Investigating Quasi-Monte Carlo (QMC) methods for Geant4/Gate simulations in medical physics

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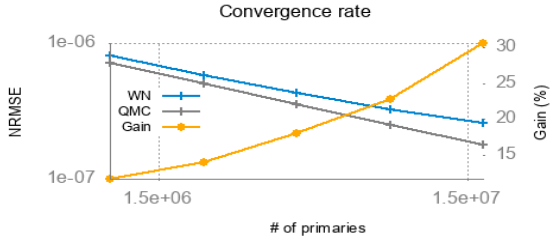
Background: Monte Carlo simulations with Geant4/Gate [1] are notoriously slow to converge. Indeed, the simulation engine performs numerous random sampling of distributions during particle tracking. In Geant4, the pseudo-random number generator draws independent samples from a canonical uniform distribution that are later transformed to target specific distribution. However, it is not optimal and it is known that *quasi-random* (QMC) sequences could speedup convergence rates [2]. QMC introduces correlation between samples, so that the sampling space is filled more homogeneously leading to error and variance reduction. It is however unclear how and if QMC samplers can be integrated within Geant4.

Material and Methods: We compared Sobol's [3] low discrepancy sequence (QMC) to conventional white noise sampling. Sobol's sampler in dimension d generates samples sequentially in the domain $[0,1)^d$. A "dimension" corresponds here to a given atomic stochastic task (AST) during particle tracking. We modified the CLHEP random engine to identify all ASTs and replace them with QMC. We restricted d to the first *23* dimensions (including rejection loops), the other being conventional whitenoise. Evaluation was performed with 140 keV gamma source in a waterbox with Compton scattering only (up to 1 order) and no secondaries.

Results and conclusion:

The fig1 depicts convergence rates for both methods, showing better convergence, with an expected gain of *50%* from 1e8 primaries. QMC integration error is related to discrepancy through the Koksma-Hlawka inequality. Our preliminary results tend to show that integrating low-discrepancy samplers in the framework of Geant4 is feasible. Works are ongoing to extend to multiple processes, considering secondaries and advanced samplers [4].



[1] D. Sarrut et al., Medical Physics, 41(2014) 064301.
[2] H. Niederreiter. Random Number Generation and quasi-Monte Carlo Methods. Society for Industrial and Applied Mathematics (SIAM) (1992)
[3] I.M. Sobol', USSR Computational Mathematics and Mathematical Physics, 7 (1967).
[4] L. Paulin et al. ACM Transactions on Graphics, 41 (2022).