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Well-tempered metadynamics: a smoothly-converging and tunable free-energy method ALESSANDRO BARDUCCI, GIOVANNI BUSSI, MICHELE PARRINELLO, ETH Zurich — We present [1] a method for determining the free energy dependence on a selected number of order parameters using an adaptive bias. The formalism provides a unified description which has metadynamics and canonical sampling as limiting cases. Convergence and errors can be rigorously and easily controlled. The parameters of the simulation can be tuned so as to focus the computational effort only on the physically relevantregions of the order parameter space. The algorithm is tested on the reconstruction of alanine dipeptide free energy landscape. [1] A. Barducci, G. Bussi and M. Parrinello, Phys. Rev. Lett., accepted (2007).

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