From Slices to Volumes: Unveiling the Geometry of High-Dimensional Energy Landscapes

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The energy landscape represents a central paradigm in physics, providing a conceptual and quantitative framework recapitulating the observed states of many-body systems and their response to perturbations, in and out of equilibrium. The high-dimensional geometry of energy surfaces, which is controlled by a plethora of critical points and their associated basins of attraction, escapes our intuition and, in most cases, analytical tractability, making it difficult to quantify their complexity. In this talk, I will describe an efficient approach to map the energy landscape accurately and, by "slicing" the energy surface, I will provide evidence that optimization methods widely used in computational studies (e.g., of supercooled liquids and atomic clusters) destroy any resemblance of the true landscape geometry [1]. Then, I will discuss the challenges inherent to measuring the volume of basins of attraction [2], and I will introduce an efficient Monte Carlo method for the computation of the volumes of high-dimensional bodies with arbitrary shape [3]. This approach will enable us to (i) gain unprecedented insight into the structure of basins of attraction [2, 3], (ii) quantify the number of minima in the energy landscape of soft sphere packings (and thus their entropy) [4, 5]; (iii) reveal hierarchies and unexpected regularities in the energy landscape of soft sphere packings [2, 4, 5]. I will conclude by highlighting challenges and promising future directions for these measurements.

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3. S. Martiniani, K. J. Schrenk, J. D. Stevenson, D. J. Wales, D. Frenkel, "Structural analysis of high dimensional basins of attraction", Phys. Rev. E 94, 031301 (2016)

4. S. Martiniani, K. J. Schrenk, J. D. Stevenson, D. J. Wales, D. Frenkel, "Turning intractable counting into sampling: computing the configurational entropy of three-dimensional jammed packings", Phys. Rev. E 93, 012906 (2016)

5. S. Martiniani, K. J. Schrenk, K. Ramola, B. Chakraborty, D. Frenkel, "Numerical test of the Edwards conjecture shows that all packings become equally probable at jamming", Nature Physics, 13, 848-851 (2017)