Linux for Scientific Computing

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Things you should know if you're thinking about using Linux for Scientific Computing

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Random thoughts on things you should know if you're thinking about using Linux for Scientific Computing

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Why?

Scientific research is one of the first areas where Linux has had a major impact on production, mission-critical computing.

Features of scientific computing

- Floating point performance is everything
  (well, almost everything)

- Users write their own codes
- Legacy Fortran is common

- Full-featured user-friendly GUI interface not required

- Goal is science, not computer science.

Who are the foolish zealots?

- Data analysis in experimental physics
  - Cern, Fermilab, SLAC, Brookhaven, DESY; Astrophysics

- Parallel computing on clusters
  - Sometimes called “Beowulf” clusters
  - Mini-supercomputers

- Thousands of random apps powered by graduate students

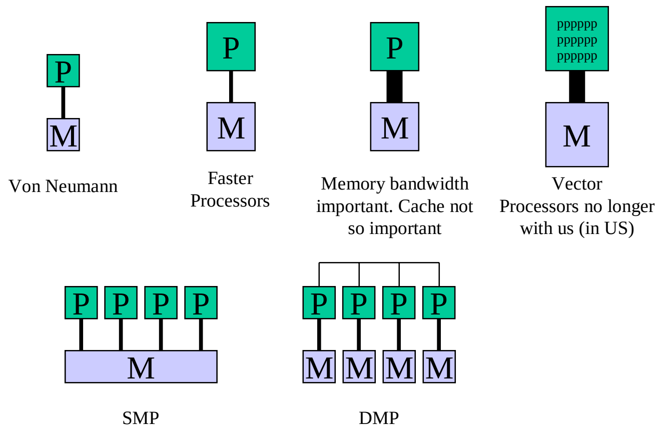
Outline

- Why Linux?
- Hardware
  - Computer architecture
  - Processors
  - Benchmarks
- Serial computation
  - Compilers
  - Libraries
- Parallel computation
  - SMP
  - Clusters

Why Linux?

- Access to cheap hardware
- Control
- Availability of software
- Convergence
- Access to cheap graduate students
- Alternative to NT

Computer architecture for HPSC



Processor support in Linux

- These supported processors are useful for scientific computing:
  - **x86**
  - **Alpha**
  - Sparc/Sparc64
  - PowerPC
  - MIPS
- Coming up:
  - Power 3
  - Merced

Which processor?

- Three important criteria
  - Cost
  - Performance
  - Availability of software

Measuring Performance

- Peak
- Linpack
- STREAM (memory bandwidth)
- SPEC
- NPB and NSB

Current Peak Rates

Name	MHz	Flop/cycle	Peak Mflop/s
Alpha 21264	677	2	**1354**
Alpha 21164	600	2	1200
Power 3	233	4	932
Sparc	450	2	900
PIII	550	1	550
R10K	250	2	500

Linpack

- The Linpack benchmark solves a dense linear algebra problem -- BLAS 3
- Can be run in serial or parallel
- Because BLAS 3 can be blocked, Linpack effectively runs in cache and gets a very high percentage of peak.
- Linpack is important for two reasons:
  - Good basic test of whether a machine (parallel) can run or not
  - Basis of Top 500 list (www.top500.org)

STREAM Benchmark

- Measures memory bandwidth
- http://www.cs.virginia.edu/stream
- Developed by John McCalpin
- 4 Tests
  - Copy (A = B)
  - Scale (A = s*B)
  - Add (A = B + C)
  - Triad (A = B + s*C)

Stream Results

Processor	**MHz**	**Peak** (Mflop/s)	**Triad** (2*MW/s)
Alpha 21264	500	1000	331
Alpha 21164	533	1066	73
Pentium II	400	400	79
Ultrasparc (UE10K)	400	400	74
MIPS (O2K)	300	600	48
Power-3	200	800	~250
Cray C90		1000	2375

SPEC95

- SPEC = Standard Performance Evaluation Corporation
- http://www.spec.org

- SPECint95
  - 8 integer-intensive codes written in C
- SPECfp95
  - 10 floating point-intensive codes written in Fortran
  - All are scientific computations.

SpecFP 95

Processor	MHz	SPECfp95	SPECint95
Alpha 21264	500	**48.4**	23.6
Power 3	200	27.6	12.5
Ultrasparc	450	27.0	19.7
MIPS	250	23.2	15.1
Athlon	650	22.4	**29.4**
PIII/500	500	15.1	21.6
Alpha 21164	533	**14.1**	16.8

Multiprocessor machines

- x86/Alpha/Sparc/MIPS all available in SMPs
  - Cache coherent shared memory
  - Single copy of operating system
  - Well-supported by Linux up to about 4 processors
- OS support is not the limiting factor.
  Memory bandwidth is.
  - Low-end SMPs share memory through a bus
  - Nearly saturated by one processor. Two or more processes compete for memory bandwidth.
  - Expect 1.5x speedup max on Intel or current Alpha.

Software

- Compilers
- Libraries
- 3rd party software

Compilers

- Old standbys, available on all platforms
  - C: gcc
  - C++: g++
  - Fortran 77: g77
- Open source but:
  - g++ doesn't handle complex C++ (e.g. heavy use of expression templates)
  - g77 is Fortran 77 only
  - no parallelization for SMPs
  - generated code is not very fast

x86 Compilers

- **Portland Group** (www.pgroup.com)
  - Fortran 90/95/OpenMP parallelization/Better performance (~10%)/HPF
- **Kuck and Associates** (www.kai.com)
  - Better C++/OpenMP parallelization
- **NAG** (www.nag.com)
  - Fortran 90/95/Tends to be picky
- **Absoft** (www.absoft.com)
  - F90/95/Includes IMSL (RH 5.2?)
- **Fujitsu** (www.tools.fujitsu.com)
  - C/C++/F90/F95

Alpha compilers

- Compaq/DEC compilers are available
  - Better performance (optimized for Alpha)
  - Full Fortran 90 (available now)
    - http://www.digital.com/fortran/linux/
  - C/C++ later
- NAG
  - Fortran 95

Other compilers

- Ultrasparc
  - Nothing more available
- MIPS
  - Nothing more available
- Power-3
  - IBM is looking into putting AIX compilers under Linux

NAS Parallel Benchmarks

- Developed at NASA Ames Numerical Aerodynamic Simulation facility.
- Designed to measure performance of parallel computers
- 8 codes: 5 kernels and 3 pseudo-applications represent a CFD workload.
- 5 sizes: S, W, A, B, C.
- Two versions
  - NPB 1: pencil and paper (algorithm specified)
  - NPB 2: specified by source code
- NAS Serial Benchmarks (NPB 2-serial) are single processor versions of NPB 2.

A Few NSB results

Proc	**MHz**	**Cmplr**	**OS**	**FP Avg**
21264 ds20	500	DEC	Tru64	182.1
21264 ds10	466	DEC	Tru64	141
21264 xp	500	DEC	Tru64	**154.1**
21264 xp	500	DEC	Linux	**132.1**
21264 xp	500	gcc	Linux	**100.0**
21164	600	DEC	Tru64	65.9
PII	400	PGI	Linux	53.4
Celeron	400	PGI	Linux	45.1

- see http://www.nersc.gov/research/ftg/pcp/performance.html

Basic Free Numerical Libraries

There are many free libraries. Some of the more important (and industrial strength) ones are:

- Optimized BLAS for x86
  - http://www.cs.utk.edu/~ghenry/distrib
- FFTW: Fastest Fourier Transform in the West
  - http://www.fftw.org

Don't use numerical recipes!

Basic libraries - Commercial

- X86
  - NAG (www.nag.com).
  - IMSL (www.vni.com/products/imsl)
- Alpha
  - Compaq Portable Math Library (CPML) -- libm replacement
  - Compaq Extended Math Library (CXML)

More software

Two excellent sources of information.

- Scientific Applications on Linux at Kachinatech:
  - http://sal.kachinatech.com
- Steven Baum's Linux List
  - http://stommel.tamu.edu/~baum/linuxlist/linuxlist/node6.html

Parallelism

- 2 types of concurrency in parallel applications
  - Embarassing parallelism
    - Little/no coupling between tasks
    - Independent processes can be executed in parallel
    - seti@home; analysis of event data from colliders; monte carlo simulations.
  - Everything else
    - parallelism is fine-grained
    - data distribution is fine-grained
    - frequent communication
    - main application focus of the rest of this talk

Parallelism

Three viable programming models

- Compiler-generated parallel code
  - SMP only
  - Not (yet?) widely used with Linux
- Threads
  - SMP only
  - Not widely used for scientific computing
- Message passing
  - Distrbuted memory or SMP
  - Widely used on clusters

- Non-viable alternatives: HPF, distributed shared memory

Compiler parallelization

- Compiler detects concurrency in loops and distributes work in a loop to different threads.

```
for (i = 0; i < 1000000; i++)
   a[i] = c[i] * (b[i+1] - 2b[i] + b[i-1]);
```

- Requires cache-coherent shared memory in general
- Compiler is usually assisted by compiler directives.
- OpenMP is the standard for Fortran and C
  - KAI
  - Portland group

Message Passing

- Programming model:
  - Separate processes with separate address spaces
  - Communication by cooperative send/receive
  - Mixed MPI/threads possible in theory, but not supported in Linux implementations.
- MPI (Message Passing Interface) is the industry standard.
- PVM should be used only when MPI can't do the job.
- Hardware
  - Distributed memory (cluster)
  - Shared memory
  - Mix of shared/distributed

Clusters

- A *cluster* is a collection of interconnected computers used as a unified computing resource. (Pfister)
- Clusters can offer
  - High performance
  - Large capacity
  - High availability
  - Incremental growth
- Clusters used for
  - Scientific computing
  - Making movies
  - Commercial servers (web/database/etc)

“Beowulf” clustering

- Clustering of x86-based Linux machines for scientific computing was popularized by the Beowulf project at Caltech/JPL.

- “Beowulf-class” is a slippery term, but usually implies:
  - Off-the-shelf parts
  - Low cost LAN
  - Open source OS

- National labs are looking at highly-scalable non-beowulf clusters for next generation of supercomputing.

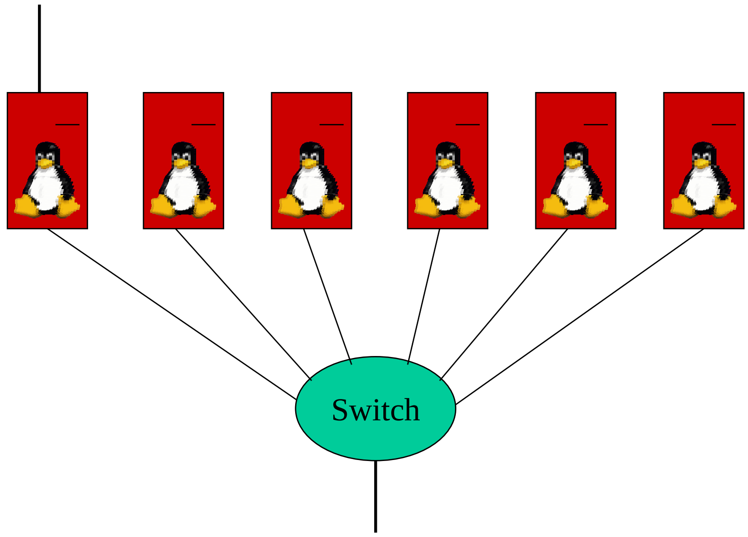
How to build a cluster

- Building/maintaining a cluster is a lot of work

- Type of cluster depends on the type of job.
- Tightly coupled applications have more stringent requirements.

- Expect a flood of software and documentation to appear over the next year that makes it much easier to put together clusters.

Architecture



Network setup

- Private network
  - Cluster security/setup/administration much easier
  - Application cannot interact with outside world
- Public network
  - Security/setup/administration difficult. IP addresses needed.
  - Interaction possible
- Firewall
  - Most flexible
  - Experts only

Local install or diskless?

- Local install
  - Most natural if you’re used to installing desktops
  - N separate copies of Linux to maintain
  - Works best in completely homogeneous system

- Diskless install
  - 1 copy of Linux to maintain
  - Requires special tools to manage
  - For many applications, scales up to 32 or 64 nodes

Node classification

- Interactive nodes
  - Attached to external network
  - Compile/edit/debug
- Fileserver nodes
  - Global file systems (e.g. home directories)
  - Remote filesystems for diskless clients
- Other service nodes
  - Batch server/YP server/Security server
- Compute nodes
  - Space-shared by parallel applications

Other cluster infrastructure

- YP (NIS) for user management
- BOOTP for IP address management
- Global filesystem.
  - Necessary and expected
  - Most important unsolved problem of clusters.
  - No viable solution except NFS
  - See http://pdsf.nersc.gov/talks/nfs/index.html

Other Hardware

- Network
  - Fast ethernet. By far the most common.
  - Gigabit ethernet. Expensive, not much faster
  - Myrinet. Network of choice for high-end clusters. $1500-$2000/node. Scalable.
  - New networks on horizon: Giganet, Servernet II
  - Virtual Interface Architecture may make high performance networks more accessible and available.
- Serial console management
  - Cyclades, Rocketport (comtrol.com) multiport serial cards

Other software

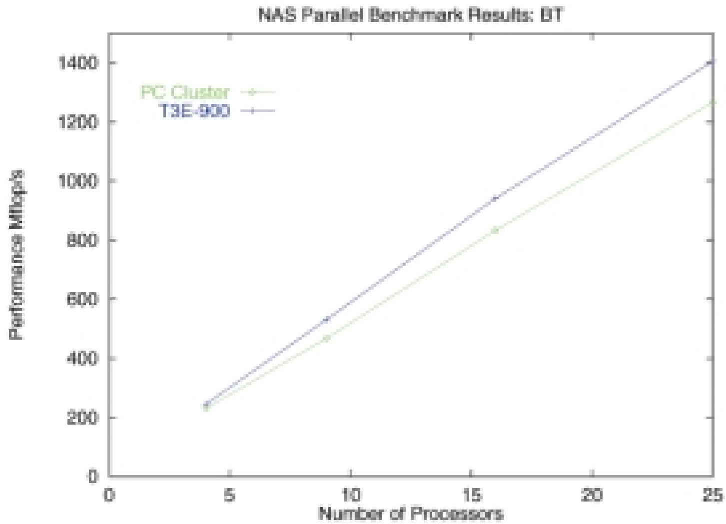
- MPI
  - Get MPICH from http://www.mcs.anl.gov
  - LAM is another free implementation, but no compelling reason to use it.
- PBS
  - Batch management system developed at NASA Ames
  - Space shares the cluster; manages multi-user system
  - Easily integrated with MPICH
  - http://pbs.mrj.com

Task Farms

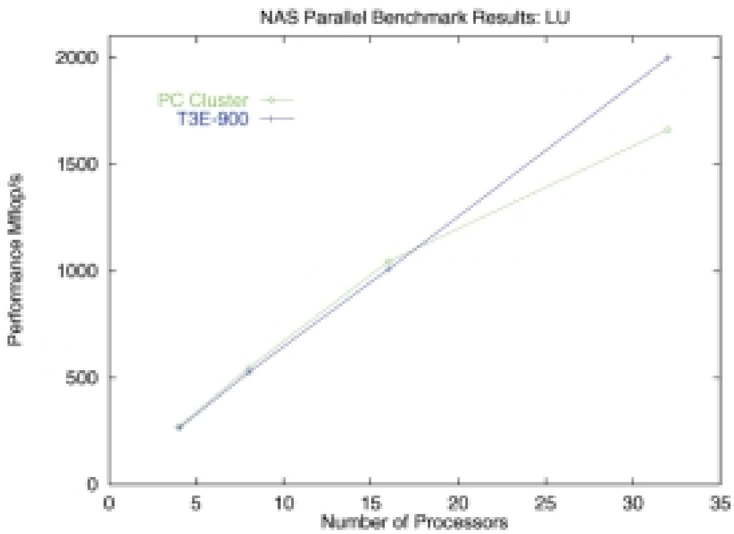
How would you do things differently for a task farm (embarassingly parallel application)?

- Consider MOSIX to transparently load balance processes
- Switched network not necessary

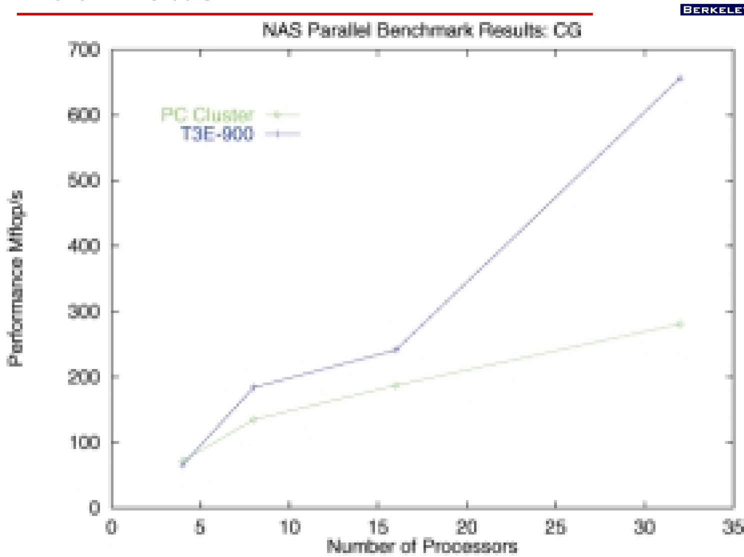
Good news



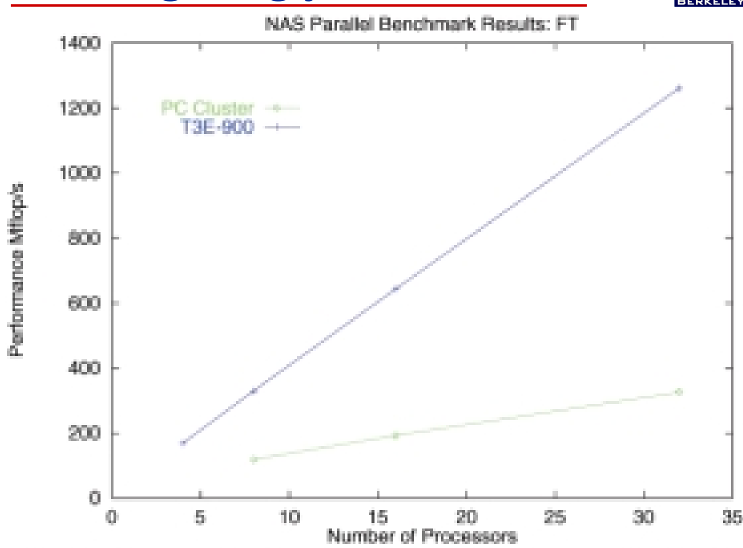
More good news



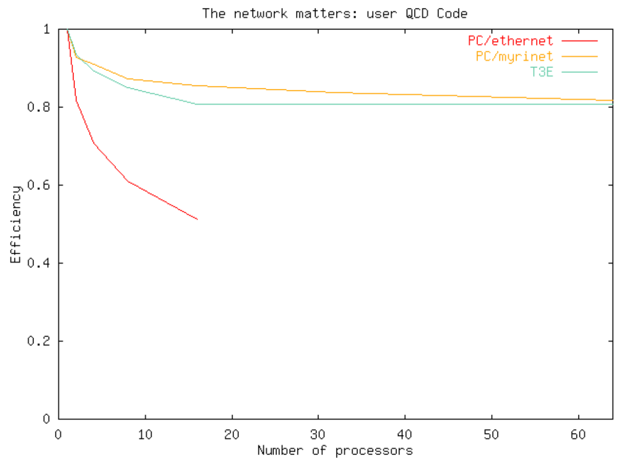
Bad News



Downright Ugly



The Network Matters



More info on clusters

- **How to Build a Beowulf**. Sterling Becker, et. al. MIT Press, 1999
- **In Search of Clusters**. Gregory Pfister. Prentice Hall, 1998 (2nd edition)
- The Beowulf mailing list: “subscribe” to beowulf-request@beowulf.gsfc.nasa.gov
- HOWTO: http://www.beowulf-underground.org/doc_project/index.html

Open source presentation

http://www.nersc.gov/~wcs