POP-ART: thermodynamically correct activated event sampling in complex materials\textsuperscript{1} M.V. CHUBYNSKY, Université de Montréal, Montréal, QC, Canada, HENK VOCKS, Universiteit Utrecht, Utrecht, The Netherlands, NORMAND MOUSSEAU, Université de Montréal, G.T. BARKEMA, Universiteit Utrecht — Dynamics of complex systems with a rugged energy landscape can be represented as a sequence of rare activated events during which the system jumps between different potential energy minima. The activation-relaxation technique (ART)\textsuperscript{[1]} is an efficient method of sampling such events; however, because of an unknown bias in selecting these events it cannot easily provide thermodynamical information. We present a modification of ART, the properly obeying probability ART (POP-ART)\textsuperscript{[2]}. POP-ART combines short molecular dynamics runs with ART-like activated moves, with an additional accept/reject step designed to satisfy detailed balance and thus reproduce correct thermodynamics. Both correctness and efficiency of the method have been tested using a variety of systems. We mention briefly some ways of extending the approach to obtain correct dynamics as well.

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