GROMACS - Feature #1053

L-BFGS doesn't use constraints or call do_em_step

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>In Progress</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>future</td>
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<td>Difficulty:</td>
<td>uncategorized</td>
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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