Parallel I/O using standard data formats in climate and NWP

Project ScalES funded by BMBF

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Outline

Thanks to

- Uwe Schulzweida, MPIM
- Mathias Pütz, IBM
- Christoph Pospiech, IBM
- Colleagues at DKRZ

ScalES (4hpc) Parallel I/O

Targets

- Scalability of Earth System Models
- Usability of Infrastructure Components
- Portability of Implemented Solutions
- Solutions Prepared for Future Computer Development
- Free Availability for the Modelling Community

Atmospheric and Oceanographic Data

Constraints

- Large amounts of data
- Comparable small spatial extent ($O(2,3)$)
- Large Time extent ($O(8)$)
- Large Number of variables ($O(3)$)

… continued …

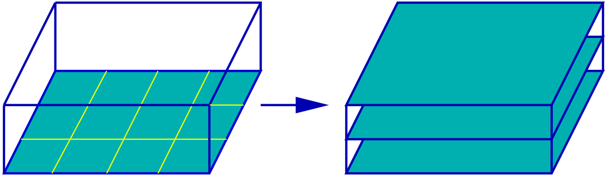
Requirements

- long term storage of metadata and data
- standardization
- compression

Solutions

- WMO GRIB standard
- lowest entropy data subsampling
- two stage compression: lossy entropy based and lossless compression of result *image* — metadata uncommpressed!

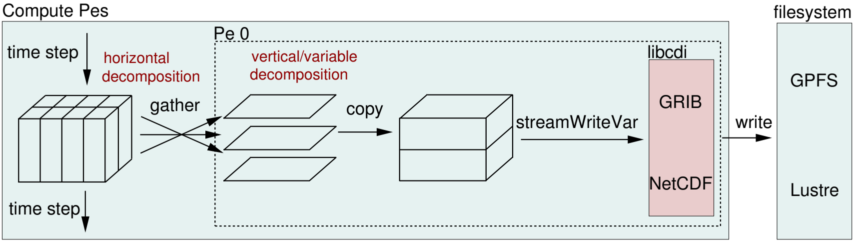
... continued



Problem

- model decomposition is based on two-dimensional horizontal slicing
- storage unit of model data is based on vertical slicing
- requires transpose and data gathering

File writing in ECHAM AS-IS



- All processes are compute processes.
- After one I/O timestep all processes gather their data on process 0.
- Process 0 writes the data to the filesystem.
- All processes compute till the next I/O timestep.

Problem

All processes wait until process 0 has written the data.

Solution strategy

1. decompose I/O in a way that all variables are distributed over the collector/concentrator PEs (I/O PEs)

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3. instead of doing I/O, copy data to buffer and continue simulation

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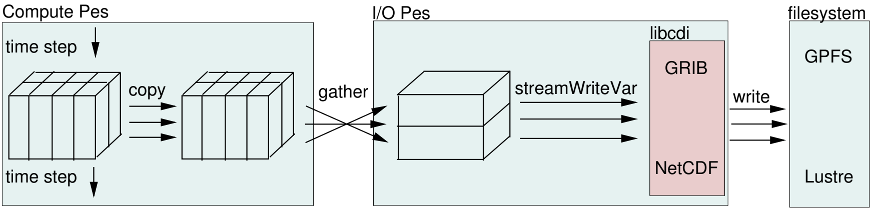
First five steps runs fine, but the last one makes a lot of trouble!

File writing in ECHAM TO-BE

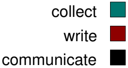


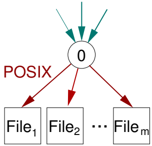
- After calculating one I/O timestep the compute processes copy their data to a buffer and go on calculating till the next I/O timestep.
- I/O processes fetch the data using MPI one sided communication.
- Gather and transpose of the data is based on callback routines supplied by the model.

Most important property

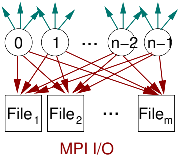
Compute processes are not disturbed by file writing.

Algorithm alternatives

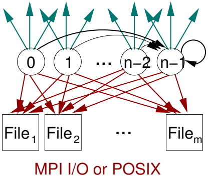




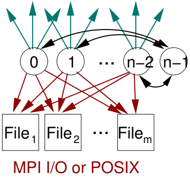
(a) *Classic serial*, no comm.



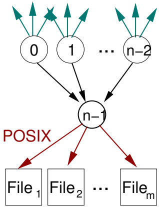
(b) *MPI writer*, no visible comm.



(c) *Offset sharing*, comm. offsets

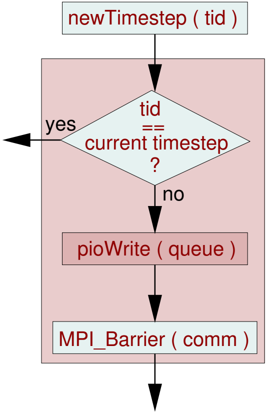


(d) *Offset guard*, comm. offsets



(e) *POSIX writer*, comm. data

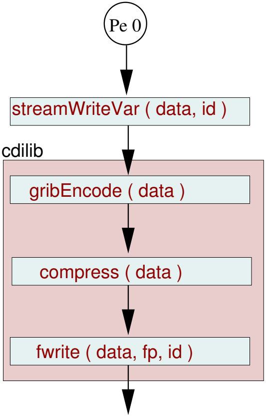
Timesteps



Characteristics

- Within files data have to be ordered by time.
- In case of serial writing is a natural barrier between the timesteps.
- When writing in parallel buffering of data is necessary for performance.
- Buffers have to be flushed after each I/O timestep to keep data in right time order.

Program flow (1), Classic serial



Collect and write serial using fwrite.

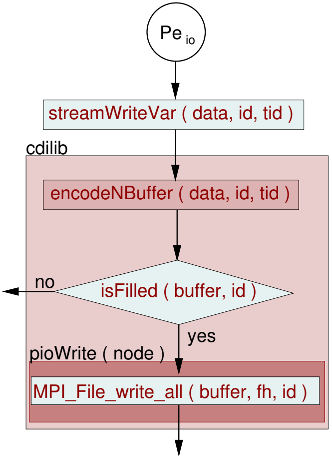
Advantages

- No communication is needed.
- Simple algorithm.
- Simple multi-file handling.

Disadvantages

- Does not scale.

Program flow (2), MPI writer (1)



Collect and write parallel using MPI_File_write_all.

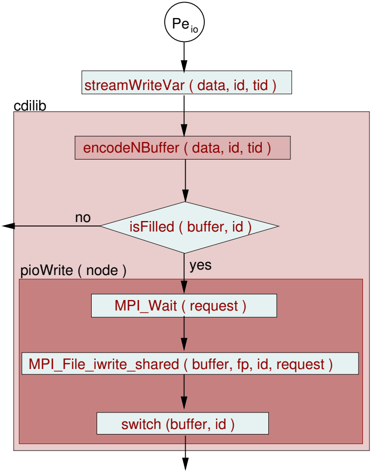
Advantages

- No user visible communication between I/O processes is needed.
- Straight forward implementation.
- Performs best of all MPI file writing routines.

Disadvantages

- Collective call, doesn't work for inhomogenous allocation of variables per process/file.

Program flow (3), MPI writer (2)



Collect and write parallel using MPI_File_iwrite_shared.

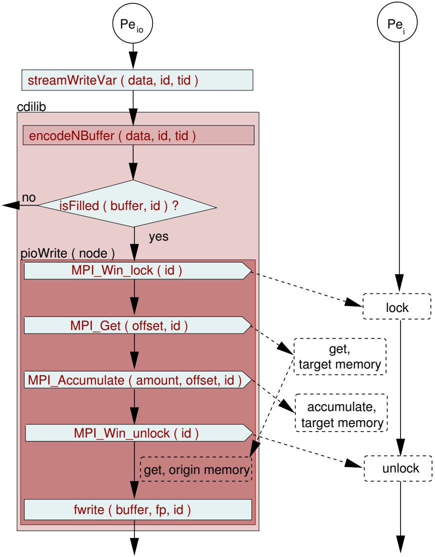
Advantages

- No user visible communication between I/O processes is needed.
- Use of double buffering is possible.

Disadvantages

- Very bad performance on GPFS.

Program flow (4), Offset sharing



Collect and write parallel, communicate file offsets using MPI RMA with passive target:

Advantages

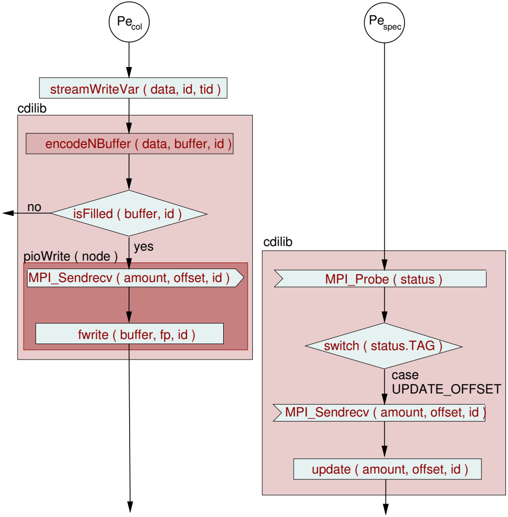
- All collectors write.
- Use of POSIX AIO possible.

Disadvantages

- Complex locking is needed, performance is bad.

Remark: double buffering not done yet.

Program flow (5), Offset guard



Collect and write parallel using one process to administrate file offsets.

Advantages

- Performs best of tested versions.
- Use of POSIX AIO possible.

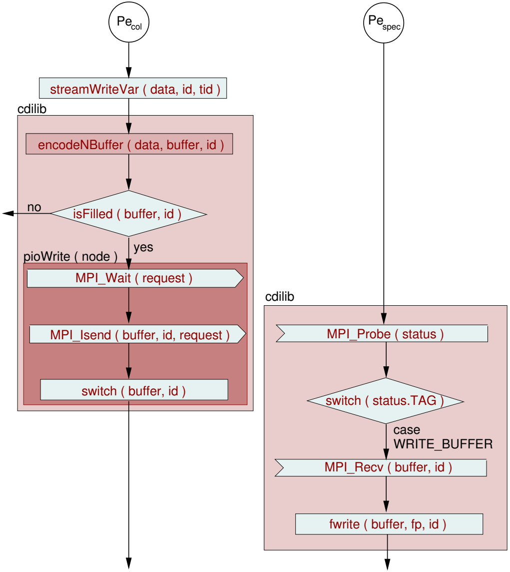
Disadvantages

- One process is idle most of the time.
- Problems if I/O PEs span over different nodes.

Remark: double buffering not done yet.

Program flow (6), Posix writer

Timings | Run fwrite | Run aio_write



Collect parallel and write serial using fwrite.

Advantages

- Use of POSIX AIO possible.
- Use of double buffering possible.
- Use one writer process for each file possible. This would probably gain performance. Furthermore these processes could be located on different nodes.

Disadvantages

- The buffer has to be communicated.
- With one writer process speedup limited.

Parallel performance profile analysis

We made several runs with the tools SCALASCA and TAU. Some of the results follow on the next slides. For these runs we let the processes write 5.9 GB distributed to 10 files.

Remark

The instumentation of the code increased the runtime of the programs up to 130%!

MPI writer, MPI_File_iwrite_shared

MPI writer

8 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$ (s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	1370.2	100.0	8	171.3	100.0	100.0
grbEncode	674.2	49.2	8	84.3	49.2	
MPI_File_iwrite_shared	58.9	4.3	8	7.4	4.3	96.7
MPI, other	592.0	43.2	8	74.0	43.2	

16 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$ (s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	2190.8	100.0	16	136.9	100.0	100.0
grbEncode	611.5	27.9	16	38.2	27.9	
MPI_File_iwrite_shared	550.2	25.1	16	34.4	25.1	97.4
MPI, other	972.5	44.4	16	60.8	44.4	

POSIX writer, aio_write, 5 output streams

POSIX writer

4 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	1582.3	100.0	4	395.6	100.0	100.0
grbEncode	540.4	34.2	3	180.1	45.5	96.6
MPI_Wait	606.3	38.3	3	202.1	51.1	
MPI_Recv	161.3	10.2	1	161.3	40.8	92.9
aio_suspend	206.0	13.0	1	206.0	52.1	

8 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	3695.3	100.0	8	461.9	100.0	100.0
grbEncode	539.5	14.6	7	77.1	16.7	97.5
MPI_Wait	2645.6	70.6	7	373.3	80.8	

Offset guard

Offset guard

4 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	875.7	100.0	4	218.9	100.0	100.0
grbEncode	540.4	61.7	3	180.1	82.3	
fseek/fwrite	74.3	8.5	3	24.8	11.3	95.9
MPI_Barrier	15.2	1.7	3	5.1	2.3	
MPI_Probe	218.3	27.9	1	218.3	99.7	99.7

32 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	1646.5	100.0	32	51.5	100.0	100.0
grbEncode	544.1	33.1	31	17.6	34.1	
fseek/fwrite	590.0	35.8	31	19.0	37.0	92.1

POSIX writer, fwrite

POSIX writer

4 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	822.7	100.0	4	206.2	100.0	100.0
grbEncode	540.7	65.6	3	180.2	87.4	
MPI_Wait	46.0	5.6	3	15.3	7.4	95.3
MPI_Barrier	2.8	0.3	3	0.92	0.5	
MPI_Recv	162.0	19.7	1	162.0	78.6	98.9
fwrite	41.8	5.1	1	41.8	20.3	

32 Pes

Routines, functions	Time(s)	%	#	$\frac{\text{Time}}{\#\text{Pes}}$(s)	%	$\sum_{\text{Pe}_i}$
cdiWrite	3855.1	100.0	32	120.5	100.0	100.0
grbEncode	543.9	14.1	31	17.6	14.6	

Timings for Power6, AIX, IB

Target: 2 GB/s

write method	# Pes	# collectors	# writers	[MB/s]
Classic serial, fwrite	1	1	1	148
MPI writer,	4	4	4	234
MPI_File_iwrite_shared	8	8	8	281
	16	16	16	338
	32	32	32	322
Offset guard, fwrite	4	3	3	240
	8	7	7	498
	16	15	15	829
	32	31	31	946
POSIX writer, fwrite	4	3	1	257
	8	7	1	450
	16	15	1	411
	32	31	1	482

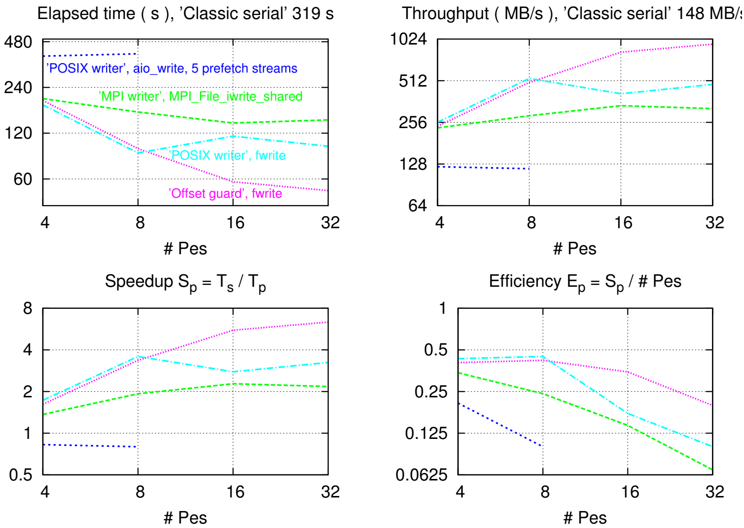
Timings for Opteron, Linux, IB

Linux cluster test: 16 MB buffer, 10 files, 49 GB in total

write method	# nodes	# PEs	throuput [MB/s]
Classic serial, fwrite	1	1	89
MPI writer,	1	8	386
MPI_File_iwrite_shared	2	16	612
Offset guard, fwrite	1	8	375
	2	16	558
POSIX writer, fwrite	1	8	142
	2	16	254

Not all possibilities might be fully optimized.

Comparison



Elapsed time (s), 'Classic serial' 319 s
480
240
120
60
'POSIX writer', aio_write, 5 prefetch streams
'MPI writer', MPI_File_iwrite_shared
'POSIX writer', fwrite
'Offset guard', fwrite
4
8
16
32
Pes
Throughput (MB/s), 'Classic serial' 148 MB/s
1024
512
256
128
64
4
8
16
32
Pes
Speedup $S_p = T_s / T_p$
8
4
2
1
0.5
4
8
16
32
Pes
Efficiency $E_p = S_p$ / # Pes
1
0.5
0.25
0.125
0.0625
4
8
16
32
Pes

Some initial conclusions

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Some initial conclusions

- For our kind of models sufficient write speed on a single IBM node to go on for the next months
- RDMA concept is meeting the expectations - may need more RMA Windows.
- Did part of MPI developers work on very unusual usage model of MPI-IO ...
- Expect them to take over and beat our results by at least a factor of ?.