GROMACS - Feature #1377

Replica exchange if replicas not in ascendent T

11/07/2013 08:17 AM - David van der Spoel

Status: Feedback wanted
Priority: Low
Assignee: David van der Spoel
Category: mdrun
Target version: 
Difficulty: uncategorized

Description
From gmx-developers

I found that when doing replica exchange, serious problems will happen if temperatures of replicas are not in ascent order. For example, the temperature of replica 1 is 500K while the one in replica 2 is 300K, then even if the exchange request is denied (as shown in the log file), two copies are still exchanged.

I suggest to modify line 1258~1259:

```
if( destinations[i] != i)
bAnyReplicaExchanged = TRUE;
```

into

```
if( destinations[i] != re->ind[i])
bAnyReplicaExchanged = TRUE;
```

because if temperatures of replicas are not in ascent order, re->ind[i] is not equal to i, while in line 978, destinations[i] are initialized as re->ind[i].

Associated revisions

Revision 4406c454 - 06/18/2014 01:12 AM - Erik Lindahl

Disabled replica exchange when T not in order

There are issues when the replica property is not increasing with the replica index. This patch has a partial fix. But since there are still issues, unordered replicas now lead to a fatal error.

Fixes #1377.

Change-Id: I272d9831df85fdc18c1b2fe5724cbfc06e73444e

History

#1 - 06/11/2014 11:58 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1377.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: l272d9831df85fdc18c1b2fe5724cbfc06e73444e
Gerrit URL: https://gerrit.gromacs.org/3574

#2 - 06/11/2014 11:59 PM - Erik Lindahl

- Status changed from New to Fix uploaded

David - please check this fix before the upcoming release if you can; you're probably the one of us with most REMD experience.

#3 - 06/12/2014 05:29 PM - David van der Spoel

- File redmine-1377.tgz added

The attached script verifies that the error message about incorrect order of temperature works. It can be used for developing a better solution.

#4 - 06/15/2014 10:49 AM - David van der Spoel
Once [https://gerrit.gromacs.org/#/c/3574/](https://gerrit.gromacs.org/#/c/3574/) is accepted, the problems associated with a non-ascending T range will be caught by mdrun. Therefore changing this to a feature request, since it would be nice if one could run

```
mdrun -replex -s *.tpr
```

#5 - 06/18/2014 08:00 AM - Erik Lindahl
- Status changed from Feedback wanted to Resolved
- % Done changed from 0 to 100

Applied in changeset 4406c454582db94df45f2d37d46acc8d092a10bf.

#6 - 06/18/2014 08:14 AM - David van der Spoel
- Status changed from Resolved to Feedback wanted

Changing status again, due to my previous comment. We can of course decide not to implement the feature. No strong feelings there, but imagine that one wants to do a large REMD calculation with different reference T and P, it might be rather complicated to sort the tpr files in the right order then.

#7 - 06/22/2014 10:11 PM - Erik Lindahl
- Priority changed from Normal to Low

#8 - 06/23/2016 03:48 PM - Mark Abraham
- Target version deleted (5.x)

The general case of multi-dimensional replica exchange, or multiple replicas at a control-variable point needs a much more flexible implementation than either requiring sorting on the mdrun command line, or doing it internally. I would much prefer scrapping -multi in favour of -multidir (so the GROMACS code and user organization both become simpler), and an .mdp setting that names the eligible exchange partners somehow. This could be done via something like

```
exange-variable = temperature
exchange-scheme  = adjacent
```

for convenience.

Files

redmine-1377.tgz  150 KB  06/12/2014  David van der Spoel