

Internal Feedback Round

- ☒ P1: "The Collection of all Forces acting on all atoms is called the Forcefield and forms the primary assumption of each MD simulation." The ForceField is the assumption that potential energy can be approximated by analytic functions with empirical parameters. Therefore, the quoted text is misleading.

No changes were applied. The collection of all terms and parameters is the collection of the potentials. The collection of the potentials is the collection of the forces ($F=dU/dr$). The introduction is intended to be brief and is not suitable for explaining concepts in detail.
- ☒ P2: Correction: Spelling error: effects -> affect.

Correction conducted.
- ☒ P2: "especially" appears to be excessive. "These limitations affect the physical realism of MD simulations, with the accurate treatment of protonation state fluctuations being a prominent problem in the study of biological systems. ..."

No changes were applied. Protonation is the most frequent reaction that occurs. Important for all processes, including those requiring chemistry. E.g., catalytic reactions often feature protonation/deprotonation of solvent molecules before catalysis.
- ☒ P7: No numbering on Fig 5.

Revision incorporated. Merged the subfigures into one figure and changed the caption.
- ☒ P7: First correction: Otherwise, A trajectory ... -> Otherwise, a trajectory.

Correction conducted.
- ☒ P8: "Assuming, N particles the motions governing particle movement [...]." Difficult to understand the meaning. Perhaps: "motions" -> laws or equations.

Revision incorporated. The sentence was indeed convoluted. Changed to: "Assuming N particles, the particle movement depends on the forces F on each particle and the potential energy function [...]"
- ☒ P8: Next sentence: "The potential energy function is also called the forcefield ..." - This might lead to confusion.

Revision incorporated. The two are equivalent terms as described above. I changed it to 'total potential energy function'.
- ☒ P8 (Also P16,23,27): GMX help link: if "documentation/2018" is switched to "current" it should point to the newest GMX documentation.

Revision incorporated. cmdline changed to <https://manual.gromacs.org/current/user-guide/cmdline.html>. manual changed to <https://manual.gromacs.org/current/reference-manual/index.html>. mdoptions changed to <https://manual.gromacs.org/current/user-guide/mdp-options.html>. gmx mdrun changed to <https://manual.gromacs.org/current/onlinehelp/gmx-mdrun.html>.
- ☒ P9: Table, First line: Missing a period after the sentence defining .tpr.

Revision incorporated.
- ☒ P33: Left side, under figure: separation line appears to be in code format.

Temporary fix applied. Cause unknown, but placing [H] after the \begin figure statement resolved the issue (no line at all). It might be advisable to try LiveCOMS new cls/bst file to determine if that resolves the issue. I suspect the bug may stem from the LiveCOMS setup.
- ☒ P25: MBAR method: Do we actually use MBAR here, as gmx bar presumably only uses BAR?

No changes were applied. BAR is a special case of MBAR, so technically by stating MBAR, BAR is included.
- ☒ AMBER, NAMD, etc. are mentioned, so they need to be cited.

Revision incorporated. Citations were at the end of the sentence. Now they are moved to the specific simulation software for clearer citation.
- ☒ Modeling "histidine" can be achieved with MD packages that have implemented constant pH simulations. Not strictly necessary to mention.

No changes were applied. I believe this provides excessive detail for a feature/phenomenon that is not important for the tutorial itself.
- ☒ Figure 44 is too small in the PDF. Make it single column.

Revision incorporated. Image is now a single-column figure.
- ☒ The Medium link to the SMILES tutorial does not work. Instead, I can access the blog via [...].

Revision incorporated. New link: <https://luis-vollmers.medium.com/tutorial-to-smiles-and-canonical-smiles-explained-with-examples-fbc8a46ca29f>.
- ☒ The right figure of Figure 48 is the zoomed-in view of the left instead of another docking result. Include this in the caption as well.

Revision incorporated.
- ☒ On page 54: "Therefore, it is recommended not to use mv rather than rm" -> I assume the "not" here is a typographical error?

Revision incorporated.
- ☒ Figures 54-57 use inconsistent color schemes. Distinguish different repeats but always use light blue for compound 0156 and orange for 1258.

Revision incorporated. I used the green/purple combination and employed different line/marker styles to distinguish runs. The result appears more professional.