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On-the-fly uncertainty quantification: algorithms and applications

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Quantification of all sources of uncertainties when modeling a physical system is essential to build an accurate digital twin and make informed decisions in an operational situation [1]. In uncertainty quantification of numerical simulation models, the classical approach for estimating distribution function or quantile function of a model output variable requires availability of an entire sample of the studied variable (i.e. the outputs of all the simulation model runs) [2]. This approach is not suitable at exascale as large ensembles of simulation runs would need to gather and store a prohibitively large amount of data [3]. For quantile estimation, this problem can be solved thanks to an on-the-fly (also called iterative or recursive) approach based on the Robbins-Monro algorithm [4]. An algorithm has been proposed for quantile function estimation in the context of uncertainty quantification [5]: it aims to estimate quantiles (at orders ranging from 5% to 95%) from samples of limited size (a few hundred observations). We illustrate it on toy functions and real application cases. We also provide some implementation elements inside the python package 'IterativeStatistics' [6] (which includes other statistics as mean, variance, covariance and first-order Sobol' index). This package is integrated into the Melissa system (on-line processing of data produced from large scale ensemble runs [7,8]) and will be also integrated into the SALOME platform [9] soon.

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[2] R. Smith. *Uncertainty quantification*, SIAM, 2014.

[3] A. Ribés, T. Terraz, Y. Fournier, B. Iooss and B. Raffin. Unlocking large scale uncertainty quantification with in-transit iterative statistics, In: *In situ visualization for computational science*, H. Childs, J. Bennet and C. Garth (Eds), Springer, 2022.

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[6] <https://pypi.org/project/iterative-stats/>

[7] T. Terraz, A. Ribés, Y. Fournier, B. Iooss and B. Raffin. Large scale in transit global sensitivity analysis avoiding intermediate files, SC17 (The International Conference for High Performance Computing, Networking, Storage and Analysis), November 2017

[8] <https://gitlab.inria.fr/melissa>

[9] <https://www.salome-platform.org/?lang=fr>

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