A new paradigm for petascale Monte Carlo simulation: Replica exchange Wang–Landau sampling*

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Abstract. We introduce a generic, parallel Wang–Landau method that is naturally suited to implementation on massively parallel, petaflop supercomputers. The approach introduces a replica-exchange framework involving densities of states that are determined iteratively for overlapping sub-windows in energy space, each via traditional Wang-Landau sampling. The advantages and general applicability of the method are demonstrated using thousands of cores for several quite different systems (possessing either discrete or continuous degrees of freedom) including those with complex free energy landscapes and topological constraints.