

GROMACS - Feature #912

include list of compiler flags in the binary version information

04/03/2012 03:27 PM - Szilárd Páll

Status:	Closed
Priority:	High
Assignee:	Erik Lindahl
Category:	build system
Target version:	4.6
Difficulty:	uncategorized
Description	
It would be highly beneficial to have the full list of compiler options recorded in the binaries and printed in the version information and/or the log file. This will enable identifying performance issues caused by incorrect or sub-optimal compiler optimizations (e.g. on Bulldozer -march=bdver1).	

Associated revisions

Revision 5ba7125c - 06/16/2012 10:02 PM - Erik Lindahl

New CPU detection & AVX/SSE code, removed raw assembly files.

Removed all raw assembly files and deprecated altivec support. Removed support for NASM and other assemblers, and replaced previous SSE detection code with a new module using CPUID instead. Added detection for SSE2, SSE4.1, AVX 128-bit with FMA, and AVX 256-bit. Added Cmake detection of build platform based on CPUID, and output this to the log file. The executables now compare the compile-time platform and selected acceleration with the run-time platform and most suitable acceleration and warns the user if they do not match. The compiler detection code has also been reordered slightly to produce more readable warnings when OpenMP is not available, and correctly disable pragma warnings.

Added intrinsics code and math functions for SSE2, SSE4.1, AVX128/256 both in single and double precision. All math functions and permutation code have been tested & verified. Single precision math functions are correct apart from the least significant bit, and double precision has roughly twice the accuracy.

This has forced me to temporarily disable the SSE & Fortran acceleration. SSE will be added back soon based on new intrinsics-only kernels currently in testing, and we will test if Fortran still makes sense then.

Finally, the patch includes a modification to gmx_rmsdist where a regression issue was introduced recently by using sqrtf() for the norm function. This caused the intel compiler to produce slightly different results at high optimization levels, which got evident here.

Closes #926 - Raw assembly code has been removed.
Refs #923 - Old kernels removed, new will be added shortly.
Fixes #914 - Cmake now does architecture-specific optimization.
Fixes #912, #913
Fixes #857 - We detect rdtscp support with CPUID and use it if possible.
Fixes #750
Closes #537, #574 - AltiVec is now deprecated.

Change-Id: Icfca5a940762f8d82ae67b59c65b2d2ac683256d

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History

#1 - 04/16/2012 05:05 PM - Rossen Apostolov

- Assignee changed from Rossen Apostolov to Erik Lindahl
- Priority changed from Normal to High

#2 - 06/23/2012 06:54 PM - Roland Schulz

- Status changed from New to Closed

Fixed by 5ba7125c.