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

| Status:   | Closed          |
| Priority: | Low             |
| Assignee: | Berk Hess       |
| Category: | mdrun           |
| Target version: | 5.0           |
| Difficulty: | uncategorized |

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 be 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: I00833f92fd468924f61879aff8b7c85fe79d3c2e

History

#1 - 05/02/2014 07:50 PM - Chris Neale

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

#2 - 06/10/2014 12:54 PM - Berk Hess

- Category set to mdrun
- Status changed from New to Feedback wanted
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?

#3 - 06/10/2014 01:16 PM - Chris Neale
I would much prefer the fatal error to the unexpected (though documented in the log file) behaviour.

#4 - 06/10/2014 02:43 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1494.
Uploader: Berk Hess (hess@kth.se)
Change-id: I00833f92fd468924f1879aaffb7c85fe79d3c2e
Gerrit URL: https://gerrit.gromacs.org/3565

#5 - 06/10/2014 02:46 PM - Berk Hess
- Status changed from Feedback wanted to Fix uploaded
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/

#6 - 06/10/2014 03:25 PM - Mark Abraham
- Description updated
Edited description. Berk's fix resolves the issue as far as I can see.

#7 - 06/12/2014 12:56 AM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#8 - 06/12/2014 01:00 AM - Berk Hess
- % Done changed from 0 to 100
Applied in changeset ec74f52659425aa6df35fbca95c018124d156f14a.

#9 - 06/12/2014 02:44 PM - Erik Lindahl
- Status changed from Resolved to Closed