Gromacs - Bug #1
Logfiles grow to several gigabytes
08/29/2005 08:20 PM - Erik Lindahl

Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: mdrun
Target version: CVS

Affected version - extra info:

Description
In some cases mdrun reports frequent constraint (LINCS) errors, but the program still doesn't crash. This will lead to logfiles that are several gigabytes in size, and eventually occupy the entire filesystem.

A good solution would be to count the number of errors generated, and eventually stop even if they are not critical.

Associated revisions
Revision 2c59f6de - 05/22/2014 06:23 AM - Mark Abraham
Refactor string handling for GPU usage report

This prepares for future addition of reporting the list of available compatible GPUs in the auto-selection case, which is needed for gmx tune-pme to function well. Current outputs are only of IDs of available GPUs, or IDs of those that will be used. The latter depends on the number of PP ranks, so it doesn't help gmx tune-pme find out how to run the optimization. At some point, delegating this kind of task to hwinfo called from gmx tune-pme might be preferable.

The only functionality changes here are of reporting GPU ids by referring to them as IDs, and the string of the ones used is of style "0,1,4" rather than 

Change-Id: lc37989ce2f9e639f6f450e1b5457ea7e07b3849b

History
#1 - 08/30/2005 03:27 PM - Erik Lindahl
Fixed by implementing a 10,000-limit to the LINCS warnings, after which the program quits.