Use of GB in parallel and/or with all-vs-all kernels needs a mention in the manual

05/17/2011 11:25 AM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: documentation
Target version: future

Description
Currently, I think the manual makes no mention of any of the details of running Generalized Born calculations in parallel, nor about the use of the all-vs-all loops.

In particular, GB simulations without cut-offs using those loops silently trigger PD, which is confusing when PD-related error messages subsequently result. There's been at least one gmx-users thread because of it.

I think the correct person to whom to assign this is Per Larsson, but I don't think he's currently on the Redmine manual project. I'll email him so it comes to his attention.

Related issues:
Related to Gromacs - Feature #1292: mdrun features to deprecate for 5.0

Related to Gromacs - Feature #753

Closed 12/02/2012

History
#1 - 09/09/2011 03:15 AM - Mark Abraham
- Assignee set to Erik Lindahl
- Target version changed from 5.0 to 4.5.5

I got no reply from Per, so assigning to Erik instead.

#2 - 09/20/2011 05:18 PM - Rossen Apostolov
I contacted Per again, hope he'll include it.

#3 - 11/23/2011 07:25 PM - Szilárd Pál
- Target version changed from 4.5.5 to 4.5.6

#4 - 04/13/2012 03:10 PM - Rossen Apostolov
- Status changed from New to In Progress
- Assignee deleted (Erik Lindahl)

Below is what Per sent me about it. Where should we put that though, in the mdp-parameters section?

"Note: In some cases it is preferable to run implicit solvent simulations with longer cutoffs than for explicit solvent. Gromacs therefore comes with the option to run with infinite cutoffs using special optimized all-vs-all loops for implicit solvent. These loops are silently triggered by setting all relevant cutoffs to 0 in the mdp-file

nstlist = 0
rlist = 0
rcoulomb = 0
rvdw = 0
rgbradii = 0

It is possible to use the all-vs-all loops for parallel computations, but that will trigger particle decomposition rather than domain decomposition."
Parallel all-vs-all calculations are quite fast for small to medium sized systems, but performance will be drastically reduced as the system size is increased.

To run a parallel implicit-solvent calculation with domain decomposition, the cut-offs have to be finite.

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#5 - 04/13/2012 04:05 PM - Justin Lemkul
It seems to me that this discussion is relevant in section 3.16, where PD is introduced. It is stated in section 3.15 that particle decomposition is useful "for a few special cases." I think that's what's being referred to. It would also be worth mentioning the fact that PD and all-vs-all kernels are not just relevant to GB simulations, but also those done in vacuo. Perhaps the text can be generalized in that way, with forward references to sections regarding GB simulations and the appropriate .mdp settings.

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#6 - 01/17/2013 09:53 PM - Mark Abraham
- Assignee set to Mark Abraham
- Target version changed from 4.5.6 to 4.5.7

#7 - 04/29/2013 06:54 PM - Mark Abraham
- Target version changed from 4.5.7 to 4.6.2

#8 - 04/29/2013 06:54 PM - Mark Abraham
- Target version changed from 4.6.2 to 4.6.3

#9 - 06/26/2013 12:46 AM - Mark Abraham
- Target version changed from 4.6.3 to future

It seems we may as well deprecate GB, since it received no maintenance in the pre-4.6 cycle and isn't likely to get any this year either.

#10 - 04/16/2014 01:18 PM - Rossen Apostolov
- Related to Feature #1292: mdrun features to deprecate for 5.0 added

#11 - 04/16/2014 01:19 PM - Rossen Apostolov
- Related to deleted (Feature #1292: mdrun features to deprecate for 5.0)

#12 - 04/16/2014 01:19 PM - Rossen Apostolov
- Related to Feature #1292: mdrun features to deprecate for 5.0 added

#13 - 04/16/2014 01:22 PM - Rossen Apostolov
- Status changed from In Progress to Resolved

added the issue as related to #1292, resolving here

#14 - 05/12/2014 10:24 AM - Rossen Apostolov
- Status changed from Resolved to Closed

#15 - 05/23/2014 02:02 PM - Rossen Apostolov
- Project changed from Documentation to Gromacs
- Category changed from manual and in-source to documentation

the issue was moved to project "Gromacs", category "documentation", and the original sub-project "Documentation" was removed.