

## GROMACS - Bug #37

### Implicit water constraints silently break conjugate gradient minimization

12/16/2005 11:39 PM - Mark Abraham

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> mdrun	
<b>Target version:</b> 3.3	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	
<b>Description</b>	
<p>There was some discussion on gmx-users of systems solvated in water that users were trying to use CG energy minimization on. They ran into problems with grompp such as</p> <p>"processing coordinates... double-checking input for internal consistency... ERROR: can not do Conjugate Gradients with constraints (201522)"</p> <p>which was thought to be caused by the implicit constraints in the rigid water model, since the user had specified no constraints in the .mdp file. One user reported that adding "-DFLEXIBLE" to their .mdp file allowed CG EM to run.</p> <p>See discussion at <a href="http://www.gromacs.org/pipermail/gmx-users/2005-December/018714.html">http://www.gromacs.org/pipermail/gmx-users/2005-December/018714.html</a> and <a href="http://www.gromacs.org/pipermail/gmx-users/2005-December/018750.html">http://www.gromacs.org/pipermail/gmx-users/2005-December/018750.html</a></p> <p>David Mobley and I thought that explicit discussion of this in the manual should be considered -</p> <ol style="list-style-type: none"><li>1) in the CG section, a note that rigid water models won't work because of the explicit constraints, and the need to overcome this with -DFLEXIBLE, if suitable</li><li>2) a mention of water constraints in the constraints section(s)</li><li>3) a more descriptive error message when using grompp to set up CG with EM if the constraints are only associated with a rigid solvent</li></ol> <p>Any of the above will help a user recognise the problem.</p>	

#### History

##### #1 - 02/22/2006 10:14 PM - David van der Spoel

I don't understand point two below, but have updated both the error message in grompp and the manual.

##### #2 - 02/23/2006 02:06 AM - Mark Abraham

(In reply to comment [#1](#))

I don't understand point two below, but have updated both the error message in grompp and the manual.

Of course... I was confusing the GROMACS usage of "restraints" and "constraints" in my mind.