Best Practice Guides

The inspiration for Best Practices documents can be found in the Atul Gawande article The Checklist, later expanded in his bestseller The Checklist Manifesto. The main goal of these documents is to reduce common errors by ensuring appropriate choices are made throughout a difficult task.

For our purposes, simulation checklists should help users avoid the most common reasons for failure or incorrect results. Checklists will typically also be accompanied by an explanation with sources, so the rest of the document can go into more detail on best practices and cover more possible failure modes and how to avoid them. One can divide the types of errors that are made performing molecular simulations into (a) mistakes experienced researchers often make, (b) mistakes new users often make, even after having received solid training in fundamentals of molecular simulation. Most checklists will be focused on these types of failures. A third type (c), would involve preventing mistakes of naive users who do not understand the basic principles of molecular simulation. These will usually require special documents aimed at novice users which serve as prerequisites for more detailed documents.

Review Criteria

- Would following the checklists help users avoid significant potential errors in simulation? Will the errors be profound and/or frequent?
- Are all assertions well sourced in published data (which may, in some cases, include data created for the document)?
- Are the explanations clear enough for researchers with only moderate training in simulation?

Living Reviews

Perpetual reviews, like standard reviews, except that they can be updated as information comes out, and can be responsive to community input, and remain up to date on the current state of the field as it evolves. An example of this process can be found at in Mobley et al. review, which was originally an "Annual Reviews in Biophysics" article, but is now being updated regularly.

Review Criteria

- Do the authors properly include information from the recent literature, such as from the last 6 to 12 months?
- Have the authors removed data that is out of date, and qualified information that has been disproven?

- Do the authors include data and viewpoints that are contradictory to their own?

Comparisons of molecular simulation programs

Simulation comparison papers describe attempts to perform the same calculation with a range of different simulation programs. Such comparison should be updated periodically with different versions of the same programs (or potentially additional programs).

Review Criteria

- Does the paper include developers or advanced users of all programs being compared to ensure that comparisons are fair?
- Are best practices being used in the simulation comparisons?

Tutorials

Tutorials are articles that come accompanied by web pages with walkthroughs and downloadable files to work with. These take users through specific tasks or sequences of tasks to help them learn how to do these tasks on their own for other applications or purposes. Tutorials should endeavor to not just cover the specific task at hand, but also highlight how the steps might need to be modified (or additional care might need to be taken at particular points) to handle more general cases. Tutorials for specific software packages must provide instructions and files for the current version of the software. The submission of existing tutorials, so long as they meet journal standards, is explicitly welcomed, to encourage the highest quality tutorials by providing some degree of academic credit for these important and time-consuming efforts.

Review Criteria

- Are files to run the simulations posted online in a permanent (or nearly so) way.
- Are the tutorials helpful and educational?
- Do they include enough information on how to generalize the approach to handle other cases, and highlight major issues to consider?