Gromacs - Bug #1117
Feature # 1292 (Closed): mdrun features to deprecate for 5.0
Feature # 1500 (New): Post-5.0 feature clean-up plan

ensemble-averaged distance restraints is probably broken
01/14/2013 12:18 AM - Mark Abraham

Status: Blocked, need info
Priority: Low
Assignee: 
Category: 
Target version: future
Affected version - extra info: 
Affected version: 4.6.1

Description
This feature predates a lot of parallelism implementations and (IIRC) the REMD implementation (with which it shares the use of -multi), so the assumptions under which it was written are probably broken by now. I suspect, but cannot test, that it does not work with more than one process per simulation.

If this isn't important functionality for anyone, it might not make the cut for 5.0

Associated revisions
Revision 64600020 - 01/14/2013 12:21 AM - Mark Abraham
Updated code checks with distance restraints

Ensemble-averaged distance restraints require -multi, and it is also reasonable to do REMD with distance restraints, which also requires -multi. So checks for the ensemble-averaging case need to be more sensitive to their context.

In fact, ensemble-averaging is probably functional only with PD and one processor per system, since that was probably all that was available when it was built.

Fixes #613, refs #1117
Change-Id: Ia6f1bb4eb82eab3c7c249638cd3a5a5d1f707132

History

#1 - 05/22/2013 05:50 AM - Mark Abraham
- Target version changed from future to 5.0
- Affected version set to 4.6.1

That is, might get axed for 5.0

#2 - 05/13/2014 10:08 AM - Mark Abraham
Unless someone is able to give me an ensemble-averaging input set that works on ~4.6, then I won't be able to take any responsibility for what might happen to this code in the future from side effects of other changes ;-) 

#4 - 06/12/2014 12:08 AM - Erik Lindahl
Nobody seems interested in helping with it, so I think it's time we kill the feature ;-) 

#5 - 08/08/2014 04:14 PM - dawei li
As mentioned elsewhere, current distance restraints doesn't support DD. However, it works fine if only opemmp (plus GPD) is used to do parallel run, per my test.
It seems not hard to improve the code so that restraints energy is communicated between copies using MPI and each copy only use (openmp+GPU).

I need this feature very much. Otherwise I have to use Charmm, which is too slow.
Is there any possibility to fix this instead of drop it? Thanks.

#6 - 08/08/2014 04:24 PM - Mark Abraham

dawei li wrote:

As mentioned elsewhere, current distance restraints doesn't support DD. However, it works fine if only opemmp (plus GPD) is used to do parallel run, per my test.
It seems not hard to improve the code so that restraints energy is communicated between copies using MPI and each copy only use (openmp+GPU).

I need this feature very much. Otherwise I have to use Charmm, which is too slow.
Is there any possibility to fix this instead of drop it? Thanks.

I don't understand what you have tested that works and what you think is broken but perhaps fixable. What is "GPD?"

One major barrier to anybody fixing anything is lack of a small-ish test case that someone would like to have working. Providing that would be a useful first step to seeing what is wrong and might be fixable.

#7 - 08/11/2014 04:18 PM - dawei li
Sorry for the typo. I means GPU.

This one works on both 4.6 and 5.0: simple distance (disre = simple) restraints and use only OPENMP for parallel. Hybrid code using both CPU and GPU is fine too.

For DD, both 4.6 and 5.0 require that two atoms from one restrained pair must be within the same domain. That is, you can't use MPI when doing restraints simulations.

So, the most easy way to include ensemble averaged restraints is to require number of copies equal to number of MPI ranks.

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**#8 - 08/16/2014 03:27 PM - Mark Abraham**

dawei li wrote:

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This one works on both 4.6 and 5.0: simple distance (disre = simple) restraints and use only OPENMP for parallel. Hybrid code using both CPU and GPU is fine too.

For DD, both 4.6 and 5.0 require that two atoms from one restrained pair must be within the same domain. That is, you can't use MPI when doing restraints simulations.

So, the most easy way to include ensemble averaged restraints is to require number of copies equal to number of MPI ranks.

OK, that confirms my suspicion, so I will make explicit the requirement that ensemble averaging works only with a single domain per simulation.

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**#9 - 12/21/2014 12:35 PM - Mark Abraham**

- Target version changed from 5.x to 5.1

I will do for 5.1 what I suggest in comment 8

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**#10 - 01/08/2015 11:57 AM - Mark Abraham**

Mark Abraham wrote:

dawei li wrote:

Sorry for the typo. I means GPU.

This one works on both 4.6 and 5.0: simple distance (disre = simple) restraints and use only OPENMP for parallel. Hybrid code using both CPU and GPU is fine too.

For DD, both 4.6 and 5.0 require that two atoms from one restrained pair must be within the same domain. That is, you can't use MPI when doing restraints simulations.
You can use MPI, you just can't have more than one domain (= MPI rank) per simulation. For a multi-simulation with distance restraints and not replica-exchange, you thus must have as many MPI ranks as simulations, so that each simulation has one rank and thus one domain.

So, the most easy way to include ensemble averaged restraints is to require number of copies equal to number of MPI ranks.

OK, that confirms my suspicion, so I will make explicit the requirement that ensemble averaging works only with a single domain per simulation.

This is already true, I fixed it in 64600020
dawei, what is stopping you from running ensemble-averaged restraints? What error message do you get? You need to compile with MPI, set up a multi-simulation, and run with GMX_DISRE_ENSEMBLE_SIZE environment variable equal to the number of simulations. I can't test that, because nobody has provided a set of inputs that should work. If it's important to be able to run this kind of simulation, please provide a set of inputs (e.g. Verlet-scheme .tpr files) that you think should work. Otherwise, it's not worth my time to do anything other than remove the feature. :-)

#11 - 06/05/2015 07:33 PM - Erik Lindahl
- Status changed from New to Blocked, need info
- Target version changed from 5.1 to future

No feedback in five months, so this will no longer be relevant for 5.1, and unless there is feedback I'd suggest we axe the feature for 6.0.