Swiss National Supercomputing Centre

Optimizing IO Performance in ECHAM5-HAM

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Background

CSCS is Switzerland's national HPC resource

- provides resource and assistance to all educational institutions
- provide computer resource from MeteoSwiss
- support various disciplines (computational chemistry, CFD, climate)
- offer different project sizes (small, large, ALPS)

Advanced Large Projects in Supercomputing

- large amounts of computational and technical resource over 2 years
- 4 projects approved for January 2007 start
  - CFD
  - computational biology
  - computational chemistry
  - climate modelling

ALPS Climate Project

"Climate change and the hydrological cycle from global to European/alpine scales".

- Principal Investigator : Dr. Ulrike Lohmann (ETHZ)

Project goals include:

- development of high-resolution climate modelling system
- prediction of extreme weather events

Use of ECHAM5-HAM(Version 5.3.02)

- 500 years of integration at T63L31
- 100 years of integration at T106L31
- 2.35M CPUh (out of 3.75M CPUh allotted)
- Optimizing ECHAM5-HAM is HIGHLY desirable

Code Specifics (at T63L31 on Cray XT3)

ECHAM5 with aerosol and atmos. chemistry modules added

- 36 additional tracers

normal domain decomposition used

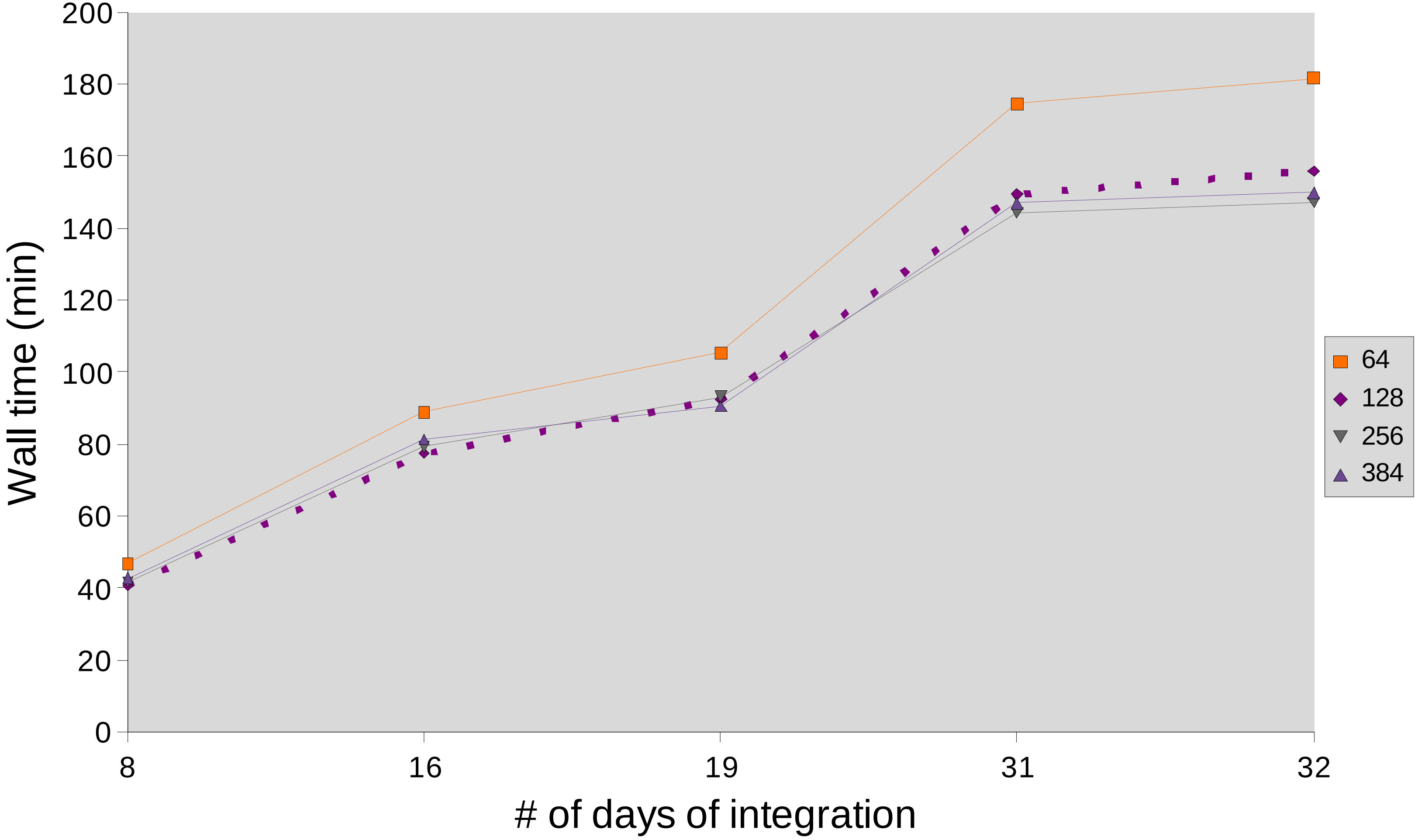
- minimum of 32 single-core nodes (memory)
- maximum of 384 single-core nodes (discretization)

single IO node used with NetCDF output format

data nudging used for SST, VOR, STP and DIV

6-hourly output frequency

ECHAM5-HAM


Wall time (min)
200
180
160
140
120
100
80
60
40
20
0
8
16
19
31
32
# of days of integration
64
128
256
384

Performance Analysis Continued...

for 1 month integration on 128 CPU (no optimizations)

- ➔ **34%** walltime is IO activity
  - concentrated in output of large diagnostic files
  - data nudging input not so significant
- ➔ **17%** walltime is MPI activity
  - barriers
  - synchronizations
  - collective communication calls

Our Goal? - ***Minimize the computational significance of IO***

How do we proceed?

- find optimal NetCDF chunk size
- exploit Lustre filesystem
- use IOBUF

Default IO Design

IO node strategy used

global domain is broken into number sub-domains that are distributed to worker nodes

At an “output event”, IO node will

- collect worker sub-domains
- create corresponding global domain
- output data to hard disk

simple, efficient with little interruption to compute node workload

targeted for shared memory platform with small # of nodes

- concern for large distributed memory platforms
- could add additional IO nodes (complexity, development time)

IO performance in default code

- Output per month is ~32.5GB data
  - translates to average output rate of ~32.5 MB/sec
  - system's maximum output rate is ~250 MB/sec

NetCDF Chunk Size

Diagnostic data output is the most computationally expensive

Diagnostic data output consists of :

- output of approx. 32.5 GB
- data written to 12 principal NetCDF files (files over 0.1 GB)
- adding a time slice of a 3D array (~ 4.4MB for T63L31)
- high frequency of these writes

Let's perform quick analytical test

- use IO pattern described above
- include 124 writes (corresponds to 31-day month)
- add some NetCDF performance tuning
  - no pre-filling of variables
  - vary size of write “chunks”
- measure average bandwidth of outputting 32.5GB in 12 files

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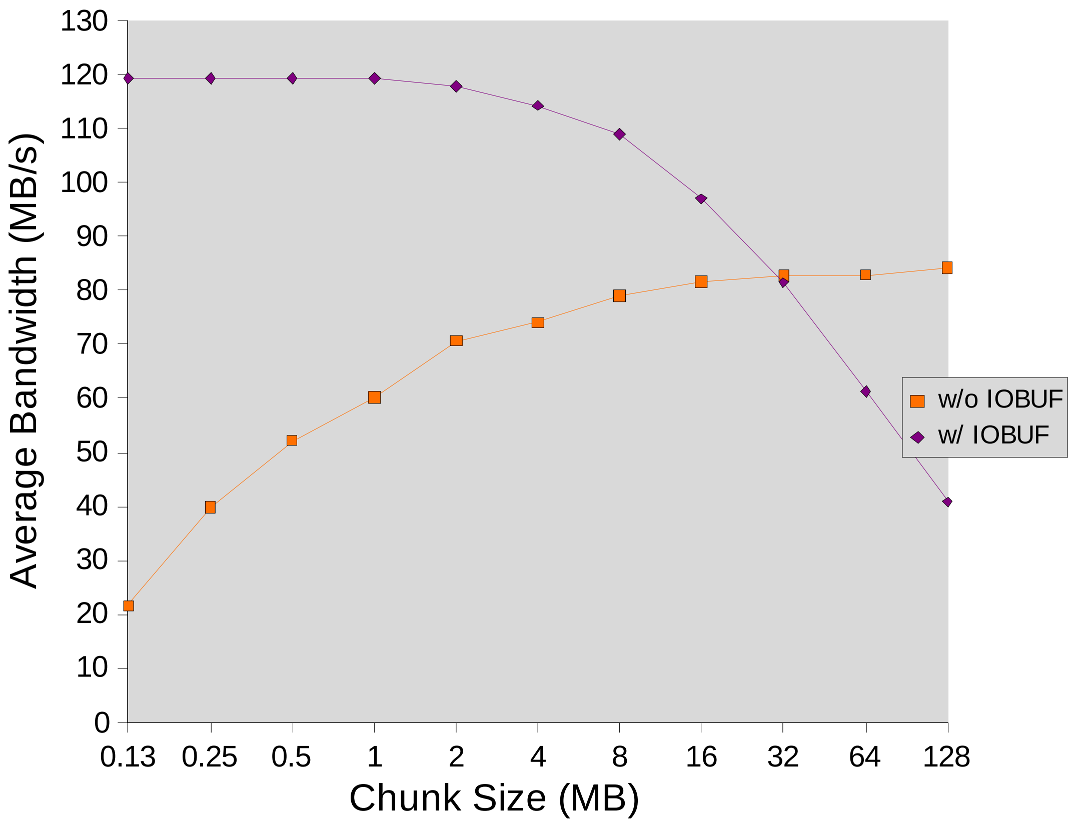
NetCDF Chunk Size



No CRAY XT-IOBUF

- output rate increases with chunk size
- 128MB optimal chunk size

With CRAY XT-IOBUF

- huge performance increase
- inverse chunk size relation
- 0.5MB optimal chunk size

***performed on a separate, dedicated system**

Lustre parallel filesystem

virtual high-speed file interface system. Composed of

- metadata server (MDS)
- object data servers (OSS)
- object storage targets (OSTs)

achieves high-throughput via

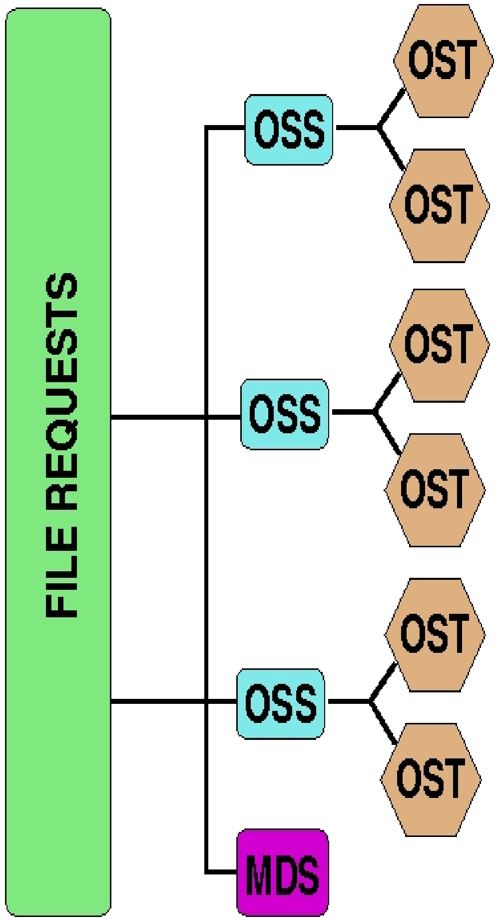
- splitting of meta-data and “real” data operations
- data striping

optimal Lustre settings are important

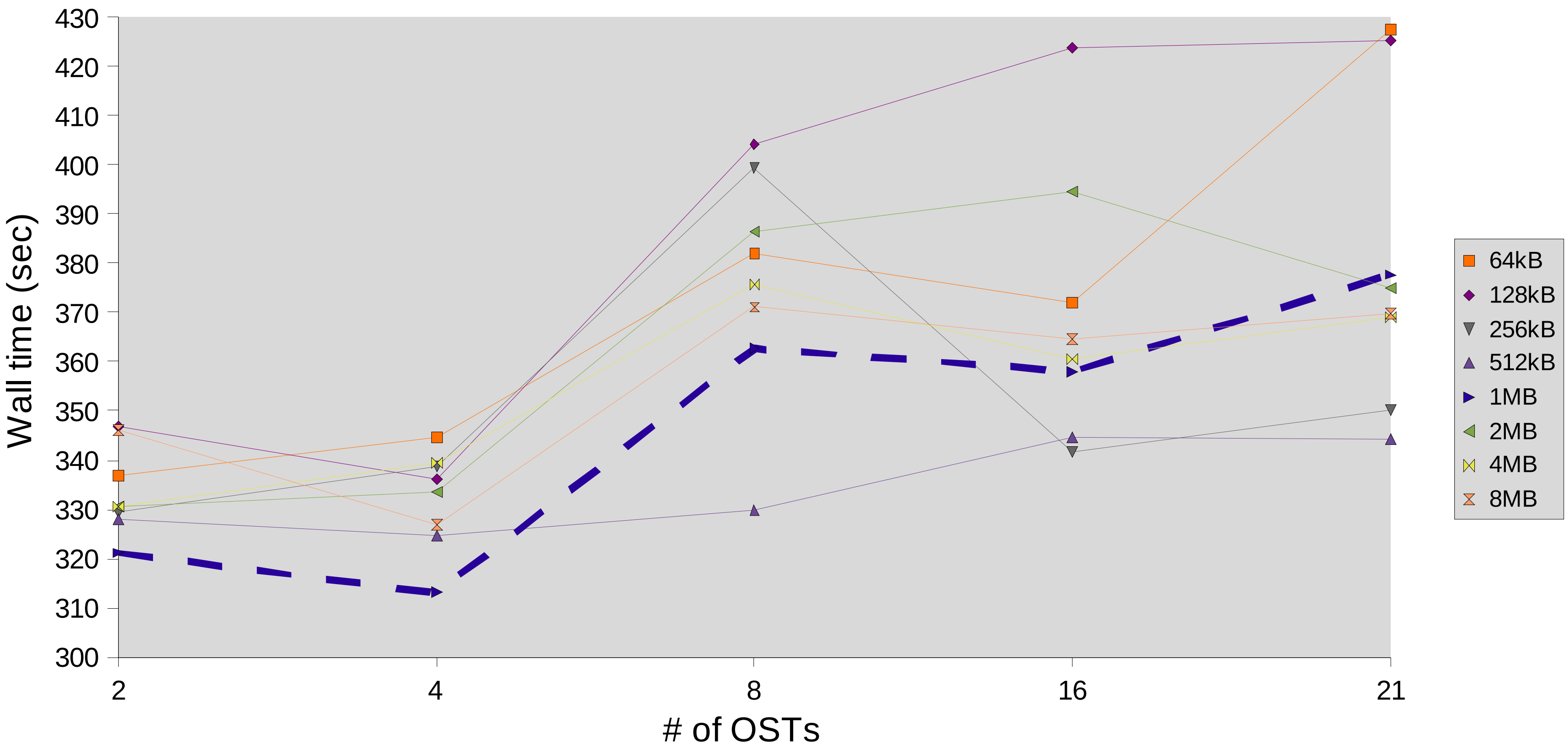
- application dependent
- system dependent

Conduct test

- 1 day of integration in ECHAM5-HAM on “PALU”
- vary stripe size from 64kB to 8MB
- vary OST number from 2 to 21

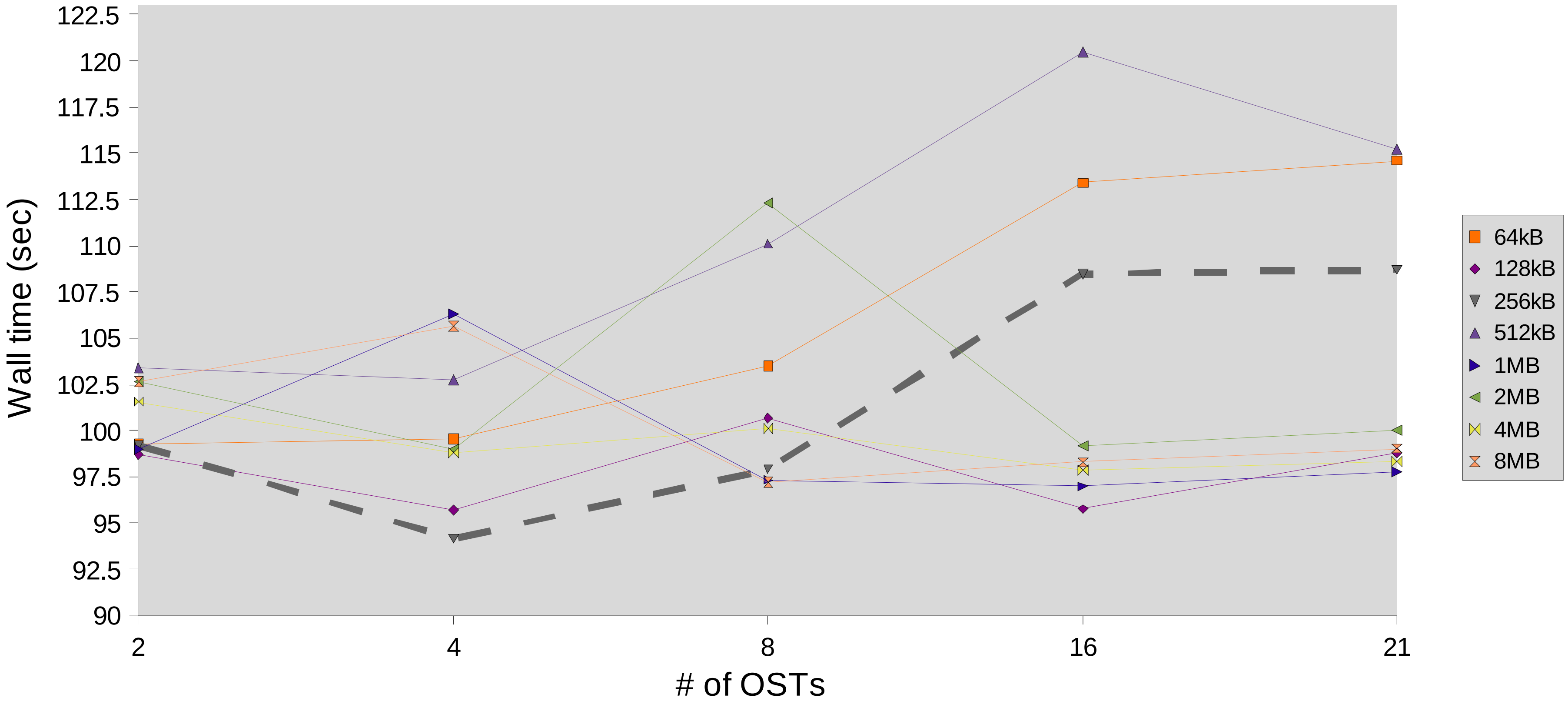


Lustre - 32kB



- possible 3-24% drop in average execution time using optimal settings
- performance drop between 4 and 8 OSTs
- 4 OSTs with 1MB stripes chosen

Lustre - 128MB



- Again best performance is with 4 OSTs
- settings still significant (2-13% drop in average execution time)

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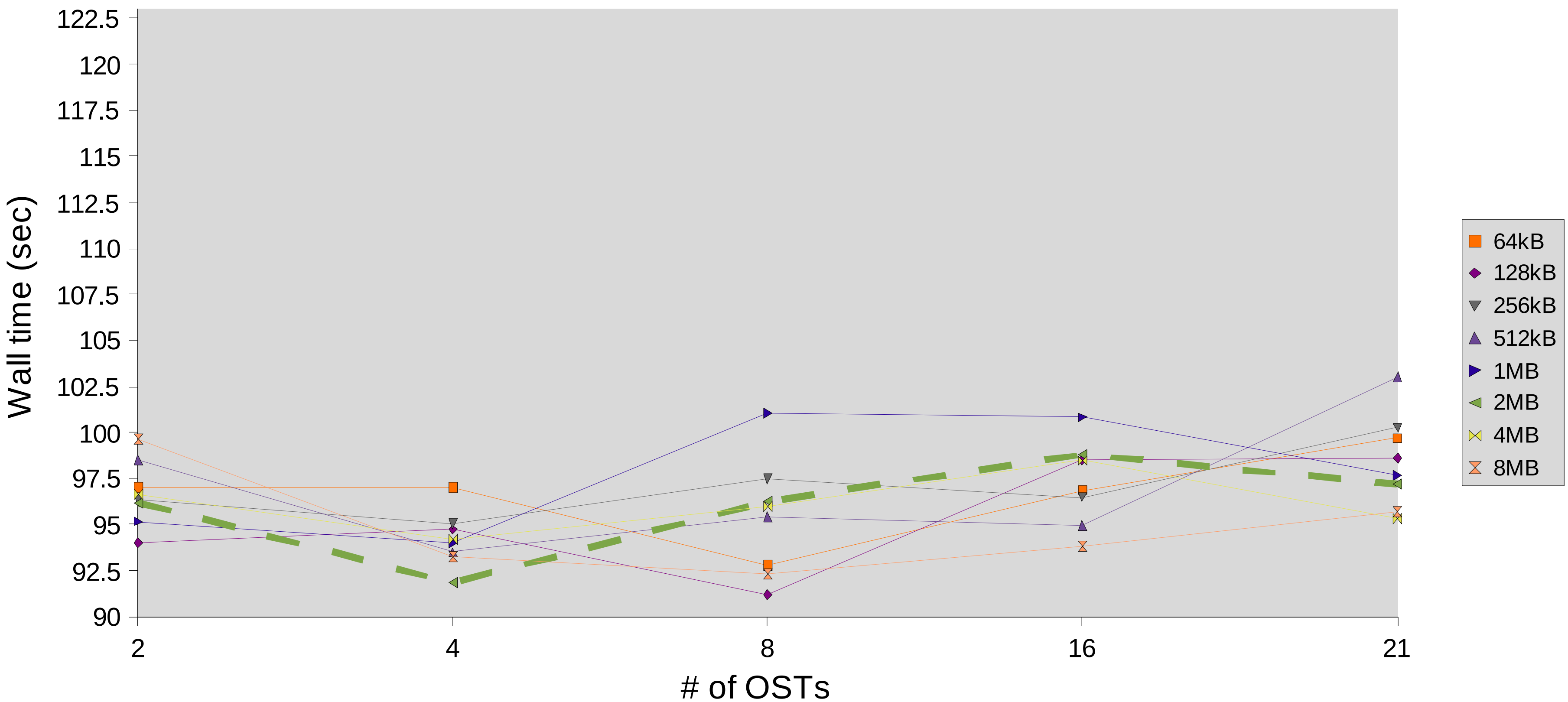
Lustre - 512kB



- IOBUF lessens impact of Lustre settings
- only 2-6% possible drop in average execution time

XT-IOBUF Library

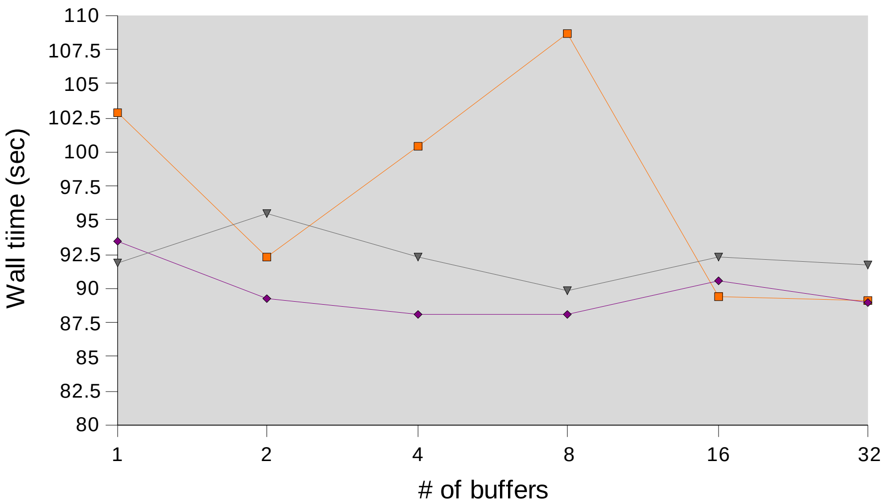
- intercepts IO calls made on the compute nodes
- user can specify:
  - size and number of buffers
  - filetype to be buffered
  - shared/not shared
  - flush frequency
- INTENDED USE: Gather “small-block” writes to reduce flush frequency from compute nodes
- limited value for “large-block” writes

Conduct tests

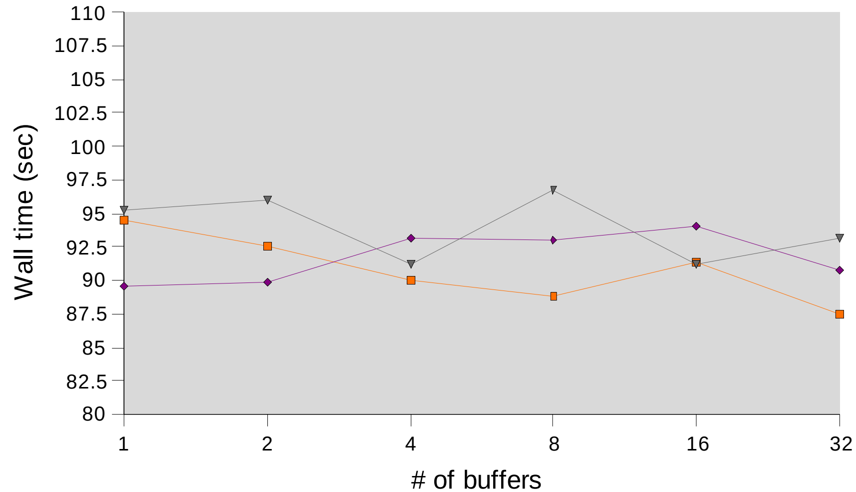
- 1 model day of integration in ECHAM5-HAM
- vary number of buffers from 1 to 32
- vary buffer size from 5MB to 20MB each
- use 4 OSTs with 1MB stripes

IOBUF

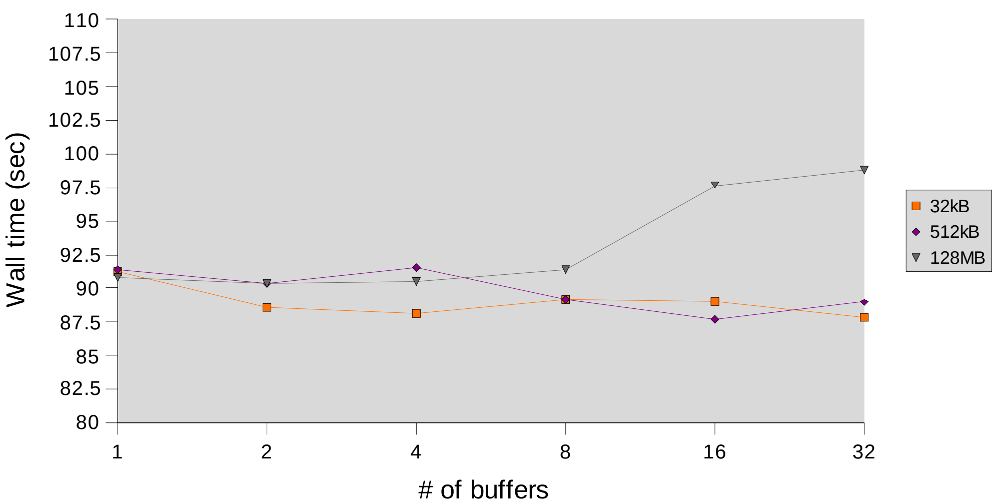
Performance with 5MB buffers



Performance with 10MB Buffers



Performance with 20MB Buffers



Observations

- more virtual buffer space leads to better performance
- only 2-5% change in average execution time

Final Configurations

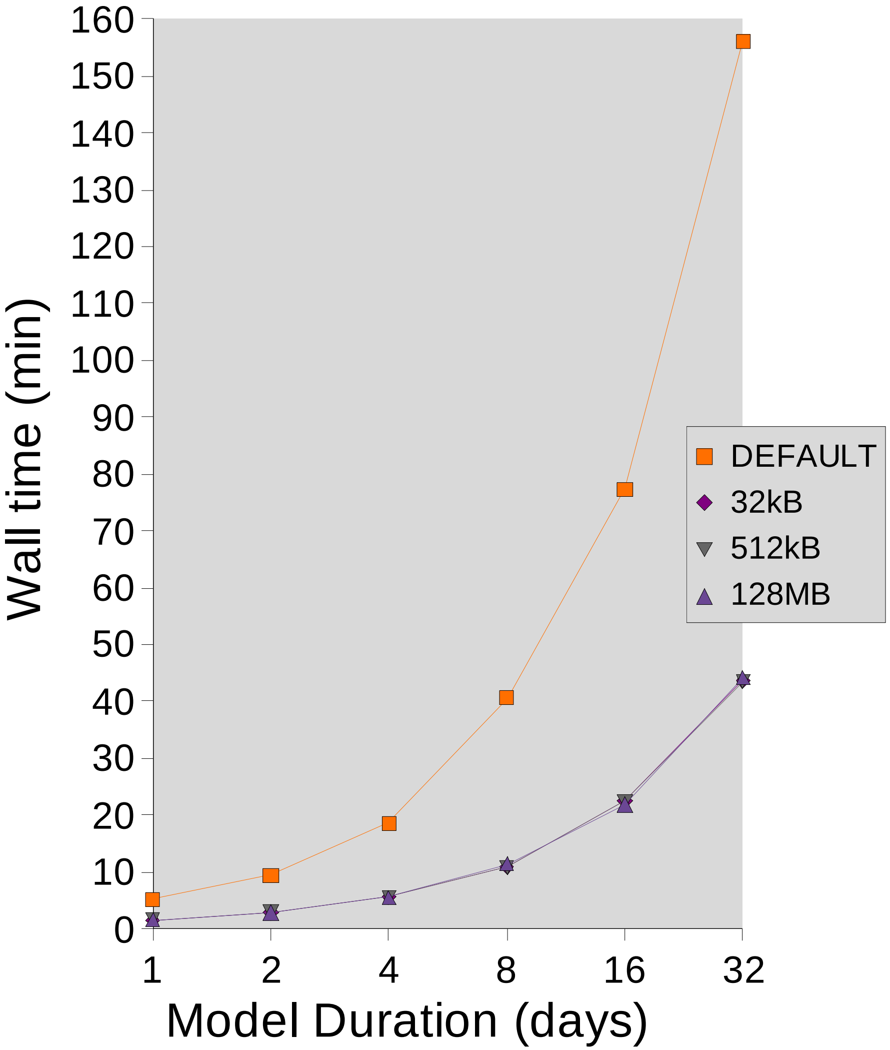
32kB chunk size	✓ 4 OSTs with 1MB stripes ✓ thirty-two 20MB buffers for IOBUF
512kB chunk size	✓ 4 OSTs with 2MB stripes ✓ eight 5MB buffers for IOBUF
128MB chunk size	✓ 4 OSTs with 256kB stripes ✓ no IOBUF for NetCDF output

*** IOBUF used to buffer STDOUT and input nudging data in all cases**

**** 128 single-core CPUs used**

***** 6-hourly output**

FINAL RESULTS



Execution times (32 days, 128 CPU)

no aggresive opt	149 min
aggresive opt + Lustre config	51 min
optimal chunksize + IOBUF	44 min
remove NetCDF sync (add Massoc)	38 min

Results achievable with “user” or “vendor” approaches

1 month of integration takes ~112 min on NEC SX-6 (8 CPU)
dedicated queue

Final Performance

Total execution time (32 days, 256 CPU)

compiler opt + Lustre config optimal chunksize & IOBUF	35 min
remove NetCDF sync (add Massoc)	28 min
remove IEEE compliance	26.5 min

IO Significance (1 month, 128 CPU)

no optimizations	33%
with compiler opt	21%
in final configurations	<11%

Final Performance

Communication costs are more important

no optimizations	17%**
with compiler opt	57%
in final configurations	~55%

Barriers and collective communication calls are most significant (~17.5% and ~12% respectively)

Communication optimization is now vital

- barrier reduction
- removal of collective communication calls

****of total wall time for run**

Acknowledgements

many thanks to the following...

CSCS

Dr. Neil Stringfellow
Mr. Hussein Harake

Cray

Mr. Roberto Ansaloni
Ms. Nina Suvanphim
Ms. Tricia Balle

MPI

Dr. Luis Kornblueh

IES-Ispra

Ms. Silvia Kloster