GROMACS - Feature #2946
Enable AWH periodicity for pull-geometry=direction

05/09/2019 11:49 AM - Semen Yesylevskyy

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2019.3</td>
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<tr>
<td>Difficulty:</td>
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Description
Since "period" keyword is now removed from awh it is not clear for the user how to define the periodic awh coordinate. Intuitively one may try direction-periodic, but again, this geometry is now not supported. The grompp also reports nothing about detecting periodicity in awh coordinates, so it is absolutely obscure for the user what is going on under the hood.
I can't figure out myself how to enable periodicity and suspect that other users will encounter exactly the same problem.

Associated revisions

**Revision 11be00e4 - 06/11/2019 09:20 AM - Berk Hess**
Allow AWH geometry 'direction' to be periodic
When an AWH dimension with pull geometry 'direction' has an interval length (nearly) matching the periodic unit cell dimension, it is now made periodic.
Fixes #2946
Change-Id: 9a09b8eb7464e04bd3d7205934bceb590e531f5

**Revision 14daed33 - 11/26/2019 08:47 AM - Berk Hess**
Fix issues with AWH with periodic pulling
Removed fatal error with AWH with periodic pull-geometry 'direction' when the distance was within 2% of half the box size.
Changed an assertion failure when the AWH interval was larger than the box size to a fatal error.
Clarified the documentation for pull geometry 'direction-periodic'.
Refs #2946
Change-Id: 447a9a490a5883139aefc268fd367b28249591fbc

History

**#1 - 05/10/2019 09:52 AM - Semen Yesylevskyy**
Digging the source code shows that function get_pull_coord_period() deduces periodicity for direction-periodic geometry:

```c
if (pcrd_params->eGeom == epullgDIRPBC)...```
However, direction-periodic is now forbidden for awh, so this code is dead and will never be called.

**#2 - 05/10/2019 05:00 PM - Paul Bauer**
The code is only left in master because the changes from 2019 have not been merged in yet. In 2019 this code path has been removed already.

**#3 - 05/11/2019 10:42 AM - Semen Yesylevskyy**
Ok, but what about the question itself - how can the user define the periodic awh coordinate, say, across the simulated membrane? When doing umbrella sampling this is done by -cycl flag to gmx wham, but it is completely obscure how to achieve the same with awh.

**#4 - 05/13/2019 11:11 AM - Berk Hess**
The only AWH dimensions that are periodic are dihedrals. Maybe this should be added to the documentation.
But I don't know what you mean exactly with periodic. I would argue that pull geometry "direction-periodic" is "less periodic" than "direction", since it
unwraps the distance, "direction" is purely periodic. The distance for geometry "direction" is computed taking PBC into account, but AWH currently does not make such a coordinate periodic. I think AWH could actually do this. We should either have a check to disallow the AWH interval to be as large as the box or implement periodicity.

**#5 - 05/13/2019 12:37 PM - Semen Yesylevskyy**

Under periodicity I mean making start and end points of interval the same point in PMF computation (an equivalent of -cycl option of gmx wham). Direction-periodic allowed doing this accross the box in awh. Now this possibility is lost and this is a big omission in functionality. For example awh is now useless for lipid membranes where both sides of the membrane are the same medium (and one uses -cycl in gmx wham).

Thus my suggestion is to keep this possibility. Ideally it should be an option awh1-dim1-cycl which works exactly the same as -cycl flag for wham.

**#6 - 05/13/2019 01:02 PM - Berk Hess**

- Tracker changed from Bug to Feature
- Subject changed from Not clear how to define periodic awh coordinate to Enable AWH periodicity for pull-geometry=direction
- Affected version deleted (2019.2)

OK. But you are then asking for the same thing I suggested: make pull geometry "direction" periodic in AWH when needed. I will try to implement that. For a proper set up case this just means setting the period in the AWH code, but some checks might be needed to catch malformed setups.

**#7 - 05/13/2019 01:06 PM - Berk Hess**

One limitation is that you can't have pressure scaling for the periodic dimension.

**#8 - 05/13/2019 01:16 PM - Semen Yesylevskyy**

Is there a possibility to allow periodicity for arbitrary pull vectors (not aligned with one of the axes?). I'm not aware of internals of course, but spanning the whole box and only along one of the axes seems to be unnecessarily strict limitation. From the point of view of the user all methods of computing PMF (umbrella sampling-wham, awh) should be able to produce comparable results. In wham one can define any pull vector. It would be very nice to be able doing the same in awh.

**#9 - 05/13/2019 03:13 PM - Berk Hess**

- Category set to mdrun
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Target version set to 2019.3

I uploaded a fix that makes direction periodic when needed, please test.

**#10 - 05/14/2019 09:36 AM - Semen Yesylevskyy**

- File bug.zip added

It doesn't work for me. See attached example. The box size on Z is 10.9827 and awh range is (-6:6). In log file there is still no periodicity:

```plaintext
awh1-dim1:
   coord-provider   = pull
   coord-index      = 1
   start            = -6
   end              = 6
   period           = 0
```

I also tried exact value of 5.49135 - still no periodicity.

(tested with release-2019 branch from git)

**#11 - 05/14/2019 09:40 AM - Berk Hess**

You need to get the change from gerrit, e.g.:
git fetch "ssh://hess@gerrit.gromacs.org/gromacs" refs/changes/20/11020/5 && git checkout FETCH_HEAD

**#12 - 05/15/2019 09:02 AM - Semen Yesylevskyy**

Yes, it seems to work correctly now on my system.

**#13 - 06/11/2019 09:30 AM - Berk Hess**

- Status changed from Fix uploaded to Resolved
#14 - 06/11/2019 12:02 PM - Paul Bauer
- Status changed from Resolved to Closed

Files

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<td>2.02 MB</td>
<td>05/14/2019</td>
<td>Semen Yesylevskyy</td>
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