An algorithm of embedding proteins into the membranes, which is now integrated into mdrun, comes from the paper of Wolf et al, J Comp Chem 31 (2010) 2169-2174. However, this algorithm of squeezing protein and growing it back in the membrane was proposed by us much earlier in 2007: S.O. Yesylevskyy, "ProtSqueeze: simple and effective automated tool for setting up membrane protein simulations", Journal of chemical information and modeling 47 (5), 1986-1994. The paper of Wolf gives no credit to our work, while the algorithm is essentially the same. I already sent a request to the authors of Wolf's paper concerning possible violation of scientific ethics in this case. Taking into account wide spread of this methodology provided by Gromacs, the question of priority becomes sensible. The manual should mention both works. Our work should be mentioned as the first publication of "squeezing-growing" algorithm. The works of Wolf should be mentioned as an implementation of this algorithm, which is used in mdrun.

Associated revisions
Revision ea690000 - 06/07/2016 03:40 PM - Semen Yesylevskyy
Added manual section about embedding proteins to membranes.

Fixes #1932
Change-Id: i0511576f06be35f1727a22c0d1e5f655f1ae06d

History
#1 - 03/29/2016 04:24 PM - Semen Yesylevskyy
The authors of Wolf's paper agree to put a reference to my paper to the documentation of g_membed and confirm that they just missed our work at the time of implementing their g_membed code.

#2 - 03/30/2016 04:20 PM - Erik Lindahl
- Tracker changed from Bug to Feature
- Subject changed from Incorrect citations for the membrane protein embedding algorithm to More citations for membrane protein embedding algorithms
- Category set to documentation
- Status changed from New to In Progress
- Priority changed from Normal to Low

Hi Semen!

Great to hear that it appears to be resolved already. The policy we try to follow for the citations printed to the log file is that we provide a reference to a paper describing the actual implementation in GROMACS, so an interested user can learn more about the choices, and hopefully that paper in turn cites other work. This provides an incentive to actually contribute and integrate concrete code, although it's a bit of a trade-off since we don't have a chance to act like judges about the relative importance of prior work inside the log file. Sadly, it has probably happened to all of us that we miss to cite some important prior work in a paper.

From my point of view, the best option in cases like this is to contribute e.g. to the LaTeX manual and write an expanded section describing what the
algorithms do in detail, with proper citations to both the history, the first papers describing the algorithms, as well as the GROMACS implementation(s).

Dear Erik,

I will be happy to contribute such section to the manual. Does it make sense for me to register as a developer and make a commit or it is better just to send you the text? I'm not familiar with LaTeX, so the later would be probably more efficient.

Upload a patch to gerrit.gromacs.org, and it will undergo peer review. This will likely take a while since people are very busy with the upcoming release right now, but it will eventually get in (and the more receptive authors are to comments, the quicker it usually is).

Sending me stuff directly is pretty much guaranteed failure since I try to focus my attention on stuff only I can do, so it will get buried in the other 200+ emails I get per day, and then nothing happens :-)