**GROMACS - Bug #3225**

**gmx angle tool erroneously calculate torsion angles (dihedrals) near 180 degrees boundary**

11/29/2019 07:49 PM - Boris Timofeev

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
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<tr>
<td>Assignee:</td>
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<tr>
<td>Category:</td>
<td>analysis tools</td>
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<tr>
<td>Target version:</td>
<td>2019.5</td>
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<td>Affected version - extra info:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>2016.6</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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**Description**

I found that gmx angle calculate torsion angles erroneously. This effect is particularly sharp near the 180 degree sign change boundary. For example, if the measured torsion angles are -179 and 179, then the correct average of the torsion angles must be 180 (or -180), but not an arithmetic average zero at all. The following workaround is proposed to solve this problem.

On each step we calculate the delta - an angle of rotation from one state to another in the range [-PI, PI]. One can generally sum the differences from the first point and calculate the average as the first point + (sum of differences)/N

When calculating the average value, the first angle is taken as the base value, and then at each sum accumulation step we take the delta of the current and basic value given to range [-PI, PI]. This delta is added to the base value. The base value is updated and added to the middle integrator.

On the example of [-179, 179] degrees:
- Base: -179;
- Delta = 179 - (-179) = 358;
- => in range [-PI, PI]: Delta = 2
- Second point = Base + Delta = -179 + (2) = -181
- Sum = -179 + -181 = -360
- Base = -181;
- Average = (-360/2) = -180.
- The average given to range [-PI, PI] = 180

On example [-1, 1] degrees:
- Base: -1;
- Delta = 1 - (-1) = 2;
- => in range [-PI, PI]: Delta = 2
- Second point = Base + Delta = -1 + 2 = 1
- Sum = -1 + 1 = 0
- Base = 1
- etc.
- Average = 0/2 = 0.

**Associated revisions**

Revision 63a8c475 - 12/16/2019 10:30 AM - Paul Bauer
Fix torsion angle calculation
Fix originally contributed by Boris Timofeev.

Fixes #3225

Change-Id: l4862679e4aae514736df530ef44bf3b85928

Revision 511d9576 - 12/17/2019 09:56 AM - Paul Bauer
Fix formatting error
Fix originally proposed by Boris Timofeev.

02/22/2020
More precisely, the error is not in calculating torsion angles, but in calculating their average.

please check out https://gerrit.gromacs.org/c/gromacs/+/14661

It's ok, as I see

Boris, Can you please try running the fixed version to confirm that it works? Thanks!

file 6gmy.pdb, chain A, for all models (1-10), for index preparation see #3206

DATASET
H2_C2_N3_C4
178.717 -179.92 178.643 178.034 178.979 178.137 178.662 177.061 178.342 179.86

Before patch
Select a group: Selected 212: 'H2_C2_N3_C4'
Reading frame  0 time  0.000   '', 701 atoms
Reading frame  9 time  0.000   WARNING: all CONECT records are ignored
Last frame      9 time  0.000
Found points in the range from 356 to 359 (max 360)
< angle > = 142.651
< angle^2 > = 31911.3
Std. Dev. = 107.526
Order parameter S^2 = 0.999753

After patch
Select a group: Selected 212: 'H2_C2_N3_C4'
Reading frame  0 time  0.000   '', 701 atoms
Reading frame  9 time  0.000   WARNING: all CONECT records are ignored
Last frame      9 time  0.000
Found points in the range from 356 to 359 (max 360)
< angle > = 178.651
< angle^2 > = 31917
Std. Dev. = 0.829602
Order parameter S^2 = 0.999753

Now it's work fine.

And please correct the typo originating from migration from char * to std::string in pdbio.cpp:

02/22/2020
#9 - 12/20/2019 11:25 AM - Paul Bauer

- **Status changed from Resolved to Closed**

## Files

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<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
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<td>anadih.patch</td>
<td>6.17 KB</td>
<td>11/29/2019</td>
<td>Boris Timofeev</td>
</tr>
<tr>
<td>pdbio.patch</td>
<td>890 Bytes</td>
<td>12/10/2019</td>
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