MICROCANONICAL ENSEMBLE OUT OF EQUILIBRIUM

R. Belousov [1,*], J. Elliott [1], F. Berger [2], L. Rondoni [3], and A. Erzberger [1*]

¹European Molecular Biology Laboratory, Meyerhofstrasse 1, 69117 Heidelberg, Germany
²Utrecht University, 3584 Utrecht, The Netherlands and
³Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Turin, Italy

Introduced by Boltzmann under the name "monode," the microcanonical ensemble serves as the fundamental representation of equilibrium thermodynamics in statistical mechanics by counting all realizations of a system's states. Ensemble theory connects this idea with probability and information theory, leading to the notion of Shannon-Gibbs entropy and, ultimately, to the principle of maximum caliber describing *trajectories* of systems–in and out of equilibrium. While the latter phenomenological generalization reproduces many results of nonequilibrium thermodynamics, given a proper choice of observables, its physical justification remains an open area of research. What is the microscopic origin and physical interpretation of this variational approach? What guides the choice of relevant observables? We address these questions by extending Boltzmann's method to a microcanonical caliber principle and counting realizations of a system's trajectories–all assumed equally probable. Maximizing the microcanonical caliber under the imposed macro- and microscopic constraints, we systematically develop generalized detailed-balance relations, clarify the statistical origins of inhomogeneous transport, and provide an independent derivation of key equations from stochastic thermodynamics. This approach introduces a *dynamical* ensemble theory for nonequilibrium steady states in spatially extended and active systems. While verifying the equivalence of ensembles, e.g. those of Norton and Thevenin, our framework highlights differences between nonequilibrium regimes not evident in the traditional formulation of the maximum-caliber principle that we validate in stochastic simulations. The microcanonical ensemble, originally conceived by Boltzmann as the "monode," represents the cornerstone of equilibrium statistical mechanics. By enumerating all possible realizations of a system's microscopic states, it provides the fundamental connection between microscopic dynamics and macroscopic thermodynamics. The development of ensemble theory has further bridged this connection with probability and information theory, giving rise to the Shannon-Gibbs entropy and, more recently, to the principle of maximum caliber for describing system trajectories - both in and out of equilibrium. While the maximum caliber principle has proven successful in reproducing many nonequilibrium thermodynamic results when appropriate observables are chosen, its physical foundations remain incompletely understood. The microscopic origin and interpretation of this variational approach, the criteria for selecting relevant observables, and the distinction between different nonequilibrium regimes are key questions that persist. In this work, we address these fundamental questions by extending Boltzmann's original counting method to develop a microcanonical caliber principle for nonequilibrium systems. Our approach counts trajectory realizations under the fundamental assumption of equal a priori probabilities, then maximizes the microcanonical caliber subject to both macroscopic and microscopic constraints.

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[1] A. Author et al., *Title of the simulation validation paper*, Journal Name **Volume**, Page (Year).

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* roman.belousov@embl.de