An Efficient Approach to Surrogate Modeling with Application to Molecular Dynamics

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Outline

1. Introduction
   (a) Need for Surrogates - especially for complex models to enable forward UQ, sensitivity studies, calibration, and experimental design (Include citations).
   (b) Computational Hurdles: Polynomial Chaos and GP can be computationally intractable and suffer from the curse of dimensionality (Include plots for PCE to motivate dimension reduction with citations for both PCE and GP).
   (c) Sensitivity analyis - a potent tool for dimension reduction. However, SA can be computationally prohibitive. In fact, there are studies demonstrating the use of surrogates to reduce costs associated with SA (include citations).
   (d) DGSM - brief introduction and citations.
   (e) Key contributions of the paper: 1) Methodology that exploits DGSM to reduce the dimensionality of the problem and thus enables efficient construction of surrogates. 2) Application of the proposed methodology to investigate relative importance of parameters in the stillinger-weber potential, commonly used for studying phonon transport in silicon. Further, construct a reasonably accurate PC surrogate in the reduced space and demonstrate computational advantage of this approach. .
2. Background
   (a) DGSM
   (b) PCE
3. Methodology/Algorithm
4. Motivating Examples
   (a) Borehole: Screening, Convergence, Verification
   (b) Elliptic PDE: Screening, Convergence, Verification
   (c) Non-linear Oscillator: Screening, Convergence, Verification
5. Application: Phonon Transport in a Si bar
   (a) Include all details pertaining to the MD simulation: system, simulation, ensembles, etc.
   (b) Results
6. Discussion

(a) Methodology is agnostic to the choice of surrogate.

(b) As required for a PCE, the uncertain parameters need not be independent.

(c) Strategy depends on the application - methodology could be implemented sequentially or adaptively.