Institutional Standards: The Critical Missing Piece

http://www.esp.org/rjr/nist2003.pdf

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Abstract

In 1990, an NSF Invitational Workshop on Scientific Database Management brought together database experts and domain scientists to consider and document the challenges of scientific database management. Nearly fifteen years later, many of those challenges are still unmet. The problem is especially acute in biomedical research, where genome-project-driven technologies have unleashed a flood of data into a community (or rather a set of communities) with major sociological and structural impediments to effective large-scale data management.

Unlike "big-instrument, single-data-source" science (e.g., high-energy physics), most public-sector biomedical research occurs as "small-instrument, multi-data-source" science in small, investigator-initiated projects at universities or independent research organizations. Multi-source data from these smaller projects then, ideally, flow together into larger national or international resources (e.g., GenBank). The GenBank model, however, is only applicable to normal or paradigmatic science in the Kuhnian sense. In pre-paradigm fields or to fields undergoing paradigm-shifts, efforts to apply the GenBank model (by proposing national data standards and repositories) will fail. Even in some normal science fields (e.g., functional tomography of the brain), efforts to apply the GenBank model will experience difficulties because of the limitations of the current scientific publishing model (e.g., total transfer of copyright to the journal publisher).

In "small-instrument, multi-data-source" science budgets are small and the allocation for local data management is usually inadequate. Resources for extending the local project to include support for participation in a national data repository are usually non-existent.

As noted in the NSF Workshop, the relational data model is an inadequate abstraction for representing many kinds of biological data (e.g., pedigrees, taxonomies, maps, metabolic networks, food chains). Efforts to deploy object-oriented DBMS have not met with widespread success. Compromise efforts to force complex biological data structures into relational models have resulted in locally effective kludges that do not admit ready integration into larger data collections. The effective use of taxonomies in bio databases quickly results in the need for tri-state logic, something not easily implemented with commercial RDBMS.

National efforts to close many of these gaps in effective bio data management will founder on problems of scale. How will the development of a national data standard help a small-RO1 PI who can barely afford any information infrastructure, much less generic systems that interoperate well with large communities? How can an individual researcher hope to address problems resulting from the current science publishing model? What systems are readily available to help a researcher comply with government requirements to share data while also complying with other government requirements to protect human-subjects privacy? The answer to these, and other challenges, will lie in the development of institutional standards for IT support of grant-funded research. These institutional standards are indeed the critical missing piece.

Goal:

To identify opportunities for information science (IS) standards and standards development to facilitate bioscience and biomedical research.

Purposes:

To define the current and emerging state of information science (IS) standards related to bioscience and biomedical research, and

To identify barriers and gaps to, and opportunities and pathways for, IS standards development and implementation to enhance bioscience and biomedical research.

Scope:

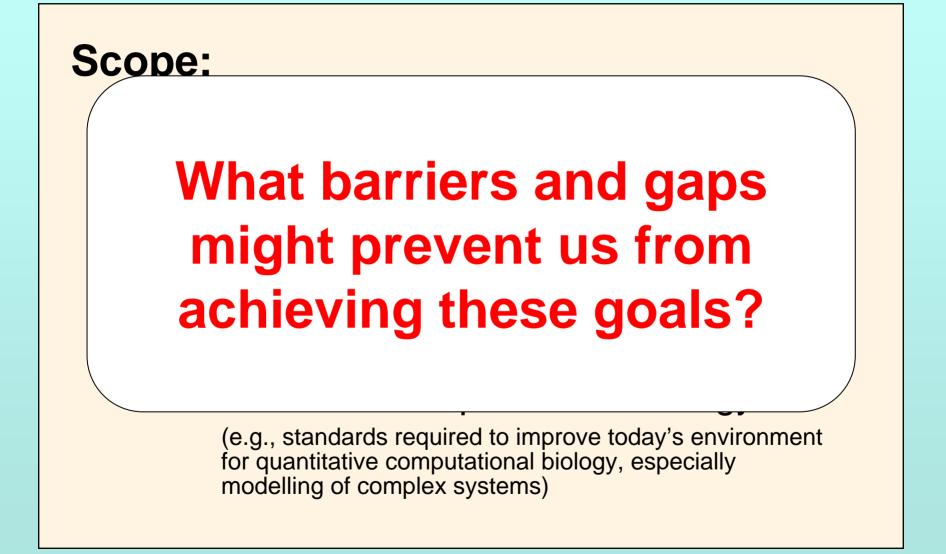
 Biomedical Data Integration Standards (e.g., ontology, data format, nomenclature)

Networked Science

(e.g., IS standards to harness teragrid-scale computing)

Quantitative Computational Biology

(e.g., standards required to improve today's environment for quantitative computational biology, especially modelling of complex systems)



Caution from the Present

Resource Inadequacy:

 Current government spending on biomedical information infrastructure is far too low to achieve the solutions many have envisioned.

Scientific Database Management

Final Report

edited by

James C. French, Anita K. Jones, and John L. Pfalz

Report of the Invitational NSF Workshop on Scientific Database Management 12–13 March 1990 Charlottesville, Virginia Anita K. Jones, Chairperson Technical Report 90-21 August 1990



CS-90-21

J.C. French, A.K. Jones and J.L. Pfaltz, Scientific Database Management (Final Report), August 1990.

ftp://ftp.cs.virginia.edu/pub/techreports/CS-90-21.ps.Z

CS-90-22

J.C. French, A.K. Jones and J.L. Pfaltz, Scientific Database Management (Panel Reports and Supporting Material), August 1990

ftp://ftp.cs.virginia.edu/pub/techreports/CS-90-22.ps.Z

Two major conclusions:

The single unifying cry of the workshop is that existing data models are inadequate for science data needs. (p. 6)

Two major conclusions:

- The single unifying cry of the workshop is that existing data models are inadequate for science data needs. (p. 6)
- The data source dimension (e.g., single or multi-source), which is not generally mentioned in the database literature, may present the most fundamental challenge. (p. 3)



Problems:

- Resource-adequacy problems
- Database Problems
- Data-source Problems

Solutions:

- More Resources
- Better Database Products
- Institutional Support for Biomedical IT

Resource Problems



Resource-adequacy problems

Current levels of government spending are woefully inadequate to meet the needs of public-sector biomedical research.

Rhetorical Question

Which is likely to be more complex:

 identifying, documenting, and tracking the whereabouts of all parcels in transit in the UPS system at one time

Rhetorical Question

Which is likely to be more complex:

- identifying, documenting, and tracking the whereabouts of all parcels in transit in the UPS system at one time
- identifying, documenting, and analyzing the structure and function of all individual genes in all economically significant organisms; then analyzing all significant gene-gene and gene-environment interactions in those organisms and their environments

Business Factoids

Five years ago, United Parcel Service:

- used redundant multi-terabyte databases to track all packages in transit
- had 4,000 full-time employees dedicated to IT
- spent one billion dollars per year on IT
- had an income of 1.1 billion dollars, against revenues of 22.4 billion dollars

Business Comparisons

Company	Revenues	IT Budget	Pct
Chase-Manhattan	16,431,000,000	1,800,000,000	10.95 %
AMR Corporation	17,753,000,000	1,368,000,000	7.71 %
Nation's Bank	17,509,000,000	1,130,000,000	6.45 %
Sprint	14,235,000,000	873,000,000	6.13 %
IBM	75,947,000,000	4,400,000,000	5.79 %
MCI	18,500,000,000	1,000,000,000	5.41 %
Microsoft	11,360,000,000	510,000,000	4.49 %
United Parcel	22,400,000,000	1,000,000,000	4.46 %
Bristol-Myers Squibb	15,065,000,000	440,000,000	2.92 %
Pfizer	11,306,000,000	300,000,000	2.65 %
Pacific Gas & Electric	10,000,000,000	250,000,000	2.50 %
Wal-Mart	104,859,000,000	550,000,000	0.52 %
K-Mart	31,437,000,000	130,000,000	0.41 %

Appropriate funding level:

- approx. 5-15% of research funding
- *i.e.*, 1 3 billion dollars per year

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- *i.e.*, 1 3 billion dollars per year

Source of estimate:

- Experience of IT-transformed industries.
- Current support for IT-rich biological research.

Warning:

Until more resources become available, finding true SOLUTIONS to biomedical-IT problems will be impossible.

- Experience of IT-transformed industries.
- Current support for IT-rich biological research.

Resource Solutions

Solutions might occur at many levels:

- Industry partnerships?
- Agency initiatives, like BISTI or caBIG?
- Agency infrastructure support, like CCSGs?
- Leverage investments by working at the INSTITUTIONAL level (e.g., caBIG)

Database Problems



Database problems

Scientific data are not standard business data. Better formal data models are required. Schema flexibility is essential. More complex logic is needed.

Database I Basics

Business Databases:

- FACTS
- REAL OBJECTS
- CLOSED UNIVERSE
- DEDUCTIVE REASONING
- CENTRALLY OPERATED

Business Databases:

- FACTS
- REAL OBJECTS
- CLOSED UNIVERSE
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Scientific Databases:

- OBSERVATIONS
- HYPOTHETICAL OBJECTS
- OPEN UNIVERSE
- INDUCTIVE REASONING
- TOTALLY DECENTRALIZED

Facts:

- SOLID
- STABLE
- GLOBALLY CONSISTENT
- STAND ALONE

Observations:

- SOFT
- CONSTANTLY CHANGING
- MUTUALLY INCONSISTENT
- REQUIRE REFERENCES

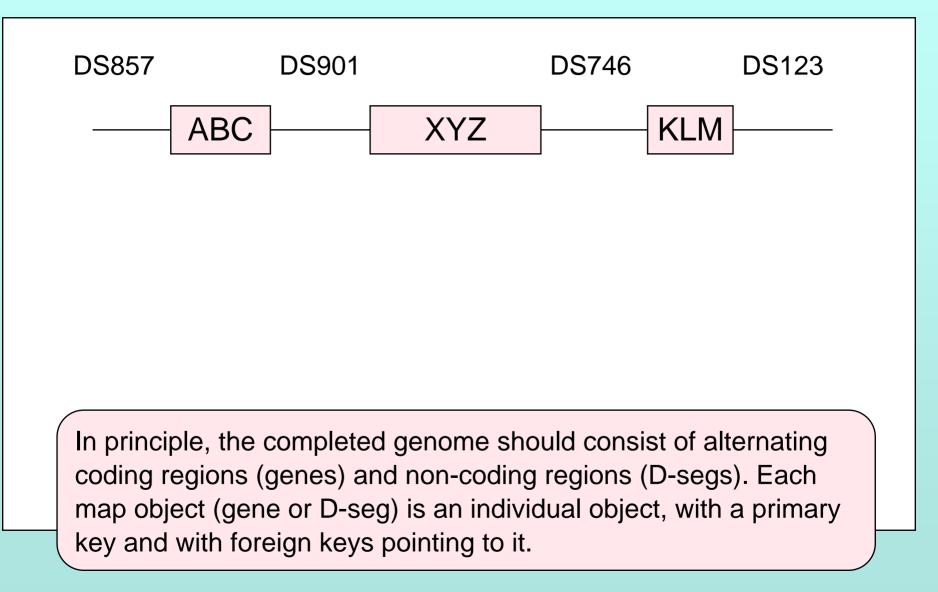
Real Objects:

- CONCRETE
- STABLE (or known instability)
- IMMUTABLE (more or less)

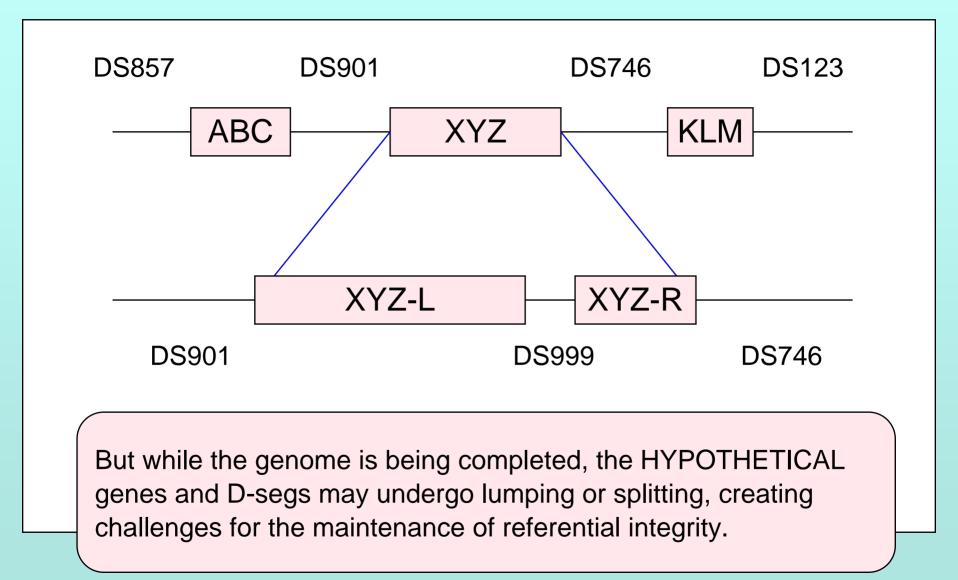
Hypothetical Objects:

- INSUBSTANTIAL
- UNSTABLE
- HIGHLY MUTABLE (lumping and splitting)

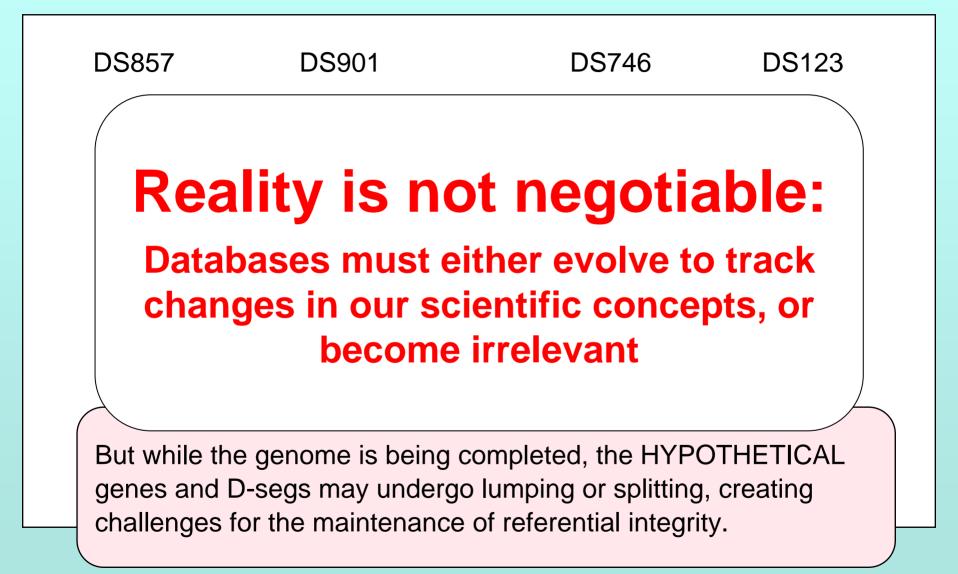
GDB Example:



GDB Example:



GDB Example:



Closed Universe:	Open Universe:
Who, of the registrants for this meeting, came to the meeting?	

Relational Databases

Closed Universe:

Who, of the registrants for this meeting, came to the meeting?

Who, of the registrants for this meeting, did not come to the meeting?

Open Universe:

Relational Databases

Closed Universe:

Who, of the registrants for this meeting, came to the meeting?

Who, of the registrants for this meeting, did not come to the meeting?

Open Universe:

Who else did not come to the meeting?

Relational Databases

Deductive Reasoning:

- DETERMINISTIC
- WELL ESTABLISHED ALGORITHMS (formal logic)

Inductive Reasoning:

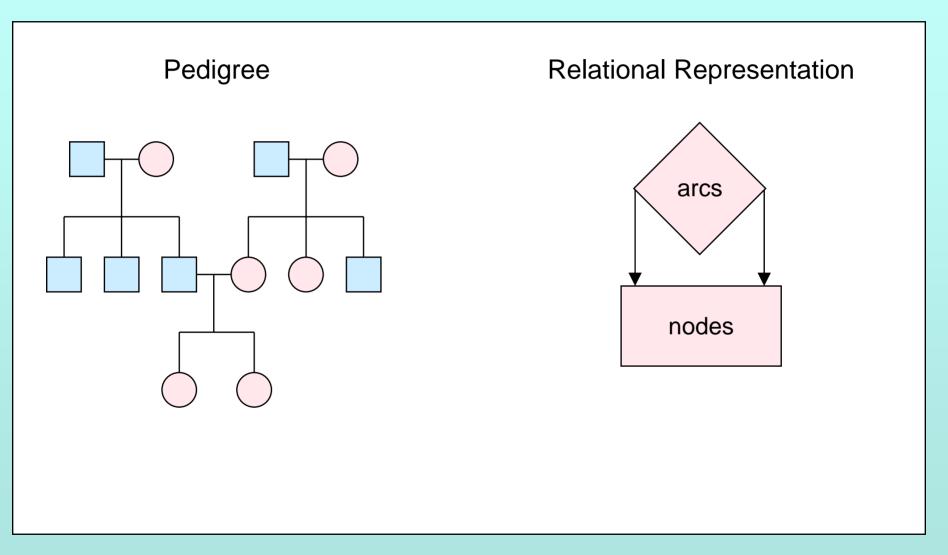
- PROBABALISTIC
- METHODS STILL DEBATED (almost at the metaphysical level)

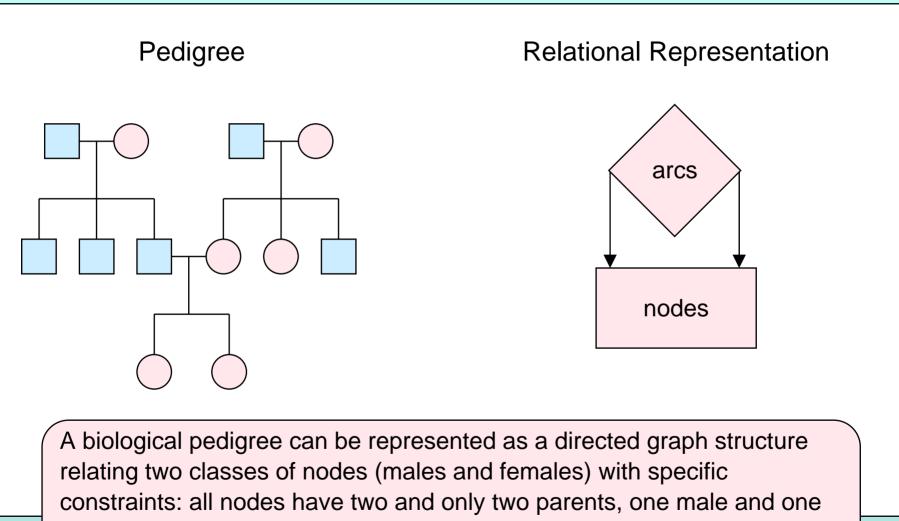
Database II Data Models

Data-model Challenges

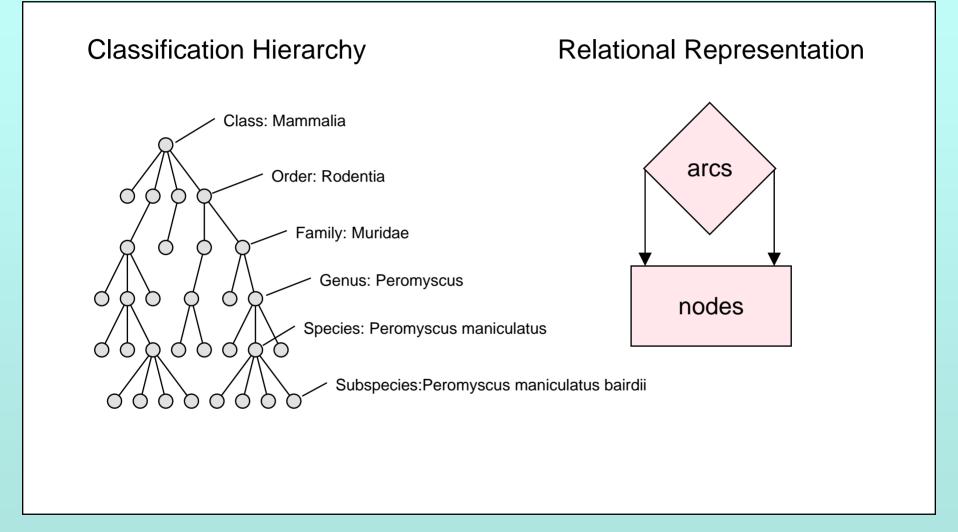
Many bio-data problems involve:

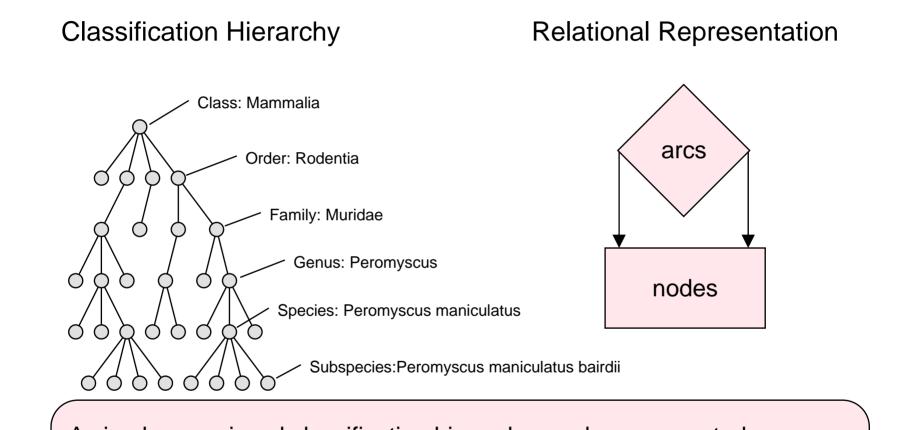
- Graphs: pedigrees, taxonomies, partial orderings, etc...
- Repeat time series observations, with inconsistent results
- Provisional conclusions
- Universal linking tables





female. In a relational database, this graph can be represented as a pair of tables.





A simple organismal classification hierarchy can be represented as a single-rooted, connected, directed graph structure with the specific constraint: all nodes have one and only one parent. In a relational database, this graph can be represented as a pair of tables.

Classification Hierarchy

Relational Representation

Graph problem:

Any graph can be represented in a relational database as a pair of tables. Enforcing the constraints for a particular graph, however, requires complex procedural code.

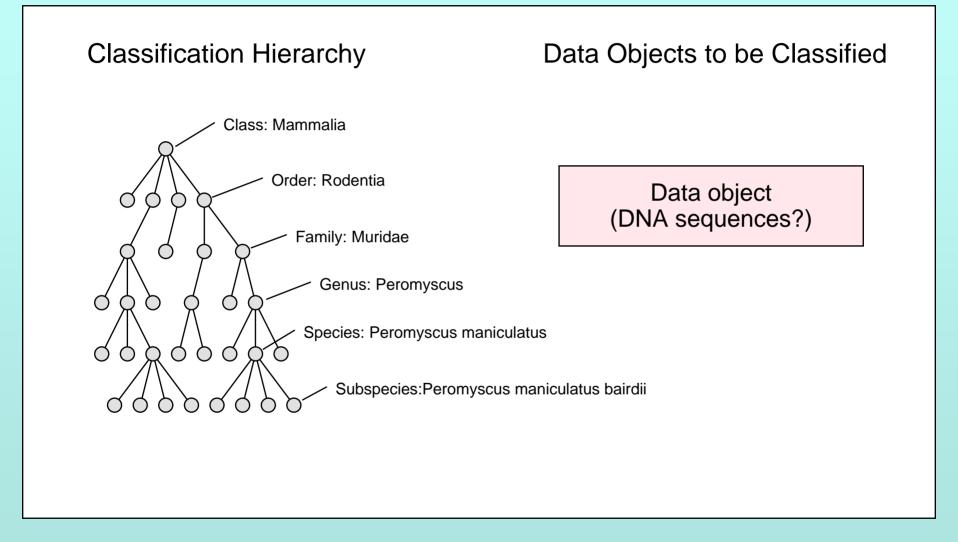
single-rooted, connected directional graph structure with the specific constraint: all nodes have one and only one parent. In a relational database, this graph can be represented as a pair of tables.

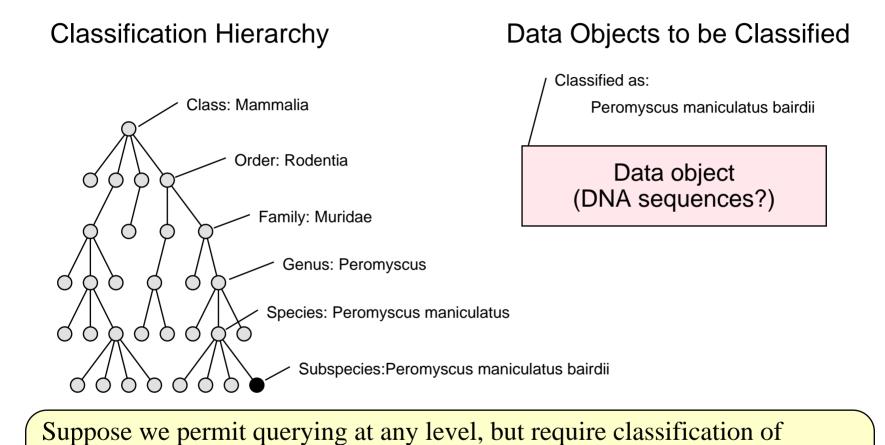
Classification Hierarchy

Relational Representation

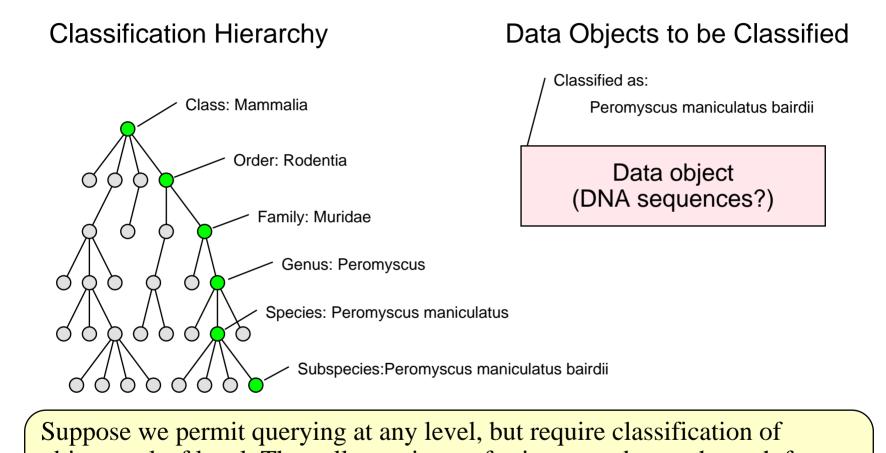
Graph solutions needed: It would be nice if database products included a CREATE GRAPH operator, including the ability to declare constraints to be maintained (e.g., directed, acyclic, connected, tree, etc)

single-rooted, connected directional graph structure with the specific constraint: all nodes have one and only one parent. In a relational database, this graph can be represented as a pair of tables.

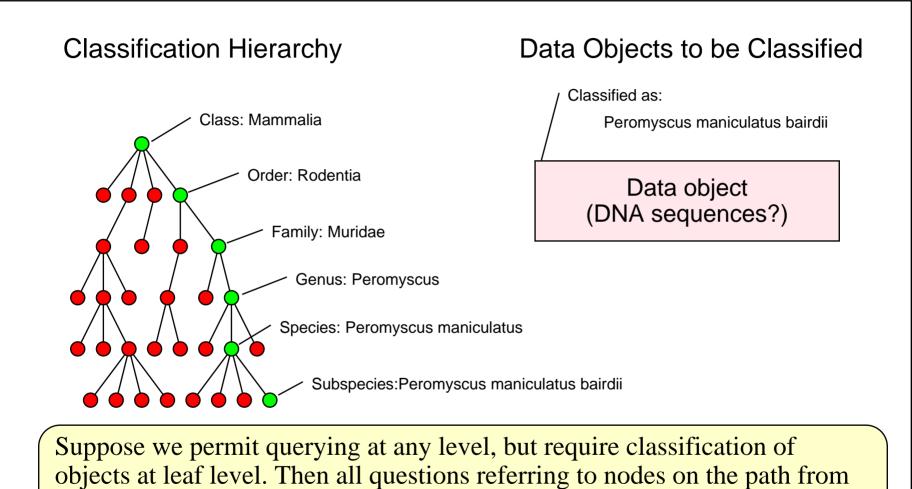




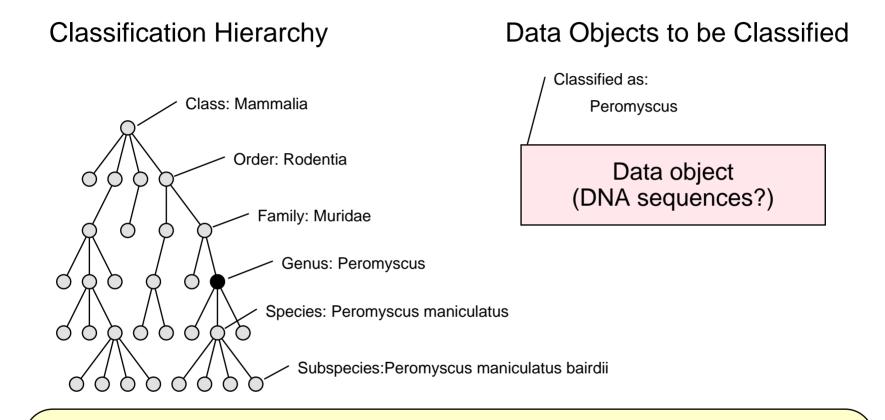
objects at leaf level.



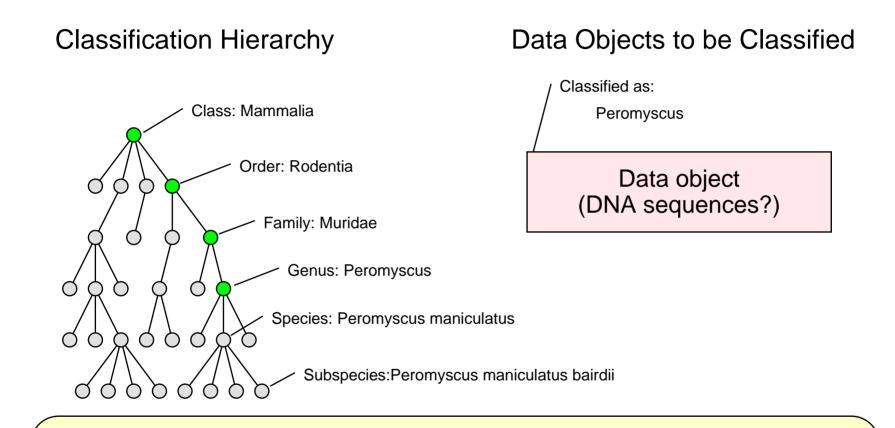
objects at leaf level. Then all questions referring to nodes on the path from the classification point to the top return **TRUE**,



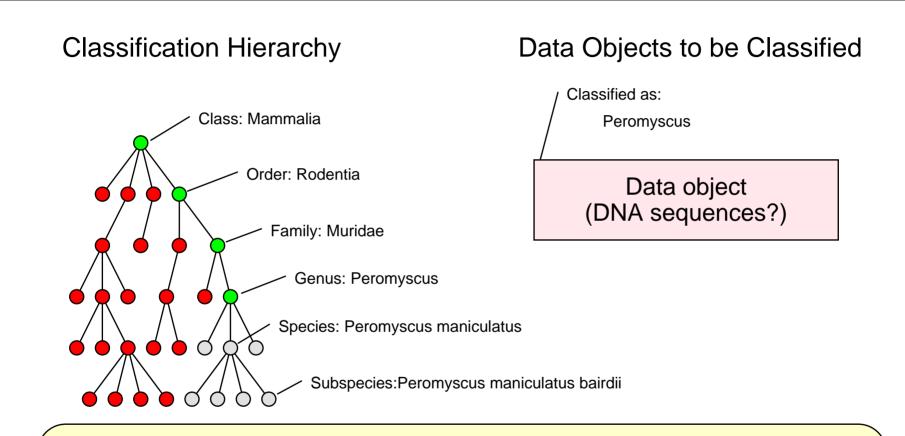
the classification point to the top return **TRUE**, all others **FALSE**.



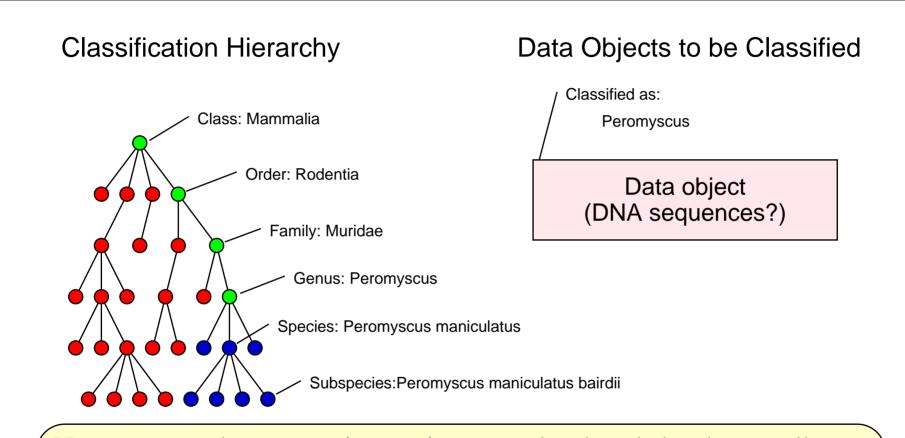
Now, suppose the we permit querying at any level, and also that we allow classification of objects at any level.



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Classification Hierarchy

Data Objects to be Classified

Tri-state logic required: If hierarchical classification schemes are used, then tri-state logic may be required.

Now, suppose the we permit querying at any level, and also that we allow classification of objects at any level. Then all questions referring to nodes on the path from the classification point to the top return **TRUE**, all questions referring to nodes lateral to this path return **FALSE**, and all questions referring to nodes below the classification point return **MAYBE**.

Database III Data Integration

Data Integration Crisis

Adequate connections among data objects in different databases do not exist.

Without adequate connectivity, much of the value of the data will be lost.

Data Integration Goals

Achieve conceptual integration of biomedical data.

Provide technical integration of both data and analytical resources to facilitate conceptual integration.

Data Integration Impediments

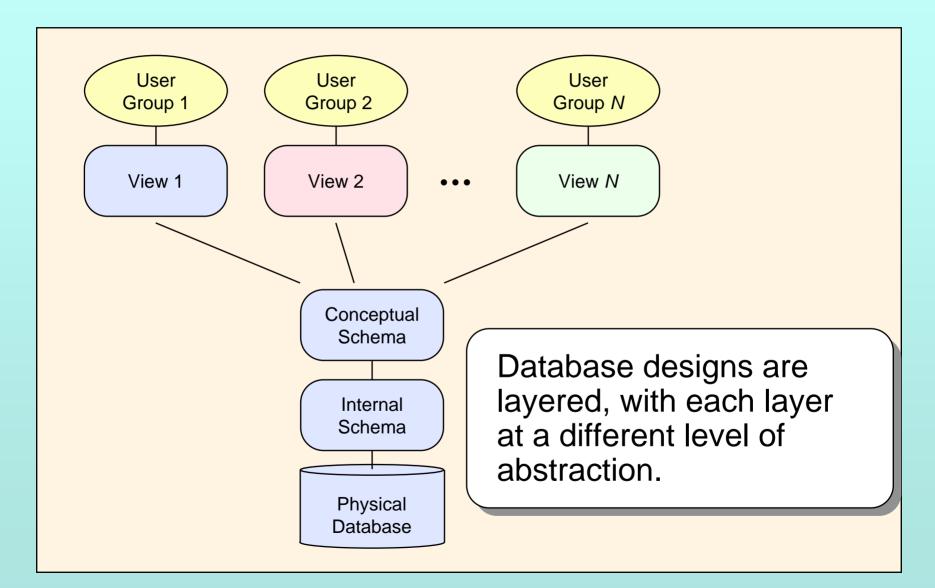
Technical: Integrating distributed, heterogeneous databases is not easy.

Sociological: Local incentives encourage competition, not cooperation.

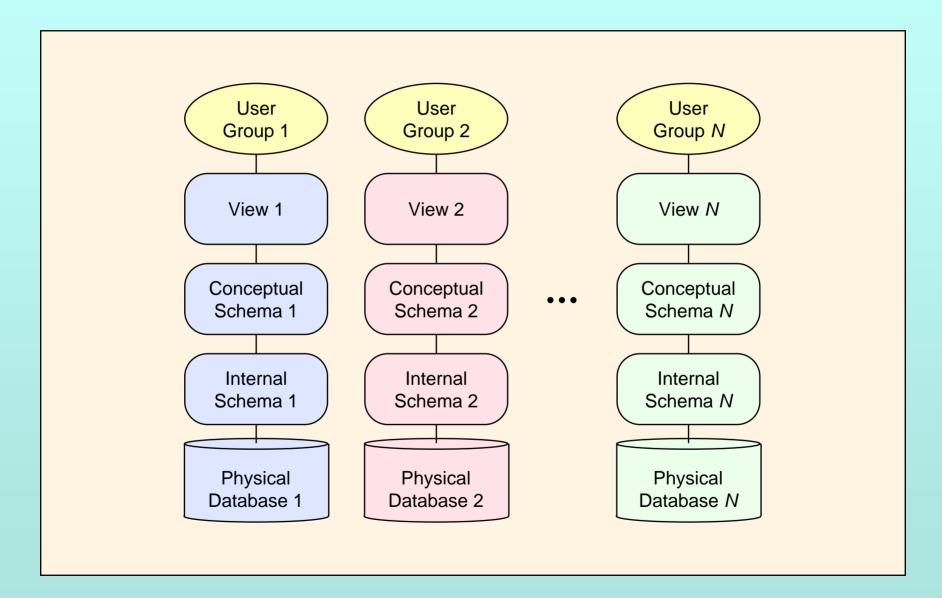
Conceptual: Semantic mismatches exist among databases.

Technical Impediments

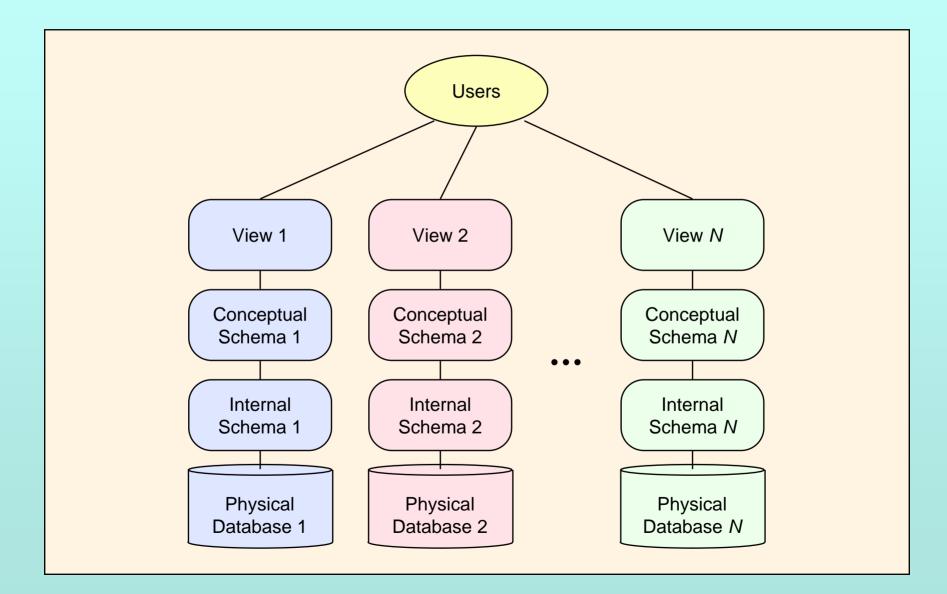
Multiple Views



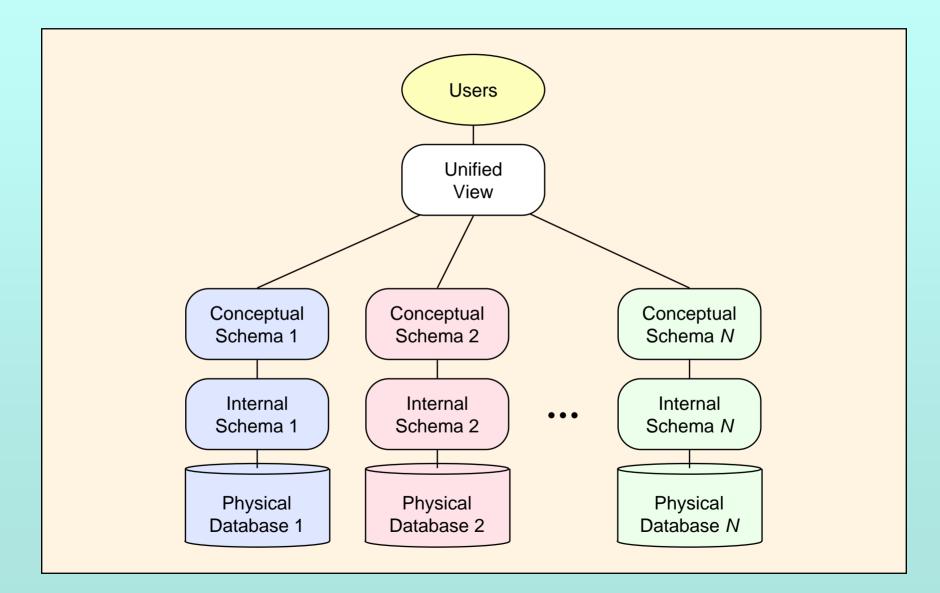
Multiple Databases



Current Situation

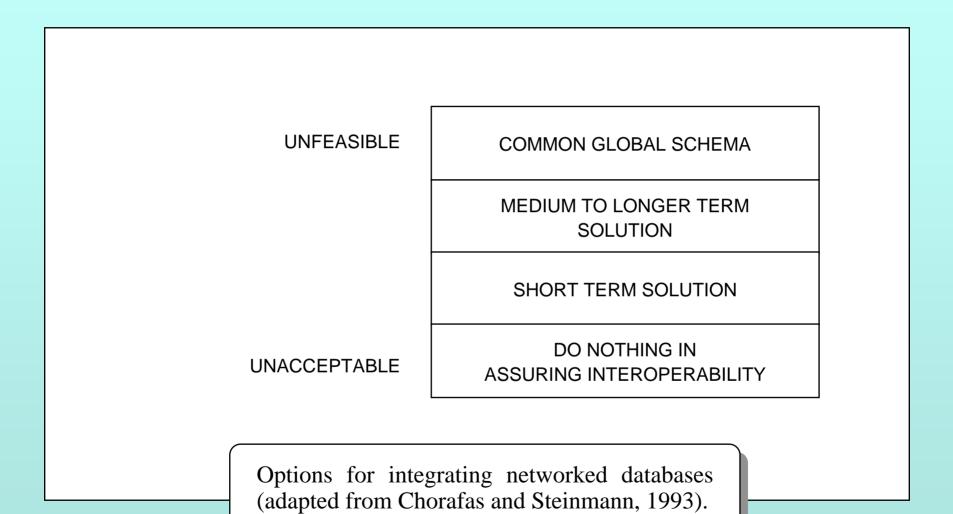


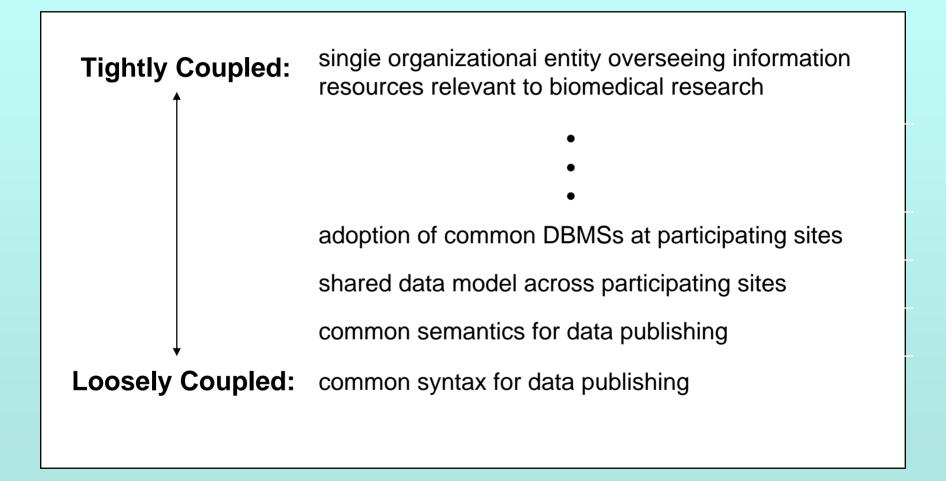
Desired Situation



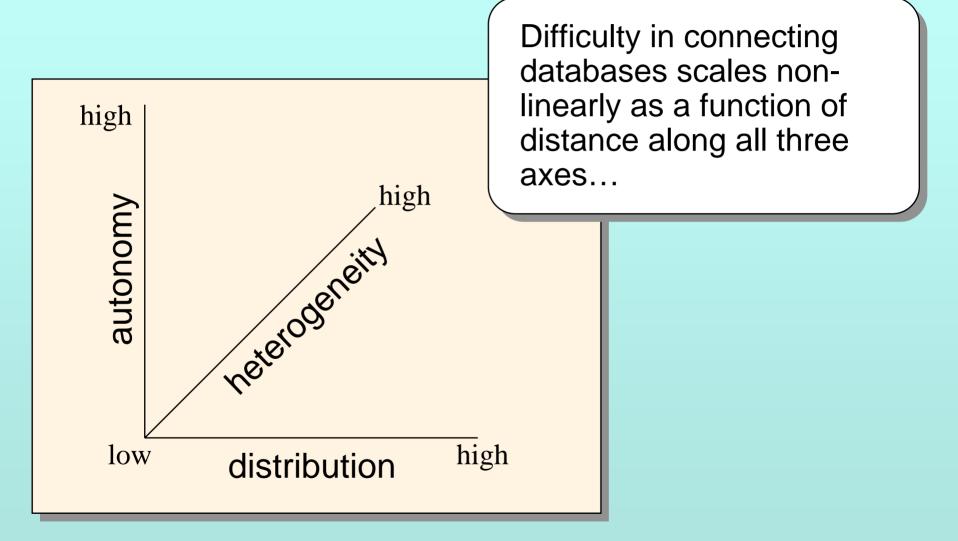
We must begin to think of the computational infrastructure of genome research as a federated information infrastructure of interlocking pieces.

Report of the Invitational DOE Workshop on Genome Informatics, 26-27 April 1993, Baltimore, Maryland

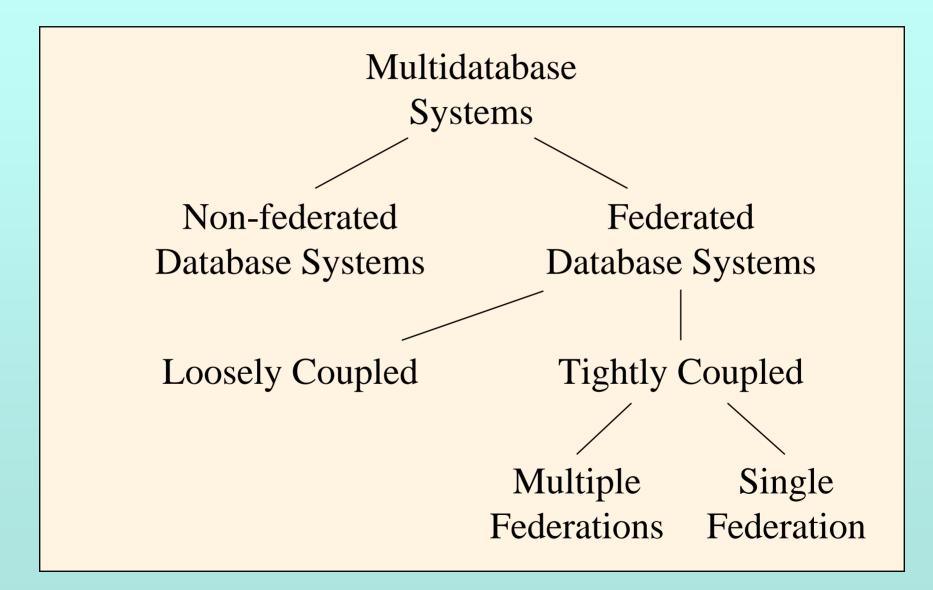


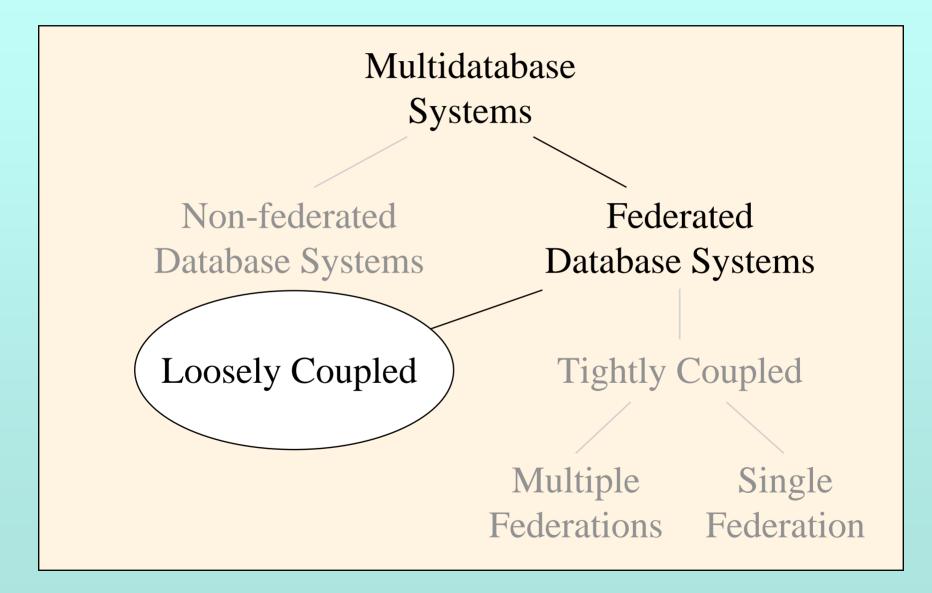


Difficulty Dimensions

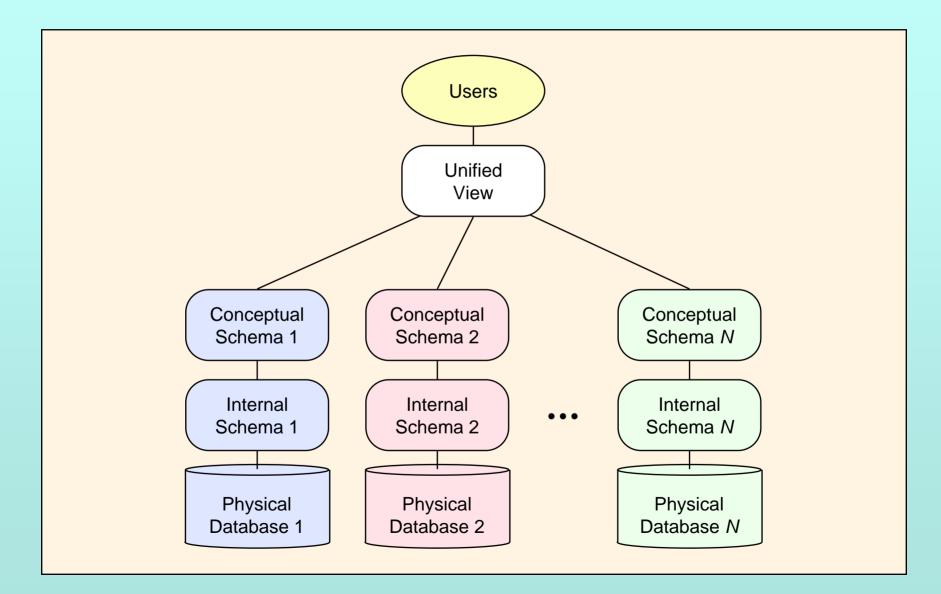


- A *multidatabase system* (MDBS) supports simultaneous operations on multiple (perhaps different) component databases.
- A federated database system (FDBS) has autonomous components, whereas non-federated database systems are unitary.
- A federated system with no strong central federation management is considered *loosely coupled*.
- One with strong central management and with federation database administrators controlling access to the components is *tightly coupled*.
- A *single federation* allows only one centrally managed federated schema; a *multiple federation* allows multiple centrally managed schemas.

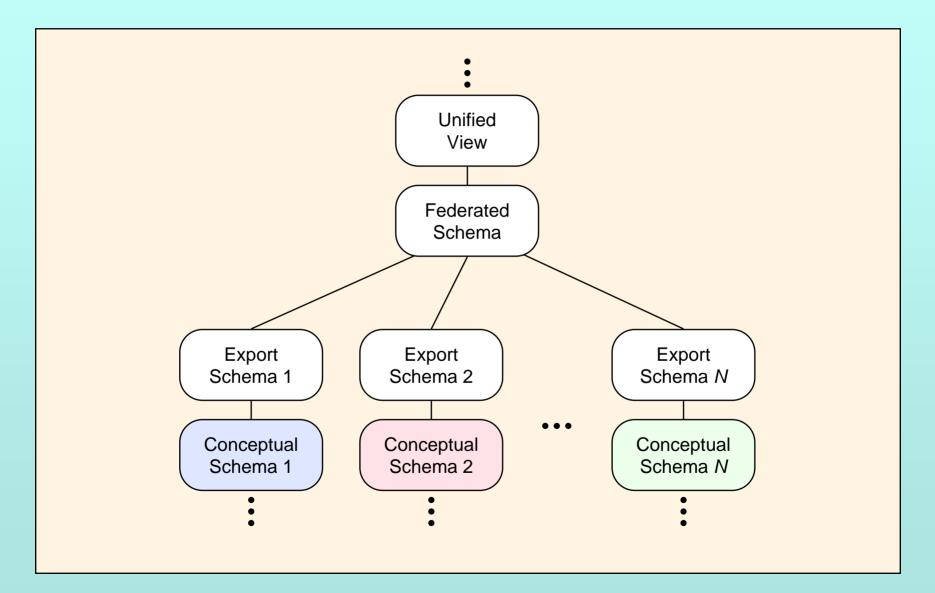




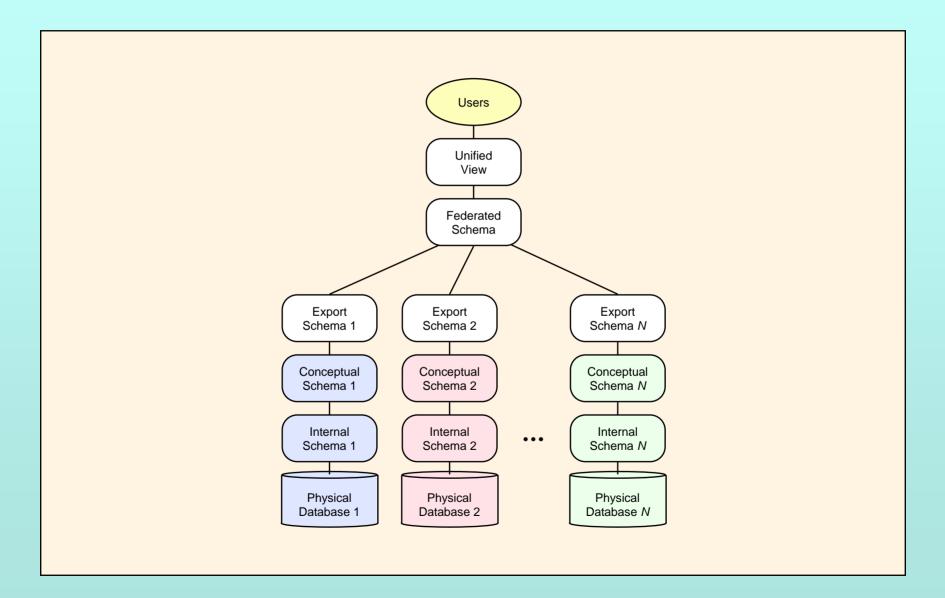
Desired Situation



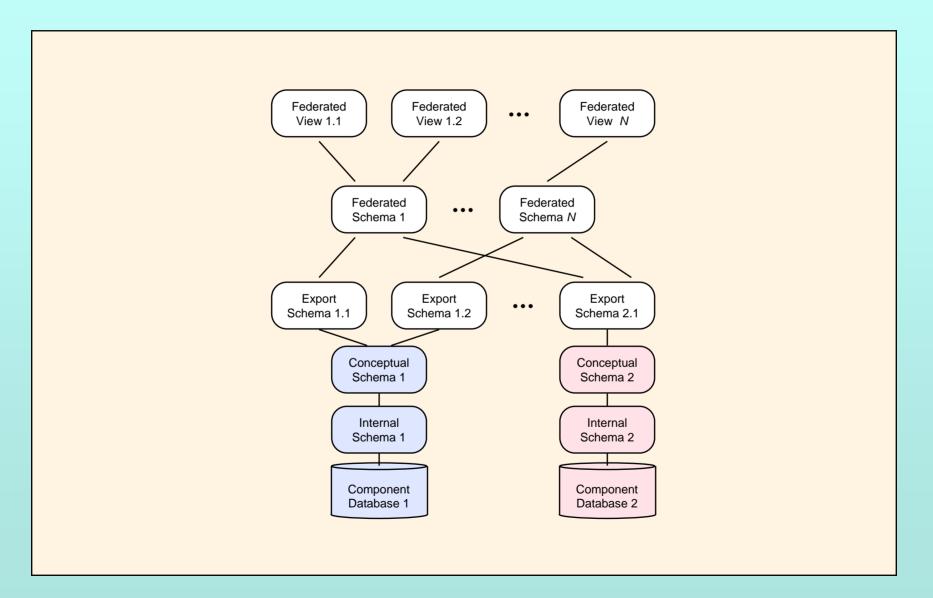
More Layers



Federated Schema



Multiple Federations



Schema Change

Schema-change Issues

Problems occur at many levels:

- Bio-database schemas evolve at a high rate (cf. failure of IGD as cited by Stein).
- We need systematic support for inter-database referential integrity.
- We need support for intra-database referential integrity following lumping or splitting actions.
- More issues...

Schema-change Issues

Problems occur at many levels:

Schema Evolution:

Schemas of scientific databases evolve at a high rate. Without tools to support referential integrity in the face of these changes, long-term data integration is impossible.

More issues...

Database Solutions

Database Solutions

Solutions might occur at many levels:

- Development of more sophisticated products by vendors.
- Adoption of consistent (if inadequate) methods in the meanwhile.
- Facilitate equivalent solutions across grants by providing equivalent infrastructure support at the institutional level.

Data Source Problems

Topics

Data-source problems

Biology is a small-instrument, multi-source science.

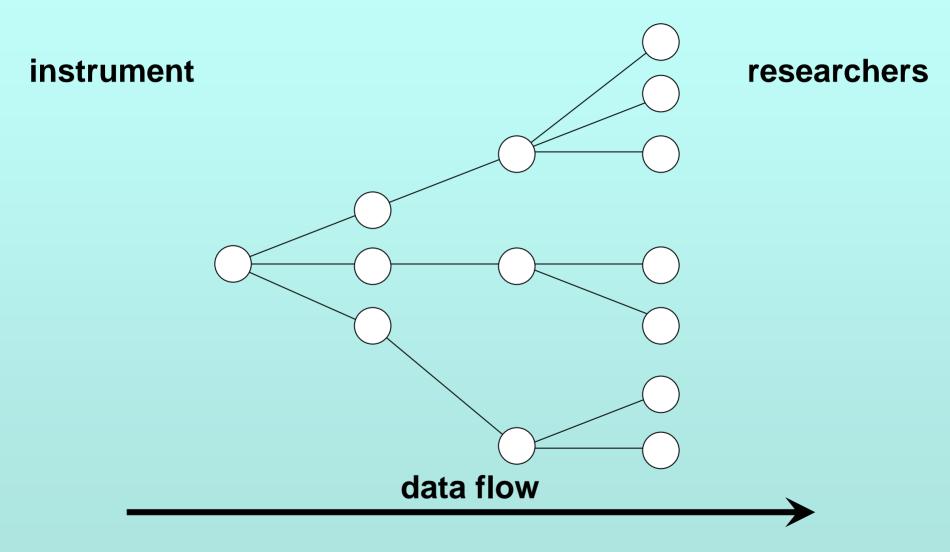
Integrating multi-source data is hard.

Consistency flows in the wrong direction.

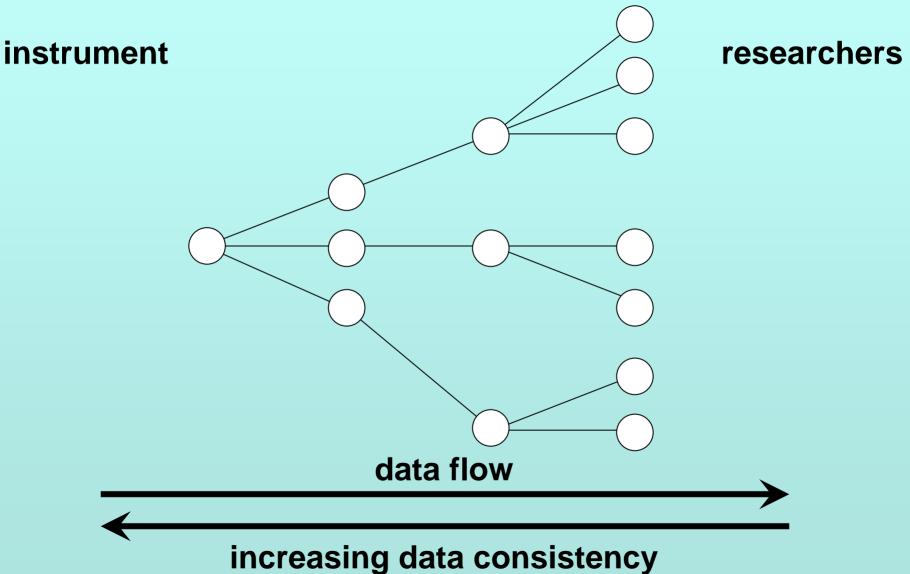
GenBank is a false model.

Source I Basics

Single-instrument Science



Single-instrument Science



Single-instrument Science

instrument

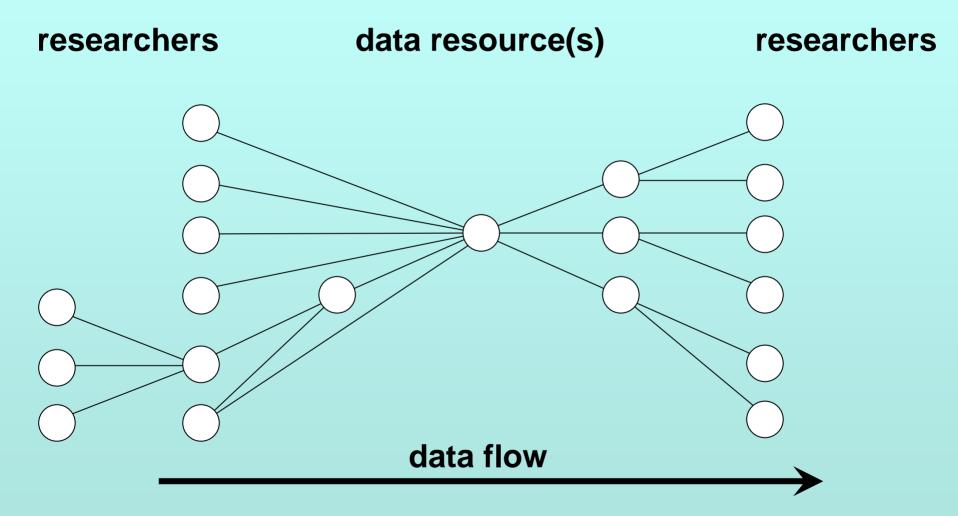
RIGHT WAY:

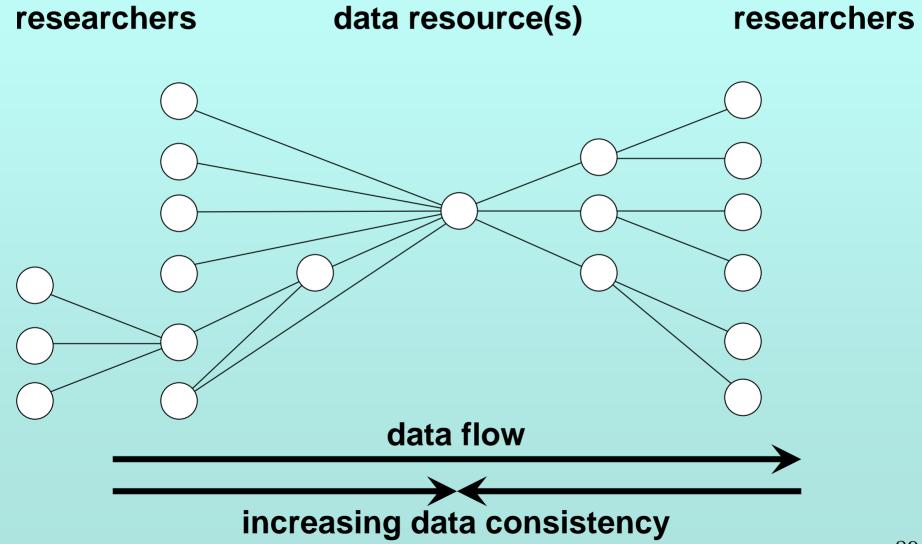
With single-source science, data is MOST consistent nearest the source, making integration unnecessary (but making the need for path documentation high).

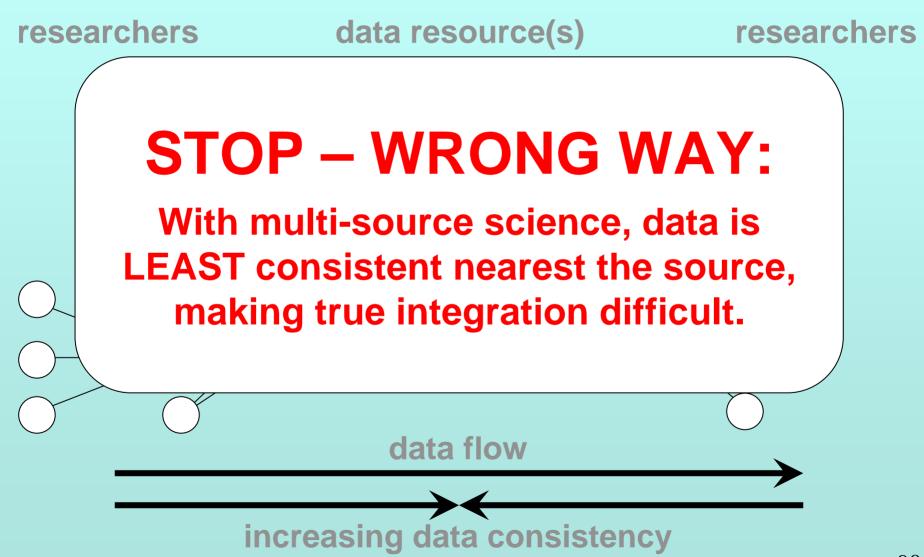
data flow

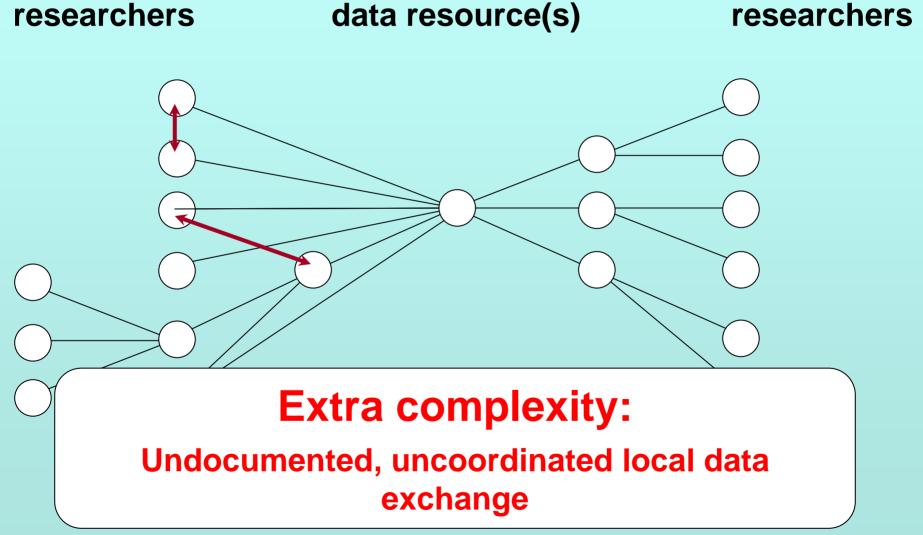
increasing data consistency

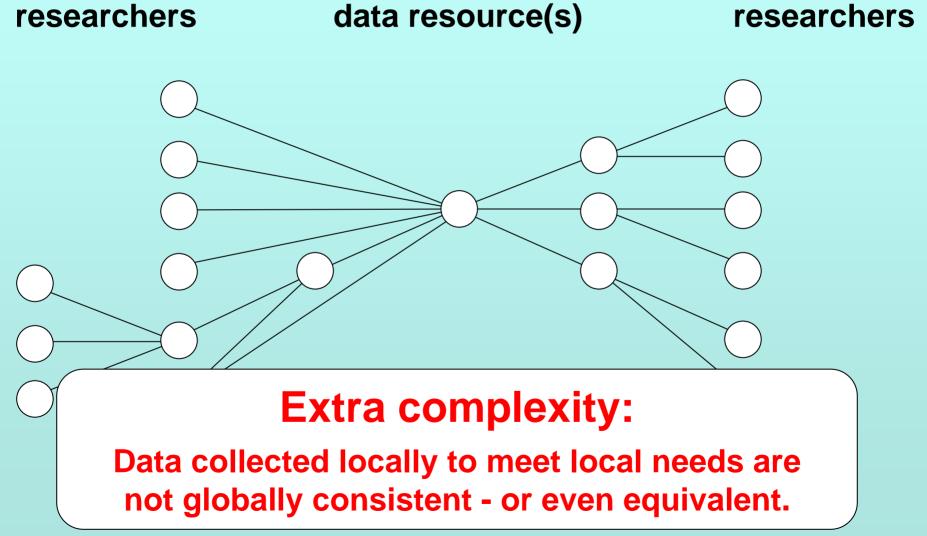
researchers

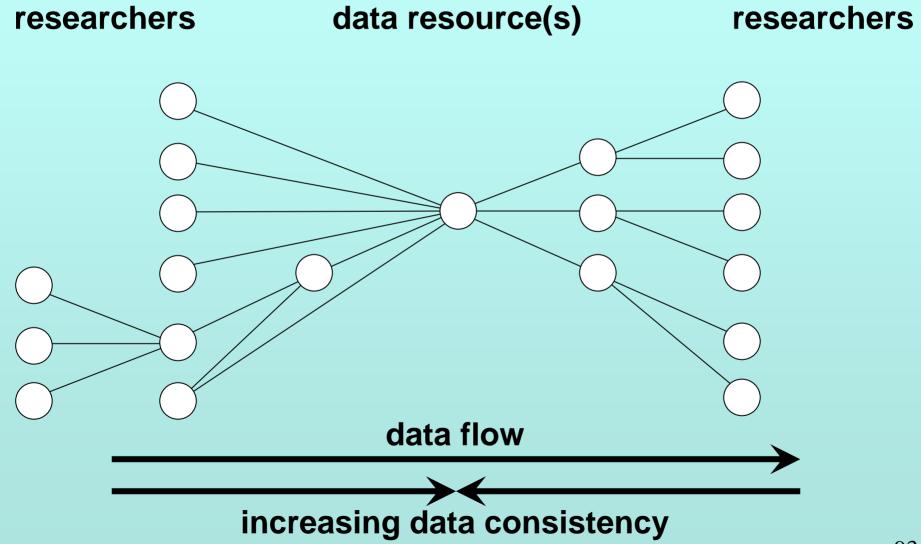












Source II Scope

Data-source Scope Issues

Problems occur at many levels:

- Integrating sequence data into GenBank
- Connecting GenBank with other genomic resources
- Connecting genomic data with other biological data
- Connecting all biological data with medical data
- Connecting all biomedical data with...

Source III Solution: GenBank

GenBank as a False Model

- Classic Kuhnian paradigm science
- Simple, unambiguous data type (string)
- Symbiotic relationship with publishers
- Sequences are nouns, not verbs

Source IV Real Solutions

Data-source Solutions

Institutional Solutions:

- Getting from RO1 science to international standards is too big a step
- We need solutions at the research institution level.
- Biomedical research organizations need to provide coherent support for biomedical IT, just as they do for biomedical bench research.
- Integrating institutional solutions is feasible; integrating individual lab solutions is not.

Institutional Support

Strategic Planning for IT Support of Grant-funded Research

(http://www.esp.org/rjr/briite-01.pdf)

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> rrobbins@fhcrc.org (206) 667 2920

Strategic Planning for IT Support of Grant-funded Research

Eh?

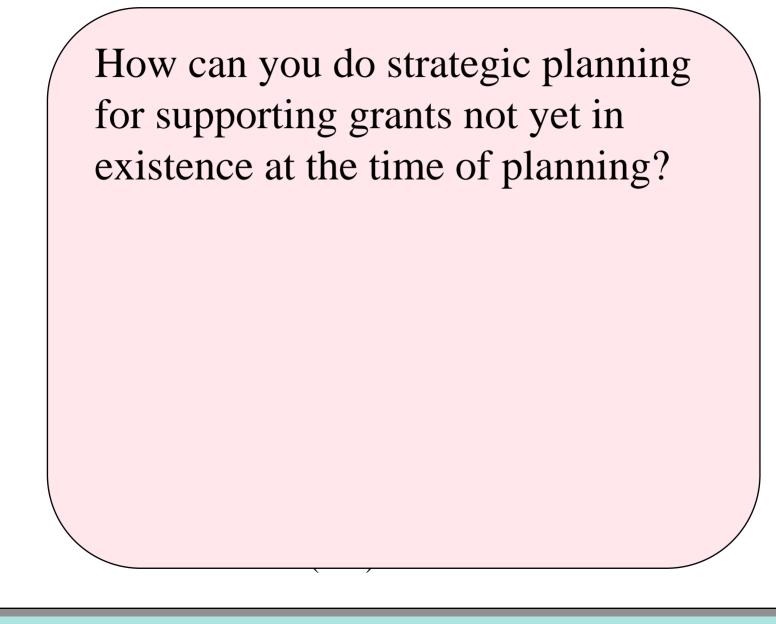
Strategic Planning: >= 5 years Grant-funded: <= 5 years

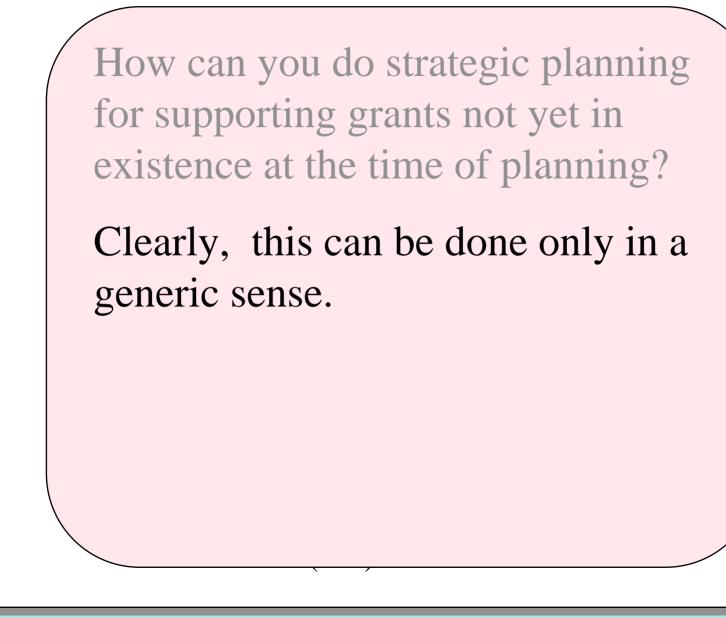
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NIST Workshop: Information Science Standards to Enable Biomedical Research

4-5 November 2003





How can you do strategic planning for supporting grants not yet in existence at the time of planning?

Clearly, this can be done only in a generic sense.

But what is the essence of generic support for IT support of grant-funded research?

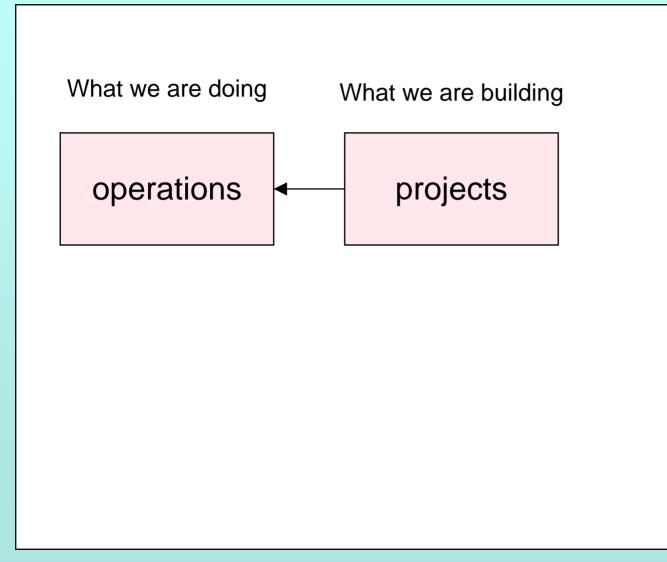
How can you do strategic planning
Is it perhaps,
CENTRALIZED SUPPORT FOR
DISTRIBUTED COMPUTING
support for 11 support of grant-
funded research?

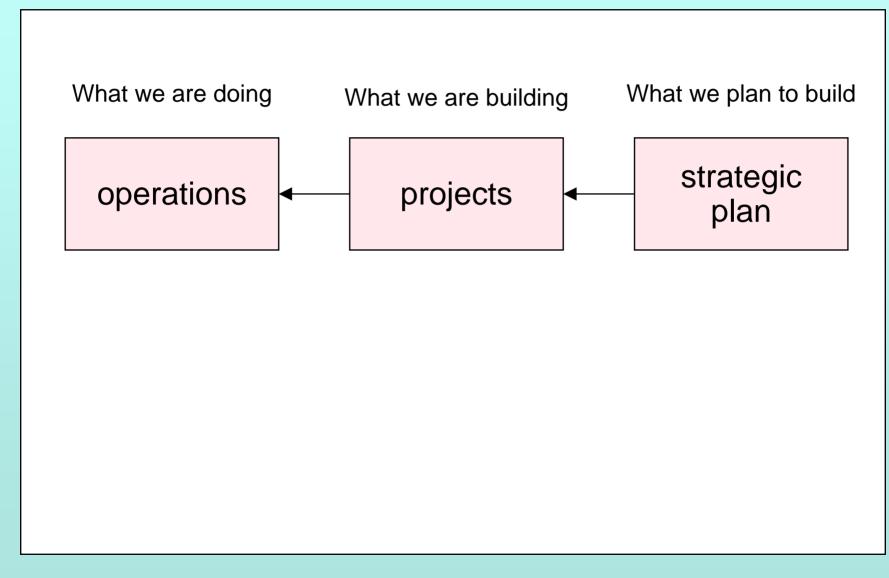
Strategic Planning for grant-funded research requires *fourth-box* thinking: a strategic architectural vision in response to some driving question.

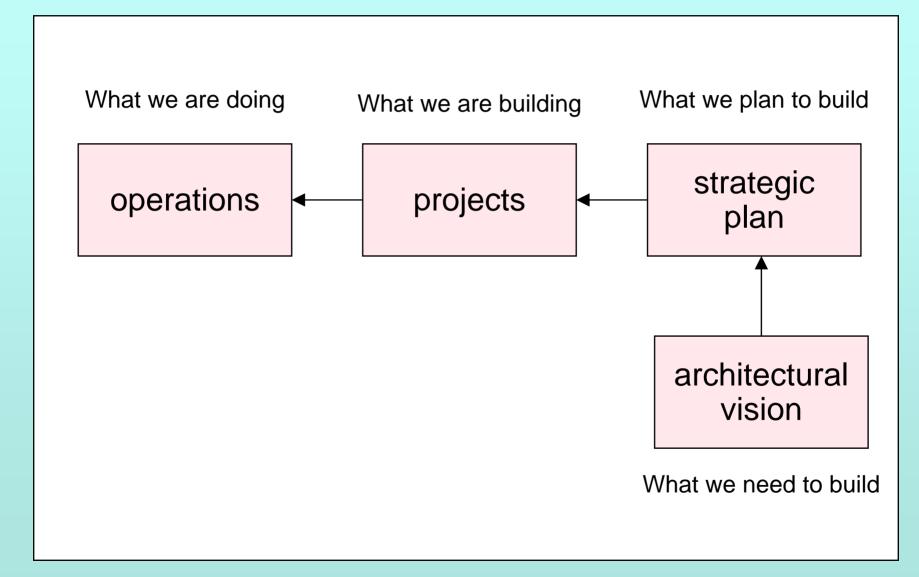
Strategic Planning

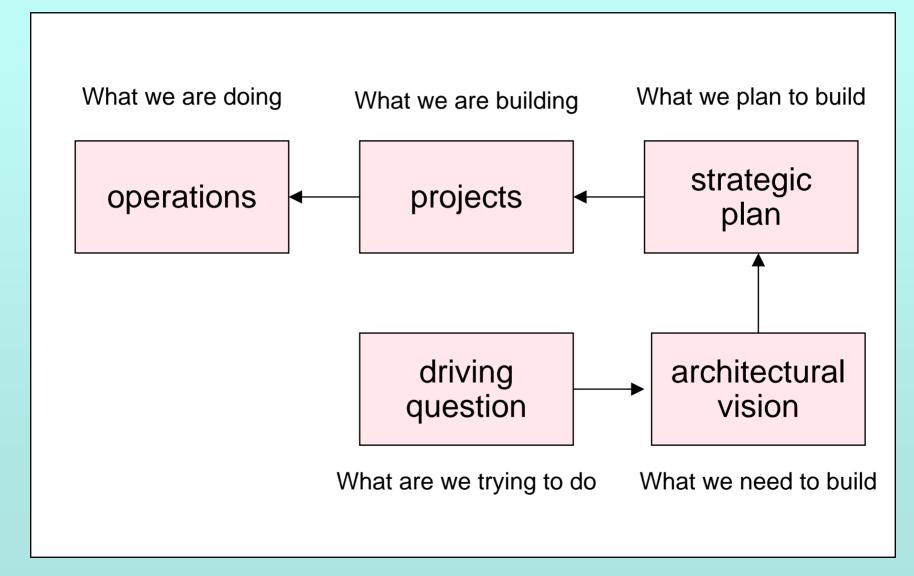
What we are doing

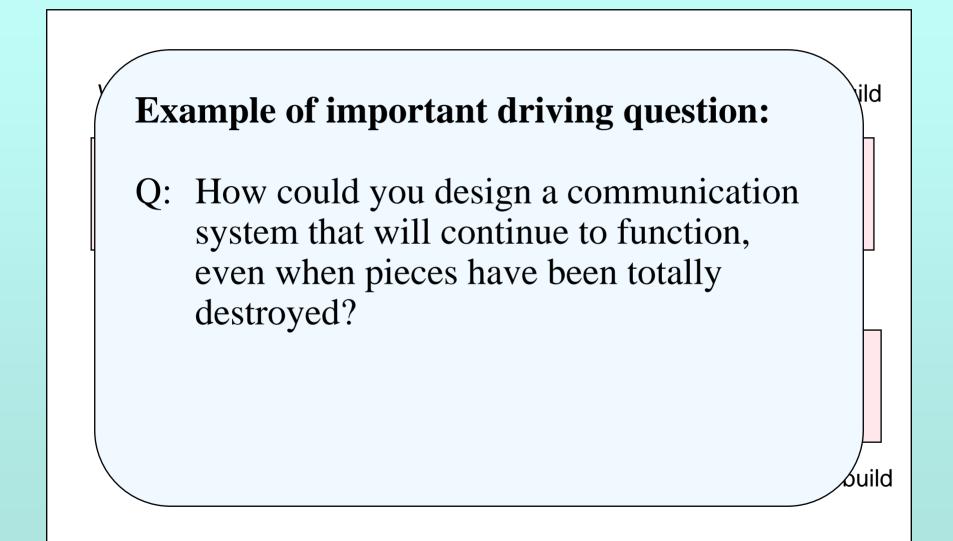
operations

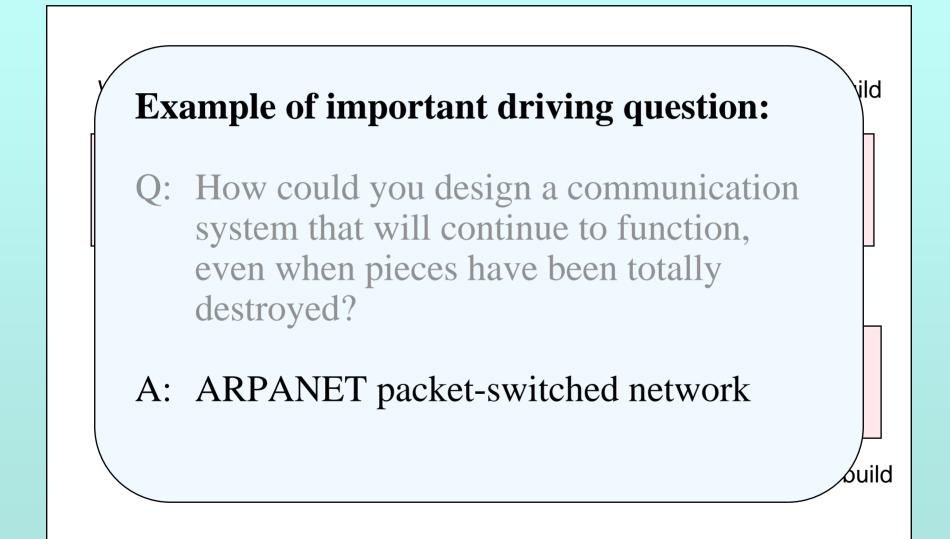


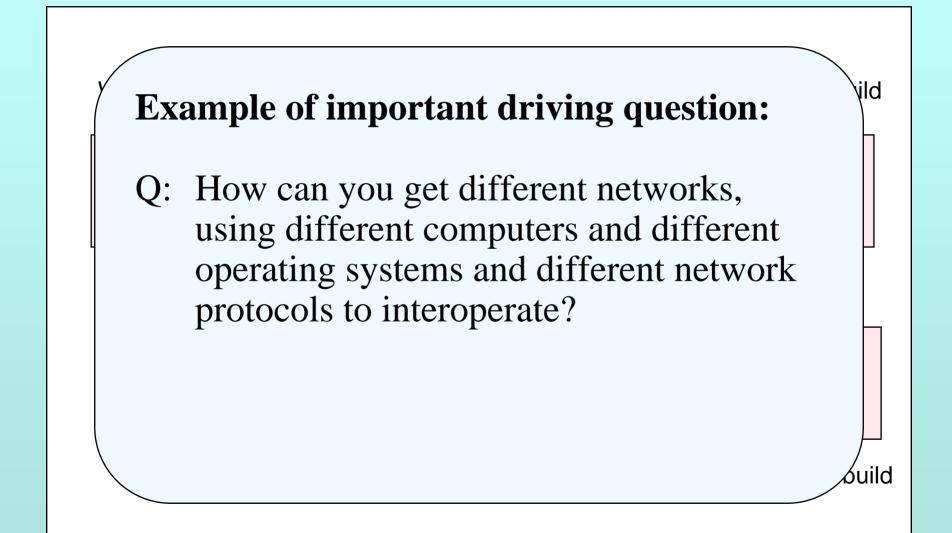


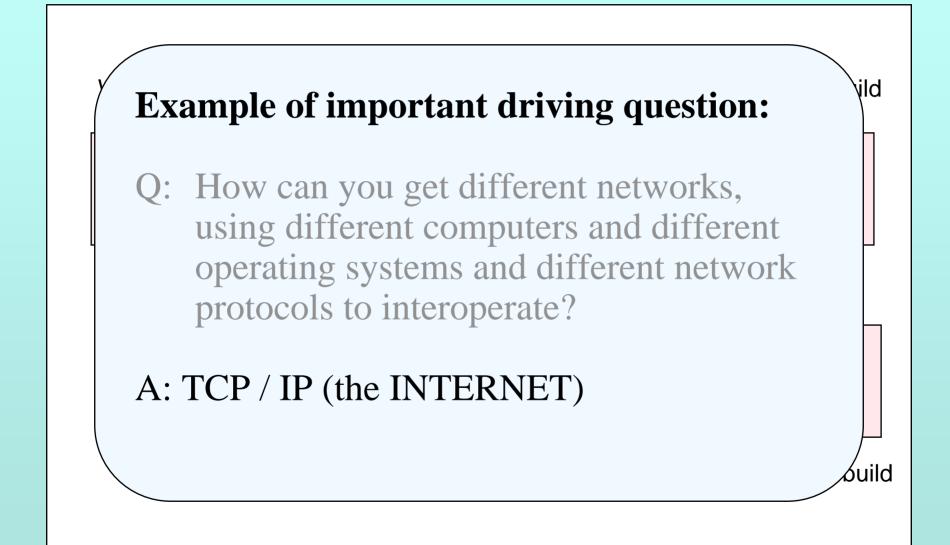


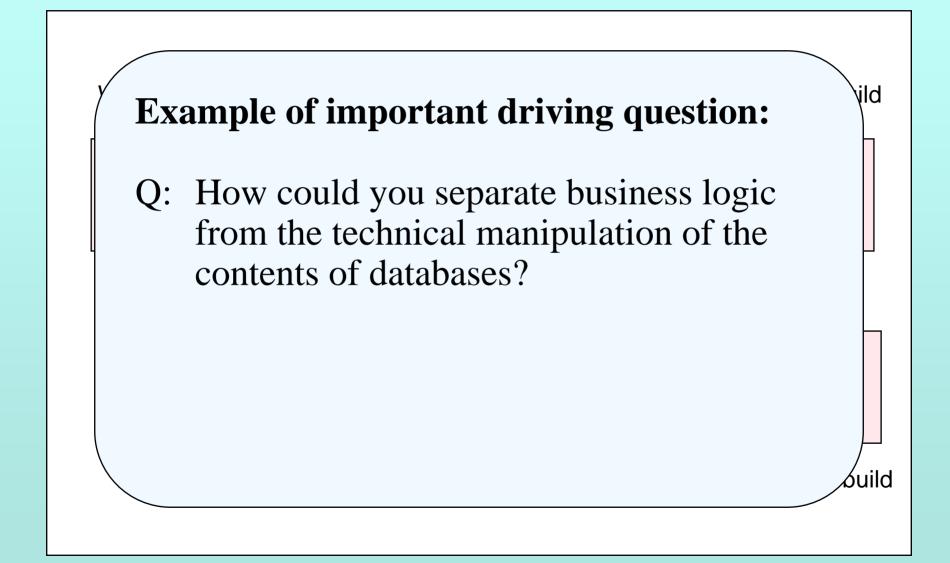


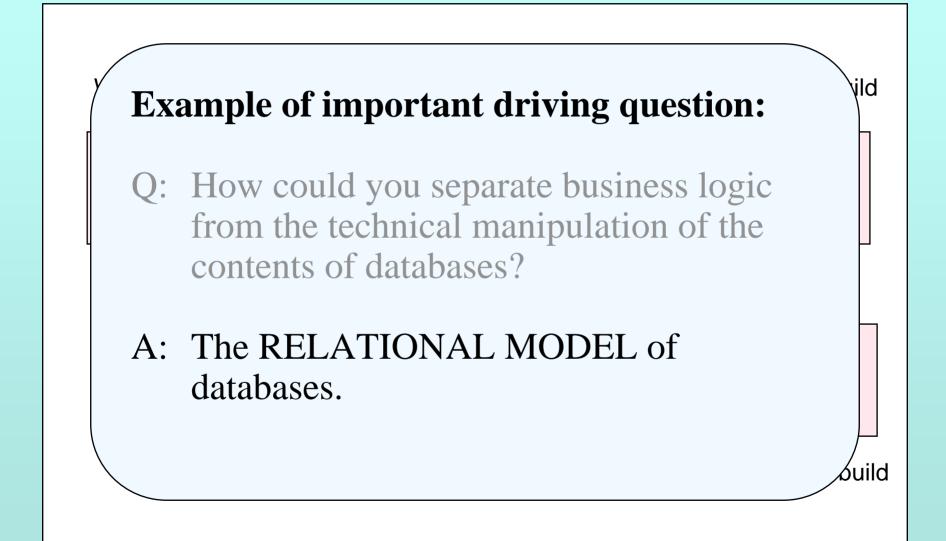


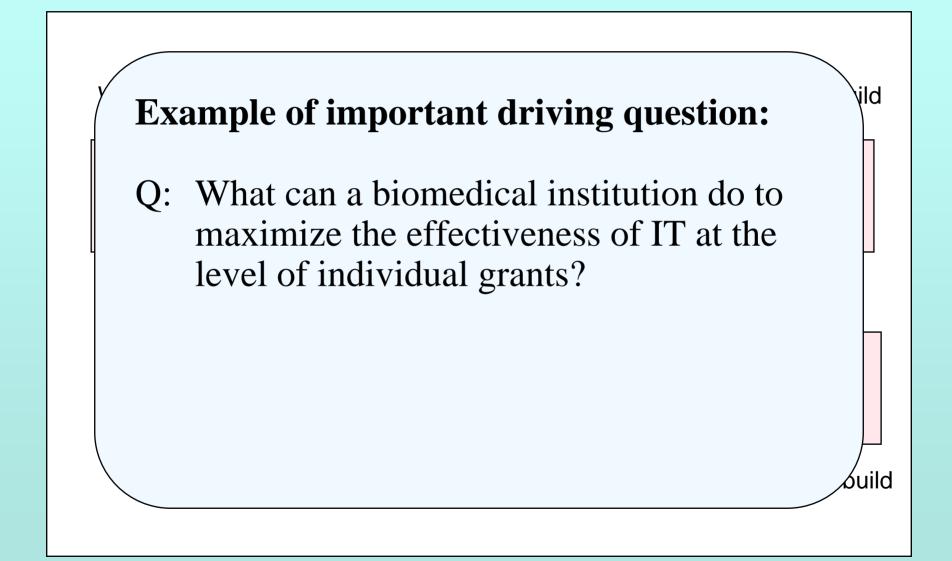










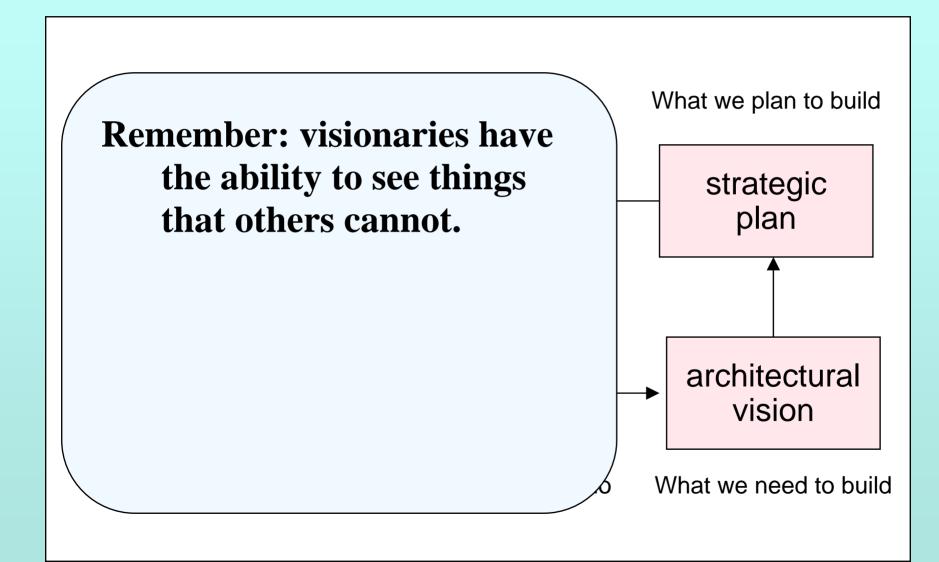


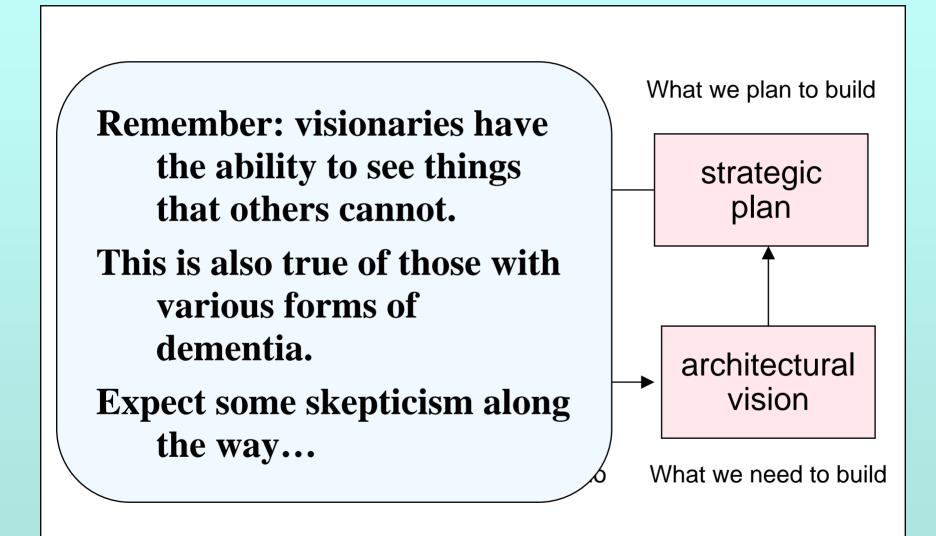


- Q: What can a biomedical institution do to maximize the effectiveness of IT at the level of individual grants?
- A: That's the question for this meeting. A strong case can be made for centralized support of distributed computing.

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TCP / IP networking and RDBMS are two of the most useful tools in the history of IT.

What can we learn from the history of their development?

• Truly valuable IT comes from a driving question, informing an architectural vision.

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- Truly valuable IT comes from a driving question, informing an architectural vision.
- You must know your GOAL and handle the trade-offs accordingly.
- The resulting architectural vision may have a NEWSPEAK flavor.
- Ultimately, the results are stunning in their power, flexibility, and extensibility.

TCP/IP & RDBMS Pattern

- Formulate driving question
- Develop vision of what might be
- Explore logical consequences of vision
- Prototype
- Expand/extend/revise vision
- Prototype
- Repeat...

Patience is a Virtue

Internet Time:

• A sustained explosion of growth and technical innovation...

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- A sustained explosion of growth and technical innovation...
- after 35 years of patient, painstaking planning, testing, and development.

Patience is a Virtue

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- A sustained explosion of growth and technical innovation...
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Conceptually, packet-switched networking began in 1960; the idea of internetworking was created in the 1970s; the whole thing took off in 1995...

BRIITE Challenge

BRIITE Challenge

- Confirm driving question
- Begin to plan architectural vision
- Identify possible components
- Describe ideal functions of components
- Imagine how functions might be achieved
- Assess how design might affect function
- Consider how components might interact
- Repeat as necessary

Possible Modules

Possible Modules

- Basic Infrastructure
- Authorization, Authentication, Auditing
- Digital Publishing Support
- Scientific Database I: Data Models & Design
- Scientific Database II: Data Integration
- Scientific Database Support III: Community Databases
- Scientific Database Support IV: Public dB Integration

Possible Modules

- Clinical Research I: Research Access to Clinical Data
- Clinical Research II: Research Trials
- Clinical Research III: Controlled Vocabularies
- Clinical Research IV: Specimen Management
- Clinical Research V: Tumor / Disease Registries
- Laboratory Information Management Systems
- Shared Resource Support

Possible Methods

- Top down: ideal solutions
- Bottom up: current problems
- Iterative: both, back and forth...

Top-down Example

Authorization, Authentication, etc.

Every administrator of a computer resource needs some way to identify users, to authorize them to access the resource, to authenticate them when they access the resource, and to log and audit them when they use the resource. In a typical academic environment, there are many, many different approaches to handling these tasks.

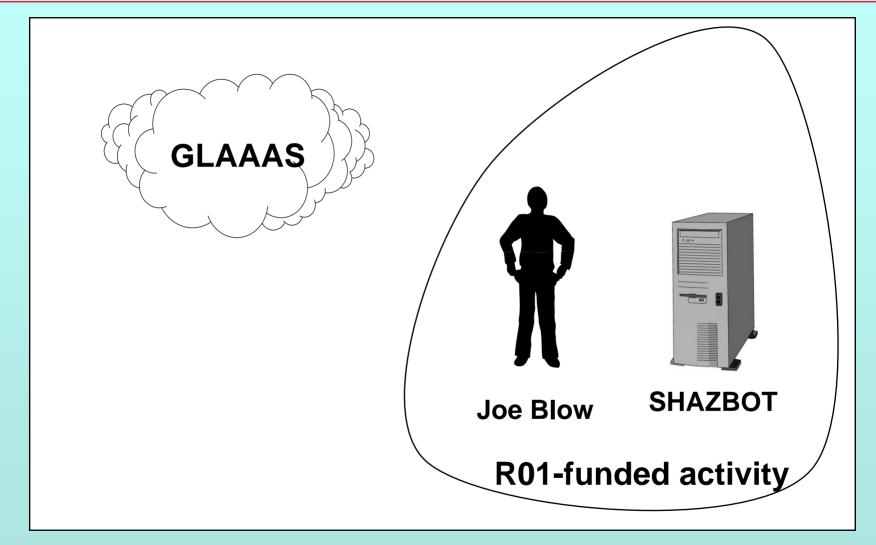
What if, once upon a time in the future, there were to be a system called GLAAAS...

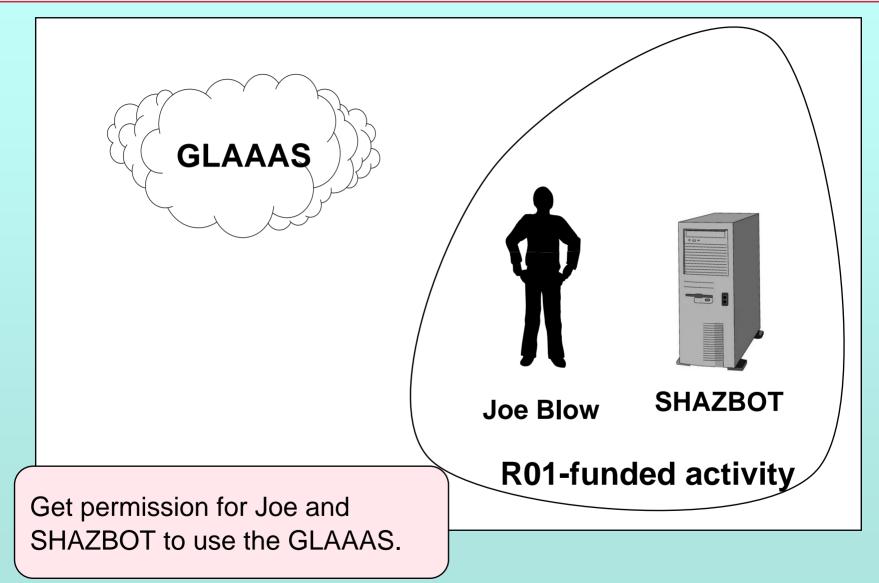
GLAAAS

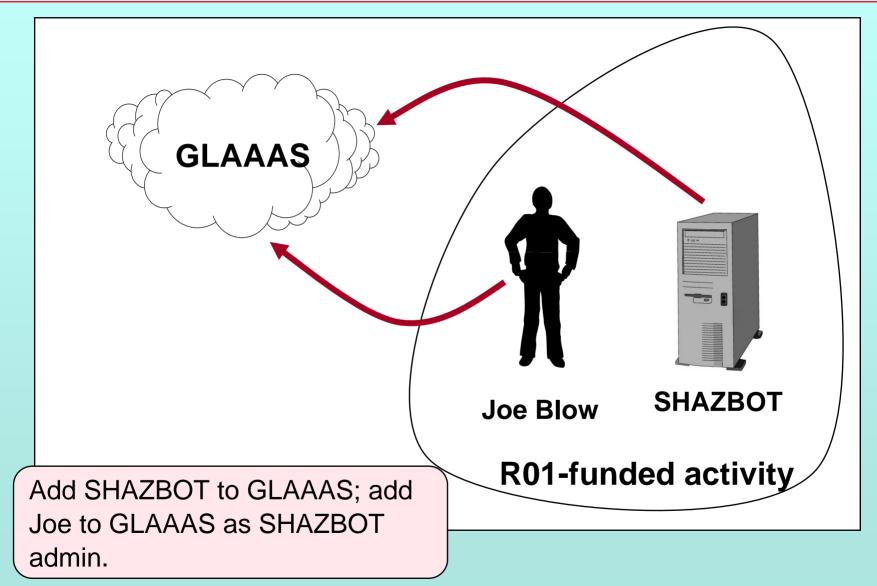
GLAAAS is a GLobal Authorization, Authentication, and Auditing System that can be used to assign, track, and audit permissions to use IT resources on any server that participates in GLAAAS.

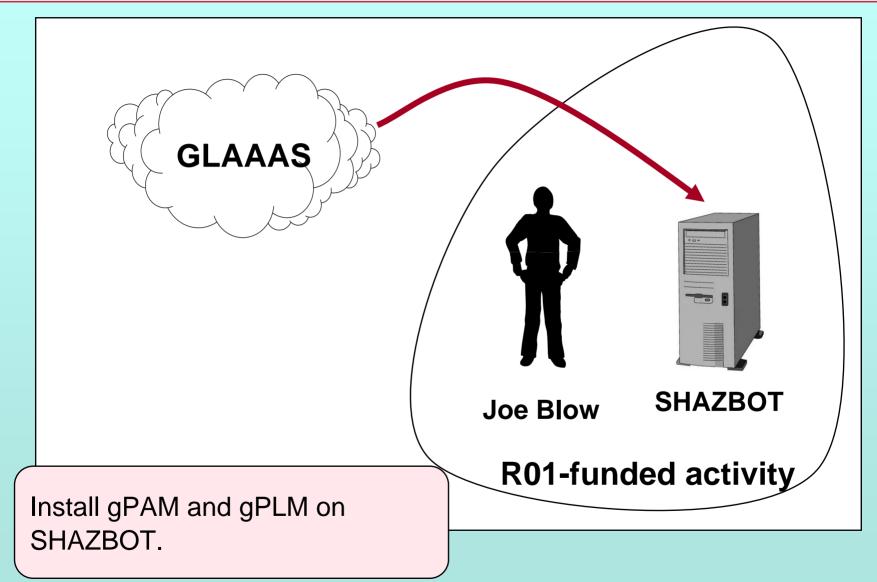
GLAAAS works with any operating system and makes almost no demands on the configuration of any participating server.

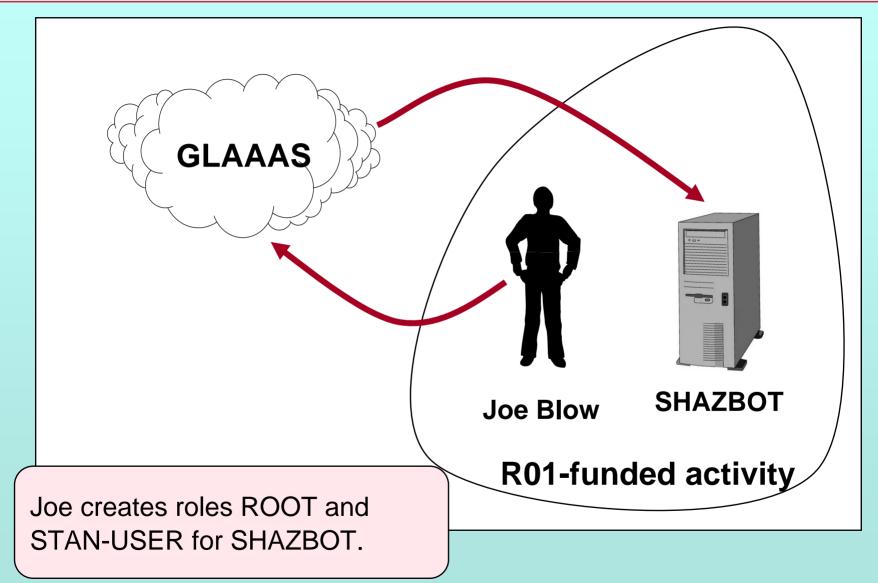
GLAAAS provides gPAMs (general pluggable authentication modules) and gPLMs (general pluggable logging modules) to all participating servers.

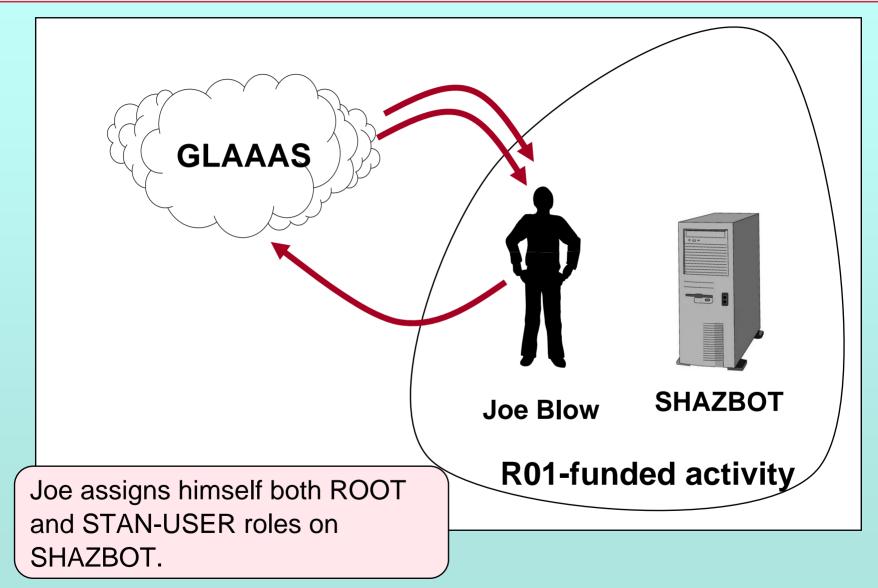


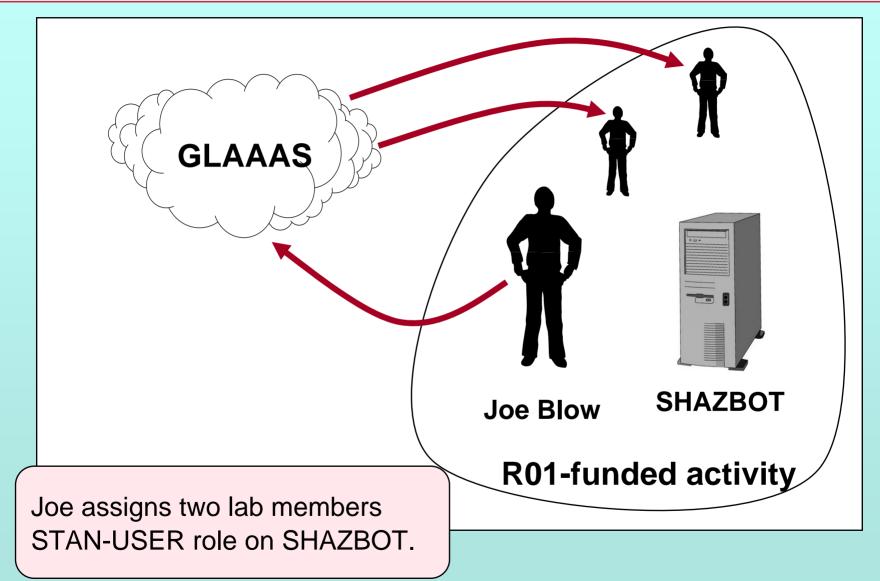


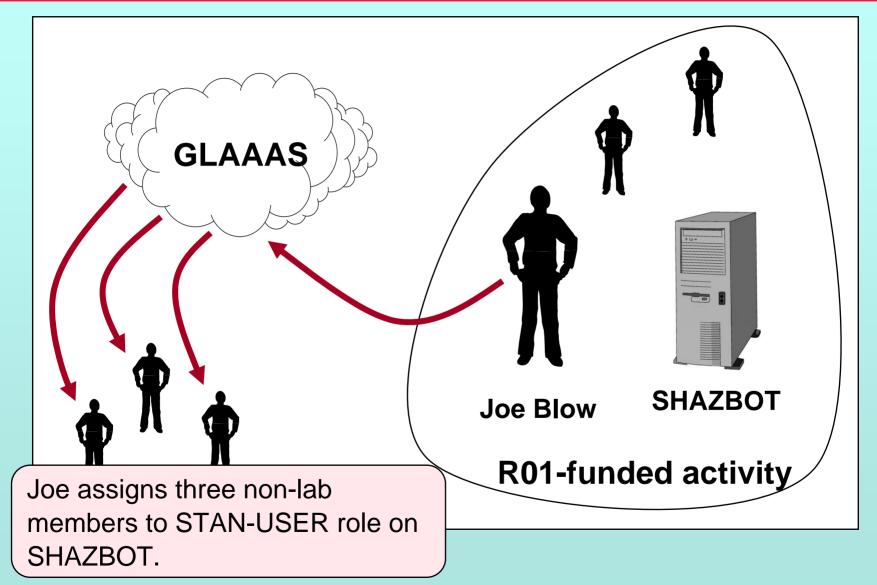


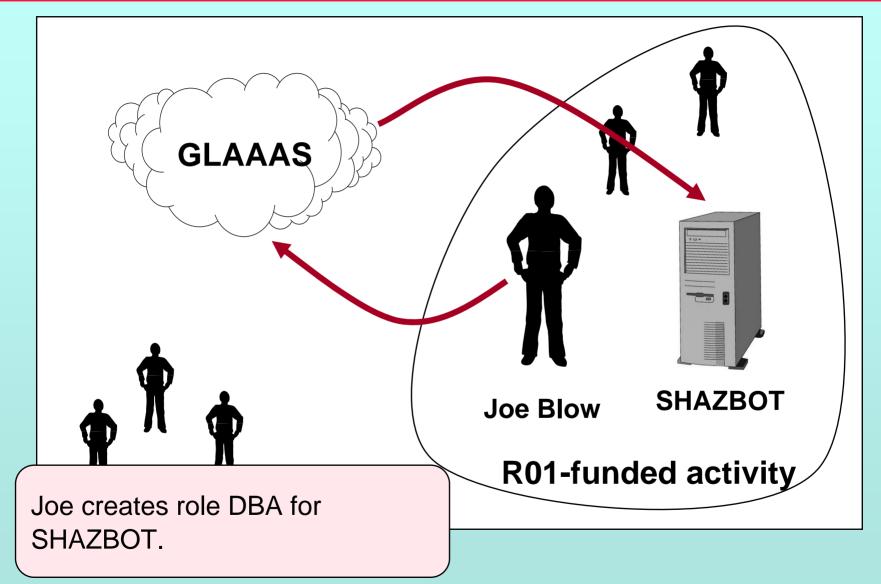


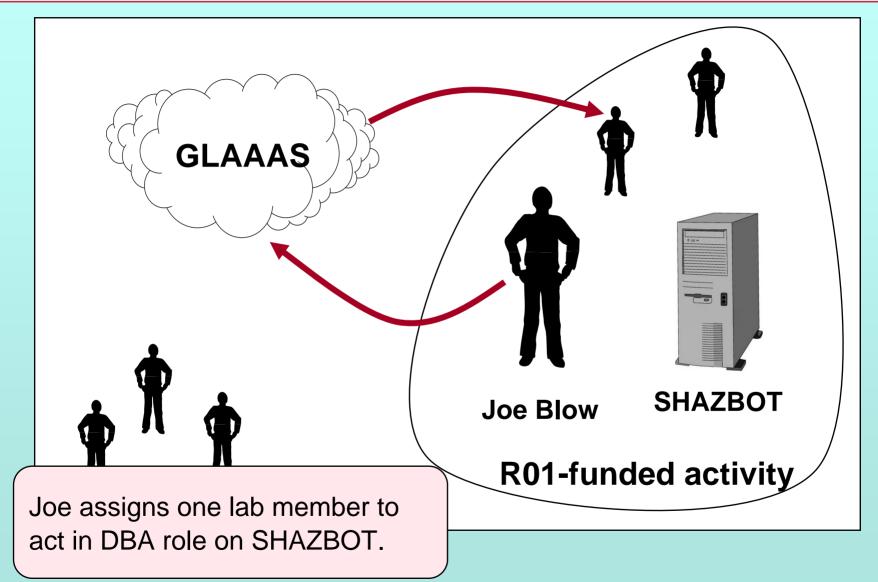


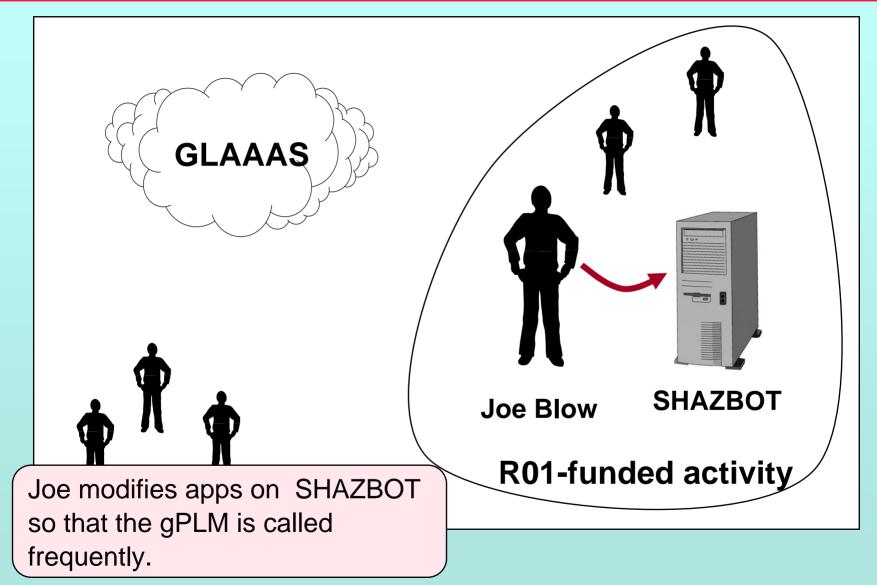


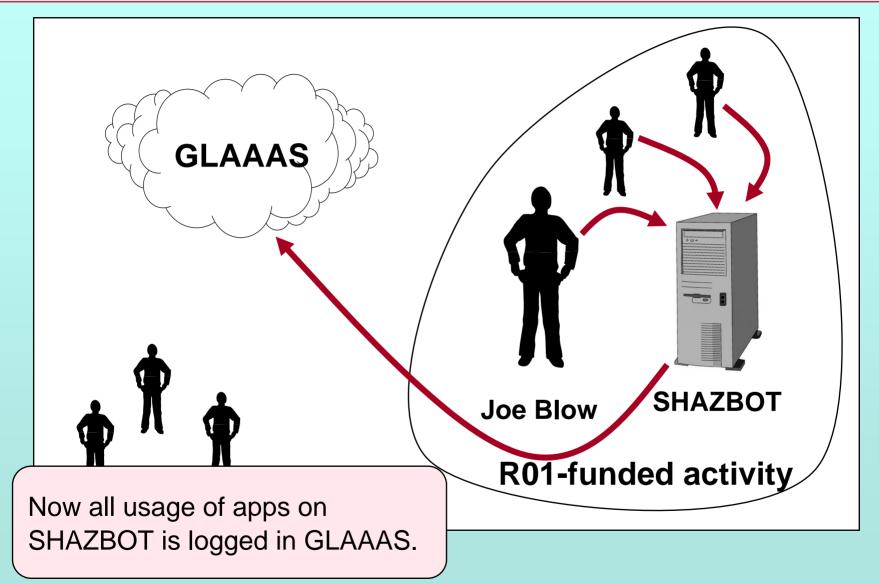


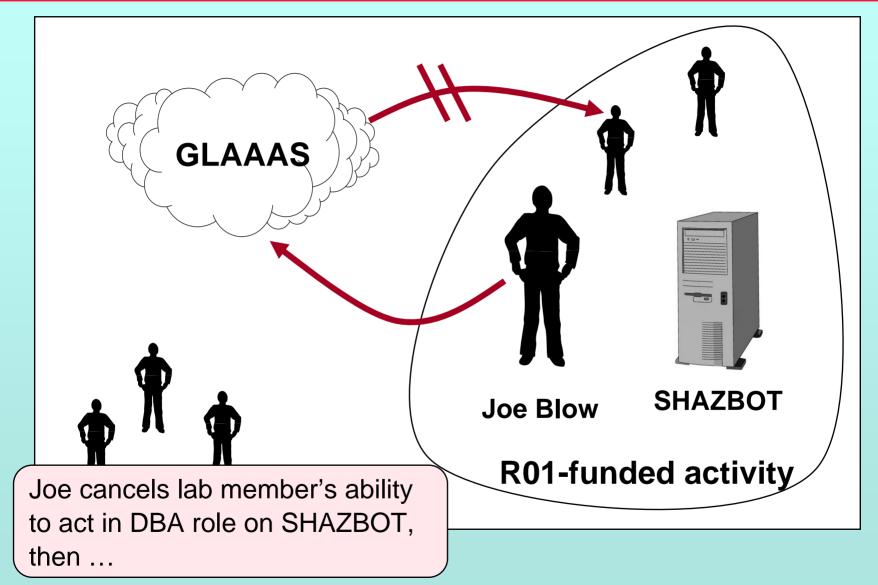


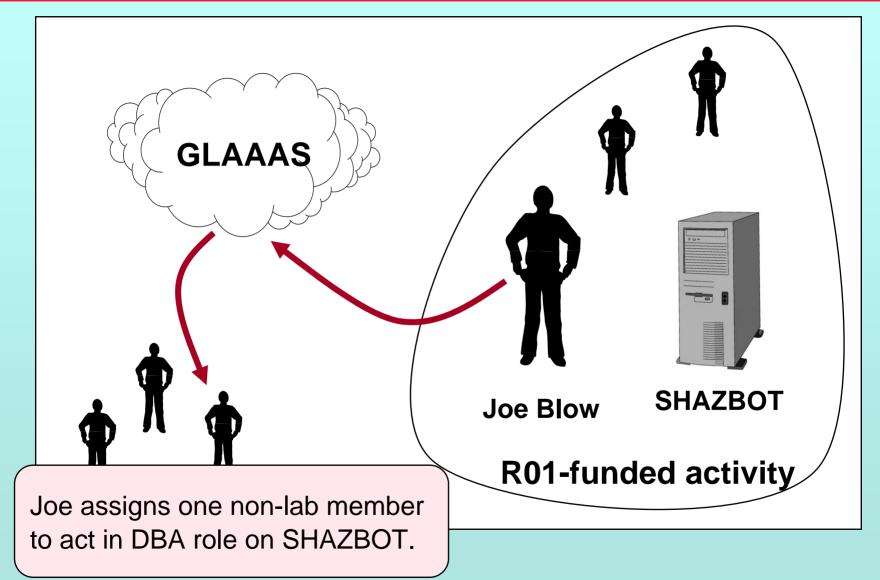












GLAAAS

All of these changes in authorization, authentication, and logging for SHAZBOT occur without any USER having to make any changes to his/her account and without any effect on the user's permissions or access on any other system.

USERs assigned multiple roles on a machine can request a change to a different authorized role at any time, without having to reauthenticate. USERs can be simultaneously connected in multiple roles, if needed.

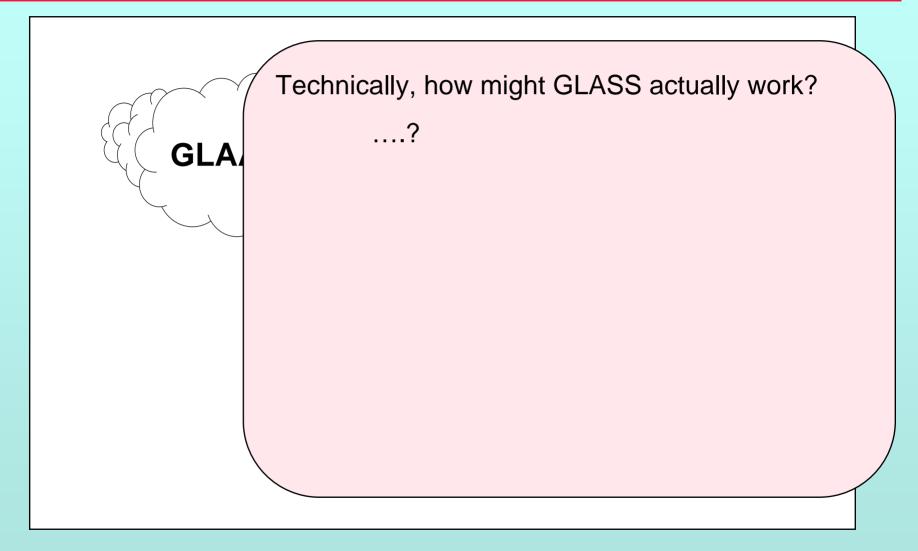
GLA



Provide truly GLOBAL support, by working with similar systems at other campuses?

Support the management of GROUPS of people, so that permission could be granted to the right group, but the responsibility for maintaining the group is no longer the system administrator's?

....?



Slides:

http://www.esp.org/rjr/nist2003.pdf