

Advancing Science Through Grid

Techscan notes
On Major Laboratories

Guidelines

- Things to watch out for:
 - Major motivation
 - Major thrusts
 - Timeline (*cannot get much info*)
 - Outcome expected

Argonne National Lab, USA

- **FY2004-2008 Institutional Plan** (published 2003)
- Relevant visionary strategic goals
 - Nanoscale and innovative materials
 - Computational biology for fundamental understanding of living systems
 - Realize full potential of scientific simulation to solve mission-related problems, through leading-edge research on systems architecture and software, parallel programming and numerical tools, distributed computing, and computational science apps
 - Optimize the operation of national user facilities to perform research in fundamental science and other areas
- Core areas:
 - Nanoscience & nanotechnology
 - Bioscience
 - National security
 - Environmental research
 - Advanced scientific computing

ANL – Needs

- Multi-disciplinary, complex system, nanosciences pushing compute requirement
- “Computing, computational science, and communications and IT will advance rapidly, will become seamlessly intertwined with experimental science, and will thereby revolutionize many fields of research and applications...”
 - **Virtual Fab Lab** (computational techniques for nanoscale simulation)
- **Petaflops** computing requirement
 - To solve problems in **biology**, high energy physics, climate modeling, **computational chemistry**, **chemical engineering**, subsurface modeling, **biomedical computing**, astrophysics...
 - New software infrastructure
 - Novel interfaces to integrate resources into emerging national computational grids; high-level tools
 - Systems integration strategies to enable scaling of the system
 - Available in 2007/2008

ANL: Thrusts

- Spearhead development of the grid tools, middleware, and services needed for large scale collaborative problem solving.
- Coupling workstations and parallel computers, large databases, virtual-reality devices, and other resources worldwide promises tremendous advances in scientific problem solving
- IT to
 - Improve lab-wide access to data supporting both R&D and ops
 - Simplify user access to operational and administrative info
 - Facilitate migration of existing incompatible business apps to more open, integrated, web-based solutions

ANL Grid Activities

- DOE Science Grid
 - Globus™ (e.g. GridFTP)
 - GRIDS Center (NSF Middleware Initiative)
 - CoG Kits: Enabling Middleware for Designing Science Applications, Web Portals, and Problem-Solving Environments
 - GrADS (Grid Application Development Software)
 - High-Performance Data Grid Toolkit: Enabling Technology for Wide Area Data-Intensive Applications
 - Access Grid
 - [iVDGL](#) (International Virtual Data Grid Laboratory)
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- Particle Physics Data Grid Collaboratory Pilot
 - Earth System Grid
 - Proteomics Data Grid, Biotechnology Data Grid
 - Management and processing of large data sets

Lawrence Livermore Nat'l Lab, USA

- 2020 Foresight (published Jan 2000)
- Simulation is an integral part of virtually every major program; a principle tool for scientific discovery and analysis
- Vastly improve computer simulations
 - High-end scientific computer simulations
 - Fundamental properties of materials, complex environ processes, biological systems
 - Simulation of complex systems
 - Sensors for data gathering and require fusion and interpretation of massive amounts of data
 - National security, crisis management, homeland security, healthcare, smart spaces...
 - Use of powerful model-development and data analysis tools

Lawrence Livermore Nat'l Lab, USA

- Prediction (10-20 years): **teraops capability in desktop computers**
- Use in environmental/biological/astrophysical simulations
- **Vastly improved capabilities to manage, fuse and display data**
- Automating setup
- Robust scalable numerical algorithms

Sandia National Lab, USA

- Annual report 2003-2004
- Multi-program science-based engineering lab
 - Multi/cross-disciplinary research
 - Modeling/simulation; engineering & advanced manufacturing; biotechnology; materials science; microtechnologies; sensors; micro/nano/info/bio/cogno interfaces
 - Security/defence technology
- 40 teraops system (Red Storm)
- Quantum computing

Oak Ridge Nat'l Lab, USA

- HPC program
 - Terescale computing
 - High performance storage systems
 - High performance networking research
 - Software tools and applied mathematics
 - Visualization
 - Virtual labs (HFIR Neutron Scattering Instruments , microscopy)
- Complex systems; computational materials science; network and cluster computing; systems and operations; computational biology; computational mathematics; statistics and data science; scientific apps support; computational chemical sciences; climate dynamics

NCSA, USA

- Focus areas
 - Cluster computing
 - Cyberinfrastructure
 - Data analysis
 - Grids
 - NCSA application technologies
 - Visualization and VR
- Grid related
 - grid performance optimization
 - node performance tuning
 - parallel system performance
 - performance tools for parallel & grid computing