

## GROMACS - Feature #921

### Default index groups and selections

04/15/2012 08:07 PM - Teemu Murtola

<b>Status:</b>	Blocked, need info	
<b>Priority:</b>	Normal	
<b>Assignee:</b>		
<b>Category:</b>	selections	
<b>Target version:</b>		
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
<p>When the selection code was originally integrated into Gromacs, Berk expressed a wish that it would not use hard-coded default index groups like Gromacs currently uses. So I implemented a mechanism where the default index groups for selections are created from a defselections.dat file: selections in this file are parsed, and an index group is generated from each selection that evaluates to a non-zero number of atoms. I believe that the default index group generation code has been updated since, but the defselections.dat file has not. It would be best to unify the handling of the default groups for 5.0.</p> <p>Questions to address:</p> <ul style="list-style-type: none"><li>• Is the defselections.dat the way to go forward for selections?</li><li>• Is something extra needed, e.g., in the form of selection methods, to express the current default groups as selections? Note that groups based on residue names do not need to be generated as it is trivial to select them using selections. Also note that regex-based selections (which the current defselections.dat uses) are not currently easily available on Windows.</li><li>• Should all default index group generation code be replaced with this approach? This requires some handling for the residue name based groups.</li><li>• It could also be possible to take variables declared in defselections.dat and make those available to user selections, e.g., to allow defining a "protein" keyword by simply adding such a variable to this file. This requires some implementation work, but should be doable.</li></ul>		
<b>Related issues:</b>		
Related to GROMACS - Task #1323: determine future of existing tools for		<b>New</b>

### Associated revisions

#### Revision 30ceea84 - 12/30/2013 03:29 PM - Teemu Murtola

Initialize default index groups for C++ tools

If an index file is not explicitly provided, initialize default index groups using the old analyse() method for the new C++ tools. This is better than nothing, and keeps the default groups in sync.

Also some clean-up for related code in TrajectoryAnalysisCommandLineRunner.

Temporary fix for #921.

Change-Id: I4f9d2586a0446302ce0a2d9326d2fd4c85b02ef0

### History

#### #1 - 04/26/2013 05:48 AM - Teemu Murtola

- Status changed from New to Accepted

#### #2 - 04/26/2013 05:48 AM - Teemu Murtola

- Status changed from Accepted to In Progress

Nothing is done, working around the workflow limitation to get this into blocked state.

#### #3 - 04/26/2013 05:48 AM - Teemu Murtola

- Status changed from In Progress to Blocked, need info

**#4 - 12/25/2013 07:53 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#921](#).  
Uploader: Teemu Murtola ([teemu.murtola@gmail.com](mailto:teemu.murtola@gmail.com))  
Change-Id: I4f9d2586a0446302ce0a2d9326d2fd4c85b02ef0  
Gerrit URL: <https://gerrit.gromacs.org/2934>

**#5 - 01/01/2014 06:54 AM - Teemu Murtola**

- *Tracker changed from Task to Feature*
- *Project changed from Next-generation analysis tools to GROMACS*
- *Subject changed from Default index groups and selections in 5.0 to Default index groups and selections*
- *Category set to selections*
- *Target version changed from 5.0 to 5.x*

No comments in more than a year; nothing is going to happen for the foreseeable future. For now, changed things such that the default index groups are initialized using the old analyse() method also for the selection-enabled tools.

**#6 - 07/11/2016 08:27 PM - Mark Abraham**

- *Target version deleted (5.x)*