GROMACS - Bug #1893

grompp fails to warn about .mdp values with the wrong type

01/27/2016 03:16 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.1.2</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>at least 5 and 5.1</td>
</tr>
<tr>
<td>Affected version:</td>
<td>5.0</td>
</tr>
</tbody>
</table>

**Description**

For example,

```
init_lambda_values = 0.35
```

is silently interpreted as 0.

**Related issues:**

Related to GROMACS - Feature #1026: request for gen_vel to work with multiple... New

**Associated revisions**

**Revision 937fd932 - 01/27/2016 10:54 PM - Mark Abraham**

Make sc-power an integer like it needs to be

This means it can pass the new check.

Refs #1893

Change-Id: I652f383e5914a6475e1640ec8842b7b6cfc8f1d3

**Revision d0071abf - 02/03/2016 01:41 PM - Mark Abraham**

Fix grompp not warning when .mdp values have wrong types

With old code, e.g. `init_lambda_state = 0.35` was silently interpreted as 0.

Added some comments and TODOs.

Added unit tests for some simple parts of the functionality that needed to be fixed. Extended the interface of warninp_t to permit sound testing.

Fixes #1893

Change-Id: I425798daa8ed3a391cde49ba4a2d3d352d682f8f

**Revision fe436f74 - 02/02/2017 10:35 PM - Mark Abraham**

Clarify use of tau-p and pcoupltype

grompp used to permit "tau-p = 5 5" which is misleading. The recent fix for #1893 leads to the user receiving a grompp warning, so this improves the docs to make clear that pressure coupling is not implemented like temperature coupling (where different time constants might be used).

Refs #1893

Change-Id: I8328b30a12689795c7af2d12dfc94db11b78a03a

**History**
#1 - 01/27/2016 03:22 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1893.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: i425798daa8ed3a391cde49ba4a2a233d52d682f8f
Gerrit URL: https://gerrit.gromacs.org/5588

#2 - 01/27/2016 10:54 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1893.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: i652f383e5914a6475e1640ec8842b7bcf8f1d3
Gerrit URL: https://gerrit.gromacs.org/5590

#3 - 02/03/2016 01:45 PM - Mark Abraham
- Status changed from New to Resolved

Applied in changeset d0071abfbebdc0a14c184707actf09737f4c4c832.

#4 - 02/03/2016 01:50 PM - Mark Abraham
- Status changed from Resolved to Closed

#5 - 02/05/2016 06:57 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #1893.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: i8328b30a12689795c7af2d12dfc94db11b78a03a
Gerrit URL: https://gerrit.gromacs.org/5618

#6 - 11/17/2016 04:38 PM - Mark Abraham
- Related to Feature #1026: request for gen_vel to work with multiple temperature coupling groups at different temperatures added

#7 - 02/02/2017 10:35 PM - Gerrit Code Review Bot
Gerrit received a related patchset '3' for Issue #1893.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: gromacs~release-5-1~I8328b30a12689795c7af2d12dfc94db11b78a03a
Gerrit URL: https://gerrit.gromacs.org/5618