Applying Many-Body Expansion aiming to make Ab Initio Molecular Dynamics more efficient

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In this present work we present a methodology that aims to apply the many-body expansion to decrease the computational cost of ab initio molecular dynamics, keeping acceptable accuracy on the results. We implemented this methodology in a program which we called ManBo.

In the many-body expansion approach, we partitioned the total energy E of the system in contributions of one body, two bodies, three bodies, etc., until the contribution of the Nth body [1-3]:

$E = E_1 + E_2 + E_3 + ...E_N$

The E_1 term is the sum of the internal energy of the molecules; the term E_2 is the energy due to interaction between all pairs of molecules; E_3 is the energy due to interaction between all trios of molecules; and so on. In Manbo we chose to truncate the expansion in the contribution of two or three bodies, both for the calculation of the energy and for the calculation of the atomic forces. In order to partially include the many-body interactions neglected when we truncate the expansion, we can include an electrostatic embedding in the electronic structure calculations, instead of considering the monomers, pairs and trios as isolated molecules in space.

In simulations we made we chose to simulate water molecules, and use the Gaussian 09 as external program to calculate the atomic forces and energy of the system, as well as reference program for analyzing the accuracy of the results obtained with the ManBo.

The results show that the use of the many-body expansion seems to be an interesting approach for reducing the still prohibitive computational cost of ab initio molecular dynamics. The errors introduced on atomic forces in applying such methodology are very small. The inclusion of an embedding electrostatic seems to be a good solution for improving the results with only a small increase in simulation time. As we increase the level of calculation, the simulation time of ManBo tends to largely decrease in relation to a conventional BOMD simulation of Gaussian, due to better scalability of the methodology presented.

References

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