Gromacs - Task #1696

FFTW auto-build and advice is no longer generally applicable

03/03/2015 02:53 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<td>Priority:</td>
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<tr>
<td>Assignee:</td>
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<td>Target version</td>
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**Description**

Recent testing on Haswell suggests both that use of hyperthreads and FFTW compiled with AVX can be beneficial, so we need to try to update our build-own-fftw and build-system advice to be a bit more applicable. (Rossen should have some of our own performance results here, but I haven't seen them yet.)

In particular, Cray's modified FFTW might have properties different from standard FFTW, and it would be nice to have a hint in the install guide about which is best to use, and the best way to configure and run on Crays.

**Associated revisions**

Revision 31bdfce0 - 06/16/2015 10:25 PM - Erik Lindahl

Updated FFTW recommendations in install-guide.

Both SSE2 and AVX should be used, and there is now info about the upcoming FFTW-3.3.5 with more SIMD support, as well as a link to an unofficial prerelease on the gmx site.

Fixes #1696.

Change-id: l6413d5e0e06c78a3c9f62acbf6fa0bfc1bd0a561

**History**

#1 - 04/14/2015 02:30 PM - Mark Abraham

- Description updated

#2 - 06/06/2015 11:22 PM - Justin Cook

I've notified a developer about the questions in this bug and will provide feedback when possible.

Thanks.

#3 - 06/12/2015 11:35 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1696.

Uploader: Erik Lindahl (erik.lindahl@gmail.com)

Change-id: l6413d5e0e06c78a3c9f62acbf6fa0bfc1bd0a561

Gerrit URL: https://gerrit.gromacs.org/4713

#4 - 06/12/2015 11:36 PM - Erik Lindahl

- Status changed from New to Fix uploaded
#5 - 06/16/2015 10:25 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#6 - 06/16/2015 10:25 PM - Erik Lindahl
- Status changed from Resolved to Closed