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 31bdfe0 - 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: i6413d5e0e06dcb8ab74620b0f0a561

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: i6413d5e0e06dcb8ab74620b0f0a561
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