compute globals should not have logic about which integrator is in use

11/23/2015 05:44 PM - Mark Abraham

Status: New
Priority: Normal
Assignee:
Category:
Target version: 5.1.2
Affected version -
extra info:

Affected version: 5.1

Description

In 488464e7, we removed the iterative cases for the md-vv integrator. This exposed a bug that I suspect has been there ever since the first implementation of md-vv.

It affects users doing replica exchange at the first successful exchange (#1848). Successful exchange triggers an extra call to compute_globals() (line 969 of md.c) to re-calculate KE-like quantities. If the integrator is not one of the VV flavors, then we segfault in global_stat (line 229 of stat.cpp) because such integrators are (erroneously) hard coded to collect the force virial when it is not required by the caller (who passed a NULL for it to be stored in). This inadvertently worked before removing constraint iteration, because bFirstIterate was FALSE for this call to global_stat(), which meant that the erroneous dereference of fvir didn't happen.

It also affects mdrun -rerun because that uses the same call to compute_globals().

When I removed the iteration code, I made a mental approximation of "all integrators now have one iteration, so bFirstIterate can be assumed to be true" which is valid, except that this particular call to compute_globals() is unusual, and inadvertently relied on the fact that the flag to indicate that this was a first iterate was (of course) not set.

There was also a test for bTemp || !bVV in global_stat, which didn't hurt because we passed ekind and bTemp was true (in at least this call to compute_globals()). So we don't segfault... but whether we trash data we intended to keep is pretty much unknowable in the current state of do_md().

I think the correct design is for integrators to pass the flags they want, and the global communication code do only what's asked directly of it.

I'll upload a patch that fixes this for release-5-1, where the bug is reported.

There remains the issue of bEkinAveVel in global-stat() which can wait to be cleaned up in master branch.

Related issues:

- Related to Gromacs - Bug #1848: Segfault with replica exchange at first succe... Resolved
- Related to Gromacs - Task #1793: cleanup of integration loop New

History

#1 - 11/23/2015 05:49 PM - Mark Abraham
- Target version set to 5.1.2

#2 - 11/23/2015 05:51 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #1858.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-id: i0fbc62a9732dac186aeeb887445c0bb848151c4fd
Gerrit URL: https://gerrit.gromacs.org/5371

#3 - 11/23/2015 05:52 PM - Mark Abraham
- Related to Bug #1848: Segfault with replica exchange at first successful exchange added
In `do_md` without VV, `compute_globals` is always called with the temp flag on.
In `minimize.c` it's always off.
So apparently the temperature summation for minimization is harmless.
But that conditional should and can also be changed, although we should do that in master.

Berk Hess wrote:

In `do_md` without VV, `compute_globals` is always called with the temp flag on.
In `minimize.c` it's always off.
So apparently the temperature summation for minimization is harmless.
But that conditional should and can also be changed, although we should do that in master.

OK. I think we also over-use `CGLO_PRESSURE`

Gerrit received a related patchset '1' for Issue #1858.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-id: I1f9583991608ffdd655439fd3f5b5ec861ec64
Gerrit URL: https://gerrit.gromacs.org/5379

- Related to Task #1793: cleanup of integration loop added