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How much precision is not enough in the computer molecular simulations?

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Computer simulations are a basic and often the only available instrument, when studying the complex phenomena of molecular interactions and molecules formation in contemporary nano-scale biological sciences. Modern simulations incorporate complicated underlying mathematics, extraordinarily large numbers of engaged numerical values, extremely small time steps and really huge numbers of iterations. Besides, the systems under simulation are chaotic by nature.

These circumstances lead to an increasing necessity to reconsider the impact of computational precision on the simulation accuracy, particularly when the behavior of individual molecules and/or atoms is in the focus of attention. This is especially true in the cases of widely adopted simulation software packages, where the pursuit of performance gain and the robust statistical indicators, used to assess the validity of the result, as a rule, neglect the above impact. The explanation for such an attitude comes from the theoretical considerations about the so-called "computed chaos". It is assumed that distinct trajectories produced by running the same simulation on the same setup, but with different computational precisions are equally valid as long as they belong to the attractor of the simulated system.

This paper presents a thorough experimental study on whether neglecting the computational precision is appropriate in some special and important cases such as very long-term simulations or simulations of non-equilibrium processes. A well known molecular simulations software package has undergone a significant replacement of its standard floating-point arithmetic with an originally developed special one – a combination of infinite precision operations inside the computationally intensive kernels and specific rounding schemes outside them.

The results, obtained by run-time monitoring of the floating-point performance and posterior trajectory analysis, show cases of dramatic impact of precision on the final simulation outcome.