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First principles molecular dynamics on a large scale

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Abstract:

Over the past decade a revolution has taken place in how we do large scale molecular dynamics. While previously first principles accuracy was solely the purview of explicit electronic structure methods such as density functional theory, the new approaches have allowed the extension of highly accurate, first principles simulations to the atomic scale, where electrons are not treated explicitly any more, and therefore hundreds of thousands of atoms can be simulated. These quantum mechanically accurate force fields and interatomic potentials are fitted to electronic structure data and at first used techniques inspired by those used in machine learning and artificial intelligence research: neural networks, kernel regression, etc. It is a quickly moving field, and - having learned key lessons about representation, symmetry and regularisation - there appears to be some semblance of convergence between the diverse methods, which now also include polynomial expansions carried to high dimension.