

## GROMACS - Bug #2693

### Several memory leaks in mdrun

10/12/2018 04:03 PM - Paul Bauer

<b>Status:</b> New	
<b>Priority:</b> Normal	
<b>Assignee:</b>	
<b>Category:</b> mdrun	
<b>Target version:</b> future	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> hard
<b>Affected version:</b> git master	
<b>Description</b>	
<p>When trying to run simulations through the new API, several issues are reported on the ASAN build that point to severe memory leaks within mdrun. I attached a log file for</p> <pre>valgrind --leak-check=full bin/gmxapi-test</pre> <p>I have a patch that fixes some of the direct leaks, but I'm out of my depth for most of the stuff.</p>	

#### Associated revisions

##### Revision 0926c8a6 - 12/17/2018 02:34 PM - Kevin Boyd

Fix memory leak at end of do\_md

Without domain decomposition, the atomtypes field of localtop is dynamically allocated and needs freeing after mdrun

Refs #2693

Change-Id: I45d18c503a87832332868e7fb9b63720548f243c

##### Revision 9ccd7f2b - 12/17/2018 02:49 PM - Kevin Boyd

Fix memory leaks in ns cleanup

Added some missing sfrees to cleanup function

refs #2693

Change-Id: I1e1455794778139d3a3866e00c05f4ed97aea07c

##### Revision 29da602d - 12/28/2018 11:20 AM - Kevin Boyd

Change t\_extmass pointers to std::vector

Using std::vector in t\_extmass fixes a leak in do\_md.

Used arrayRefs to view arrays in NHC\_trotter

Refs #2693

Change-Id: I6bd84952fb7a470879ddd665183680c865e22fc2

#### History

##### #1 - 10/12/2018 04:16 PM - Mark Abraham

Yes, that's one of about 50 reasons we're not able to support an API in a useful way in GROMACS 2019. :-)

I'm not sure whether we have blanket suppressions somewhere for ASAN (more particularly, LeakSanitizer), but we certainly could. But I doubt there's a good way to separate the leaks from mdrun from any caused by the memory management in gmxapi.

**#2 - 10/29/2018 11:00 AM - Paul Bauer**

- Target version changed from 2019 to future

Those are not going to be fixed in 2019.

**#3 - 12/16/2018 12:11 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '2' for Issue [#2693](#).  
Uploader: Kevin Boyd ([kevin.boyd@uconn.edu](mailto:kevin.boyd@uconn.edu))  
Change-Id: gromacs~master~l2a74543c3d393fca2a8e44e02e00c5daa68df922  
Gerrit URL: <https://gerrit.gromacs.org/8830>

**#4 - 12/16/2018 12:46 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2693](#).  
Uploader: Kevin Boyd ([kevin.boyd@uconn.edu](mailto:kevin.boyd@uconn.edu))  
Change-Id: gromacs~master~l1e1455794778139d3a3866e00c05f4ed97aea07c  
Gerrit URL: <https://gerrit.gromacs.org/8831>

**#5 - 12/17/2018 12:24 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '3' for Issue [#2693](#).  
Uploader: Kevin Boyd ([kevin.boyd@uconn.edu](mailto:kevin.boyd@uconn.edu))  
Change-Id: gromacs~master~l45d18c503a87832332868e7fb9b63720548f243c  
Gerrit URL: <https://gerrit.gromacs.org/8832>

**#6 - 12/18/2018 04:22 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2693](#).  
Uploader: Kevin Boyd ([kevin.boyd@uconn.edu](mailto:kevin.boyd@uconn.edu))  
Change-Id: gromacs~master~l6bd84952fb7a470879ddd665183680c865e22fc2  
Gerrit URL: <https://gerrit.gromacs.org/8847>

**Files**

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