

GROMACS - Feature #1932

More citations for membrane protein embedding algorithms

03/29/2016 02:33 PM - Semen Yesylevskyy

Status:	Closed
Priority:	Low
Assignee:	
Category:	documentation
Target version:	2016
Difficulty:	uncategorized
Description	
<p>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.</p> <p>However, this algorithm of squeezing protein and growing it back in the membrane was proposed by us much earlier in 2007:</p> <p><i>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.</i></p> <p>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.</p> <p>Taking into account wide spread of this methodology provided by Gromacs, the question of priority becomes sensible.</p> <p>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.</p>	

Associated revisions

Revision ea690f00 - 06/07/2016 03:40 PM - Semen Yesylevskyy

Added manual section about embedding proteins to membranes.

Very short paragraph referencing needed papers and linking to user guide for details.

Fixes #1932

Change-Id: I0511576f06be35f1727a22c0d1e5f6552f1ae06d

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 logfile is that 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 logfile. 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).

#3 - 03/30/2016 08:28 PM - Semen Yesylevskyy

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.

#4 - 03/31/2016 08:05 PM - Erik Lindahl

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 :-)

#5 - 03/31/2016 08:06 PM - Gerrit Groenhof

Hi Semen,

As agreed, we have submitted a corrigendum to the JCC paper. I should get the proofs soon.

On topic: There seems to be no manual entry for `membed` option yet. The question is do we want to have one? if yes, then obviously with a reference to Semen's prior work too.

#6 - 04/01/2016 02:11 PM - Semen Yesylevskyy

Hi Gerrit,

As far as I understand there is no separate `g_membed` in gromacs =>5.1.2. There is an option in `mdrun` which is currently documented as this:

"The option `-membed` does what used to be `g_membed`, i.e. embed a protein into a membrane. The data file should contain the options that where passed to `g_membed` before. The `-mn` and `-mp` both apply to this as well."

There is also a description here: <http://manual.gromacs.org/documentation/5.1.2/user-guide/mdrun-features.html>

I propose to add both references to the later page and add a link to this page to the `mdrun` help message (which is rather puzzling for unaware user otherwise).

I think it worse describing the method briefly in the manual. "Special topics" seems to be a right place.

#7 - 04/01/2016 03:13 PM - Semen Yesylevskyy

I've committed a patch for user guide. I hope that I understand correctly how it works.

Concerning changes in the manual - should I commit to master branch or to the manual branch?

#8 - 04/02/2016 10:51 AM - Semen Yesylevskyy

I also made a patch to the manual with very brief section, which cites both papers. However my knowledge of LaTeX is almost zero and I can't understand why it doesn't compile. I would appreciate if somebody will review this commit.

#9 - 04/03/2016 06:59 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#1932](#).

Uploader: Semen Yesylevskyy (yesint4@yahoo.com)

Change-Id: I0511576f06be35f1727a22c0d1e5f6552f1ae06d

Gerrit URL: <https://gerrit.gromacs.org/5764>

#10 - 06/07/2016 04:07 PM - Semen Yesylevskyy

- Status changed from *In Progress* to *Resolved*

Applied in changeset [ea690f00d05614bc5673cf113166808f686b8584](#).

#11 - 06/23/2016 11:11 AM - Mark Abraham

- Status changed from *Resolved* to *Closed*

- Target version set to 2016