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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 2)

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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 manuscript entitled "Accurate Sampling with Noisy Forces from Approximate Computing" deals with the interesting and timely topic of using modern hardware efficiently in molecular simulations by decreasing the precision with which numbers are represented. The introduction is clear, well written and to the point. The writing in the rest of the manuscript is also good, with only a couple of small issues listed at the end of this report for the authors' reference. In my opinion, the manuscript can be published after some minor revisions.

My main issue is that it becomes only gradually clear that no approximate computation is actually performed in this work. Rather, forces that might be obtained from approximate computation are modelled in a specific way - by adding white noise. There is nothing wrong with that, but it should be made more clear earlier on. Even the title makes the reader expect actual approximate computing. Related to this, there is a larger assumption built into the whole thing that forces coming from approximate computing will, in fact, have the form of the exact forces plus white noise. This might very well be true, but it is a rather strong assumption and should be

discussed in more detail. If it is not valid in practice, this paper is very relevant to approximate computing. These two points should be addressed before the manuscript is published.

If the authors claim that even the tail of the Maxwell distribution comes out accurately from the noisy calculation, perhaps Figure 3 could be presented on logarithmic scale?

Additionally, here are some suggestions that would, in my opinion, improve the paper for the authors to consider. It would help clarity if the authors specified explicitly early in the paper that the approximate computing applies specifically to the calculation of forces. At the beginning of Section 2, it would be helpful to state that double precision is the most common standard for accurate numerical computation.

Typos to correct:
line 82: "a MD simulations"
line 102: "thitherto"

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