Gromacs - Bug #1507
Support large systems with TNG
05/22/2014 08:39 AM - Roland Schulz

<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>Magnus Lundborg</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
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<tr>
<td>Target version:</td>
<td>5.0</td>
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<tr>
<td>Affected version</td>
<td>5.0</td>
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<td>extra info:</td>
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**Description**
Currently TNG is prohibitive slow for very large systems. I gave up waiting after ~10min to write a file for a system containing 2M atoms. The problem is that several functions search large tables for every atom in the system. E.g. tng_chain_residue_find (O(N^2), N: residues) or tng_residue_atom_w_id_add (O(NM) N: total number of atoms, M: atoms per residue). It seems, TNG needs to be profiled for a large system, and those searches need to be replaced with hash-table lookups.

**Associated revisions**
Revision 4aa9a806 - 06/24/2014 09:25 PM - Magnus Lundborg
Improved check to decide if to add chain/residue.
Together with the latest TNG library updates this fixes #1507
Change-Id: lea7160cc1194fc398f9c4db0cc66f4bd43ce724a

**History**
#1 - 05/22/2014 08:49 AM - Rossen Apostolov
There was a bug causing that and it was fixed in 1d33dec1ff75, release-5-0.

#2 - 05/22/2014 08:49 AM - Rossen Apostolov
- Status changed from New to Feedback wanted

#3 - 05/22/2014 09:05 AM - Roland Schulz
I tested with recent master which already included this fix.

#4 - 05/22/2014 09:57 AM - Rossen Apostolov
can you send me your inputs? because I've tried with the lignocellulose 3.3M and it seemed to work fine

#5 - 06/05/2014 11:35 AM - Rossen Apostolov
Can you send/upload a test case to check?

#6 - 06/17/2014 12:35 PM - Rossen Apostolov
- Status changed from Feedback wanted to Accepted

#7 - 06/19/2014 10:57 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1507.
Uploader: Magnus Lundborg (magnus.lundborg@sciifelab.se)
Change-Id: lea7160cc1194fc398f9c4db0cc66f4bd43ce724a
Gerrit URL: https://gerrit.gromacs.org/3625

#8 - 06/19/2014 11:14 PM - Erik Lindahl
- Target version set to 5.x

#9 - 06/20/2014 04:45 PM - Erik Lindahl
- Status changed from Accepted to Fix uploaded

#10 - 06/24/2014 09:58 PM - Magnus Lundborg
- Status changed from Fix uploaded to Resolved

#11 - 06/26/2014 10:15 PM - Erik Lindahl
- Status changed from Resolved to Closed

#12 - 07/15/2014 06:48 AM - Teemu Murtola
- Tracker changed from Feature to Bug
- Category set to core library
- Target version changed from 5.x to 5.0
- Affected version set to 5.0