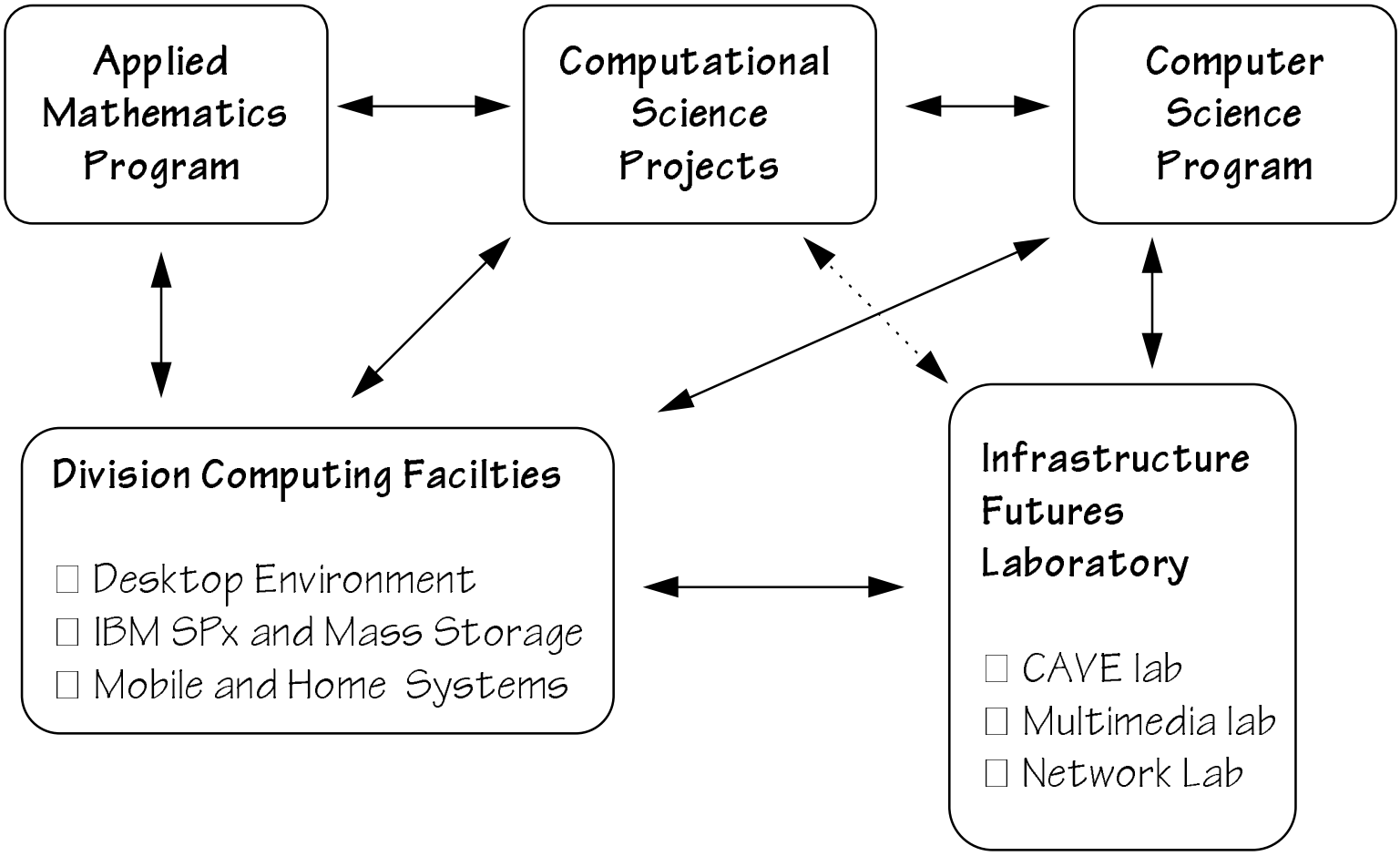
Mathematics and Computer Science Division Structure



Research Program Components

- mathematics of physical systems
- computational science applications
- computational differentiation and sensitivity analysis
- numerical solutions of partial differential equations
- large-scale optimization
- numerical linear algebra
- automated reasoning
- wavelets and image processing
- computational support for genome initiatives
- parallel programming tools and systems software
- performance evaluation of parallel systems
- performance visualization tools
- visualization and data systems
- finite element methods
- quadrature
- approximation methods and libraries
- immersive virtual environments
- distributed collaborative research environments

MCS Computing Resources

- Divisional Computing Environment
  - workstations,fileservers and local compute servers
  - portable computing devices (laptops and PDAs)
  - home computing devices
- High-Performance Computing Research Facility
  - IBM MPP systems
  - mass storage systems
  - scientific visualization facilities
- Computing and Communications Infrastructure Futures Laboratory
  - virtual environments project (ANL-CAVE)
  - multimedia space/ video server projects
  - wireless computing and communications pilot project

ANL/IBM High-Performance Computing Research Consortium

- focus on five application areas
  - computational chemistry
  - computational biology
  - materials science
  - global change
  - stellar astrophysics
- development of software tools and systems software
- CRADA with IBM of MPP computer systems
- design, implementation and deployment of educational programs

New Projects Since Last Review

- National Energy Modeling System*
- Advanced Computational Technology Initiative
- Optimization Software Center with Northwestern*
- Automated mesh generation (new science)*
- Wavelets and Image Processing*
- Computational Medicine (new science and tech)
- National HPCC Software Exchange
- Scalable I/O Initiative*
- CAVE: Virtual Environments project*
- Distributed Collaborative Research Environments (LabSpace project and multimedia lab)

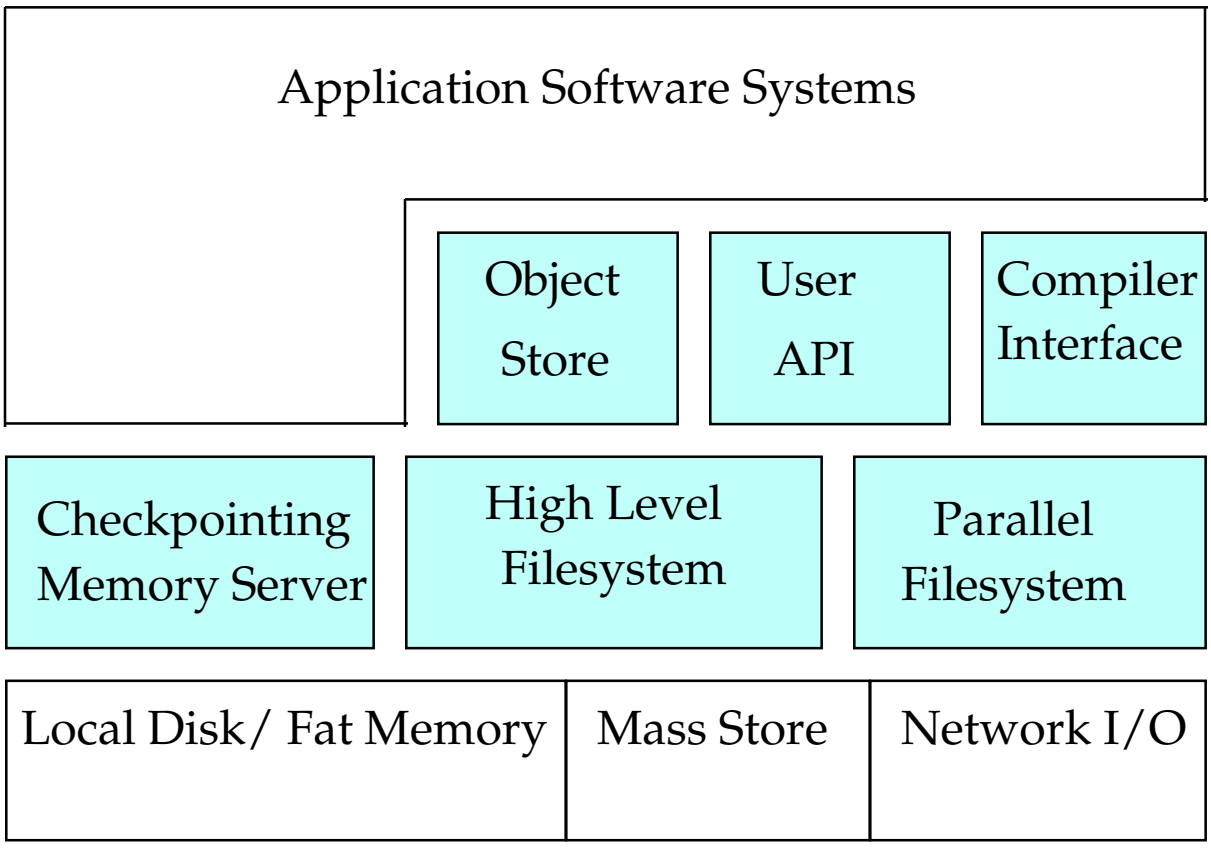
Scalable I/O Initiative

- integrated project to build parallel I/O software
- Darpa, NSF, NASA, DOE supported
- Caltech, ANL, UIUC, Uof Washington, Rice, Arizona, PNL, NASA Langley, JPL, CMU, Princeton, etc.
- $10 M budget over 3 years
- ANL will lead software integration activity, $700K /year
- IBM, Intel, Cray,Convex all involved
- @ANL (Foster, Gropp, Lusk, Stevens)

Scalable I/O Initiative

- Development and integration of software to support parallel I/O
- Focus on I/O for tightly coupled massively parallel computers
- Builds on NSL-unitree and vendor provided parallel filesystems
- Test innovative approaches to the I/O problem at full scale, on real applications
- 18 applications projects, Intel and IBM testbeds
- Perforamnce characterization is important

Scalable I/O System Architecture



ISDN Pilot Project

- Extending ANL LAN to researcher homes
- Seamless computing from lab to home
- Plan to test voice, video and data transparency
- Evolution beyond SLIP at 14.4 Kbps
- Testbed for ISDN hardware/software
- NeXT, Sun, SGI, IBM PC and Mac hardware
- MCS, ECT, Ameritech, Gandalf, Network Express et al.

Argonne Digital Infrastructure

- ATM desktop and back bone networks
- FCS streaming data channels for RT data
- Central data stores (AFS service, archival service, database & indexing services)
- Digital/analog video distribution/switching
- ISDN integration (LAN extensions, end user PTP WANs)
- Wireless LANs (integration with wired networks)
- WAN (smds, atm, etc.)

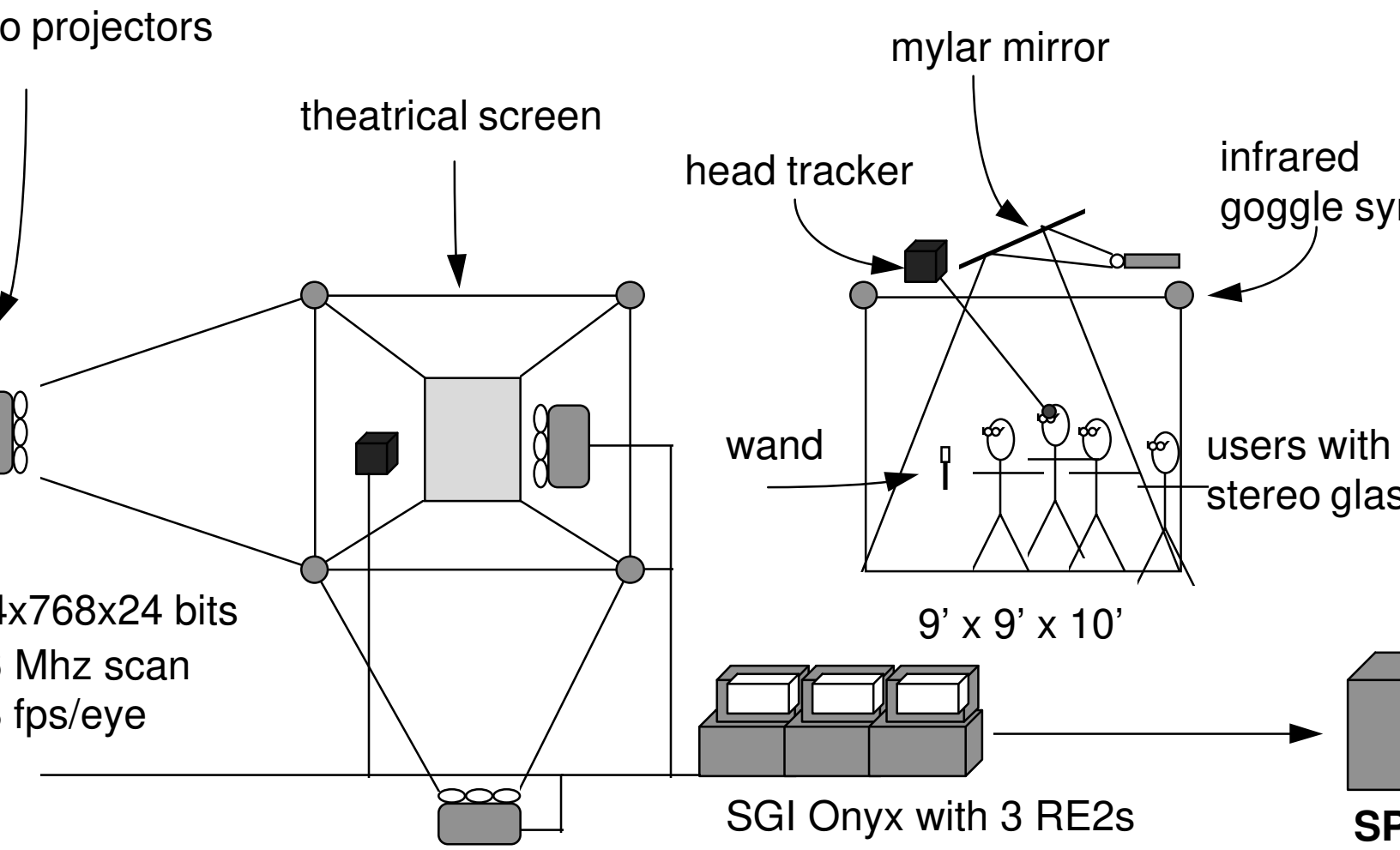
What is the CAVE ?

- Multipassenger high-end virtual environment
- Immersive realtime interactive
- Designed for large-scale applications
- Designed to interface to supercomputers
- Handful of CAVEs under development

Cave Automatic Virtual Environment (CAVE)

- multiviewer virtual reality environment
- walkin 10'x10' cube (Holodeck like)
- 3-4 planes of 1024x768x32 bit realtime stereo images
- provides peripheral vision and significantly more resolution than helmet based systems
- applications visualization (biology, materials, astrophysics, etc.)
- CAVEs at ANL, UIC, NCSA, ARPA
- UIC, ANL, NCSA, SGI, IBM, et al.

CAVE Architecture



How the CAVE fits into NII

- Improved output bandwidth for supercomputing apps
- Expands user interface for non-computing people
- Supports virtual prototyping
- Supports remote training and education
- Supports telepresence applications
- New user interface frontier

Argonne Demonstration Applications

- Interactive molecular modeling and docking (Bash et al.)
- Metal casting and transparent mold (Domanus et al.)
- Interactive grinder with heat model (Canfield et al.)
- Dynamic mesh generation w/FEM model (Freitag, Plassmar
- Interactive reactor vessel (EBR) (Hudson et al.)
- others under development

CAVE Technology Research Issues

Recording and play back of CAVE experiences

Integration of video as texture maps

Improved linkage of the CAVE to parallel supercomputers

CAVE-to-CAVE communications

Support for more than one virtual viewpoint

Heads up display and user sampling of 3D fields

Support for 3D menus and icons

Help systems and support for "Guided Tours"

Improved navigation paradigms for virtual spaces

Improved tracking and control, sonic imaging, and feedback

Improvements of display technology (support for HDTV)

- Goal: to run teraFLOPS applications in the `National Machine Room` with interactive immersive visualization via CAVEs @ San Diego Supercomputing Conference in December 1995.
- Needs:
  - distributed parallel applications
  - parallel programming tools ported to the NMR
  - performance monitoring tools
  - interactive immersive virtual environments
  - interactive application benchmarks
  - SW tools for managing cluster computing applications
  - SW tools for parallel/distributed I/O mapped on NMR
  - HIGH PERFORMANCE LOW LATENCY "`superVROOMnet`"
  - ideas and algorithms for managing latency
  - 30 site gang scheduling mechanisms
  - wide area implementations of collective communications

Acknowledgments

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- CAVE technology originally developed at the Electronic Visualization Laboratory, UIC

Strategy for the National Information Infrastructure

Leverage

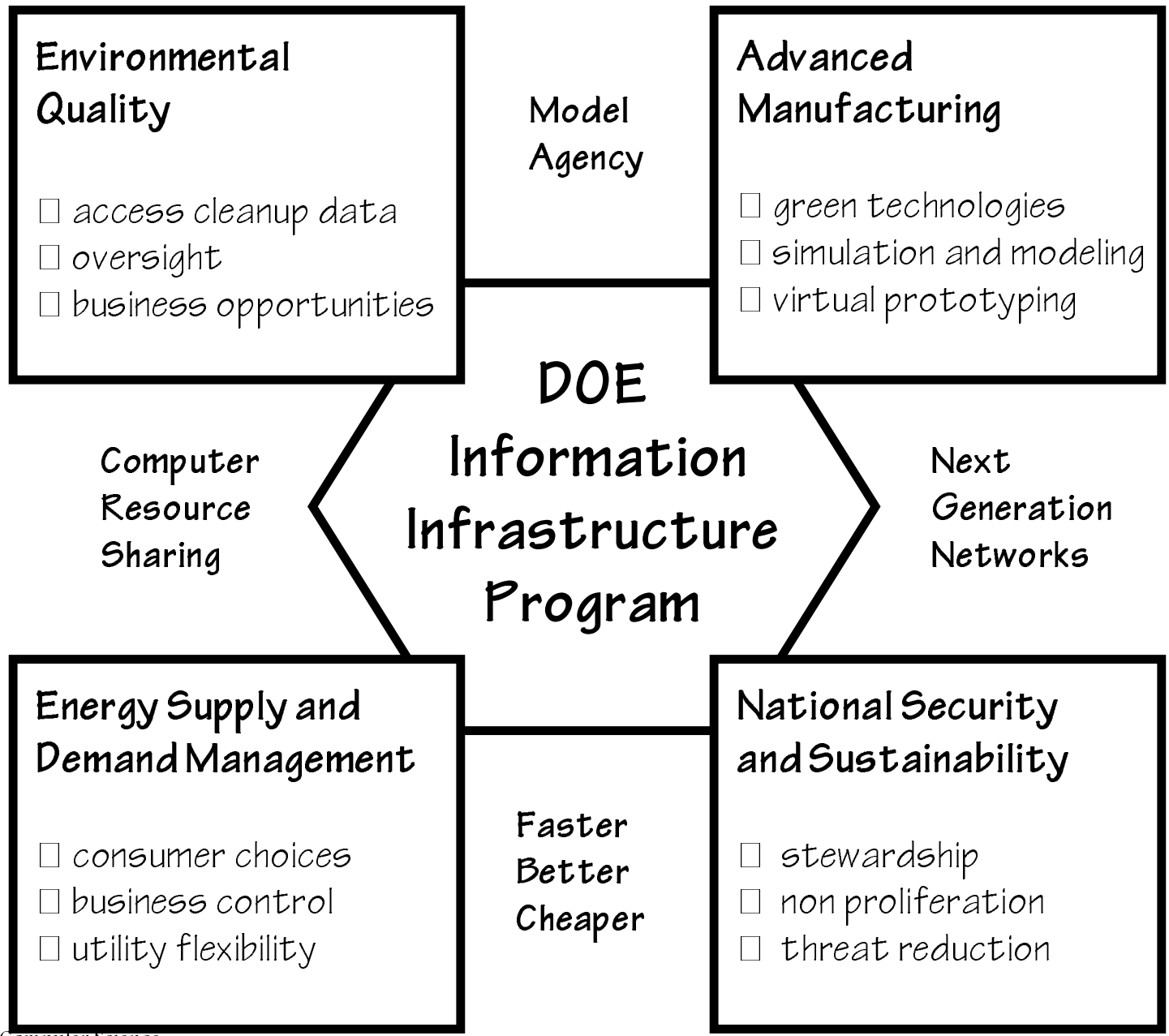
- basic research and development program
- HPCC program, facilities and relationships (ANL Focus)

Focus on DOE relevant programs

- ER research and development programs (DOE Focus)
- Environment
- Energy supply and demand management (DOE Focus)

Build new technology base

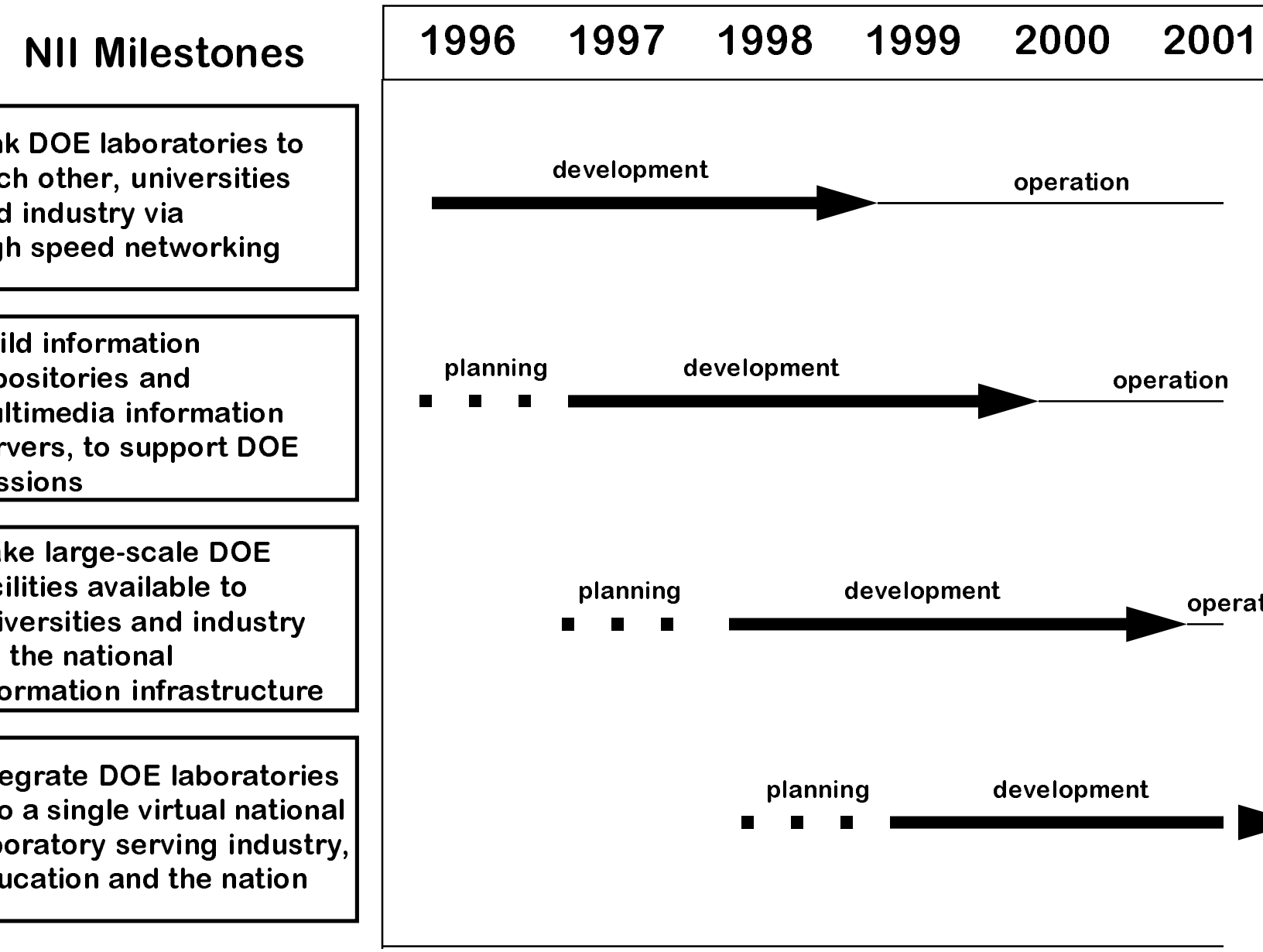
- multimedia x supercomputing x virtual environments (DOE Focus)
- integration of narrowband, wideband and broadband networks
- digital libraries and cyberspace tools
- telepresence/ remote operation monitor and control (DOE Focus)


Environmental Quality
access cleanup data
oversight
business opportunities
Model Agency
Advanced Manufacturing
green technologies
simulation and modeling
virtual prototyping
DOE Information Infrastructure Program
Computer Resource Sharing
Next Generation Networks
Energy Supply and Demand Management
consumer choices
business control
utility flexibility
Faster Better Cheaper
National Security and Sustainability
stewardship
non proliferation
threat reduction

Overview of Program

- Scope of NII program
  - existing and future HPCC work
  - information infrastructure technology and applications component
  - government information services component
- Focus:
  - DOE mission critical programs
  - DOE outreach activities
  - technology research and development
- Leverages existing infrastructure and HPCC research programs
- DOE's contribution to a multiagency program

Timeline for Implementation of DOE Information Infrastructure



DOE NII Program Layers

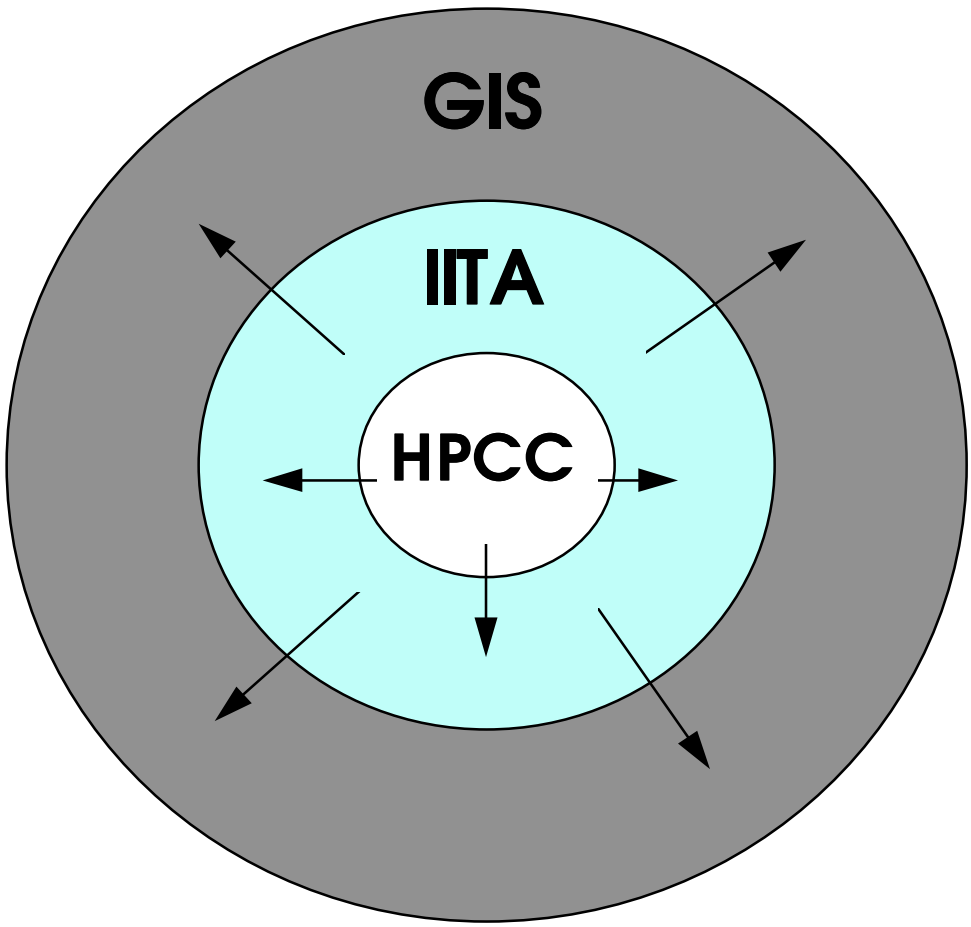
NII subsumes HPCC program

echnology flows from the
PCC programs to the IITA
nd GIS programs.

= Government
rmation Services

= Information
astructure Technology
Applications

C = High Performance
puting and Communications



Advanced HPCC Program

- Applications driven by core DOE mission areas
  - development of environmentally sound energy sources
  - environmental restoration and monitoring
  - stockpile stewardship & virtual prototyping
  - basic science and technology
- Advanced computational and communications technology research and development
- Centers for user and development of HPCC systems
- Methods development for information intensive computing systems
- Testbeds for information infrastructure development
- Participation in multiagency petaFLOPS initiative

Information Infrastructure Technology and Applications

- Develop technology base for NII applications
  - information analysis and navigation tools
  - databases and storage environments
  - collaboration and telepresence technologies
  - internetworking and information surety
- Focus on "National Challenge" problems
  - energy demand management
  - environmental monitoring
  - education and outreach
  - medical databases and electronic imaging
  - agile manufacturing and electronic commerce
- Develop NII testbeds linking DOE resources and facilities
- Develop collaborative environments for DOE and industry

Government Information Services

- Targets for DOE information services
  - general public and state and local governments
  - businesses, hospitals, libraries and schools
  - DOE offices and laboratories
- Goals for GIS
  - greater energy efficiency
  - improved environmental quality
  - access to software, data and facilities
  - access to business opportunities
  - better education and training
- Based on distributed Internet resources
- Provides DOE's electronic window to the world

NII Technology Development Projects

- support of two types of applications
- internal DOE applications: state-of-the-art technical solutions for DOE specific missions as prototypes for other agencies
- external applications: developed specifically for deployment external to DOE
- leverage DOE expertise and resources with emerging commercial technology
- utilize DOE's unique position in the research community

Future DOE Computing Environment

- Integrated Computational Science Environments
  - control and monitoring of computations (e.g. workstation, PDA)
  - computational engines and mass storage environments (distributed)
  - visualization and shared immersive displays
  - postprocessing and annotation tools
  - high-performance communications system
- Joint development of new supercomputing hardware/softwar based on strong computing science research programs
- Joint development of new communications technologies based on strong computer science programs
- Joint development of applications and programming tools and environments

World Class Research Programs

- Increase research support for computer science needed to develop HW/SW technology for computational science and information infrastructure applications
- Develop long-term support for computational science programs started under the HPCC program
- Revitalize the DOE applied mathematics program with a new set of goals and program links
- Benchmark DOE research programs against other agencies
- Encourage stronger Inter-agency relationships

Education and Training

- Develop a visible program to use the NII to help train the next generation of computational scientists for DOE and the country
- Expand educational program to all of science and technical training (e.g. partner with DoEd ?)
- Encourage innovative partnerships between DOE laboratories and universities and industry to "field test" new educational technology
- Increase support for graduate students and post-doctoral positions

Benefits to DOE

- New foundation for departmental openness
- Provides new ways of doing business that:
  - save money and improve capability
  - improve service and visibility to the public
  - makes DOE more responsive to future challenges
- Continues historical leadership in science and technology including critical computing and communications technologies
- Necessary for DOE mission critical applications

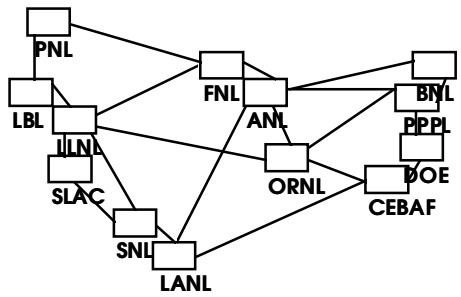
Example Projects

The purpose of the examples are to illustrate the types of programs that could be supported under a DOEwide NII program

- DOE meta-laboratory system
- DOE Internet science education program
- DOE system wide environmental contamination and cleanup databases
- Remote operation and access to DOE facilities
- DOE - Industrial Partner infrastructure linkage

DOE Meta-Laboratory System

NII testbed linking major DOE sites



- Gigabit/s networks
- Shared filesystems
- Shared computing facilities
- Common user simulation environment
- Mechanisms for supporting shared DOE databases
- Distributed collaborative work environments

Creates the foundation for virtual laboratories and ad hoc teaming for rapid problem solving

DOE Internet Based Science Education Program

- Laboratory/K-12/University partnership
- Provides high-quality interactive science programs/courses
- Supports mentoring by real scientists
- Integrated with existing DOE educational programs
- Available to all via the internet/NII
- Supports multiple types of programming and media

Environmental Databases

- Open databases of DOE sites and environmental status
- Provides public access to modeling and analysis environments and data
- Acts as a model for other agencies
- Integrated with DOE public communications (Office of Public Affairs)
- Provides multiple levels of interpretation to public and business
- Can be used in education and training
- Supports DOE science programs and public outreach

On-line Facilities

Makes DOE's unique large-scale facilities more accessible and valuable by putting them on-line

- Supports remote operation and telepresence
- Facilitates private use of DOE resources via public Internet networks
- Educational use of DOE facilities
- Includes: X-ray sources, microscopes, accelerators, neutron sources, databases, etc.

Provides a way to embed DOE infrastructure in to the national industrial and educational infrastructures

DOE-Industrial Partner Linkage

Creating strong infrastructure connections between DOE laboratories and industrial partners

- Distributed collaborative work environments
- Common user simulation environment
- Mechanisms for supporting sharing databases
- Gigabit/s networks
- Shared filesystems
- Shared computing facilities
- Online rapid prototyping facilities

Creates the foundation for DOE-Industry teaming for advanced industrial problem solving