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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<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.

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: I40e0bd35225170e13a18ee54f6798470e697f29d

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: I40e0bd35225170e13a18ee54f6798470e697f29d
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