Gromacs - Feature #1494

request for changes to repl_ex_nst to issue a warning, rather than a note

05/02/2014 07:48 PM - Chris Neale

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<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
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**Description**

Using gromacs 4.6.1, I set -replex 250 but got exchanges every 300 steps instead. I gather that this is because nstcalcenergy now defaults to 100 (see issue 695 for resetting of repl_ex_nst to be a multiple of nstcalcenergy).

In the log file, I have:

NOTE: nstcalcenergy changes repl_ex_nst to 300

However, I didn't notice this for quite some time. It's not a big problem, and I know that you try not to out-think the user, but the combination of the code resetting variables on the fly and developers making changes to defaults can lead to users not getting what they intend (and not knowing so).

For instance, in gromacs 4.5.5, nstcalcenergy defaulted to -1 (in src/kernel/readir.c):

```
ITYPE ("nstcalcenergy", ir->nstcalcenergy, -1);
```

Such that it was then reset to 10, which is what made me think that I could do exchanges every 250 steps.

However, in gromacs 4.6.1, nstcalcenergy now defaults to 100 (in src/kernel/readir.c):

```
ITYPE ("nstcalcenergy", ir->nstcalcenergy, 100);
```

Leading to my confusion.

I think that a warning is better (causing the job to stop without -maxwarn being set sufficiently high), plus a detailed description of what is going on, so that the user at least knows what they are getting.

Thank you,

Chris.

**Associated revisions**

Revision ec74f525 - 06/12/2014 12:56 AM - Berk Hess

Decoupled repl_ex_nst from nstcalcenergy

The replica exchange frequency is automatically changed by mdrun to a multiple of nstcalcenergy, which is annoying. It turns out that it doesn't need to be a multiple, so this changing has been removed.

Fixes #1494

Change-Id: i00833f92f4d468924f61879aff8b7c85fe79d3c2e
strikeout text was not intentional in the above comment. Somewhat ironically, it was auto-formatted based on the negative sign ;)

But the replica exchange frequency is an option of mdrun, which doesn't have a terminate on warning option. The only option is to make it a fatal error. Would you prefer this?

I would much prefer the fatal error to the unexpected (though documented in the log file) behaviour.

Initially I thought that repl_ex_nst wouldn't need to be linked to nstcalcenergy, then I thought it should, because of global signalling. But the global signalling doesn't need to happen at repl_ex_nst steps, so it's fine anyhow. I pushed up a patch which completely removes the issue: https://gerrit.gromacs.org/#/c/3565/

Edited description. Berk's fix resolves the issue as far as I can see.

Applied in changeset e074f5259425aa6d36fbc95c018124d156f14a.

- Status changed from Resolved to Closed