

GROMACS - Feature #2886

Feature # 2816 (New): GPU offload / optimization for update&constraints, buffer ops and multi-gpu communication

CUDA version of SETTLE

03/08/2019 04:20 PM - Artem Zhmurov

Status:	New
Priority:	Normal
Assignee:	Artem Zhmurov
Category:	core library
Target version:	2020
Difficulty:	uncategorized
Description	
Initial implementation that works as a separate instance, i.e. is be able to copy coordinates and velocities to and from GPU, handle PBC, compute virial. The infrastructure that maintains coordinates, velocities and PBC is temporary and will be removed when it is integrated with other parts of the GPU-only loop. GPU version is enabled by setting the environment variable "GMX_SETTLE_GPU".	
TODO:	
<ul style="list-style-type: none">• Stand-alone module that is enabled using environment variables.• A version of algorithm for derivatives.• Unify virial reduction with LINCS• Unify SettleParameters and their initialization with CPU version• Better integration with CPU version (e.g. checks for input consistency)	
Related issues:	
Related to GROMACS - Feature #2885: CUDA version of LINCS	New
Related to GROMACS - Feature #2887: CUDA version of Leap Frog algorithm	New
Related to GROMACS - Feature #2888: CUDA Update and Constraints module	New

Associated revisions

Revision 02a92f23 - 04/30/2019 05:19 PM - Artem Zhmurov

CUDA version of SETTLE algorithm with basic tests

CUDA-based GPU implementation of SETTLE. This is a part of all-GPU loop. Can work isolated from other parts of the code since coordinates are copied to (from) device before (after) SETTLE kernel call. The velocity update as well as virial evaluations can be enabled.

To enable, set GMX_SETTLE_GPU environment variable.

Limitations:

1. Does not work when domain decomposition is enabled.
2. Projection of the derivative is not implemented.
3. Not fully integrated/unified with the CPU version.

TODOs:

1. Multi-GPU case.
2. Better virial reduction. This is a more general feature, not only related to constraints.
5. More cleanup in constr.cpp needed.
6. Better unit tests.

Refs #2816, #2886

Change-Id: I218e1bf1f86a2351e189e3c27f950f45c06135a4

Revision 1b64f6aa - 07/04/2019 08:23 AM - Artem Zhmurov

Use reallocateDeviceBuffer(...) in CUDA version of SETTLE

Refs #2886 and #2888

Change-Id: la45254a24eda8e6ad151b1f4c6583b1a2c926004

Revision d1f2302e - 08/09/2019 05:35 PM - Artem Zhmurov

Refactoring of the SETTLE tests

Current version of tests for CUDA version of SETTLE was a quick addition to the old tests, with direct comparison of the GPU implementation with the old original CPU-based implementation. This commit rearranges the test structure, making it possible to apply the same set of tests to both implementations. There are no changes to the tests themselves. Currently, comparison tests will run twice and will dry-run on CUDA builds without CUDA-capable devices.

TODO: Add comparison with pre-computed values for coordinates, velocities and virial. Remove the CPU vs GPU comparison tests.

Refs #2886, #2888.

Change-Id: lfc6af9af6c93787b919b785348f9f4547b6c267

Revision 7bd1c817 - 08/13/2019 04:13 PM - Artem Zhmurov

Make use of reference data in SETTLE tests

As a temporary measure, the CPU and GPU versions of SETTLE were tested against each other. Making use of the reference data framework allows to test them against precomputed values. Now, the final positions, velocities and virial are properly tested in CPU and, if available, in GPU versions.

Refs. #2886, #2888.

Change-Id: l8e54e1a741263b8bf9774a21141c527f58130fa9

History

#1 - 03/08/2019 05:06 PM - Artem Zhmurov

- Related to Feature #2885: CUDA version of LINCOS added

#2 - 03/11/2019 11:52 AM - Artem Zhmurov

- Description updated

#3 - 03/11/2019 11:53 AM - Artem Zhmurov

- Related to Feature #2887: CUDA version of Leap Frog algorithm added

#4 - 03/11/2019 11:54 AM - Artem Zhmurov

- Related to Feature #2888: CUDA Update and Constraints module added

#5 - 03/13/2019 01:40 PM - Artem Zhmurov

- Description updated

#6 - 10/02/2019 12:02 PM - Artem Zhmurov

- Description updated