Future Directions in HPC and Grids
Numerical Relativity as Driver
US Status Report: personal perspective

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The Challenges
Comp. Science as “Third Pillar”

• Applications
• Data
• Communities

GWEN
Gravitational Wave European Network
From Astrophysical Theory to Detection and Understanding

Data Tsunami
Huge Black Hole Collision Simulation

- **Data Tsumani**
  - Smarr: supercomputers as petabyte generators
    - Num. Rel.: $10^6$ sims for GW param space, each 25TB
      - How to retrieve, track, manage?

- **Many components developed by distributed collaborations**
  - How to build codes for modern environments?

- **Many computational resources available**
  - How to find best ones to start?
  - How to distribute work? Interact w/code?

- **Time-changing computations!**
  - Multiscale, multiphysics: low efficiency
  - Adapt, monitor changes?

- **Interact with experiments? Coming!**
Almost Meeting Demand Now...

From Horst Simon

This is log scale!

Projected gap

Other Facilities:
DOE: NLCF
NSF: NCSA, PSC, SDSC
NASA: Columbia

Similar story! Worries!
Ubiquitous sensors and high-resolution detectors, can couple observation-driven computation and analysis, particularly in response to transient phenomena.

Explosive growth in resolution of sensors and scientific instruments creates unprecedented volumes of experimental data.

PITAC (Reed)
Collaborations for Complex Problems

**NASA Neutron Star Grand Challenge**
- 5 US Institutions
- Attack colliding neutron star problem

**EU Astrophysics Network, GWEN**
- 10 EU Institutions
- 3 years
- Continue these problems

**NSF Black Hole Grand Challenge**
- 8 US Institutions
- 5 years
- Attack colliding black hole problem

Examples of Future of Science & Engineering
- Require large scale data, simulations, beyond reach of existing supercomputers
- Require large geo-distributed cross-disciplinary collaborations
- Require Grid technologies

*Grids are not a substitute for SC’s!*
Sputnik: October 4, 1957
System trends towards Petascale

- **Processors**
  - Moore’s Law slowing, typical efficiencies lower than ever.
  - Heat!! Memory Bandwidth!!

- **System Taxonomy**
  - Commodity
  - Hybrid
  - Custom
  
  “Challenge: Prove efficiency of petascale system is bounded away from zero” Mike Heath

- **Power consumption impact**
  - Large systems using order MWatts of power.
  - Prevents dense packaging of HPC systems.
  - Adds facility costs

- **Worries**: we will need something new! Who is funding this? See “High End Crusader”, HPCWire
Note similarity with DEISA!
Computational Devices Scattered Across the World
- Compute servers (double every 18 months)
- Networks (double each 9 months)
- Sensors (exploding field)

How to take advantage of this for science, engineering, business, art?
- Harness multiple sites and devices
- Deploy cyberinfrastructure: Globus, Unicore, many others

Worries in US!
- DOE, NSF cyberinfrastructure funding

Gordon Bell Prize, 2001
Computational Science Software

• There is a crisis in computational science software
  – many years of inadequate investments
  – lack of useful tools
    • Cactus, Samrai, Overture, etc desperately needed
  – dearth of widely accepted standards and best practices
  – paucity of third party software vendors
    • DARPA survey: only handful could possibly scale to petascale
• Improvement in computational science software is needed urgently along multiple dimensions
• Half-life
  – few years for machines
  – decades for software!!

Source: Dan Reed
IT Funding Crisis in US

• Computing growth path in doubt
• Academic IT funding at Darpa down 50% in 3 years
• NASA downsizing IT
• DOE, NIH facing cuts
• NSF in disarray – funds 86% of IT research
  - success rate drops below 15%

An Endless Frontier Postponed

Next month, U.S. scientists Vinton G. Cerf and Robert E. Kahn will receive computing’s highest prize, the A. M. Turing Award, from the Association for Computing Machinery. Their Transmission Control Protocol (TCP) created in 1973, became the language of the Internet. Twenty years later, the Mosaic Web browser gave the Internet its public face. TCP and Mosaic illustrate the nature of computer science research, combining a quest for fundamental understanding with considerations of use. They also illustrate the essential role of government-sponsored university-based research in producing the ideas and people that drive innovation in information technology (IT).

Recent changes in the U.S. funding landscape have put this innovation pipeline at risk. The Defense Advanced Research Projects Agency (DARPA) funded TCP. The shock of the Soviet satellite Sputnik in 1957 led to the creation of the agency, which was charged with preventing future technological surprises. From its inception, DARPA funded long-term unclassified IT research in academia, even during several wars, to leverage all the best minds. Much of this

Lazowska, Patterson

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Recommendations

• Good advice for all from PITAC, others
Recommendation

The Federal government must rebalance research and development investments to:

a) create a new generation of well-engineered, scalable, easy-to-use software suitable for computational science that can reduce the complexity and time to solution for today’s challenging scientific applications and can create accurate simulations that answer new questions;

b) design, prototype, and evaluate new hardware architectures that can deliver larger fractions of peak hardware performance on scientific applications; and

c) focus on sensor- and data-intensive computational science applications in light of the explosive growth of data.
Lessons Not Learned

- Panel on Large Scale Computing in Science and Engineering, interagency, 1982
- From Desktop to Teraflop: Exploiting the U.S. Lead in High Performance Computing, NSF, 1993
- Information Technology Research: Investing in Our Future, PITAC 1999
- The Biomedical Information Science and Technology Initiative, NIH, 1999
- Making IT Better, National Academies, 2000
- Embedded Everywhere, National Academies, 2001
- High-Performance Computing for the National Security Community, DOD, 2002
- Knowledge Lost in Information, NSF, 2003
- Revolutionizing Science and Engineering Through Cyberinfrastructure, 2003
- A Science-Based Case for Large-Scale Simulation (ScALES), DOE, 2003
- Supercharging U. S. Innovation & Competitiveness, Council on Competitiveness, 2004
- Getting up to Speed: the Future of Supercomputing, National Academies, 2004
Futures

I can assure you that despite the recent set backs, the government is still fully committed to a digital future.
NSF, NASA

• DARPA High Productivity Computing Systems
  – 3 phase program over 8 years 2002-2010
    • aiming at comprehensive, balanced environments with > 4 PFlops
  – Aims to develop disruptive technologies for future generations of HPC applications
    • hardware
    • software
  – Currently Phase II: Sun, IBM, Cray
  – Phase III will have two vendors
EU GridLab Project
Tools for New Paradigms on Grids

Application

“Is there a better resource I could be using?”
“Where are my data?”

GAT_FindResource( )

Grid Application Toolkit (GAT)

GLOBUS (v1, 2, 3, 4, …) UNICORE
Other Grid Infrastructure?

Monitoring Security Notification Data Management
Profiling Resource Management
Information Application Management
Logging Migration

SOAP WSDL CORBA OGSA Other

SOAP
WSDL
CORBA
OGSA
Other

GLOBUS (v1, 2, 3, 4, …)
UNICORE
Other Grid Infrastructure?
GGF SAGA-RG

• GAT evolves into GGF standard
  – Numerous attempts to address: GAT most ambitious, but also CoG, DRMAA, GridRPC, many others  
    www.gridlab.org/GAT

• SAGA: Simple API for Grid Applications
  – Bringing all these efforts together
  – Chicago, Berlin, Brussels, LSU, Berkeley, Seoul, and Chicago in June, 2005

• GGF focussing now on standardization
  – SAGA API spec done
  – Much momentum in SAGA now

forge.gridforum.org/projects/saga-rg
Task Farming, Spawning & Migration

Main Cactus BH Simulation starts in Berkeley

Dozens of small jobs sent out to test parameters

Data returned for main job

Huge job generates remote data to be visualized in Baltimore: lambda on demand!
• UCoMS (Petroleum Engineering)
  – Deploy sensor networks across Gulf
  – Data collected to provide input to simulations, tasks farmed out
  – Results collected (transmitted back)
  – http://www.ucoms.org

• SCOOP (Ocean Observing)
  – Data coming in from sensors all over Gulf Realtime Operational Grid
  – Feeds in to models on Grid sites
Summary

- Apps challenge HPC, Grids for years to come
- Some challenges partially met, many not
  - Hardware: C
  - Networks: B
  - Software: D
  - Funding (US): F
- Many new application types coming
- DEISA, others, EU 7th Framework poised to fill some of the void, take some leadership
  - But: Grids do not replace supercomputers!! EU still has no SC Center

Old Europe??