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Monte Carlo and Molecular Dynamics in the Multicanonical Ensemble: Connections between Wang-Landau Sampling and Metadynamics THOMAS VOGEL, DANNY PEREZ, CHRISTOPH JUNGHANS, Los Alamos National Laboratory — We show direct formal relationships between the Wang-Landau iteration [PRL 86, 2050 (2001)], metadynamics [PNAS 99, 12562 (2002)] and statistical temperature molecular dynamics [PRL 97, 050601 (2006)], the major Monte Carlo and molecular dynamics work horses for sampling from a generalized, multicanonical ensemble. We aim at helping to consolidate the developments in the different areas by indicating how methodological advancements can be transferred in a straightforward way, avoiding the parallel, largely independent, developments tracks observed in the past.

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