

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)"

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

Class3D

job	binary	hardware	Tasks / threads	Nodes	pool	Runtime h:m	
job039	basic	gpu	5 / 1 / 4 gpu	1	30	7:57	
job066	basic	Skylake	9 / 6	3	30	34:32	
job067	accelerated	Skylake	9 / 6	3	30	8:47	

Refine3D

job	binary	hardware	Tasks / threads	Nodes	pool	Runtime h:m	
job030	basic	gpu	5 / 1 / 4 gpu	1	30	16:16	
job069	accelerated	Skylake	11 / 6	3	30	35:00	