HYBRID UNCERTAINTY QUANTIFICATION TECHNIQUES FOR REACTIVE TRANSPORT APPLICATIONS

Xiao Chen, Lawrence Livermore National Laboratory, 925-422-6037, chen73@llnl.gov

1. Xiao Chen, Lawrence Livermore National Laboratory
2. Brenda Ng, Lawrence Livermore National Laboratory
3. Yunwei Sun, Lawrence Livermore National Laboratory
4. Charles Tong, Lawrence Livermore National Laboratory

This work presents a novel hybrid intrusive/non-intrusive approach for building multi-physics simulators embedded with uncertainty quantification (UQ) capabilities. This hybrid approach offers the flexibility over pure intrusive or non-intrusive approach by incorporating a "mix-and-match" philosophy whereby each individual physics module may be equipped with the best UQ method (intrusive or non-intrusive) available to it, and by seamlessly "gluing" these modules together to facilitate forward and inverse uncertainty propagation through the multi-physics model. We demonstrate its viability by formulating, implementing, and analyzing our hybrid UQ method on a two-dimensional nonlinear multi-species reactive flow-transport model, discretized by the finite-element method. The hydraulic conductivity field is represented by the Karhunen-Loeve expansion. The hydraulic head, specific flux, flow concentration and reaction rates are expressed by the polynomial chaos expansion.