



ExaQUTE

Exascale Quantification of Uncertainties for
Technology and Science Simulation

Recent advancements in high performance computing (HPC) will soon allow for the use of exascale systems in industrial practice, bringing the immense computational power of today's machines to real engineering applications. The ExaQUTE project aims at exploiting such systems, pushing our current physics simulation capabilities by performing Uncertainty Quantification (UQ) and Optimization Under Uncertainties (UQQ).

If we analyze the performance of current simulation tools, nowadays we can use numerical methods to accurately simulate and predict the behavior of a real phenomenon (for instance the interaction of structures and fluids, such as a building and the wind), provided that the values of relevant parameters at the initial state from external contributions to the system are known beforehand. This type of analysis can be costly for large and accurate cases, such as a whole high-rise building, but it is still doable with our current technology.

Why dealing with uncertainty?

Uncertainty comes into play when some of the input parameters of our problem are not exactly known a priori. Then, since the inputs for the simulation are not exact, the solution of the problem we are simulating will not be the exact one. What if we had to make decisions worth millions of euros based on something that we do not know at its fullest?

The approach of ExaQUTE to overcome this situation implies performing a large number of repeated simulations with similar but different input and boundary parameters, as opposed to running only one huge simulation. This strategy will allow to exploit our supercomputers by performing parallel calculations

Tossing a coin

A way to visualize the concepts of uncertainty and parallelism is by thinking of the example of tossing a coin. In an ideal set up, when tossing a coin a set number of times, and always in the same exact way, it would land on the same side every single time. However, in reality, there are many factors that are uncertain, such as the action of the air when the coin is moving, or shaking the hand. This leads to a certain proportion of heads and tails that will depend on all the external factors that contribute to the system. To obtain these exact percentages, one should think that the more throws, the more accurate the result.

For the sake of argument, consider that a hundred throws are enough to fully describe this behavior. In case you are asked to do this experiment by yourself, it will take you some time to toss the coin repeatedly until reaching the 100th experiment. If instead, 99 colleagues come to help you, you will have the analysis finished in one single go. This is the concept of parallelism.

Following the coin example, ExaQUTE aims at understanding the relation between the uncertainty (shaking of the hand, action of air) and final result (head or tail), in the smallest possible amount of time (parallelism).

Optimize the simulation results while taking into account uncertainty

Moreover, provided that we are able to model an uncertain phenomenon such as wind, in the same way as the coin example, how can we use this knowledge in engineering? How can we exploit the uncertain solution? Is it possible to use this result to optimize the shape of buildings accordingly?

ExaQUTE will answer this final question by combining the concept of uncertainties with optimization. Typically, optimization is used to find the optimal design that yields the best performance for a given analysis with a specific set of inputs and parameters. This, however, may result in fragile designs that are only adequate for the set of conditions they were conceived for. In this regard, the information given by uncertainty quantification allows us to converge to a final robust design which takes into account a wide range of different and uncertain conditions.

