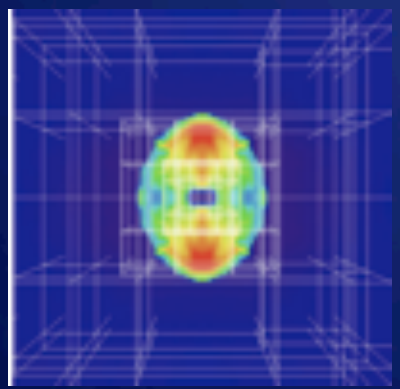
Data- and Compute-Driven Transformation of Modern Science

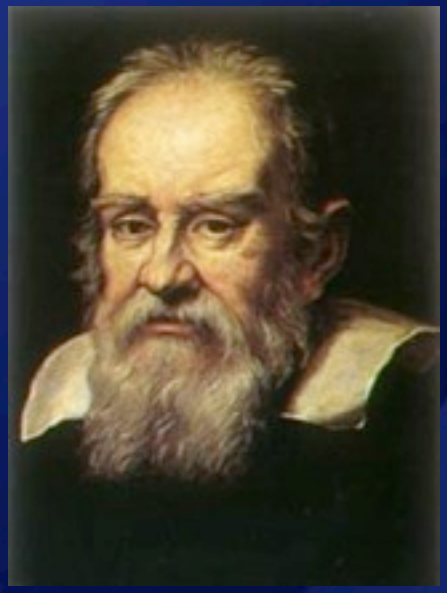
Edward Seidel

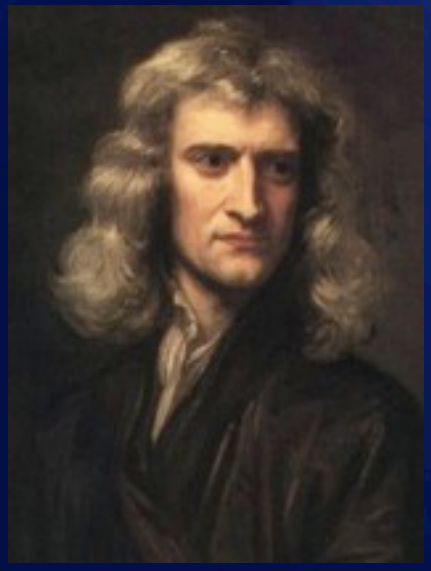
Assistant Director, Mathematical and Physical Sciences, NSF



1

Profound Transformation of Science
Gravitational Physics

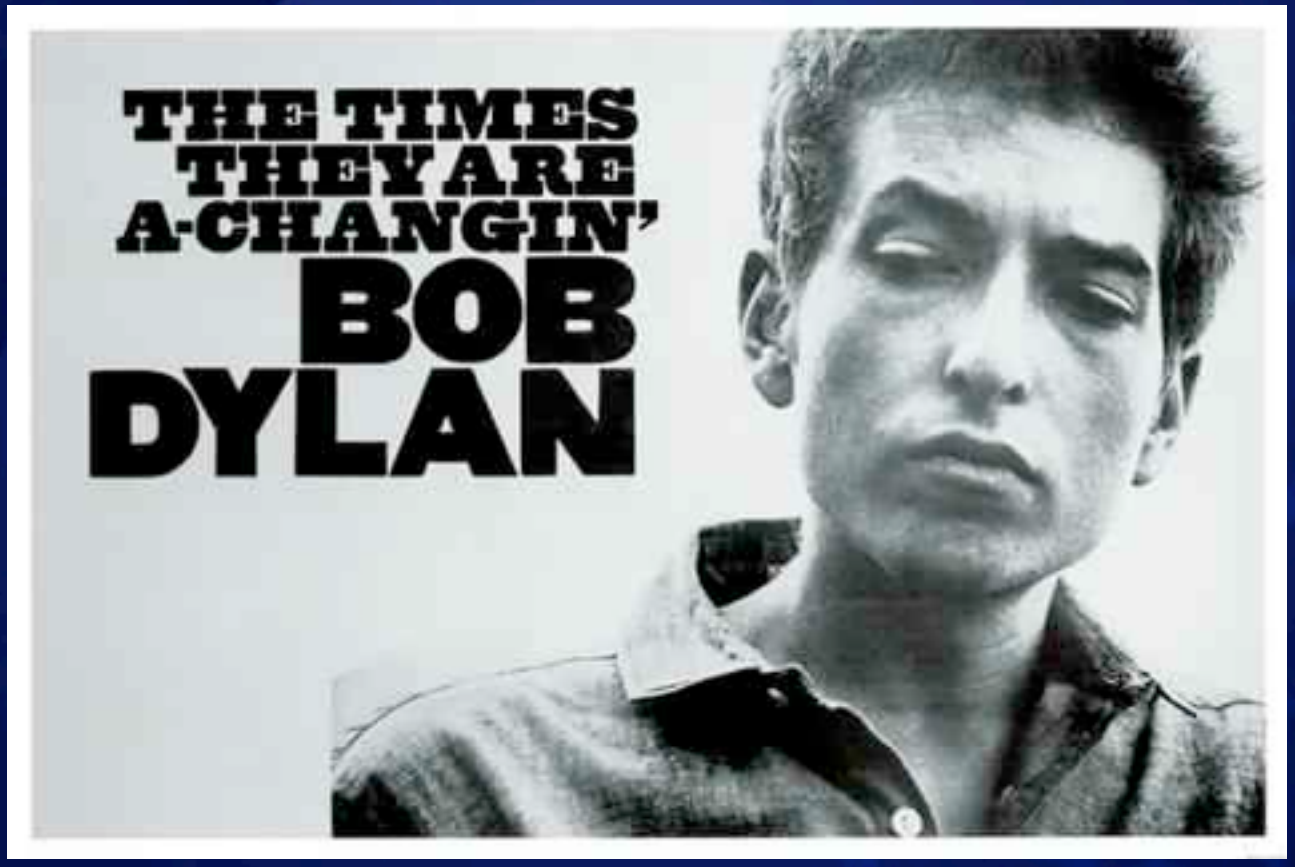




- Galileo, Newton usher in birth of modern science: c. 1600
- Problem: single "particle" (apple) in gravitational field (General 2 body-problem already too hard)
- Methods
  - Data: notebooks (Kbytes)
  - Theory: driven by data
  - Computation: calculus by hand (1 Flop/s)
- Collaboration
  - 1 brilliant scientist, 1-2 student

2

Part 1: Changing Cultures and Methodologies of Science…and the crises they create…



3

Profound Transformation of Science

Collision of Two Black Holes

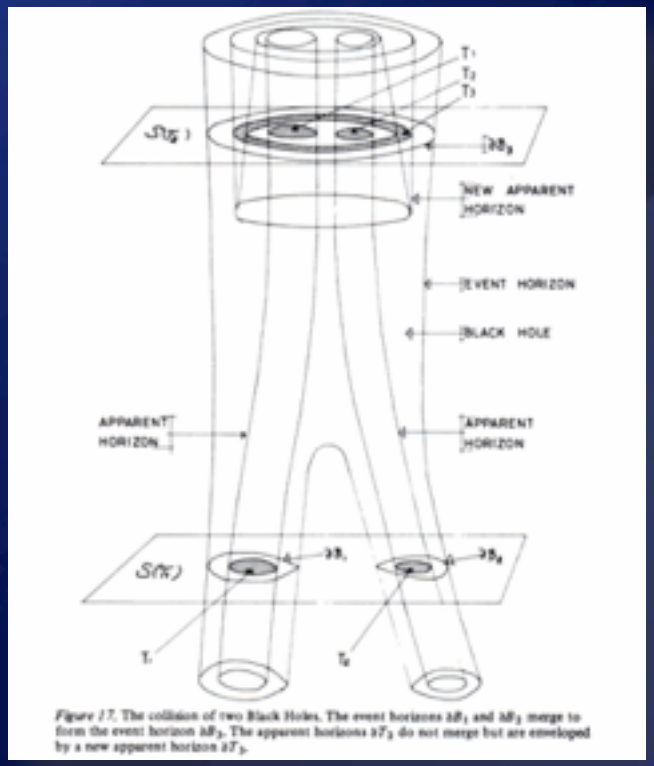
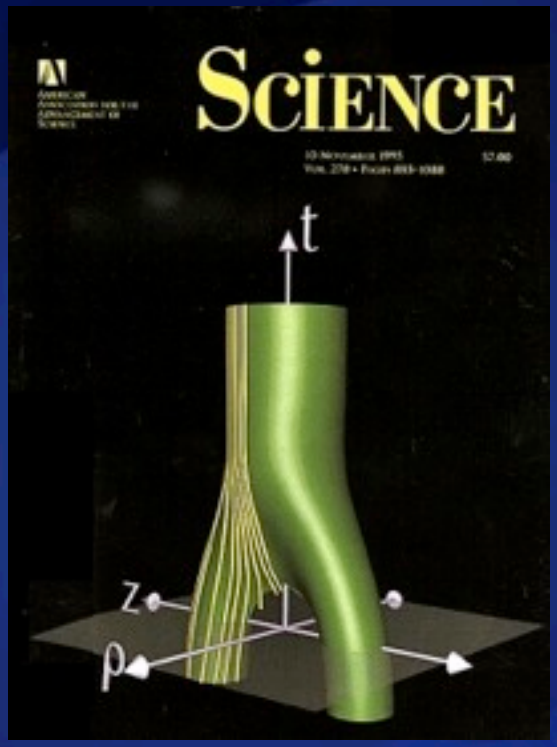
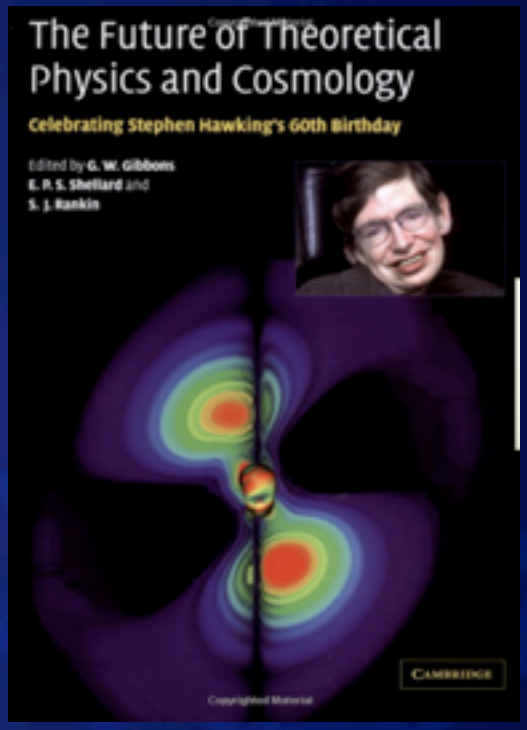


Figure 17. The collision of two Black Holes. The event horizons ΔB_1 and ΔB_2 merge to form the event horizon ΔB_3. The apparent horizons ΔT_1 do not merge but are enveloped by a new apparent horizon ΔT_3.





1972: Hawking. 1 person, no computer 50 KB

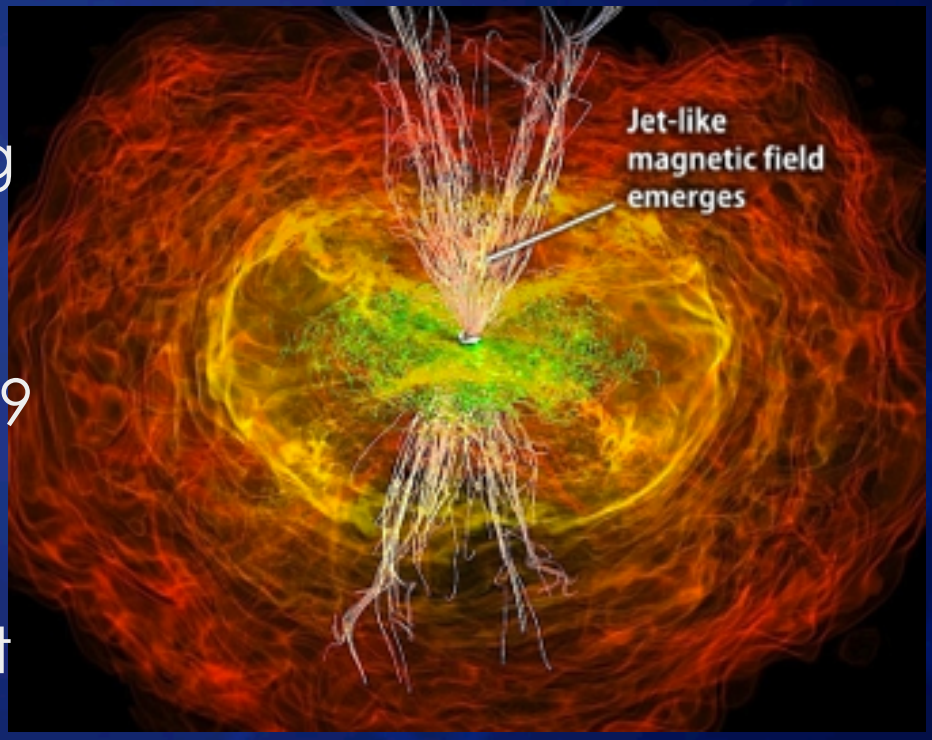
1995: 10 people, large computer, 50MB

1998: 15 people, larger computer, 50GB

Community Einstein Toolkit

"Einstein Toolkit : open software for astrophysics to enable new science, facilitate interdisciplinary research and use emerging petascale computers and advanced CI."

- Consortium: 67 members, 29 sites, 11 countries
- Simulation credits: Luciano Rezzolla, Max Planck Institut für Gravitationsphysik (Albert-Einstein-Institut)



Community + software + algorithms + hardware + …

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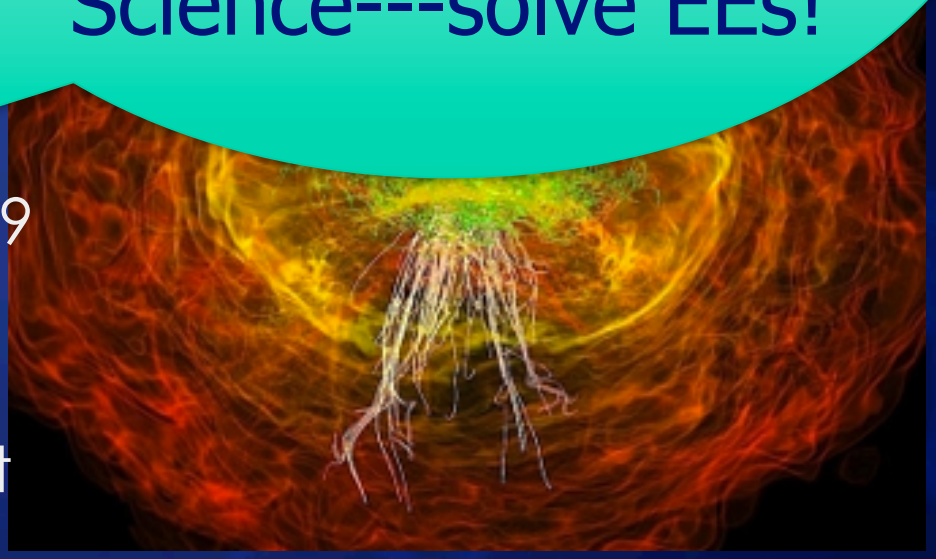
Many groups can do this: field explodes! Major triumph of Computational Science---solve EEs!



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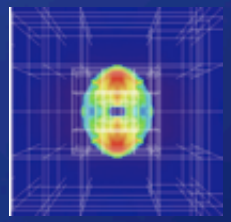
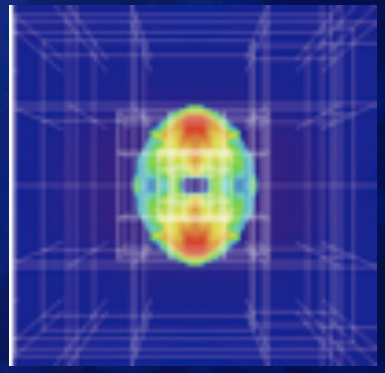


Just ahead: Complexity of Universe

LHC, Gamma-ray bursts!

- Gamma-ray bursts!
  - Now: complex problems in relativistic astrophysics
  - Relativity, hydrodynamics, nuclear physics, radiation, neutrinos, magnetic fields: globally distributed collab!
  - Scalable algorithms, complex simulation codes, viz, PFlops*week, PB output!
- Gravity and general relativity are transformed
  - 4 centuries of small science, small data culture
  - 2-3 decades of radical change in both data (factors of 1000 per~5 years) and collaboration

LIGO



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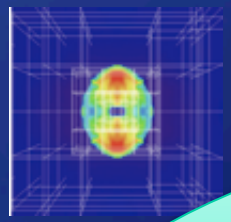

Just ahead: Complexity of Universe

...ma-ray bursts!

New era of science after a century! Data- and compute-dominated gravitational wave astronomy!

- ...
  - ...
  - ...
  -

Transient & Data-intensive Astronomy

- New era: seeing events as they occur
  - (Almost) here now
    - ALMA, EVLA in radio
    - Ice Cube neutrinos
  - On horizon
    - 24-42m optical?
    - Indo-US transient collaboration
    - Indigo?
    - LSST
    - SKA = exabytes
- Simulations integrate all physics

Astronomy 1500-2010 was passive. No longer!

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Will require integration across disciplines, end-to-end

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Communities need to share data, software, knowledge, in real time

Big Data vs The Long Tail of Science

- Many "Big Data" projects are "special"
  - Tend to be highly organized, have singular sources of data, professionally curated, a lot attention paid to them
- What about the "Long Tail" (the other 99%)?
  - Thousands of biologists sequencing communities of organisms
  - Thousands of chemist and materials scientists developing a "materials genome"
  - Millions of people "Tweeting"…
  - Characteristics:
    - Heterogeneous, perhaps hand generated
    - Not curated, reused, served, etc…

MATERIALS GENOME

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How do we harness the power of this long tail?

MATERIALS GENOME

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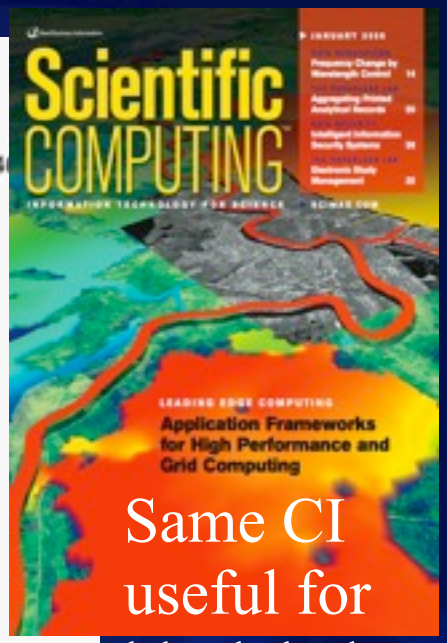
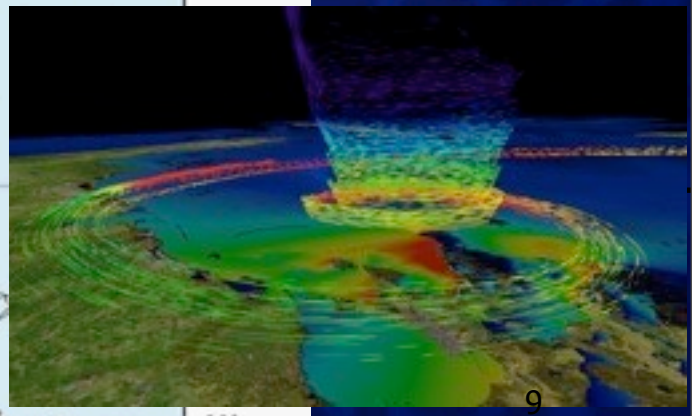
Grand Challenge Communities Combine it All...

Where is it going to go?



Same CI useful for black holes, hurricanes



9

Grand Challenge Communities for

- Require many disciplines, all scales of collaborations
  - Individuals, groups, teams, communities
  - Multiscale Collaborations: Beyond teams
- Are dynamic and highly multidisciplinary
  - Time domain astronomy, emergency forecasting, metagenomincs, materials genome…
- Drive sharing technologies and methodologies
- Researchers collaborate, work by sharing data. Places requirements on:
  - Software, networks, collaborative environments, data, sharing, computing, etc
  - Scientific culture, reproducibility, access, university structures
  - "Publications." What is a modern publication?

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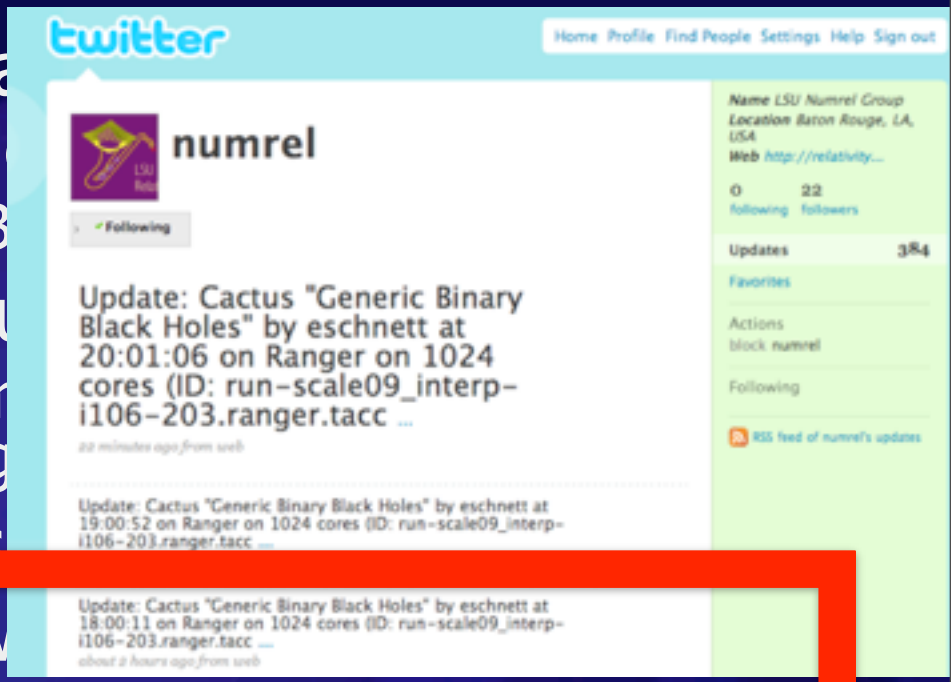

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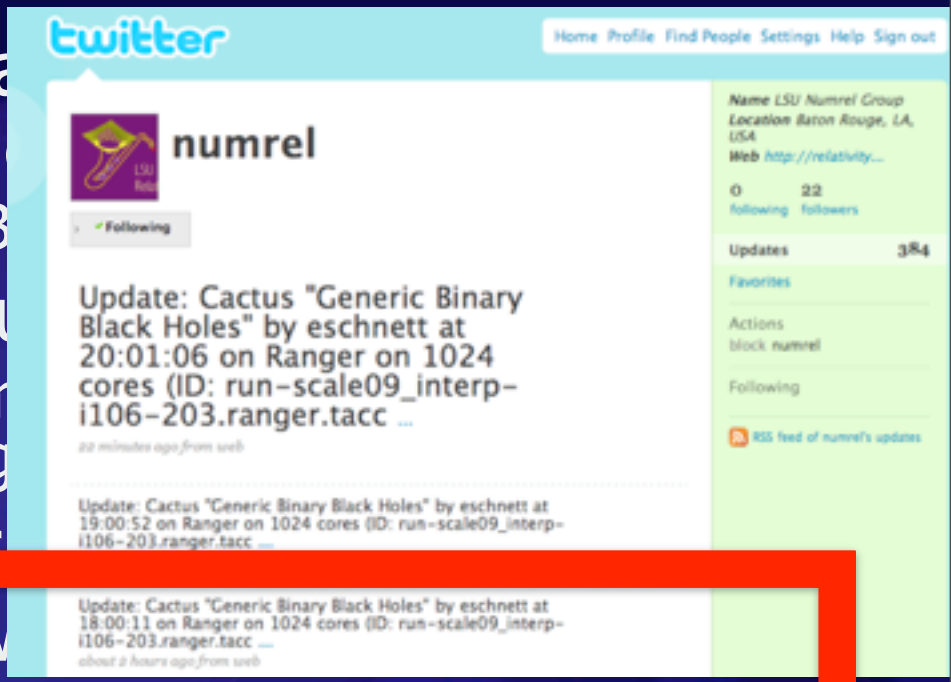

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Grand Challenge Communities for

Social, behavioral and economic sciences will be critical in helping us understand these issues…

- R… a…
- A… B… u…
- D…
- R… requirements on:
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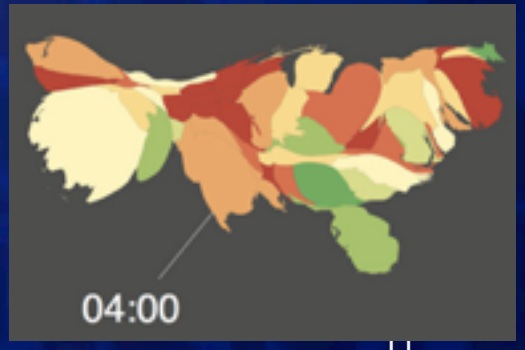
Scenarios like this in all fields

MATERIALS GENOME

CineGrid



Framing the Challenge: Science and Society Transformed by Data

- Modern science
  - Data- and compute-intensive
  - Integrative, multiscale
  - 4 centuries of constancy, 4 decades 10^{9-12} change!
- Multi-disciplinary Collaborations
  - Individuals (Galileo!)
  - Groups, teams, Grand Challenge Communities
  - Big Data + Long Tail
- Sea of Data
  - Age of Observation

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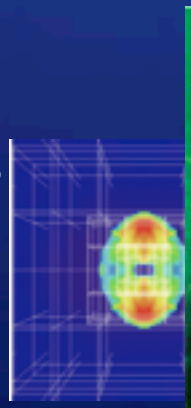

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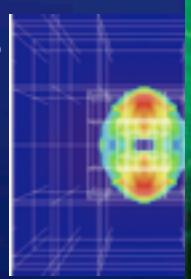

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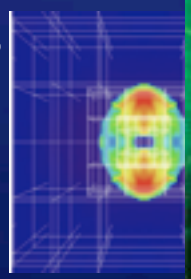

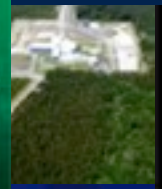

Framing the Challenge:
Society Transformed by Data

We still think like this…

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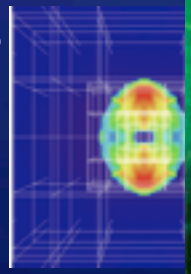

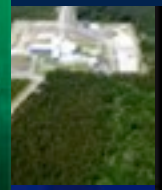

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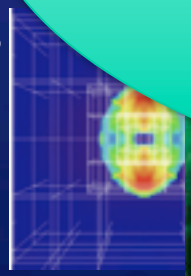
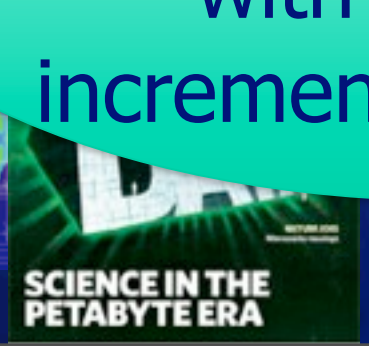
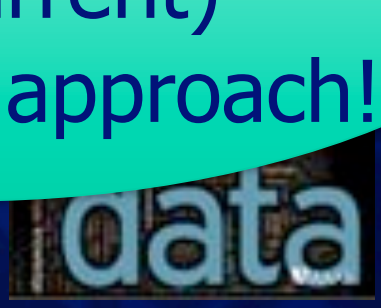
…But such radical change cannot be adequately addressed with (current) incremental approach!







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We still think like this…

Students take note!

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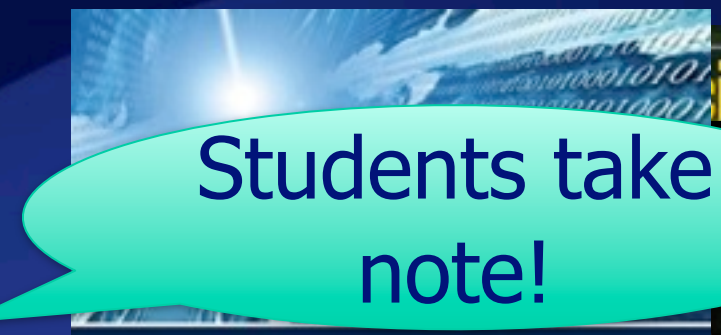

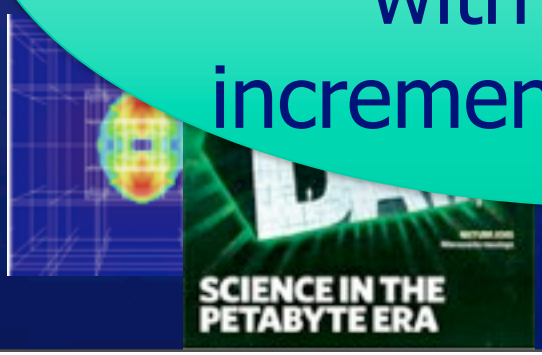

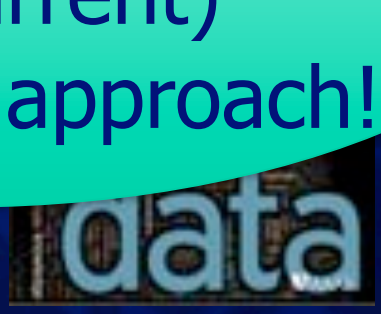

Part 2: Crises to Deal With

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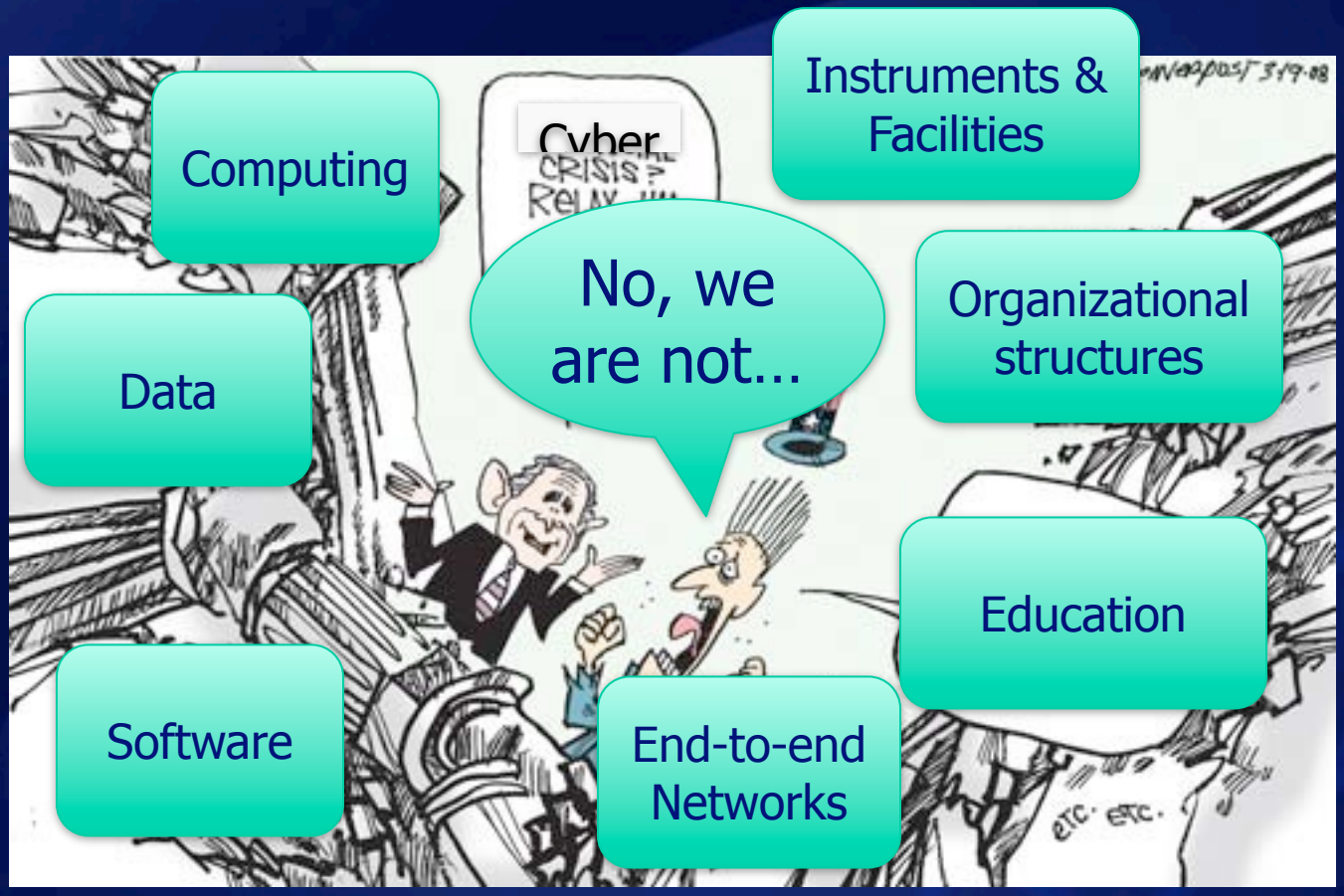
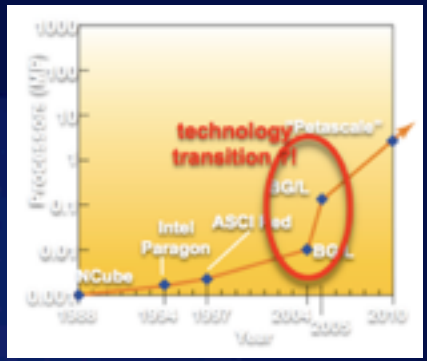
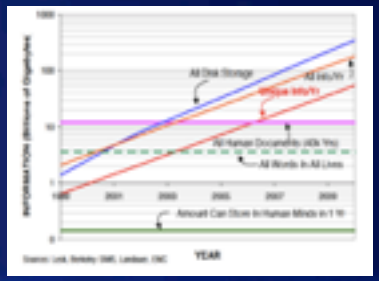
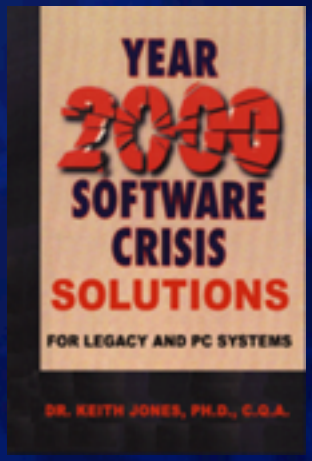


Three Crises

- Computing Technology
  - Multicore: processor is new transistor
  - Programming model, fault tolerance, etc
  - New models: clouds, grids, GPUs,… where appropriate
- Data, provenance, and visualization
  - Generating more data than in all of human history: preserve, mine, share?
  - How do we create "data scientists"?
- Software
  - Complex applications on coupled compute-data-networked environments, tools needed
  - Modern apps: 10^6+ lines, many groups contribute, take decades







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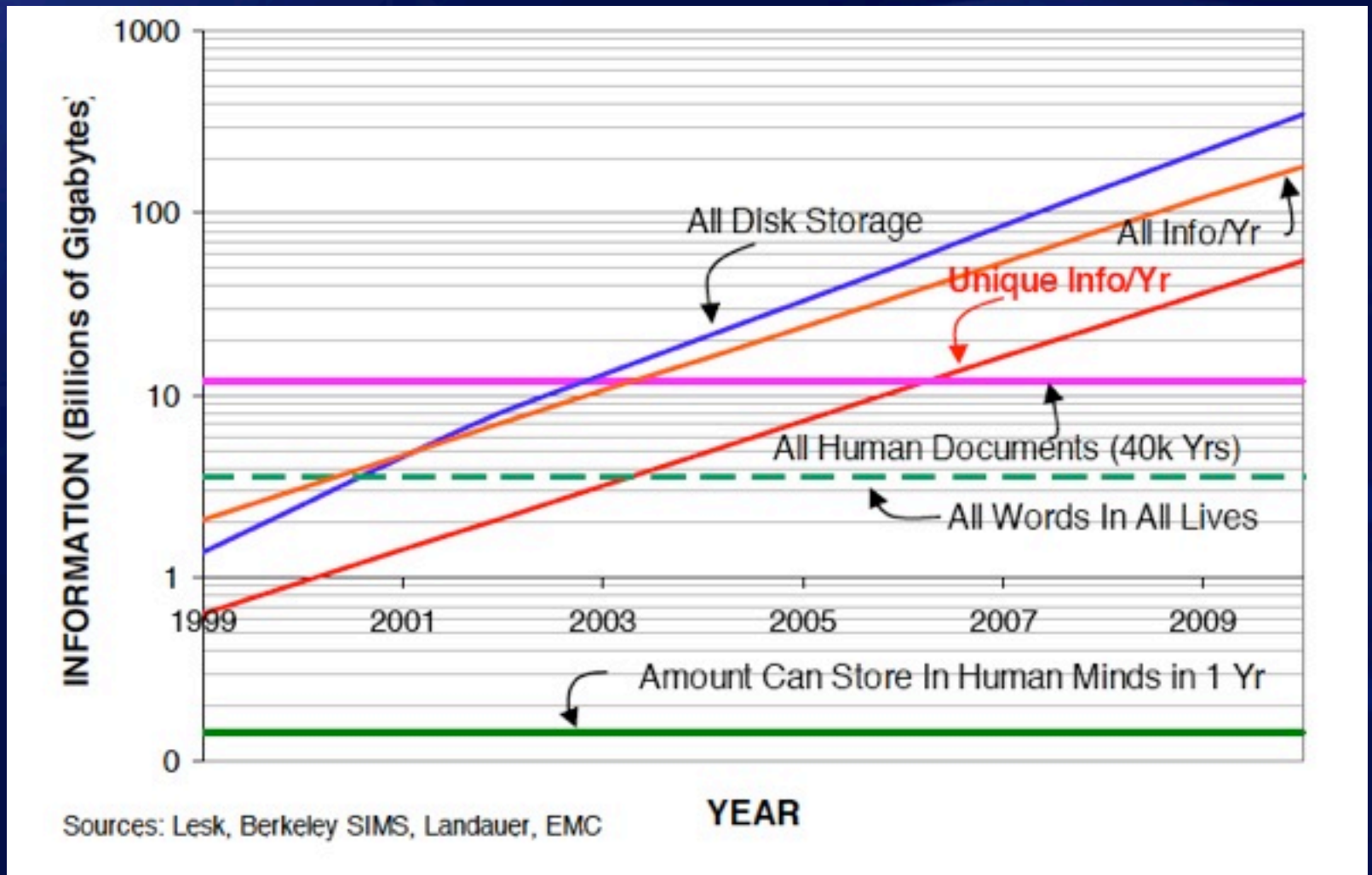
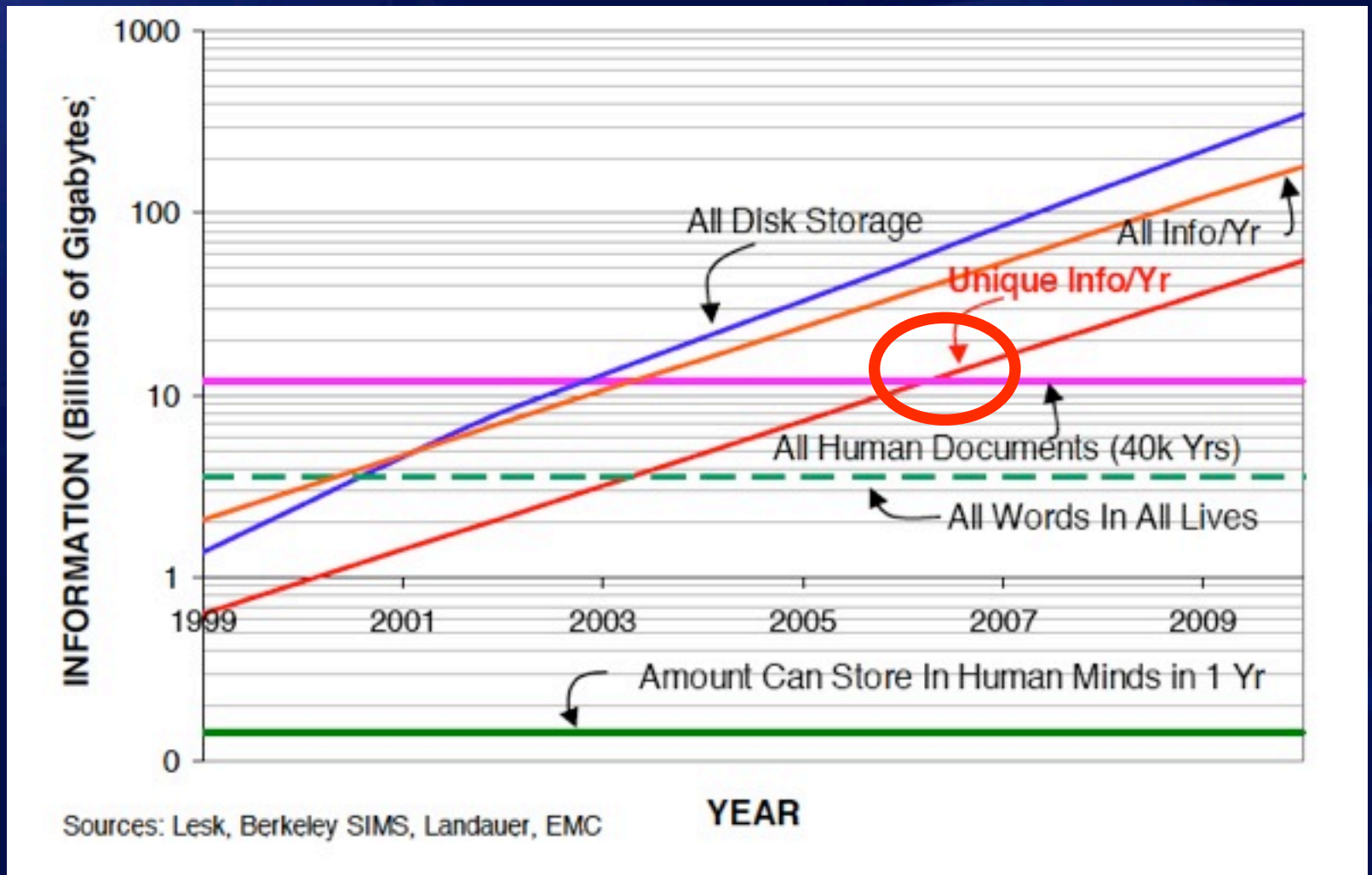
Data Crisis: Information Big Bang



Scientific Computing and Imaging Institute, University of Utah

Data Crisis: Information Big Bang



Data Crisis: Information Big Bang

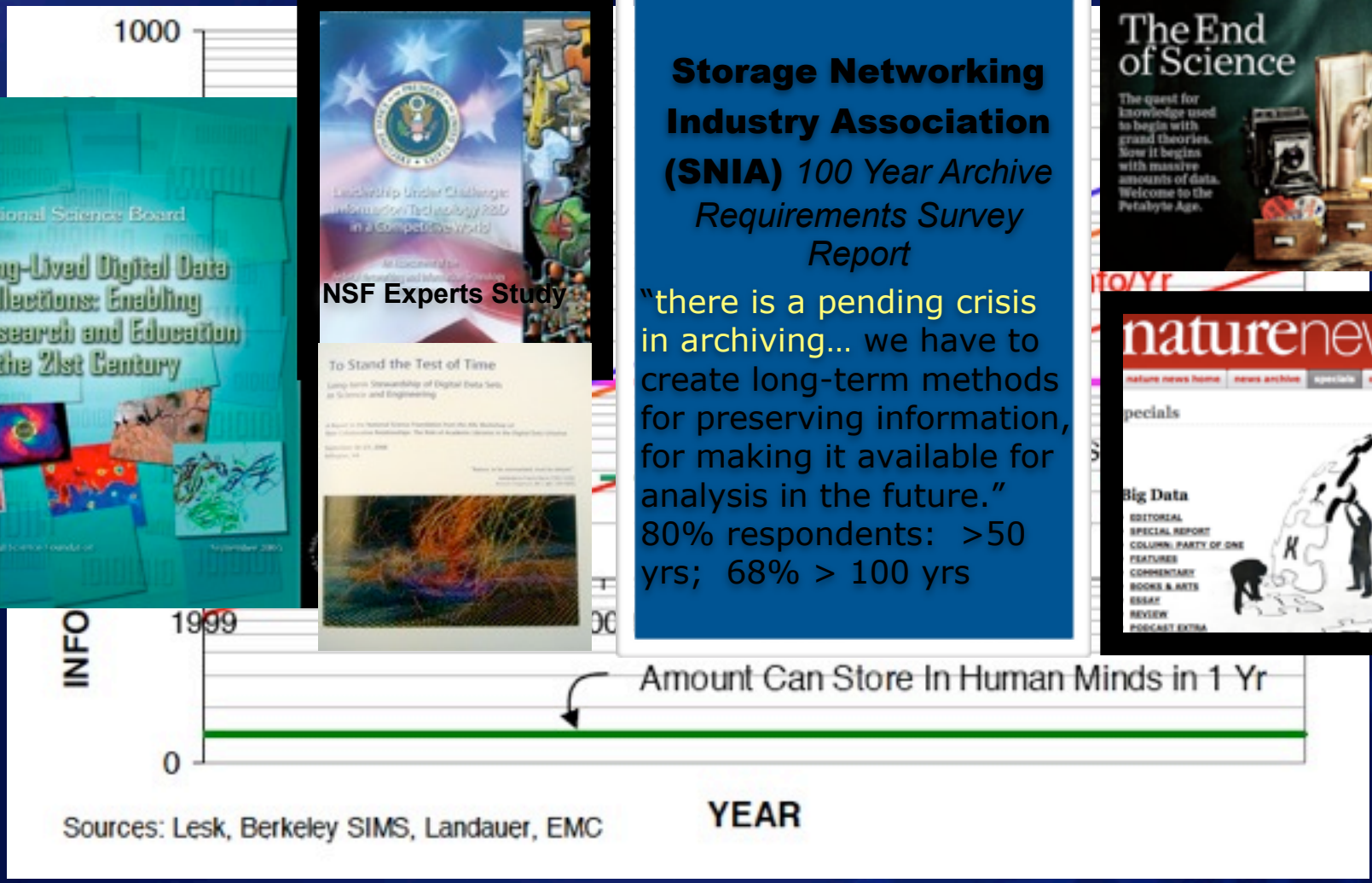
PCAST Digital Data

Industry

Wired, Nature

Storage Networking Industry Association (SNIA) *100 Year Archive Requirements Survey Report*

"there is a pending crisis in archiving… we have to create long-term methods for preserving information, for making it available for analysis in the future."
80% respondents: >50 yrs; 68% > 100 yrs



Scientific Computing and Imaging Institute, University of Utah

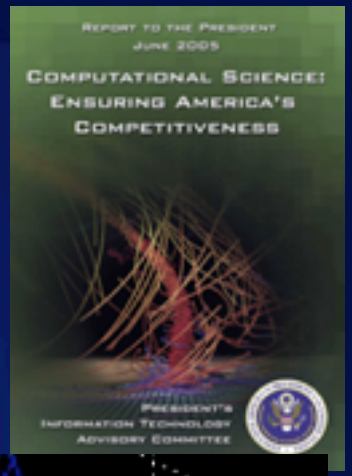
Two More Crises

- Organization for Multidisciplinary & Computational Science
  - "Universities must significantly change organizational structures: multidisciplinary & collaborative research are needed [for US] to remain competitive in global science"
  - "Itself a discipline, computational science advances all science…inadequate/outmoded structures within Federal government and the academy do not effectively support this critical multidisciplinary field"
- Education
  - The CI environment is running away from us!
  - How do we develop a workforce to work effectively in this world?
  - How do we help universities transition?

16

Two More Crises

- Organization for Multidisciplinary & Computational Science
  - "Universities must significantly change organizational structures: multidisciplinary & collaborative research are needed [for US] to remain competitive in global science"



- Education
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  - How do we help universities transition?

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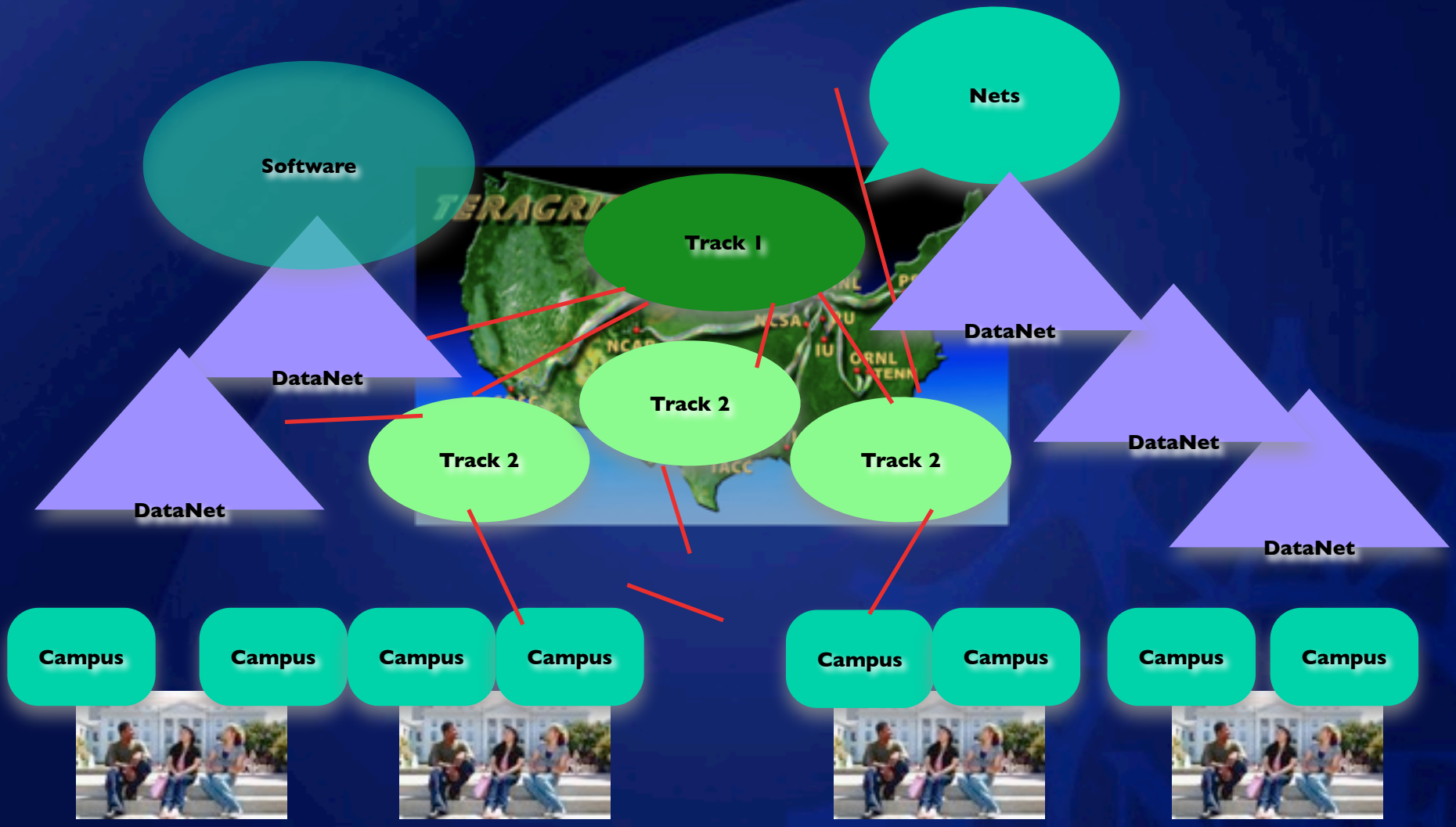
NSF Vision and US National CI Blueprint



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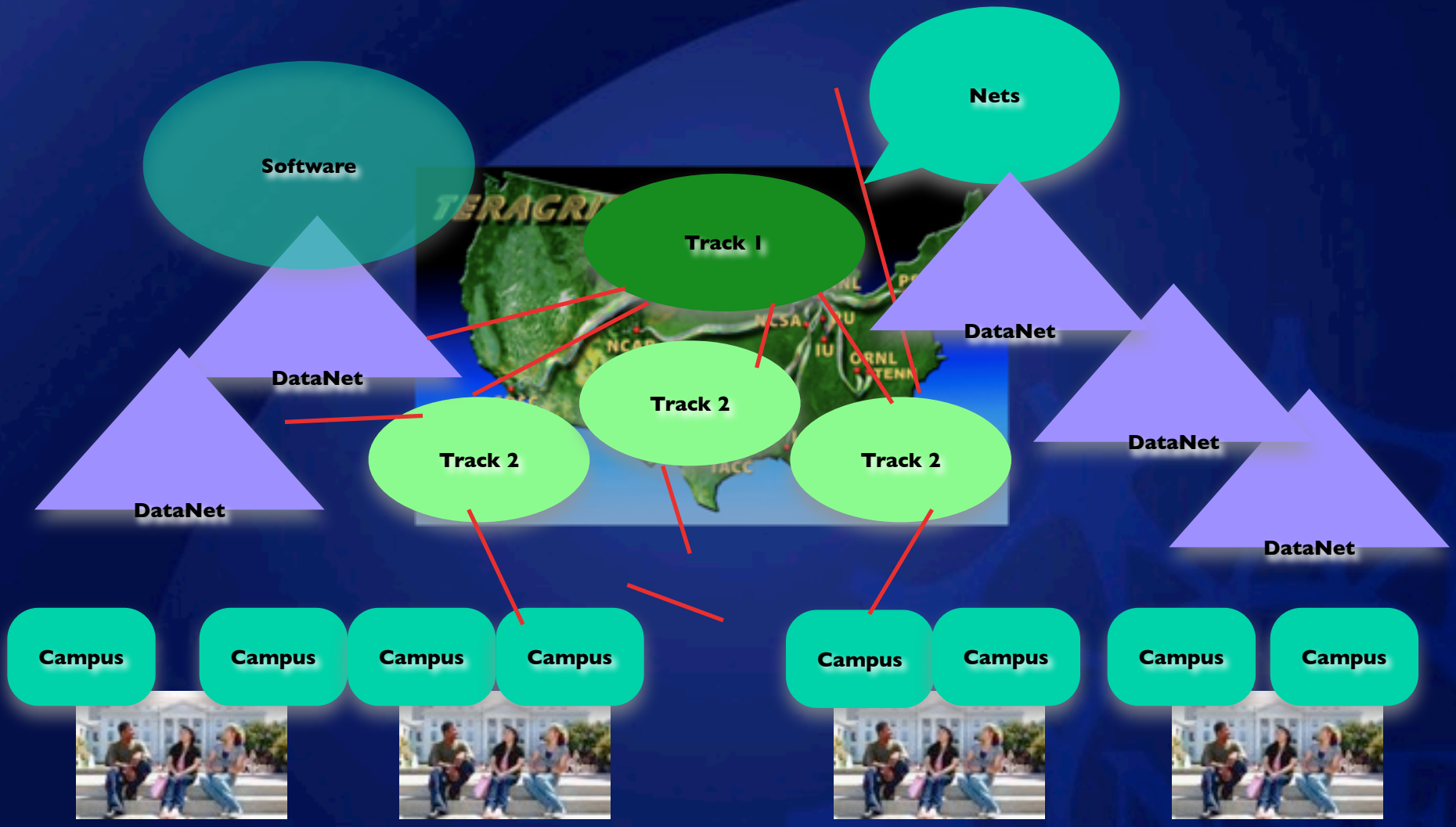
NSF Vision and US National CI Blueprint



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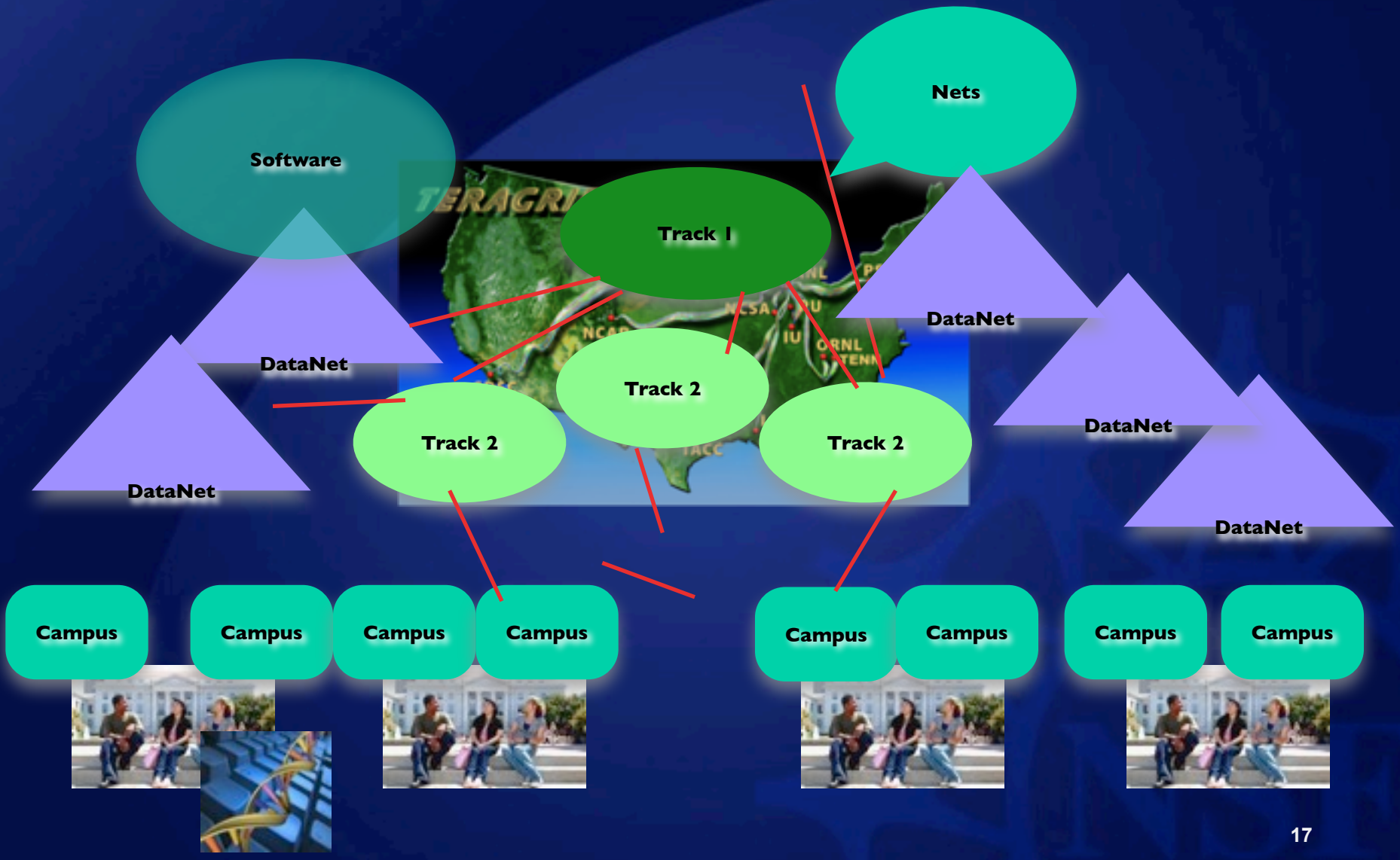

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NSF Vision and US National CI Blueprint

Software

Nets

Track 1

DataNet

DataNet

DataNet

DataNet

Track 2

Track 2

Track 2

Campus

Campus

Campus

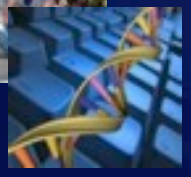
Campus

Campus

Campus

Campus

Campus



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NSF Vision and US National CI Blueprint

Education Crisis: I need all of this to start to solve my problem!

DataNet

DataNet

DataNet

Track 1

Track 2

Track 2

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Campus

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17

NSF Vision and US National CI Blueprint

Education Crisis: I need all of this to start to solve my problem!

DataNet

DataNet

Nets

Track 1

Tra

DataNet

Science demands integration of all components of this ecosystem..

Campus

Campus

Campus

Campus

Campus

17

NSF Vision and US National CI Blueprint

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DataNet

DataNet

DataNet

Track 1

Track 2

Track 2

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Campus

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Campus

Campus

17

NSF Vision and US National CI Blueprint

Education Crisis: I need all of this to start to solve my problem!

Software

neon
National Ecological Observatory Network, Inc.

Nets

Science is becoming unreproducible in this environment. Validation? Provenance? Reproducibility?

DataNet

DataNet

Campus

Campus

Campus

Campus

Campus

Campus

17

The Opportunity!

XSEDE
Extreme Science and Engineering Discovery Environment

- We have critical elements in place for an architecture
  - NSF XSEDE architecture can connect…
    - Campus Bridging: campus to national CI…
      - Campus Assets: MRI, Instruments, DNA sequencers…
      - Campus: InCommon, Gateways, Open Science Grid
      - Campus Applications: SI2, SAGA, etc…
      - Networks: end-to-end connectivity
      - Middleware, e.g. Globus Online
    - Facilities to campuses…
      - MREFC: telescopes, accelerators, light sources, …"More silicon than Steel"
      - NEON, OOI, LSST, etc…how to integrate?
    - International (e.g., LHC), Commercial (e.g., Clouds) to local
  - XSEDE can enable…

Dumped On by Data? Scientists Say a Deluge Is Drowning Research

18

Part 3: Recommendations

19

ACCI Task Force Reports

- Final recommendations presented to the NSF Advisory Committee on Cyberinfrastructure Dec 2010
- More than 25 workshops and Birds of a Feather sessions, 1300 people involved
- Final reports on-line

"Permanent programmatic activities in Computational and Data-Enabled Science & Engineering (CDS&E) should be established within NSF." Grand Challenges Task Force

"NSF should establish processes to collect community requirements and plan long-term software roadmaps" Software Task Force

"NSF should fund interdisciplinary research on the science of broadening participation" Cyberlearning Task Force

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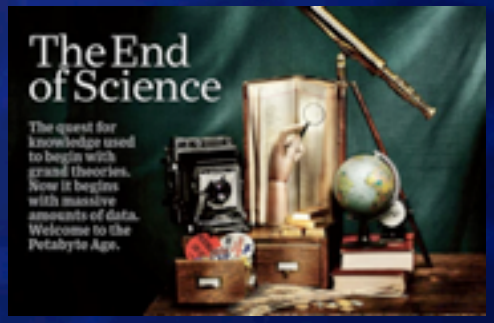
Part 4: Focus on Data

21

The Shift Towards a "Sea of Data"
Implications

- Science & society are now data-dominated
  - Experiment, computation, theory
  - Fourth paradigm
  - US mobile phone traffic exceeded 1 exabyte!
- Classes of data
  - Collections, observations, experiments, simulations
  - Software
  - Publications
- Totally new methodologies
  - Algorithms, mathematics, culture
- Data become the medium for
  - Multidisciplinarity, communication, publication…science [22]



The Shift Towards a "Sea of Data" Implications

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  - [illegible]
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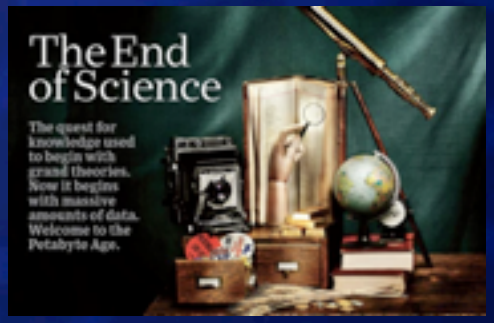
Fundamental questions become focused around data: How to remove boundaries? How to incentivize sharing?



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How do we attribute credit for this new publication form? How are data peer reviewed? What is a publication in the modern data-rich world?

22

Recent NSF Activities on Data Policy and Implementation

23

Fundamental points on data and publication policy

- Communities work together/advance through sharing of data, pubs & software (which is data)
- Publicly funded scientific data and publications should be available, and science benefits
- There has to be a place to keep data, and a way to access it
- There needs to be an affordable, sustainable cost model for this

24

Fundamental points on data and publication policy

- Communities work
  sharing of data, p
- Publicly funded s
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- There has to be a pl
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What data must be made available? Raw data? Peer reviewed? When is it available? 6 months? 1 year? After publication?

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Where is it placed? Author web site? Library? NCSA? EU repository?

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Who pays? Agency? The Institution? What is the cost model? What is reasonable?

Where is it placed? Author web site? Library? NCSA? EU repository?

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Fundamental points on data and publication policy

How long is it made available? How do we enforce/serve it post-award?

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- The pla

Where is it placed? Author

There is great variability in requirements across science communities: app driven concept

24

Changes Coming at NSF for Data!

- Data are becoming:
  - Primary means of communication through sharing
  - Major product of research (including publication)
- Long-standing NSF Policy on Data:
  - "Investigators are expected to share with other researchers, at no more than incremental cost and within a reasonable time, the primary data... created or gathered in the course of work under NSF grants"
- NSF now requires a Data Management Plan (DMP):
  - 2-page supplement to the proposal
    - subject to peer review; criterion for award
  - Not possible to submit proposals without DMP
- National Science Board beginning to examine policy

25

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Sharing data, software will be needed for both interdisciplinary work and reproducibility. We need a national data infrastructure!

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Critical Lessons to Take Home

- Comprehensive approach needed to address complex problems of 21st century
  - All elements must be addressed, not just a few; can't even start to address problems without all
  - Many exponentials: data, compute, collaborate
- Data-intensive science increasingly dominant
  - Modern data-driven CI presents numerous crises, opportunities; long tail and grand challenge communities
  - Impacts CI from campus to facility
  - Policy changes needed; publication, reproducibility
- Academia and Agencies must address
  - Rethinking Academic Structures, Curriculum, P&T