SuperComputing Applications and Innovation

I/O: State of the art and Future developments

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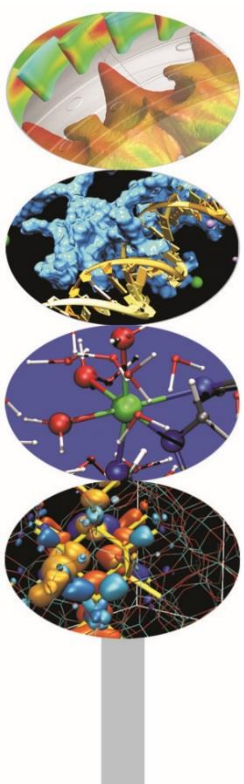


Cineca
TRAINING
High Performance
Computing 2016

Some questions

- Just to know each other:
  - ✓ Why are you here?
  - ✓ Which is the typical I/O size you work with?
    - GB?
    - TB?
  - ✓ Is your code parallelized?
  - ✓ How many cores are you using?
  - ✓ Are you working in a small group or you need to exchange data with other researchers?
  - ✓ Which language do you use?

“Golden” rules about I/O

- Reduce I/O as much as possible: only relevant data must be stored on disks
- Save data in binary/unformatted form:
  - ✓ asks for less space comparing with ASCI/formatted ones
  - ✓ It is faster (less OS interaction)
- Save only what is necessary to save for restart or check-pointing, everything else, unless for debugging reason or quality check, should be computed on the fly.
- Dump all the quantities you need once, instead of using multiple I/O calls: if necessary use a buffer array to store all the quantities and the save the buffer using only a few I/O calls.
- Why?

What is I/O?

- ✓ Raw data
- ✓ **`fwritef, fscanf, fopen, fclose, WRITE, READ, OPEN, CLOSE`**
- ✓ Call to an external library: MPI I/O, HDF5, NetCDF, ecc…
- ✓ Scalar/parallel/network Filesystems
  1. I/O nodes and Filesystem cache
  2. I/O network (IB, SCSI, Fibre, ecc..)
  3. I/O RAID controllers and Appliance (Lustre, GPFS)
  4. Disk cache
  5. FLASH/Disk (one or more Tier)
- ✓ Tape

Latencies

- I/O operations involves
  - ✓ OS & libraries
  - ✓ IO devices (e.g. RAID controllers)
  - ✓ Disks
- I/O latencies of disks are of the order of microseconds
- RAM latencies of the order of 100-1000 nanoseconds
- FP unit latencies are of the order of 1-10 nanoseconds
- → I/O very slow compared to RAM of FP unit

Architectural trends

Peak Performance	↑	Moore law
FPU Performance	↔	Dennard law
Number of FPUs	↑	Moore + Dennard
App. Parallelism	↑	Amdahl's law

Architectural trends

		2020 estimates
Number of cores	↑	10^9
Memory x core	↓	100Mbyte or less
Memory BW/core	↓	500GByte/sec
Memory hierachy	↑	Reg, L1, L2, L3, …

Architectural trends

2020 estimates

Wire BW/core	1GByte/sec
Network links/node	100
Disk perf	100Mbyte/sec
Number of disks	100K

What is parallel I/O?

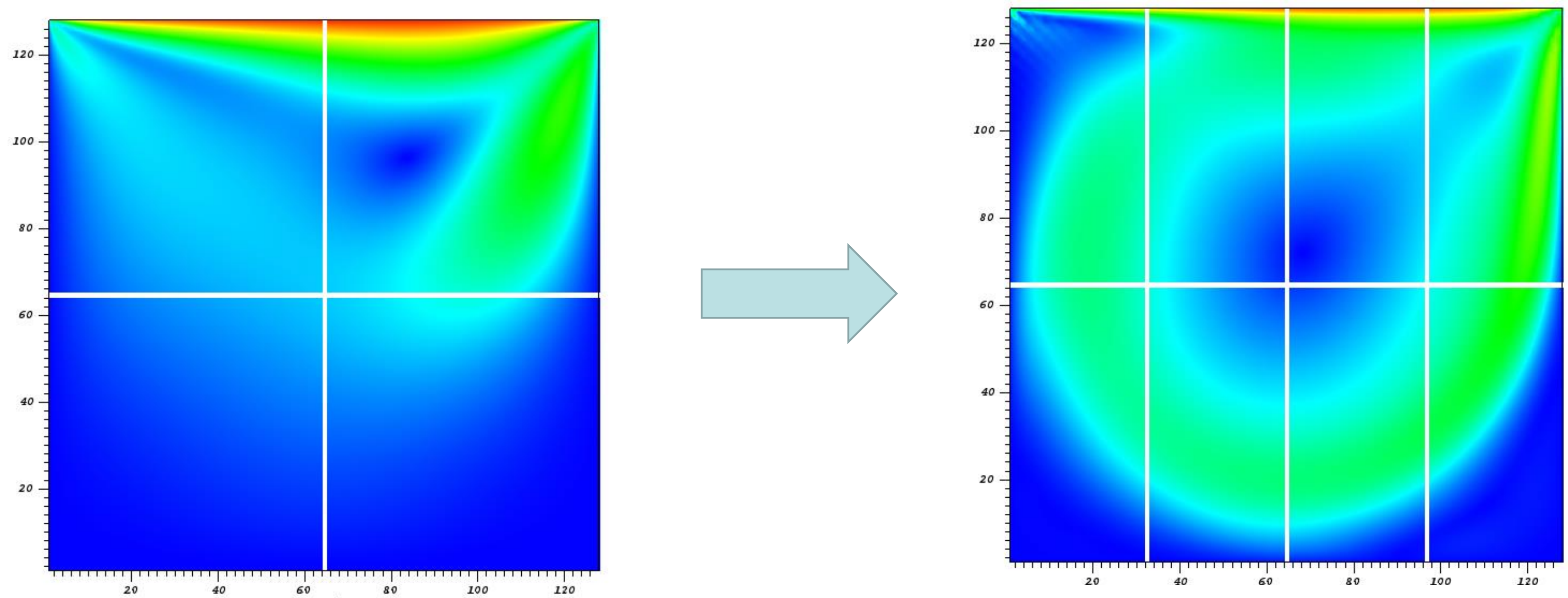
- A more correct definition in the afternoon
- Serial I/O
  - ✓ 1 task writes all the data
- Parallel I/O
  - ✓ All task write its own data in a different file
  - ✓ All task write its own data in a single file

- MPI/IO, HDF5, NetCDF, CGNS,……

Why parallel I/O?

- New Architectures: many-many core (up to 10^9)
- As the number of task/threads increases I/O overhead start to affect performance
- I/O (serial) will be a serious bottleneck
- Parallel I/O is mandatory else no gain in using many-many core
- Other issues:
  - ✓ domain decomposition
  - ✓ data format: ASCII vs binary
  - ✓ endianess
  - ✓ blocksize
  - ✓ data management

I/O: Domain Decomposition



- I want to restart a simulation using a different number of tasks: three possible solutions
  - ✓ pre/post processing (merging & new decomposition)
  - ✓ serial dump/restore
  - ✓ Parallel I/O

I/O: ASCII vs. binary/1

- ASCII is more demanding respect binary in term of disk occupation
- Numbers are stored in bit (single precision floating point number → 32 bit)

- 1 single precision on disk (binary) → 32 bit
- 1 single precision on disk (ASCII) → 80 bit
  - 10 or more **`char`** (**`1.23456e78`**)
  - Each char asks for 8 bit

✓ Not including spaces, signs, return, …
✓ Moreover there are rounding errors, …

I/O: ASCII vs. binary/2

- Some figures from a real world application
- **`openFOAM`**
- Test case: 3D Lid Cavity, 200^3, 10 dump

- Formatted output (ascii)
  - ✓ Total occupation: 11 GB
- Unformatted output (binary)
  - ✓ Total occupation: 6.1 GB

- A factor 2 in disk occupation!!!!

I/O: endianess

- IEEE standard set rules for floating point operations
- But set no rule for data storage
- Single precision FP: 4 bytes (**B0**,B1,B2,B3)
  - ✓ Big endian (IBM): **B0** B1 B2 B3
  - ✓ Little endian (INTEL): B3 B2 B1 **B0**
- Solutions:
  - ✓ Hand made conversion
  - ✓ Compiler flags (intel, pgi)
  - ✓ I/O libraries (HDF5)

I/O: blocksize

- The blocksize is the basic (atomic) storage size
- One file of 100 bit will occupy 1 blocksize, that could be > 4MB

```
ls -lh TEST_1K/test_1
-rw-r--r-- 1 gamati01  10K 28 gen 11.22 TEST_1K/test_1
…
du -sh TEST_1K/test_1
512K       TEST_0K/test_1
…
du -sh TEST_1K/
501M       TEST_10K/
…
```

- Always use **tar** commando to save space

```
ls -lh test.tar
-rw-r--r-- 1 gamati01 11M  5 mag 13.36 test.tar
```

I/O: managing data

- TB of different data sets
- Hundreds of different test cases
- Metadata
- Share data among different researchers
  - ✓ different tools (e.g. visualization tools)
  - ✓ different OS (or dialect)
  - ✓ different analysis/post processing

- You need a common "language"
  - ✓ Use I/O libraries
  - ✓ Invent your own data format

Some figures/1

Simple CFD program, just to give you an idea of performance loss due to I/O.

- 2D Driven Cavity simulation
- 2048*2048, Double precision (about 280 MB), 1000 timestep
- Serial I/O = 1.5''
  - ✓ 1% of total serial time
  - ✓ 16% of total time using 32 Tasks (2 nodes) → 1 dump = 160 timestep
- Parallel I/O = 0.3'' (using MPI I/O)
  - ✓ 3% of total time using 32 Tasks (2 Nodes) → 1 dump = 30 timestep
- An what using 256 tasks?

Some figures/2

Performance to dump huge file using Galileo: same code with different I/O strategies….

- RAW (512 files, 2.5GB per file)
  - Write: 3.5 GB/s
  - Read: 5.5 GB/s
- HDF5 (1 file, 1.2TB)
  - Write: 2.7 GB/s
  - Read: 3.1 GB/s
- MPI-IO (19 files, 64GB per file)
  - Write: 3.1 GB/s
  - Read: 3.4 GB/s

Some strategies

I/O is the bottleneck → avoid when possible
I/O subsystem work with locks → simplify application
I/O has its own parallelism → use MPI-I/O
I/O is slow → compress (to reduce) output data
Raw data are not portable → use library
I/O C/Fortran APIs are synchronous → use dedicated I/O tasks

Application DATA are too large → analyze it "on the fly", (e.g. re-compute vs. write)

At the end: moving data

- Now I have hundreds of TB. What I can do?
  - Storage using Tier-0 Machine is limited in time (e.g. PRACE Project data can be stored for 3 Month)
  - Data analysis can be time consuming (eyen years)
  - I don’t want to delete data
  - I have enough storage somewhere else?

How can I move data?

Moving data: theory

- BW requirements to move Y Bytes in Time X

Bits per Second Requirements

	1H	8H	24H	7Days	30Days
10PB	25,020.0 Gbps	3,127.5 Gbps	1,042.5 Gbps	148.9 Gbps	34.7 Gbps
1PB	2,502.0 Gbps	312.7 Gbps	104.2 Gbps	14.9 Gbps	3.5 Gbps
100TB	244.3 Gbps	30.5 Gbps	10.2 Gbps	1.5 Gbps	339.4 Mbps
10TB	24.4 Gbps	3.1 Gbps	1.0 Gbps	145.4 Mbps	33.9 Mbps
1TB	2.4 Gbps	305.4 Mbps	101.8 Mbps	14.5 Mbps	3.4 Mbps
100GB	238.6 Mbps	29.8 Mbps	9.9 Mbps	1.4 Mbps	331.4 Kbps
10GB	23.9 Mbps	3.0 Mbps	994.2 Kbps	142.0 Kbps	33.1 Kbps
1GB	2.4 Mbps	298.3 Kbps	99.4 Kbps	14.2 Kbps	3.3 Kbps
100MB	233.0 Kbps	29.1 Kbps	9.7 Kbps	1.4 Kbps	0.3 Kbps

moving data: some figures/1

- Moving outside CINECA
  - ✓ **`scp`** → 10 MB/s
  - ✓ **`rsync`** → 10 MB/s
- I must move 50TB of data:
  - ✓ Using **`scp`** or **`rsync`** → 60 days
- No way!!!!!
- Bandwidth depends on network you are using. Could be better, but in general is even worse!!!

moving data: some figure/2

- Moving outside CINECA
  - **`gridftp`** → 100 MB/s
  - **`globusonline`** → 100 MB/s
- I must move 50TB of data:
  - Using **`gridftp/globusonline`** → 6 days
- Could be a solution…

- Note
  - We get these figures between CINECA and a remote cluster using a 1Gb Network

moving data: some hints

- **Size matters**: moving many little files cost more then moving few big files, even if the total storage is the same!
- Moving file from Fermi to a remote cluster via Globusonline

Size	Num. Of files	Mb/s
10 GB	10	227
100 MB	1000	216
1 MB	100000	61

✓ You can loose a factor 4, now you need 25 days instead of 6 to move 50TB!!!!!

moving data: some hints

- ✓ Plan your data-production carefully
- ✓ Plan your data-production carefully (again!)
- ✓ Plan your data-production carefully (again!)
- ✓ Clean your dataset from all unnecessary stuff
- ✓ Compress all your ASCII files
- ✓ Use **`tar`** to pack as much data as possible
- ✓ Organize your directory structure carefully
- ✓ Syncronize with **`rsync`** in a systematic way
- ✓ One example:
  - We had a user who wants to move 20TB distributed over more then 2’000’000 files…
  - **`rsync`** asks many hours (about 6) only to build the file list, without any synchronization at all