GROMACS - Feature #1053
L-BFGS doesn't use constraints or call do_em_step

11/30/2012 07:20 PM - Mark Abraham

Status: In Progress
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: future
Difficulty: uncategorized

Description
http://lists.gromacs.org/pipermail/gmx-developers/2012-November/006433.html

Associated revisions
Revision 1f387a48 - 01/15/2013 12:36 AM - Mark Abraham
Added fatal error for constraints + L-BFGS minimizer
Refs #1053
Change-Id: I0fd609918927883fc9ec20d0599a48e396d81d94

History
#1 - 01/15/2013 12:40 AM - Mark Abraham
- Status changed from New to In Progress

https://gerrit.gromacs.org/2049 prevents people generating garbage, at least.

Once that commit's in, I will re-target this patch to future, unless you're keen to fix it for 4.6.1, Berk.

#2 - 01/17/2013 09:42 PM - Mark Abraham
- Target version changed from 4.5.6 to future

#3 - 01/18/2013 11:00 AM - Berk Hess
- Tracker changed from Bug to Feature