FEASST: Free Energy and Advanced Sampling Simulation Toolkit

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The Free Energy and Advanced Sampling Simulation Toolkit (FEASST) is a free, open-source, modular program to conduct molecular and particle-based simulations with Metropolis, Wang-Landau and Transition-Matrix Monte Carlo. Simulations may be conducted in the microcanonical, canonical and (semi-)grand canonical ensembles. Particle models include hard spheres, square wells, patchy particles, and Lennard-Jones with Yukawa, long-range corrections, Gaussians, point charges and Ewald. Features in development include expanded ensembles in temperature or alchemical transformations, configurational bias, geometric cluster algorithm, aggregation volume bias, confinement, and Mayer sampling. FEASST is implemented in C++ and may be imported as a module within Python. The code is available at https://pages.nist.gov/feasst and https://github.com/usnistgov/feasst.