e-Science, Archives and the Grid

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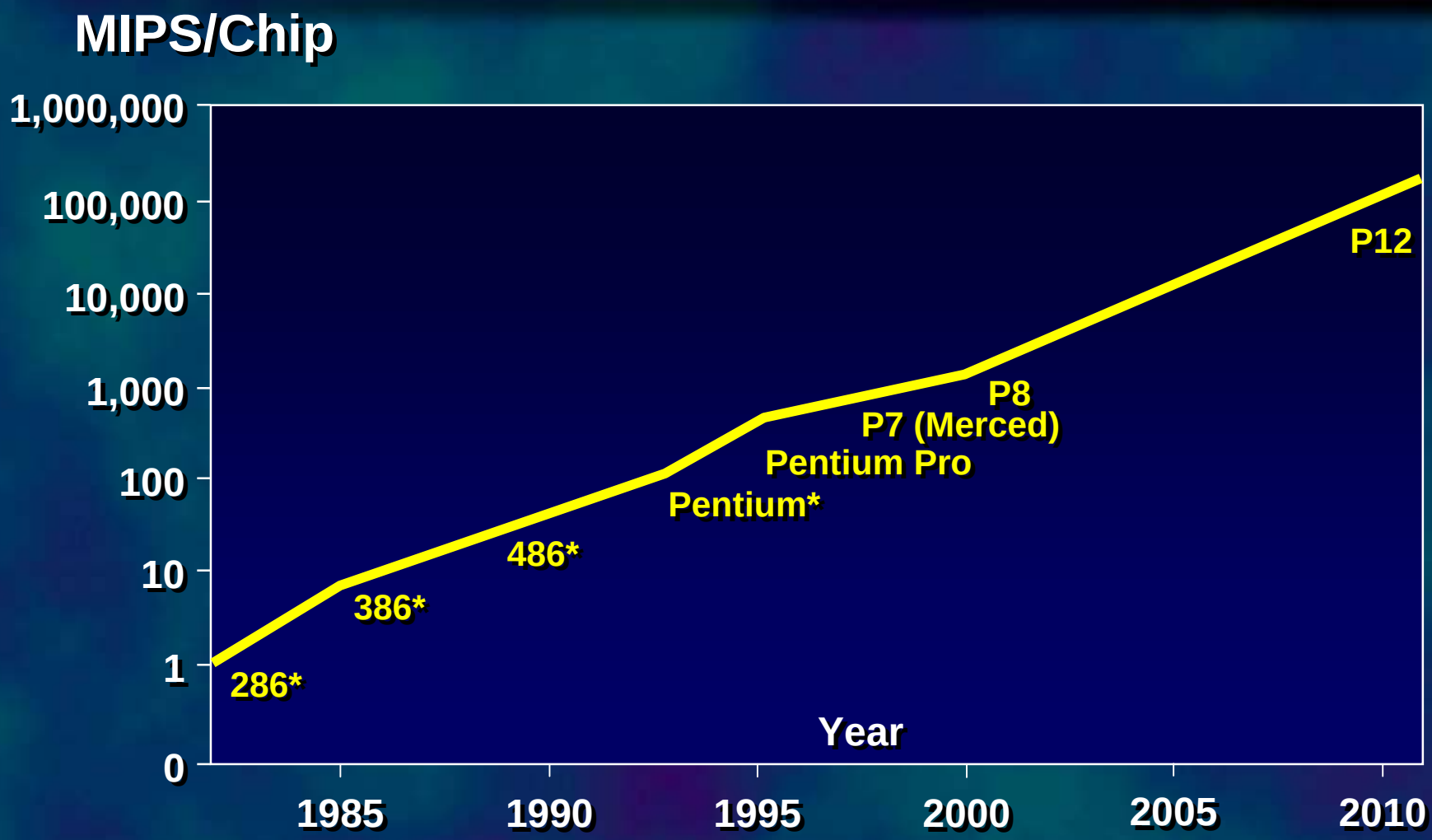
Outline

- Technology Trends
- What is e-Science?
- What is ‘the’ Grid?
- Present Grid Projects

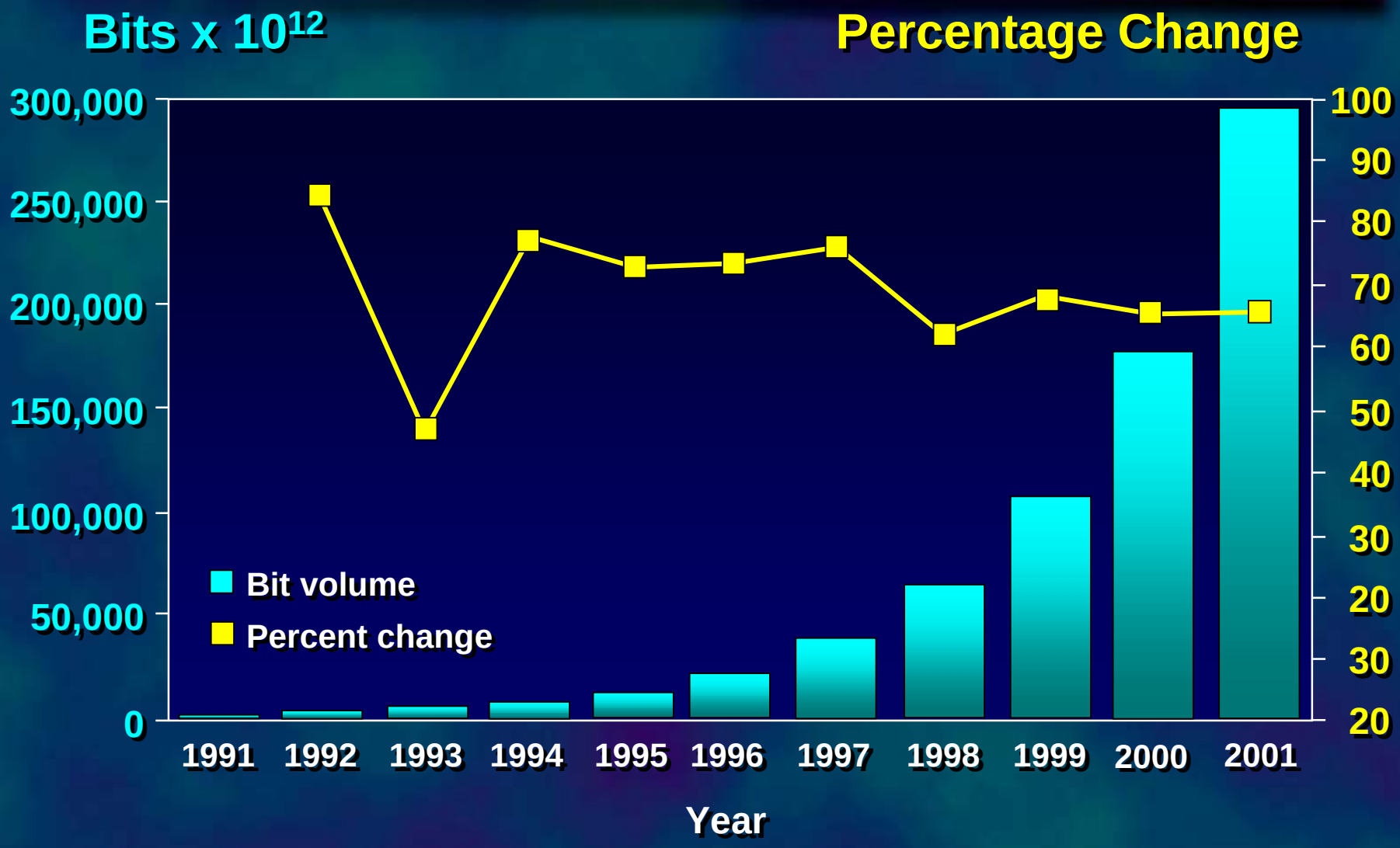
Increase in MIPS per Chip



MIPS - Millions of instructions per second

*Pentium, 286, 386 and 486 are registered trademarks of Intel Corp.

Growth of DRAM use



e-Science

‘e-Science is about global collaboration in key areas of science, and the next generation of infrastructure that will enable it.’

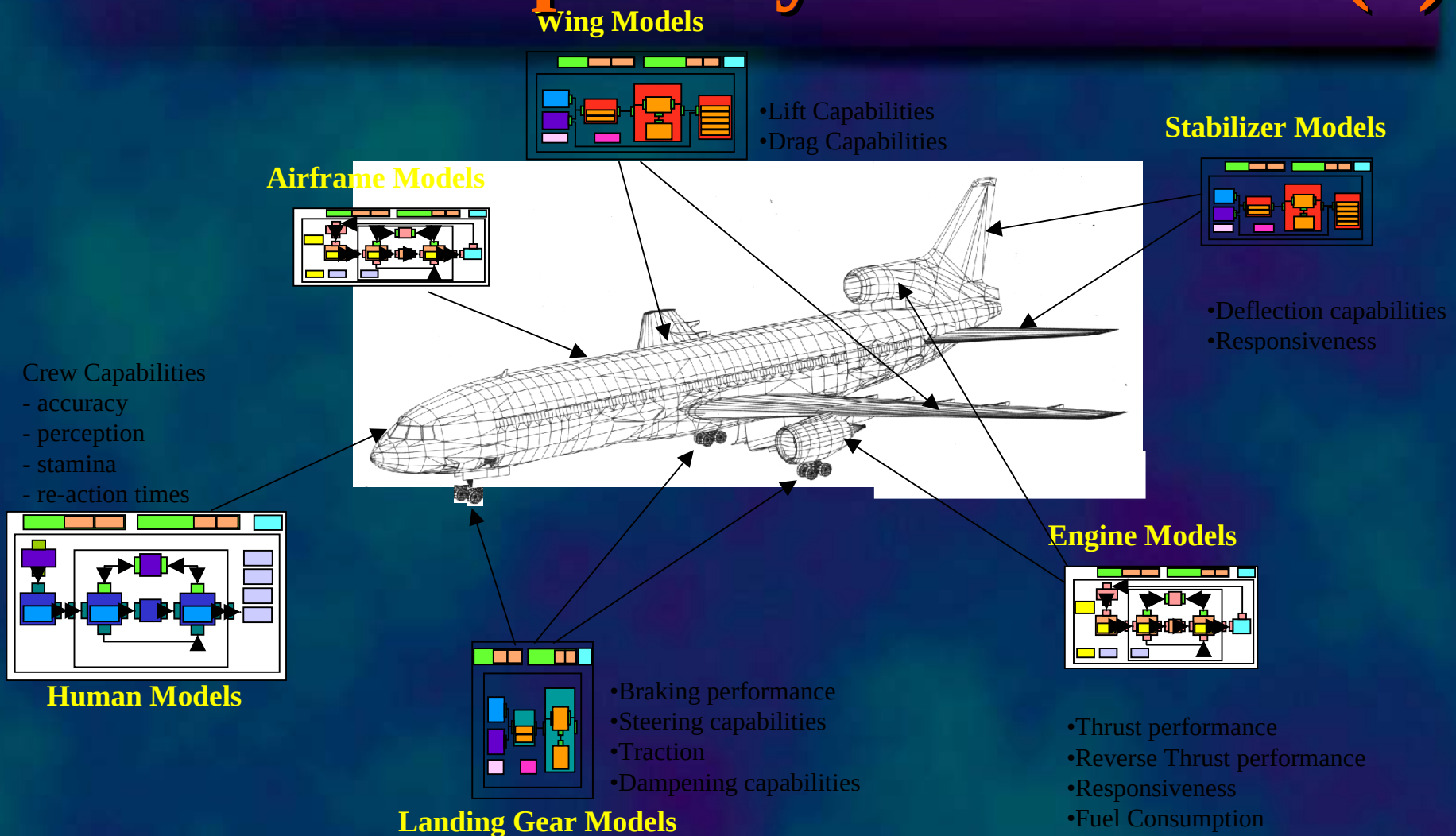
‘e-Science will change the dynamic of the way science is undertaken.’

John Taylor
Director General of Research Councils
Office of Science and Technology

NASA's IPG

- The vision for the *Information Power Grid* is to promote a revolution in how NASA addresses large-scale science and engineering problems by providing *persistent infrastructure* for
  - "highly capable" computing and data management services that, on-demand, will locate and co-schedule the multi-Center resources needed to address large-scale and/or widely distributed problems
  - the ancillary services that are needed to support the workflow management frameworks that coordinate the processes of distributed science and engineering problems

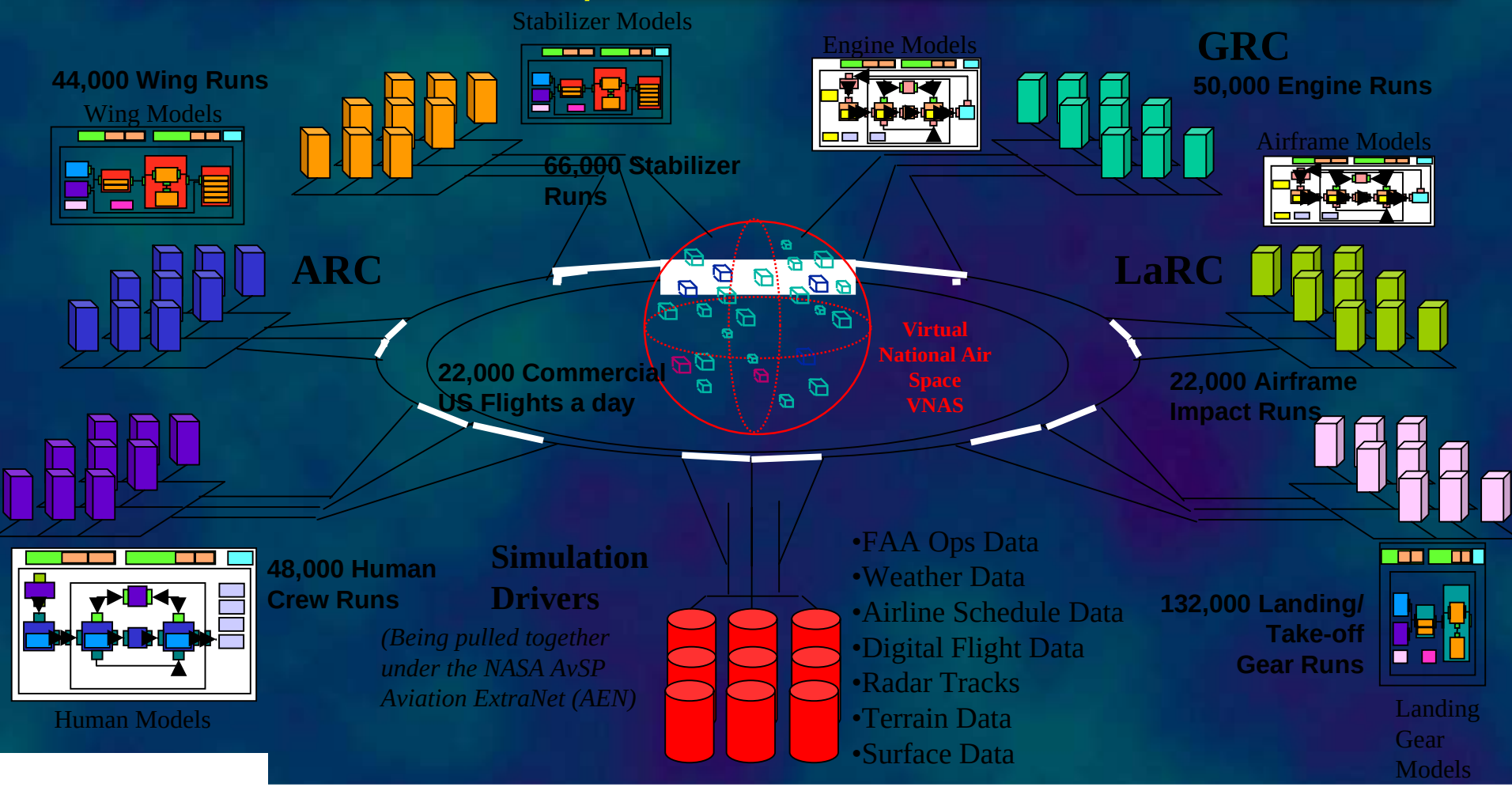
Multi-disciplinary Simulations (1)



Whole system simulations are produced by coupling all of the sub-system simulations

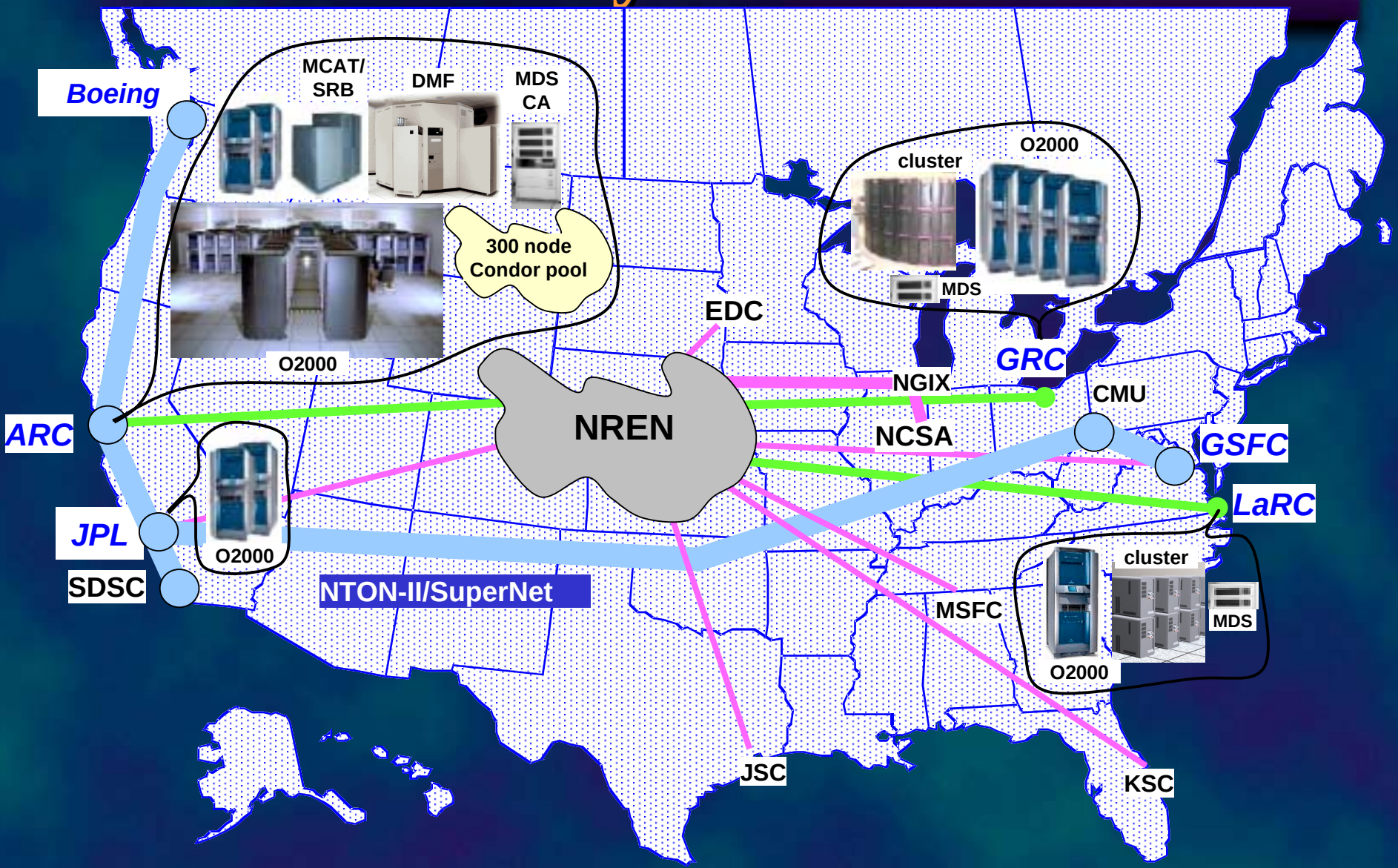
Multi-disciplinary Simulations (2)

National Air Space Simulation Environment



Many aircraft, flight paths, airport operations, and the environment are combined to get a virtual national airspace

IPG Baseline System



e-Science Examples

- Bioinformatics/Functional genomics
- Collaborative Engineering
- Medical/Healthcare informatics
- Earth Observation Systems
- TeleMicroscopy
- Virtual Observatories
- Robotic Telescopes
- Particle Physics at the LHC

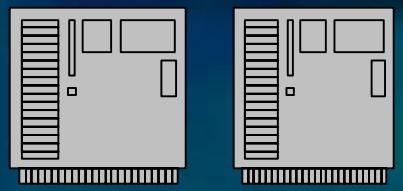
What is the Grid?

• Computing cycles, Data Storage, Bandwidth and Facilities viewed as commodities as in Electric Power Grid

• Need software and hardware infrastructure to support ‘Grid’ model of ‘Information Utilities’ on demand

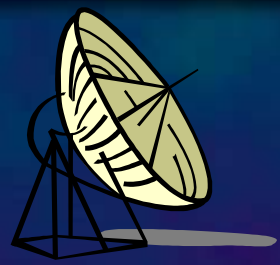
• Grid offers uniform access to more than just html pages and information

The GRID Vision

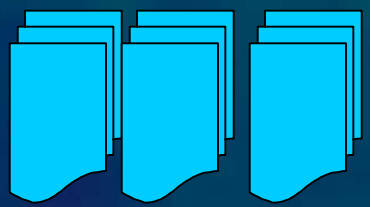


Computing resources

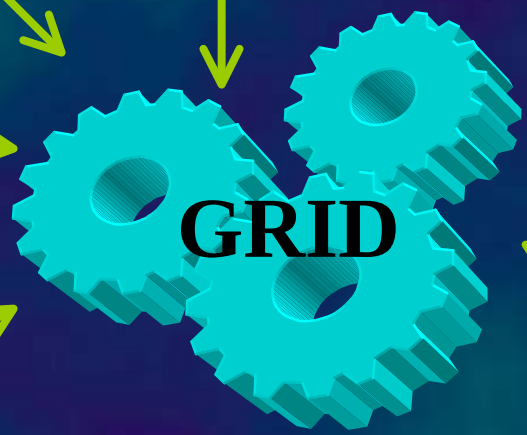
Complex problem



Instruments



Data



GRID

Knowledge

Solution

People

The Challenge of the Grid

- The Grid is an emergent infrastructure capable of delivering dependable, pervasive and uniform access to a set of globally distributed, dynamic and heterogeneous resources
- Problems of scalability, interoperability, fault tolerance, resource management and security
- A useful abstraction of the Grid architecture is in terms of a three layered model going from data and computation to information and knowledge

Data, Information and Knowledge

- Data

  Uninterpreted bits and bytes

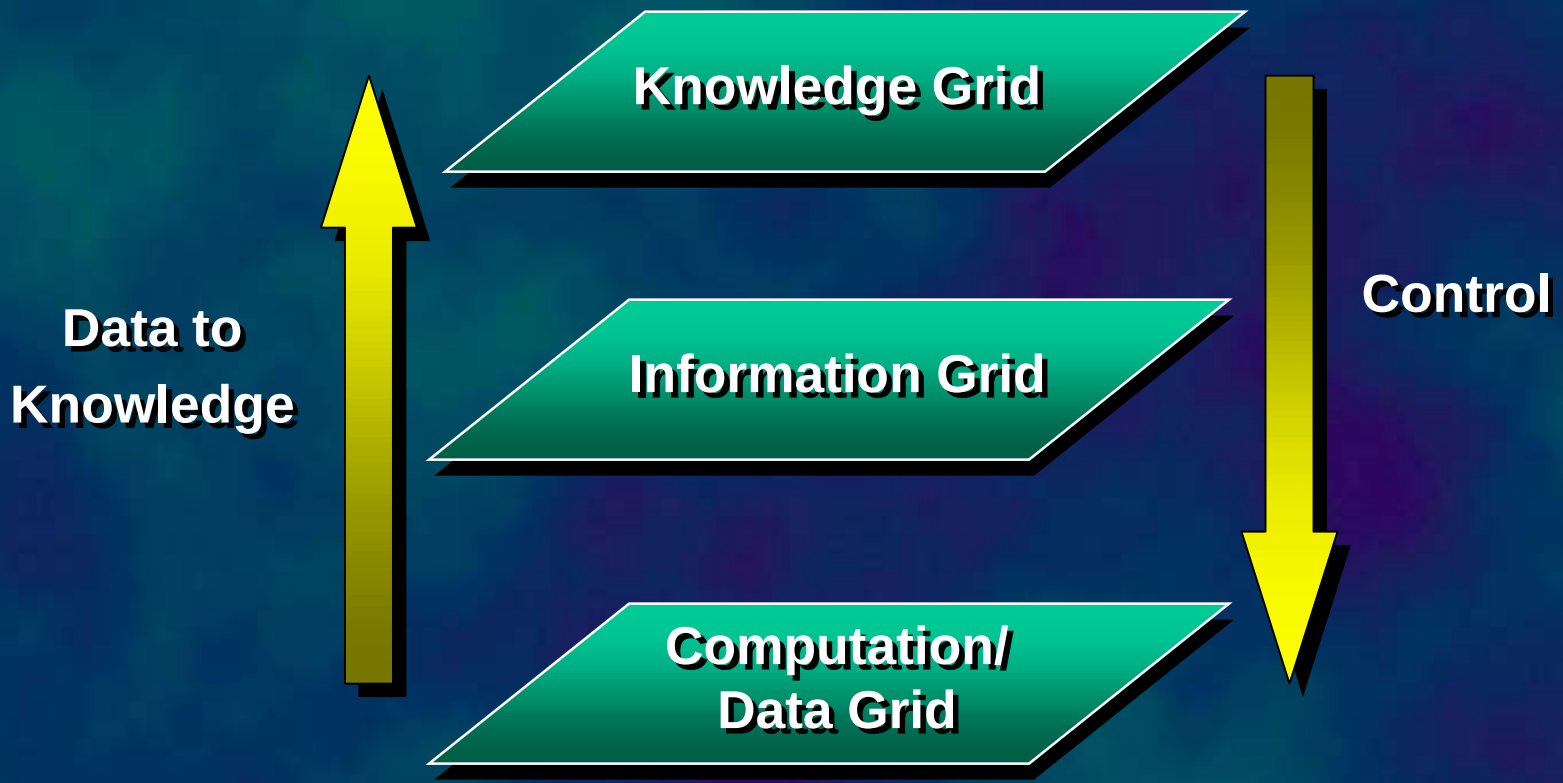
- Information

  Data equipped with meaning

- Knowledge

  Information applied to achieve a goal, solve a problem or enact a decision

Three Layer GRID Abstraction



US Grid Projects

- NASA Information Power Grid
- DOE Science Grid
- NSF National Virtual Observatory
- NSF GriPhyN
- DOE Particle Physics Data Grid
- NSF Distributed Terascale Facility
- DOE ASCI Grid
- DOE Earth Systems Grid
- DARPA CoABS Grid
- NEESGrid
- DOH BIRN
- NSF iVDGL

EU Grid Projects

- DataGrid (CERN, ..)
- EuroGrid (Unicore)
- DataTag (TTT…)
- Astrophysical Virtual Observatory
- GRIP (Globus/Unicore)
- GRIA (Industrial applications)
- GridLab (Cactus Toolkit)
- CrossGrid (Infrastructure Components)
- EGSO (Solar Physics)

National Grid Projects

- UK e-Science Grid
- Japan – Grid Data Farm, ITBL
- Netherlands – VLAM, PolderGrid
- Germany – UNICORE, Grid proposal
- France – Grid funding approved
- Italy – INFN Grid
- Eire – Grid proposals
- Switzerland - Grid proposal
- Hungary – DemoGrid, Grid proposal
- ApGrid
- ……

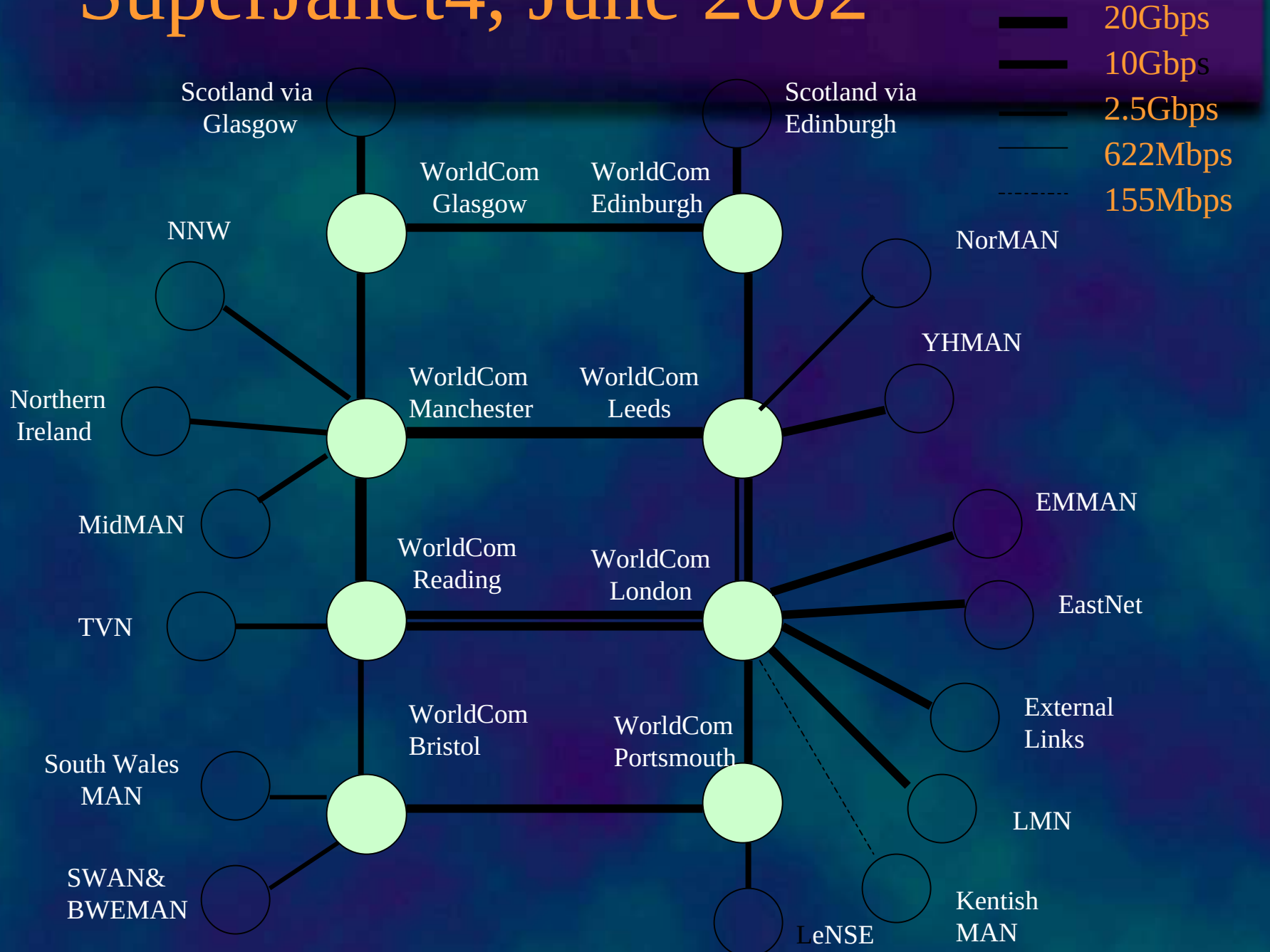
UK e-Science Initiative (1)

- £120M 3 Year Programme to create the next generation IT infrastructure to support e-Science and Business
- SR2000 – Funded UK e-Science Grid and Grid Support Centre, e-Science Application research projects and industrial collaboration
- SR2002 – Bidding for additional funding to extend scope of e-Science programme
- Essential that UK plays a leading role in Global Grid development with the USA, EU and Asia

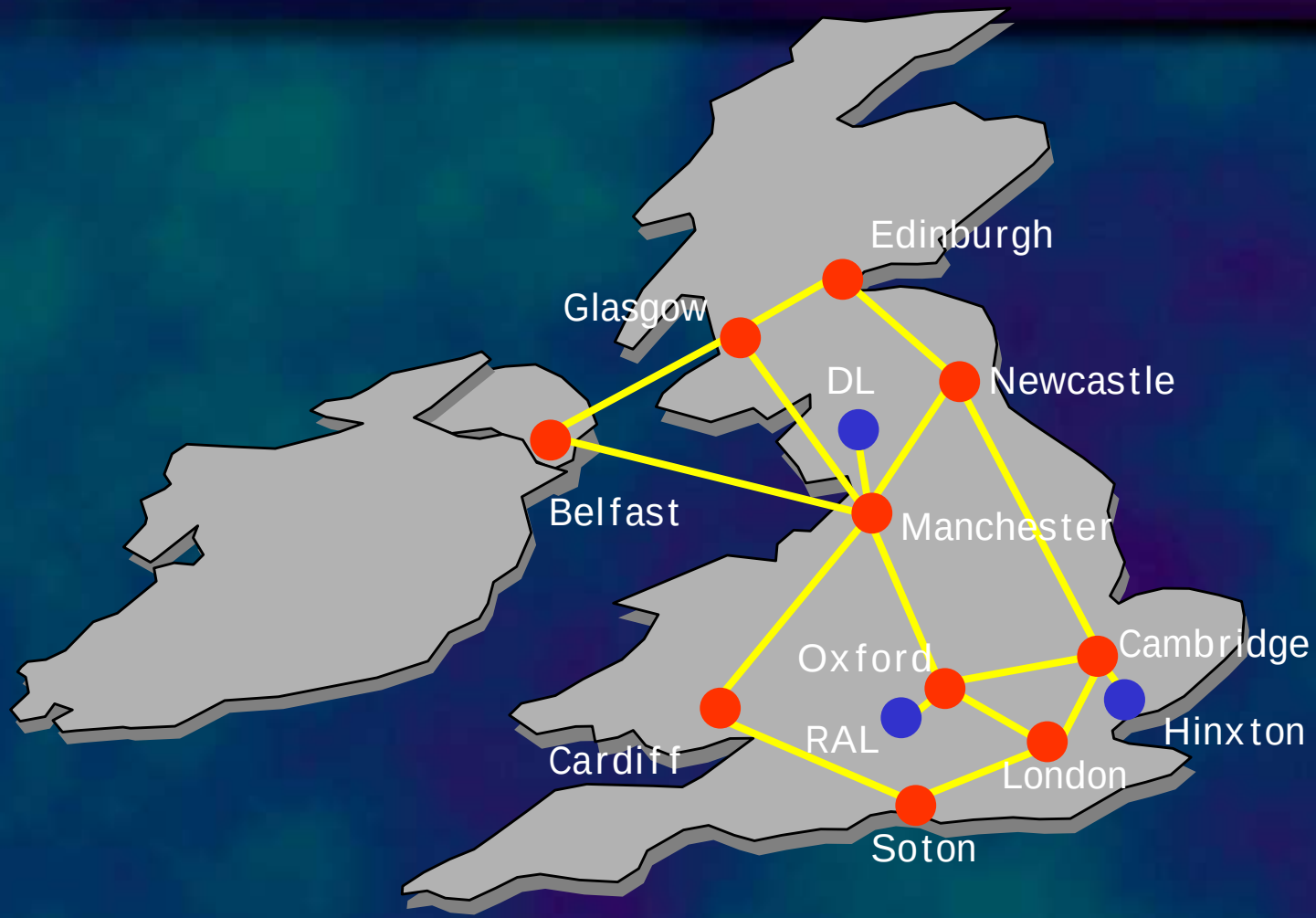
UK e-Science Initiative (2)

- £120M Programme over 3 years
- £75M is for Grid Applications in all areas of science and engineering
- £10M for Supercomputer upgrade
- £35M for development of ‘industrial strength’ Grid middleware
  - Require £20M additional ‘matching’ funds from industry

SuperJanet4, June 2002



UK e-Science Grid



Centres will be Access Grid Nodes

- Access Grid will enable informal and formal group to group collaboration
- It enables:
  - Distributed lectures and seminars
  - Virtual meetings
  - Complex distributed grid demos
- Improves user experience (“sense of presence”) - natural interactions (natural audio, big display)

Manchester Access Grid Node

Generic Grid Middleware

- All e-Science Centres will donate resources to form a UK ‘national’ Grid
- All Centres will run same Grid Software
  - Starting point will be based on Globus, Storage Resource Broker and Condor
- Work with Global Grid Forum and major computing companies to move Grid software on towards realizing VO vision

Globus Grid Middleware

- Single Sign-On
  - Proxy credentials, GRAM
- Mapping to local security mechanisms
  - Kerberos, Unix, GSI
- Delegation
  - Restricted proxies
- Community authorization and policy
  - Group membership, trust
- File-based
  - GridFTP gives high performance FTP integrated with GSI

Storage Resource Broker (1)

- Open Source software developed by Reagan Moore and the DICE group at the San Diego Supercomputer Center
- SRB approach separates organization of distributed digital objects into a collection from their physical storage location

  - Metadata catalog to manage attributes about digital objects

  - Data handling system to manage interaction with remote storage systems

Storage Resource Broker (2)

- SRB allows access through federated servers
  - file systems, databases, archival systems
- Collection-based data handling system
- Extensible collection attributes
- Extensible support for access to any type of storage system
- SRB only interim solution – need well-defined Grid middleware interface to Databases

IBM Grid Press Release

Irving Wladawsky-Berger

(Lead for IBM Corporate on Grid)

- ‘Grid computing is a set of research management services that sit on top of the OS to link different systems together’
- ‘We will work with the Globus community to build this layer of software to help share resources’
- ‘All of our systems will be enabled to work with the grid, and all of our middleware will integrate with the software’

EPSRC e-Science Projects (1)

- **Comb-e-Chem**:Structure-Property Mapping
  - Southampton, Bristol
- **DAME**: Distributed Aircraft Maintenance Environment
  - York, Oxford, Sheffield, Leeds
- **Reality Grid**: A Tool for Investigating Condensed Matter and Materials
  - QMW, Manchester, Edinburgh, IC, Loughborough, Oxford

EPSRC e-Science Projects (2)

- **My Grid**: Personalised Extensible Environments for Data Intensive *in silico* Experiments in Biology
  - Manchester, EBI, Southampton, Nottingham, Newcastle, Sheffield
- **GEODISE**: Grid Enabled Optimisation and Design Search for Engineering
  - Southampton, Oxford, Manchester
- **Discovery Net**: High Throughput Sensing Applications
  - Imperial College

Comb-e-Chem: Structure-Property Mapping

- Goal is to integrate structure and property data sources within knowledge environment to find new chemical compounds with desirable properties
- Accumulate, integrate and model extensive range of primary data from combinatorial methods
- Support for provenance and automation including multimedia and metadata
- Southampton, Bristol, Cambridge Crystallographic Data Centre
- Roche Discovery, Pfizer, IBM

MyGrid:An e-Science Workbench

- Goal is to develop ‘workbench’ to support:
  - Experimental process of data accumulation
  - Use of community information
  - Scientific collaboration
- Provide facilities for resource selection, data management and process enactment
- Bioinformatics applications
  - Functional genomics, database annotation
- Manchester, EBI, Newcastle,Nottingham, Sheffield, Southampton
- GSK, AstraZeneca, Merck, IBM, Sun, ...

PPARC e-Science Projects

- **GridPP**
  - links to EU DataGrid, CERN LHC Computing Project, U.S. GriPhyN and PPGrid Projects
- **AstroGrid**
  - links to EU AVO and US NVO projects
- **VISTA**
  - under consideration

Support for e-Science Projects

- ‘Grid Starter Kit’ available from July 2001
- Set up Grid Support Centre

  - International dimensions: EU DataGrid, and US iVDGL projects
- Grid Network Team will identify bottlenecks and elucidate Testbed requirements
- Training Courses and Research Seminars

  - Coordinated by National e-Science Centre

The Grid and Virtual Organisations

[Foster and Kesselman – 'Take 2']

The Grid is a software infrastructure that enables flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions and resources

- includes computational systems and data storage resources and specialized facilities
- enabler for transient 'virtual organisations'

➢ Must also address access to digital archives