Gromacs - Bug #1004

Memory leaks in trajectory I/O proportional to size of the trajectory
09/13/2012 05:25 AM - Teemu Murtola

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.5.6</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>4.5-4.5.5</td>
</tr>
</tbody>
</table>

**Description**

In several text-based trajectory I/O routines, there are memory leaks that are proportional to the number of frames read/written (as well as to the number of unique strings in the file). At least some of these have been introduced when static variables have been changed to non-static (previously, the memory was allocated only once and referenced from the static variable until the program ended). For reading, the common problem is that symtab.h is used to store the strings read, and it is typically allocated anew and initialized for each frame. Need to still analyze whether this is possible to fix without reintroducing global variables or large changes in the trajectory I/O calls.

For PDB writing, there is a separate problem: residuetypes.dat is read and parsed each time a PDB frame is written to output, and the memory used for this is leaked. The memory leak should be straightforward to fix, but we really should not do the read/parse operation more than once, which requires more changes...

Found in https://gerrit.gromacs.org/#/c/1427/, where reading of .gro files and writing of .pdb files cause these leaks; other text-based formats are probably also affected.

**Associated revisions**

Revision 3b8e1cd9 - 09/13/2012 06:52 AM - Teemu Murtola
Fix some memory leaks.
Fixes part of #1004.
Change-Id: i22280999c5c3c40e8efae45461bd53bae8e2ff40

Revision 3b8e1cd9 - 09/13/2012 06:52 AM - Teemu Murtola
Fix some memory leaks.
Fixes part of #1004.
Change-Id: i22280999c5c3c40e8efae45461bd53bae8e2ff40

Revision ad406a3a - 09/16/2012 08:43 PM - Teemu Murtola
Fix insolidangle selections near poles.
- Correctly treat cases where a point is so close the one of the poles that it completely covers one or more bins in the zenith angle direction.
- Adjust update_surface_bin() to be more robust to rounding errors and easier to understand by simplifying the code used for wrapping angles to [-pi, pi] interval. Problems were triggered here by the first change.
- Update comments.
Fixes #1004.

Change-Id: i2707f775793fabb64ea197bd85bfe68d6a933

Revision ad406a3a - 09/16/2012 08:43 PM - Teemu Murtola

Fix insolidangle selections near poles.
- Correctly treat cases where a point is so close the one of the poles that it completely covers one or more bins in the zenith angle direction.
- Adjust update_surface_bin() to be more robust to rounding errors and easier to understand by simplifying the code used for wrapping angles to [-pi, pi] interval. Problems were triggered here by the first change.
- Update comments.

Fixes #1004.
Change-Id: i2707f775793fabb64ea197bd85bfe68d6a933

History

#1 - 09/16/2012 12:27 PM - Teemu Murtola
The linked 3b8e1cd9 fixes the mentioned memory leaks in .gro reading and .pdb writing for 4.5.6. Other formats should also be checked.

#2 - 09/18/2012 12:46 PM - Teemu Murtola
Went through the occurrences of t_symtab in the source. Based on reviewing the code, both .g96 and .pdb formats suffer from the same problem: when reading a trajectory in either of these formats, t_symtab is initialized anew on each frame in read_g96_conf() and read_pdbfile(), and is never freed. There are only a few calls to these functions, all from confio.c, pdbio.c or trxio.c, so it should be possible to fix this without affecting a lot of code. It is not possible to fix this without changing the interface to these functions, but previous fixes to read_g96_conf() have already changed the signature from 4.5.5, so user code will anyways be affected.

There are also smaller memory leaks for other formats in read_stx_conf() (also related t_symtab not being freed), but that should typically occur only once in a program, so it's not worth fixing before 5.0. In particular because it would require quite large changes, since read_stx_conf() is used quite a lot.

#3 - 09/18/2012 01:46 PM - Teemu Murtola
- Status changed from New to Closed
- Assignee set to Teemu Murtola
- Target version set to 4.5.6
- Affected version - extra info changed from 4.5 and later to 4.5.4-5.5

Actually, the .g96 and .pdb trajectory reading does work, but the code is so convoluted that it was hard to see that from the outset... The symtab is still allocated for each frame, but it is not used since a specially prepared t_atoms structure is passed in. I think the issues worth fixing for 4.5.6 are now
fixed. This code would benefit from a lot of clean-up in 5.0. In particular, there are so many overlapping interfaces to the system (and a lot of them are in installed headers) that is difficult to see interactions between the parts.

#4 - 07/17/2013 07:20 AM - Teemu Murtola
- Category set to core library
- Affected version set to 4.5.5