GROMACS - Task #1805

Difficult to find gmx select documentation

08/13/2015 12:21 PM - Viveca Lindahl

Status:	Closed	
Priority:	Normal	
Assignee:	Viveca Lindahl	
Category:	selections	
Target version:	5.1.2	
Difficulty:	uncategorized	

Description
I find it difficult to find the gmx select syntax. I end up googling it and wind up here: http://www.gromacs.org/Documentation/Gromacs_Utilities/g_select where I read that

g_select -select 'help all'

should give me the docs. On my (master-based) gmx doing

gmx select -select 'help all'

gives a syntax error.

To get to the docs I need a tpr and do 'gmx select -s topol.tpr' and then 'help' and then e.g.'help syntax'. It would be much better if 1) I get info about how to reach the docs directly from 'gmx select -h' and 2) if I can go through the docs without providing any input. |

Associated revisions

Revision b8019378 - 08/13/2015 02:01 PM - Mark Abraham

Make it easier to find selection help

Fixes #1805

Change-Id: Ie09baa75601f6ba3e8e514f78e3bae34e7327f86

Revision c99cdd50 - 08/13/2015 05:17 PM - Mark Abraham

Make it easier to find selection help

Now the command-line reference part of the user guide has a TOC entry
that has the magic work "selection" in it.

Fixes #1805

Change-Id: Ib99840ab1f3fd72a52f28ffa1e06ee1242fa4310

History

#1 - 08/13/2015 01:51 PM - Justin Lemkul

The "problem" (if it can be called that) is that the selection mechanism is gradually being introduced into multiple tools; the help info is no longer unique to gmx select, which in old versions as g_select, was the only tool that used the selection syntax. Now, others (e.g. gmx distance) use it, too. So what you want is

```
gmx help selections
```

which can then be used to find syntax, examples, etc. Much of the information on the wiki is getting outdated, and I haven't had time to keep up with that as I once did, but of course others can add to it with new information that they learn :)

#2 - 08/13/2015 01:54 PM - Mark Abraham

gmx help selections is the new magic thing. Let me see if I can make this easier in both 5.0 and 5.1 branches

#3 - 08/13/2015 01:59 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1805.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: Ie09baa75601f6ba3e8e514f78e3bae34e7327f86
Gerrit URL: https://gerrit.gromacs.org/4990

#4 - 08/13/2015 02:10 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1805.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Ib99840ab1f3fd72a52f28ffa1e06ee1242fa4310
Gerrit URL: https://gerrit.gromacs.org/4991

#5 - 08/13/2015 02:10 PM - Teemu Murtola

Note that in 5.1, you can just read all the information that is available in the selection help directly from the user guide.

#6 - 08/13/2015 04:21 PM - Mark Abraham

Teemu Murtola wrote:

> Note that in 5.1, you can just read all the information that is available in the selection help directly from the user guide.

Indeed, although 4991 makes it easier to find it in the TOC

#7 - 08/13/2015 05:31 PM - Mark Abraham

- Status changed from New to Resolved

- % Done changed from 0 to 100

Applied in changeset b80193784dd4ac929f18c30031a91141e650baa9.

#8 - 01/12/2016 08:29 PM - Teemu Murtola

- Status changed from Resolved to Closed

- Target version set to 5.1.2