

GROMACS - Bug #14

Rahman Parrinello barostat not accurate for the anisotropic case.

09/15/2005 08:03 PM - Ramon Garcia

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| Status: Closed | |
| Priority: Normal | |
| Assignee: Erik Lindahl | |
| Category: mdrun | |
| Target version: CVS | |
| Affected version - extra info: | Difficulty: uncategorized |
| Affected version: | |
| Description | |
| <p>The implementation of the Rahman Parrinello barostat does not match the one published in M. Parrinello, A. Rahaman J. Appl. Phys vol 52 n 12 page 7182</p> <p>For the case where only isotropic pressure is applied, the implementation is correct. However, when there is an non isotropic stress tensor, Gromacs uses an incorrect generalization that consists in replacing the pressure by the stress tensor in the formula:</p> $W_{\text{box}} = (\text{pressure_observed} - \text{pressure}) \text{box}^{-1} * \text{volume}$ <p>This seems a natural generalization. In fact first paper anticipating the Rahman Parrinello thermostat (PRL vol 45, n 14, pg 1196) suggested this extension. But the paper (earlier mentioned) that developed the method gives a different formula.</p> <p>A posible solution is to support isotropic pressure only, even when allowing box deformations. This is done by DL_POLY. In fact, the review article of Nose and Klein (Molecular Physics, vol 50, n 5 pg 1055) cited by Gromacs does not mention how to implement a barostat to a stress tensor. Furthermore according to the paper by Rahman and Parrinello, if a external stress tensor is applied, both the hydrostatic pressure and the tensor have to be specified. So ref_p for the anisotropic case would need 7 components, one for the isotropic pressure and 6 for the external stress tensor.</p> | |

History

#1 - 09/15/2005 09:05 PM - Erik Lindahl

Hi Ramon,

Thanks for the report. This will *probably* not be fixed right now, since Michael Shirts is working on a complete overhaul of the Parinello-Rahman (and Anderson) pressure scaling.

The problem is that to conserve enthalpy we cannot reformulate the equation of motion from scaled to normal coordinates like we do now. It also requires velocity verlet integration, which in turn means we need the velocity constraint correction step in Lincs and Settle (Rattle). Too many things depending on each other...

Nevertheless, I'll try to have a look at the article.

#2 - 07/23/2007 04:15 PM - David van der Spoel

I'm closing this bug, it has now been listed as a development target at the gromacs wiki:

<http://wiki.gromacs.org/index.php/Barostat>