

GROMACS - Bug #321

cg / steep minimizations do not write modified configurations to trajectory

05/05/2009 04:31 AM - Heiko Lammert

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>In the trr trajectory written during a minimization, using cg or steep, all frames except the last one are identical to the starting configuration. The minimization itself does work, as the energy decreases and a modified final configuration is found and written.</p> <p>Observed in Gromacs 4.0.3 on x86-64 running Linux, on a single CPU.</p> <p>do_cg() in minimize.c gets a t_state state_global. Modified configurations are stored in a local copy, s_min->s. Frames are written using write_traj(), which calls fwrite_trn() for the unmodified state_global.</p> <p>Only after the minimization loop, copy_em_coords_back() is called for not-parallel runs (if (!PAR), which updates state_global from s_min->s. The final frame is written after this, using the modified state_global.</p> <p>The same problem exists in do_steep().</p> <p>Possible fix:</p> <p>Calling copy_em_coords_back() after each iteration inside the minimization loop produces trajectories with updated configurations.</p>	

History

#1 - 05/05/2009 12:58 PM - Berk Hess

I fixed it.
Note that this problem only occurred when not running in parallel.

Berk