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POP-ART: thermodynamically correct activated event sampling in complex materials[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) [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) [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.
[1] G.T. Barkema and N. Mousseau, Phys. Rev. Lett. 77, 4358 (1996)
[2] H. Vocks, M.V. Chubynsky, G.T. Barkema and N. Mousseau, J. Chem. Phys., accepted

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Mykyta Chubynsky
Université de Montréal, Montréal, Québec

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