GROMACS - Bug #716

Memory leak in g_rms when using the -prev flag

03/02/2011 05:53 PM - Daniel Larsson

Status:	Closed		
Priority:	Low		
Assignee:	David van der Spoel		
Category:			
Target version:	future		
Affected version - extra info:	4.5.3 and earlier	**Difficulty:**	uncategorized
Affected version:	5.0		

Description
g_rms eats up all system memory and crashes when analyzing long and large trajectories using the -prev flag.

Associated revisions

Revision d40ce2b8 - 06/09/2014 09:42 PM - Rossen Apostolov

Issue a warning for using gmx_rms -prev with large trajectories.

Refs #716.

Change-Id: l607d6a63259e0dd9de7c8c99e4917bbe9f37ff8e

History

#1 - 04/11/2012 12:13 PM - Rossen Apostolov

- Assignee set to David van der Spoel

- Priority changed from Normal to High

- Target version set to 4.5.6

#2 - 04/12/2012 09:07 PM - David van der Spoel

- Priority changed from High to Low

- Target version changed from 4.5.6 to 5.0

To fix this would require a large amount of work. This can be postponed to a later release when we do more modularization.

#3 - 05/23/2014 01:31 AM - Erik Lindahl

- Affected version set to 5.0

Rossen: I would consider removing the -prev feature for now.

#4 - 05/23/2014 01:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #716.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: l607d6a63259e0dd9de7c8c99e4917bbe9f37ff8e
Gerrit URL: https://gerrit.gromacs.org/3491

#5 - 05/23/2014 01:50 PM - Rossen Apostolov

I added only a warning because in most cases it will work fine despite the memory requirements.

#6 - 06/12/2014 01:59 AM - Erik Lindahl

- Target version changed from 5.0 to future

#7 - 12/31/2017 12:10 AM - Erik Lindahl

- Status changed from New to Closed

No point in keeping this open. As the C++ underpinnings are maturing it's time to reimplement many of these tools, and then we should be strict about not allowing any memory leaks. However, we won't touch the old tools.