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# Cluster performance, how to get the most out of Abel

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# Introduction

- Smarte queueing
- Smart job setup
- Scaling
- Effective IO
- Big data handling
- Compiler usage
- Programming for the future

# Smart queueing

# Smart queueing

- Exclusive or none-exclusive ?
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- Exclusive
  - --ntasks-per-node=16 (or 20 for rack 31)
  - --nodes=n
- None-exclusive
  - --ntasks=m

# Smart job setup

- Ask only for what you really need
- Stage data smart
- Carefully consider the IO load
- Have you control over scaling and input ?
- What happen if your job crashes or is killed ?
- What about log files ?

# Ask only for what you need

- Queue system allocate and prioritise based on your footprint
- Footprint is based on
  - number of cores/nodes
  - Memory
  - Wall time

- Large footprint means longer wait time in queue

# Stage data smart

- /work is faster and larger than /cluster
- There is NO backup on /work
- $SCRATCH is on /work
- $SCRATCH is deleted when job is finished
- /work/users/<your user name> is available
  - Files are kept for 45 days, no backup
- /project is slow, stage files on /work

# Carefully consider the IO load

- /project is slow and not part of Abel
- /cluster is backed up and high performance
- /work is not backed up and has even higher performance
- Backup cannot tackle millions of files
- Small log files are ok on /cluster/home
- Large files should be on /work
  - $SCRATCH for temporary scratch files
  - /work/user/<username> for log files
- Files on /work/users are **deleted** after 45 days
  - Touching the files does not prevent this !

# Carefully consider the IO load

- /cluster and /work file system are unhappy with millions of small files

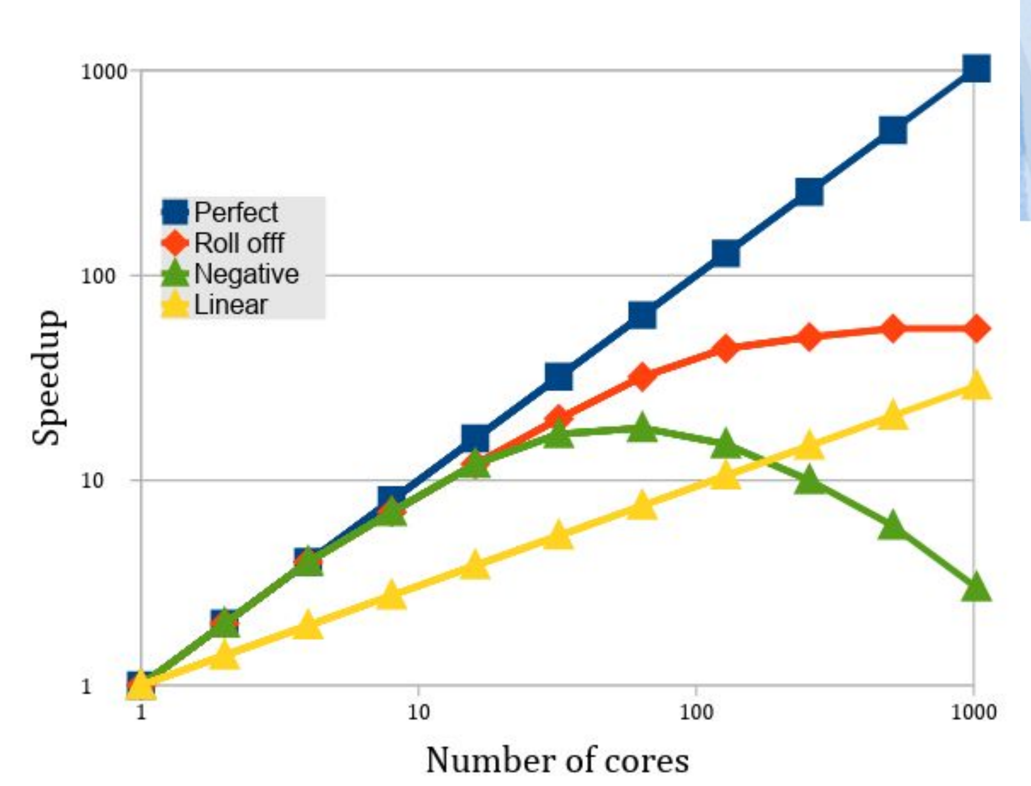
- If you use millions of temporary files ask for local scratch named $LOCALTMP
  - --gres=localtmp:x (x is in GiB)
  -

- Backup system are unhappy with millions of small files
  - Use a directory called nobackup or /work

# Have you control over scaling and input ?

- Does your application scale ?
- Does it scale to the core count you request?
- Does it scale with the given input ?

- OpenMP threads
- MPI ranks
- Hybrid (multi threaded
  - MPI executables)



# MPI Vs OpenMP

- MPI stands for Message Passing Interface. It is a set of API declarations on message passing (such as send, receive, broadcast, etc.), and what behavior should be expected from the implementations.
  - Many nodes many threads
  - OpenMPI is MPI (not OpenMP)

- OpenMP is an API which is all about making it (presumably) easier to write shared-memory multi-processing programs.
  - One node many threads

# What happen if your job crashes or is killed ?

- If you application crashes everything works as if it terminated normally
-
- If your job is killed (memory, time limit etc)
  - chkfile <file> work as expected
  - Directory $SCRATCH is removed
  - Files on $SCRATCH are lost
  -

# What about log files ?

- Log files can reside on /cluster/home or /work
  - No need to use $SCRATCH for them
  - Logs of reasonable size on $SUBMITDIR

- If log files are written to $SCRATCH remember to use chkfile

- Log files are required when reporting problems (RT)

# Effective IO

- How much IO is your application doing ?
- Few large files or millions of small files ?
- Where are the files placed ?
- Copying of files
- Archiving many files to one large
- Do the files compress ?
  - Not all files compress well

# Effective IO

- /work and /cluster are global parallel file systems, BeeGFS.
- In order to make it coherent locks and tokens are needed.
- Any operation must be locked to prevent corruption if more than one writer want to update a file
- All parallel file systems struggle to cope with huge amount of metadata updates.
- They love few large files !

# Effective IO

- Use $SCRATCH or /work/users/ during runs
- Use $LOCALTMP for millions of files
  - Make a tar archive of these before moving them to /work or /cluster
- Stage files from /projects to /work/users
  - /project has limited bandwidth

# Big data handling

- Few large files or millions of small files ?
- BeeGFS can handle large files easy
  - Bandwidth like 8-10 GiB/s
  - /work have higher bandwidth than /cluster

- Use infiniband if possible
  - scp file.ext  <host ib ip number>:
  - Doubles the transfer speed

# Big data handling

- Many small files are problematic
- Backup system struggle with millions of files
- BeeGFS struggle with metadata of millions of entries
- Make archives of directories with large number of files
- Use local scratch or temporal storage of possible
  - These sizes are relatively small
  - Tar directory to a single large file

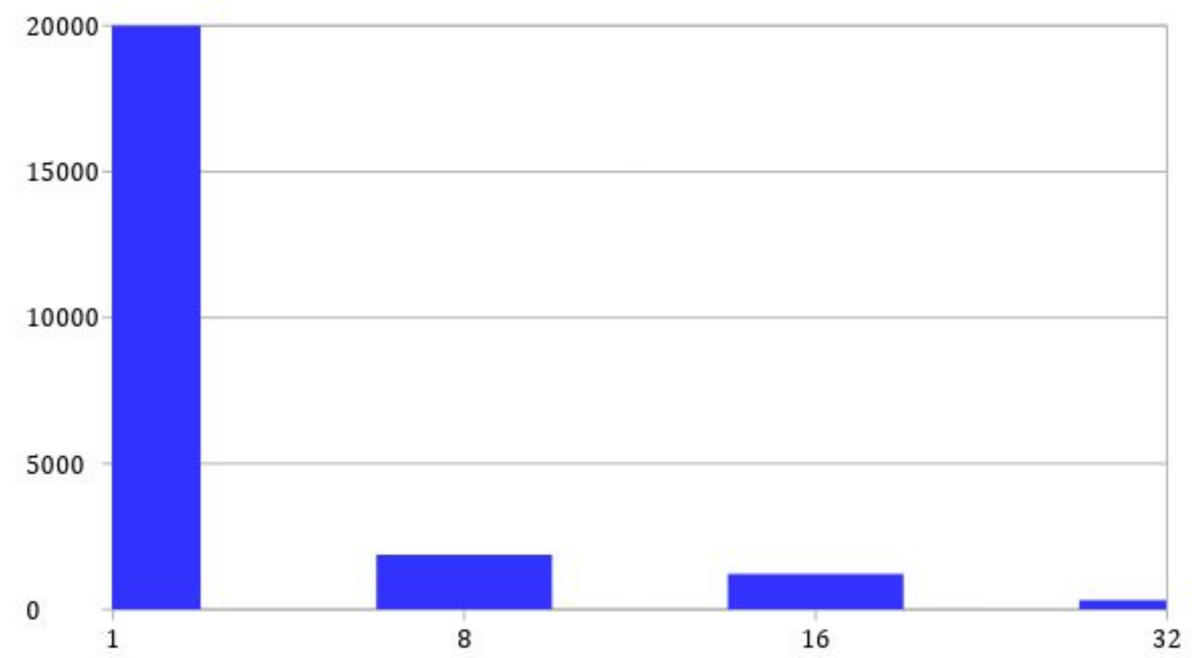
- Mount an image on /work as a file system
  - Require help from support team

# Big data handling

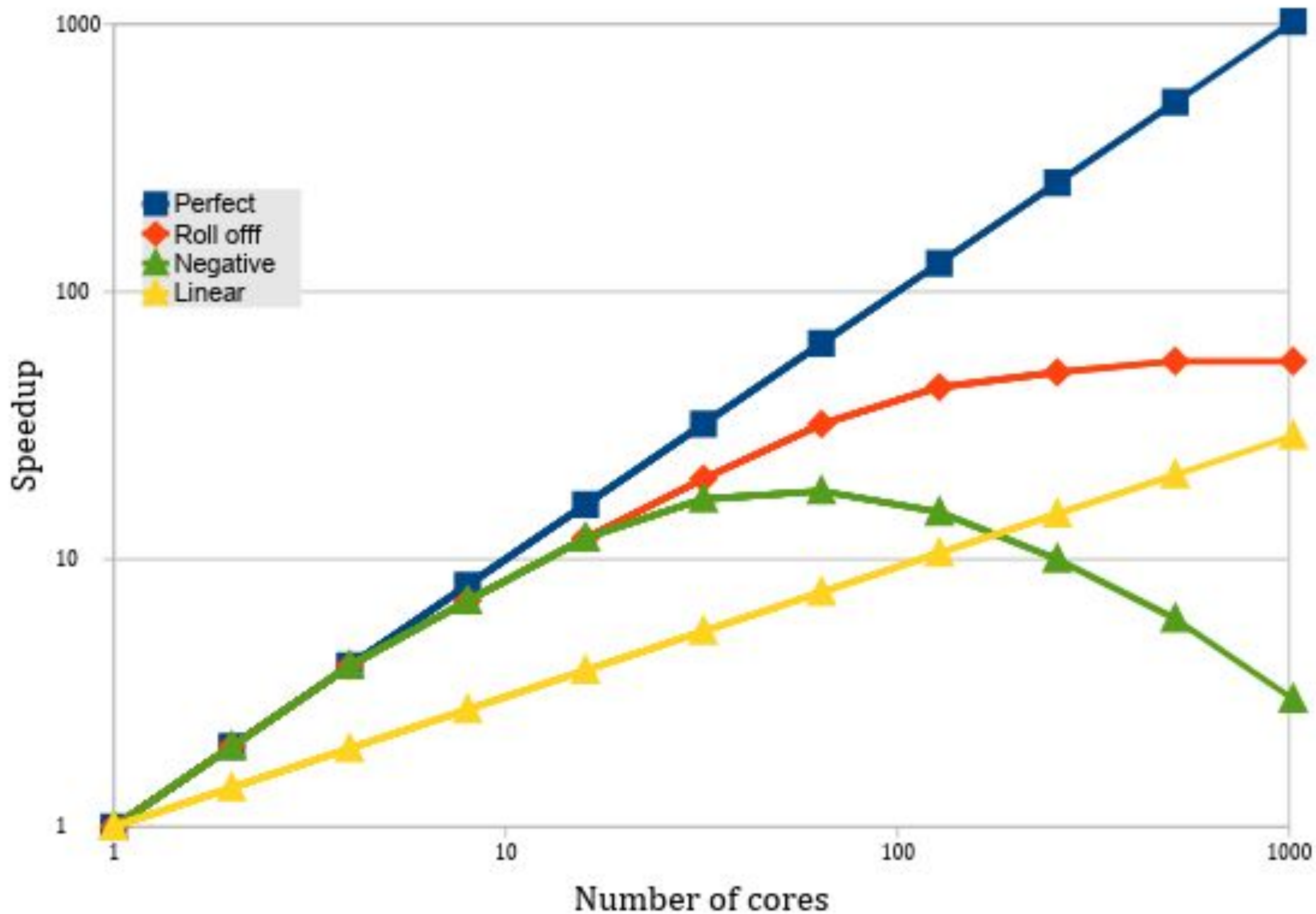
- Copying of millions of files are slow
- Rsync may take hours
- Option to use parallel rsync

- 1: rsync
- 

2-32 : parsync

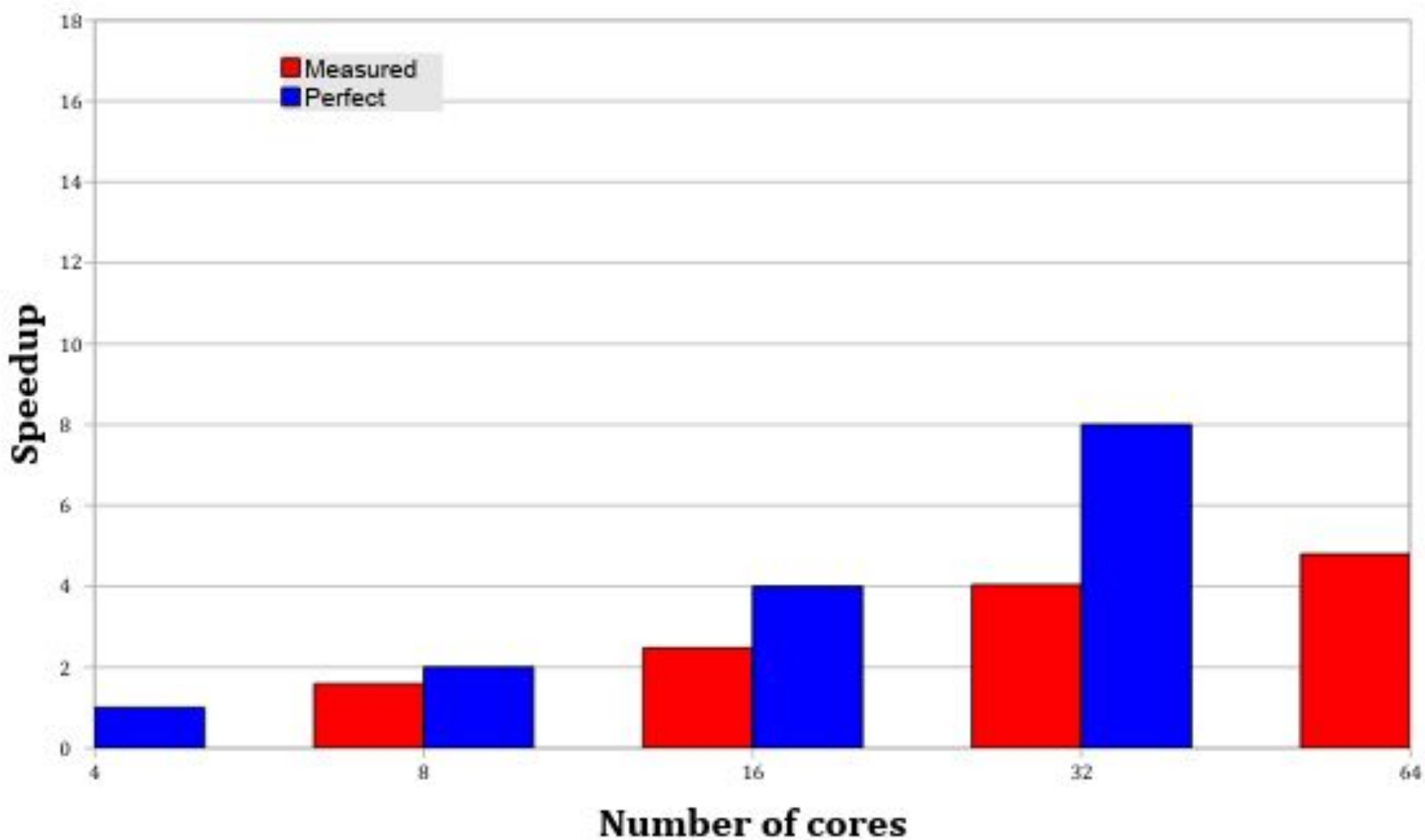


# Scaling



Perfect
Roll offf
Negative
Linear
1000
100
10
1
Speedup
1
10
100
1000
Number of cores

# Scaling



Measured
Perfect
18
16
14
12
10
8
6
4
2
0
Speedup
4
8
16
32
64
Number of cores

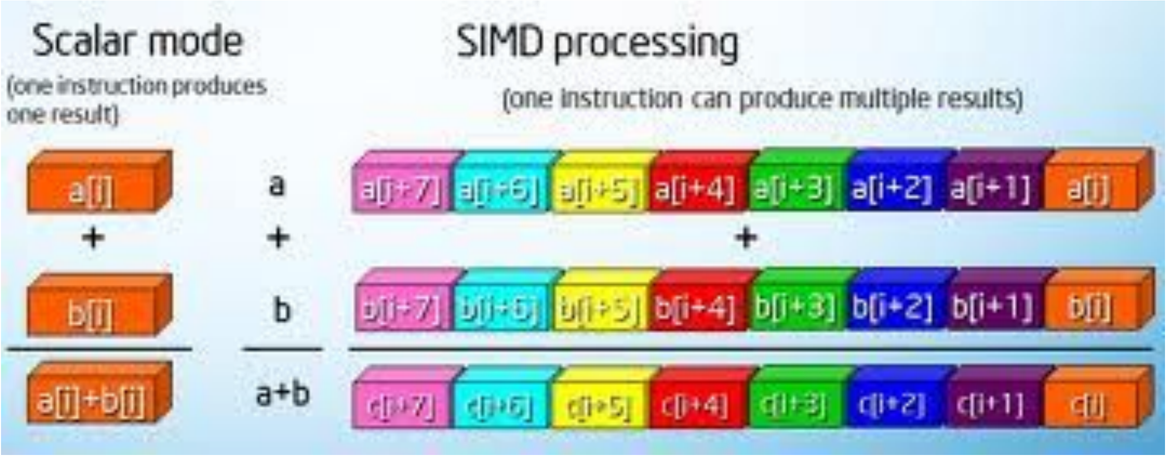
# Scaling

- How does your application scale ?
- Is it dependent on input ?
- Are you running at the sweet spot ?
- Threads ?
- MPI ?
- Hybrid ?
- Will your application scale to more than 120 threads to use the new Intel Knights Landing processor ?

# Compiler usage

- Parallel – 16 to 20 cores in a node
  - Vectorisation
  - OpenMP
  - MPI

- More and more focus on vectorisation



# Programming for the future

- Pure MPI may yield too many ranks
  - Large memory demand
- Pure threads may scale weakly
  - OpenMP scaleing is often limited
- Hybrid multi threaded MPI

- One MPI rank per core, 2-32 threads per core

# Programming for the future

- Vectorization vital for performance
  - Scalar code perform at 1/16 performance

- OpenMP 4.0 introduces SIMD directives

- All OpenMP programming facilities now apply to SIMD

- Vectorization is made easier with OpenMP, just like threading was made simpler.

# Programming for the future

- OpenMP SIMD - vectorization
- Single program, multiple data
- Vector units are becoming increasingly more important
- AVX / AVX2 256 bits = 4 dp and 8 sp floats
- AVX512 has 512 bits vector = 8 dp and 16 sp floats
- Vector fused multiply add double vector performance

# Programming  - Intel tuning tools

- Tuning tools
- Compiler – *only time the source code is read*
- MPI library – *can provide vital statistics*
- Vector Advisor - *vectorization*
- Thread Inspector - *Threads*
- Vtune Amplifier – *CPU / memory performance*
- Trace Analyser – *MPI calls*

# Questions ?