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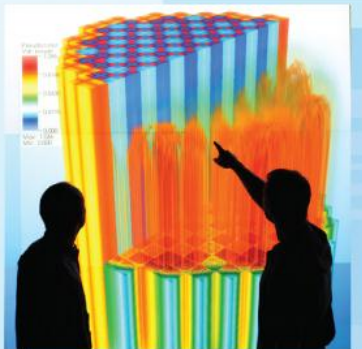

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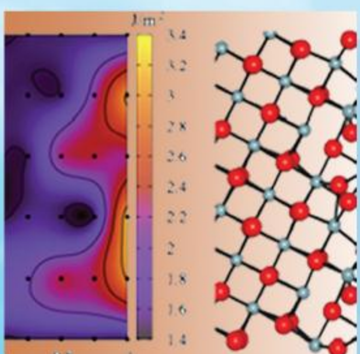

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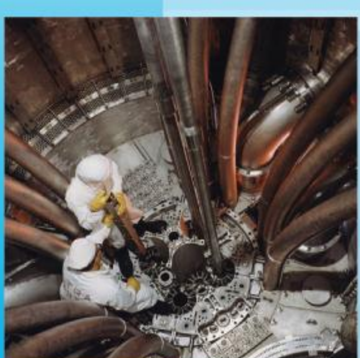

Plant operational data

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Investigation of Advanced UQ for CRUD Prediction with VIPRE

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Investigation of Advanced UQ for CRUD Prediction with VIPRE

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Abstract

This document summarizes the results from a level 3 milestone study within the CASL VUQ effort. It demonstrates the application of "advanced UQ," in particular dimension-adaptive p-refinement for polynomial chaos and stochastic collocation. The study calculates statistics for several quantities of interest that are indicators for the formation of CRUD (Chalk River unidentified deposit), which can lead to CIPS (CRUD induced power shift).

CASL-U-2011-0194-000

Acknowledgment

The author thanks Brian Adams for supplying the VIPRE models and executables used in this study and Yixing Sung for guidance on modifying the VIPRE source code.

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1 Background

Stochastic expansion methods are attractive methods for uncertainty quantification due to their fast convergence properties. For smooth functions (i.e., analytic, infinitely-differentiable) in L^2 (i.e., possessing finite variance), exponential convergence rates can be obtained under order refinement for integrated statistical quantities of interest such as mean, variance, and probability. Two stochastic expansion methods are of interest: nonintrusive polynomial chaos expansion (PCE), which computes coefficients for a known basis of multivariate orthogonal polynomials, and stochastic collocation (SC), which forms multivariate interpolation polynomials for known coefficients.

Within the DAKOTA project, recent research in stochastic expansion methods has focused on automated polynomial order refinement ("p-refinement") of expansions to support scalability to higher dimensional random input spaces [4, 3]. By preferentially refining only in the most important dimensions of the input space, the applicability of these methods can be extended from $O(10^0) - O(10^1)$ random variables to $O(10^2)$ and beyond, depending on the degree of anisotropy (i.e., the extent to which random input variables have differing degrees of influence on the statistical quantities of interest (QOIs)). Thus, the purpose of this study is to investigate the application of these adaptive stochastic expansion methods to the analysis of CRUD using the VIPRE simulation tools for two different plant models of differing random dimension, anisotropy, and smoothness.

2 Computational Experiments

The previous VIPRE CRUD study [2] demonstrated fast PCE convergence for the four variable "Plant A" problem, but results were less conclusive for the more challenging ten variable "Plant B" problem. Here we take a closer look at the convergence behavior for these two problems using a variety of algorithms from DAKOTA [1]. Starting with parameter studies, we explore the behavior of mass evaporation response metrics over the parameter ranges of the random variables. Next, we compare the performance of uncertainty quatification (UQ) methods, including Latin hypercube sampling (LHS) with uniform refinement and stochastic expansions (PCE or SC) with uniform or adaptive refinement. An important goal is to demonstrate the ability of the adaptive refinement strategies to detect anisotropy and preferentially refine in the most important stochastic dimensions, thereby improving scalability to higher dimensional UQ problems.

2.1 Plant A

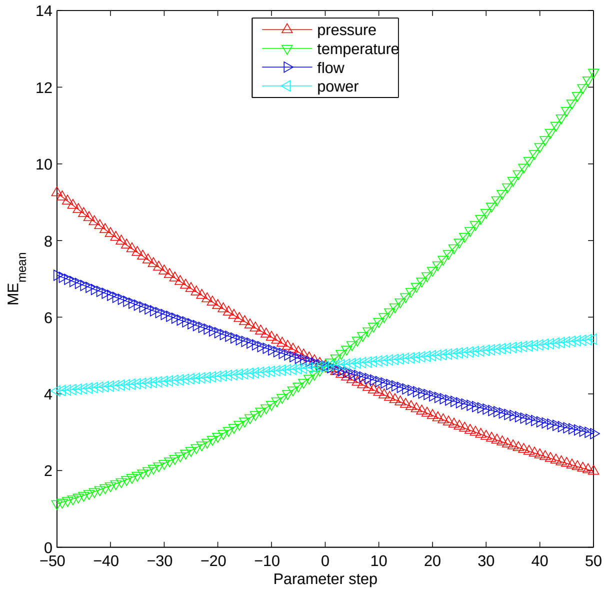
Studies for Plant A include the effect of four random variables: pressure, temperature, flow, and power. Each of these is modeled using a truncated normal distribution [2]. Metrics involve the mass evaporation rate "m-dot-e" (abbreviated ME hereafter) over a set of spatial nodes, where nonzero mass evaporation at a node indicates localized boiling, an indicator for CRUD formation.

2.1.1 Parameter studies

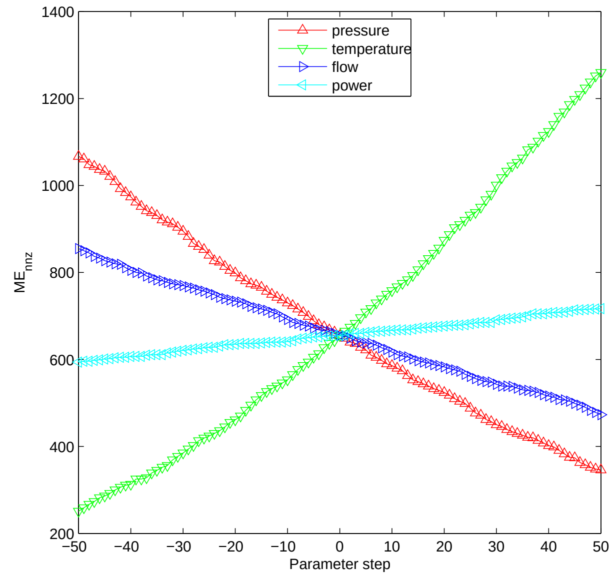
Figure 1 shows the results of a centered parameter study, which provides a set of one-dimensional slices through each of the four response surfaces for each of the four variables. Its primary purpose is to assess the smoothness of the different response metrics, although it also provides a partial view of global sensitivity. The parameter ranges are centered at the mean values and extend to the truncated normal bounds. It is evident that that there is a spectrum of smoothness from ME_{mean} and ME_{max} (which appear very smooth) to ME_{nnz} (which displays moderate noise) to ME_{meannz} (which displays significant noise). It is also evident that there is mild anisotropy in the importance of the random variables and that global sensitivity over the input ranges provided can be ranked in descending order as temperature, pressure, flow, and power.

2.1.2 Uncertainty quantification

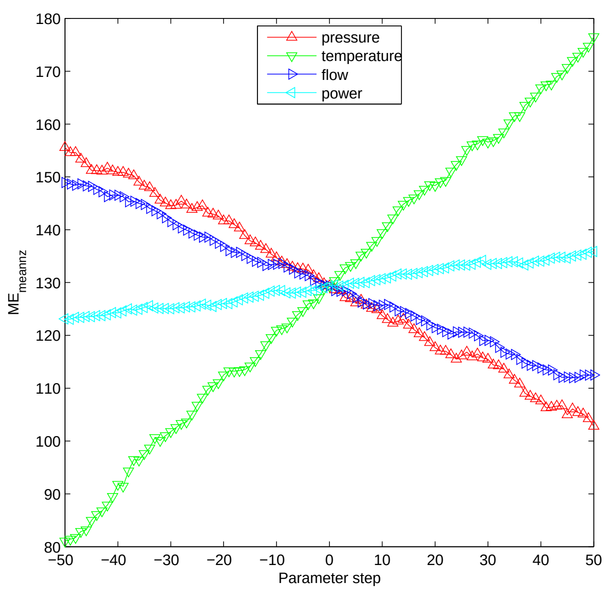
There are several different options for defining the grids within the stochastic domain, including unstructured grids from random sampling or structured grids from tensor-product quadrature, cubature, or Smolyak sparse grids. In this study, we focus on LHS using unstructured grids, uniform refinement of PCE and SC using isotropic sparse grids, and adaptive refinement of PCE and SC using generalized sparse grids [5].



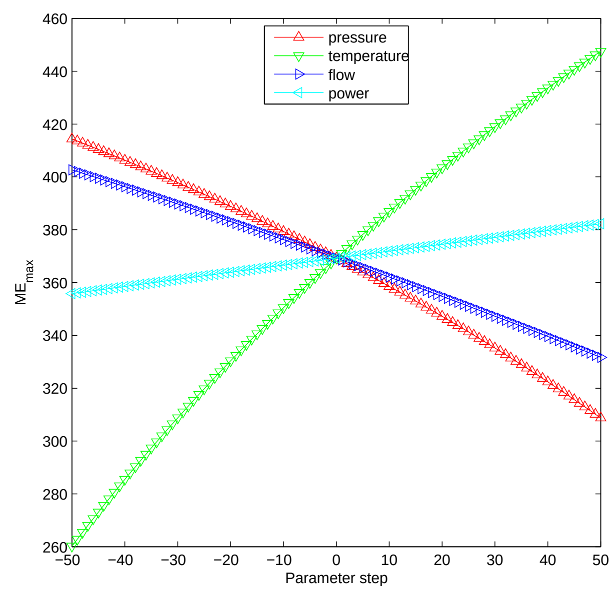
(a) ME_{mean}



(b) ME_{nnz}



(c) ME_{meannz}



(d) ME_{max}

Figure 1. Assessment of response smoothness for Plant A using a centered parameter study.

Table 1 shows results for uniform refinement for LHS, PCE, and SC. These results differ slightly from those in [2] due to modifications to VIPRE to increase the output precision of the mass evaporation rate to full double precision (since highly resolved stochastic expansions are extracting high-order modes, it is important for loss of precision to not induce or conceal these modes). Comparing, for example, σ for ME_{mean}, it appears that four digits of accuracy (3.203) are achieved in fewer than 1000 evaluations for PCE and SC, but will require greater than 100000 LHS evaluations.

Tables 2 and 3 shows results for adaptive refinement of ME_{mean} and ME_{max}, respectively, using PCE and SC on generalized sparse grids (GSG) [5]. Different rows correspond to different convergence tolerances within the adaptive procedure, applied to the change in the response variance for each algorithm iteration. In the latter ME_{max} case, a convergence tolerance of 1.e-4 was not quite achievable due to the restricted range (levels 0 through 5 only) of nested Genz-Keister rules for transformed normals.

Since a “truth” reference solution is not readily available, we instead investigate relative convergence; in particular, the absolute value of the change in statistical QOI versus the total evaluations required for a particular level within the refinement study. The relative convergence of σ for ME_{mean} and ME_{max} is shown in Figure 2 for LHS and uniform and adaptive refinement of stochastic expansions. For these two smooth metrics, it is evident that the stochastic expansion approaches with global basis polynomials achieve a much higher rate of convergence than LHS, as expected. In addition, the adaptive refinement approaches outperform the uniform refinement despite the lack of strong anisotropy in the importance of the four random variables.

Table 1. Plant A four variable problem, uniform refinement. Stochastic expansions employ isotropic sparse grids, global basis polynomials, and nested quadrature rules for transformed Askey distributions (Genz-Keister for normal).

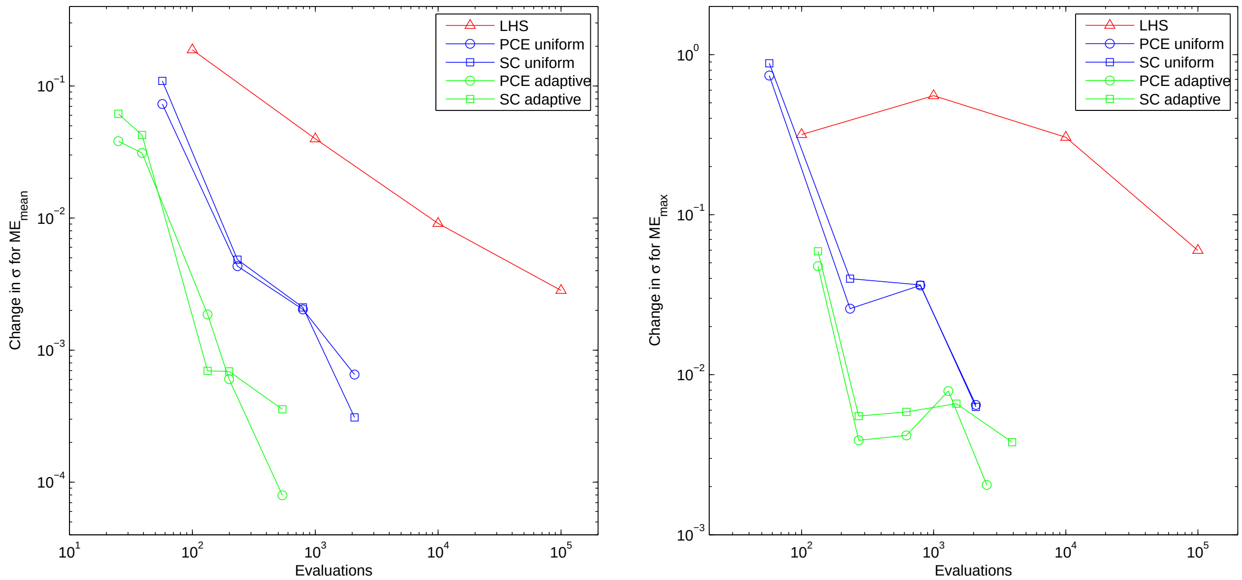
UQ	Fn	ME_{mean}		ME_{nnz}		ME_{meannz}		ME_{max}	
Method	Evals	μ	σ	μ	σ	μ	σ	μ	σ
LHS	10	5.2024283	3.0484628	676.50000	286.18225	128.44912	25.756736	362.90413	51.316263
LHS	100	5.3811040	3.2365378	689.95000	296.55767	129.20760	26.014010	364.30704	51.633028
LHS	1000	5.3537813	3.1966980	688.34200	292.56409	129.15964	25.493298	364.29270	51.078414
LHS	10000	5.3541864	3.2058056	688.43740	292.96176	129.14142	25.414158	364.32952	50.774176
LHS	100000	5.3549242	3.2029750	688.35309	292.71069	129.15984	25.454925	364.31772	50.833965
PCE L1	9	5.3659585	3.1364040	687.66667	290.37055	129.38399	25.611976	364.34780	50.188754
PCE L2	57	5.3622758	3.2093874	685.83687	292.53889	129.76796	25.889725	364.30435	50.929430
PCE L3	233	5.3554087	3.2050689	687.80375	292.85255	129.31060	25.359233	364.30650	50.903587
PCE L4	793	5.3524636	3.2030337	689.83644	295.20852	128.92811	24.983725	364.31110	50.867450
PCE L5	2089	5.3549595	3.2036871	688.70472	292.87033	129.05825	25.560947	364.31107	50.873928
SC L1	9	5.3659585	3.1011071	687.66667	289.43950	129.38399	25.613615	364.34780	50.060639
SC L2	57	5.3622758	3.2102752	685.83687	292.79278	129.76796	25.861697	364.30435	50.944095
SC L3	233	5.3554087	3.2054364	687.80375	292.66517	129.31060	25.320585	364.30650	50.904241
SC L4	793	5.3524636	3.2033290	689.83644	294.92151	128.92811	24.895490	364.31110	50.867862
SC L5	2089	5.3549595	3.2036382	688.70472	292.68151	129.05825	25.483007	364.31107	50.874157

Table 2. Plant A four variable problem, adaptive refinement of ME_{mean} using generalized sparse grids, global basis polynomials, and nested quadrature rules for transformed Askey distributions (Genz-Keister for normal).

UQ Approach	Conv Tol	Fn Evals	ME_{mean} μ	σ
PCE GSG	10	9	5.3659585	3.1364040
PCE GSG	1	25	5.3656145	3.1746208
PCE GSG	1e-1	39	5.3629245	3.2056836
PCE GSG	1e-2	133	5.3549026	3.2038212
PCE GSG	1e-3	199	5.3539898	3.2032185
PCE GSG	1e-4	541	5.3520119	3.2032980
SC GSG	10	9	5.3659585	3.1011071
SC GSG	1	25	5.3656145	3.1627265
SC GSG	1e-1	39	5.3629245	3.2052408
SC GSG	1e-2	133	5.3549026	3.2045450
SC GSG	1e-3	199	5.3539898	3.2038557
SC GSG	1e-4	541	5.3520119	3.2034992

Table 3. Plant A four variable problem, adaptive refinement of ME_{max} using generalized sparse grids, global basis polynomials, and nested quadrature rules for transformed Askey distributions (Genz-Keister for normal).

UQ Approach	Conv Tol	Fn Evals	ME_{max} μ	σ
PCE GSG	10	57	364.30435	50.929430
PCE GSG	1	133	364.31150	50.881781
PCE GSG	1e-1	271	364.31023	50.877890
PCE GSG	1e-2	621	364.30900	50.873714
PCE GSG	1e-3	1293	364.31124	50.865815
PCE GSG	2e-4	2525	364.31102	50.867865
SC GSG	10	57	364.30435	50.944095
SC GSG	1	133	364.31150	50.885042
SC GSG	1e-1	271	364.31023	50.879527
SC GSG	1e-2	621	364.30900	50.873670
SC GSG	1e-3	1485	364.31168	50.867080
SC GSG	2e-4	3929	364.31179	50.870868



(a) ME_{mean} **(b)** ME_{max}

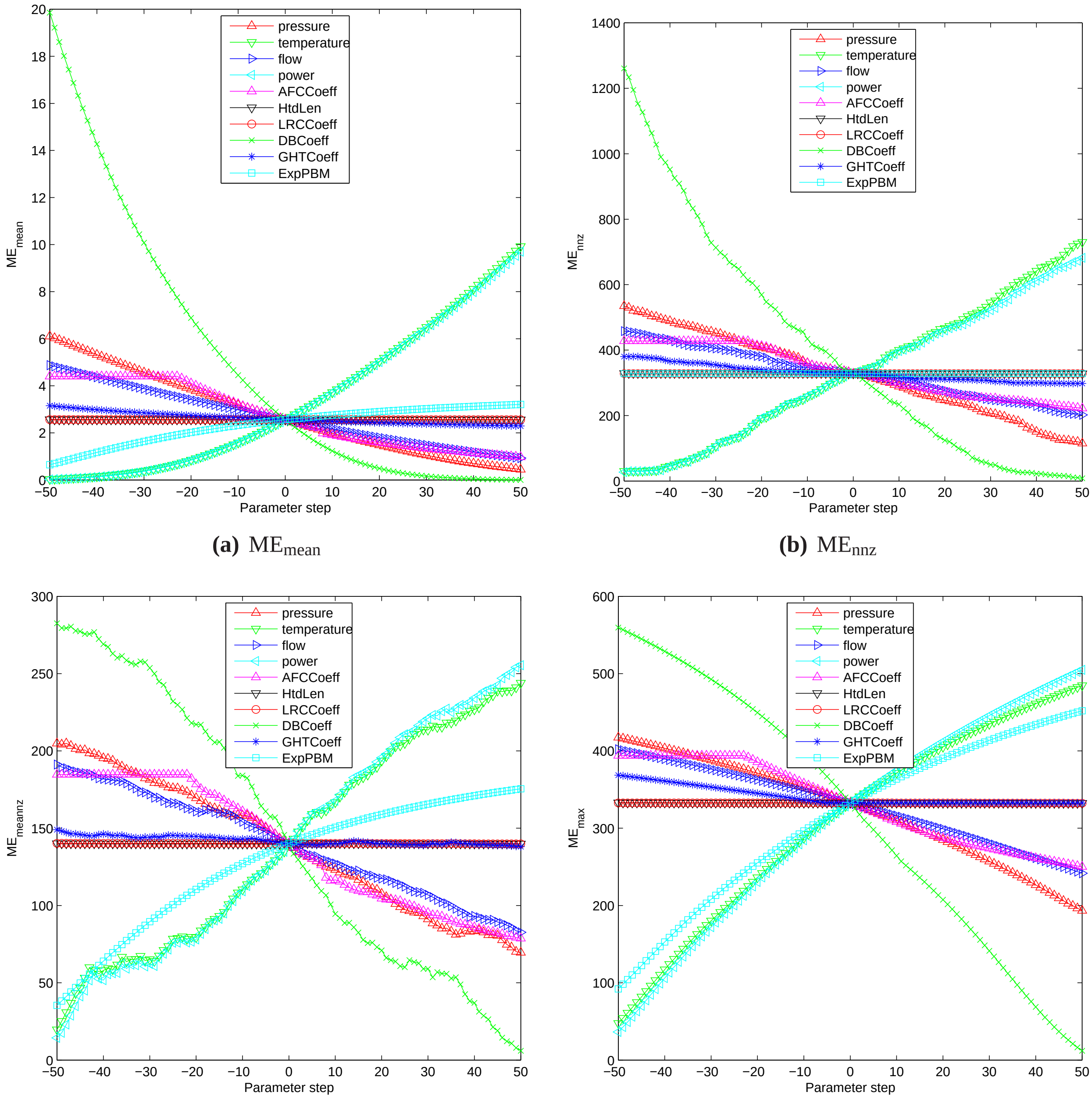
Figure 2. Relative convergence of standard deviation using LHS, PCE/SC uniform refinement, and PCE/SC adaptive refinement.

2.2 Plant B

As compared to Plant A, Plant B introduces six "model form" random variables (AFCCoeff, HtdLen, LRCCoeff, DBCoeff, GHTCoeff, and ExpPBM), all uniformly distributed about a nominal value [2]. These augment the previous pressure, temperature, flow, and power random variables, which are again modeled as truncated normal distributions (although the distribution parameters differ in general for the different plant).

2.2.1 Parameter studies

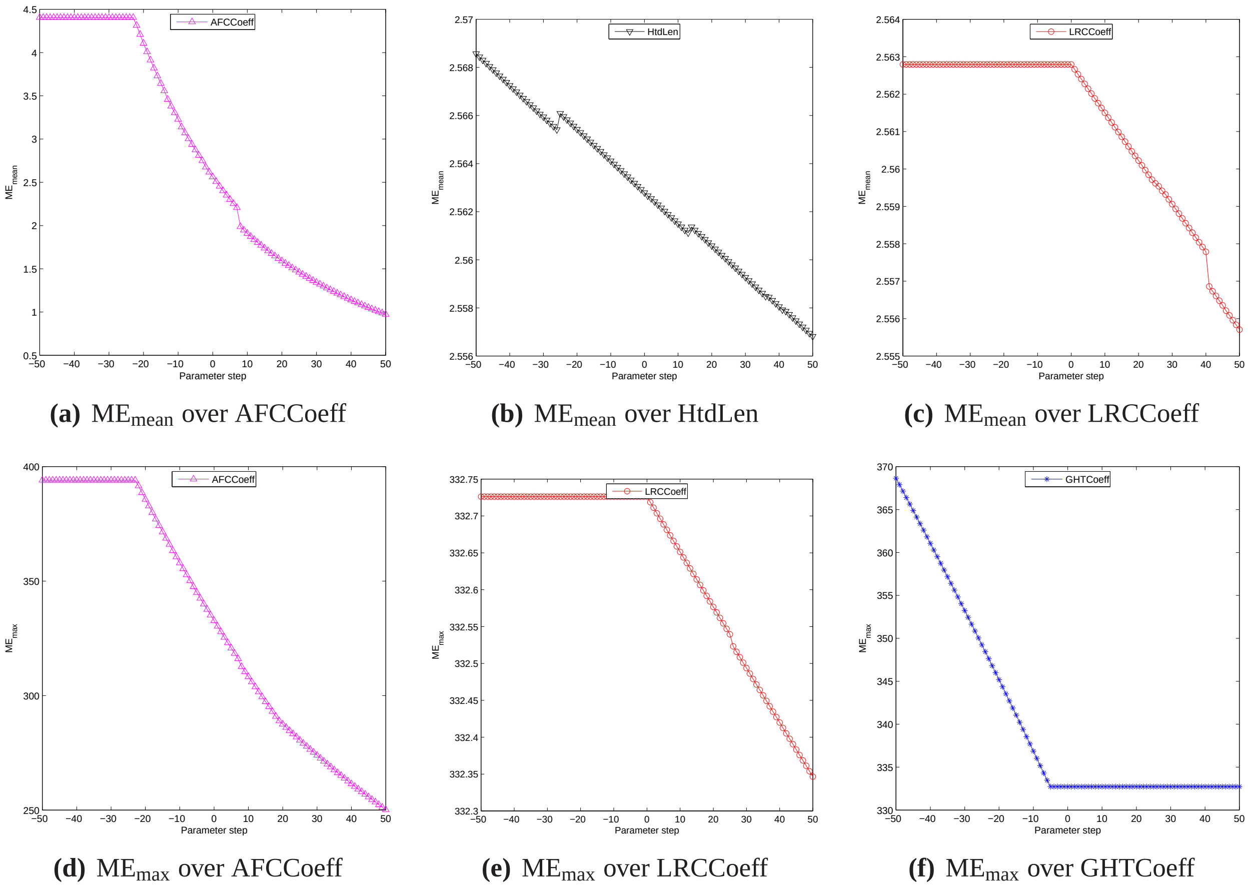
Figure 3 shows the results of another centered parameter study, where the one-dimensional slices for the four response metrics are now shown for each of the ten variables. The parameter ranges are centered at the mean values and extend approximately to the truncated normal or uniform bounds. A spectrum of smoothness is again evident, ranging from ME_{mean} and ME_{max} (which appear relatively smooth) to ME_{nnz} (which displays moderate noise) to ME_{meannz} (which displays significant noise). Upon closer inspection of ME_{mean} and ME_{max} in Figure 4, however, it is evident that these response functions now contain discontinuities with respect to some of the model form variables. The combination of higher random dimensionality and discontinuous response functions makes the uncertainty quantification much more challenging for stochastic expansion methods based on global polynomial basis functions. In terms of the relative importance of the different parameters, significant anisotropy is now present as the global sensitivity of several of the six



(a) $\mathrm{ME}_{\mathrm{mean}}$ **(b)** $\mathrm{ME}_{\mathrm{nnz}}$

(c) $\mathrm{ME}_{\mathrm{meannz}}$ **(d)** $\mathrm{ME}_{\mathrm{max}}$

Figure 3. Assessment of response smoothness for Plant B using a centered parameter study.



(a) ME_{mean} over AFCCoeff **(b)** ME_{mean} over HtdLen **(c)** ME_{mean} over LRCCoeff

(d) ME_{max} over AFCCoeff **(e)** ME_{max} over LRCCoeff **(f)** ME_{max} over GHTCoeff

Figure 4. Nonsmoothness within ME_{mean} and ME_{max} for selected model form variables.

model form parameters is much lower than that of the four operational parameters.

2.2.2 Uncertainty quantification

Table 4 shows results for uniform refinement for unstructured or isotropic structured grids. As for Plant A, these results differ slightly from those in [2] due to modifications to VIPRE to increase the output precision of the mass evaporation rate. It is evident that convergence has been impeded by the discontinuities in the response surfaces shown previously in Figure 4. Discontinuities are known to induce Gibbs oscillation in global polynomial approximations, which leads to slow convergence in integrated L^2 measures. Significant oscillation is evident in the convergence of mean and standard deviation for ME_{nnz}, ME_{meannz}, and ME_{max}. Only ME_{mean} apppears to be reasonably well behaved.

Table 5 shows results for adaptive refinement of ME_{mean} variance using PCE or SC on generalized sparse grids, where different rows correspond to refinement convergence tolerances in the

Table 4. Plant B ten variable problem, uniform refinement. Stochastic expansions employ isotropic sparse grids, global basis polynomials, and nested quadrature rules for transformed Askey distributions (Genz-Keister and Gauss-Patterson for normal and uniform).

UQ	Fn	ME_{mean}		ME_{nnz}		ME_{meannz}		ME_{max}	
Method	Evals	μ	σ	μ	σ	μ	σ	μ	σ
LHS	10	6.4583938	7.1019694	492.80000	439.37375	141.90488	121.92322	293.98242	243.18689
LHS	100	6.0354837	7.9765695	482.62000	472.57435	137.08093	105.22836	299.28587	205.55896
LHS	1000	5.8417074	7.5517979	481.49300	461.27668	139.93617	103.14638	305.62411	199.51242
LHS	10000	5.8388456	7.7294552	481.06170	465.54077	139.55339	102.98826	305.70088	198.93159
LHS	100000	5.8346719	7.6948522	481.33838	466.77452	139.05364	102.81946	305.01128	199.11421
PCE L1	21	6.0963634	6.7580396	438.50000	427.34519	137.44868	121.72384	282.75861	241.06341
PCE L2	249	5.8492224	7.7725066	515.52214	477.76385	126.67750	110.29644	309.72904	197.55537
PCE L3	2121	5.8408327	7.6841480	461.88990	462.81354	144.82442	113.66851	302.09471	213.25019
PCE L4	14329	5.8606195	7.7018543	465.61125	483.94538	152.11892	104.51174	308.94206	199.65995
SC L1	21	6.0963634	6.3818259	438.50000	423.18019	137.44868	122.15485	282.75861	236.31031
SC L2	249	5.8492224	7.8040605	515.52214	458.45618	126.67750	104.88659	309.72904	191.24337
SC L3	2121	5.8408327	7.6704579	461.88990	464.31351	144.82442	106.60457	302.09471	207.06866
SC L4	14329	5.8606195	7.6832159	465.61125	476.35690	152.11892	91.743840	308.94206	189.09085

Table 5. Plant B ten variable problem, adaptive refinement of ME_{mean} using generalized sparse grids, global basis polynomials, and nested quadrature rules for transformed Askey distributions (Genz-Keister and Gauss-Patterson for normal and uniform).

UQ	Conv	Fn	ME_{mean}	
Approach	Tol	Evals	μ	σ
PCE GSG	10	25	6.0985463	6.8213492
PCE GSG	1	49	6.0175205	7.5473652
PCE GSG	1e-1	169	5.8002740	7.5976745
PCE GSG	1e-2	535	5.8408538	7.7749293
PCE GSG	1e-3	3159	5.8402871	7.7141125
PCE GSG	1e-4	11953	5.8300648	7.6895616
SC GSG	10	25	6.0985463	6.4485081
SC GSG	1	65	5.8128055	7.4332141
SC GSG	1e-1	205	5.8626848	7.7592240
SC GSG	1e-2	719	5.8413910	7.7641182
SC GSG	1e-3	3933	5.8523593	7.6913452
SC GSG	1e-4	15805	5.8307209	7.6860392

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range of 10 to 10^{-4}. When erroneous oscillations are being induced due to discontinuities, one might conjecture that use of greedy adaptive algorithms (such as generalized sparse grids) could be counter-productive since selecting the refinement increments that induce the largest changes in the statistical QOI could be the ones that are most dominated by numerical instability or approximation error. However, it is evident that the generalized sparse grid procedure does reasonably well in capturing an accurate solution and does not fall victim to chasing errors.

Similar to Figure 2, Figure 5 shows relative convergence of σ for ME_{mean} for LHS and uniform and adaptive refinement of stochastic expansions. It is evident that the relative convergence rate is more rapid for uniform refinement of PCE/SC than for LHS, and that the initial rate for adaptive refinement is more rapid than uniform refinement. However, the relative convergence trajectory for adaptive refinement becomes noisy as the convergence tolerance is tightened, indicating some sensitivity to the nonsmoothness in this problem. The most refined LHS and adaptive PCE/SC results agree that $(\mu, \sigma) = (5.83, 7.69)$ when rounded to three digits. Thus, it appears that the adaptive PCE/SC results are more converged than the most resolved uniform refinement results (L4 in Table 4), where both sets are obtained for comparable expense.

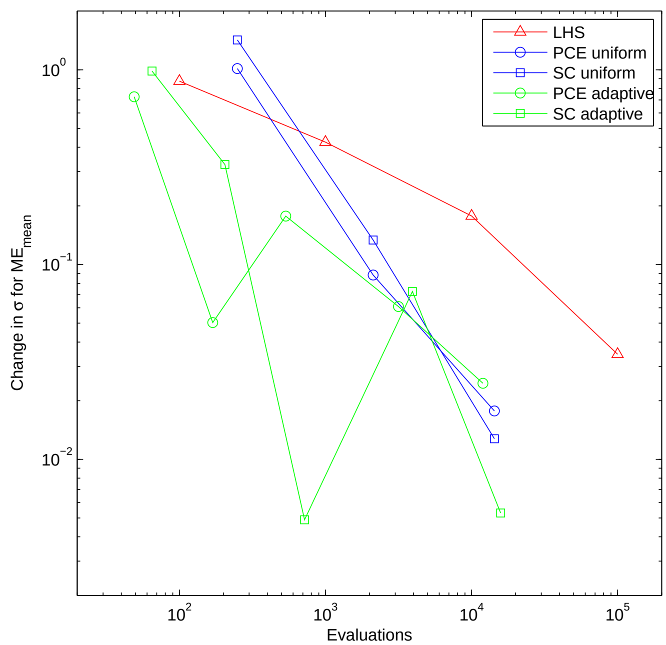

Figure 5. Relative convergence of ME_{mean} standard deviation using LHS, PCE/SC uniform refinement, and PCE/SC adaptive refinement.

3 Observations

Deployment of advanced UQ methods to uncertainty quantification of CRUD has led to the following primary observations:

- Centered parameter studies uncovered important information related to smoothness of the four response metrics, anisotropy in random variable importance, and discontinuities with respect to model form parameters. This insight helped guide study selection and explain observed differences in algorithm performance.
- Stochastic expansion methods for UQ (PCE and SC) exploit smoothness when present to provide more rapid convergence than random sampling approaches (e.g., LHS). For smooth Plant A metrics, PCE and SC were clearly superior, and for Plant B, PCE and SC were still more efficient than LHS despite the impediment of approximating discontinuous functions with smooth global basis polynomials.
- Adaptive p-refinement has been shown to be more efficient than uniform p-refinement for smooth problems that exhibit anisotropy. However, some caution is warranted when applying adaptive p-refinement methods to problems that are nonsmooth. In particular, greedy adaptive algorithms that select increments that induce the greatest change in statistical QOIs cannot discern among increments that increase accuracy through resolution and increments that might induce greater oscillation or numerical error. In the current studies, some sensitivity of the adaptive algorithms to nonsmoothness was detected, although they were still the top performers for both smooth and nonsmooth cases.
- Adaptive h-refinement is expected to be an effective option for dealing with nonsmooth response variations such as the discontinuities observed with the model form parameters used with Plant B. Initial capabilities have been developed for dimension-adaptive h-refinement using local bases (linear value-based or cubic gradient-enhanced) within global sparse grids; however, enabling local refinement based on local error estimates is expected to extract the full potential from adaptive h-refinement formulations. These capabilities are currently under development.

In addition, the following details were observed:

- Sharp discontinuities (Figure 4 for Plant B) appear to be more problematic that small-scale noise (Figure 1(b,c) for Plant A and Figure 3(b,c) for Plant B) in terms of their effect on PCE/SC convergence behavior (comparing noisy ME_{nnz} and $ME_{meannnz}$ metrics in Table 1 versus Table 4). The smoothing of noise on top of global trends is an interesting topic for future study.
- For PCE and SC techniques based on sparse grids (that extract high order modes from evaluations at precise Gauss points), it is important to pay attention to the precision of the input pre-processing and output post-processing. LHS is less sensitive to this issue. Since VIPRE

is a Fortran program that uses fixed formatting, increasing the input/output precision requires modifications to the VIPRE source code. While issues with output precision were addressed, similar issues with input precision (only 5 digits were allowed following the decimal) were not discovered until after the numerical studies were completed. Future studies should address this; it is expected that the convergence behavior for higher order grids could be further improved.

- For Plant B, comparing LHS and uniform refinement for ten input variables displays a cross-over where LHS initially appears better for low samples, but the faster convergence of stochastic expansions appears to result in greater accuracy for higher samples. This is as expected, as relative efficiency comparisons between these methods are dimension dependent. Since the convergence rate of random sampling is slow but dimension independent and the convergence rate of stochastic expansions is fast but dimension dependent, this cross-over point will tend to shift to the right as dimension increases. A goal of adaptive refinement is to reduce this dependence on dimensionality by reducing the effective dimension through preferential refinement.

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