How to simulate molecular dynamics the "right" way

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Numerical methods are often used to solve many differential equations in science and engineering. One application is in Molecular Dynamics (MD), where numerical methods are used to study the motions of atoms and molecules and their properties.Unfortunately, traditional numerical methods do not respect the mathematical properties of the MD equations, such as conservation of energy and volume-preservation.

In this talk, I will discuss about "symplectic methods" for simulating MD and their advantages over traditional numerical methods.

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