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Rare event uncertainty quantification based on Hamiltonian MCMC approaches and the Approximate Sampling Target with Post-processing Adjustment (ASTPA) framework

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A new framework for computationally efficient rare event uncertainty quantification and reliability estimation is presented in this work, having exceptional performance, particularly in complex and most general static and dynamic cases of high-dimensionality, multi-modality, and very low failure probabilities. The introduced methodology is termed *Approximate Sampling Target with Post-processing Adjustment* (ASTPA) and comprises a sampling and a post-processing phase. The sampling target in ASTPA is constructed by appropriately combining the multi-dimensional random variable space with a cumulative distribution function that utilizes the limit-state function. Although the method is general and can be related to any appropriate sampling scheme, it is very efficiently supported by Hamiltonian Markov Chain Monte Carlo approaches and particularly our newly developed *Quasi-Newton mass preconditioned Hamiltonian MCMC* (QNp-HMCMC) approach. As with any HMCMC method, samples are produced based on Hamiltonian dynamics concepts, yet, in contrast to typical cases, quasi-Newton principles are now consistently used to guide the samples and form the preconditioned mass matrix that is eventually used in the final non-adaptive stage of the sampling algorithm. Alternative HMCM variants are also studied, and their characteristics and performance are compared and explained. Having acquired the samples, an adjustment step then follows, without involving any extra model calls, in order to accurately estimate the probability of failure. An original *inverse importance sampling* procedure is devised for this ASTPA phase, taking its name from the fact that importance sampling principles are exploited based on the already available samples. Due to this post-processing stage, an approximate analytical expression for the uncertainty of the computed estimation can also be derived, showcasing significant accuracy with numerical results. The suggested methodology can also work directly for first-passage dynamic problems and non-Gaussian multi-dimensional domains, hence, when a transformation to the favorable and preferred Gaussian space cannot be achieved, the probability of failure can still be effectively quantified. Finally, the capabilities and efficiency of the suggested approach are demonstrated and compared against Subset Simulation in a series of challenging low- and high-dimensional static and dynamic problems, with emphasis on newly introduced highly nonlinear multi-modal test examples.

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