GROMACS - Feature #2888

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

CUDA Update and Constraints module

03/08/2019 04:22 PM - Artem Zhmurov

Status:	New
Priority:	High
Assignee:	Artem Zhmurov
Category:	
Target version:	2020
Difficulty:	uncategorized

Description

- ~~LINCS for non-water constraints.~~
- ~~SETTLE for water constraints.~~
- ~~Leap frog integrator.~~
- ~~Merge of the three into single module.~~
- Remove the scaffolding from LINCS, SETTLE and Leap-Frog:
    - ~~Coordinates, velocities, forces management.~~
    - PBC management.
    - Virial reduction.
    - ~~Update tests.~~
    - ~~Remove Impl.~~
    - ~~Template computeVirial and updateVelocities~~
    - ~~Remove the D2D copy for the coordinates (xp->x)~~

Subtasks:

Task # 3114: Possible improvements to update-constraints	**New**
Feature # 3162: Add virtual site support to GPU version of update-constraints.	**New**
Bug # 3163: gpuupdate / task assignment stabilization	**New**
Task # 3167: GPU update path user documentation	**New**
Feature # 3168: GPU update release notes	**New**
Bug # 3182: pressure coupling buggy with GPU update	**New**

Related issues:

Related to GROMACS - Feature #2885: CUDA version of LINCS	**New**
Related to GROMACS - Feature #2886: CUDA version of SETTLE	**New**
Related to GROMACS - Feature #2887: CUDA version of Leap Frog algorithm	**New**
Related to GROMACS - Task #2936: introduce check that CPU-GPU transfers are m...	**New**
Related to GROMACS - Task #3171: schedule CPU H2D force contribution in separ...	**New**
Related to GROMACS - Task #3195: assess nightly master failures	**New**

Associated revisions

Revision 1c8eb7c5 - 06/18/2019 11:24 AM - Artem Zhmurov

Combine CUDA Leap-Frog, LINCS and SETTLE. I.

This is the first step in combining constraints and integrator
into "UpdateAndConstraints" module. The initial merge does not
imply any performance optimisation or code clean-up. Hence, this
patch keeps all the temporary infrastructure that was built
around SETTLE, LINCS and Leap-Frog to allow them to function as
a separate units. In the following commits, this infrastructure
will be removed and these three implementations will be more closely
integrated. To enable, set GMX_UPDATE_CONSTRAIN_GPU environment
variable. Note, that environment variables GMX_LINCS_GPU,
GMX_SETTLE_GPU and GMX_INTEGRATE_GPU will no longer work.

Refs #2816, #2888

Change-Id: I8730aad0ecaa0230686fe89d1157b0da2f01f7bc

Revision fb7a59cd - 07/03/2019 09:42 AM - Artem Zhmurov

Combine CUDA Leap-Frog, LINCS and SETTLE. II.

Stand-alone CUDA implementations of Leap-Frog, LINCS
and SETTLE required additional scaffolding for integration
and testing. The most prominent part of this is the
management of coordinates, velocities and forces, which
is removed in this commit. Management of periodic boundary
conditions and virial reduction will be removed in
following commits.

Refs #2816, #2888

Change-Id: I4c65a6c7088fd8059f4e7fa3cb4637cb2af79ebc

Revision 747c371c - 07/03/2019 01:01 PM - Artem Zhmurov

Memory management fixes in CUDA version of LINCS

This fix is to prepare LINCS to run with DD.

1. The masses array size depends on the current number of atoms
rather than on the number of constraints.
2. The size of other arrays should be based on the number of
threads launched on the GPU, which include padding added to
align coupled constraints with the thread blocks. Also
renamed variable according to conventions.

Refs #2885 and #2888

Change-Id: I20cb53ebc6da6a1ff2ee1e385613b27c4a01d11f

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

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

Refs #2886 and #2888

Change-Id: Ia45254a24eda8e6ad151b1f4c6583b1a2c926004

Revision 6385f296 - 07/05/2019 11:05 AM - Artem Zhmurov

Remove PImpl scaffolding from CUDA version of LINCS

The CUDA implementation of LINCS was initially introduced as a
stand-alone feature. This required hiding CUDA-specific variables
and subroutines into the private implementation subclass. Since the
LINCS is not a part of Update and Constraints module, this is no
longer required and can be removed.

Refs #2816, #2888

Change-Id: I9698224d4702dfb8d99106999335c62e83a511df

Revision b1150eee - 07/26/2019 10:20 AM - Artem Zhmurov

Remove PImpl scaffolding from CUDA version of SETTLE

GPU version of SETTLE was implemented as a class with private
implementation so it will be possible to initialize on
non-CUDA hosts. Now, the implementation can be hidden
inside the Update and Constraints PImpl so that the CUDA
specific types and calls can be exposed in SETTLE and
private implementation is no longer needed there.

Refs #2816, #2888

Change-Id: I4c78f2629be34b42bb5f4f7d34970c3e41515691

Revision 1bfc9ba5 - 08/06/2019 03:52 PM - Artem Zhmurov

Remove PImpl scaffolding from CUDA version of Leap-Frog

Private implementation in CUDA version of Leap-Frog was
used to introduce this integrator as a stand-alone unit.

Now it is merged with constraints, PImpl is no longer
needed.

Refs #2816, #2888

Change-Id: Iea82abef016b7e15b9be44a0e1b446e12e582d3c

Revision b1be1e72 - 08/08/2019 11:13 AM - Artem Zhmurov

Refactor Leap-Frog tests and connect them to CPU version

This introduces test data object and runners to the Leap-Frog
tests, which are now connected to the CPU version of Leap-Frog.
This also makes possible to include tests based on the reference
values, which are needed to make sure that the temperature and(or)
pressure control works fine in new implementations.

Refs. #2816, #2888.

Change-Id: Id2d934c43138889ad178a94126cab4da2895bb5a

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
is 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: Ifcb6af9af6c93787b919b785348f9f4547b6c267

Revision 0cd72f2b - 08/09/2019 07:59 PM - Artem Zhmurov

Prepare Update and Constraints for Domain Decomposition

Initial GPU-based version of the update and constraints was not
designed to run with the Domain decomposition. This introduces a
couple of fixes to the memory management that should alow the
module to work with the DD enabled. The memory buffers are now
re-allocated at the set(...) stage, if so needed.

Refs. #2816, #2888.

Change-Id: I155884f5797252cf048a6400a2dd7b042d355b7e

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 agains 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: I8e54e1a741263b8bf9774a21141c527f58130fa9

Revision 1fbaf8ff - 08/16/2019 11:29 AM - Artem Zhmurov

Remove PImpl scaffolding from CUDA version of SETTLE

GPU version of SETTLE was implemented as a class with private

implementation so it will be possible to initialize on non-CUDA hosts. Now, the implementation can be hidden inside the Update and Constraints PImpl so that the CUDA specific types and calls can be exposed in SETTLE and private implementation is no longer needed there.

Refs #2816, #2888

Change-Id: I4c78f2629be34b42bb5f4f7d34970c3e41515691

Revision 3d35e919 - 08/16/2019 11:29 AM - Artem Zhmurov

Remove PImpl scaffolding from CUDA version of Leap-Frog

Private implementation in CUDA version of Leap-Frog was used to introduce this integrator as a stand-alone unit. Now it is merged with constraints, PImpl is no longer needed.

Refs #2816, #2888

Change-Id: Iea82abef016b7e15b9be44a0e1b446e12e582d3c

Revision 039709b7 - 08/16/2019 11:29 AM - Artem Zhmurov

Prepare Update and Constraints for Domain Decomposition

Initial GPU-based version of the update and constraints was not designed to run with the Domain decomposition. This introduces a couple of fixes to the memory management that should alow the module to work with the DD enabled. The memory buffers are now re-allocated at the set(...) stage, if so needed.

Refs. #2816, #2888.

Change-Id: I155884f5797252cf048a6400a2dd7b042d355b7e

Revision 4b07f76f - 08/26/2019 03:07 PM - Artem Zhmurov

Add temperature coupling to CUDA Leap-Frog integrator

Velocity rescaling added to the integrator. None, one, or multiple rescaling groups are supported. Tests that include temperature coupling are added.

NoseHoover temperature control is not implemented.

Refs. #2887, #2888.

Change-Id: I1e6850eeb74de829554260fba6a6e6c1c63ceb46

Revision 7ddb7204 - 09/03/2019 06:49 AM - Artem Zhmurov

Add Parrinello-Rahman pressure coupling to CUDA Leap-Frog integrator

Parrinello-Rahman isotropic pressure coupling scheme is now added to CUDA version of the Leap-Frog integrator. The Leap-Frog tests are updated to check the new addition.

Refs. #2887, #2888.

Change-Id: Icf42667621c16a994e68baf5158ea4abac387928

Revision 79aab161 - 10/02/2019 07:07 PM - Artem Zhmurov

Eliminate D2D copy in update constraints

The intermediate coordinates (x' or xp) are only needed inside the update-constraints module (for the constraints algorithms) and never used outside. Hence, the xp variable can be used to save the coordinates before update, while x stores the final coordinates. This way, there is no need to make a D2D xp->x copy after applying the constraints, since x will have the correct data.

Refs. #2888, #3114.

Change-Id: l363b633976a236a8e2bf2137c21d3bf0a765cb06

Revision f310be38 - 10/16/2019 01:54 AM - Szilárd Páll

Trigger synchronizer when local forces are ready

The sycnhronizer is created and managed in StatePropagatorDataGpu and is
passed to the nonbonded mdoule at the f buffer ops init.

Refs #2888 #3126

Change-Id: le9bf0b6cd8511fe282e377e48f3940e591db214c

Revision 7bbfb57c - 10/16/2019 10:21 AM - Artem Zhmurov

Link GPU force producer and consumer tasks

The GPU event synchronizer that indicates that forces are ready
for a consumption is now passed to the GPU update-constraints.
The update-constraints enqueue a wait on the event in the update
stream before performing numerical integration and constraining.
Note that the event is conditionally returned by the
StatePropagatorDataGpu and indicates that either the reduction of
forces on the GPU or the H2D copy is done, depending on offload
scenario on a current timestep.

Refs. #2816, #2888, #3126.

Change-Id: lc12b0c55b75ec5f0c31ce500a2760fb4d5cf3b91

History

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

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

#2 - 03/11/2019 11:54 AM - Artem Zhmurov

- Related to Feature #2886: CUDA version of SETTLE added

#3 - 03/13/2019 01:37 PM - Artem Zhmurov

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

#4 - 03/13/2019 07:10 PM - Artem Zhmurov

- Description updated

I have LINCS with some tests for it, SETTLE with some tests for it and Leap-Frog integrator with some tests for it. Now I combine them into one
"Update and Constrain" module. Any ideas for the test that the merge was successful?

#5 - 03/13/2019 07:12 PM - Artem Zhmurov

- Subject changed from CUDA GPU-only loop to CUDA Update and Constraints module

- Description updated

#6 - 03/21/2019 08:43 PM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue [#2888](#).
Uploader: Artem Zhmurov (zhmurov@gmail.com)
Change-Id: gromacs~master~l8730aad0ecaa0230686fe89d1157b0da2f01f7bc
Gerrit URL: https://gerrit.gromacs.org/9329

#7 - 03/21/2019 10:35 PM - Artem Zhmurov

- Description updated

#8 - 03/22/2019 02:10 PM - Artem Zhmurov

- Description updated

#9 - 04/24/2019 11:32 PM - Artem Zhmurov

- Description updated

#10 - 04/24/2019 11:32 PM - Artem Zhmurov

- Description updated

#11 - 04/29/2019 11:10 AM - Szilárd Páll

- Related to Task #2936: introduce check that CPU-GPU transfers are made between arrays of compatible types added

#12 - 08/08/2019 10:47 AM - Artem Zhmurov

- Description updated

#13 - 09/19/2019 02:13 PM - Artem Zhmurov

- Description updated

#14 - 10/08/2019 03:09 PM - Artem Zhmurov

- Description updated

#15 - 10/22/2019 12:20 AM - Szilárd Páll

- Related to Task #3171: schedule CPU H2D force contribution in separate stream added

#16 - 11/01/2019 09:22 PM - Szilárd Páll

- Related to Task #3195: assess nightly master failures added