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

Description
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 do_update_md, 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:

\[ m \cdot \frac{d^2 s}{dt^2} = h^{-1} f - m \cdot G^{-1} \frac{dG}{dt} \frac{ds}{dt} \]

\[ s = \text{coordinates in the box frame} \]
\[ h = \text{box matrix, transposed of Gromacs box} \]
\[ G = h^t \]

Looking at Gromacs code in do_update_md and parrinellorahman_pcoupl and comparing to the equation above we see that the velocity is defined as:

\[ v_i = h \frac{ds_i}{dt} \]

therefore, the updating of the coordinates should be

\[ \frac{dx_i}{dt} = d(h s_i)/dt = \frac{dh}{dt} s_i + h \frac{ds_i}{dt} = \frac{dh}{dt} h^{-1} x_i + v_i = M x_i + v_i \]

(the last step assumes that \( \frac{dh}{dt} h^{-1} \) is symmetric)

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

### Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>patch_update</td>
<td>2 KB</td>
<td>10/10/2005</td>
<td>Ramon Garcia</td>
</tr>
<tr>
<td>patch_update</td>
<td>1.98 KB</td>
<td>10/10/2005</td>
<td>Ramon Garcia</td>
</tr>
</tbody>
</table>