

## GROMACS - Feature #2885

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

### CUDA version of LINCS

03/08/2019 04:19 PM - Artem Zhmurov

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	Artem Zhmurov
<b>Category:</b>	core library
<b>Target version:</b>	2020
<b>Difficulty:</b>	uncategorized
<b>Description</b> Adapt the LINCS constraints to work efficiently on CUDA-enabled GPUs.  TODO: <ul style="list-style-type: none"><li><del>A separate class that contains the logic.</del></li><li>Reduction for the virial using shuffle.</li><li>PLINCS.</li><li>Many-GPU version.</li><li>Free energy.</li></ul> Ideas for kernel improvement: <ul style="list-style-type: none"><li>Use analytical solution for matrix A inversion (for small matrices of H-bonds constraints), inverted matrix itself can be reused rather than recomputed.</li><li>Move more data to local/shared memory and try to get rid of atomics (at least on the device level).</li><li>Use locality of coupled constraints better (maybe go from block-sync to warp-sync)</li><li>Introduce mapping of thread id to both single constraint and single atom, thus designating Nth threads to deal with Nat &lt;= Nth coupled atoms and Nc &lt;= Nth coupled constraints.</li></ul> Testing: <ul style="list-style-type: none"><li><del>Initial integration to the constraints test.</del></li><li>Add bigger systems to test virial reduction and overall redistribution of constraints among threads.</li><li>Generalization of tests for different platforms.</li></ul> Current version of the code is in gerrit change 9193 ( <a href="https://gerrit.gromacs.org/#/c/9193/">https://gerrit.gromacs.org/#/c/9193/</a> ).	
<b>Related issues:</b>	
Related to GROMACS - Feature #2886: CUDA version of SETTLE	<b>New</b>
Related to GROMACS - Feature #2887: CUDA version of Leap Frog algorithm	<b>New</b>
Related to GROMACS - Feature #2888: CUDA Update and Constraints module	<b>New</b>

### Associated revisions

#### Revision 0a1aae78 - 04/28/2019 05:29 PM - Artem Zhmurov

CUDA version of LINCS constraints.

Implementation of the LINCS constraints for NVIDIA GPUs. Currently works isolated from the other parts of the code: coordinates and velocities are copied to and from GPU on every integration timestep. Part of the GPU-only loop. Loosely based on change 9162 by Alan Gray. To enable, set the environmental variable GMX\_LINCS\_GPU.

Limitations:

1. Works only if the constraints can be split in short uncoupled groups (currently < 256, designed for H-bonds constraints).
2. Does not change the matrix inversion order for constraints triangles.
3. Does not support free energy computations.

4. Assumes no communications between domains (i.e. assumes that there is no constraints connecting atoms from two different domains).
5. Number of thread per blocks should be a power of 2 for reduction of virial to work.

TODOs:

1. Move more data from the global memory to local.
2. Change .at() to []
3. Add sorting by the number of coupled constraints to decrease warp divergencies.
4. numAtoms should be changeable (for multi-GPU case).

Refs #2816, #2885

Change-Id: I3c975cf898053b7467bcd30459e60ce2c8852be6

#### **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

## **History**

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

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

### **#2 - 03/08/2019 05:06 PM - Artem Zhmurov**

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

### **#3 - 03/08/2019 05:06 PM - Artem Zhmurov**

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

### **#4 - 03/08/2019 05:11 PM - Artem Zhmurov**

- Description updated

### **#5 - 03/12/2019 01:33 PM - Artem Zhmurov**

- Description updated