Hi,

When applying the dihedral_restraints option in my topology file, it yields a grompp fatal error.

Topology insertion (after [dihedrals]):

```plaintext
; Include forcefield parameters
#include "./chalc.ff/forcefield.itp"

[moleculetype ]
; Name nrexcl
1PE 3

[ atoms ]
...
[ bonds ]
...
[ dihedral_restraints ]
; ai aj ak al phi dphi kfac
5 1 2 3 90 0 1
```

Error:

Fatal error:
Incorrect number of parameters - found 2, expected 3 or 6 for Dih. Rest..

I have also tried the insertion with 6 parameters, but grompp just finds 5.
Change-Id: I356e14541d4aaffad054d5ecfb8a9e3cb04cd25f

History

#1 - 03/20/2017 07:14 PM - Marcelo Depolo Poleto
The right insertion is below:

```
[ dihedral_restraints ]
; ai aj ak al phi dphi kfac
5 1 2 3 90 0 1
```

#2 - 03/21/2017 11:00 AM - Mark Abraham
- Description updated

#3 - 03/21/2017 11:09 AM - Mark Abraham
- Status changed from New to Feedback wanted
- Target version set to 2016.4

I think this input is ill-formed. The following snippet from our regression tests works:

```
[ dihedral_restraints ]
; i j k l type phiA dphiA kfacA phiB dphiB kfacB
1410 1393 1391 2610 1 38 0 0.00 38 0 41.84
1393 1391 2610 2604 1 111 0 0.00 111 0 41.84
1391 2610 2604 2606 1 -39 0 0.00 -39 0 41.84
```

The type column is required, even though only one function type is currently implemented. With your input, grompp is interpreting 90 as the function type and then being unable to find all 3 of phi, dphi and kfac, nor two such sets of 3 for a dual-topology setup.

#4 - 03/21/2017 11:25 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2144.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~Iac28e88e966f1c2b7a8e533e97abe94173470eb
Gerrit URL: https://gerrit.gromacs.org/6534

#5 - 03/21/2017 02:19 PM - Marcelo Depolo Poleto
What is the use for two dihedral restraints (A and B)?

The error message is also confusing: it says it expects 3 or 6 parameters, but with TYPE required, they become 4 or 7 respectively.

#6 - 03/21/2017 07:52 PM - Mark Abraham
Marcelo Depolo Poleto wrote:

What is the use for two dihedral restraints (A and B)?

As I hinted, in a dual-topology setup used for free-energy calculations, the same .mdp describes two topologies for the same system. Even if the configurations don't change, you can simply change parameters (or e.g. morph one halide to another, etc.)

The error message is also confusing: it says it expects 3 or 6 parameters, but with TYPE required, they become 4 or 7 respectively.

Yeah I see how that could be confusing. The parameters are specific to the function type, though, which is consistent with the organization of Table 5.5 in the manual. I'll think about what might be improved in the error message

#7 - 09/12/2017 11:55 AM - Mark Abraham
- Target version changed from 2016.4 to 2016.5

#8 - 12/12/2017 12:26 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2144.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2018~I356e14541d4aaffad054d5ecfb8a9e3cb04cd25f
Gerrit URL: https://gerrit.gromacs.org/7334

02/20/2020
#9 - 12/12/2017 12:27 PM - Mark Abraham
- Status changed from Feedback wanted to Fix uploaded
- Target version changed from 2016.5 to 2018-beta3

I improved the error message

#10 - 12/12/2017 10:53 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#11 - 12/12/2017 10:53 PM - Erik Lindahl
- Status changed from Resolved to Closed