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

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.
#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: I0fbce62a9732dac186acec687445d8848151c4fd
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

#4 - 11/24/2015 09:42 PM - Berk Hess
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.

#5 - 11/24/2015 09:45 PM - Mark Abraham
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

#6 - 11/24/2015 11:58 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1858.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I1f9583991608ffdd655439f0c3df5bec861ec64
Gerrit URL: https://gerrit.gromacs.org/5379

#7 - 11/25/2015 12:31 AM - Mark Abraham
- Related to Task #1793: cleanup of integration loop added

#8 - 12/10/2015 03:24 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1858.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I7f99eba36184f564108c38865e21f1bc55354
Gerrit URL: https://gerrit.gromacs.org/5435

#9 - 12/11/2015 09:30 AM - Mark Abraham
- Status changed from New to Resolved

Applied in changeset ed86315f3d58c7b42334c220f3aed8a13e2be9cb.

#10 - 01/12/2016 04:23 PM - Mark Abraham
- Status changed from Resolved to Closed