

## Understanding Molecular Simulation From Algorithms To Applications

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Molecular Dynamics Molecular dynamics is a technique for computing the equilibrium and non-equilibrium properties of classical\* many-body systems. \* The nuclear motion of the constituent particles obeys the laws of classical mechanics (Newton). References: 1) Computer Simulation of Liquids, M.P. Allen & D.J. Tildesley, Clarendon, Oxford, 1987.

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