GROMACS - Bug #3120

Uninitialized energy and virial contributions with PME on GPU on PME-only rank

10/04/2019 12:54 PM - Berk Hess

Status: Closed
Priority: High
Assignee: mdrun
Category: mdrun
Target version: 2019.5
Difficulty: uncategorized

Affected version - extra info:

Affected version: 2019.4

Description
The struct passing data from a PME-only rank is uninitialized with PME on a GPU, which can give non-zero LJ reciprocal energy and virial contributions, which are added to the potential energy and virial.

Up till now we only observed non-zero contributions with the clang compiler for the CPU side code and only with release builds. The "random" energy and virial contributions likely don't go unnoticed and with pressure coupling we would expect a run to crash after a few steps.

Associated revisions

Revision 41bcf87d - 10/04/2019 12:55 PM - Berk Hess
Fix random energy and virial with PME on GPU on a PME-only rank

Missing zero initialization of never computed LJ PME energy and virial terms with PME on the GPU could lead to random energy, virial and pressure numbers.

The effect of this bug was that the potential and total energy could be off (not the Coulomb mesh energy). This didn't affect sampling. The pressure could be off, which would affect sampling when pressure coupling is used, but likely the simulation would explode after a few steps.

Fixes #3120

Change-Id: I309dde958f1b73e7f71f87f4f5ad016d16f8d16b

Revision 54898ee5 - 10/09/2019 10:26 AM - Berk Hess
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History

#2 - 10/04/2019 01:09 PM - Berk Hess
- Subject changed from Unitialized energy and virial contributions with PME on GPU on PME-only rank to Uninitialized energy and virial contributions with PME on GPU on PME-only rank

#3 - 10/04/2019 03:15 PM - Berk Hess
- Status changed from Fix uploaded to Resolved
Applied in changeset 41bc87d5c619598200e04db22db6e949e2c767e.

#4 - 10/09/2019 11:15 AM - Berk Hess
Applied in changeset 54898ee515142db4555c297b90ba1831d0e28208.

#5 - 11/20/2019 05:15 PM - Paul Bauer
- Status changed from Resolved to Closed