TeraGrid and High-end Computing: Lessons and Futures

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Outline

• The really big questions
  – life, the universe, and everything
    • why they matter and how we react

• TeraGrid and NCSA
  – status and directions
    • lessons and capabilities
    • applications and needs

• High-end futures
  – petascale system design
    • challenges and opportunities
  – international networks
The Big Questions

• Life and nature
  – structures, processes and interactions

• Matter and universe
  – origins, structure, manipulation and futures
  – interactions, systems, and context

• Humanity
  – creativity, socialization and community

• Answering big questions requires
  – boldness to engage opportunities
  – expandable approaches
  – world-leading infrastructure
  – broad collaborations and interdisciplinary partnerships
HPC Application Studies

• Contributors
  – Berger (NYU)
  – Ceperley (UIUC)
  – Koonin (Caltech)
  – McCurdy (LBL)
  – Mount (SLAC)
  – Ostriker (Princeton)
  – Reed (UIUC)
  – Sugar (UCSB)
  – Wilkins (Ohio State)
  – Woodward (Minnesota)

G-2 Data Analysis

- Brookhaven g-2 experiment
  - 60 scientists from 11 institutions
  - standard model testing
    - muon anomalous magnetic moments
  - large-scale cluster data analysis
    - Herzog et al (Illinois), 10X time decrease

- The story is in the data …
Evolutionary Biology

• Phylogenetic tree display
  – all known prokaryotic potassium channels
  – all potassium channels from two animals
    • *homo Sapiens* and *c. Elegans*
  – three classes of animal channels
    • voltage gated, ligand modulated and “other”

• Observations
  – Ligand modulated/voltage-gated prokaryotic
    • mingled with the animal channels
    • indicating origin in prokaryotics
  – “other” class
    • no prokaryotes, indicating an origin in eukaryotes
  – roots of two other channels (sodium and calcium)
    • arose in a region in the ligand-gated group
The Computing Continuum

- Each strikes a different balance
  - computation/communication coupling
- Implications for execution efficiency
- Applications for diverse needs
  - computing is only one part of the story!
2003 NCSA System Status: 30+TF

• Three new major computational systems
  – 17.7 TF Dell Xeon replacement for 1 TF Pentium III cluster
    • 1474 Dell servers, dual Intel Xeon 3.06 GHz nodes
    • installation in progress now and scheduled for operation in late 2003
  – TeraGrid cluster with Itanium2/Madison nodes
    • 2 TF Itanium2 systems delivered, upgraded to 1.3 GHz Madison
      – production December 2003
    • additional 8 TF of Madison in fall 2003 (production April 2004)
  – IBM p690 32p SMP systems
    • operational in spring 2003
    • 2 TF, 12 systems, 384 1.3 GHz Power4 processors
    • 4 large memory systems with 256 GB of memory

• Two other production clusters
  – 1 TF Pentium III and 1 TF Itanium

• Condor resource pools
  • parameter studies and load sharing

• ~500 TB of spinning storage
  – Brocade SAN fabric with DataDirect, IBM and LSI storage arrays

1 TF IBM Pentium III Cluster

Application scientists Login, FTP

Interactive Node

Mgmt Node

Ethernet Switch

Job Control

GPFS Testbed

/home scratch

NFS

32 Dual 1 GHz Nodes

32 Dual 1 GHz Nodes

32 Dual 1 GHz Nodes

32 Dual 1 GHz Nodes

512 Connections

Myrinet Fabric

2 Storage Nodes w/GbE

Lesson: No Receptions

National Center for Supercomputing Applications
Cluster in a Box/OSCAR

• Community code base with strong support
  – Bald Guy Software, Dell, IBM, Intel, Indiana
  – MSC.Software, NCSA, ORNL, Sherbrooke University, ...

• Six releases within the past year
  – 29,000 downloads during this period

• Recent additions
  – HDF4/HDF5 I/O libraries
  – OSCAR database for cluster configuration
  – Itanium2 and Gelato consortium integration
  – NCSA cluster monitor package (Clumon)
  – NCSA VMI 2 messaging layer
    • Myrinet, gigabit Ethernet and Infiniband
  – PVFS added for parallel filesystem

• First Annual OSCAR Symposium
  – May 11-14, 2003, Québec, CANADA
Tungsten: 17.7 TF Peak from Dell

- Dell Xeon cluster for highly scalable applications
  - successor to production 512 node/1024p Pentium III cluster
  - scalable configuration for administration and management
    - LSF, Red Hat 9, LSF, Lustre, Dell OpenManage …
- Maximize increase in capability
  - 3.06 GHz, 512 KB (L2), dual Xeon nodes
    - application interest in hyperthreading
- Increase in storage capacity and capability
  - 100-200 TB and 2GB/s per TF peak
- Scalable administration
  - 256 nodes/administration server
- Support for very large, long running applications
  - 256 node/3 TF administrative “subclusters”
  - run times of at least 1 week on 100s of nodes
    - significant numbers of nodes dedicated to projects
NCSA Tungsten: Xeon Scalable System

- 3 TF Peak/256 Nodes
- Myrinet Fabric
- Installation begins August 2003
- Applications Testing Subcluster
- 64 x Dell PowerEdge 1750 Installed July 2003
- Force 10 GbE Fabric
- 106 Dell Storage Nodes
- DataDirect Networks, 122 TB Usable Storage
- Other NCSA Systems

Long-term Allocations
NCSA System Integration

TeraGrid

- "Mercury"
  - 8 TF Madison
  - ~670 Nodes
  - Fall 03

- "Titan"
  - IA-64 Linux
  - 1 TF

- "Copper"
  - Power4 AIX
  - 2 TF
  - Operational Q1 03

- "Titan"
  - Itanium2
  - 2 TF
  - Installation

- "Platinum"
  - IA-32 Linux
  - 1 TF

GbE/10GbE Fabric

- Mass storage
  - Upgrade FY03
  - 4-SGI
  - 1 Pt
  - 1 Titan
  - 14 (26)

- Tier 3
  - Mass Storage
  - SGI O2000
  - Retire FY’03

- Short term working storage
- Long term working storage

- Tier 2
  - Long term

- Tier 3
  - Long term

- IA-64
  - FS

- IA-32
  - FS

- AIX
  - FS

- All other systems on Myrinet

National Center for Supercomputing Applications
Science and Engineering Grids

[Diagram showing a map of the United States with a network of connections indicating the NSF TeraGrid Backbone and other key nodes such as Caltech, SDSC, Argonne, NCSA, StarLight, A-WIRE, and PSC. The map highlights TeraGrid Partners, Alliance Partners, NPACI Partners, and Abilene Backbone with different line colors and symbols.]
TeraGrid Objectives

• **Enable and empower new science**
  – “traditional” supercomputing made simpler
    • remote access to data and computers
  – distributed data archive access/correlation
  – remote rendering and visualization
  – remote sensor and instrument coupling

• **Deploy a balanced, distributed system**
  – not a “distributed computer” but rather
  – a distributed “system” using Grid technologies
    • computing and data management
    • visualization and scientific application analysis

• **Define an open and extensible infrastructure**
  – an “enabling cyberinfrastructure” for scientific research
  – extensible beyond original sites with additional funding
    • NCSA, SDSC, ANL, Caltech, PSC, …
TeraGrid Components and Partners

- Intel/HP Itanium Processor Family™ nodes
  - Itanium2/3 IA-64 processors for commodity leverage
- IBM Linux clusters
  - open source software and community
- Very high-speed network backbone
  - high bandwidth for rich interaction and tight coupling
- Large-scale storage systems
  - hundreds of terabytes of secondary storage
- Grid middleware
  - Globus, data management, …
- Next-generation applications
  - breakthrough versions of today’s applications
  - but also, reaching beyond “traditional” supercomputing
Extensible TeraGrid Facility (ETF)

**CALTECH**: Data collection analysis
- 0.4 TF IA-64
- IA32 Datawulf
- 80 TB Storage

**ANL**: Visualization
- 1.25 TF IA-64
- 96 Viz nodes
- 20 TB Storage

**SDSC**: Data Intensive
- 4 TF IA-64
- DB2, Oracle Servers
- 500 TB Disk Storage
- 6 PB Tape Storage
- 1.1 TF Power4

**NCSA**: Compute Intensive
- 10+ TF IA-64
- 128 large memory nodes
- 230 TB Disk Storage
- GPFS and data mining

**PSC**: Compute Intensive
- 6 TF EV68
- 71 TB Storage
- 0.3 TF EV7 shared-memory
- 150 TB Storage Server

Legend:
- Cluster
- Visualization Cluster
- Storage Server
- Shared Memory
- Disk Storage
- Backplane Router

Extensible Backplane Network


National Center for Supercomputing Applications
NCSA TeraGrid: 10.6 TF IPF and 230 TB

Phase One (Dec ’03 Production)
- 2.6 TF
- 1.3 GHz Itanium2
- 256 nodes (3 MB cache)
- 2p 1 GHz
- 4 or 12 GB memory
- 73 GB scratch
- 268 2x FC

Phase Two (Apr ’04 Production)
- 1.5 GHz Itanium2 nodes
- 667 nodes (6 MB cache)
- Intel Tiger2 (IBM)

40 Gb/s TeraGrid Network

Myrinet Fabric

Force10 GbE Fabric

IBM FastT Storage
230 TB

Brocade FC Fabric

NCSA: Compute Intensive

National Center for Supercomputing Applications
TeraGrid Network Backbone

Qwest 40 Gb/s Backbone

Qwest 40 Gb/s Backbone

StarLight
International Optical Peering
(see www.startap.net)

I-WIRE
Multiple Carrier Hubs

$7.5M Illinois DWDM Initiative

National Center for Supercomputing Applications
Large Hadron Collider: 2007

ALICE:

LHC Project Structures
LHC Excavated Structures
LHC Completed Structures (CE)
LHC Completed Structures (CV, EL, HM)

ATLAS

CMS

TOTEM

LHCb: B-physics

National Center for Supercomputing Applications
CMS Data Preparations

- **Data and software testing challenge**
  - test and validate analysis software
    - 100,000,000 events

- **Testing approach**
  - particle-detector interaction simulator (CMSIM)
    - energy deposition in the detector
  - ORCA (Object Reconstruction for CMS Analysis)
    - reconstruct QCD background sample
  - tracks and reconstructed particles, ready for analysis

- **Computing, storage and networking**
  - 2,600,000 SUs on the TeraGrid
    - 400 processors through April 2005
  - 1,000,000 SUs on IA-32 cluster
  - 1 TB for production TeraGrid simulations
    - 400 GB for data collection on IA-32 cluster
  - 2-5 MB/s throughput between NCSA and Caltech
GriPhyN: CMS Data Reconstruction

1) Launch secondary job on WI pool; input files via Globus GASS
2) Master starts reconstruction jobs via Globus jobmanager on cluster
3) 100 Monte Carlo jobs on Wisconsin Condor pool
4) 100 data files transferred via GridFTP, ~ 1 GB each
5) Secondary Condor job on WI pool
6) Master Condor job running at Caltech
7) GridFTP fetches data from UniTree
8) Processed objectivity database stored to UniTree
9) Reconstruction job reports complete to master

Source: Scott Koranda, Miron Livny and many others
Building Something New

One Organization (merge institutions)
- One sysadmin team
- One management team
- Distributed machine room, centralized control
  e.g., Google data centers

The TeraGrid (A Grid hosting environment)
- Single development environment
- Single stack to learn
- Develop here, run there
- Run here, store there

Very Loose Collaboration (current situation)
- Different MPIs
- Hit-and-miss Grid software:
  - Globus version?
  - Condor-G?
  - G2?
- Unique development environment

Not a Grid
Applications are developed for the Grid because the barriers are low and the return large

Not a Grid, but with significant user investment, Grid applications can be developed

Source: TG Team

National Center for Supercomputing Applications
Grids and Capability Computing

• **Not an “either/or” question**
  – each addresses different needs
  – both are part of an integrated solution

• **Grid strengths**
  – coupling *necessarily* distributed resources
    • instruments, archives, and people
  – eliminating time and space barriers
    • remote resource access and capacity computing
  – *Grids are not a cheap substitute for capability HPC*
    • the latency/bandwidth continuum rules

• **Capability computing strengths**
  – supporting foundational computations
    • terascale and petascale “nation scale” problems
  – engaging tightly coupled teams and computations
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High-end Computing Challenges

- Funding and long-term R&D
  - ☻ and ☹
- Time to solution
  - too difficult to program and to optimize
  - better programming models/environments needed
- Often, efficiency declines with more processors
  - adversely affects time to solution and cost to solution
- Support overhead for system parallelism
  - management of large-scale concurrency
- Processor-memory latency and bandwidth
  - can be constraining for HEC applications
    - scatter-gather and global accesses
- I/O and data management
  - volume and transfer rates
- Power consumption, physical size and reliability
HPC Clusters

✓ Processors
  ✓ x86, Itanium, Opteron, …

✓ Memory systems
  ✓ the jellybean market
    • memory bandwidth 😞

✓ Storage devices
  ✓ vibrant storage market

• Interconnects
  ✓ Ethernet (10/100, GbE, 10GbE)
  ✓ Infiniband (maybe)
    • Myrinet, Quadrics, SCI, … 😞
Node Interconnects (2003)

- **2p Node**
  - ~$5K
  - 9.6GFLOP/s

- **On board Gigabit Ethernet**
  - ~$1000/port
  - MPI:
    - BW ~115 MB/s
    - RT time ~52 usec

- **InfiniBand**
  - ~$1700-2000/node
  - MPI:
    - BW ~760 MB/s
    - RT time ~12 usec

- **Myrinet**
  - ~$1700/node
  - MPI:
    - BW ~220 MB/s
    - RT time ~12 usec
Computing On Toys

- Sony PlayStation2 features
  - 6.2 GF peak
  - 70M polygons/second
  - 10.5M transistors
  - superscalar RISC core
  - plus vector units, each:
    - 19 mul-adds & 1 divide
    - each 7 cycles
  - $199 retail
    - loss leader for game sales
- 70 unit cluster at NCSA
  - Linux software and vector unit use
    - over 0.5 TF peak but difficult to program
  - vector assembly code
    - linear algebra libraries (BLAS1, 2, 3)
    - adaptive version selection
  - application porting atop vector code
    - MILC QCD (conjugate gradient dominated)
      - primary PACI cycle consumer
Trans-Petascale Vision

• **Multiple petabyte data archives**
  – 1-10 petabytes of secondary storage
  – tens to hundreds of petabytes of tertiary storage

• **DWDM terabit wide area networks (WANs)**
  – hundreds to thousands of lambdas
    • each operating at >10 Gb/s

• **Petascale computing systems**
  – dense, low-power packaging
  – memory access optimized

• **Responsive environments**
  – ubiquitous, mobile information sharing

• **Coupled by distributed Grid infrastructure**
GLORIAD

- **GLObal RLing Network for Advanced Applications Development**
  - Russia-China-USA science and education Network
    - 10 Gb/s transglobal network led by NCSA
    - builds on NCSA-led USA-Russia NaukaNet project
  - **Funding (beginning in 2004, we hope)**
    - cooperatively funded by USA, China and Russia.
      - USA commitment anticipated at $2.5M annually
    - example applications
      - HEP, ITER, IVO, climate change, nanomaterials
The Computing Continuum

It’s weird (and cool) all along the curve!

- **Power/Node**
  - Embedded Sensors

- **Memory/Node**
  - Petascale Systems

- **Cost/System**
  - Terascale Clusters
Building A Petaflop System

• **Technology trends**
  – dual-core processors
    • IBM Power4 and SUN UltraSPARC IV
    • quad-core is coming …
  – reduced power consumption (e.g, Intel Banias)
    • laptop and mobile market drivers
  – increased I/O and memory interconnect integration
    • PCI Express, Infiniband, …

• **Let’s look forward five years to 2008**
  – 4-way or 8-way cores (4 or 8 processors/chip)
  – ~10 GF cores (processors)
  – 4-way nodes (4, 4-way cores/node)
  – Infiniband-like interconnect
Building A Petaflop System

• With 10 GF/processors
  – 100K processors are required
  – 6200 nodes (4-way with 4 cores each)

• Power consumption
  – more than a portable generator
  – but, quite a bit less than a nuclear plant

• Software challenges
  – reliability and recovery

• Cost of a petaflop system, O($100M)
  – value of scientific breakthroughs … priceless
Very Large Scale Implications

- Single node failure during application execution
  - causes blockage of the overall simulation
  - data is lost and must be recovered/regenerated
  - key physics require neighbor exchanges
  - each spatial cell exists in one processor memory
- ~10^6 hours for component MTTF
  - sounds like a lot until you divide by 10^5!
- It’s time to take RAS seriously
  - systems do provide warnings
    - soft bit errors – ECC memory recovery
    - disk read/write retries, packet loss
  - status and health provide guidance
    - node temperature/fan duty cycles
- We have to expect components to fail!
- Software and algorithmic responses
  - diagnostic-mediated checkpointing and algorithm-based fault tolerance
  - domain-specific fault tolerance and loosely synchronous algorithms
Physics Challenges

• Much more mass than we can see
  – more than 80-90% of believed mass is not visible
  • rotation curves in spiral galaxies
  • globular clusters and gas by elliptical galaxies
  • gravitational lensing by clusters

• In addition, expansion is accelerating
  – dark energy unexplained
  • vacuum energy (cosmological constant)
  • dynamic field (quintessence)

• Possible missing mass candidates
  – baryonic
    • Massive Compact Halo Objects (MACHOS)
  – non-baryonic
    • Weakly Interacting Massive Particles (WIMPS)

• Recent experiment/theory interactions
  – Wilkinson Microwave Anisotropy Probe (WMAP)

  • universe is 13,400 ± 300 million years old and flat

Bridle et al, Science March 7 2003

Galaxies

Large Scale Filaments
Our immediate neighborhood we know intimately. But with increasing distance our knowledge fades. ...The search will continue. The urge is older than history. It is not satisfied, and it will not be denied.

*Edwin Hubble*