Aldolase performance benchmarks

Source

RELION version: 3.1-beta-commit-9090fd
Precision: BASE=double, CUDA-ACC=single

Binaries:

Basic = Intel 2018 compiler but no cmake options
Accelerated = CC=mpiicc CXX=mpiicpc cmake -DCUDA=OFF -DALTCPU=ON -DCudaTexture=OFF -DMKLFFT=ON -D CMAKE_C_FLAGS="-O3 -ip -g -xCOMMON-AVX512 -restrict " -D CMAKE_CXX_FLAGS="-O3 -ip -g -xCOMMON-AVX512 -restrict " -DGUI=OFF -D CMAKE_BUILD_TYPE=Release ..

Currently Loaded Modules:
1) binutils/.2.30-GCCcore-7.3.0 (H)
2) GCCcore/7.3.0
3) icc/2018.3.222-GCC-7.3.0-2.30
4) ifort/2018.3.222-GCC-7.3.0-2.30
5) iccifort/2018.3.222-GCC-7.3.0-2.30
6) impi/2018.3.222-iccifort-2018.3.222-GCC-7.3.0-2.30
7) iimpi/2018b
8) imkl/2018.3.222-iimpi-2018b
9) intel/2018b

Hardware:

Broadwell = scarf17
Skylake = scarf18. 24 cores / node. 192 GB RAM per node.
Details at https://www.scarf.rl.ac.uk/scarf_hardware.html

OS

Login node:
Linux scarf.rl.ac.uk 3.10.0-1062.9.1.el7.x86_64 #1 SMP Fri Dec 6 15:49:49 UTC 2019 x86_64 x86_64 x86_64 GNU/Linux
PRETTY_NAME="CentOS Linux 7 (Core)"
Skylake compute node:
Linux cn846.scarf.rl.ac.uk 3.10.0-1062.18.1.el7.x86_64 #1 SMP Tue Mar 17 23:49:17 UTC 2020 x86_64 x86_64 x86_64 GNU/Linux
PRETTY_NAME="CentOS Linux 7 (Core)"

Cascade Lake nodes

RELION version 3.1.2-commit-dcab79 was built on the nextgenio Cascade Lake cluster. This is a slightly more recent version of RELION with a number of minor fixes, but it should not affect the benchmark timings significantly. Relion was built with acceleration options:

cmake -DTIFF_INCLUDE_DIR=/home/software/tiff/4.0.10/include
-DTIFF_LIBRARY=/home/software/tiff/4.0.10/lib/libtiff.so.5 -DALTCPU=ON -DMKLFFT=ON
-DFORCE_OWN_TBB=ON
-DCMAKE_INSTALL_PREFIX=/lustre/home/nx04/nx04/mfarsara/build/relion ..

The --cpu option was used at runtime for some, but not all, benchmarks. This is slightly different to SCARF where two different binaries were used.

Class 2D

job	binary	hardware	Tasks / threads	Nodes	pool	Runtime h:m	
job025	basic	Broadwell	9 / 6	3	3	27:17	
job063	basic	Skylake	9 / 6	3	3	23:12	Change CPU
job064	basic	Skylake	9 / 6	3	12	23:06	Change pool
job065	accelerated	Skylake	9 / 6	3	12	6:40	Change binary
job077	basic	Cascade	9 / 2	1	12	21 hrs (16 iterations)	
job079	accelerated	Cascade	9 / 2	1	12	2.5 hrs (5 iterations)	Change binary
job080	accelerated	Cascade	17 / 4	2	12	2.5 hrs (2 iterations)	No hyperthr.

Jobs 077, 079, 080 killed by system crash.

Class3D

job	binary	hardware	Tasks / threads	Nodes	pool	Runtime h:m	Top class

job039	basic	gpu	5 / 1 / 4 gpu	1	30	7:57	0.49
job066	basic	Skylake	9 / 6	3	30	34:32	0.45
job067	accelerated	Skylake	9 / 6	3	30	8:47	0.37
job075	basic	Cascade	9 / 2	1	30	1.7 days (17 iterations)	0.46

The column “Top class” shows the fraction of particles in the top class. This shows that the way a job is run can have an effect on the scientific results.
Job075 killed by system crash. Was not converged in terms of class occupancies.

Refine3D

job	**binary**	**hardware**	**Tasks / threads**	**Nodes**	**pool**	**Runtime h:m**	**Unmasked resolution**
job030	basic	gpu	5 / 1 / 4 gpu	1	30	16:16	4.55
job069	accelerated	Skylake	11 / 6	3	30	35:00	4.55
job073	basic	Cascade	33 / 2	2	30	2 days (11 iterations)	4.62

The non-accelerated run on CLX did not complete. From the reported resolution, it was getting close after 2 days and 11 iterations.