GROMACS - Bug #901

Dispersion correction incorrect with energy minimization

03/18/2012 09:52 AM - David van der Spoel

Status:	Closed		
Priority:	Normal		
Assignee:	Berk Hess		
Category:	mdrun		
Target version:	4.5.6		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

The dispersion correction term is multiplied by the number of processors in parallel energy minimization runs. This could be due to the fact that term is summed into the potential energy before evaluating global_stat in the function evaluate_energy in minimize.c. Since this does not affect the minimization it is not very important, but as soon as force fields start to reproduce meaningful energies it will be important.

Associated revisions

Revision c19645bf - 04/26/2012 02:40 PM - Berk Hess

fixed dispersion correction with parallel EM

With EM the energy and pressure dispersion correction terms
were multiplied by the number of nodes. Fixes #901

Change-Id: I289ac0de7d7a9c1f72e939b840c549c1cb49a52a

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History

#1 - 04/11/2012 10:56 AM - Rossen Apostolov

Do we want this fixed for 4.5.6?

#2 - 04/26/2012 08:27 PM - David van der Spoel

- Status changed from New to Closed

Fixed in commit I289ac0de.