

## GROMACS - Task #2658

### Secondary structure assignment via DSSP as native gromacs code

10/01/2018 09:54 AM - Christian Blau

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	Christian Blau
<b>Category:</b>	analysis tools
<b>Target version:</b>	future
<b>Difficulty:</b>	simple
<b>Description</b>	
<p>The GROMACS do_dssp analysis tool enables secondary structure analysis over a trajectory.</p> <p>The tool, however depends on a call to the externally to be installed dssp tool, which is maintained here:</p> <p><a href="https://github.com/cmbi/xssp">https://github.com/cmbi/xssp</a></p> <p>User regularly complained about the challenge to get dssp set up correctly, and the main branch is currently broken from Ubuntu 18.04.</p> <p>The current do_dssp implementation calls dssp and writes and parses back a dssp output file for every trajectory frame.</p> <p>A GROMACS native dssp implementation will</p> <ul style="list-style-type: none"><li>greatly facilitate use of secondary structure assignment for trajectories, because it ships "out of the box" * speed up the analysis too, because no writing and reading of temporary files is needed * is a requirement for driving simulations to secondary structure targets, with a secondary structure assignment that can run in simulation time</li></ul> <p>The current xssp suite that includes dssp has a boost license that should allow the modification of their code for our purposes, however, okay from the software maintainers is still pending.</p>	

#### History

##### #1 - 10/01/2018 09:58 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '2' for Issue [#2658](#).  
Uploader: Christian Blau ([cblau@gwdg.de](mailto:cblau@gwdg.de))  
Change-Id: gromacs~master~la7b7bea83a6f82e2d38d1dcf1bd316516001b029  
Gerrit URL: <https://gerrit.gromacs.org/8458>

##### #2 - 10/09/2018 03:20 PM - Alexey Shvetsov

Hi!

Does someone already working on native dssp code?

##### #3 - 10/09/2018 04:23 PM - Mark Abraham

Yes, Christian has a draft of an import of xssp. If you're interested to collaborate, I'm sure he'd consider tagging you on gerrit.

##### #4 - 10/09/2018 04:51 PM - Christian Blau

Mark Abraham wrote:

Yes, Christian has a draft of an import of xssp. If you're interested to collaborate, I'm sure he'd consider tagging you on gerrit.

Tagged Alexey Shvetsov in gerrit draft.