## GROMACS - Bug #1020

### g_enemat options

10/06/2012 12:07 PM - Justin Lemkul

<table>
<thead>
<tr>
<th>Status</th>
<th>Closed</th>
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<tr>
<td>Priority</td>
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</tr>
<tr>
<td>Assignee</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version</td>
<td>4.6</td>
</tr>
<tr>
<td>Affected version</td>
<td>4.5.5</td>
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<td>Difficulty</td>
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### Description

There are two command line options for g_enemat that are overlapping:

```
{ "-lj", FALSE, etBOOL, {&bLJSR},"extract Lennard-Jones SR energies"),
{ "-lj", FALSE, etBOOL, {&bLJLR},"extract Lennard-Jones LR energies"),
```

It would also be preferable to standardize the naming of energy terms to more clearly specify SR vs LR. For instance, Buckingham terms are `-bhamsr` and `-bhamlr`, which I think is very clear, but then (aside from the above-mentioned identical names for LJ terms), `-coul` vs. `-coulr` for Coul-SR vs Coul-LR is not very clear.

### Associated revisions

Revision 7ec19728 - 11/12/2012 12:00 PM - David van der Spoel
Fixes #1020 options in g_enemat
Disentangled the options for selecting energy terms.
Change-Id: l8b2979a32e75a9e6a0eb641c0965089db5318f69

### History

#### #1 - 10/18/2012 12:20 AM - Roland Schulz
What names do you suggest? And should this only be fixed for 4.6 or also for 4.5.6? It might be not such a good idea to change the options name for 4.5.x. So the coul. part I wouldn't change there but the lj might be good to change in also for 4.5.6. Should we use ljlr and ljlsr? And for 4.6 coullr and coulrsr? But coulrlr is difficult to read.

#### #2 - 10/18/2012 12:34 AM - Justin Lemkul
I'd say we could target 4.6 rather than 4.5.6. I suspect it's a fairly minor problem, since no one has ever complained on the mailing list (to my knowledge). I happened across it while looking into something else. In any case, I'm a fan of clarity and the mash-up of letters doesn't strike me as particularly attractive, but I'd say perhaps the best options would make use of underscores, i.e. `-lj_sr`, `-lj_lr`, `-coul_sr`, and `-coul_lr`.

#### #3 - 12/28/2012 08:14 PM - Erik Lindahl
- Status changed from New to Closed