Journal	Computation (https://www.mdpi.com/journal/computation) (ISSN 2079-3197)
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Title	Accurate Sampling with Noisy Forces from Approximate Computing
Authors	Varadarajan Rengaraj , Michael Lass , Christian Plessl * , Thomas D Kuehne
Abstract	In scientific computing, the acceleration of atomistic computer simulations by means of custom hardware is finding ever growing application. A major limitation, however, is that the high efficiency in terms of performance and low power consumption entails the massive usage of low-precision computing units. Here, based on the approximate computing paradigm, we present an algorithmic method to rigorously compensate for numerical inaccuracies due to low-accuracy arithmetic operations, yet still obtaining exact expectation values using a properly modified Langevin-type equation.

Author's Reply to the Review Report (Reviewer 1)

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* Author's Notes to Reviewer

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English language and style	( ) Extensive editing of English language and style required ( ) Moderate English changes required (x) English language and style are fine/minor spell check required ( ) I don't feel qualified to judge about the English language and style

	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	(x)	( )	( )	( )
Are the results clearly presented?	(x)	( )	( )	( )
Are the conclusions supported by the results?	(x)	( )	( )	( )

Comments and Suggestions for Authors

The authors present a study on how to account for noise introduced by approximate force calculations due to low machine precision. In modern science, existing algorithms are often ported to accelerator devices such as GPUs and FPGAs, which on the one hand yields a much higher execution speed per unit of consumed energy (and money spent), but on the other hand often sacrifices the precision of the computations to some degree (e.g., single-precision floating point units in common GPUs). Therefore, the subject of the study is very important for the transition towards sustainable and energy-efficient computational sciences.

The article is well written, all methods used are sound, and the obtained results are clearly communicated. Therefore, I can recommend the publication of the manuscript in "Computation".

I only have a few suggestions which might improve the article:

(*) The Figures show that the computations with the newly developed methods almost yield the exact results, i.e., the random noise on the forces is indeed very well compensated for. However, I (and probably also many other readers) am wondering what the effect of this random noise would be if no compensation is active. I strongly recommend to add curves to the Figures (at least to Figure 1 and 2) where the simulation results with random noise and without any mitigation (i.e., standard time integration) are shown. Only then, it will be possible to see how much the newly developed approach actually improves the results.

(*) In general, I recommend to use SI units in scientific articles. While in some fields of science the use of certain non-SI units is very common, these units are rarely known in other fields of science, and a reader from such a field will struggle to correctly interpret the numbers. In the present manuscript, this concerns "Angstrom" and "eV". I recommend to replace these units by pm (or nm) and kJ/mol.

(*) In all four figures, it would be good to have insets which zoom in to "critical regions" (probably the first maximum/minimum in all four cases). With the current presentation style, it is hardly able to judge how much the approximative curves deviate from the correct result.

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