GROMACS - Bug #552

sundry documentation issues

09/09/2010 06:11 AM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Rossen Apostolov
Category: documentation
Target version: 
Affected version - extra info: 
Affected version: N/A

Description

- The manual section in forcefields.tex on optimizing Fourier transforms is out of date. 11 and 13 are no longer accepted, and I understand there are situations under which using optimize_fft is known not to be useful
- 3.15 Parallelization needs to mention threading, and that threading and MPI cannot coexist (as I understand things)
- grompp should flag the user when the estimated PME load is outside the recommended 25%-33% zone. A comment with "note" severity seems in order to me.
- Appendix A1 should refer to the wiki page
- Appendix A3 needs to mention threads as well as MPI, and A3.1 is approaching obsolescence
- Appendix A4, the list of influential environment variables, is probably complete as far as it goes, but it seems a bit weird to list DUMPNL and not the ones for limiting solvent and kernel optimization, or DD-debugging, etc.
- Appendix A5 should be superseded by something on the wiki, or mention threads

Associated revisions

Revision 10384720 - 04/07/2011 03:34 PM - Justin Lemkul
Updates to the environment variables section of the manual.
I organized the list so it wasn't such a mash-up of random things, incorporating sections and adding a few useful environment variables.
Addresses a small part of IssueID #552

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Revision 8fe4088b - 06/17/2014 02:01 PM - Rossen Apostolov
Small changes in appendix A of the manual.
Final fixes #552.
Change-Id: l8e7939ae70eb14d2e1fc0a25b50774d472889bd1

Revision 6d6547c1 - 06/20/2014 10:04 AM - Rossen Apostolov
Removed unused parameters and cleanup of inputrec.
Removed optimize_fft, dihre_fc, nstcheckpoint.
Fixes #820, related to #552.

Change-Id: i8d1c3700834e5575972165410b3b29cbb56cba53

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**History**

#1 - 09/09/2010 08:57 PM - Berk Hess

MPI and threads are basically the same thing in version 4.5. There is a Gromacs library that does MPI through threads, so you don't need to compile in an external library and you don't need mpirun. But everything still uses MPI and the same parallelization scheme. This should be indeed be mentioned in the manual.

`grompp` prints a note when the pme load is more than 50%. Between 33% and 50% is fine when running on something like 1 to 4 cores inside a machine. Generating a note for something that you might actually want in many cases in not convenient. On the other hand the parallel performance might be lower, so I might want to reconsider this.

Berk

#2 - 09/10/2010 11:59 AM - Berk Hess

Just to be sure I ran the villin benchmark with different cut-off and grid spacings. On 4 cores of my Intel Core i7 the speed is significantly higher with a cut-off of 0.8 and a grid of 48^3. For those settings `grompp` reports a pme load of 0.52, but it turns out to be something like 0.47 (AMD is somewhat slower with PME though). I did not try even shorter cut-off's, since that would be bad for the LJ accuracy.

So we have the problem that serial or SMP PME is often fastest with a PME load of 50% or more, whereas highly parallel simulations run better with 25% to 33%. I don't know if we want `grompp` to print a note anyhow for the range from 33% to 50% (currently only above 50%). Do you have any suggestion?

PS We hope to resolve this in the future through combining MPI and "real" multi-threading.

Berk

#3 - 09/13/2010 11:08 AM - David van der Spoel

(In reply to comment #0)

- The manual section in `forcefields.tex` on optimizing Fourier transforms is out of date. 11 and 13 are no longer accepted, and I understand there are situations under which using `optimize_fft` is known not to be useful

Where does this notion come from? I couldn't find it on the fftw website. Or is it something that gromacs actively disallows?

- 3.15 Parallelization needs to mention threading, and that threading and MPI cannot coexist (as I understand things)
- `grompp` should flag the user when the estimated PME load is outside the recommended 25%-33% zone. A comment with "note" severity seems in order to me.
- Appendix A1 should refer to the wiki page

There is no wiki page anymore, that is [www.gromacs.org](http://www.gromacs.org) is now a wiki.

- Appendix A3 needs to mention threads as well as MPI, and A3.1 is approaching obsolescence
- Appendix A4, the list of influential environment variables, is probably complete as far as it goes, but it seems a bit weird to list DUMPNL and not the ones for limiting solvent and kernel optimization, or DD-debugging, etc.

I added some, but the DD ones are really incomprehensible to most people.

- Appendix A5 should be superseded by something on the wiki, or mention threads
It's not really wrong, is it?

#4 - 09/20/2010 04:08 PM - Rossen Apostolov
changing to minor severity (but should fix it soon :) )

#5 - 02/23/2011 03:00 AM - Szilárd Pál
- Target version deleted (CVS)

#6 - 04/11/2012 11:28 AM - Rossen Apostolov
- Project changed from GROMACS to Documentation
- Category deleted (documentation)

Moved to documentation

#7 - 05/23/2014 02:02 PM - Rossen Apostolov
- Project changed from Documentation to GROMACS
- Category set to documentation
- Affected version set to N/A

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

#8 - 06/05/2014 01:42 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #552.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-id: 8d1c3790634e5575972165410b93b29cb56c6ba53
Gerrit URL: https://gerrit.gromacs.org/3549

#9 - 06/17/2014 02:02 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #552.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-id: b8e7939ae70eb14d2e1fd0a25b50774d472889bd1
Gerrit URL: https://gerrit.gromacs.org/3605

#10 - 06/17/2014 02:02 PM - Rossen Apostolov
- Status changed from New to Fix uploaded
- Assignee changed from David van der Spoel to Rossen Apostolov

#11 - 06/17/2014 03:00 PM - Rossen Apostolov
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 8fe4088bf76d1f72847fe43e388e06f414f8ce83

#12 - 06/17/2014 03:01 PM - Rossen Apostolov
- Status changed from Resolved to Closed