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Coding Considerations for Standalone Molecular Dynamics Simulations of Atomistic Structures

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Abstract : The laws of Newtonian mechanics allow ab-initio molecular dynamics to model and simulate particle trajectories in material science by defining a differentiable potential function. This paper discusses some considerations for the coding of ab-initio programs for simulation on a standalone computer and illustrates the approach by C language codes in the context of embedded metallic atoms in the face-centred cubic structure. The algorithms use velocity-time integration to determine particle parameter evolution for up to several thousands of particles in a thermodynamical ensemble. Such functions are reusable and can be placed in a redistributable header library file. While there are both commercial and free packages available, their heuristic nature prevents dissection. In addition, developing own codes has the obvious advantage of teaching techniques applicable to new problems.

Keywords : C language, molecular dynamics, simulation, embedded atom method
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