GROMACS - Task #1069
Appendix A overhaul
12/11/2012 08:08 PM - Justin Lemkul

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>documentation</td>
</tr>
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<td>Target version:</td>
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<td>Difficulty:</td>
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### Description

Before we release an official 4.6 version, Appendix A of the manual needs a major revision. Specific tasks:

1. Section A.3 may need revisions based on more modern requirements (Minimum recommended/necessary gcc/icc/whatever? Is Fortran relevant? CUDA/GPU requirements?)
2. Section A.3.1 needs to at least reflect the fact that some functions are no longer in network.h
3. Section A.4 may need updating as (I think) more environment variables have been added since I wrote the new section
4. Section A.5 needs to be scrapped and completely overhauled to describe the new hybrid parallelization scheme

I’ll assign this to Mark for now to be delegated as needed. I’m happy to help, as well, if there are things I can do.

### Associated revisions

**Revision c64f4e5d - 01/07/2013 05:33 PM - Justin Lemkul**

Extended environment variable documentation.

Several items have yet to be described or are only partially described, as the authors of that code will have to contribute that information.

Partial fix for #1069.

Change-Id: I9221d932dd26a73bad7ee42d099109086de29e97

**Revision ff2f6cd7 - 03/05/2013 04:37 PM - Justin Lemkul**

Revisions to environment variable section.

Also removed env. vars. that were not specific to Gromacs, per previous feedback.

Partial fix for #1069.

Change-Id: Idd6cb4ce37c7359020e23254c4b93407a37b89e

**Revision d708c6b1 - 05/25/2014 12:58 AM - Rossen Apostolov**

Simplified section “Porting”.

Fixes #1069.

Change-Id: I01578dfe27585f5c5cc81ce9f564e9586c60a3ed

### History

**#1 - 01/07/2013 02:07 PM - Mark Abraham**

Justin Lemkul wrote:

Before we release an official 4.6 version, Appendix A of the manual needs a major revision. Specific tasks:

A.1 and the start of A.2 also need total re-writes.

1. Section A.3 may need revisions based on more modern requirements (Minimum recommended/necessary gcc/icc/whatever? Is Fortran relevant? CUDA/GPU requirements?)
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Agreed all need extensive work.

A.3.1 will disappear.

If Justin could start on A.4, that would be great. grep, sort and uniq should be good to find the new variables and let you make at least a stub gerrit patch with as much as you can put together and TODOs elsewhere. If the use of any variables isn't clear from the code, then I will nag the authors to comment their code and update that gerrit patch.

For A.5 I am tempted to remove much of the related wiki material and put it here, and replace the wiki material with something simpler (per #1076) that references this section. There's no getting away from the fact that getting near-maximum performance will require user investment, but we don't want to force alphabet soup on people who just want to know whether X exists.

#2 - 01/07/2013 02:08 PM - Mark Abraham
Berk can you please edit manual section A.2 on single or double precision, to reflect any changes relevant with the use of Verlet kernels?

#3 - 01/07/2013 02:12 PM - Justin Lemkul
Mark Abraham wrote:

Justin Lemkul wrote:

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Will do. I will try to have something uploaded to Gerrit in the next day or two.

For A.5 I am tempted to remove much of the related wiki material and put it here, and replace the wiki material with something simpler (per #1076) that references this section. There's no getting away from the fact that getting near-maximum performance will require user investment, but we don't want to force alphabet soup on people who just want to know whether X exists.

Definitely agree. The learning curve nowadays is a bit steeper (by necessity) so whatever baseline information we can provide will be useful.

#4 - 01/07/2013 05:37 PM - Justin Lemkul
Updated environment variables posted in https://gerrit.gromacs.org/#/c/1998/. I tried to add Mark as a reviewer, but for some reason Gerrit says he's not valid. Added reviewers who should be able to contribute to the noted TODO items (mostly in CUDA and GPU stuff that's over my head at the moment).

#5 - 01/18/2013 03:26 PM - Erik Lindahl
- Target version changed from 4.6 to 4.6.1

#6 - 01/18/2013 03:40 PM - Justin Lemkul
We're planning to release 4.6 without an accompanying manual?

#7 - 01/21/2013 10:05 AM - Berk Hess
I pushed up an update to the installation section: https://gerrit.gromacs.org/#/c/2107/
I think we should avoid putting too much detail in there, as this stuff is more suited for a wiki.

#8 - 01/21/2013 10:49 AM - Berk Hess
- Status changed from Feedback wanted to In Progress

I added more information and the term mixed precision in the install section of the pdf manual: https://gerrit.gromacs.org/#/c/2107/
I don't think it occurs anywhere else in the pdf manual.
I also updated: http://www.gromacs.org/Documentation/Terminology/Precision
We should check if there are more places where single precision is mentioned.

#9 - 02/18/2013 04:06 PM - Berk Hess
I think I addressed most, if not all of this, but I wasn't aware of the redmine issue.
Can we close this?

#10 - 02/18/2013 07:25 PM - Justin Lemkul
I think the only item that really remains to be addressed is in Appendix A.3. I'm not sure the requirements listed there are correct any more, and perhaps we should specify some minimum version numbers? I know that becomes a slippery slope in a sense, but we do know of real issues with some older versions of gcc and icc. I don't think it's quite correct any more to simply say "you need a C compiler." Also, we should probably remove A.3.1 altogether. After that, I think the Appendix is reasonably up-to-date.

#11 - 04/29/2013 08:05 PM - Mark Abraham
- Target version deleted (4.6.1)

#12 - 05/23/2014 02:29 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1069.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-id: I01578dfe27585f5c5cc81ce9f9564e9586c60a3ed
Gerrit URL: https://gerrit.gromacs.org/3492

#13 - 05/23/2014 02:30 PM - Rossen Apostolov
- Status changed from In Progress to Fix uploaded

I simplified section A3 in the 5-0 branch, we can leave 4-6 as is.

#14 - 05/25/2014 01:15 AM - Rossen Apostolov
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset d708c6b1324168d07c9c1c6c18601d250b62d394.

#15 - 06/05/2014 11:35 AM - Rossen Apostolov
- Status changed from Resolved to Closed