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# Smart use of Density Functional Theory calculations to drive Newtonian dynamics

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We present a method for adaptively creating and sampling a database of density functional calculations in order to simulate large, complex atomistic systems at finite temperatures. The database consists of configurational/cluster-to-force maps and has a metric property via the Kabsch algorithm which we exploit in structuring the database for efficiency and accuracy. Details of the formulation including the correlation between local configuration size and force accuracy, will be discussed, as well as a number of practical applications of the method.

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