

## GROMACS - Bug #2392

### mdp field 'define' does not correctly handle inputs that used to work

01/23/2018 11:55 AM - Mark Abraham

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Mark Abraham	
<b>Category:</b> preprocessing (pdb2gmx,grompp)	
<b>Target version:</b> 2018.1	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018	

#### Description

As reported by Joshua Mitchell on gmx-users:

It seems that preprocessor variables can no longer be given values in the MDP as of GROMACS 2018? So in 2016 I could do

```
define = -DPOSRES -DPOSRESFC=500.0
```

and then in the posres ITP:

```
#ifndef POSRESFC
#define POSRESFC 1000.0
#endif
```

```
[ position_restraints ]
; atom type  fx  fy  fz
1  1 POSRESFC POSRESFC POSRESFC
4  1 POSRESFC POSRESFC POSRESFC
7  1 POSRESFC POSRESFC POSRESFC
....
```

And this would let me set the position restraint force constants from the MDP, which was very convenient. I'm pretty sure I got this trick from MARTINI so I'm not the only person who uses it. Frustratingly, in 2018 that little equal sign causes the whole MDP define line to be ignored, causing position restraints to fail silently. So I've spent all day trying to figure out why it looked like my position restraints aren't working!

I think this could trick a lot of people, especially newer users trying out MARTINI. Is the old behaviour coming back?

#### Associated revisions

##### Revision c5fe4494 - 02/26/2018 12:09 PM - Mark Abraham

Permit define .mdp field to assign values

It is intended that the "define" .mdp field can set preprocessor variables to values, but this got broken in some clean up. Added a test to cover it.

Fixes #2392

Change-Id: I16a3705a0d59a912a8eb7bfad0b472f12d2dc377

#### History

#1 - 01/23/2018 11:56 AM - Mark Abraham

I suspect this is related to whether the string intended to be passed to the preprocessor contains any '=' symbol. I did do some clean-up here since 2016 branch. There are some TODO items in the test coverage, IIRC.

**#2 - 02/19/2018 03:21 PM - Mark Abraham**

I'll try to work on this for 2018.1, but i have other things to tackle this week, first.

**#3 - 02/23/2018 12:03 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2392](#).

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Change-Id: gromacs~release-2018~116a3705a0d59a912a8eb7bfad0b472f12d2dc377

Gerrit URL: <https://gerrit.gromacs.org/7616>

**#4 - 02/23/2018 12:03 PM - Mark Abraham**

- Status changed from New to Fix uploaded

**#5 - 02/26/2018 02:15 PM - Mark Abraham**

- Status changed from Fix uploaded to Resolved

Applied in changeset [c5fe449463a24eb44843352b031fbc7515081532](#).

**#6 - 03/02/2018 03:52 PM - Mark Abraham**

- Status changed from Resolved to Closed