HIGH DIMENSIONAL MODEL REPRESENTATIONS (HDMR): CONCEPTS AND APPLICATIONS

Genyuan Li, Sheng-Wei Wang and Herschel Rabitz[†]
Department of Chemistry, Princeton University
Princeton, New Jersey 08544

Abstract

A general set of quantitative model assessment and analysis tools, termed High Dimensional Model Representations (HDMR), have been introduced recently for improving the efficiency of deducing high dimensional input-output system behavior. HDMR techniques are based on optimization and projection operator theory, which can dramatically reduce the sampling effort for learning the input-output behavior of high dimensional systems (i.e., a reduction of effort from exponential scaling to only polynomic complexity). HDMR can be applied for different purposes: construction of a computational model directly from lab/field data, creating an efficient fully equivalent operational model for an existing mathematical model, identification of key model variables, global uncertainly assessments, efficient quantitative risk assessment, etc. In one domain of applications significant computational enhancements have been observed in certain atmospheric model calculations.

The performance of long-term simulations with high resolution 3-D global chemistry-transport models (3-D GCTMs) is central to revealing the effects of natural and human-induced changes of trace constituents in the troposphere. A major difficulty in executing GCTMs for long-term and multi-scenario simulations arises from the computational burden of the chemical

[†]Author to whom correspondence should be addressed

kinetics calculations involved. The kinetics can consume as much as 90% of the total CPU time in simulations employing detailed non-methane hydrocarbon chemistry. This computational burden arises from the chemical rate equations involving many species and being stiff, such that they require the use of elaborate numerical integration schemes (e.g., the Gear-type implicit solvers). Furthermore, typical 3-D GCTM simulations can call on a kinetic package $\sim 10^9$ times / year. Even the best advanced numerical algorithms are extremely expensive for solving the kinetic equations directly within the 3-D models. This situation will become even more severe as additional chemical species and reactions are included to make the models more comprehensive and realistic.

In order to circumvent this computational difficulty, parameterized polynomial expansions or interpolative look-up tables have been introduced to fit the results by solving the chemistry rate equations "off-line". The fits may then be employed for the chemical kinetics component of the 3-D calculations [1, 2, 3, 4, 5, 6]. Spivakovsky *et al.* [3] used high-order polynomials to express the input-output chemical kinetic response through least squares fitting. Turányi [4] extended the approach of Spivakovsky *et al.* by expressing the chemical kinetic input-output relation as an expansion in orthogonal polynomials. Klonecki and Levy [5, 7] used standard high-dimensional look-up tables to perform chemical kinetic calculations of CO-CH_4-NO_x-H_2O chemistry in 3-D GCTM ozone simulations. One major problem associated with these approaches is that without the possibility of simplification, the number of times the chemistry rate equations need to be solved to obtain the fits grows exponentially with respect to the dimension of the system (i.e., the number of chemical species). This comment may be understood from consideration of the effort required to deduce the chemical kinetic input-output mapping by sampling with s points for each of the n input variables (e.g., initial chemical species concentrations) corresponding to a computational cost scaling of $\sim s^n$. Realistically, one may expect s to be approximately $10 \sim 20$ and n to be $10 \sim 10^2$ or larger in typical chemical systems. Furthermore, the evaluation of a new point by interpolation in an n-dimensional space for $n \gg 10$ would be difficult with a standard interpolative look-up table. Therefore, these traditional approaches would be prohibitive in high-dimensional chemical systems such as non-methane hydrocarbon chemistry.

A general set of quantitative model assessment and analysis tools, termed High Dimensional Model Representations (HDMR), have been introduced recently for improving the efficiency of deducing high dimensional input-

output (IO) system behavior, and then can be used to relieve the computational burden of 3-D GCTMs. HDMR is an expansion in terms of correlated functions with increasing dimension which capture the chemical kinetic input-output relationships. In this fashion the original high-dimensional interpolation problem is broken into a set of low-dimensional pieces which may be efficiently handled. HDMR can be used to directly calculate output species concentrations and related chemical properties at a given reaction time based on the initial input species concentrations. There are many attractive features of HDMR including: (a) operations that only involve very rapid and stable algebraic manipulations, (b) accuracy comparable to conventional chemistry solvers, while attaining very significant computational savings, and (c) full variable coverage for high-dimensional systems.

HDMR can be applied for different purposes. For instance, construction of a computational model directly from lab/field data, creating an efficient fully equivalent operational model for existing mathematical model, identification of key model variables, global uncertainly assessments, efficient quantitative risk assessment, etc. In one domain of applications significant computational enhancements have been observed in certain atmospheric model calculations.

1 Theoretical Basis of HDMR

Many problems in science and engineering reduce to the need for finding an efficiently constructed map of the relationship between sets of high dimensional input and output system variables. The system may be described by a mathematical model (e.g., typically a set of differential equations), where the input variables might be specified initial and boundary conditions, parameters as well as functions residing in the model, and the output variables would be the solutions to the model or a functional of it. The IO behavior may also be based on observations in the laboratory or field where a mathematical model cannot readily be constructed for the system. In this case the system is simply considered as a black box. The inputs consist of the measured laboratory or field (control) variables and the output(s) is the observed system response. Regardless of the circumstances, the input is often very high dimensional with many variables even if the output is only a single quantity. We refer to the input variables collectively as $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ with $n \sim 10^2 - 10^3$ or more, and the output as $f(\mathbf{x})$. For simplicity in the remainder of the paper and without loss of generality, we shall refer to the

system as a model regardless of whether it involves modeling, laboratory experiments or field studies.

A general set of HDMR mathematical analysis tools have been introduced for improving the efficiency of deducing high dimensional IO system behavior [8, 9, 10, 11, 12, 13]. Since the influence of the predictor variables on the response variable can be independent and/or cooperative, it is natural to express the output $f(\mathbf{x})$ as a hierarchical correlated function expansion in terms of the input variables as follows:

$$\begin{aligned} f(\mathbf{x}) &= f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) + \sum_{1\le i<j<k\le n} f_{ijk}(x_i, x_j, x_k) \\ &+ \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n). \end{aligned} \tag{1}$$

Here f_0 denotes the mean value of $f(\mathbf{x})$ over the entire domain Ω of $\mathbf{x}$. The first order ($l = 1$) function $f_i(x_i)$ represents the effect of input variable x_i acting independently, although generally nonlinearly, upon the output $f(\mathbf{x})$. The second order ($l = 2$) function $f_{ij}(x_i, x_j)$ describes the cooperative effects of the input variables x_i and x_j upon the output $f(\mathbf{x})$. The higher-order terms reflect the cooperative effects of increasing numbers of input variables acting together to influence the output $f(\mathbf{x})$. The last term $f_{12\ldots n}(x_1, x_2, \ldots, x_n)$ gives any residual dependence of all the input variables locked together in a cooperative way to influence the output $f(\mathbf{x})$.

The basic conjecture underlying HDMR is that the component functions in Eq. (1) arising in typical real problems will not likely exhibit high order l cooperativity among the input variables such that the significant terms in the HDMR expansion are expected to satisfy the relation: $l \ll n$ for $n \gg 1$. Experience shows that an HDMR expression to 2nd order

$$f(\mathbf{x}) \approx f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) \tag{2}$$

often provides a satisfactory description of $f(\mathbf{x})$ for many high dimensional systems. Broad evidence from statistics supports this conjecture where it is rarely found that more than input variable covariance (i.e., variable pair cooperativity) arises to a significant degree. HDMR attempts to exploit this observation to efficiently determine high dimensional input-output system mapping. The presence of only low order variable cooperativity does not necessarily imply a small set of significant variables nor does it limit the nonlinear nature of the input-output relationship.

1.1 Determination of HDMR Component Functions

This valuable property of inputs cooperativity for high dimensional systems may be utilized only if the proper formulas of the HDMR component functions can be found. *The critical feature of HDMR expansion is that its component functions* f_0, $f_i(x_i), f_{ij}(x_i, x_j), \cdots$ *are optimal choices tailored to a given* $f(\mathbf{x})$ *over the entire desired domain* Ω *of* $\mathbf{x}$ *such that the high order terms in the expansion are negligible.* A particular component function $f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l})$ ($l = 0, 1, \ldots, n-1$ with f_0 corresponds to $l = 0$) of HDMR expansion is obtained by an optimization procedure that minimizes the functional

$$\min_{f_{i_1 i_2 \ldots i_l}} \int_{\Omega} w_{i_1 i_2 \ldots i_l}(\hat{\mathbf{x}}, \mathbf{u}) \Big[f(\mathbf{u}) - f_0 - \sum_{i=1}^{n} f_i(u_i) - \sum_{1 \le i < j \le n} f_{ij}(u_i, u_j) - \cdots - \sum_{i_1 i_2 \ldots i_l} f_{i_1 i_2 \ldots i_l}(u_{i_1}, u_{i_2}, \ldots, u_{i_l}) \Big]^2 \mathrm{d}\mathbf{u} \tag{3}$$

under a suitable specified condition which guarantees all the component functions to be determined step by step. Here, $\hat{\mathbf{x}} = (x_{i_1}, x_{i_2}, \ldots, x_{i_l})$, $\mathrm{d}\mathbf{u} = \mathrm{d}u_1 \mathrm{d}u_2 \cdots \mathrm{d}u_n$, and $w_{i_1 i_2 \ldots i_l}(\hat{\mathbf{x}}, \mathbf{u})$ may be considered as a weight function.

Different weight functions will produce distinct, but formally equivalent HDMR expansions, all of the same structure as Eq. (1). There are two commonly used HDMR expansions: Cut- and RS(Random Sampling)-HDMR which are two extreme cases of different HDMR expansions. Cut-HDMR depends on the value of $f(\mathbf{x})$ at a specified reference point $\bar{\mathbf{x}}$ while RS-HDMR depends on the average value of $f(\mathbf{x})$ over the whole domain Ω.

1. Cut-HDMR

When ordered sampling for output $f(\mathbf{x})$ at chosen points of $\mathbf{x}$ is possible (e.g., for lab data with controlled values of $\mathbf{x}$), then a Cut-HDMR expansion can be constructed. For Cut-HDMR, first a reference point $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_n)$ is selected in the domain Ω. The optimal component functions of Cut-HDMR in Eq. (1) possess the following structure:

$$f_0 = f(\bar{\mathbf{x}}), \tag{4}$$

$$f_i(x_i) = f(x_i, \bar{\mathbf{x}}^i) - f_0, \tag{5}$$

$$f_{ij}(x_i, x_j) = f(x_i, x_j, \bar{\mathbf{x}}^{ij}) - f_i - f_j - f_0, \tag{6}$$

$$\cdots\cdots$$

where

$$\begin{aligned}(x_i, \bar{\mathbf{x}}^i) &= (\bar{x}_1, \ldots, \bar{x}_{i-1}, x_i, \bar{x}_{i+1}, \ldots, \bar{x}_n), \\ (x_i, x_j, \bar{\mathbf{x}}^{ij}) &= (\bar{x}_1, \ldots, \bar{x}_{i-1}, x_i, \bar{x}_{i+1}, \ldots, \bar{x}_{j-1}, x_j, \bar{x}_{j+1}, \ldots, \bar{x}_n).\end{aligned}$$

The last term $f_{12\ldots n}(x_1, x_2, \ldots, x_n)$ is determined by the difference between $f(\mathbf{x})$ and all other component functions in Eq. (1).

The above formulas can be readily obtained simply by substituting $(x_{i_1}, x_{i_2}, \ldots, x_{i_l}, \bar{\mathbf{x}}^{i_1 i_2 \ldots i_l})$ with different sets of $\{i_1, i_2, \ldots, i_l\} \subset \{1, 2, \ldots, n\}$ for $\mathbf{x}$ on the both sides of Eq. (1) and using the specified condition: a component function of Cut-HDMR vanishes when any of its own variables takes the value of the corresponding element in $\bar{\mathbf{x}}$, i.e.,

$$f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l})|_{x_s = \bar{x}_s} = 0, \quad s \in \{i_1, i_2, \ldots, i_l\} \tag{7}$$

which defines an orthogonal relation between two different component functions of Cut-HDMR as

$$f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) f_{j_1 j_2 \ldots j_k}(x_{j_1}, x_{j_2}, \ldots, x_{j_k})|_{x_s = \bar{x}_s} = 0. \tag{8}$$

$$s \in \{i_1, i_2, \ldots, i_l\} \bigcup \{j_1, j_2, \ldots, j_k\}$$

The Cut-HDMR component functions $f_i(x_i), f_{ij}(x_i, x_j), \cdots$ are typically provided numerically at discrete values of the input variables x_i, $x_j, \cdots$ producing from the resultant output function $f(\mathbf{x})$ for employment of the R.H.S. of Eqs. (4)-(6). Notice that the Cut-HDMR component functions are defined along some *cut* lines, planes, subvolumes, etc. across the reference point $\bar{\mathbf{x}}$ in Ω. This is the name Cut-HDMR coming from.

Since all the component functions are obtained by minimization procedures, they are optimal choices for a given output $f(\mathbf{x})$, and thus only low order terms of Cut-HDMR expansion are needed to give a good approximation for $f(\mathbf{x})$. Numerical data tables can be constructed for these component functions, and the values of $f(\mathbf{x})$ for an arbitrary point $\mathbf{x}$ are determined from these tables by performing only low dimensional interpolation over $f_i(x_i), f_{ij}(x_i, x_j), \cdots$. If each input variable takes s values, the required model runs to construct the $f_i(x_i)$, $f_{ij}(x_i, x_j)$ ... tables are

$$1 + ns + \frac{n(n-1)s^2}{2} + \cdots,$$

which are only polynomial functions of n and s. As only low dimensional tables are necessary, the saving of sampling for large n is significant compared to traditional s^n sampling. Thus, Cut-HDMR renders the original exponential difficulty to a problem of only polynomic complexity.

2. RS-HDMR

For RS-HDMR, the component functions are determined through an averaging processes on a set of randomly sampled points over the entire domain Ω, and this procedure is likely to be most appropriate for generating an HDMR from lab/field data.

For RS-HDMR, we first rescale variables x_i such that $0 \leq x_i \leq 1$ for all i. The output function $f(\mathbf{x})$ is then defined in the unit hypercube $K^n = \{(x_1, x_2, \ldots, x_n) | 0 \leq x_i \leq 1, i = 1, 2, \ldots, n\}$. The component functions of RS-HDMR possess the following forms:

$$f_0 = \int_{K^n} f(\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{9}$$

$$f_i(x_i) = \int_{K^{n-1}} f(\mathbf{x}) \mathrm{d}\mathbf{x}^i - f_0, \tag{10}$$

$$f_{ij}(x_i, x_j) = \int_{K^{n-2}} f(\mathbf{x}) \mathrm{d}\mathbf{x}^{ij} - f_i(x_i) - f_j(x_j) - f_0, \tag{11}$$

$$\cdots\cdots$$

where $\mathrm{d}\mathbf{x}^i$ and $\mathrm{d}\mathbf{x}^{ij}$ are just the product $\mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n$ without $\mathrm{d}x_i$ and $\mathrm{d}x_i, \mathrm{d}x_j$, respectively. Similarly, the last term $f_{12\ldots n}(x_1, x_2, \ldots, x_n)$ is determined from the difference between $f(\mathbf{x})$ and all other component functions in Eq. (1).

Considering that the domain Ω is a unit hypercube, f_0 is actually the average value of $f(\mathbf{x})$ over the whole domain in contrast with f_0 of Cut-HDMR which is the value of $f(\mathbf{x})$ at the specified single reference point $\bar{\mathbf{x}}$.

All the above formulas can be readily obtained simply by integrating the both sides of Eq. (1) with respect to different sets of input variables $\{x_{i_1}, x_{i_2}, \ldots, x_{i_l}\}$ $(l = n, n-1, \ldots, 1)$, and using the specified condition: the integral of a component function of RS-HDMR with respect to any of its own variables is zero, i.e.,

$$\int_0^1 f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) \mathrm{d}x_s = 0, \qquad s \in \{i_1, i_2, \ldots, i_l\} \tag{12}$$

which defines the orthogonal relation between two different RS-HDMR component functions as

$$\int_{K^n} f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) f_{j_1 j_2 \ldots j_k}(x_{j_1}, x_{j_2}, \ldots, x_{j_k}) \mathrm{d}\mathbf{x} = 0. \tag{13}$$

$$\{i_1, i_2, \ldots, i_l\} \neq \{j_1, j_2, \ldots, j_k\}$$

Evaluations of the high dimensional integrals in RS-HDMR expansion may be carried out by Monte Carlo random sampling integration since it is the most viable algorithm for this purpose [14], and this is the name RS(Random Sampling)-HDMR coming from.

According to the above formulas one can see that all the component functions of Cut- and RS-HDMR expansions can be directly constructed from the values of output $f(\mathbf{x})$ either at some ordered or randomly generated points of $\mathbf{x}$, which makes the construction of f_0, $f_i(x_i)$,$f_{ij}(x_i, x_j)$, ... simple and straight forward.

1.2 Projector Theory for HDMR

To have a better understanding of the concepts of HDMR expansions, it may be viewed from another perspective. The component functions of HDMR can be obtained through application of a suitably defined set of linear operators $\wp_0, \wp_i \ (i = 1, 2, \ldots, n)$, $\wp_{ij} \, (1 \leq i < j \leq n), \ldots$:

$$\begin{aligned} \wp_0 \, f(\mathbf{x}) &= f_0, & (14) \\ \wp_i \, f(\mathbf{x}) &= f_i(x_i), & (15) \\ \wp_{ij} \, f(\mathbf{x}) &= f_{ij}(x_i, x_j), & (16) \\ &\cdots. \end{aligned}$$

It has been proven that all the operators for Cut- and RS-HDMR expansions are commutative projection operators and they are mutually orthogonal to one another, i.e., they obey

1. Idempotency:

$$\wp^2_{i_1 i_2 \ldots i_l} = \wp_{i_1 i_2 \ldots i_l}, \quad \{i_1, i_2, \ldots, i_l\} \subset \{1, 2, \ldots, n\} \tag{17}$$

where $0 \leq l \leq n$, and $\wp_0$ corresponds to $l = 0$.

2. Orthogonality:

$$\wp_{i_1 i_2 \ldots i_l} \wp_{j_1 j_2 \ldots j_k} = 0. \quad \{i_1, i_2, \ldots, i_l\} \neq \{j_1, j_2, \ldots, j_k\} \tag{18}$$

3. Resolution of the identity:

$$\sum_{l=0}^{n} \sum_{i_1 i_2 \ldots i_l} \wp_{i_1 i_2 \ldots i_l} = \mathbf{1}, \tag{19}$$

where $\mathbf{1}$ denotes the identity operation.

The projectors act on a linear space $\mathcal{F}$ composed of all n-variable functions $f(\mathbf{x})$. Each projector $\wp_t$ provides an approximation $\wp_t f(\mathbf{x})$ for $f(\mathbf{x})$, and has its range Φ_t which is a subspace of the linear space $\mathcal{F}$. Any function $f(\mathbf{x}) \in \Phi_t$ is invariant upon the action of $\wp_t$, i.e.,

$$\wp_t f(\mathbf{x}) = f(\mathbf{x}), \qquad \forall f(\mathbf{x}) \in \Phi_t. \tag{20}$$

This implies that upon the action of $\wp_t$ there is no error for any function $f(\mathbf{x}) \in \Phi_t$. The larger the range Φ_t is, the better approximation $\wp_t$ produces.

Two projectors $\wp_i$ and $\wp_j$ are mutually orthogonal if

$$\wp_i \wp_j = \wp_j \wp_i = 0. \tag{21}$$

This is equivalent to

$$\Phi_i \cap \Phi_j = 0. \tag{22}$$

A sum of two mutually orthogonal projectors $\wp_i + \wp_j$ is also a projector whose range is $\Phi_i + \Phi_j$ which is larger than anyone of Φ_i and Φ_j. Therefore, $\wp_i + \wp_j$ has a better accuracy than any single $\wp_i$ and $\wp_j$.

Any set of commutative projectors generate a *distributive lattice* whose elements are obtained by all possible combinations (Boolean addition and multiplication) of the projectors in the set. In particular, the lattice has a unique *maximal* projector $\mathcal{M}$ which provides the algebraically best approximation to all n-variable functions $f(\mathbf{x})$ in $\mathcal{F}$ [15]. The range of the maximal projector $\mathcal{M}$ for the lattice generated by mutually commutative projectors $\{\wp_1, \wp_2, \ldots, \wp_s\}$ is the union of all the ranges Φ_t, i.e.

$$\Phi_{\mathcal{M}} = \Phi_1 \cup \Phi_2 \cup \cdots \cup \Phi_s. \tag{23}$$

When the projectors are mutually orthogonal, the maximal projector is simply their sum

$$\mathcal{M} = \sum_{i=1}^{s} \wp_s, \tag{24}$$

and the range $\Phi_{\mathcal{M}}$ is $\sum_{i=1}^{s} \Phi_i$. As more orthogonal projectors are retained in the set, the resultant approximation obtained by its maximal projector $\mathcal{M}$ becomes better.

For instance, if we choose the subset $\mathcal{S}_1 = \{\wp_0, \wp_i\,(i = 1, 2, \ldots, n)\}$ of the above mutually orthogonal projectors to generate a lattice, its maximal projector is simply the sum of all these projectors:

$$\mathcal{M}_1 = \wp_0 + \sum_{i=1}^{n} \wp_i, \tag{25}$$

and the best approximation of $f(\mathbf{x})$ by the projectors in this lattice is

$$\begin{aligned} f(\mathbf{x}) \approx \mathcal{M}_1\, f(\mathbf{x}) &= \wp_0\, f(\mathbf{x}) + \sum_{i=1}^{n} \wp_i\, f(\mathbf{x}) \\ &= f_0 + \sum_{i=1}^{n} f_i(x_i), \end{aligned} \tag{26}$$

which is the first order HDMR approximation for $f(\mathbf{x})$. Similarly, for the subset $\mathcal{S}_2 = \{\wp_0, \wp_i\,(i = 1, 2, \ldots, n), \wp_{ij}\,(1 \le i < j \le n)\}$, the best approximation of $f(\mathbf{x})$ is given by

$$\begin{aligned} f(\mathbf{x}) \approx \mathcal{M}_2\, f(\mathbf{x}) &= \wp_0\, f(\mathbf{x}) + \sum_{i=1}^{n} \wp_i\, f(\mathbf{x}) + \sum_{1 \le i < j \le n} \wp_{ij}\, f(\mathbf{x}) \\ &= f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \le i < j \le n} f_{ij}(x_i, x_j), \end{aligned} \tag{27}$$

which is the second order HDMR approximation for $f(\mathbf{x})$, and so on.

As $\mathcal{S}_1$ is a subset of $\mathcal{S}_2$, and $\mathcal{M}_2$ is the maximal projector in the lattice generated by $\mathcal{S}_2$, then $\mathcal{M}_2$ is better than $\mathcal{M}_1$, i.e., the second order approximation of HDMR is better than the first order one. General speaking, higher order HDMR approximations are never worse than lower order HDMR approximations even through they may not improve much in some cases. This implies that adding a new orthogonal projector into a sum of orthogonal projectors always produces a new projector with a better accuracy no matter

how better it is. Finally, as the sum of all projectors of HDMR expansion is the identity, the full HDMR expansion is exactly equal to $f(\mathbf{x})$.

It can be also proven that the range for projector $\wp_0 + \wp_i$ is any constant and any function of variable x_i, and the range for $\wp_0 + \sum_{i=1}^{n} \wp_i$ is any constant and any linear combination of functions with one variable x_i $(i = 1, 2, \ldots, n)$. Similarly, the range for projector $\wp_0 + \sum_{i=1}^{n} \wp_i + \sum_{1 \le i < j \le n} \wp_{ij}$ is any constant and any linear combination of functions with one or two variables x_i, x_j $(1 \le i < j \le n)$. As $f(x_i, \bar{\mathbf{x}}^i)$ is a one variable function, it is invariant to projector $\wp_0 + \sum_{i=1}^{n} \wp_i$, i.e., there is no error for 1st order Cut-HDMR approximation of $f(\mathbf{x})$ whenever the point $\mathbf{x}$ is located on a cut line across the reference point $\bar{\mathbf{x}}$ in Ω. Similarly, $f(x_i, x_j, \bar{\mathbf{x}}^{ij})$ is a two variable function, and thus there is no error for 2nd order Cut-HDMR approximation of $f(\mathbf{x})$ whenever the point $\mathbf{x}$ is located on any cut line or plane across the reference point $\bar{\mathbf{x}}$ in Ω. In summary, there is no error for lth order Cut-HDMR approximation of $f(\mathbf{x})$ whenever the point $\mathbf{x}$ is located on any k $(k \le l)$-dimensional subvolume across the reference point $\bar{\mathbf{x}}$ in Ω.

1.3 The Properties of HDMR Expansions

The following properties of HDMR are important for its application in different scientific problems.

1.3.1 Fast convergence of HDMR expansions

As mentioned above, HDMR expansions converge fast. This property can be demonstrated below. Suppose an output $f(\mathbf{x})$ defined in a unit hypercube of $\mathbf{x}$ can be expanded as a convergent Taylor series at reference point $\bar{\mathbf{x}}$, i.e.,

$$f(\mathbf{x}) = f(\bar{\mathbf{x}}) + \sum_{i=1}^{n} \frac{\partial f(\bar{\mathbf{x}})}{\partial x_i}(x_i - \bar{x}_i) + \sum_{i,j=1}^{n} \frac{1}{2!} \frac{\partial^2 f(\bar{\mathbf{x}})}{\partial x_i \partial x_j}(x_i - \bar{x}_i)(x_j - \bar{x}_j) + \cdots. \quad (28)$$

Then the component functions f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j), \cdots$ in Cut-HDMR given by Eqs. (4)-(6) have clear mathematical meaning. As shown above, $f_0 = f(\bar{\mathbf{x}})$. Since $f_i(x_i) = f(x_i, \bar{\mathbf{x}}^i) - f(\bar{\mathbf{x}})$, substituting $(x_i, \bar{\mathbf{x}}^i)$ for $\mathbf{x}$ and subtracting $f(\bar{\mathbf{x}})$ from the both sides of Eq. (1) gives $f_i(x_i)$. As all the terms containing $x_j (j \ne i)$ vanish, the first order component function $f_i(x_i)$ is the sum of *all* the Taylor series terms which contain and only contain variable x_i. Similarly, the second order component function $f_{ij}(x_i, x_j)$ is the sum of *all* the Taylor series terms which contain and only contain variables x_i and x_j,

etc. Thus, the infinite number of terms in the Taylor series are partitioned into finite different groups and each group corresponds to one Cut-HDMR component function. Or we say in other way that each component function of Cut-HDMR is composed of an infinite sub-class of the full multi-dimensional Taylor series. Therefore, any truncated Cut-HDMR expansion gives a better approximation of $f(\mathbf{x})$ than any truncated Taylor series because the latter only contains a finite number of terms of Taylor series. Furthermore, considering that $0 \leq x_i \leq 1\,(i = 1, 2, \ldots, n)$ and $(x_i - \bar{x}_i) < 1$, the high order Cut-HDMR component functions are usually smaller than low order ones because the high order component functions are composed of the product $\prod_{s=1}^{l}(x_{i_s} - \bar{x}_{i_s})^{k_s}$ with larger l. This may not be a strict proof in mathematics, but it gives us some idea why Cut-HDMR expansion converges fast.

Moreover, the sub-classes of Taylor series corresponding to different component functions of Cut-HDMR do not overlap one another, which is the basis for the orthogonal relation between two Cut-HDMR component functions.

Other HDMR expansions possess the same property as Cut-HDMR because a one-to-one relationship between two different HDMR expansions can be established. Thus, if Cut-HDMR converges at certain order, so do the other HDMR expansions.

1.3.2 Invariance of conservation laws for HDMR approximations

If a set of outputs $\{f^{(1)}(\mathbf{x}), f^{(2)}(\mathbf{x}),\ldots, f^{(s)}(\mathbf{x})\}$ obey a set of linear-superposition conservation laws, their HDMR approximations at any order also obey these conservation laws, i.e., if

$$\sum_{i=1}^{s} w_{ki} f^{(i)}(\mathbf{x}) = c_k, \qquad k = 1, 2, \ldots, m \tag{29}$$

where w_{ki} and c_k are two sets of constants, then

$$\sum_{i=1}^{s} w_{ki}\Big[\mathcal{M}_l f^{(i)}(\mathbf{x})\Big] = c_k, \quad k = 1, 2, \ldots, m; \quad l = 0, 1, \ldots, n \tag{30}$$

here

$$\mathcal{M}_l = \wp_0 + \sum_{i=1}^{n} \wp_i + \cdots + \sum_{i_1 i_2 \ldots i_l} \wp_{i_1 i_2 \ldots i_l}, \tag{31}$$

and $\mathcal{M}_l f^{(i)}(\mathbf{x})$ denotes the l-th order HDMR approximation for $f^{(i)}(\mathbf{x})$. This property can be proven by applying operator $\mathcal{M}_l$ to the both sides of Eq. (29)

and using the identity

$$\mathcal{M}_l c = c, \qquad c \text{ being a constant.} \tag{32}$$

The invariance of conservation laws is very useful for the application of HDMR in physics, chemistry and other scientific disciplines where conservation laws (e.g., mass, energy, momentum conservations, etc.) are important.

1.3.3 Decomposition of variance by RS-HDMR

Using the orthogonality property of RS-HDMR component functions it can be proven that the total variance σ_f^2 of $f(\mathbf{x})$ caused by all input variables may be decomposed into different kinds of its input contributions: due to the x_i independent action σ_i^2, the x_i and x_j pair correlated action σ_{ij}^2, etc.

$$\begin{aligned}
\sigma_f^2 &= \int_{K^n} \Big[f(\mathbf{x}) - \bar{f}\Big]^2 d\mathbf{x} = \int_{K^n} \Big[f(\mathbf{x}) - f_0\Big]^2 d\mathbf{x} \\
&= \int_{K^n} \Big[\sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) + \cdots\Big]^2 d\mathbf{x} \\
&= \sum_{i=1}^{n} \int_0^1 f_i^2(x_i)\mathrm{d}x_i + \sum_{1\le i<j\le n} \int_0^1 \int_0^1 f_{ij}^2(x_i, x_j)\mathrm{d}x_i\mathrm{d}x_j + \cdots \\
&= \sum_{i=1}^{n} \sigma_i^2 + \sum_{1\le i<j\le n} \sigma_{ij}^2 + \cdots,
\end{aligned} \tag{33}$$

where $\bar{f}$ is the mean value of $f(\mathbf{x})$ over the whole domain Ω. This property is useful for global uncertainty analysis because the above decomposition is valid over the whole domain. According to the magnitudes of σ_i^2, σ_{ij}^2, etc., it is easy to find out how the output uncertainty is influenced by the input uncertainties, which are the key input variables and what kinds of cooperativities exist.

1.4 Approximate and Advanced HDMR

1.4.1 Approximate formulas for RS-HDMR component functions

The direct determination of the component functions of RS-HDMR at different values of $x_i, x_j, \ldots$ by Monte Carlo integration requires a huge amount of random sampling. For instance, different Monte Carlo random samples for

$f(x_i, \bar{\mathbf{x}}^i)$ at different fixed values of x_i are needed to determine $f_i(x_i)$ [16]. To reduce sampling effort, the RS-HDMR component functions may be approximated analytically and numerically.

1. Analytical approximation

The RS-HDMR component functions may be approximated by some known functions, like orthogonal polynomials, spline functions, or even simply polynomial functions. For example,

$$f_i(x_i) \approx \sum_{r=1}^{k} \alpha_r P_r(x_i), \tag{34}$$

$$f_{ij}(x_i, x_j) \approx \sum_{r=1}^{l} \sum_{s=1}^{l} \beta_{rs} P_{rs}(x_i, x_j), \tag{35}$$

where α_r, β_{rs} are constant coefficients, and $P_r(x_i)$, $P_{rs}(x_i, x_j)$ are one and two variable orthogonal polynomials, respectively. Our task is to determine all the constant coefficients. Using the orthogonality property of orthogonal polynomials, the coefficients are given by

$$\alpha_r = \frac{\int_{K^n} f(\mathbf{x}) p_r(x_i) d\mathbf{x}}{\int_0^1 p_r^2(x_i) \mathrm{d}x_i}, \tag{36}$$

$$\beta_{rs} = \frac{\int_{K^n} f(\mathbf{x}) p_{rs}(x_i, x_j) d\mathbf{x}}{\int_0^1 \int_0^1 p_{rs}^2(x_i, x_j) \mathrm{d}x_i \mathrm{d}x_j}. \tag{37}$$

As no restriction is posed on the values of the elements of $\mathbf{x}$ for $f(\mathbf{x})$ in the above integrals, only one set of random samples for $f(\mathbf{x})$ are necessary to determine all the coefficients, and consequently all the component functions of RS-HDMR. The sampling effort is then dramatically reduced.

2. Numerical approximation

The RS-HDMR component functions may be also approximated numerically by using kernel smoothers. For instance, the first and second order RS-HDMR component functions are given by

$$f_i(x_i) \approx \int_{K^n} f(\mathbf{u}) k\Big(\frac{|x_i - u_i|}{\lambda}\Big) d\mathbf{u} - f_0 \tag{38}$$

$$\begin{aligned} f_{ij}(x_i, x_j) &\approx \int_{K^n} f(\mathbf{u}) \Big[k\Big(\frac{|x_i - u_i|}{\lambda_1}\Big) k\Big(\frac{|x_j - u_j|}{\lambda_2}\Big)\Big] d\mathbf{u} \\ &- f_i(x_i) - f_j(x_j) - f_0, \end{aligned} \tag{39}$$

where λ, λ_1 and λ_2 are window-widths, and $k(t)$ is certain kernel function. One example of kernel smoothers is given below [17]:

$$k(t) = \begin{cases} \frac{3}{4}(1-t^2), & \text{for } |t| \leq 1; \\ 0, & \text{otherwise.} \end{cases} \tag{40}$$

Similarly, as no restriction is posed on the values of the elements of $\mathbf{x}$ for $f(\mathbf{x})$ in the above integrals, only one set of random samples for $f(\mathbf{x})$ are necessary to determine all the component functions of RS-HDMR at different values of the elements of $\mathbf{x}$. The sampling effort is also dramatically reduced.

1.4.2 Monomial preconditioning Cut-HDMR

As argued earlier, very often the high order HDMR terms are small thereby making low (usually, first and second) order HDMR approximations satisfactory for practical purposes. However, in some cases the first or second order HDMR approximations may not provide desired accuracy, and higher order HDMR approximations might have to be considered. For Cut-HDMR the higher order terms demand a polynomially increasing number of data samples and possibly large computer storage. If the higher order component functions of Cut-HDMR can be approximately represented in a similar fashion as those for the zeroth, first and second order component functions, then higher order approximations of Cut-HDMR can be included without dramatically increasing the number of experiments or model runs as well as reducing computer storage requirements. One way to realize this idea is to represent a high order Cut-HDMR component function as products of low order Cut-HDMR component functions and some known functions of the remained input variables. For instance, a third order Cut-HDMR component function can be approximated as

$$\begin{aligned} f_{ijk}(x_i, x_j, x_k) &\approx \varphi_{ijk}(x_i, x_j, x_k)\bar{f}_0 + \varphi_{jk}(x_j, x_k)\bar{f}_i(x_i) + \varphi_{ik}(x_i, x_k)\bar{f}_j(x_j) \\ &+ \varphi_{ij}(x_i, x_j)\bar{f}_k(x_k) + \varphi_k(x_k)\bar{f}_{ij}(x_i, x_j) + \varphi_j(x_j)\bar{f}_{ik}(x_i, x_k) \\ &+ \varphi_i(x_i)\bar{f}_{jk}(x_j, x_k), \end{aligned} \tag{41}$$

where $\varphi_i(x_i), \varphi_j(x_j), \ldots, \varphi_{ijk}(x_i, x_j, x_k)$ are some known functions (e.g., the products of monomial $(x_i - b_i)$, $(x_j - b_j)$ and $(x_k - b_k)$), and $\bar{f}_0$, $\bar{f}_i(x_i)$, $\ldots$, $\bar{f}_{jk}(x_j, x_k)$ are similar to the zeroth, first and second order Cut-HDMR component functions. Thus, the 3-dimensional numerical table for $f_{ijk}(x_i, x_j, x_k)$ is replaced by some 1- and 2-dimensional numerical tables. The saving is

large especially for high order component functions. Using projector theory, an approach named as *monomial preconditioning* Cut-HDMR has been developed for this purpose [18].

1.4.3 Multiple Cut-HDMR

The basic principles of HDMR may be extended to more general cases. Multiple Cut-HDMR is one of these extensions where several lth order Cut-HDMR expansions at different reference points $\mathbf{a}(1), \mathbf{a}(2), \ldots, \mathbf{a}(m)$ are constructed, and $f(\mathbf{x})$ is approximately represented not by one but by all m Cut-HDMR expansions:

$$f(\mathbf{x}) \approx \sum_{k=1}^{m} w_k(\mathbf{x}) \Big[f_0^{(k)} + \sum_{i=1}^{n} f_i^{(k)}(x_i) + \cdots + \sum_{i_1 i_2 \ldots i_l} f_{i_1 i_2 \ldots i_l}^{(k)}(x_{i_1}, \ldots, x_{i_l}) \Big]. \quad (42)$$

The coefficients $w_k(\mathbf{x})$ possess the properties

$$w_k(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ is on any cut subvolume} \\ & \text{of } k\text{th point expansion,} \\ 0, & \text{if } \mathbf{x} \text{ is on any cut subvolume} \\ & \text{of other points expansions,} \end{cases} \quad (43)$$

$$\sum_{k=1}^{m} w_k(\mathbf{x}) = 1. \quad (44)$$

The properties of the coefficients $w_k(\mathbf{x})$ imply that all other Cut-HDMR expansions vanish except one when $\mathbf{x}$ is located on any cut line, plane or higher dimensional ($\leq l$) subvolumes through that reference point, and then the multiple Cut-HDMR expansion reduces to single point Cut-HDMR expansion. As mentioned above, lth order Cut-HDMR approximation does not have error when $\mathbf{x}$ is located on these subvolumes. When m Cut-HDMR expansions are used to construct a multiple Cut-HDMR expansion, the no error region is m times of that for a single reference point Cut-HDMR expansion. Therefore, the accuracy will be improved.

Different ways may be used to define $w_k(\mathbf{x})$. For example, the metric distances $\rho_k^{i_1 i_2 \ldots i_l}$ from point $\mathbf{x}$ to an l-dimensional subvolume with variables $\{x_{i_1}, x_{i_2}, \ldots, x_{i_l}\}$ across reference point $\mathbf{a}(k)\,(k = 1, 2, \ldots, m)$

$$\rho_k^{i_1 i_2 \ldots i_l}(\mathbf{x}) = \Big[\sum_{\substack{i=1 \\ i \notin \{i_1, i_2, \ldots, i_l\}}}^{n} [x_i - a_i(k)]^2 \Big]^{\frac{1}{2}} \qquad \{i_1, i_2, \ldots, i_l\} \subset \{1, 2, \ldots, n\} \quad (45)$$

can be used to define

$$\bar{w}_k(\mathbf{x}) = \prod_{\substack{s=1 \\ s\neq k}}^{m} \prod_{i_1 i_2 \ldots i_l} \rho_s^{i_1 i_2 \ldots i_l}(\mathbf{x}), \tag{46}$$

$$w_k(\mathbf{x}) = \frac{\bar{w}_k(\mathbf{x})}{\sum_{s=1}^{m} \bar{w}_s(\mathbf{x})}. \tag{47}$$

It can be readily proven that the defined $w_k(\mathbf{x})$ satisfies the required properties if different reference points $\mathbf{a}(k)$ do not share any coordinate. When $\mathbf{a}(k)$s do have the same values for some elements, modified definitions for $w_k(\mathbf{x})$ may be used.

1.4.4 HDMR with discrete input variables

HDMR can treat continuous as well as discrete input variables. The notion of inherently discrete variables refers to those that are naturally discrete or sampled in that fashion (e.g., socio-economic variables such as residences, families, ethnicities, occupations, income and age levels, etc.) A potentially serious difficulty in treating inherently discrete data arises since there is often no *a priori* means to order the input data. Without some identified rational ordering, the output $f(\mathbf{x})$ will likely appear as random over the domain Ω, and this behavior would prevent an efficient use of coarse sampling for interpolation. A good ordering of the input variables is defined as one that produces well-behaved "smooth" property variations $f(\mathbf{x})$ over the domain Ω. A rational ordering of the variables can be found, based on the first order HDMR component functions $f_i(x_i)$. The observed output due to the discrete values of each input variable may be used to produce a monotonic output variation with respect to a suitable ordering of the input variables. It is then natural to expect that the remaining behavior over the second, or possibly third, order HDMR output surfaces will be regular, if not monotonic. This variable ordering is crucial to make feasible the physical interpretation of the discrete input variables, and to allow ready use of the HDMR formulations. The discrete input variable capabilities of HDMR have been successfully tested recently with analogous problems involving protein mutations where the discrete variables are the amino acid residues.

1.4.5 Functional HDMR

If inputs for a system consist of a set of functions, i.e., the input vector $\mathbf{x}(t) = (x_1(t), x_2(t), \ldots, x_n(t))$, then the system output becomes a functional. One approach to this functional mapping problem is to assume that a discretization of the following form is valid

$$x_i(t) = \sum_{k=1}^{N_i} c_{ik}\phi_k(t), \tag{48}$$

where $\{\phi_k(t)\}$ is a family of orthogonal functions. Then any "functional" becomes a "function" of the parameters c_{ik} and then the HDMR formulas can be applied to it. This approach has been successfully implemented for an atmospheric radiative heating problem where the inputs consisted of species and temperature profiles as functions of altitude.

1.5 Applications of HDMR

1.5.1 Construction of observation-based models directly from lab/field data

An important application of HDMR is to model construction from lab/field data. In many cases where a large amount of experimental or field data are available, the mathematical model to treat these data cannot be readily constructed due to the complexity and uncomplete knowledge of the system. The models people used to describe the system are often so poor that they can neither reproduce the measured data nor provide reasonable prediction of the system behavior.

For such systems the HDMR technologies are powerful tools for model construction either by Cut-HDMR if ordered sampling is possible or by RS-HDMR when the available data can be considered as produced randomly. After HDMR expansion given by Eq. (1) has been constructed, the accurate reproduction of the measured data and the reasonable prediction of the output $f(\mathbf{x})$ for a given input $\mathbf{x}$ can be obtained.

The HDMR expansion serves as a mathematical model, with specific advantages over those generated by mechanistic or conventional statistical approaches: 1) it does not rely on any constraining physical, chemical and other theoretical assumptions. Its accuracy only depends on the quantity and quality of the data. This is especially useful when we do not have a

thorough understanding of the system; 2) it can also be used for statistical analysis of its own quality, thereby placing quantitative flags on the resultant predictions, to indicate whether additional measurements are needed; 3) it may be improved *continuously* without discarding the original learned terms by simply adding more new terms into the expansion when the information about new input variables is identified; 4) it can provide a better understanding of the physical content of the system such that a mechanistic model may be properly constructed/refined.

1.5.2 Construction of a fully equivalent operational model

An intriguing application of HDMR is to model or its component replacement by highly efficient equivalent forms. This operation takes advantage of the fact that complex models are typically broken into various submodels (e.g., involving chemistry, mechanical coupling, mass transport, etc.). The submodels of an overall model are often treated by numerical splitting techniques, thus isolating them for efficient replacement with equivalent HDMRs. The HDMR expansions for these submodels are constructed from off-line submodel runs. After the component functions $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$ for a submodel are obtained, they may be reused as a basis to predict output behavior at any other point $\mathbf{x}$ in the desired region Ω called upon by additional execution of the submodel. The HDMR expansion obtained in this way corresponds to a fully equivalent operational model (FEOM) which could replace the original submodels. This logic will be most appreciate for model components that involve very large numbers of computational operations which are repeated many times in executing the overall model (e.g., chemistry in a chemistry-transport model). The computational saving using a FEOM can be dramatic. Preliminary applications to atmospheric modeling lead to a computational saving by a factor of $\sim 10^3$ [11, 12].

This replacement can even be applied to an entire model. A FEOM for a transport-biochemical model to simulate the bioremediation of trace metals and/or radionuclides in soil and groundwater systems was constructed [19].

1.5.3 Global uncertainty assessment and identification of key variables and their interrelationship

As mentioned in Sec. 1.3.3, the individual component functions of RS-HDMR expansion have a direct statistical correlation interpretation, that permits the

output variance σ_f^2 to be decomposed into its input variable contributions σ_i^2, σ_{ij}^2, etc.

The information gained from this decomposition can be most valuable for attaining a physical understanding of the origins of output uncertainty. Since no restriction are placed on the form of HDMR component functions, a fully global uncertainty assessments can be achieved. The computational savings and the thoroughness of the sampling arise from HDMR decomposition into a set of low dimensional functions which can be exhaustively sampled. Furthermore, we have already commented that the HDMR component functions have a unique correlation function interpretation. Combing the decomposition property of the total variance σ_f^2 into its subcomponents σ_i^2 and σ_{ij}^2 etc., it is feasible to identify which model input variables are important and how they interrelate with each other. The resultant information will provide suggestions for modification of the model and additional laboratory or field studies to best improve the quality of the model.

1.5.4 Efficient quantitative risk assessments

For a quantitative risk assessment it is generally necessary to reconsider the original set of input variables and split them into two components ($x_1, x_2, \ldots, x_s$; $y_1, y_2, \ldots, y_r$; $s + r = n$) where the set $\{x_i\}$ will be referred to as scenario variables under human control (e.g., industrial emissions, etc.) and the set $\{y_j\}$ corresponds to all other model variables (e.g., chemical rates, transport coefficients, unidentified factors, etc.) which are present and subject to some degree of uncertainty. Typically, risk is associated with identifying whether the output $f(\mathbf{x}, \mathbf{y})$ exceeds (or goes below) a critical value f_c. The risk is defined as the probability $P(f > f_c)$ for this event to occur while simultaneously taking into account the uncertainty amongst the model input variables $\{y_j\}$. Thus the risk is defined as

$$R = \int H[f(\mathbf{x}, \mathbf{y}) - f_c] \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \tag{49}$$

and the variance of the risk is

$$\sigma_R^2 = \int H[f(\mathbf{x}, \mathbf{y}) - f_c] H[f(\mathbf{u}, \mathbf{y}) - f_c] \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} - R^2, \tag{50}$$

here $H(z)$ is a Heaviside function

$$H(z) = \begin{cases} 1, & z \geq 0; \\ 0, & z < 0. \end{cases} \tag{51}$$

The probability distribution for $\{y_j\}$ is folded into the transformation of the variables to form a unit hypercube. We may take special advantage of the HDMR expansions in evaluating risk, and variance around the risk, in a quantitative fashion. These tasks are facilitated by the ability to rapidly evaluate $f(\mathbf{x}, \mathbf{y})$ from Eq. (1) and thorough the full coverage of the space $\{\mathbf{x}, \mathbf{y}\}$ that this permits. In addition, it will be possible to determine the portion of the scenario variables $(x_1, x_2, \ldots, x_s)$ which contribute independently or in a correlated fashion to the risk. *The analysis will not only provide the risk R, but also a quality assurance on the risk through its variance σ_R^2 due to the model variables $\{y_j\}$ and their uncertainty.*

2 Illustrations of HDMR Applications

Some examples of HDMR applications related to atmospheric modeling are given below.

2.1 Atmospheric Radiation Transport

The radiation transport component of atmospheric modeling codes is typically a major contributor to the overall execution time. FEOMs were constructed as a high speed replacement for traditional transport modules. The input information to the FEOM test was the atmospheric water vapor and temperature profiles as a function of altitude as well as the surface temperature and albedo. The FEOM operates by identifying how these latter variables impact the heating rate as a function of altitude. The FEOM was shown to be better than 97% accurate over a broad input variable range, while simultaneously being approximately 10^3 times faster than traditional radiation transport module it replaced [12].

2.2 Atmospheric Chemistry Modeling

A major portion of the computational effort in simulations by 3-D chemistry-transport models is consumed in chemical kinetics calculations which repeatedly solve coupled ordinary differential equations. To relieve this computational burden, the HDMR techniques can be used to create a high-speed FEOM for chemical kinetics calculations. The initial development of FEOM atmospheric modeling was successfully tested in a photochemical box-model

study of 46 input variables where the FEOM technique produced accurate chemical species concentrations, while being orders of magnitude faster than a conventional stiff equation solver [11].

A preliminary FEOM has also been successfully tested in 3-D global chemistry-transport model (GCTM) ozone simulations for CO-CH_4-NO_x-H_2O chemistry [20], where the dynamic ranges of the chemical species concentrations are far broader than in the above study. The FEOMs were constructed for all GCTM model levels, all 12 months of the year, every 10 degrees of latitude, for two types of surface albedo, and for the entire range of tropospheric values of H_2O, CO, NO_x and O_3. The resultant FEOMs were then used to predict the chemical ozone production and destruction rates based on the mixing ratios of the four tracers (O_3, NO_x, CO and H_2O) in each of the tropospheric grid boxes during GCTM ozone simulations. The results show that the predicted ozone production and destruction rates using the FEOMs were more accurate than those obtained by traditional 4-way interpolative look-up tables. Furthermore, the simulated global ozone fields using FEOMs in the GCTM ozone simulation are closer to the observations from ozonesonde data than those obtained by the traditional 4-way interpolative look-up tables (see Figure 1).

2.3 Uncertainty Analysis of Bioremediation Modeling

RS-HDMR has been successfully applied to analyze the results of a mathematical model for identifying relevant variables in simulating bioremediation of trace metals/radionuclides in groundwater [19]. The challenge in heavy metal bioremediation modeling is to meaningfully represent the effects of biogeochemistry on the speciation and transport of trace metals/radionuclides in groundwater system. Due to significant uncertainties present in the rates of the relevant biogeochemical reactions, it is essential to quantify the contributions of these input variable uncertainties upon the model output uncertainty and also identity the key biogeochemical variables and their interrelationships. Twenty input variables, including eight oxidation rates of electron acceptors and twelve second order chemical reaction rates were selected to perform nonlinear HDMR uncertainty assessments for several model outputs including the total precipitation, accumulated flux and concentration of radionuclides.

An uncertainty assessment based on the HDMR methodology was conducted by performing selected model simulations with randomly generated

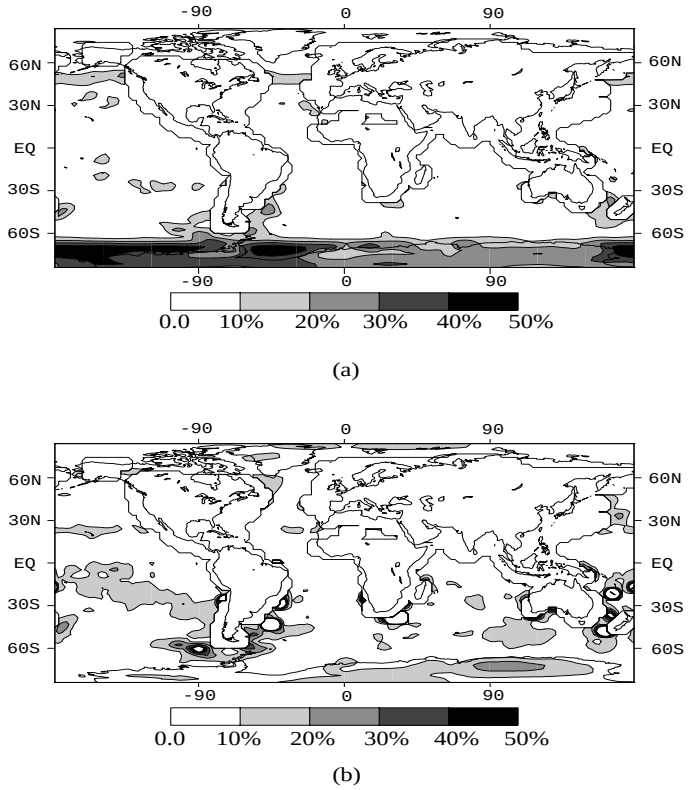

Figure 1: Percentage deviation from the exact solution of the ozone net chemical tendency (production - destruction) predicted by (a) the 4-way look-up table (b) the FEOM approximation in the surface level during February. The FEOM results are overall more reliable.

points in the twenty dimensional input-variable space. Thee resultant model outputs and associated random inputs were used to construct the component functions of the RS-HDMR expansion. Consequently, the total variance of model outputs was decomposed into its input variable contributions according to Eq.(33). By only performing a few hundred model simulations, we were able to satisfactorily identify the key variables from the 1st order (independent) variances σ_i, which accounted for most variation in the model

outputs. Also, the relative order of the 2nd order covariances was obtained. Moreover, from the functional behavior of the 1st- and 2nd-order component functions for the key variables, we are able to reveal the nonlinear relationships between model inputs and outputs (see Figure 2).

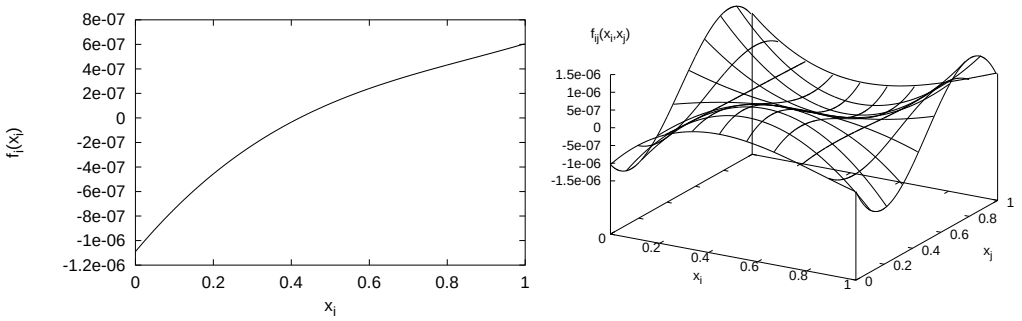

Figure 2: The functional behavior of typical 1st (left) and 2nd order (right) HDMR component functions from bioremediation where x_i and x_j are rate constants in the model.

3 Conclusions

A general set of quantitative model assessment and analysis tools, termed High Dimensional Model Representations (HDMR), have been introduced and successfully applied to relieve the computational burden of 3-D global chemistry-transport model simulations.

HDMR can be applied for other purposes, like construction of a computational model directly from lab/field data, identification of key model variables, global uncertainly assessments, and efficient quantitative risk assessment, etc.

HDMR techniques are quite generic in many areas involving experimentation, plant operations, and modeling. Essentially the same methodology being developed for these chemical applications may be transferable to even broader classes of problems of equal significance in other domains. The diverse applications of HDMR can, in turn, stimulate further development of the primary chemical/physical applications.

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