GROMACS - Bug #2409

PME gather CUDA kernel failing on Fermi

02/14/2018 04:12 PM - Szilárd Páll

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Aleksei lutinov</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
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<td>Target version:</td>
<td>2018.1</td>
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<tr>
<td>Affected version</td>
<td>uncategorized</td>
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<td>Affected version</td>
<td>2018</td>
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Description
For inputs larger than ~350k:

Error while launching kernel pme_gather_kernel: invalid configuration argument

Reproduced on C2070 and GTX 580.

Associated revisions
Revision fa92dbed - 02/16/2018 10:53 AM - Aleksei lutinov

Fix PME for large systems with Fermi GPUs
PME spread/gather CUDA kernel scheduling did not account for compute capability limitations. Realistically this has only caused it to fail on CC 2.x with input systems larger than $2^{18} \approx 262k$ atoms. This is now fixed for all CUDA architectures.

Fixes #2409
Change-Id: i59295b5d53a341d08a221ae6b52e1db9f1e80107

History
#1 - 02/14/2018 06:33 PM - Aleksei lutinov
- Assignee set to Aleksei lutinov
- Target version set to 2018.1

Thanks, reproduced on C2075 on gromacs3!

#2 - 02/15/2018 01:10 PM - Mark Abraham
- Subject changed from PME gathee CUDA kernel failing on Fermi to PME gather CUDA kernel failing on Fermi

#3 - 02/15/2018 02:48 PM - Gerrit Code Review Bot
Gerrit received a related patchset '3' for Issue #2409.
Uploader: Aleksei lutinov (a.yupinov@gmail.com)
Change-Id: gromacs~release-2018~I59295b5d53a341d08a221aebb52e1db9f1e80107
Gerrit URL: https://gerrit.gromacs.org/7584

#4 - 02/16/2018 11:00 AM - Aleksei lutinov
- Status changed from New to Resolved

Applied in changeset fa92dbed34ec7b916f4aa2dd6f17c1b08a8ede0a.

#5 - 02/16/2018 03:26 PM - Mark Abraham
- Status changed from Resolved to Closed

#6 - 02/16/2018 03:38 PM - Aleksei lutinov
One thing TO DO here would be to have a huge input system sanity test, but Szilard brought up a good point that such a thing would fail for many users due to memory usage, and maybe should be an internal project rather. Not important anyway.

#7 - 02/16/2018 06:07 PM - Mark Abraham

NB we have the GMX_DEVELOPER_BUILD cmake configuration that could be used to enable such things. And of course we'd generate the contents of such a test system rather than store the coordinates.

#8 - 02/16/2018 06:37 PM - Szilárd Páll

Mark Abraham wrote:

NB we have the GMX_DEVELOPER_BUILD cmake configuration that could be used to enable such things. And of course we'd generate the contents of such a test system rather than store the coordinates.

That could indeed be useful.

On a side-note it seems to me that it would be quite appropriate for Google test (and/or CTest) to support subsets of tests to not be compulsory and by default issue only warning/note when such a test fails; these tests can be turned compulsory and warnings emitted as failures in our controlled CI environment. This way a test that fails due to out-of-memory error (because the user's browser chews up 1.65 of the 2 Gb GPU memory) won't mark a unit test failed in the users' hands, but if it terminates with some weird error we may still learn about it. Can this be done with the available features?