**GROMACS - Feature #1577**

**Extend flat-bottom position restraints**

08/15/2014 12:17 AM - Justin Lemkul

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Justin Lemkul</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.1</td>
</tr>
<tr>
<td>Difficulty:</td>
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**Description**

I received a request from another group to implement the cylindrical position restraints along x and y. The current code assumes the cylinder is aligned along z. The code changes should be fairly minimal, and this would be a useful feature as the planar geometry already allows for planes perpendicular to any axis.

**Associated revisions**

Revision cb466e44 - 09/10/2014 07:17 AM - Justin Lemkul

Added flat-bottom cylindrical restraints in x and y.

The code previously only allowed the long axis of the cylinder to be aligned along z. This patch allows the cylinder to be aligned along any axis.

Old topologies and .tpr files will still work for all geometries with g values from 2 to 5, as 2 is now just a synonym for a z-directional cylinder. The new values are g=6 for x, g=7 for y, and g=8 for z. The manual has been updated to reflect these changes.

Introduced a new static function that computes forces and energy for the flat-bottom restraint.

Refs #1577

Change-Id: l40e0bd35225170e13a18ee54f6798470e697f29d

**History**

#1 - 08/15/2014 01:15 AM - Gerrit Code Review Bot

Gerrit received a related patchset ‘1’ for Issue #1577.
Uploader: Justin Lemkul (jalemkul@vt.edu)
Change-Id: l40e0bd35225170e13a18ee54f6798470e697f29d
Gerrit URL: https://gerrit.gromacs.org/3894

#2 - 08/17/2014 01:17 AM - Justin Lemkul

- Status changed from New to In Progress

#3 - 06/16/2015 11:04 PM - Erik Lindahl

- Status changed from In Progress to Resolved

#4 - 06/16/2015 11:04 PM - Erik Lindahl

- Status changed from Resolved to Closed

#5 - 07/11/2016 07:46 PM - Mark Abraham

- Target version changed from 5.x to 5.1