

GROMACS - Bug #18

Implement position rescaling with Rahman Parrinello barostat.

10/10/2005 05:27 PM - Ramon Garcia

Status: Closed	
Priority: Low	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: CVS	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>Although there is some ongoing work to enhance the barostat with Gromacs, the current barostat can be made more accurate with a painless change. In <code>do_update_md</code>, modify the updating of the coordinates to include the change of the box. In fact, I believe that not doing so was a misunderstanding of the equations. The differential equation of the coordinates, in the box reference frame is:</p> $m_i d^2s_i/dt^2 = h^{(-1)} f_i - m_i G^{(-1)} dG/dt ds_i/dt$ <p>s = coordinates in the box frame h = box matrix, transposed of Gromacs box $G = h^t t$</p> <p>Looking at Gromacs code in <code>do_update_md</code> and <code>parrinellorahman_pcoupl</code> and comparing to the equation above we see that the velocity is defined as:</p> $v_i = h ds_i/dt$ <p>therefore, the updating of the coordinates should be</p> $dx_i/dt = d(h s_i)/dt = dh/dt * s_i + h * ds_i/dt = dh/dt * h^{(-1)} * x_i + v_i = M * x_i + v_i$ <p>(the last step assumes that $dh/dt * h^{(-1)}$ is symmetric)</p>	

History

#1 - 10/10/2005 05:29 PM - Ramon Garcia

Created an attachment (id=3)
Patch to implement the feature described.

Do patch < the_patch in the directory of update.c

#2 - 10/10/2005 07:16 PM - Ramon Garcia

Created an attachment (id=4)
Small correction to the previous patch.

#3 - 10/12/2005 10:22 PM - Erik Lindahl

Hi Ramon,

Thanks - we'll look into this later. We just have to stabilize 3.3 first, and then get back to working in the head branch (where this will go).

#4 - 07/23/2007 04:38 PM - David van der Spoel

This bug goes the same fate as 14 but its contents have been copied to the wiki.

Files

patch_update
patch_update

2 KB
1.98 KB

10/10/2005
10/10/2005

Ramon Garcia
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