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Parallel Adaptive Monte Carlo Optimization, Sampling, and Integration in C/C++, Fortran, MATLAB, and Python SHASHANK KUMBHARE, AMIR SHAHMORADI, University of Texas — At the foundation of predictive science lies the scientific methodology, which involves multiple steps of observational data collection, developing testable hypotheses, and making predictions. Once a scientific theory is developed, it can be cast into a mathematical model whose parameters have to be fit via observational data. This leads to the formulation of a mathematical objective function for the problem at hand, which has to be then optimized to find the best-fit parameters of the model or sampled to quantify the uncertainties associated with the parameters, or integrated to assess the performance of the model. Toward this goal, a highly customizable, user-friendly high-performance parallel Monte Carlo optimizer, sampler, and integrator library is presented here, which can be used on a variety of platforms with single to many-core processors, with interfaces to popular programming languages including C/C++, Fortran, MATLAB, and Python.

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