Responses to Reviewer 2

Hello Cibran Lopez and IonRepo, here are my comments on your manuscript and code submitted to Journal of Open Source Software.

The motivation described in the manuscript for implementing this code is clear. Employing the k-means clustering method, this code is able to perform accurate analysis of the diffusion paths of the particles, particularly, a completely unsupervised analysis can be enabled for the ion-hopping problems. I think this implementation is important for high-throughput screening of fast-ion conductors since the diffusion issue is usually materials dependent, thus this code can be used to automate the analysis faster.

However, I found this code has not be well implemented yet, which prevented me from running the examples. Thus I'd like to invite the authors to complete the implementation so that we can test the examples and our own projects.

A: We thank the Reviewer for their careful and comprehensive reading of our work and for their very useful and insightful comments that have allowed us to significantly improve the readability of our article and the user-friendliness of our IonDiff software.

1 On the Manuscript

On line 32, I think it omitted "they" between "valuable" and "since"

A: We thank the Reviewer for having spotted this gramatical error. In the revised version of our manuscript, that sentence has been corrected.

Lines 88-89 claimed that the time cost of "self" and "distinct" were roughly the same. Could authors provide some benchmarks to evidence it? I feel it's surprising because the "distinct" part is associated to many particles correlation and should intuitively take more time than "self" part.

A: The time spent by the IonDiff software in computing the "self" and "distinct" parts of the ionic diffusion coefficient is roughly the same. Once every particle displacement is stored, estimating cross-particle terms only requires accessing the memory more frequently, rather than performing more windowing calculations. Since this is not the most important capability of the IonDiff software, we have not included any benchmark validation test in this regard, and the particular claim has been removed.

Authors are invited to compare their code to other commonly used code to demonstrate it's beyond the state of the art.

A: The most important feature of our implementation is the unsupervised and parameter-free identification of ionic diffusion events and many-ion diffusing correlations from molecular dynamics simulation data, which, to the best of our knowledge, has not been previously implemented in any other code. Consequently, comparisons with other codes are not possible in this regard. For consistency reasons, our previous claim that "the IonDiff implementation outperforms standard evaluation algorithms" has been removed in the revised version of our manuscript.

A separate section of "A statement of need" should be included in the paper to meet the requirement of JOSS.

A: We thank the Reviewer for having spotted this absence. A "Statement of need" section has been added to

the revised software paper (this was somehow embedded in the original Introduction section).

2 On Code Implementation

The 'sklearn' PyPI package is deprecated, use 'scikit-learn' rather than 'sklearn' for pip commands.

A: We thank the Reviewer for this advice, which has been very useful. In the revised version of our software documentation, this detail has been updated.

It seems that pip3 install -r requirements.txt doesn't really install the code because python3 cli.py identify_diffusion –MD_path examples failed. Thus, I cannot confirm the claimed functionality and the performance of the code.

A: We are sorry about this incident. Those execution lines have been tested to work in several different computers. However, in order to facilitate the execution and transferability of the IonDiff software, this has been added to PyPI, thus it can be installed via pip (see updated **README** file). Therefore, now IonDiff can be used both as a python library or a command-line tool (illustrated in the *examples* folder).

3 On Documentation

The documentation is not available for this code, which makes it user-unfriendly. However, it's required for the publication at JOSS. I suggest authors implement the documentation by creating html web-pages including the details about the installation, the license of the code, the execution of code and the basic tutorials.

A: The Reviewer is totally right. The documentation for the code's functionalities has been created through ReadTheDocs and now can be found in the GitHub site and PyPI (https://pypi.org/project/IonDiff/). As well, new Jupyter Notebooks tutorials have been added to the *examples* folder, better exemplifying the usage of the code.

Here, I also linked this GitHub issue to JOSS Review checklist (comment) so that the authors can track the status of this review report.

A: We thank the reviewer for their very useful and constructive comments, which have significantly improved the readability of our article and the user-friendliness of our IonDiff software.