Gromacs - Task #1852
Remove group scheme
11/10/2015 07:57 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>New</th>
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<tbody>
<tr>
<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>mdrun</td>
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<td>Category:</td>
<td>mdrun</td>
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<td>Target version:</td>
<td>2016</td>
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Description
This can be done once we've

- deployed new SIMD layer (work in gerrit now)
- deployed new Verlet kernel generation (TODO after the above)
- decided how to read tables from grompp or mdrun for the Verlet scheme (some work in Gerrit now)
- got GPU and CPU kernels working for user tables (some work in Gerrit now, none for CPU)
- got no-PBC simulations working (in Gerrit now)

Anything else?

We can remove AdResS in advance, for the little bit that that helps.

Associated revisions
Revision 85d918db - 11/15/2015 08:18 PM - Mark Abraham
Remove AdResS

This feature will disappear with the group scheme, so we might as well get it out of the way first. Doing this removal on its own might help re-implement some time, if someone was keen.

Removed bVir, bPress, bSurft fields of t_mdebin, because all MD algorithms now support such calculations.

gmx grompp now issues a fatal error if the main adress .mdp option is on, and otherwise ignores the obsolete fields (like we do with other .mdp options we've removed).

mdrun can read old .tpr files, but issues a fatal error if AdResS was active in them.

gmx dump and gmx compare ignore all AdResS related fields.

Other tools can still read such .tpr files for their other content.

Removed Sebastian Fritsch from GROMACS 2016 contributor list, since he only worked on AdResS features. Christoph Junghans made other contributions that are still useful, and so remains.

Removed obsolete literature references

Also fixed some incorrect doxygen of init_forcerec().

Part of #1852

Change-Id: 122fa0fe480148aeda0ace194646a5ec2f3d20a8c
We're not likely to have any kind of twin-range / MTS support by the time we ship GROMACS 2016, so there's a bunch of old .tprs that can no longer be run. I don't think it is wise to run pre-4.6 .tpr files that happen to use a single-range scheme that happens to fit the requirements of the Verlet scheme, because any such simulations were semantically different (no buffer) and can't be compared with new ones. Defaulting them to a no-buffer version of the Verlet scheme is not terrible, but such simulations are arguably wrong, and they still always get a potential shift and so aren't readily comparable. So, I think there is a serious case for mdrun in GROMACS 2016 to refuse to run all pre-4.6 .tpr files. I see this very much as a step in the direction of "correct by default," and I'd certainly put that objective before "forward compatible .tpr files." (Of very much secondary concern is that this lets us remove small amounts of code that supports reading such files.)