Add CMake support for external LAPACK libraries

Hi,

could you please add support for external LAPACK libraries in CMake, as was the case with autotools? Currently only the Apple and Intel proprietary libraries seem to be supported.

I'd think that support should be added for at least GotoBLAS and ATLAS, out of which the latter is more important due to its free license. I'd like to compile the Fedora packages against ATLAS.

Hi,

Unfortunately it seems that this report want unnoticed and we're planning to release 4.5.2 in a matter of minutes/hours. Unless you or someone else can contribute with a patch in max 30min this will not make it into the release.

Otherwise, I can look into this after the release.

Cheers,

Szilard

Hi,

Intel & apple are a bit special since we use those accleration libraries for FFTs; the BLAS support is just a bonus.

Normal simulations never use BLAS/LAPACK - it is only sparse matrix diagonalization for normal modes that benefit from it.

The big problem with BLAS is that there's no standard for the library names, so the only thing the option really does is to disable the corresponding built-in functions. Then the user will have to set the external libraries themselves, and I'm not sure how easy that is to do in cmake.

Anyway - i'm not sure the small gain is worth the effort and extra dependencies for you!

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#2 - 10/29/2010 05:27 PM - Erik Lindahl

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#3 - 01/24/2011 01:28 PM - Mark Abraham
There's some CMake updates from Christoph that improve things on the detection front. 26d8c915b3c0 in master or 36aa859b in release-4-5-patches.

Do these meet your desires, Jussi?

#4 - 01/24/2011 02:26 PM - Jussi Lehtola
Yes, looks like it should do the trick. I haven't tried it myself, though.

#5 - 02/23/2011 03:11 AM - Szilárd Páll
- Category changed from mdrun to build system
- Status changed from New to Feedback wanted
- Target version changed from 4.5.1 to 4.5.4

#6 - 06/08/2011 03:25 PM - Szilárd Páll
- Assignee set to Christoph Junghans
- Target version changed from 4.5.4 to 4.5.5

#7 - 06/08/2011 03:38 PM - Christoph Junghans
- Status changed from Feedback wanted to Closed
- % Done changed from 0 to 100

Done a long time ago, closing.