

GROMACS - Bug #1071

segfault in grompp with pulling and free-energy (if foreign_lambda empty)

12/12/2012 02:05 PM - Anonymous

Status: Closed	
Priority: Normal	
Assignee: Michael Shirts	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 4.6	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
With pulling and free_energy=yes, grompp gives as segfault if mdp option foreign_lambda is empty. If foreign_lambda = 0 (for example), no error occurs. Because foreign_lambda is empty by default, this error is likely to occur.	

Associated revisions

Revision 99faecfa - 12/14/2012 05:38 PM - Michael Shirts

Fixes redmine issue #1071

Fixes issue where pull code can crash grompp if foreign_lambda is not defined in the mdp. Some simplification of code path for initialization of lambda as a side product.

Change-Id: I6c6a0c1591cc332efddb769f3552c0379e7dc708

Revision 60790b19 - 12/19/2012 12:22 AM - Christoph Junghans

Merge "Fixes redmine issue #1071" into release-4-6

History

#1 - 12/12/2012 09:38 PM - Anonymous

Please use

```
grompp -p topol000 -n index000 -c umb_start000.pdb -f lambda
```

With

```
foreign_lambda = 0
```

the segfault disappears.

#2 - 12/12/2012 09:50 PM - Anonymous

- File error.tar.bz2 added

#3 - 12/29/2012 08:40 PM - Erik Lindahl

- Status changed from New to Closed

Merged into git 11 days ago. Jochen: Please reopen if it is not working.

Files

error.tar.bz2	2.54 MB	12/12/2012	Anonymous
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