Abstract Submitted
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A new graph-matching-based algorithm to study dynamical processes[1] FAUSTO MARTELLI, HSIN-YU KO, ROBERTO CAR, Princeton University — We present a new algorithm to identify and quantify the degree of local order in dynamical systems. To each particle site we associate a given number of neighboring sites the positions of which define the nodes of a pattern graph. We match this graph with a graph describing the geometry of an ordered reference system. The degree of overlap is obtained by recursively maximizing a score function having a value ranging from 0 (in the case of a completely disordered system) to 1 (in the case of a perfect crystal). While typically order parameters are tailored to specific cases, our approach is general and could be applied to different areas of condensed matter physics. Here we illustrate the approach with applications to atomic and molecular fluids, namely melting of Lennard Jones particles, direct crystallization of supercooled water and melting of Yukawa crystals.

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Fausto Martelli
Princeton University

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