HPC Best Practices

Ontario Summer School on
High Performance Computing

Scott Northrup
SciNet HPC Consortium
Compute Canada

June 28th, 2012

Outline

1. Work-flow
2. Batch Computing
3. Data Management
   - File Systems and I/O
   - Data Management
   - Parallel I/O
4. Development Overview
   - Compilers
   - Libraries
5. Performance Analysis

Acknowledgments

Contributing Material

- HPC Best Practices - G. Baolai, SHARCNET
- The Parallel File System and I/O - R. van Zon, SciNet
- Monitoring Job Efficiently - R. van Zon, SciNet
- Profiling and Tuning - L. J. Dursi, SciNet
- Tuning MPI - L. J. Dursi, SciNet

Work-flow

Typical Simulation/Analysis Work-flow

- pre-process (grid creation, partitioning)
- solve/analysis
- postpones (data-mining, generate plots)

Work-flow

Typical Simulation/Analysis Work-flow

- pre-process (grid creation, partitioning)
- solve/analysis
- postpones (data-mining, generate plots)

Automate

- learn and use script languages (bash, python)
- use scheduler efficiently (job size, dependencies)
- add data management into work-flow from beginning

Batch Computing

Batch computing

SciNet systems are batch compute clusters

- Computing by submitting batch jobs to the scheduler.
- When you submit a job, it gets placed in a queue.
- Job priority is based on allocation and fairshare.
- When sufficient nodes are free to execute a job, it starts the job on the appropriate compute nodes.
- Jobs remain 'idle' until resources become available.
- Jobs can be temporarily 'blocked' if you submit too much.

Batch computing

Components

Torque: Resource manager providing control over batch jobs and distributed compute nodes.

Moab: A policy-based job scheduler and event engine that enables utility-based computing for clusters.

Fairshare: Mechanism using past utilization for prioritization.

Job cycle

Preparation

- Compile
- Test on devel node
- Determine resources
- Write job script

llsubmit
qsub

Job cycle

Preparation

- Compile
- Test on devel node
- Determine resources
- Write job script

llsubmit
qsub

Monitor

- Job queued?
- When will it run?
- What else is queued?
- Efficiency?

qstat -f
checkjob
showstart
showbf
showq

Job cycle

Preparation

- Compile
- Test on devel node
- Determine resources
- Write job script

llsubmit
qsub

Monitor

- Job queued?
- When will it run?
- What else is queued?
- Efficiency?

qstat -f
checkjob
showstart
showbf
showq

Control

- Cancel job
- Ssh to nodes
- Interactive jobs
- Debug queue

canceljob
top
qsub -I
qsub -q debug

Job cycle

Preparation

- Compile
- Test on devel node
- Determine resources
- Write job script

llsubmit
qsub

Monitor

- Job queued?
- When will it run?
- What else is queued?
- Efficiency?

qstat -f
checkjob
showstart
showbf
showq

Control

- Cancel job
- Ssh to nodes
- Interactive jobs
- Debug queue

canceljob
top
qsub -I
qsub -q debug

Reports

- Check .o/.e *jobname*.{o,e}
- usage stats on Scinet web portal

showstats -u

Monitoring not-yet-running jobs

qstat and checkjob

- Show torque status right away on GPC: qstat
- Show moab status (better): checkjob *jobid*
- See more details of the job: checkjob -v *jobid* (e.g., why is my job blocked?)

showq

- See all the jobs in the queue: showq (from gpc or tcs)
- See your jobs in the queue: showq -u *user*

showstart and showbf

- Estimate when a job may start: showbf
- Estimate when a queued job may start: showstart *jobid*
- Estimates only!

Monitoring running jobs

checkjob

- checkjob *jobid*

showq

- showq -r -u $USER

ssh

- ssh *node* (node name from checkjob)
- top: shows process state, memory and cpu usage

Job stdout/stderr files

- {jobname}.o{jobid}
- {jobname}.e{jobid}

Top example

```
gpc-f103n084-$ ssh gpc-f109n001
gpc-f109n001-$ top
```

```
top - 21:56:45 up  5:56,  1 user,  load average: 5.55, 1.73, 0.88
Tasks: 234 total,   1 running, 233 sleeping,   0 stopped,   0 zombie
Cpu(s): 11.4%us, 36.2%sy,  0.0%ni, 52.2%id,  0.0%wa,  0.0%hi,  0.2%si,  0.0%st
Mem:  16410900k total,  1542768k used, 14868132k free,        0k buffers
Swap:        0k total,        0k used,        0k free,   294628k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+   P COMMAND
22479 ljdursi   18   0  108m 4816 3212 S 98.5  0.0   1:04.81  6 gameoflife
22480 ljdursi   18   0  108m 4856 3260 S 98.5  0.0   1:04.85 13 gameoflife
22482 ljdursi   18   0  108m 4868 3276 S 98.5  0.0   1:04.83  2 gameoflife
22483 ljdursi   18   0  108m 4868 3276 S 98.5  0.0   1:04.82  8 gameoflife
22484 ljdursi   18   0  108m 4832 3232 S 98.5  0.0   1:04.80  9 gameoflife
22481 ljdursi   18   0  108m 4856 3256 S 98.2  0.0   1:04.81  3 gameoflife
22485 ljdursi   18   0  108m 4808 3208 S 98.2  0.0   1:04.80  4 gameoflife
22478 ljdursi   18   0  117m 5724 3268 D 69.6  0.0   0:46.07 15 gameoflife
 8042 root       0 -20 2235m 1.1g  16m S  2.3  6.8   0:30.59  8 mmfsd
10735 root      15   0  3792  452  372 S  1.3  0.0   0:16.80  0 cat
```

Top example

```
gpc-f103n084-$ ssh gpc-f109n001
gpc-f109n001-$ top
```

```
top - 21:56:45 up  5:56,  1 user,  load average: 5.55, 1.73, 0.88
Tasks: 234 total,   1 running, 233 sleeping,   0 stopped,   0 zombie
Cpu(s): 11.4%us, 36.2%sy,  0.0%ni, 52.2%id,  0.0%wa,  0.0%hi,  0.2%si,  0.0%st
Mem:  16410900k total,  1542768k used, 14868132k free,        0k buffers
Swap:        0k total,        0k used,        0k free,   294628k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+   P COMMAND
22479 ljdursi   18   0  108m 4816 3212 S 98.5  0.0   1:04.81  6 gameoflife
22480 ljdursi   18   0  108m 4856 3260 S 98.5  0.0   1:04.85 13 gameoflife
22482 ljdursi   18   0  108m 4868 3276 S 98.5  0.0   1:04.83  2 gameoflife
22483 ljdursi   18   0  108m 4868 3276 S 98.5  0.0   1:04.82  8 gameoflife
22484 ljdursi   18   0  108m 4832 3232 S 98.5  0.0   1:04.80  9 gameoflife
22481 ljdursi   18   0  108m 4856 3256 S 98.2  0.0   1:04.81  3 gameoflife
22485 ljdursi   18   0  108m 4808 3208 S 98.2  0.0   1:04.80  4 gameoflife
22478 ljdursi   18   0  117m 5724 3268 D 69.6  0.0   0:46.07 15 gameoflife
 8042 root       0 -20 2235m 1.1g  16m S  2.3  6.8   0:30.59  8 mmfsd
10735 root      15   0  3792  452  372 S  1.3  0.0   0:16.80  0 cat
```

Control

canceljob

- If you spot a mistake: canceljob *jobid*

qsub for interactive and debug jobs

- -I:
  - Interactive
  - After qsub, waits for jobs to start.
  - Usually combined with:
- -q debug:
  - Debug queue has 10 nodes reserved for short jobs.
  - You can get 1 node for 2 hours, but also
  - 8 nodes, for half an hour.

Job output/error files (*.e / *.o)

```
----------------------------------------
Begin PBS Prologue Tue Sep 14 17:14:48 EDT 2010 1284498888
Job ID:      3053514.gpc-sched
Username:    ljdursi
Group:       scinet
Nodes:       gpc-f134n009 gpc-f134n010 gpc-f134n011 gpc-f134n012
gpc-f134n043 gpc-f134n044 gpc-f134n045 gpc-f134n046 gpc-f134n047 gpc-f134n048
[...]
End PBS Prologue Tue Sep 14 17:14:50 EDT 2010 1284498890
----------------------------------------
[ Your job's output here... ]
----------------------------------------
Begin PBS Epilogue Tue Sep 14 17:36:07 EDT 2010 1284500167
Job ID:      3053514.gpc-sched
Username:    ljdursi
Group:       scinet
Job Name:    fft_8192_procs_2048
Session:     18758
Limits:      neednodes=256:ib:ppn=8,nodes=256:ib:ppn=8,walltime=01:00:00
Resources:   cput=713:42:30,mem=3463854672kb,vmem=3759656372kb,walltime=00:21:07
Queue:       batch_ib
Account:
Nodes:  gpc-f134n009 gpc-f134n010 gpc-f134n011 gpc-f134n012 gpc-f134n043
[...]
Killing leftovers...
gpc-f141n054:   killing gpc-f141n054 12412

End PBS Epilogue Tue Sep 14 17:36:09 EDT 2010 1284500169
----------------------------------------
```

Data Management

Disk I/O

Common Uses

- Checkpoint/Restart Files
- Data Analysis
- Data Organization
- Time accurate and/or Optimization Runs
- Batch and Data processing
- Database

Disk I/O

Common Bottlenecks

- Mechanical disks are slow!
- System call overhead (open, close, read, write)
- Shared file system (nfs, lustre, gpfs, etc)
- HPC systems typically designed for high bandwidth (GB/s) not IOPs
- Uncoordinated independent accesses

Disk Access Rates over Time

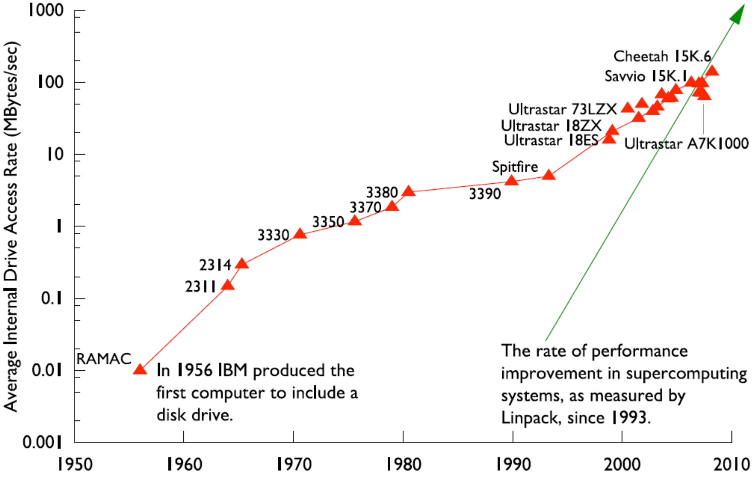


Figure by R. Ross, Argonne National Laboratory, CScADS09

Memory/Storage Latency

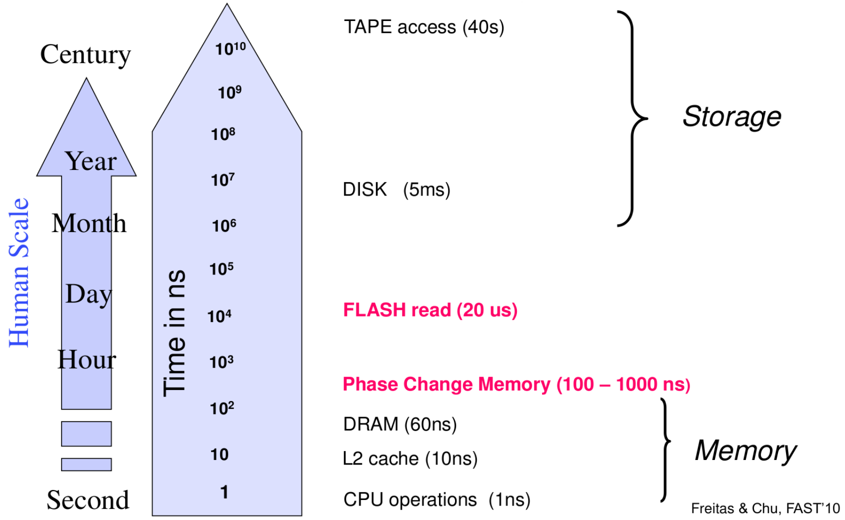


Figure by R. Freitas and L Chiu, IBM Almaden Labs, FAST'10

Definitions

IOPs

Input/Output Operations Per Second (read,write,open,close,seek)

I/O Bandwidth

Quantity you read/write (think network bandwidth)

Comparisons

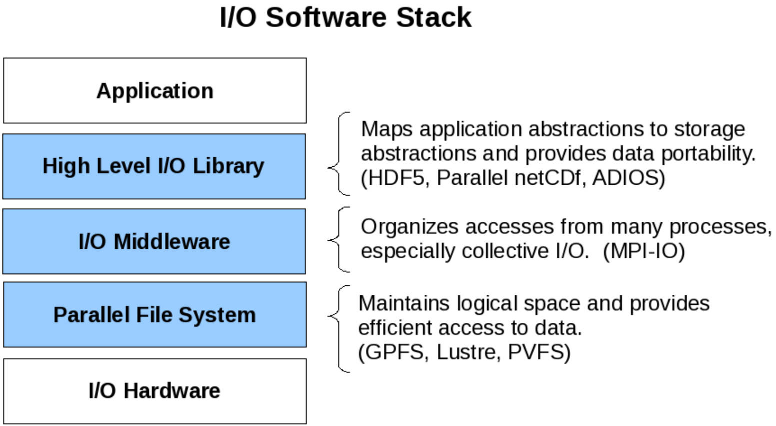
Device	Bandwidth (MB/s)	per-node	IOPs	per-node
SATA HDD	100	100	100	100
SSD HDD	250	250	4000	4000
SciNet	5000	1.25	30000	7.5

SciNet Filesystem

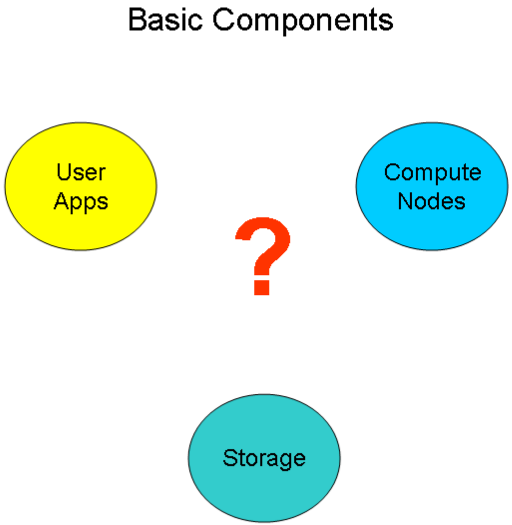
File System

- 1,790 1TB SATA disk drives, for a total of 1.4PB
- Two DCS9900 couplets, each delivering:
  - 4-5 GB/s read/write access (bandwidth)
  - 30,000 IOPs max (open, close, seek, . . .)
- Single *GPFS* file system on TCS and GPC
- I/O goes over infiniband (as of April 2012)
- File system is parallel!

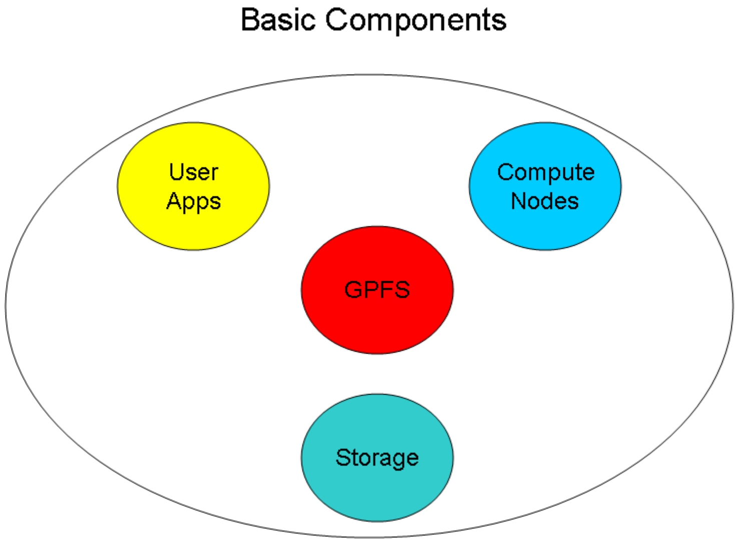
I/O Software Stack



Parallel File System

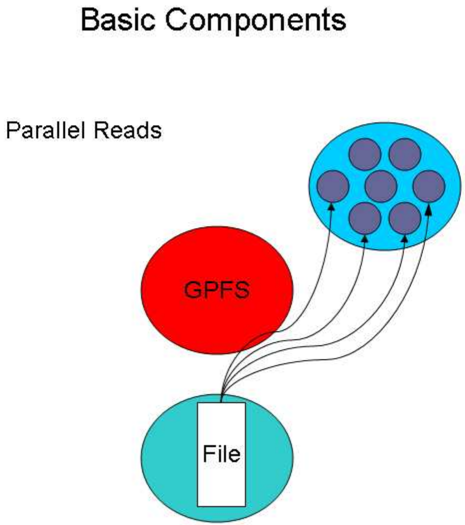


Parallel File System

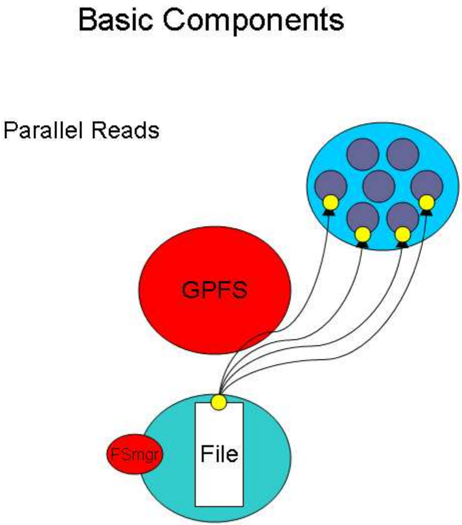


General Parallel File System

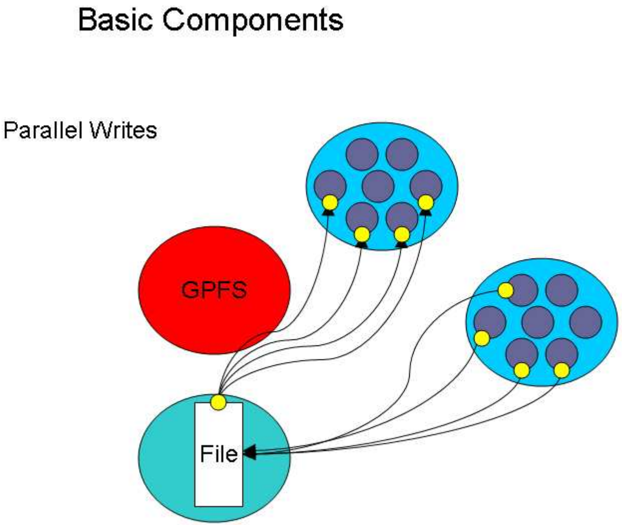
Parallel File System



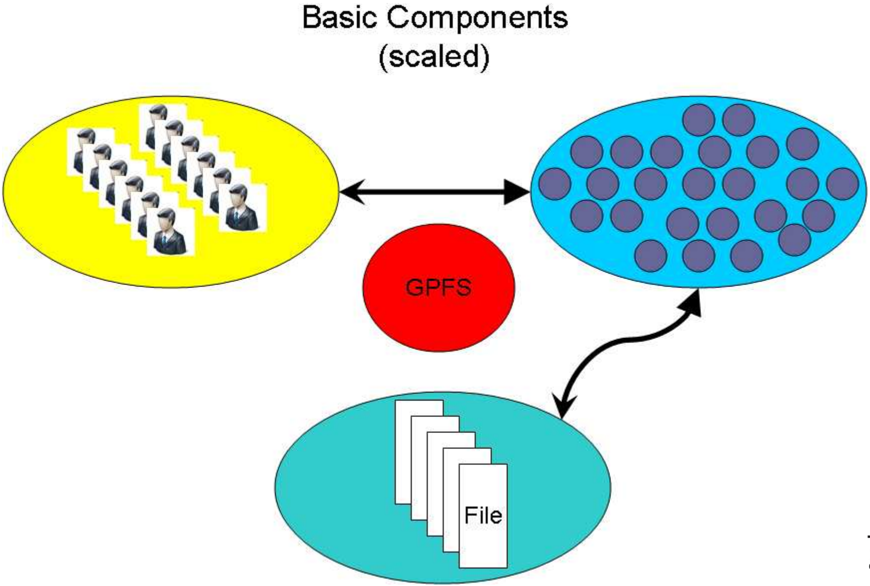
Parallel File System



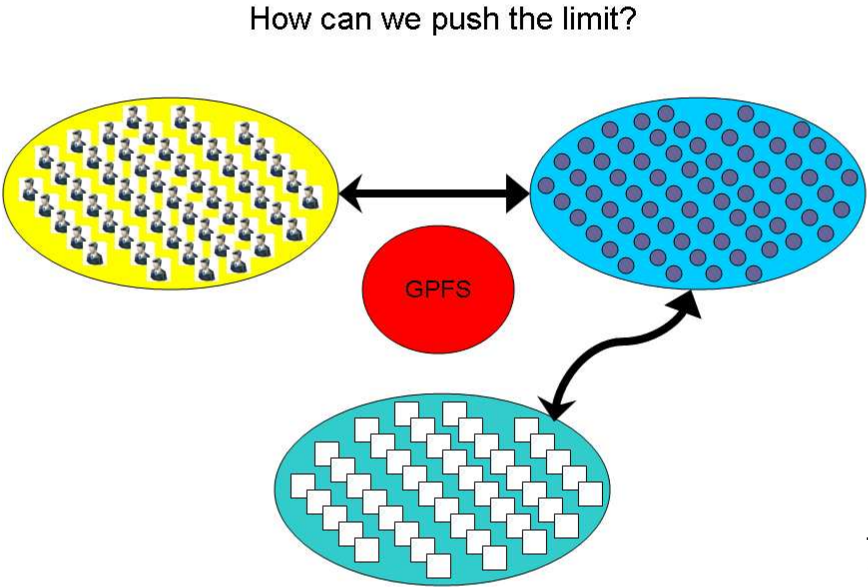
Parallel File System



Parallel File System

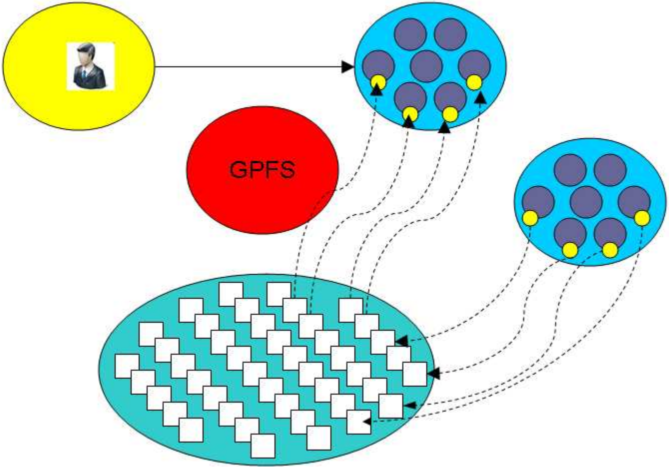


Parallel File System



Parallel File System

How can we BREAK the limit?



Parallel File System

File Locks

Most parallel file systems use locks to manage concurrent file access

- Files are broken up into lock units
- Clients obtain locks on units that they will access before I/O occurs
- Enables caching on clients as well (as long as client has a lock, it knows its cached data is valid)
- Locks are reclaimed from clients when others desire access

Parallel File System

- Optimal for large shared files.
- Behaves poorly under many small reads and writes, high IOPs
- Your use of it affects everybody!
  (Different from case with CPU and RAM which are not shared.)
- How you read and write, your file format, the number of files in a directory, and how often you `ls`, affects every user!
- The file system is shared over the network on GPC:
  Hammering the file system can hurt process communications.
- File systems are not infinite!
  Bandwidth, metadata, IOPs, number of files, space, ...

Parallel File System

- 2 jobs doing simultaneous I/O can take much longer than twice a single job duration due to disk contention and directory locking.
- SciNet: 500+ users doing I/O from 4000 nodes. That's a lot of sharing and contention!

SciNet
compute • calcul
CANADA

I/O Best Practices

Make a plan

- Make a plan for your data needs:
  - How much will you generate,
  - How much do you need to save,
  - And where will you keep it?
- Note that /scratch is temporary storage for 3 months or less.

Options?

1. Save on your departmental/local server/workstation (it is possible to transfer TBs per day on a gigabit link);
2. Apply for a project space/HPSS allocation at next RAC call (but space is very limited);
3. Change storage format.

I/O Best Practices

Monitor and control usage

- Minimize use of filesystem commands like `ls` and `du`.
- Regularly check your disk usage using /scinet/gpc/bin/diskUsage.
- Warning signs which should prompt careful consideration:
  - More than 100,000 files in your space
  - Average file size less than 100 MB
- Monitor disk actions with `top` and `strace`

- RAM is always faster than disk; think about using ramdisk.
- Use `gzip` and `tar` to compress files to bundle many files into one
- Try gziping your *data* files. 30% not atypical!
- Delete files that are no longer needed
- Do "housekeeping" (`gzip`, `tar`, delete) regularly.

I/O Best Practices

Do's

- Write binary format files
  Faster I/O and less space than ASCII files.
- Use parallel I/O if writing from many nodes
- Maximize size of files. Large block I/O optimal!
- Minimize number of files. Makes filesystem more responsive!

Don'ts

- Don't write lots of ASCII files. Lazy, slow, and wastes space!
- Don't write many hundreds of files in a 1 directory. (File Locks)
- Don't write many small files ($<$ 10MB).
  System is optimized for large-block I/O.

Data Management

Formats

- ASCII
- Binary
- MetaData (XML)
- Databases
- Standard Library's (HDF5,NetCDF)

ASCII

American Standard Code for Information Interchange

Pros

- Human Readable
- Portable (architecture independent)

Cons

- Inefficient Storage
- Expensive for Read/Write (conversions)

Native Binary

100100100

Pros

- Efficient Storage (256 x floats @4bytes takes 1024 bytes)
- Efficient Read/Write (native)

Cons

- Have to know the format to read
- Portability (Endianness)

ASCII vs. binary

Writing 128M doubles

Format	/scratch (GPCS)	/dev/shm (RAM)	/tmp (disk)
ASCII	173s	174s	260s
Binary	6s	1s	20s

Syntax

Format	C	FORTRAN
ASCII	`fprintf()`	open(6,file='test',form='formatted') write(6,*)
Binary	`fwrite()`	open(6,file='test',form='unformatted') write(6)

Metadata

What is Metadata?

Data about Data

- File System: size, location, date, owner, etc.
- App Data: File format, version, iteration, etc.

Example: XML

```
<?xml version="1.0" encoding="UTF-8" ?>
<slice_data>
  <format>UTF1000</format>
  <verstion>6.8</version>
  <img src="slice1_2010.img" alt='Slice 1 of Data'/>
  <date> January 15th, 2010 </date>
  <loc> 47 23.516 -122 02.625 </loc>
</slice_data>
```

Databases

Beyond flat files

- Very powerful and flexible storage approach
- Data organization and analysis can be greatly simplified
- Enhanced performance over seek/sort depending on usage
- Open Source Software
  - SQLite (serverless)
  - PostgreSQL
  - mySQL

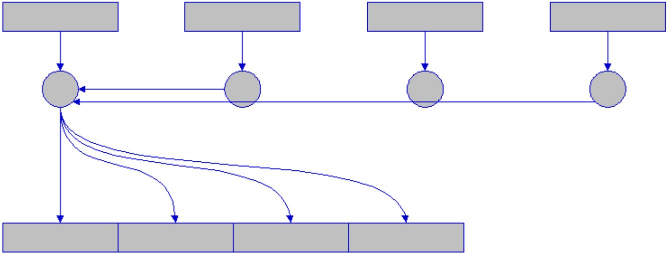
“Standard” Formats

- CGNS (CFD General Notation System)
- IGES/STEP (CAD Geometry)
- HDF5 (Hierarchical Data Format)
- NetCDF (Network Common Data Format)
- disciplineX version

Parallel I/O

Sequential I/O (only proc 0 Writes/Reads)

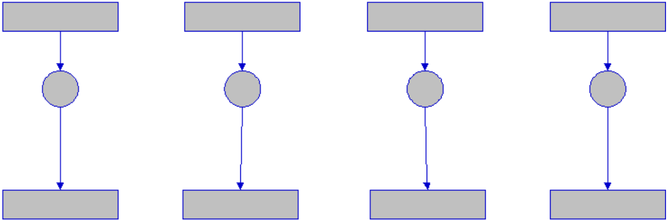
- Pro
  - Trivially simple for small I/O
  - Some I/O libraries not parallel
- Con
  - Bandwidth limited by rate one client can sustain
  - May not have enough memory on node to hold all data
  - Won't scale (built in bottleneck)



Common Ways of Doing Parallel I/O

N files for N Processes

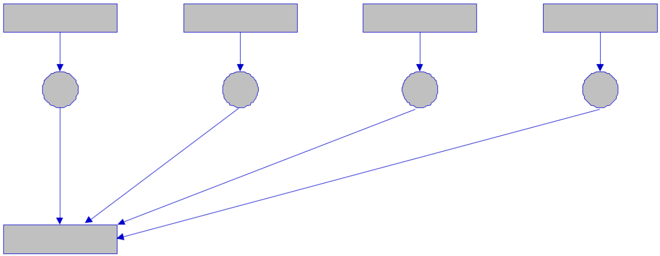
- Pro
  - No interprocess communication or coordination necessary
  - Possibly better scaling than single sequential I/O
- Con
  - As process counts increase, lots of (small) files, won't scale
  - Data often must be post-processed into one file
  - Uncoordinated I/O may swamp file system (File LOCKS!)



Common Ways of Doing Parallel I/O

All Processes Access One File

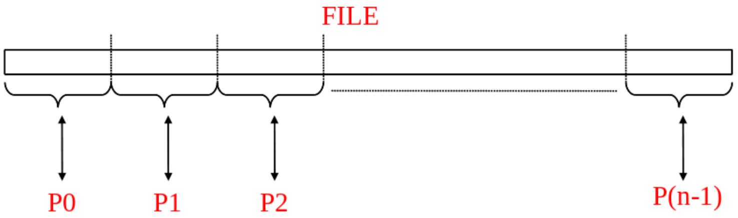
- Pro
  - Only one file
  - Data can be stored canonically, avoiding post-processing
  - Will scale if done correctly
- Con
  - Uncoordinated I/O WILL swamp file system (File LOCKS!)
  - Requires more design and thought



Parallel I/O

What is Parallel I/O?

Multiple processes of a parallel program accessing data (reading or writing) from a common file.



Parallel I/O

Why Parallel I/O?

- Non-parallel I/O is simple but:
  - Poor performance (single process writes to one file)
  - Awkward and not interoperable with other tools (each process writes a separate file)
- Parallel I/O
  - Higher performance through collective and contiguous I/O
  - Single file (visualization, data management, storage, etc)
  - Works with file system not against it

Parallel I/O

Available Approaches

- MPI-IO: MPI-2 Language Standard
- HDF (Hierarchical Data Format)
- NetCDF (Network Common Data Format)
- Adaptable IO System (ADIOS)
  - Actively developed (OLCF,SandiaNL,GeorgiaTech) and used on largest HPC systems (Jaguar,Blue Gene/P)
  - External to the code XML file describing the various elements
  - Uses MPI-IO, can work with HDF/NetCDF

Software Development

Software Development

Tools of the Trade

- Editors/IDE

Software Development

Tools of the Trade

- Editors/IDE
- Version Control

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers
- Libraries

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers
- Libraries
- Debuggers (gdb,idb, Allinea DDT)

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers
- Libraries
- Debuggers (gdb,idb, Allinea DDT)
- Memory (valgrind)

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers
- Libraries
- Debuggers (gdb,idb, Allinea DDT)
- Memory (valgrind)
- I/O (strace)

Software Development

Tools of the Trade

- Editors/IDE
- Version Control
- Build System (make)
- Compilers
- Libraries
- Debuggers (gdb,idb, Allinea DDT)
- Memory (valgrind)
- I/O (strace)
- Performance (gprof,Scalasa,IPM)

Version Control

What is it?

- A tool for managing changes in a set of files.

Version Control

What is it?

- A tool for managing changes in a set of files.
- Figuring out who broke what where and when.

Version Control

What is it?

- A tool for managing changes in a set of files.
- Figuring out who broke what where and when.

Why Do it?

- Collaboration
- Organization
- Track Changes
- Faster Development
- Reduce Errors

Collaboration

With others and yourself

Questions

Collaboration

With others and yourself

Questions

- What if two (or more) people want to edit the same file at the same time?

Collaboration

With others and yourself

Questions

- What if two (or more) people want to edit the same file at the same time?
- What if you work on SciNet and on your own computer?

Questions

- What if two (or more) people want to edit the same file at the same time?
- What if you work on SciNet and on your own computer?

Answers

Collaboration

With others and yourself

Questions

- What if two (or more) people want to edit the same file at the same time?
- What if you work on SciNet and on your own computer?

Answers

- Option 1: make them take turns
  - But then only one person can be working at any time
  - And how do you enforce the rule?

Collaboration

With others and yourself

Questions

- What if two (or more) people want to edit the same file at the same time?
- What if you work on SciNet and on your own computer?

Answers

- Option 1: make them take turns
  - But then only one person can be working at any time
  - And how do you enforce the rule?
- Option 2: patch up differences afterwards
  - Requires a lot of re-working
  - Stuff always gets lost

Collaboration

Questions

- What if two (or more) people want to edit the same file at the same time?
- What if you work on SciNet and on your own computer?

Answers

- Option 1: make them take turns
  - But then only one person can be working at any time
  - And how do you enforce the rule?
- Option 2: patch up differences afterwards
  - Requires a lot of re-working
  - Stuff always gets lost
- Option 3: **Version Control**

Organize and Track Changes

Question

Organize and Track Changes

Question

- Want to undo changes to a file
  - Start work, realize it's the wrong approach, want to get back to starting point
  - Like "undo" in an editor...
    ...but keep the whole history of every file, forever

Organize and Track Changes

Question

- Want to undo changes to a file
  - Start work, realize it's the wrong approach, want to get back to starting point
  - Like "undo" in an editor...
    ...but keep the whole history of every file, forever
- Also want to be able to see who changed what, when
  - The best way to find out how something works is often to ask the person who wrote it

Organize and Track Changes

Question

- Want to undo changes to a file
  - Start work, realize it's the wrong approach, want to get back to starting point
  - Like "undo" in an editor...
    ...but keep the whole history of every file, forever
- Also want to be able to see who changed what, when
  - The best way to find out how something works is often to ask the person who wrote it

Answer

- **Version Control**

What Software to Use

Software

- Open Source
  - Subversion, CVS, RCS
  - Git, Mercurial, Bazaar
- Commercial
  - Perforce, ClearCase

available as modules on SciNet

Version Control Software

Subversion (svn)

- Centralized Version Control
- Replaces CVS
- Lots of web and GUI integration
- Users: GCC, KDE, FreeBSD

Git

- Distributed Version Control
- *nix command line driven design model
- advanced features `git-stash`, `git-rebase`, `git-cherry-pick`
- Users: Linux kernel, GNOME, Wine, X.org

Compiler Flags and Optimizations

Numerical Libraries

Numerical Computing

Numerical Methods

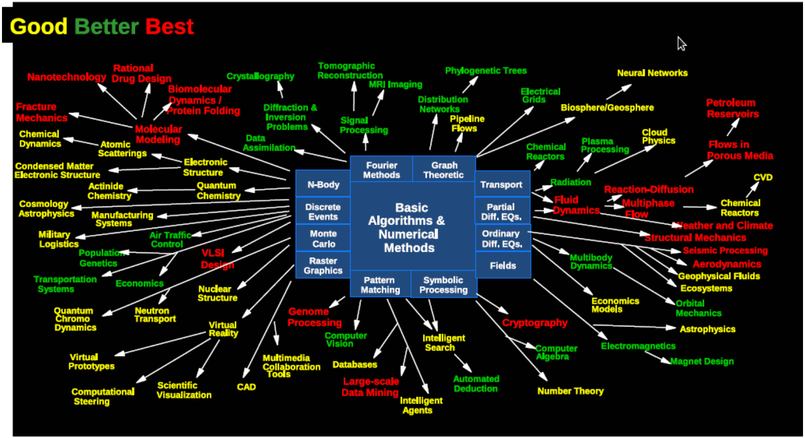
- Linear algebra
- Nonlinear equations
- Optimization
- Interpolation/Approximation
- Integration and differentiation
- Solving ODEs
- Solving PDEs
- FFT
- Random numbers and stochastic simulations
- Special functions

Numerical Algorithms

Top Ten Algorithms for Science (Jack Dongarra, 2000)

1. Metropolis Algorithm for Monte Carlo
2. Simplex Method for Linear Programming
3. Krylov Subspace Iteration Methods
4. The Decompositional Approach to Matrix Computations
5. The Fortran Optimizing Compiler
6. QR Algorithm for Computing Eigenvalues
7. Quicksort Algorithm for Sorting
8. Fast Fourier Transform
9. Integer Relation Detection
10. Fast Multipole Method

Numerical Algorithms



Argonne National Laboratory GBB

Libraries

Numerical Libraries

- BLAS (gotoblas, ATLAS)
- LAPACK (ESSL, MKL, ACML)
- ScaLAPACK
- GSL (GNU Scientific Library)
- FFTW
- PETSc
- TAO
- IMSL
- NAG

Libraries

Numerical Libraries

- BLAS (gotoblas, ATLAS)
- LAPACK (ESSL, MKL, ACML)
- ScaLAPACK
- GSL (GNU Scientific Library)
- FFTW
- PETSc
- TAO
- IMSL
- NAG

Don't re-invent the wheel!

Performance & Profiling