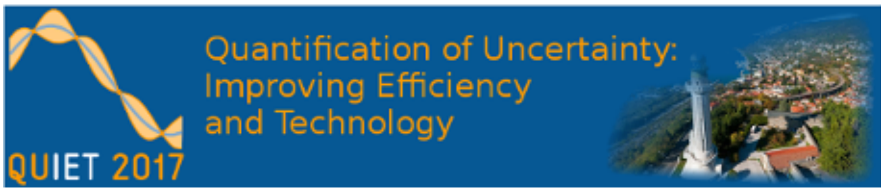

Improving Sampling-based Uncertainty Quantification Performance Through Embedded Ensemble Propagation

E. Phipps[1], M. D'Elia[1], M. Ebeida[1], and A. Rushdi[2]

[1]Sandia National Laboratories, Albuquerque, United States
[2]University of California, Davis, United States

A key component of computational uncertainty quantification is the forward propagation of uncertainties in simulation input data to output quantities of interest. Typical approaches involve repeated sampling of the simulation over the uncertain input data, and can require numerous samples when accurately propagating uncertainties from large numbers of sources. Often simulation processes from sample to sample are similar and much of the data generated from each sample evaluation could be reused.

In this talk, we explore a new method for implementing sampling methods that simultaneously propagates groups of samples together in an embedded fashion, which we call embedded ensemble propagation [3]. We show how this approach exploits properties of modern computer architectures to improve performance by enabling reuse between samples, reducing memory bandwidth requirements, improving memory access patterns, improving opportunities for fine-grained parallelization, and reducing communication costs. We describe a software technique for implementing embedded ensemble propagation based on the use of C++ templates, and demonstrate improved performance for the approach when applied to model diffusion problems on a variety of contemporary architectures.

A challenge with this method however is ensemble-divergence, whereby different samples within an ensemble choose different code paths. This can reduce the effectiveness of the method and increase computational cost. Therefore grouping samples together to minimize this divergence is paramount in making the method effective for challenging computational simulations. We also present several grouping approaches [1, 2] that attempt to minimize this divergence through surrogate models of ensemble computational cost. These approaches are developed within the context of locally adaptive stochastic collocation methods and Voronoi piecewise surrogate methods [4], and are applied to highly anisotropic diffusion problems where computational cost is driven by the number of (preconditioned) linear solver iterations, which vary widely from sample to sample.

References

[1] M. D'Elia, H. Edwards, J. Hu, E. Phipps, and S. Rajamanickam. Ensemble grouping strategies for embedded stochastic collocation methods applied to anisotropic diffusion problems. *Submitted to SIAM Journal on Uncertainty Quantification*, 2016.

[2] M. D'Elia, E. Phipps, A. Rushdi, and M. Ebeida. Surrogate-based ensemble grouping strategies for embedded sampling-based uncertainty quantification. *Submitted to SIAM Journal on Uncertainty Quantification*, 2017. `https://arxiv.org/abs/1705.02003`.

[3] E. Phipps, M. D'Elia, H. C. Edwards, M. Hoemmen, J. Hu, and S. Rajamanickam. Embedded ensemble propagation for improving performance, portability, and scalability of uncertainty quantification on emerging computational architectures. *SIAM Journal on Scientific Computing*, 39(2):C162–C193, 2017.

[4] A. Rushdi, L. Swiler, E. Phipps, M. D'Elia, and M. Ebeida. VPS: Voronoi piecewise surrogate models for high-dimensional data fitting. *International Journal for Uncertainty Quantification*, 7(1):1–21, 2017.