which results in the usage of stochastic partial differential equations. Also, in many of the applications the number of random variables is high; therefore one has to represent and integrate functions on a high-dimensional set of parameters. An elegant way of representing such functions is the Analysis of Variance expansion (ANOVA), also used in different reports under the name HDMR (high-dimensional model representation).

The idea of ANOVA (see Section 3 for the exact definition) is to expand the given multivariate function in terms of

- constant functions
- univariate functions
- bivariate functions
- etc.

In many applications the number of random parameters is prohibitively large, making the ANOVA expansion technique inefficient. Some recent advances have been made in trying to separate the important variables and then build the higher-order terms of the expansion, using only the important dimensions. A large body of work was done in this direction by Ma and Zabaras, [4]. To date, all the reports on this topic propose to only include the variables in the ANOVA expansion based on their importance; the

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unimportant variables are automatically omitted from all terms of ANOVA. However, one can easily construct an example to show that two unimportant variables can have an important interaction, e.g., $f(x_1, x_2, x_3) = \frac{1}{N^2}\sin(Nx_1x_2) + \sin(x_3)$. For large values of N the only important variable is x_3. But if we disregard the unimportant variables x_1 and x_2, we will miss the effects of their important interaction.

We propose a new method of singling out the important variables, based not only on their input, but also on the importance of their interaction. With our new proposed technique, we will be able to decide which variables to keep in each term of the ANOVA expansion of a function. This is crucial for two reasons. First, this allows us to reduce the number of variables to the necessary minimum - therefore reducing the dimension of the space over which we integrate. Secondly, we will now be able to add or remove variables from this minimum set, and we can do it for each term in the expansion. This is also very important, since some variables that are important for the first term of the ANOVA expansion, might not be important in the second term, and vice versa. Our approach will guarantee that the exact minimum of necessary calculations will be performed in computing the ANOVA expansion (and the related notion of the effective dimension) of a multivariate function. It will also guarantee, that all the important effects be captured.

We also address another pressing issue of the anchored ANOVA in its current form: the high sensitivity of the approximation error to the choice of the reference point. Such sensitivity is inacceptible in many applications, especially since the correct choice of the reference point is hard (or impossible) to make *á priori*. It is shown in [12, 10] that an incorrect choice of the reference point can lead to an unacceptible approximation error, and a class of problems with such high sensitivity to the choice of the reference point is discussed. We also point out, that with the incorrect choice of the reference point the approximation error of the truncated ANOVA expansion might even increase when more terms are included in the truncated expansion.

To that end, we propose to use the screening method prior to constructing the anchored ANOVA expansion of a multivariate function. The resulting anchored ANOVA with screening will not depend on the choice of the reference point; this approach will also allow to gain more insight into the importance of the separate inputs and their interactions, mixing well with our previous idea of tracking the important interactions. We also point out that the number r of sampling points needed for screening is always kept small, $r = 4, 5, 6$ even for problems with very large number of stochastic dimensions, [15, 11]. We will show in this report that the proposed method is computationally attractive, gives more information about the multivariate function, and there are many real life applications where the existing versions of anchored ANOVA expansion cannot be used, while our method is still applicable. In particular, in Section 3.3 we consider the dynamo action in magnetohydrodynamic flow. The current approach to describe the mechanism of full nonlinear dynamo involves the mean field theory with the first-order smoothing approximation. It has been argued recently, that some of currently omitted effects have to be included in the existing models of dynamo. We apply our method to get an insight into the dynamo mechanism by comparing the importance of different inputs and their interactions. The existing methods utilizing anchored ANOVA expansion cannot be applied to this problem, since all the separate inputs are equally unimportant (compared to their interactions). Thus, one would have to either resolve all the dimensions by some type of sparse grid collocation, which is prohibitively expensive even for $2 - D$ magnetohydrodynamics, or truncate the ANOVA expansion after the zeroth term, thus approximating the multivariate

function by its value at the reference point - and the large approximation error will disallow to reveal any information about what affects the dynamo mechanism.

2. Previous Work. When solving partial differential equations with random inputs, there often arises a problem of integrating multivariate functions. These are the integrals that can involve hundreds or even thousands of variables. The typical approach is to approximate the high-dimensional integrals by sampling the integrand functions at many points in the integration domain. However, the number of sample points needed to approximate the integrals with acceptable accuracy, increases exponentially as the dimension increases. This is known as the curse of dimensionality - see, e.g., [7] and the references therein. To further complicate the issue, in most of the real life applications leading to PDEs with random inputs, the underlying deterministic problem is also computationally expensive to solve. Thus, the number of sampling points must be reduced dramatically, and such methods as Monte Carlo or Quazi Monte Carlo are no longer affordable to use.

This has motivated a large body of research in stochastic collocation and sparse grids. In [9] the authors consider the solution of elliptic PDEs with random coefficients and forcing terms (input data of the model); they especially address the situation where the input data are assumed to depend on a moderately large number of random variables. They propose an anisotropic Sparse Grid Stochastic Collocation, which consists of a Galerkin approximation in the space variables and a collocation, in probability space, on sparse tensor product grids utilizing either Clenshaw-Curtis or Gaussian knots. The authors show that for moderately large dimensional problems, the sparse grid approach with a properly chosen anisotropy is superior to the Monte Carlo-type methods. In [6] the authors introduce the multi-element probabilistic collocation method; the method is applied to the two-dimensional Navier-Stokes equations with random inputs, in up to 50 stochastic dimensions. Naturally, the number of samples is limited in this setting, since solving the inderlying deterministic problem is costly. The authors show numerically, that while the convergence rate of their method deteriorates in 50 dimensions, the error in the mean and variance is two orders of magnitude lower than the error obtained with the Monte Carlo method using only a small number of samples.

Recently, many papers were written, focusing on one elegant way of representing functions depending on a high-dimensional set of parameters - the analysis-of-variance, ANOVA, expansion. ANOVA expansions are exact and contain a finite number of terms, while truncations of ANOVA expansions may provide good approximations with fewer terms. These expansions are constructed in such way, that the relationship between the sets of input and output variables is captured, and the hierarchy of correlations among the input variables is revealed. Namely, each new term of the ANOVA expansion contains the higher-order correlated effects of the input variables. Depending on the way that one determines the component functions (typically, as one chooses between the Lebesgue or Dirac measure to be used) there are two types of ANOVA expansions: Lebesgue ANOVA and anchored ANOVA - both defined in Section 3. In [8] the authors study the general approximation properties of ANOVA expansions for functionals of solutions of nonlinear partial differential equations. The authors demonstrate via numerical examples that whenever truncated ANOVA expansions of functionals provide accurate approximations, optimizers found through a simple surrogate optimization strategy are also relatively accurate. This study was successfully conducted in the framework of Lebesgue ANOVA - although this involves high dimensional integration even for the zeroth term of the expansion, and therefore

it is impractical in most of the applications. The alternative approach, the anchored ANOVA, is discussed, e.g., in [5], where the authors discuss the sensitivity of the approximation error to the choice of the reference point. The authors explain that the reference (or anchor) point plays an essential role in the overall efficiency and accuracy of the expansion. They discuss several different techniques of choosing the reference point, including it being randomly chosen in the high-dimensional space, or being a trial point with the output closest to mean of the function computed from a moderate number of quasi-random points, as in [12, 10]. They also consider the choice based on the optimal weights in quasi Monte Carlo methods, and conclude that this approach should only be suggested for problems that allow dimensional variable separation. The authors themselves suggest the reference point to be always taken as the center point of a sparse grid quadrature associated with the integration. This comes at no extra computational cost and is shown to perform better than most alternatives. However, this choice also isn't universally applicable and, as the authors say, there is no easy and straightforward way to correctly make this choice for general functions.

It was argued by Rabitz et al., [14], that quite often in high-dimensional models small subsets of input variables have the main impact upon the output. In that case, if one could take advantage of this fact by constructing a model representation that allows for solving (possibly several) low-dimensional problem instead of the original high-dimensional problem, it would alleviate the curse of dimensionality. Also, the ANOVA expansion of multivariate functions (or, by another terminology, HDMR - the high dimensional model representation) appears to be the natural candidate for such representation, since its terms are organized to reveal the hierarchy of correlations between the inputs. It is no surprise, therefore, that a substantial body of literature has appeared lately, addressing the issue of separating the important variables, and using only these subsets of important inputs in the multivariate function representations.

In [15] Morris proposed an effective screening sensitivity measure to identify the few important factors in models with many factors. His screening method was based on computing a number of elementary effects for each input, and then averaging them to assess the effect that the given input has upon the output. However, this global method is still rarely used, and the local methods such as One Factor at a Time (OAT) screening techniques are employed instead. The modification of the Morris's screening method was introduced in [11] - and Saltelli insists in this and his other papers that the OAT sensitivity techniques should not be used.

In [4] Ma and Zabaras develop a computational algorithm aiming to solve stochastic problems in high dimensions. This paper can be considered the current state-of-the-art result, as the authors introduce an adaptive anchored ANOVA expansion, to find the (first order) important inputs and then construct higher-order terms of ANOVA involving only these important inputs. The authors then incorporate the adaptive sparse grid collocation (ASGC) method to solve the resulting lower dimensional problems. They choose the anchor point to be the mean of the random input vector. In order to find the important dimensions in the first term of anchored ANOVA expansion (i.e. the separate inputs that have the most effect upon the output) the authors always construct the zeroth- and first-order ANOVA expansion and define the weights which measure the effect that each separate input has upon the output. If some weights are larger than the predefined threshold, the corresponding inputs are considered important. Then only these dimensions can be present in the terms of the expansion. Namely, if the important dimensions are $\{1, 3, 5\}$ then only the higher-order terms $\{13\}$, $\{15\}$, $\{35\}$, and $\{135\}$ are considered. The ASGC method

is used to resolve the important dimensions.

Several barriers to further progress still remain, when one tries to model a multivariate function in high dimensions. First, the dependence on the choice of the reference point should be avoided. No matter how sophisticated the algorithm for singling out the important dimensions, if the choice of the reference point is incorrect, the approximation error can be unacceptable and the constructed expansion will be inaccurate. Also, the incorrect choice of the reference point can affect the choice of the important dimensions: e.g., in [4] the corresponding weights depend on the value of the multivariate function at the reference point - thus choosing a different reference point may lead to treating another dimensions as important.

Secondly, it is easy to construct an example showing that an interaction of two inputs can have an important effect upon the output, even if one or even both of these inputs are not considered important (i.e. when the effect of these separate inputs upon the output is small). One such example was given in Section 1. Another example from a real life application (magnetohydrodynamics) will be considered in Section 3.3, where small perturbations of velocity and magnetic field are treated as noise. The corresponding random variables have small effects upon the output - the mean magnetic field. However, their interaction is responsible for the mechanism of full nonlinear dynamo. In this situation none of the separate inputs are important - but some of their interactions are, and therefore the existing approaches that utilize the anchored ANOVA expansion aren't applicable.

We propose a method that overcomes both of these barriers. First, we avoid the problem of choosing the reference point, by introducing the anchored ANOVA with screening. Secondly, we approach the problem of recognizing the important dimensions differently; by approximating not only the first, but also second mixed partial derivatives of the multivariate function at the screening points we are now able to find exactly which separate inputs are important and which interactions (possibly of unimportant inputs) are important as well. Thus we know exactly which dimensions need to be resolved by a sparse grid collocation method to construct an efficient and accurate truncation of the ANOVA expansion. We also obtain (without any extra computational cost) an approximation to the truncated ANOVA expansion, from which an information can be gained about the effects that separate inputs and their interactions have upon the output.

3. Analysis of Variance (ANOVA). The Lebesgue ANOVA expansion is used to represent multivariate functions in such a way, that every new term in the expansion captures higher-order interactions of the input variables.

Let $P = 1, ..., p$; for any subset of (ordered) coordinate indices $T \subseteq P$, let $|T|$ denote the cardinality of T , let $\vec{\alpha}_T \in \mathbb{R}^{|T|}$ denote the $|T|$-vector containing the components of the vector $\vec{\alpha}_T \in \mathbb{R}^p$ indexed by T , and let $A_T^{|T|}$ denote the $|T|$-dimensional unit hypercube which is the projection of the p-dimensional unit hypercube A^p onto the coordinates indexed by T. Any function $g \in L^2(A^p)$ may be written as the ANOVA expansion

$$g(\vec{\alpha}) = g_0 + \sum_{T \subseteq P} g_T(\vec{\alpha}_T), \tag{3.1}$$

where the terms in the expansion are determined recursively by

$$g_T(\vec{\alpha}_T) = \int_{A^{p-|T|}} g(\vec{\alpha}) d\vec{\alpha}_{P\setminus T} - \sum_{V\subseteq T} g_V(\vec{\alpha}_V) - g_0, \tag{3.2}$$

starting with

$$g_0 = \int_{A^p} g(\vec{\alpha}) d\vec{\alpha}. \tag{3.3}$$

The Lebesgue ANOVA expansion is useful in different settings, including the computation of global sensitivity by measuring the contribution of variance of each component function to the overall variance. However, constructing such expansion involves the evaluation of high-dimensional integrals, even for the zeroth term. It is therefore computationally expensive and impractical.

The Dirac measure is used in real life applications instead of the Lebesgue measure, leading to the anchored ANOVA (also called cut-HDMR) expansion. Consider a multivariate function $f(\bar{Y}) = f(Y_1, Y_2, .., Y_k)$ defined on a k-dimensional unit hypercube. Following the notation of [4], one chooses a reference point $\bar{\mathbf{Y}} = (\bar{Y}_1, \bar{Y}_2, .., \bar{Y}_k)$ and constructs the anchored ANOVA expansion:

$$\begin{aligned} f(\mathbf{Y}) = f_0 + \sum_{i=1}^{k} f_i(Y_i) + \sum_{1\le i_1<i_2\le k} f_{i_1 i_2}(Y_{i_1}, Y_{i_2}) \\ + \cdots + \sum_{1\le i_1<\cdots<i_s\le k} f_{i_1\cdots i_s}(Y_{i_1}, ..., Y_{i_s}) + \cdots + f_{12\cdots k}(Y_1, ..., Y_k), \end{aligned} \tag{3.4}$$

where

$$\begin{aligned} f_0 = f(\bar{\mathbf{Y}}), f_i(Y_i) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus Y_i} - f_0, \\ f_{ij}(Y_i, Y_j) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus\{Y_i,Y_j\}} - f_i(Y_i) - f_j(Y_j) - f_0, ... \end{aligned} \tag{3.5}$$

The notation $\mathbf{Y} = \bar{\mathbf{Y}}\setminus\mathbf{Y}_\mathbf{u}$ means that the components of $\mathbf{Y}$ other than those indices that belong to the set $\mathbf{u}$ are set equal to those of the reference point. This expansion only involves function evaluations at reference points, and high-dimensional integration is not needed, making the anchored ANOVA a much more efficient tool in real life computations.

3.1. Screening. Anchored ANOVA in its current form has two serious flaws, which we address here. First, the convergence properties of anchored ANOVA depend (sometimes heavily) on the choice of the reference point. It was shown in [12, 10] that a wrong choice of a reference point may lead to an unacceptable approximation error. To this end, we propose to use another technique instead of using an arbitrary reference point. We suggest that the anchored ANOVA expansion must be preceded by a screening method - the one originally introduced by Morris [15], or its modification by Campolongo, Cariboni and Saltelli, [11]. For our purposes, we will use the following formulation of Morris's screening method.

Consider the case where the region of interest is a k-dimensional unit hypercube Ω, with a regular k-dimensional p-level grid. For a function $f(\mathbf{x}) = f(x_1, x_2, .., x_k)$ define the elementary effect of x_i as

$$d_i(\mathbf{x}) = \frac{f(x_1, x_2, .., x_{i-1}, x_i + h, x_{i+1}, .., x_k) - f(\mathbf{x})}{h}, \tag{3.6}$$

where the increment is taken to be equal to the mesh size, $h = \frac{1}{p-1}$.

To generate an economical random sampling, we now construct a $(k+1)$-by-k sampling matrix $\mathbf{B}$, $\mathbf{B}_{ij} \in \{0, 1\}$, such that for every column $j = 1, 2, .., k$ there are two rows of $\mathbf{B}$ that differ only in their j-th entries. For example,

$$\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}$$

For a design matrix $h\mathbf{B}$ each experiment would provide k elementary effects, based on $k+1$ runs. These selections are not random, but a randomization algorithm for the sampling matrix was also given by Morris in [15]; however, the screening method above in sufficient for the demonstration of our approach.

Notice that the number of experiments (i.e. the number of elementary effects for each input) is small, $r = 4, 5, 6$, even for sampling the hypercubes in high dimensions, e.g. for $k = 20, 50, 100$. Note also, that the total number of needed samples of the k-dimensional space depends on both r and k, since we will be taking samples not only in these r points, but also in the neighborhood of each point.

Introducing the anchored ANOVA with screening, we change the formulation $(3.4) - (3.5)$ to

$$f(\mathbf{Y}) = \frac{1}{r} \sum_{m=1}^{r} [f_0^m + \sum_{i=1}^{k} f_i^m(Y_i) + \sum_{1 \le i_1 < i_2 \le k} f_{i_1 i_2}^m(Y_{i_1}, Y_{i_2}) \tag{3.7}$$
$$+ \cdots + \sum_{1 \le i_1 < \cdots < i_s \le k} f_{i_1 \cdots i_s}^m(Y_{i_1}, ..., Y_{i_s}) + \cdots + f_{12\cdots k}^m(Y_1, ..., Y_k)],$$

where

$$f_0^m = f(\mathbf{Y}^m), f_i^m(Y_i) = f(\mathbf{Y})|_{\mathbf{Y}=\mathbf{Y}^m \setminus Y_i} - f_0^m, \tag{3.8}$$
$$f_{ij}^m(Y_i, Y_j) = f(\mathbf{Y})|_{\mathbf{Y}=\mathbf{Y}^m \setminus \{Y_i, Y_j\}} - f_i^m(Y_i) - f_j^m(Y_j) - f_0^m, ...$$

Here $\mathbf{Y}^m$, $m = 1, .., r$ are the sampling points from the screening algorithm, and we again point out that the number of these points is small, $r \in \{4, 5, 6\}$, even for large values of k.

A clear advantage of using the screening method is that now the anchored ANOVA expansion becomes stable - in a sense that it is not sensitive to the choice of the reference point, which is hard to make *á priori*. Prescreening also reduces the approximation error of the anchored ANOVA; The cost of these improvements seems to be the increased amount of runs needed, which is prohibitive when the underlying deterministic PDE is hard to solve. However, we will show that the anchored ANOVA with screening is a strategically different approach, which in many real life applications can

even reduce the number of the needed solves of the deterministic problem. Moreover, we will demonstrate a complex real life application, where the anchored ANOVA is too computationally expensive or cannot be applied even when the number of random variables is small - and the anchored ANOVA with screening still works and captures all the important effects of the physical model.

3.2. Capturing Important Interactions. We address now the second issue of the existing approach to ANOVA (Lebesgue or anchored). Very often in high dimensional models there exist small subsets of input variables that have the main impact on the output. The idea of capturing which input variables are more "important" (i.e. have the larger impact on the output) has been investigated since Morris in [15] proposed to compute the elementary effects for each input, and then average them to assess the overall importance of the input. There have been many investigation on the subject of important variables, see, e.g., [14, 12, 4] and references therein. However, none of the existing methods goes beyond evaluating the separate effects of different inputs upon the output - and there are many situations where this could lead to either missing the important properties of the modeled problem, or to a method which is too computationally expensive.

Consider now the proposed expansion of a multivariate function $f(Y_1, Y_2, .., Y_k)$ - the anchored ANOVA with prescreening, given by (3.7) – (3.8). Following [15], we distinguish four different scenarios: for any point $\mathbf{Y} = (Y_1, Y_2, .., Y_k)$ in the hypercube, the value $\frac{\partial f}{\partial Y_i}|_{\mathbf{Y}}$ may be approximately

(a) zero over all values of $\mathbf{Y}$,

(b) a nonzero constant over all values of $\mathbf{Y}$,

(c) a nonconstant function of Y_i, or

(d) a nonconstant function of one or more $Y_j, j \neq i$.

These cases are understood as follows: (a) the input Y_i doesn't affect the output, (b) the effects of Y_i of f are linear and additive - therefore we add Y_i to the set of the important variables, (c) the effect of Y_i on f is nonlinear, and (d) Y_i is involved in interaction with another inputs.

To the best of our knowledge, all the existing methods can only be used in the cases (a) and (b) - i.e., for assessing the importance of the inputs based on their linear effect on the output. It is usually argued (see, e.g., the recently proposed method in [4]) that only the two important variables can have important interactions, therefore only such interactions need to be tracked. However, one can demonstrate that a problem can be modeled incorrectly when the effects of the interactions are omitted in such manner. For instance, consider a function

$$f(x_1, x_2, x_3) = \frac{1}{N^2} \sin(N x_1 x_2) + \sin(x_3).$$

For large values of N the only important variable (based on separate effects of different inputs upon the output) is x_3. Therefore, if we were to use the existing methods and construct the anchored ANOVA with the adaptive technique, as proposed in [4] (which is the latest and the most advanced effort to treat important variables differently in the anchored ANOVA), we would have left only two terms in the anchored ANOVA expansion (3.4). Namely, this would lead to the approximation

$$f(\mathbf{x}) = f_0 + f_3(x_3). \tag{3.9}$$

Therefore, when constructing the anisotropic sparse grid collocation method based on (3.9), one would try to resolve the x_3-dimension only. However, by taking the mixed partial derivative $\frac{\partial f^2}{\partial x_1 \partial x_2}$ one can verify that the unimportant variables x_1, x_2 have an important interaction, which needs to be tracked in order to capture the effects of the modeled problem.

This simple example shows that the case (d) must be addressed - i.e., the importance of interactions of different inputs must be also assessed. Notice also, that not only has this issue not been addressed before, but it cannot even be resolved within the mainframe of existing methods. Even the convergence properties of anchored ANOVA are sensitive to the choice of the reference point. This dependence on the choice of the reference point becomes even heavier as one tries to determine the important variables, since this is based on approximating the first partial derivatives at the reference point. Since our approach to assessing the importance of interactions will involve second mixed partial derivatives, using the anchored ANOVA in its current form will be restricted to a small class of problems where the given choice of a reference point is justified. As was discussed in [12, 10], the correct choice of a reference point can rarely be made *á priori*.

We propose to track not only the important variables, but also the variables with important interactions, therefore keeping only the necessary summands in the first three terms of ANOVA, and at not same time not loosing any properties of the modeled problem by throwing away the summands which affect the output. In order to decide which interactions are important, we propose to compute the finite difference approximations of second mixed partial derivatives of the form $\frac{\partial f^2}{\partial Y_i \partial Y_j}$, $i, j = 1, ..k$, $i < j$. Note that the anchored ANOVA with screening is employed. Hence, we propose the following algorithm for approximating the multivariate function $f(\mathbf{Y}) = f(Y_1, .., Y_k)$:

ALGORITHM 3.1.

(1) Use screening method by Morris [15] or Campolongo, Cariboni and Saltelli [11] for the random sampling of the k-dimensional hypercube Ω. At this stage, we will need to solve the underlying deterministic equations r times, $r = 4, 5, 6$.

(2) Following the screening method, compute the elementary effects of each input; for that, the multivariate function f needs to be evaluated at rk points: given each point $\mathbf{Y}^m \in \Omega$, $m = 1, .., r$, we evaluate $f(\mathbf{Y}^m + h\mathbf{e}_i)$, $i = 1, .., k$. Here $\mathbf{e}_i = (0, 0, .., 0, 1, 0, .., 0)$ is the unit vector with its i-th component equal to one. The step h is taken to be the mesh size of the screening method used. Note that the values $f(\mathbf{Y}^m)$ where obtained at the previous step of the algorithm.

(3) Given a predefined threshold value ϵ_1, we call the i-th input important and keep the corresponding summand in the second term of anchored ANOVA with screening, if

$$\sum_{m=1}^{r} |\frac{f(\mathbf{Y}^m + h\mathbf{e}_i) - f(\mathbf{Y}^m)}{h}| \geq r\epsilon_1. \tag{3.10}$$

(4) In order to find important interactions, we need to find $f(\mathbf{Y}^m + h\mathbf{e}_i + h\mathbf{e}_j)$, $i, j = 1, ..k$, $i < j$. Therefore, at this step of the algorithm $r\frac{k(k-1)}{2}$ function evaluations are needed.

(5) Given a predefined threshold value ϵ_2, we call the interaction of the ij-th inputs important and keep the corresponding summand in the third term of anchored ANOVA with screening, if

$$\sum_{m=1}^{r} |\frac{f(\mathbf{Y}^m + h\mathbf{e}_i + h\mathbf{e}_j) - f(\mathbf{Y}^m + h\mathbf{e}_i) - f(\mathbf{Y}^m + h\mathbf{e}_i) + f(\mathbf{Y}^m)}{h^2}| \geq r\epsilon_2. \quad (3.11)$$

The *total* number of function evaluations needed is $r(1 + k + \frac{k(k-1)}{2})$; however, at this cost we not only reduce the number of summands in the first three ANOVA terms to a minimum, but we are now able to capture all the key properties of the modeled problem. We now discuss the advantages of the proposed approach.

- There is no averaging of elementary effects in our algorithm, which is usually the case when screening methods are used to estimate the importance of separate inputs.
- No weights need to be computed to determine the importance of inputs or their interactions; at the same time, if needed, the weights can be easily added to the algorithm.
- The sensitivity of the expansion to the choice of the reference point is eluded. Not only this improves the approximation error of ANOVA expansion, but in many problems this also allows for the smaller effective dimension, and therefore the shorter truncation of the expansion.
- The function evaluations, although sometimes costly, can allow for the significant reduction of the number of summands in the second and, more importantly, third term of (3.7). Thus, when the construction of truncated ANOVA expansion is followed by some type of anisotropic sparse grid collocation method, the number of dimensions that need to be resolved is significantly lowered. This will be demonstrated by an example in Section 3.3.
- If the underlying deterministic problem is too computationally expensive, one sometimes cannot afford to resolve even the important dimensions. In that case, the gathered information can be intelligently used to construct an approximation to the multivariate function (or any functionals of interest) as follows:

$$f(\mathbf{Y}) \approx \frac{1}{r} \sum_{m=1}^{r} [f_0^m + \sum_{i \in S_1} f_i^m(Y_i) + \sum_{(i_1,i_2) \in S_2} f_{i_1 i_2}^m(Y_{i_1}, Y_{i_2})], \quad (3.12)$$

where S_1 is the set of important inputs, S_2 is the set of important interactions, and

$$f_0^m = f(\mathbf{Y}^m), f_i^m(Y_i) = f(\mathbf{Y}^m + h\mathbf{e}_i) - f_0^m, \quad (3.13)$$
$$f_{ij}^m(Y_i, Y_j) = f(\mathbf{Y}^m + h\mathbf{e}_i + h\mathbf{e}_j) - f_i^m(Y_i) - f_j^m(Y_j) - f_0^m.$$

Note that two unimportant inputs can have an important interaction. Note also, that even when values of k are moderate, the number of needed function evaluations $r(1 + k + \frac{k(k-1)}{2})$ is small compared to the number of function evaluations needed in a sparse grid collocation method, even when the number of important dimensions is reduced.

3.3. Computational Verification. It is unrealistic to make an assumption that in most of the real life applications the multivariate functions can be accurately approximated by the sum of constant and univariate functions. This would mean

that the ANOVA expansion can always be truncated after the second term and still accurately represent the multivariate function sought - and this is not usually the case. In particular, it was verified computationally in [8] that the summands in the third term of ANOVA are of the same order of magnitude as are those in the second term. In other words, the interactions among the inputs have the same effect upon the output, as do the separate inputs. This was calculated for the Laplace equation with small perturbation, and the number of random variables was kept as low as $k = 4$. As follows from the numerical data given in [8], the existing approaches to ANOVA expansion are costly even in this simple application, since all of the dimensions need to be resolved by some type of sparse grid technique, which is computationally expensive even for low values of k, and the adaptive anchored ANOVA described in [4], cannot be used effectively because the interactions of unimportant inputs also turn out to be important.

One of the areas of applications where our approach is not simply more effective than the existing ones, but is also the only one usable, is the modeling of turbulent fluid flows. Turbulence modeling in the setting of PDEs with random inputs has been a subject of several recent investigation - see, e.g., [1] and references therein. Typically these are settings where the underlying deterministic PDEs are expensive to solve even in the presence of turbulence modeling; also, the uncertainty can occur in the boundary data, coefficients, domain geometry and excitations, which can lead to moderate-to-high values of k. Hence, one has to try to gather as much information as possible about the importance of separate inputs and their interactions, in order to reduce the number of dimensions needed to be resolved. One cannot assume *á priori* that only the first two terms in the ANOVA expansion must be kept after the truncation, since many of the physical properties of turbulent fluid flows are subtle and cannot be captured when the ANOVA expansion is truncated too early.

We will not stop here and consider an even more complicated system of PDEs - namely, the magnetohydrodynamic (MHD) flow. When this flow becomes turbulent, all the problems of turbulent modeling of the Navier-Stokes equations are magnified many times over - see, e.g., [2, 3]. At the same time, the idea of breaking the sought quantity (for instance, the velocity field $\mathbf{u}$ or the magnetic field $\mathbf{B}$) into the sum of its mean and fluctuations, and then treating the fluctuations as noise, can be tested on a simpler application than turbulence. However, the example considered below is chosen so that it could lead to applying our approach in turbulence modeling.

We now consider the mechanism of dynamo in MHD. Assuming the fluid to be viscous and incompressible, the governing equations of MHD are the Navier-Stokes equations of fluid dynamics and Maxwell's equations of electromagnetism, coupled via the Lorentz force and Ohm's law. Let $\Omega = (0, L)^3$ be the flow domain, and $\mathbf{u}(t, \mathbf{x}), p(t, \mathbf{x}), \mathbf{B}(t, \mathbf{x})$ be the velocity, pressure, and the magnetic field of the flow, driven by the velocity body force $\mathbf{f}$ and magnetic field force $\operatorname{curl} \mathbf{g}$. Then $\mathbf{u}, p, \mathbf{B}$ satisfy the MHD equations:

$$\begin{aligned}
&\mathbf{u}_t + \nabla \cdot (\mathbf{u}\mathbf{u}^T) - \frac{1}{\mathrm{Re}}\Delta \mathbf{u} + \frac{S}{2}\nabla(\mathbf{B} \cdot \mathbf{B}) - S\nabla \cdot (\mathbf{B}\mathbf{B}^T) + \nabla p = \mathbf{f}, \\
&\mathbf{B}_t + \frac{1}{\mathrm{Re}_{\mathrm{m}}}\operatorname{curl}(\operatorname{curl} \mathbf{B}) + \operatorname{curl}(\mathbf{B} \times \mathbf{u}) = \operatorname{curl} \mathbf{g}, \\
&\nabla \cdot \mathbf{u} = 0, \nabla \cdot \mathbf{B} = 0,
\end{aligned} \tag{3.14}$$

in $Q = (0,T) \times \Omega$, with the initial data:

$$\mathbf{u}(0,\mathbf{x}) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{B}(0,\mathbf{x}) = \mathbf{B}_0(\mathbf{x}) \quad \text{in } \Omega, \tag{3.15}$$

and with periodic boundary conditions (with zero mean):

$$\Phi(t,\mathbf{x}+L\mathrm{e}_i) = \Phi(t,\mathbf{x}), i = 1,2,3, \quad \int_\Omega \Phi(t,\mathbf{x})d\mathbf{x} = 0, \tag{3.16}$$

for $\Phi = \mathbf{u}, \mathbf{u}_0, p, \mathbf{B}, \mathbf{B}_0, \mathbf{f}, \mathbf{g}$.

Here Re, $\mathrm{Re_m}$, and S are nondimensional constants that characterize the flow: the Reynolds number, the magnetic Reynolds number and the coupling number, respectively.

The dynamo theory proposes a mechanism, by which an electrically conducting fluid can maintain a magnetic field. In particular, the dynamo action of the turbulent motion can overcome the Ohmic dissipation thus providing for growing magnetic fields. When the velocity field is affected by the Lorentz forces, it leads to the coupled system of equations, as in (3.14). In that case, fully nonlinear (hydromagnetic) dynamos appear, which need to be modeled. Numerical models employed in simulation of fully nonlinear dynamos, use different assumptions about the system, sometimes very restricting. Most of the approaches to modeling dynamos utilize the mean field dynamo theory: the velocity and magnetic fields are represented as sums of their mean parts and fluctuations,

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}', \mathbf{B} = \overline{\mathbf{B}} + \mathbf{b}', \text{ and also } p = \overline{p} + p',$$

where the overbar denotes spatially or statistically averaged long-scale fields (a common approach is to use spatial ensemble averaging), and $\mathbf{u}'$ and $\mathbf{b}'$ are small-scale perturbations. The small-scale fields have zero averages, while their products in general do not.

However, there are many MHD applications where the traditional mean field dynamo theories cannot be applied, since they use the first-order smoothing approximation, see [13] and the references therein. Hence, in these applications it is not known exactly which effects should be accounted for in the dynamo theory. In particular, this can happen when the condition $\mathrm{Re_m} \ll 1$ is violated (which occurs in a number of the MHD applications, including astrophysics).

There has been a controversy regarding which effects to take into consideration when modeling dynamos. For instance, it is argued in [13] that the generally neglected Hall term in the two-fluid MHD may have a profound effect on the dynamo action. To that end, we propose to use our method to discover the mechanisms involved, and the effects that need to be accounted for. We suggest to treat the system (3.14) as PDEs with random input variables. Namely, we will treat $\mathbf{u}'$ and $\mathbf{b}'$ as noise - therefore, we get six random variables if the MHD flow is three-dimensional, and four random variables in the case of the $2-D$ MHD. We then use the proposed anchored ANOVA with screening to determine which of the random variables and which interactions have the largest effect upon the mean long-scale magnetic field $\overline{\mathbf{B}}$. We also test the assumption that the output $\overline{\mathbf{B}}$ is affected the most by the interaction of the random inputs, and not the separate inputs themselves; in particular, a term $\overline{\mathbf{u}' \times \mathbf{b}'}$ is known to give rise to an additional electromotive force in Ohm's law for the mean fields, [16]. If that is the case, then all the existing approaches, including the adaptive anchored

ANOVA of [4], are ineffective: if all the separate inputs are unimportant, the anchored ANOVA expansion has to be either truncated at the zeroth (mean value) term, or all the dimensions have to be resolved - which is too computationally expensive for systems like (3.14).

We consider a two-dimensional MHD flow, governed by (3.14) with the coupling number $S = 1$, in $\Omega = [0,1] \times [0,1]$. The Reynolds and magnetic Reynolds numbers are $Re = Re_m = 1$; the final time is $T = 0.1$, with the time step proportional to the spatial mesh size d, $\Delta t = 0.1d$. The right hand side and the boundary conditions of the deterministic problem are chosen so that its solution is a traveling wave, with the magnetic field increasing in time:

$$\mathbf{u} = \begin{pmatrix} 0.75 + 0.25\cos(2\pi(x-t))\sin(2\pi(y-t))e^{-8\pi^2 tRe^{-1}} \\ 0.75 - 0.25\sin(2\pi(x-t))\cos(2\pi(y-t))e^{-8\pi^2 tRe^{-1}} \end{pmatrix},$$
$$p = -\frac{1}{64}(\cos(4\pi(x-t)) + \cos(4\pi(y-t)))e^{-16\pi^2 tRe^{-1}},$$
$$\mathbf{B} = \begin{pmatrix} y^3 e^t \\ x^3 e^t \end{pmatrix}.$$

The small perturbations u_1', u_2', b_1', b_2' are added through the boundary conditions; namely, $u_1|_{\partial\Omega_1} = u_1|_{\partial\Omega_1} + \alpha_1\epsilon\Phi_1$, $u_2|_{\partial\Omega_2} = u_2|_{\partial\Omega_2} + \alpha_2\epsilon\Phi_2$, $b_1|_{\partial\Omega_3} = b_1|_{\partial\Omega_3} + \alpha_3\epsilon\Phi_3$, $b_2|_{\partial\Omega_4} = b_2|_{\partial\Omega_4} + \alpha_4\epsilon\Phi_4$. Here

$$\partial\Omega_1 = \{(x,y)|x = 0, 0 \le y \le 1\},$$
$$\partial\Omega_2 = \{(x,y)|0 \le x \le 1, y = 1\},$$
$$\partial\Omega_3 = \{(x,y)|x = 1, 0 \le y \le 1\},$$
$$\partial\Omega_4 = \{(x,y)|0 \le x \le 1, y = 0\}.$$

Hence, the four random variables, corresponding to the perturbations u_1', u_2', b_1', b_2', are sought in the parameter space $\Gamma^4 = \{(\alpha_1, \alpha_2, \alpha_3, \alpha_4)\} \subset [0,1]^4$. We take $\epsilon = 0.001$, and the parabolic inflows

$$\Phi_1(x,y) = \epsilon y(1-y), \qquad \Phi_2(x,y) = -\epsilon x(1-x),$$
$$\Phi_3(x,y) = -\Phi_1(x,y), \qquad \Phi_4(x,y) = -\Phi_2(x,y).$$

We now follow Algorithm 3.1: introduce a regular 4-dimensional p-level grid on Γ^4, letting $p = 4$ and $\Delta = \frac{p/2}{p-1} = \frac{2}{3}$. Using the 5×4 sampling matrix ΔB, we pick three sampling points in Γ^4, $r = 3$. Thus, the total number of sampling needed for the proposed ANOVA with screening is $r(1 + k + \frac{k(k-1)}{2}) = 33$. The increment h in the stochastic dimensions is taken small, $h = 0.1$. Following (3.10)-(3.11), we measure the effects of the small perturbations u_1', u_2', b_1', b_2' and their interactions upon the mean long-scale magnetic field $\mathbf{B}$ - see Figure 3.1.

We have repeated the computations for three successive refinements of the spatial mesh - verifying the results of Figure 3.1. Notice that the separate inputs u_1', u_2', b_1' are equally unimportant. Thus, the existing methods (e.g., [4]) will either construct the ANOVA expansion consisting only of the zeroth term, resulting in an unacceptably inaccurate approximation, or all four stochastic dimensions would need to be resolved by some sparse grid technique, resulting in a large number of needed deterministic

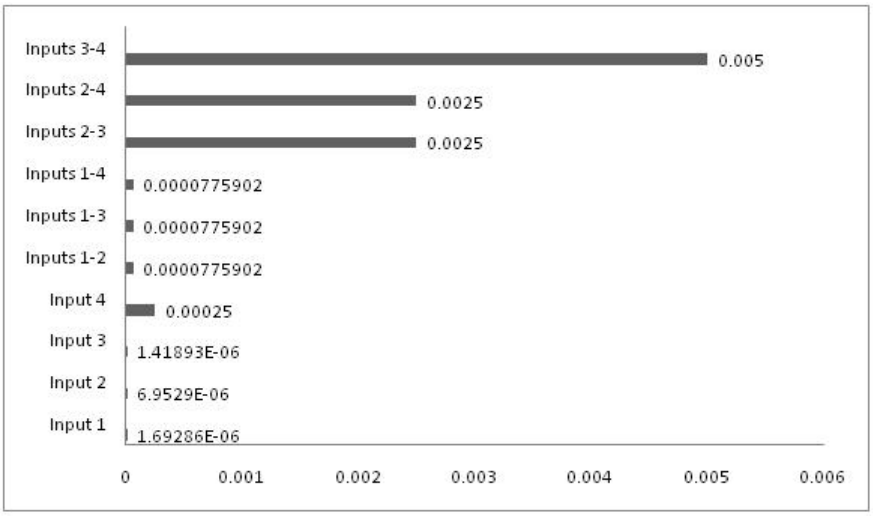

FIG. 3.1. *Importance of small perturbations of magnetic and velocity fields and their interactions*

solves (n^4, where n is the number of sparse grid points in each dimension). Our method is not only computationally attractive (only 33 samples were computed), but it also sheds light into the mechanism of dynamo, showing that although the only important separate perturbation is b_2', but the interactions of $\{u_2', b_1'\}$, $\{u_2', b_2'\}$ and especially $\{b_1', b_2'\}$ are the most important. The obtained results can already be used as an approximation of the multivariate function B, and they can also be used to decide which dimensions should be resolved by the sparse grid technique - in this case the first dimension can be omitted. Finally, our example demonstrates that the important and unimportant variables can have an important interaction (e.g., the inputs 3 and 4), and even the interaction of two unimportant variables (e.g., the inputs 2 and 3) can be important.

The advantages of the proposed method can be clearly seen even when the number of parameters is small. It was demonstrated in the example above, that sometimes the proposed method can be applied without any additional sampling, so that the sparse grid methods can be avoided. Furthermore, even with the sparse grid collocation methods employed, the proposed method reduces the amount of sampling necessary; if the 5-level sparse grid method is used with the previous versions of anchored ANOVA, the number of solves needed is $5^4 = 625$, whereas the same 5-level sparse grid technique combined with the proposed method results in $3(1 + 4 + \frac{4(4-1)}{2}) + 5^3 = 158$ solves needed. The economy in the number of solves of the underlying deterministic problem is noticeable even for the problem with four random inputs; the attractiveness of the proposed method will increase as the number of random variables is increased.

4. Future work. The proposed method can be further developed in several aspects. First, we will compare the anchored ANOVA with screening to the different strategies of choosing the anchor point in the anchored ANOVA,[5]. We aim to demonstrate the smaller approximation error when using the anchored ANOVA with screening. These results need to be tested on different types of problems, see [12].

The proposed Algorithm 3.1 for the anchored ANOVA with screening should be compared to the existing computational methodologies - e.g., that of [4]. The compar-

ison criteria should include the computational time needed, the number of samples taken in the high dimensional stochastic space, and the accuracy of the resulting ANOVA expansion. We will also investigate the class of problems, where our method is the only one available. An example of such problems is the one discussed in Section 3.3. The result of this extensive research should summarize the advantages of our method: smaller approximation error; better quality of the approximation, including capturing the effects of important interactions of the inputs upon the output; and in many cases, the overall computational attractiveness of our method, including the class of problems where there is no alternative to the proposed Algorithm 3.1, as in the MHD dynamo problem discussed above.

We also aim to investigate (both theoretically and numerically) the idea that the underlying deterministic problem can be simplified at the stage when the anchored ANOVA with screening is used to highlight the important inputs and interactions. Then the important dimensions are resolved by an ASGC-type method with the original, nonsimplified underlying problem. This will result in significant reduction of computational expenses; in particular, the underlying discretized deterministic PDE can be solved on a much coarser mesh and over a smaller period of time - at the stage when the important dimensions are sought. This idea is crucial if one wants to reduce the computational cost of the method, and we take advantage of the flexibility of the proposed algorithm. Not only the method can be used on its own, but it can be naturally combined with the sparse grid collocation technique. In the latter case, the ANOVA with screening is used as a predictor of which dimensions are important (either by themselves or in an interaction) and need to be further resolved by the ASGC method. If a multivariate function f depends on $k = 200$ variables and our method is used to find that only 100 of these variables have significant effect upon the output f, then one only needs to sample the domain $r(1 + 200 + \frac{200 \cdot 199}{2}) + n^{100}$ times instead of n^{200} times (here n is the number of ASGC sampling points in each dimension, and r is the number of samples in screening, $r = 4, 5, 6$). We will be investigating whether these first $r(1 + k + \frac{k(k-1)}{2})$ samples can be taken of a simplified deterministic problem.

When applying Algorithm 3.1 to approximating multivariate functions, one can encounter the situation where two unimportant variables have an important interaction (see, e.g., inputs 2 and 3 in Figure 3.1). This leads to another new area of potential research: we will look into the improvements on the existing sparse grid techniques. For instance, suppose that we use the ANOVA with screening as a predictor of important dimensions and then employ an ASGC method; if the dimensions x_i and x_j are unimportant but have an important interaction, they need to be resolved by the sparse grid method. However, the number of sampling points in these directions can be reduced, if they are rearranged along the line $x_i = x_j$. The creation the dimension-selective sparse grid collocation methods will allow for the reduced number of sample points in the unimportant dimensions (but with important interactions). We will show that the accuracy of the method is comparable to that of the existing sparse grid collocation techniques, but the effectiveness of the new method is improved due to the smaller number of the (rearranged) sample points.

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