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Coding considerations for standalone molecular dynamics simulations of atomistic structures

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Abstract content
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While computational materials science has grown substantially, the bulk of research output still remains largely experimental, inevitably leaving the avenue of computation largely unexplored. 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 simulation 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 library header 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. This article is written from the experiential standpoint aimed at developing atomistic and molecular dynamics simulation toolkit development through which initial simulations may be undertaken by interested researchers. The programs codes presented here have been tested successfully on Microsoft C/C++ compiler (Windows 7) and \verb+gcc+ in Ubuntu Linux with little modification for various fcc metal parameters. The outputs compare favorably with published literature sources and confirm the applicability of the software.

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