calc_fluctuation_props output

06/06/2012 03:23 AM - Mark Abraham

Status: Closed
Priority: Low
Assignee: David van der Spoel
Category: analysis tools
Target version: 4.5.6

Description

calc_fluctuation_props() in g_energy writes header output when temperature is detected in the output set, even when none of the actual fluctuation-dependent properties are. I think the line

if (tt != NOTSET)

should also test a condition that is true when at least one other variable is not NOTSET.

Associated revisions

Revision 3b218ec2 - 08/16/2012 03:33 PM - David van der Spoel

Optional computation of fluct. props in g_energy. Fixes #954

Added a command line option -fluct_props to turn on the computation of heat capacity etc. in g_energy. This prevents a warning message from appearing on the screen each time the program is run.

Change-Id: l0cac44494ec5a366762d4d0a915146298d2ce1e0

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History

#1 - 06/06/2012 08:44 AM - David van der Spoel

Do you mean this should not be printed unless one of the other variables, e.g. volume, enthalpy, total energy, is printed? Obviously this output makes sense mostly for liquids and less so for complex system.

#2 - 08/16/2012 02:15 PM - Mark Abraham
David van der Spoel wrote:

Do you mean this should not be printed unless one of the other variables, e.g. volume, enthalpy, total energy, is printed? Obviously this output makes sense mostly for liquids and less so for complex system.

Yes. One of those should be present in order for fluctuations to be calculated/printed.

#3 - 10/21/2012 12:40 PM - David van der Spoel
- Status changed from New to Closed

Fixed in gerrit 2 months ago.