

Responses to Reviewer Comments for:
Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics [Article v1.0]

by

Edward J. Maginn, Richard A. Messerly, Daniel J. Carlson, Daniel R. Roe, J. Richard Elliott

Overview

We are pleased that the manuscript has passed the technical review stage. Having addressed each of the editorial issues detailed in this document, we believe that the revised manuscript is ready for publication in the *Living Journal of Computational Molecular Science*.

Itemized List of Changes to Manuscript (Page numbers refer to revised manuscript.)

Response to Editor, Comment 1: p 1
Response to Editor, Comment 2: p 2
Response to Editor, Comment 3: Figure captions
Response to Editor, Comment 4: Figure captions
Response to Editor, Comment 5: Figure 1, p 8
Response to Editor, Comment 6: Figure 2, p 9
Response to Editor, Comment 7: Figure 8, p 12
Response to Editor, Comment 8: p 5
Response to Editor, Comment 9: pp 9, 17
Response to Editor, Comment 10: Numerous instances
Response to Editor, Comment 11: p 18
Response to Editor, Comment 12: p 19
Response to Editor, Comment 13: pp 18-20
Response to Editor, Comment 14: p 18

Editorial Issues

Comment #1

The title should be in the form: (title) [Article v1.0]

Response #1

The title now reads, “Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics [Article v1.0]”

Comment #2

In the other resources section, in the introduction, put titles in italics in references, or otherwise set them apart, additionally, it probably makes sense to list just the name of person for class notes (I'm open to other suggestions).

Response #2

Titles are italicized, and we have removed the university from the class notes list.

Comment #3

Figures should have their first sentence rephrased as the conclusion that the figure shows, so that the point the figures make is self-contained. For example, in figure 5, Figure 5: rephrase the first sentence as a conclusion, such as "viscosity obtained with the Green-Kubo relationship is only weakly dependent on system size in the range studied".

Response #3

The first sentence has been rephrased for all figure captions.

Comment #4

Generally, the figures should be examined to ensure they are self-contained. In many cases, the figures refer to the paper the figure came from itself, which is acceptable for the data on how the figures are generated, but the meaning of the figures should be self-contained in the caption. Also, thanks for seeing out permission to use those figures.

Response #4

In addition to the specific changes recommended in comments 5-7, we have gone back through all the figure captions and made a few small changes to ensure they are self-contained. For example, we now discuss the inset for Figure 10, “The inset highlights the large long-time fluctuations.”

Comment #5

Figure 1: MD and YH not defined in caption.

Response #5

MD and YH are now defined as “molecular dynamics (MD)” and “Yeh-Hummer (YH)”.

Comment #6

Figure 2: This is a bit confusing, as the linear fits are to points that appear to be outside the graph. Red dotted line does not have a label. The notation E_{tors} is not explained.

Response #6

The following explanation is included for the red dotted line and E_{tors} :

The line colors correspond to different torsional energies (E_{tors}). The dash-dotted and solid red lines represent the same simulation results averaged over one and sixty time origins, respectively.

Comment #7

Figure 8: the inset is not described as such.

Response #7

We now describe the inset as, “The inset focuses on the short-time interval where the initial plateau is observed.”

Comment #8

Table 1: Variables (such as γ and ξ) should be explicitly define in the table, not just in the context.

Response #8

In addition to γ and ξ , Table 1 now defines t, r, v, V, T , and m .

Comment #9

Section 5.4 and 6.4: Suggest something more specific than “special topics”

Response #9

The section “Special topics” is intended to be a catch-all that is primarily serving as a placeholder for future versions. We anticipate that this section will be more expansive in future versions and, thus, a more specific name would be too restrictive. However, to improve the specificity of the current version, we have included subsections 5.4.1 and 6.4.1 with the respective headers, “Considerations for membrane systems” and “Considerations for cut-off length.”

Comment #10

ACS style guide says do not leave a space between a number and a percent; this happens a number of times in the article.

Response #10

We have removed the space between a number and a percent for all instances.

Comment #11

Acknowledgements should be updated to include anyone who has contributed (other than the author and the editors) to improve the paper.

Response #11

We now acknowledge the two NIST internal reviewers, “We are grateful for the internal review provided by Alta Y. Fang and Arno R. Laesecke of the National Institute of Standards and Technology (NIST).”

Comment #12

Reference 23 has an improperly formatted DOI.

Response #12

DOI has been fixed.

Comment #13

Preference is that citations are abbreviations, but the regardless style must be consistent; there are citations that are both abbreviations and full journal entries.

Response #13

We chose to use the full journal title, and have ensured that all citations are consistent with this style choice.

Comment #14

For references 14-17, see if there is a way to split the html without losing the link (check href package options?)

Response #14

The html is now split across two lines without losing the link.