Making effective use of HPC systems

August 4-8, 2014
SDSC Summer Institute

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How do I know that I'm making effective use of my hardware?

We always want to know if we're making effective use of our hardware. This applies to your own workstation or private cluster, but even more when you're using high-end, shared resources.

This presentation won't cover everything, but it will hopefully give you an introduction to some important topics and an awareness of what's going on 'under the hood'

Focus will be on a few of the standard and widely available, yet powerful tools and utilities. We'll consider top, gprof and iostat along with the /proc and /sys pseudo file systems. We'll also discuss scalability and Amdahl's law.

Obtaining hardware info – why should I care?

- You may be asked to report the details of your hardware in a manuscript or presentation, especially if you're discussing application performance
- You'll know exactly what you're running on. Can answer questions like "Is the login node the same as the compute nodes?"
- It will give you a way of estimating performance, or at least bounds on performance, on another system. All else being equal, jobs will run at least as fast on hardware that has
  - Faster CPU clock speeds
  - Larger caches
  - Faster local drives
- You'll sound smart when you talk to other technical people
  - You: "I'm running on a dual socket node with 8-core Intel ES-2670 processors clocked at 2.6 GHz with 64 GB of DDR3-1333"
  - Your colleague: "Wow!"

Getting processor information (/proc/cpuinfo)

On Linux machines, the /proc/cpuinfo pseudo-file lists key processor information. Mostly cryptic hardware details, but also some very helpful data

```
processor       : 0 (processor number, actually refers to core)
vendor_id       : GenuineIntel
cpu family      : 6
model           : 45
model name      : Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz (processor type)
stepping        : 6
cpu MHz         : 2593.576 (nominal clock speed)
cache size      : 20480 KB
physical id     : 0
siblings        : 8
core id         : 0
cpu cores       : 8 (number of cores in processor)
apicid          : 0
initial apicid  : 0
fpu             : yes
fpu_exception   : yes
cpuid level     : 13
wp              : yes
flags           : fpu vme de … avx … (AVX capable processor)
```

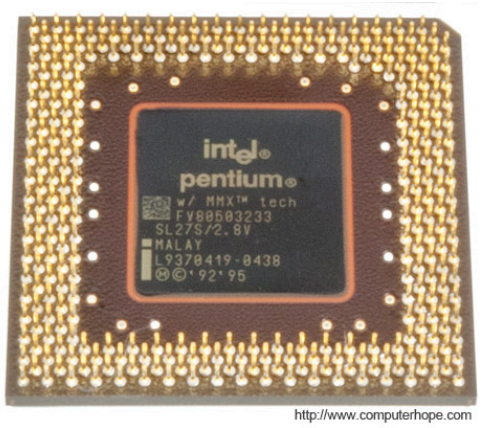
What do we mean by a pseudo-file system?

/proc and /sys are not real file systems. Instead, they're just interfaces to Linux kernel data structures in a convenient and familiar file system format.

```
$ ls -l /proc/cpuinfo
-r--r--r-- 1 root root 0 Aug  3 20:45 /proc/cpuinfo
[sinkovit@gcn-18-32 ~]$ head /proc/cpuinfo
processor : 0
vendor_id : GenuineIntel
cpu family          : 6
model               : 45
model name          : Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz
stepping  : 6
cpu MHz             : 2593.861
cache size          : 20480 KB
physical id         : 0
siblings  : 8
```

Advanced Vector Extensions (AVX)

- The Advanced Vector Extensions (AVX) are an extension to the x86 microprocessor architecture that allows a compute core to perform up to 8 floating point operations per cycle. Previous limit was 4/core/cycle
- Partial response to challenges in increasing clock speed (we're now stuck around 2.5 – 3.0 GHz)



1996 Intel Pentium 150 MHz

March 6, 2000 8:00 AM PST

AMD makes move to 1-GHz chip

By Joe Wilcox and Michael Kanellos
Staff Writers, CNET News

Advanced Vector Extensions (AVX)

- Keeping to the theme of “Am I making effective use of hardware?”, should ideally observe a 2x speedup when going from a non-AVX processor to an AVX capable processor (all else being equal)
- If not, you’re not making very effective use of your hardware and you can run just as well on a less expensive non-AVX CPU.

- Newer generations of processors are expected to have the AVX2 instructions. As you might have guessed, AVX2 cores will be capable of 16 floating point operations per cycle per core.
- Don’t get too excited. It’s difficult enough to make good use of AVX and even harder to make good use of AVX2. Need long loops with vectorizable content. Memory bandwidth not keeping up with gains in computing power.

```
...
flags : fpu vme de … avx2 … (AVX2 capable processor)
...
```

Getting processor information (/proc/cpuinfo)

Confirming number of compute cores on a node. Note that this will report virtual cores if features such as hyper-threading are enabled (not done on SDSC machines)

```
[sinkovit@gordon-ln2 ~]$ grep processor /proc/cpuinfo
processor : 0
processor : 1
processor : 2
processor : 3
processor : 4
processor : 5
processor : 6
processor : 7
processor : 8
processor : 9
processor : 10
processor : 11
processor : 12
processor : 13
processor : 14
processor : 15
```

Getting processor information (/proc/cpuinfo)

Confirming number of sockets (processors) on a node. Each processor will be labeled with a unique ‘physical id’

```
[sinkovit@gordon-ln2 ~]$ grep 'physical id' /proc/cpuinfo
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 0
physical id         : 1
physical id         : 1
physical id         : 1
physical id         : 1
physical id         : 1
physical id         : 1
physical id         : 1
physical id         : 1
```

Getting memory information (/proc/meminfo)

On Linux machines, the /proc/meminfo pseudo-file lists key memory specs. More information than you probably want, but at least one bit of useful data

```
MemTotal:       66055696 kB   (total physical memory)
MemFree:         3843116 kB
Buffers:            6856 kB
Cached:         31870056 kB
SwapCached:          1220 kB
Active:          7833904 kB
Inactive:       25583720 kB
Active(anon):     593252 kB
Inactive(anon):   949000 kB
Active(file):    7240652 kB   (pretty good approximation to used memory)
Inactive(file): 24634720 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:       2097144 kB
SwapFree:         902104 kB
Dirty:             17772 kB
Writeback:            32 kB
AnonPages:       1540768 kB
...
```

For more details, see http://www.redhat.com/advice/tips/meminfo.html

Getting memory information (/proc/meminfo)

Using a simple script, you can monitor total memory usage for all processes as a function of time. Note that there is a lot of discussion on how to precisely measure memory (http://stackoverflow.com/search?q=measuring+memory+usage). The following should be good enough if you're on a dedicated node.

```
#!/usr/bin/perl
use strict;
use warnings;
my $count = 0;
print (" time(s)    Memory (GB)\n");
while(1) {
    sleep(1);
    $count++;
    open(MI, "/proc/meminfo");
    while(<MI>) {
        if (/Active:/) {
            my (undef, $active, undef) = split();
            $active = $active /         1048576.0;
            printf("%6d       %f\n", $count, $active);
        }
    }
    close(MI);
}
```

Finding cache information

On Linux systems, can obtain cache properties through the /sys pseudo filesystem. Details may vary slightly by O/S version and vendor, but basic information should be consistent

```
$ pwd
/sys/devices/system/cpu

$ ls
cpu0   cpu12  cpu2  cpu6  cpufreq     online       probe
cpu1   cpu13  cpu3  cpu7  cpuidle     perf_events  release
cpu10  cpu14  cpu4  cpu8  kernel_max  possible     sched_mc_power_savings
cpu11  cpu15  cpu5  cpu9  offline     present      sched_smt_power_savings

$ cd cpu0/cache
$ ls
index0  index1  index2  index3

$ cd index0
$ ls
coherency_line_size  physical_line_partition  size
level                shared_cpu_list          type
number_of_sets       shared_cpu_map           ways_of_associativity
```

Cache properties – Intel Sandy Bridge (Intel Xeon E5-2670)

level	type	line size	sets	associativity	size (KB)
L1	data	64	64	8	32
L1	instruction	64	64	8	32
L2	unified	64	512	8	256
L3	unified	64	16384	20	20480

High end processor used in many Top500 supercomputers, including SDSC's Gordon system and TACC's Stampede

L1 and L2 caches are per core

L3 cache shared between all 8 cores in socket

sanity check: line size x sets x associativity = size

L2 cache size = 64 x 512 x 8 = 262144 = 256 K

Cache properties – AMD Magny-Cours (AMD Opteron Processor 6136)

level	type	line size	sets	associativity	size (KB)
L1	data	64	512	2	64
L1	instruction	64	512	2	64
L2	unified	64	512	16	512
L3	unified	64	1706	48	5118

Previous generation AMD enterprise level processor, used in SDSC's Trestles system (currently used as capacity HPC resource)

L1 and L2 caches are per core

L3 cache shared between all 8 cores in socket

sanity check: line size x sets x associativity = size

L2 cache size = 64 x 512 x 16 = 524288= 512K

Impact of cache size on performance

Based on the clock speed and instruction set, program run on single core of Gordon should be 2.26x faster than on Trestles. The larger L1 and L2 cache sizes on Trestles mitigate performance impact for very small problems.

DGSEV (Ax=b) wall times as function of problem size

N	t (Trestles)	t (Gordon)	ratio	KB
62	0.000117	0.000086	1.36	30
125	0.000531	0.000384	1.38	122
250	0.002781	0.001542	1.80	488
500	0.016313	0.007258	2.24	1953
1000	0.107222	0.046252	2.31	7812
2000	0.744837	0.331818	2.24	31250
4000	5.489990	2.464218	2.23	125000

Finding SCSI device information

SCSI (Small Computer System Interface) is a common interface for mounting peripheral, such as hard drives and SSDs. The /proc/scsi/scsi file will provide info on SCSI devices

```
// Gordon login node
$ cat /proc/scsi/scsi
Attached devices:
Host: scsi0 Channel: 00 Id: 00 Lun: 00
  Vendor: ATA      Model: INTEL SSDSA2CW08 Rev: 4PC1
  Type:   Direct-Access                    ANSI  SCSI revision: 05
```

Click to open expanded view

Intel SSDSA2CW080G3 80 GB Internal Solid State Drive - 1 x Retail Pack. 80GB SSD 320 SERIES RESELLR BOX GEN3 2.5 MLC SATA2 9.5MM SATSSD. 2.5' - SATA

Finding network information

The ip command (/sbin/ip) is normally used by sys admins, but regular users can use it to learn about networking information

```
$ /sbin/ip link
1: lo: <LOOPBACK,UP,LOWER_UP> mtu 16436 qdisc noqueue state UNKNOWN
    link/loopback 00:00:00:00:00:00 brd 00:00:00:00:00:00
2: eth0: <BROADCAST,MULTICAST,UP,LOWER_UP> mtu 1500 qdisc mq state UP qlen 1000
    link/ether 00:1e:67:29:5f:02 brd ff:ff:ff:ff:ff:ff
3: eth1: <BROADCAST,MULTICAST,UP,LOWER_UP> mtu 1500 qdisc mq state UP qlen 1000
    link/ether 00:1e:67:29:5f:03 brd ff:ff:ff:ff:ff:ff
4: ib0: <BROADCAST,MULTICAST,UP,LOWER_UP> mtu 1500 qdisc pfifo_fast state UP qlen
256
    link/infiniband 80:00:00:48:fe:80:00:0a:aa:aa:aa:aa:00:1e:67:03:00:29:5f:07
brd 00:ff:ff:ff:ff:12:40:1b:ff:ff:00:00:00:00:00:00:ff:ff:ff:ff
5: ib1: <BROADCAST,MULTICAST,UP,LOWER_UP> mtu 1500 qdisc pfifo_fast state UP qlen
256
    link/infiniband 80:00:00:48:fe:8b:bb:bb:bb:bb:bb:b1:00:02:c9:03:00:2f:7b:21
brd 00:ff:ff:ff:ff:12:40:1b:ff:ff:00:00:00:00:00:00:ff:ff:ff:ff
```

Machine info - overkill?

- We've probably gone a little deeper than is necessary for you to be an effective supercomputer user.

- Think of this as a way to round out your HPC knowledge. You're learning a little bit about the tools of the trade, getting comfortable poking around on a system, acquiring the knowledge that will make it easier to work with your sys admin and picking up the background that will help you to make intelligent decisions in the future.

Using the Linux top utility

The top utility is found on all Linux systems and provides a high level view of running processes. Does not give any information at the source code level (profiling), but can still be very useful for answering questions such as

- How many of my processes are running?
- What are the states of the processes (running, sleeping, etc.)?
- Which cores are being utilized?
- Are there any competing processes that may be affecting my performance?
- What fraction of the CPU is each process using?
- How much memory does each process use?
- Is the memory usage growing over time? (Useful for identifying memory leaks)
- How many threads are my processes using?

Customizing top

Top has the following defaults, but is easily customizable

- Processes only (no threads)
- To toggle threads display, type “H” while top is running
- Information for all users
- Can restrict to a single user by launching with “top -u username”
- Process ID, priority, ‘nice’ level, virtual memory, physical memory, shared memory, state, %CPU, %memory, CPU time, command
- To modify, type “f” while top is running and toggle fields using letters
- Update information every 3 seconds
- Change refresh rate by launching with “top -d *n*”
- Ordered by CPU usage
- Type “M” to order by memory usage

Non-threaded code

stivoknis — sinkovit@gcn-17-57:~ — ssh — 94×33

```
top - 08:37:00 up 60 days, 14:23,  1 user,  load average: 15.32, 10.36, 6.12
Tasks: 624 total,  17 running, 607 sleeping,   0 stopped,   0 zombie
Cpu(s): 68.7%us,  1.3%sy,  0.0%ni, 29.9%id,  0.1%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  66054160k total, 37885796k used, 28168364k free,     8808k buffers
Swap:  2097144k total,    13400k used,  2083744k free, 32927192k cached
```

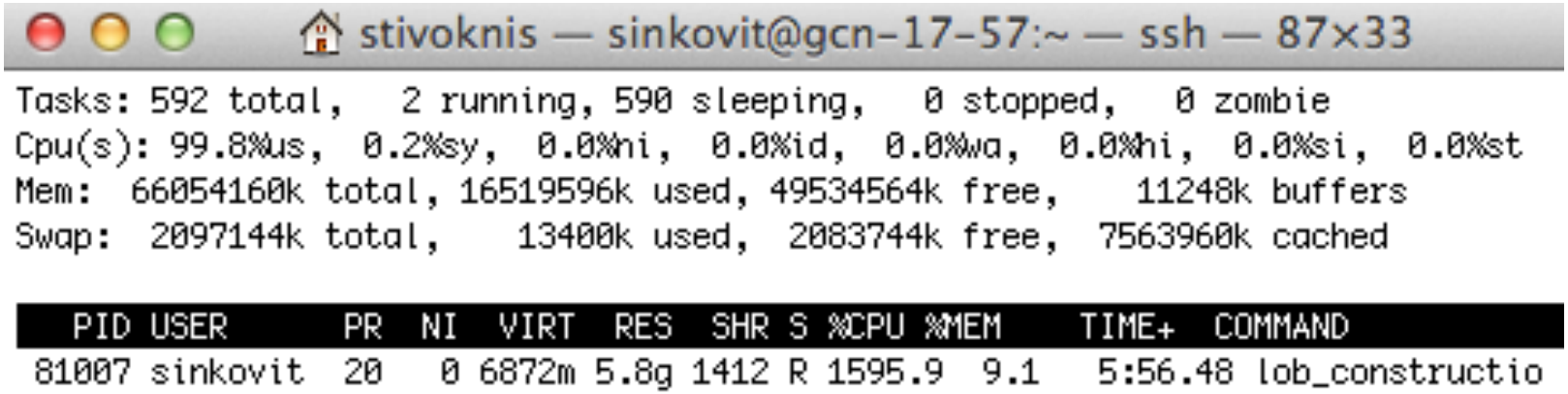
PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
70388	sinkovit	20	0	194m	76m	1612	R	100.0	0.1	1:31.06	lobfaster.pl
72547	sinkovit	20	0	120m	2976	1612	R	100.0	0.0	0:01.49	lobfaster.pl
72516	sinkovit	20	0	127m	9.9m	1608	R	100.0	0.0	0:02.09	lobfaster.pl
72526	sinkovit	20	0	121m	3388	1612	R	100.0	0.0	0:01.84	lobfaster.pl
72535	sinkovit	20	0	121m	4208	1612	R	100.0	0.0	0:01.73	lobfaster.pl
72565	sinkovit	20	0	120m	3212	1612	R	100.0	0.0	0:01.01	lobfaster.pl
72268	sinkovit	20	0	130m	12m	1612	R	98.9	0.0	0:11.96	lobfaster.pl
72359	sinkovit	20	0	123m	5976	1612	R	98.9	0.0	0:09.77	lobfaster.pl
72460	sinkovit	20	0	127m	10m	1612	R	98.9	0.0	0:08.38	lobfaster.pl
72481	sinkovit	20	0	131m	13m	1612	R	98.9	0.0	0:07.44	lobfaster.pl
72529	sinkovit	20	0	122m	4576	1612	R	98.9	0.0	0:01.82	lobfaster.pl
72439	sinkovit	20	0	130m	12m	1612	R	97.0	0.0	0:08.64	lobfaster.pl
72590	sinkovit	20	0	120m	3140	1612	R	71.7	0.0	0:00.37	lobfaster.pl
72602	sinkovit	20	0	120m	2576	1612	R	38.8	0.0	0:00.20	lobfaster.pl
72605	sinkovit	20	0	120m	2528	1600	R	34.9	0.0	0:00.18	lobfaster.pl
72608	sinkovit	20	0	119m	2340	1600	R	21.3	0.0	0:00.11	lobfaster.pl

16 processes, each using anywhere from 21.3% to 100% of a compute core.

Memory footprint (RES) is minimal, with each process only using up to 76 MB.

CPU times ranging from 0.11s (just started) to 1:31

Threaded code (thread display off)



Threaded code with thread display toggled to the “off” position. Note the heavy CPU usage, very close to 1600%

Threaded code (thread display on)

stivoknis — sinkovit@gcn-17-57:~ — ssh — 87×33

```
Tasks: 626 total,  17 running, 609 sleeping,   0 stopped,   0 zombie
Cpu(s): 15.8%us,  0.2%sy,  0.0%ni, 84.0%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  66054160k total, 17495556k used, 48558604k free,    11552k buffers
Swap:  2097144k total,    13400k used,  2083744k free,  8478752k cached
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
81007	sinkovit	20	0	6927m	5.8g	1412	R	99.5	9.2	8:37.91	lob_constructio
81096	sinkovit	20	0	6927m	5.8g	1412	R	10.5	9.2	1:13.43	lob_constructio
81105	sinkovit	20	0	6927m	5.8g	1412	R	10.5	9.2	1:13.43	lob_constructio
81107	sinkovit	20	0	6927m	5.8g	1412	R	10.5	9.2	1:13.43	lob_constructio
81097	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.40	lob_constructio
81099	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.39	lob_constructio
81100	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.44	lob_constructio
81101	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.44	lob_constructio
81102	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.43	lob_constructio
81103	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.45	lob_constructio
81106	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.44	lob_constructio
81108	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.44	lob_constructio
81109	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.29	lob_constructio
81110	sinkovit	20	0	6927m	5.8g	1412	R	10.2	9.2	1:13.39	lob_constructio
81098	sinkovit	20	0	6927m	5.8g	1412	R	9.9	9.2	1:13.44	lob_constructio
81104	sinkovit	20	0	6927m	5.8g	1412	R	9.9	9.2	1:13.38	lob_constructio

16 threads, with only one thread making good use of CPU

Total memory usage 5.8 GB (9.2% of available)

Threaded code (thread display on)

stivoknis — sinkovit@gcn-17-57:~ — ssh — 87×33

```
Tasks: 626 total,  17 running, 609 sleeping,   0 stopped,   0 zombie
Cpu(s): 90.9%us,  0.1%sy,  0.0%ni,  9.0%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  66054160k total, 17628152k used, 48426008k free,    11496k buffers
Swap:  2097144k total,    13400k used,  2083744k free,  8396488k cached
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
81007	sinkovit	20	0	7132m	6.0g	1412	R	100.0	9.5	7:54.98	lob_constructio
81110	sinkovit	20	0	7132m	6.0g	1412	R	90.4	9.5	0:51.15	lob_constructio
81096	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.17	lob_constructio
81098	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.19	lob_constructio
81099	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.14	lob_constructio
81100	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81101	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81102	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81103	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.19	lob_constructio
81104	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.14	lob_constructio
81105	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.19	lob_constructio
81106	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81107	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81108	sinkovit	20	0	7132m	6.0g	1412	R	90.1	9.5	0:51.18	lob_constructio
81097	sinkovit	20	0	7132m	6.0g	1412	R	89.8	9.5	0:51.15	lob_constructio
81109	sinkovit	20	0	7132m	6.0g	1412	R	89.8	9.5	0:51.08	lob_constructio

16 threads, all making good (but not ideal) use of the compute cores

Getting an interactive compute node

- All exercises should be run on the compute nodes, not the login nodes. You will have dedicated access to the former, while the latter are shared by all users connecting to the system. The following is aliased for the training accounts as ggn

  ```
  [gordon]$  qsub -I -q normal -lnodes=1:ppn=16:native,walltime=1:00:00
                -A PROJID
  ```

- Once you have been assigned a compute node, you can access it directly.

  ```
  $[gordon] ssh gcn-2-31

  $[gordon] more /etc/security/access.conf
  -:ALL EXCEPT root (wheel) (xsede-admin) sinkovit:ALL
  ```

Top example

- Copy the lineq_top.c file to your home directory. The program generates a random vector and matrix of rank N, calls the linear solver DGESV (Ax=b) then reports run time. Does this for 10 matrices
- Compile using the following commands

  icc -O3 -o lineq_top lineq_top.c -mkl
- Grab an interactive Gordon compute node
- Open a second terminal, login directly to compute node and launch top
  For example: ssh gcn-4-68
- On the first terminal, run program with different matrix sizes
  ./lineq_top 5000
  ./lineq_top 10000
- Monitor CPU and memory usage. Do you notice anything funny? If so, see if you can fix the problem.

Profiling your code with gprof

gprof is a profiling tool for UNIX/Linux applications. First developed in 1982, it is still extremely popular and very widely used. It is always the first tool that I use for my work.

Universally supported by all major C/C++ and Fortran compilers

Extremely easy to use

1. Compile code with -pg option: adds instrumentation to executable
2. Run application: file named gmon.out will be created.
3. Run gprof to generate profile: gprof a.out gmon.out

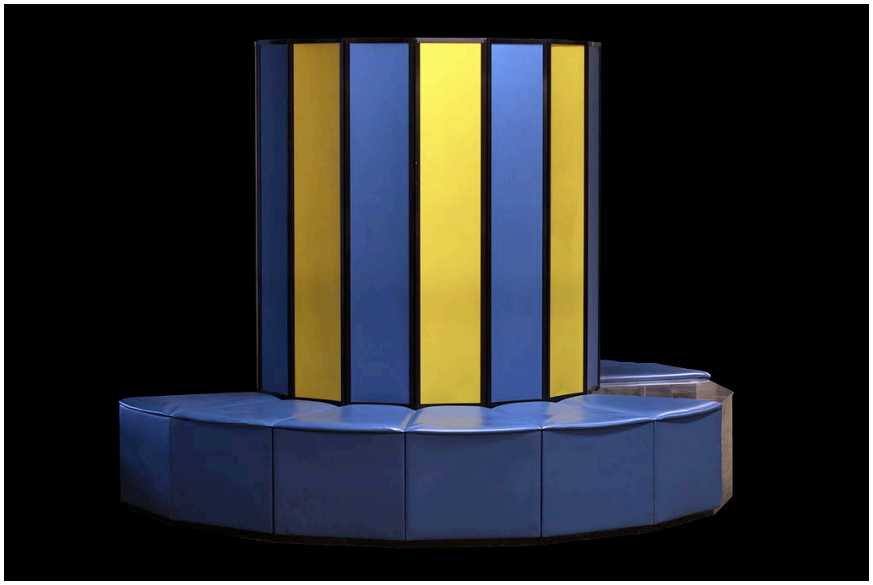
Introduces virtually no overhead

Output is easy to interpret

1982!

Worth reflecting on the fact that gprof goes back to 1982. Amazing when considered in context of the leading technology of the day

Michael Douglas as Gordon Gecko in Wall Street, modeling early 1980s cell phone. List price ~ $3000



Cray X-MP with 105 MHz processor. High end configuration (four CPUs, 64 MB memory) has 800 MFLOP theoretical peak. Cost ~ $15M

gprof flat profile

The gprof flat profile is a simple listing of functions/subroutines ordered by their relative usage. Often a small number of routines will account for a large majority of the run time. Useful for identifying hot spots in your code.

```
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  ms/call  ms/call  name
 68.60    574.72   574.72   399587     1.44     1.44  get_number_packed_data
 13.48    687.62   112.90                             main
 11.60    784.81    97.19   182889     0.53     0.53  quickSort_double
  2.15    802.85    18.04   182889     0.10     0.63  get_nearest_events
  1.52    815.56    12.71                             __c_mcopy8
  1.28    826.29    10.73                             _mcount2
  0.96    834.30     8.02    22183     0.36     0.36  pack_arrays
  0.12    835.27     0.97                             __rouexit
  0.08    835.94     0.66                             __rouinit
  0.06    836.45     0.51    22183     0.02     5.58  Is_Hump
  0.05    836.88     0.44        1   436.25   436.25  quickSort
```

gprof call graph

The gprof call graph provides additional levels of detail such as the exclusive time spent in a function, the time spent in all children (functions that are called) and statistics on calls from the parent(s)

```
index % time    self  children    called     name
[1]     96.9  112.90  699.04                 main [1]
              574.72    0.00  399587/399587      get_number_packed_data [2]
                0.51  123.25   22183/22183       Is_Hump [3]
                0.44    0.00       1/1           quickSort [11]
                0.04    0.00       1/1           radixsort_flock [18]
                0.02    0.00       2/2           ID2Center_all [19]
-----------------------------------------------
              574.72    0.00  399587/399587      main [1]
[2]     68.6  574.72    0.00  399587          get_number_packed_data [2]
-----------------------------------------------
                0.51  123.25   22183/22183       main [1]
[3]     14.8    0.51  123.25   22183          Is_Hump [3]
               18.04   97.19  182889/182889      get_nearest_events [4]
                8.02    0.00   22183/22183       pack_arrays [8]
                0.00    0.00   22183/22183       pack_points [24]
```

The value of re-profiling

After optimizing the code, we find that the function main() now accounts for 40% of the run time and would be a likely target for further performance improvements.

```
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  ms/call  ms/call  name
 41.58     36.95    36.95                             main
 26.41     60.42    23.47    22183     1.06     1.06  get_number_packed_data
 11.58     70.71    10.29                             __c_mcopy8
 10.98     80.47     9.76   182889     0.05     0.05  get_nearest_events
  8.43     87.96     7.49    22183     0.34     0.34  pack_arrays
  0.57     88.47     0.51    22183     0.02     0.80  Is_Hump
  0.20     88.65     0.18        1   180.00   180.00  quickSort
  0.08     88.72     0.07                             _init
  0.05     88.76     0.04        1    40.00    40.00  radixsort_flock
  0.02     88.78     0.02        1    20.00    20.00  compute_position
  0.02     88.80     0.02        1    20.00    20.00  readsource
```

Limitations of gprof

- grprof only measures time spent in user-space code and does not account for system calls or time waiting for CPU or I/O
- gprof has limited utility for threaded applications (e.g. parallelized using OpenMP or Pthreads) and will normally only report usage for thread 0
- gprof can be used for MPI applications and will generate a gmon.out.id file for each MPI process. But for reasons mentioned above, it will not give an accurate picture of the time spent waiting for communications
- gprof will not report usage for un-instrumented library routines
- In the default mode, gprof only gives function level rather than statement level profile information. Although it can provide the latter by compiling in debug mode (-g) and using the gprof -l option, this introduces a lot of overhead and disables many compiler optimizations.

  In my opinion, I don't think this is such a bad thing. Once a function has been identified as a hotspot, it's usually obvious where the time is being spent (e.g. statements in innermost loop nesting)

gprof example1

- Copy the gprof_ex.f file to your home directory. Compile using the following command

  ifort -pg -O3 -o gprof_ex gprof_ex.f

- Grab an interactive Gordon compute node
- Run as follows

  time ./gprof_ex 100000000

- Generate profile and examine results

  gprof gprof_ex gmon.out > profile_gp

gprof example 1 (examining call tree)

```
-----------------------------------------------
                0.85    5.23       1/1           MAIN__ [3]
[6]     12.4    0.85    5.23       1         sub1_ [6]
                4.05    0.00 100000000/100000000     f2_ [7]
                1.18    0.00 100000000/200000000     f1_ [8]
-----------------------------------------------
                4.05    0.00 100000000/100000000     sub1_ [6]
[7]      8.2    4.05    0.00 100000000         f2_ [7]
-----------------------------------------------
                1.18    0.00 100000000/200000000     sub1_ [6]
                1.18    0.00 100000000/200000000     sub2_ [9]
[8]      4.8    2.36    0.00 200000000         f1_ [8]
-----------------------------------------------
                0.39    1.18       1/1           MAIN__ [3]
[9]      3.2    0.39    1.18       1         sub2_ [9]
                1.18    0.00 100000000/200000000     f1_ [8]
-----------------------------------------------
```

- sub1 called by MAIN once
- calls f2 10^8
- calls f1 10^8

- f2 called by sub1 10^8

- f1 called by sub1 10^8
- f1 called by sub2 10^8

- sub2 called by MAIN once
- calls f1 10^8

gprof example 2

- Copy the lineq_top.c file to your home directory. Make sure that you fixed the memory leak. Compile using the following command

  icc -pg -O3 -o lineq_top lineq_top.c -mkl

- Grab an interactive Gordon compute node
- Run as follows

  export OMP_NUM_THREADS=1
  time ./lineq_top 5000

- Generate profile and examine results

  gprof lineq_top gmon.out > profile_lineq

- How does time reported by ‘time’ command compare to total time in the profile?

Torque output at glance

Torque output can give you a quick feel for memory footprint and core usage
For single node jobs, CPU time ideally should be equal to (wall time x cores/node)
In this case CPU time (7550 s) divided by wall x cores (17,776) is 0.42

```
PBS Job Id: 1398938.gordon-fe2.local
Job Name:   lob_050610
Exec host:
gcn-17-57/0+gcn-17-57/1+gcn-17-57/2+gcn-17-57/3+gcn-17-57/4+gcn-17-57/5+gcn-17-57/6+g
cn-17-57/7+gcn-17-57/8+gcn-17-57/9+gcn-17-57/10+gcn-17-57/11+gcn-17-57/12+gcn-17-57/13
+gcn-17-57/14+gcn-17-57/15
Execution terminated
Exit_status=0
resources_used.cput=02:05:50        CPU time summed across all cores
resources_used.mem=2801508kb        Real memory usage
resources_used.vmem=48536612kb
resources_used.walltime=00:18:31    Wall clock time
Error_Path: gordon-ln1.sdsc.edu:/oasis/projects/nsf/use310/sinkovit/MaoYe/order-book/
LOBFAST/lob_050610.err
Output_Path: gordon-ln1.sdsc.edu:/oasis/projects/nsf/use310/sinkovit/MaoYe/order-book/
LOBFAST/lob_050610.out
```

Manually instrumenting codes

- Performance analysis tools ranging from the venerable (gprof) to the modern (TAU) are great, but they all have several downsides
  - May not be fully accurate
  - Can introduce overhead
  - Sometimes have steep learning curves

- Once you really know your application, your best option is to add your own instrumentation. Will automatically get a performance report every time you run the code.

- There are many ways to do this and we'll explore portable solutions in C/C++ and Fortran. Note that there are also many heated online discussions arguing over how to properly time codes.

Linux time utility

If you just want to know the overall wall time for your application, can use the Linux time utility. Reports three times

- real – elapsed (wall clock) time for executable
- user – CPU time integrated across all cores
- sys – system CPU time

```
$ export OMP_NUM_THREADS=16 ; time ./lineq_mkl 30000
Times to solve linear sets of equations for n = 30000
t = 70.548615

real     1m10.733s  ← wall time
user     17m23.940s ← CPU time summed across all cores
sys      0m2.225s
```

Manually instrumenting C/C++ codes

The C gettimeofday() function returns time from start of epoch (1/1/1970) with microsecond precision. Call before and after the block of code to be timed and perform math using the tv_sec and tv_usec struct elements

```
struct timeval tv_start, tv_end;

gettimeofday(&tv_start, NULL);
// block of code to be timed
gettimeofday(&tv_end, NULL);

elapsed = (tv_end.tv_sec - tv_start.tv_sec) +
          (tv_end.tv_usec - tv_start.tv_usec) / 1000000.0;
```

Manually instrumenting Fortran codes

The Fortran90 system_clock function returns number of ticks of the processor clock from some unspecified previous time. Call before and after the block of code to be timed and perform math using the elapsed_time function (see next slide)

```
integer clock1, clock2;
double precision elapsed_time

call system_clock(clock1)
// block of code to be timed
call system_clock(clock2)

time = elapsed_time(clock1, clock2)
```

Manually instrumenting Fortran codes (cont)

Using system_clock can be a little complicated since we need to know the length of a processor cycle and have to be careful about how we handle overflows of counter. Write this once and reuse everywhere.

```
double precision function elapsed_time(c1, c2)
implicit none
integer, intent(in) :: c1, c2
integer ticks, clockrate, clockmax

call system_clock(count_max=clockmax, count_rate=clockrate)
ticks = c2-c1
if(ticks < 0) then
  ticks = clockmax + ticks
endif
elapsed_time = dble(ticks)/dble(clockrate)

return
end function elapsed_time
```

A note on granularity

Don't try to time at too small a level of granularity, such as measuring the time associated with a single statement within a loop

```
elapsed = 0.0;

for (i=0; i<n; i++) {
  w[i] = x[i] * y[i];
  gettimeofday(&tv_start, NULL);
  z[i] = sqrt(w[i]) + x[i];
  gettimeofday(&tv_end, NULL);
  elapsed += (tv_end.tv_sec - tv_start.tv_sec) +
             (tv_end.tv_usec - tv_start.tv_usec) / 1000000.0;
}
```

Although they're pretty lightweight, there is still a cost associated with calls to gettimeofday or system_clock. In addition, the insertion of these calls into loops can impact the flow and hamper optimizations by the compiler.

Amdahl's Law

Amdahl's law sets an upper limit on the speedup of a parallel code based on the serial content.

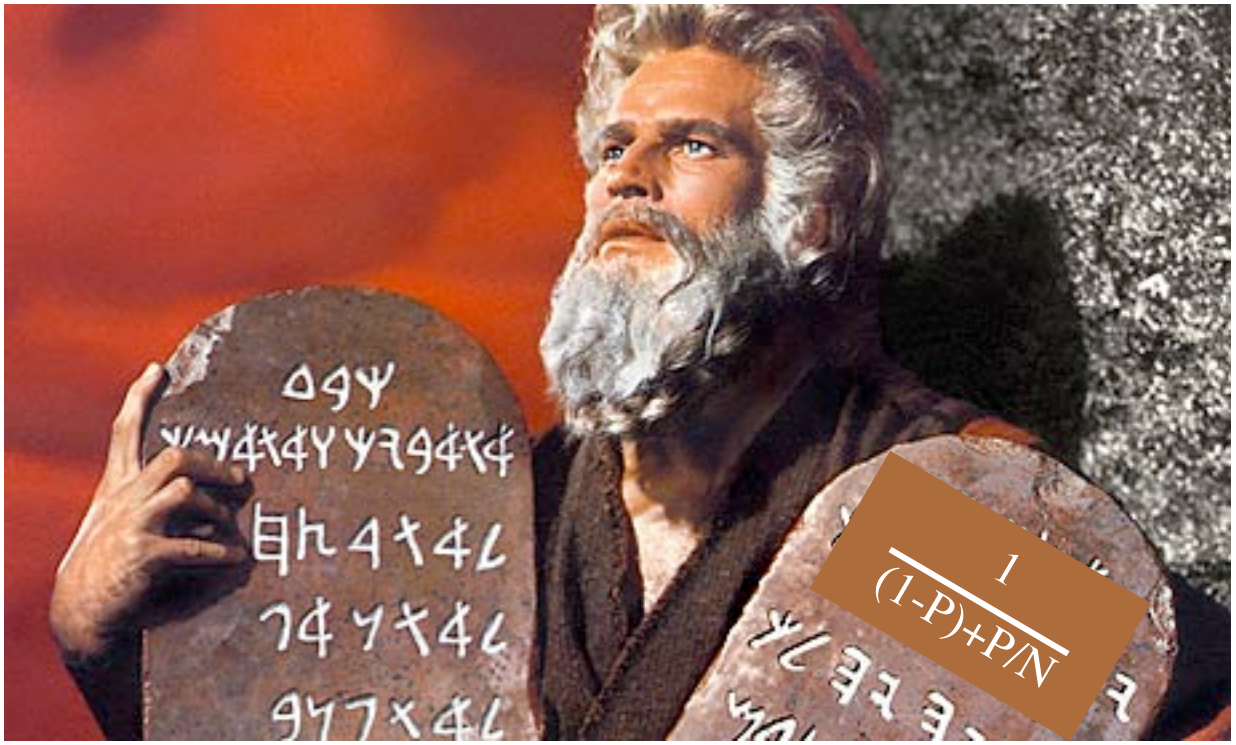
- Let P be the fraction of the code that can be run in parallel
- Let (1-P) be the serial fraction of the code
- Let N be the number of parallel threads or processes

$$S(N) = \frac{1}{(1-P) + P/N} \qquad S(\infty) = \frac{1}{(1-P)}$$

In reality, you will probably do a good bit worse than Amdahl's law due to a number of factors, most importantly

- Load imbalance – processes assigned different amounts of work
- Communications overhead – latency and bandwidth

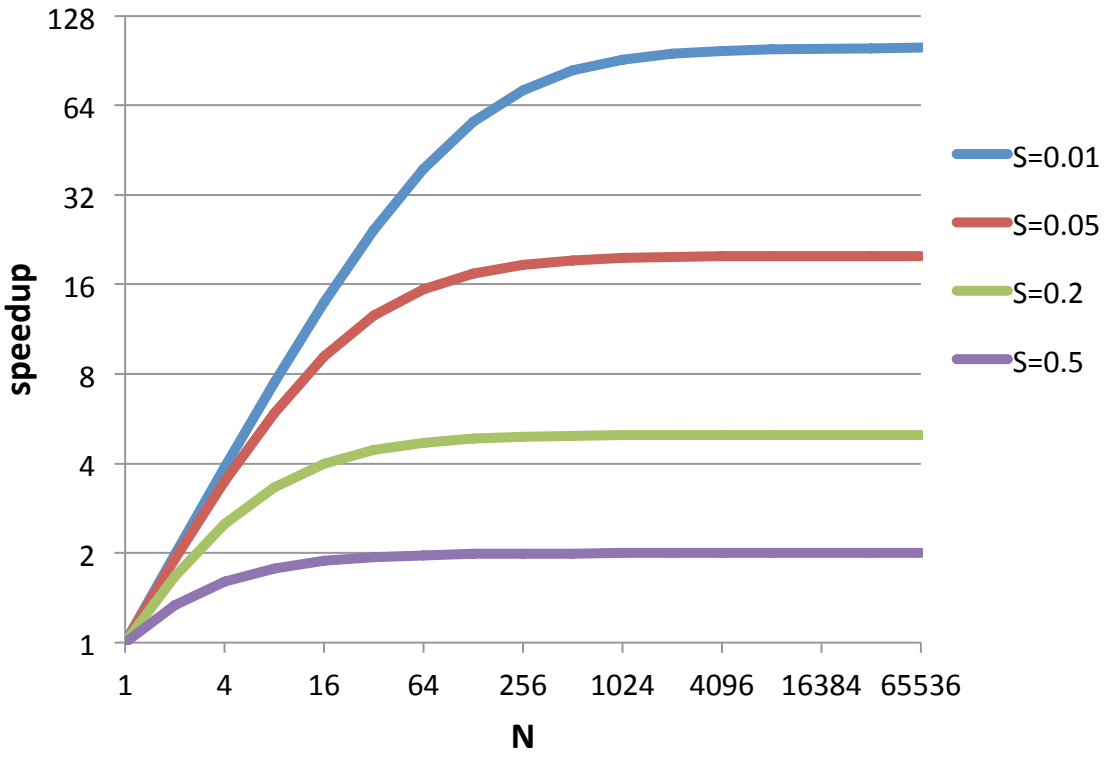
Amdahl's Law – kind of a big deal



Charlton Heston in *Moses and the Ten Commandments*, delivering a slightly updated version to the SDSC Summer Institute

Amdahl's Law

The theoretical maximum speedup, running on an infinite number of compute cores, is the inverse of the serial content. This places a very stringent bound on the benefits of parallelization



Amdahl's Law

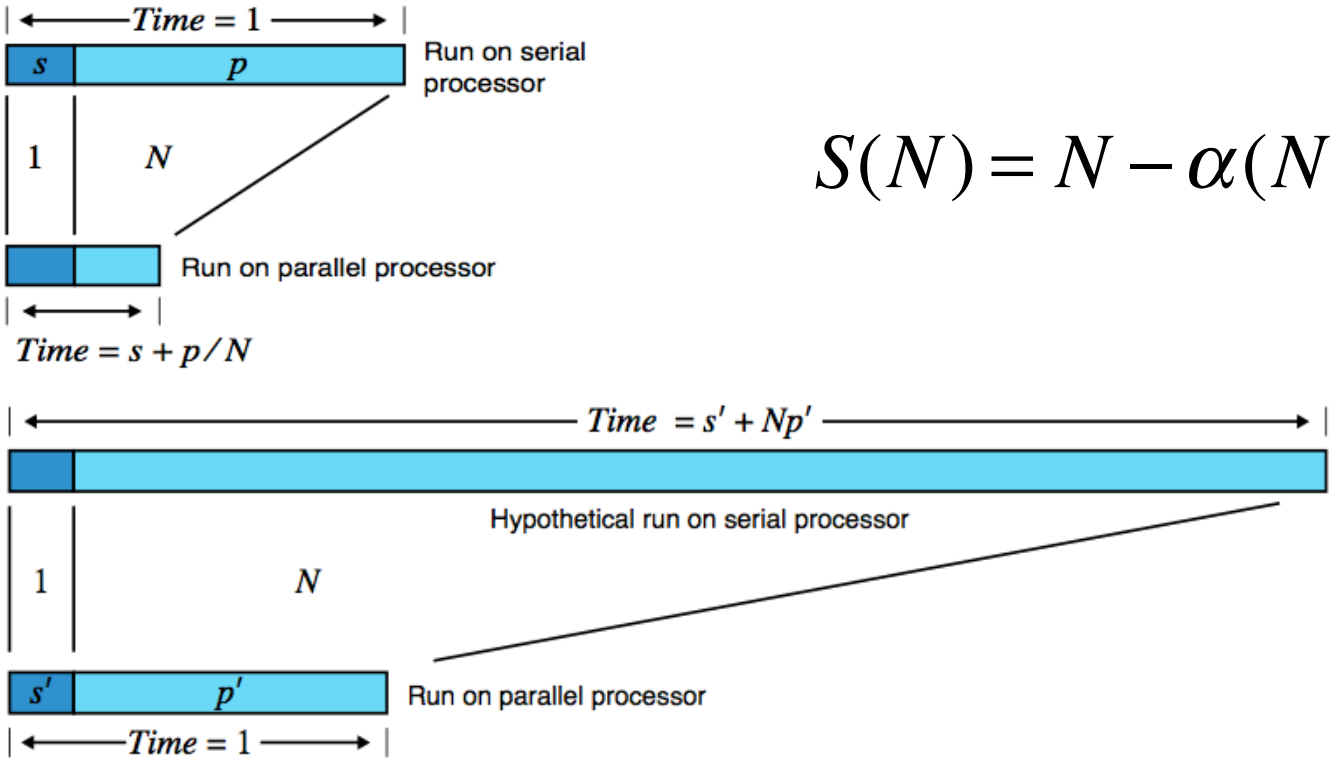
Fortunately, things aren't as gloomy as they appear. For many applications, there is a lot of work that can be done in parallel and the serial content is rather minimal

- Updating grid cells in discretized solutions of PDEs
- Calculating forces on particles in molecular dynamics, N-body problems
- Ensemble calculations – many repetitions of calculation with different data sets or slightly different input parameters

If your application falls into the last category, there is no need for you to worry about parallelization at the program level. Instead, just develop a workflow that allows you to run the serial instances of your code in parallel.

Gustafson's Law

A limitation of Amdahl's Law is that it assumes you want to run a fixed size problem on an increasing number of processors. In many real problems, you'll want to increase the problem size as the processing power grows



$$S(N) = N - \alpha(N-1)$$

Gustafson, Communications of the ACM 31(5), 1988 532-533

Strong scaling vs. Weak Scaling

The discussion of Amdahl's Law and Gustafson's Law segues into the topic of strong vs. weak scaling

- Strong scaling – how does the run time scale (decline) as the number of processors is increased? Ideally, linear speedup ($t \sim 1/N$)

- Weak scaling – how does the run time vary as the work per process stays constant while the problem size grows. Ideally, t is unchanged.

Scaling experiment

- Copy the lineq_mkl.c file to your home directory. The program generates a random vector and matrix of rank N, calls the linear solver DGESV (Ax=b) then reports run time.
- Compile using the following commands

  icc -O3 -o lineq_mkl lineq_mkl.c –mkl

- On a Gordon compute node, run with a variety of problem sizes using 1, 2, 4, 8 and 16 threads. Note the run times and any trends in scalability as the problem size is increased from N=1000 to N=10000

  export OMP_NUM_THREADS=1
  ./lineq_mkl 3000
  export OMP_NUM_THREADS=2
  ./lineq_mkl 3000
  export OMP_NUM_THREADS=4
  ./lineq_mkl 3000