

## GROMACS - Task #2686

Task # 2675 (In Progress): bonded CUDA offload task

### add tests for gpu bonded interactions

10/09/2018 09:54 PM - Szilárd Páll

<b>Status:</b>	New	
<b>Priority:</b>	Normal	
<b>Assignee:</b>		
<b>Category:</b>	testing	
<b>Target version:</b>	2020	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
In order to support quick testing of the new late-arrival bonded kernel integration, we'd benefit from mdrun-tests of bonded interactions and/or end-to-end tests with: - only offload-supported bonded interactions - supported and unsupported (including perturbed)		
<b>Related issues:</b>		
Related to GROMACS - Feature #2034: Unit tests for bonded forces		<b>New</b>

### History

#### #1 - 10/10/2018 10:11 AM - Mark Abraham

I think this will be fine, there's already e.g. alanine dipeptide in vacuo and solvent, and there's a nonanol (in vacuo?) for free-energy rerun that will be straightforward to have work.

#### #2 - 10/22/2018 12:18 PM - Mark Abraham

- Target version changed from 2019-beta1 to 2019-beta2

#### #3 - 11/05/2018 10:02 AM - Paul Bauer

- Target version changed from 2019-beta2 to 2019-beta3

Nothing has happened so far, re-targeted for beta3

#### #4 - 11/21/2018 07:56 AM - Mark Abraham

There are also bonded interaction unit tests that David wrote, but we'd need to write quite a bit of glue code for the test binary to be GPU aware and to do data transfer and kernel launch. That probably makes more sense after we've worked on the GPU infrastructure a bit more.

#### #5 - 11/21/2018 12:34 PM - Mark Abraham

- Target version changed from 2019-beta3 to 2019

This target should be reconsidered later

#### #6 - 11/29/2018 10:44 AM - Mark Abraham

- Subject changed from ensure that mrun unit tests cover bonded offload use-cases to add tests for gpu bonded interactions

- Target version changed from 2019 to 2020

There are already some bonded unit tests that David wrote, these can probably be built upon

#### #7 - 01/03/2019 01:03 AM - Szilárd Páll

- Related to Feature #2034: Unit tests for bonded forces added