## GROMACS - Bug #2489

### Handle mdp-option case "awh-nsamples-update = 0"

04/25/2018 02:34 PM - Viveca Lindahl

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Viveca Lindahl</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018.2</td>
</tr>
<tr>
<td>Affected version</td>
<td>2018.1</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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</table>

**Description**

Setting "awh-nsamples-update = 0" is accepted by grompp but leads to a floating point exception because the variable is later (in mdrun) used in a modulo operator.

**Associated revisions**

Revision cb1ac9a9 - 06/06/2018 12:51 PM - Viveca Lindahl

Make sure that the value of awh-nsamples-update is allowed

Previously, awh-nsamples-update could be set to zero, leading to division by zero. Now it results in a fatal error.

Fixes #2489

Change-Id: l65aae5d5c533b9aab7ea9aee3e317e92a926c18c

**History**

### #1 - 04/25/2018 04:04 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2489.
Uploader: Viveca Lindahl (vivecalindahl@gmail.com)
Change-Id: gromacs~master~I23dbc80992e130a28af413754d12f8fd167e7bde
Gerrit URL: [https://gerrit.gromacs.org/7794](https://gerrit.gromacs.org/7794)

### #2 - 06/05/2018 10:55 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2489.
Uploader: Viveca Lindahl (vivecalindahl@gmail.com)
Change-Id: gromacs~release-2018~I65aae5d5c533b9aab7ea9aee3e317e92a926c18c
Gerrit URL: [https://gerrit.gromacs.org/7980](https://gerrit.gromacs.org/7980)

### #3 - 06/05/2018 11:03 PM - Viveca Lindahl

- Status changed from New to Fix uploaded

### #4 - 06/06/2018 01:00 PM - Anonymous

- Status changed from Fix uploaded to Resolved

Applied in changeset cb1ac9a9b43a4d9468d3019882d2f279281ce82ca5.

### #5 - 06/07/2018 01:50 AM - Mark Abraham

- Status changed from Resolved to Closed