GROMACS - Bug #481

Normal mode analysis produces wrong output in parallel

07/28/2010 07:01 PM - Rui Rodrigues

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Normal mode analysis ("integrator = nm" in mdp) runs in parallel without any error and it finishes in about half the time when compared to serial run:
mpirun -np 2 /usr/local/gromacs/bin/mdrun_d_mpi -s nm.tpr -v -deffnm nm -mtx hessian.mtx

However, output is wrong: mdrun write multiple hessian.mtx files (one for each core), each with small size.
Also, mdrun seems to get in to some kind of race condition, because sometimes only one .mtx is produced (still, with small size).
Running g_nmeig with these "parallel" mtx results in huge all-negative eigenvalues:
g_nmeig_d -f hessian.mtx -s nm.tpr

The following gives correct output:
mdrun_d -s nm.tpr -v -deffnm nm -mtx hessian.mtx
g_nmeig_d -f hessian.mtx -s nm.tpr

Tested with gromacs 4.0.5 and 4.0.7, compiled in 64 bit, double precision, with or without mpi, in a Mac (OSX 10.5.8).

History

#1 - 07/30/2010 12:38 PM - Berk Hess

This was never intended to work in parallel,
but we forgot to add a check for that.
I made nm work in parallel for the 4.5 release.

Berk