

GROMACS - Feature #2887

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

CUDA version of Leap Frog algorithm

03/08/2019 04:21 PM - Artem Zhmurov

Status:	New	
Priority:	Normal	
Assignee:	Artem Zhmurov	
Category:		
Target version:	2020	
Difficulty:	uncategorized	
Description		
<p>The initial implementation works independently from other parts of the code, which require a temporary infrastructure to hide CUDA-specific types from CPU compiler, manage coordinates, velocities and forces, handle periodic boundary conditions. It is enabled by setting environmental variable "GMX_INTEGRATE_GPU".</p>		
TODO:		
<ul style="list-style-type: none">Initial implementation as a stand-alone class.Make sure that all not supported cases exit with error.Temperature control.Pressure control.		
Tests:		
<ul style="list-style-type: none">Tests against the exact solution of constant force case.Unify tests with the CPU version.		
Related issues:		
Related to GROMACS - Feature #2885: CUDA version of LINC5		New
Related to GROMACS - Feature #2886: CUDA version of SETTLE		New
Related to GROMACS - Feature #2888: CUDA Update and Constraints module		New

Associated revisions

Revision d061dec5 - 05/12/2019 01:44 PM - Artem Zhmurov

CUDA version of Leap-Frog integrator with basic tests

Part of the GPU-only loop. Current version is as a stand-alone module, with its own coordinate, velocities and forces data management. To activate, set environment variable GMX_INTEGRATE_GPU.

Limitations:

- Only basic Leap-Frog is implemented.
- No temperature control.
- No pressure control.

Refs #2816, #2887

Change-Id: I439d7f5fd4f69a17ca7aaa412e242ce5e3aa5dbd

Revision a80b9cef - 08/13/2019 04:14 PM - Artem Zhmurov

Make use of reference data in integrator tests

Current version of tests is based on exactly solvable model, which does not allow for testing more sophisticated cases, including when temperature or pressure control is enabled. This commit adds the tests that are based on the reference data, which can be generated for any existing use-case.

Refs. #2816, #2887.

Change-Id: I64bb2326b0adf44be8b48449ef09cd26939ea467

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

History

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

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

#2 - 03/11/2019 11:53 AM - Artem Zhmurov

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

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

- Description updated

#4 - 03/13/2019 01:37 PM - Artem Zhmurov

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

#5 - 03/21/2019 10:36 PM - Artem Zhmurov

- Description updated

#6 - 08/08/2019 10:47 AM - Artem Zhmurov

- Description updated

#7 - 10/02/2019 12:00 PM - Artem Zhmurov

- Description updated