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Dan Fay

Microsoft* **Research** Connections



MSR eScience Workshop Looking Back 8 yrs to the Beginning



Scientific Data Intensive Computing Workshop 2004

- Keynote: 20 Questions to a Better Application Jim Gray
 Online Science the New Computational Science
- Talk: Data Explosion: Astrophysics with Terabytes of Data
 Alex Szalay

Online Science the New Computational Science

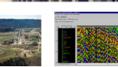
Information Avalanche

- In science, industry, government,....
 - -better observational instruments and
 - and, better simulations producing a data avalanche



- BaBar: Grows 1TB/day
 2/3 simulation Information
 1/3 observational Information
- CERN: LHC will generate 1GB/s .~10 PB/y
- VLBA (NRAO) generates 1GB/s today
- Pixar: 100 TB/Movie
- · New emphasis on informatics:
 - Capturing, Organizing,
 Summarizing, Analyzing, Visualizing





P&E Gene Sequencer Fro



Publishing Data

Roles Traditional Emerging
Authors Scientists Collaborations
Publishers Journals Project www site
Curators Libraries Bigger Archives
Consumers Scientists Scientists

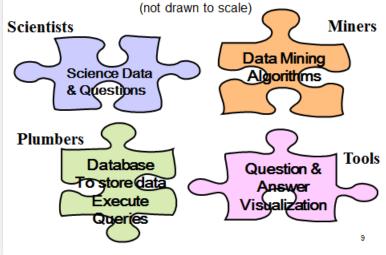
- Exponential growth:
- Projects last at least 3-5 years
- Data sent upwards only at the end of the project
- Data will never be centralized
- · More responsibility on projects
 - Becoming Publishers and Curators
 - Often no explicit funding to do this (must change)
- Data will reside with projects
 - Analyses must be close to the data (see later)
- Data cross-correlated with Literature and Metadata

Global Federations

- Massive datasets live near their owners:
 - Near the instrument's software pipeline
 - Near the applications
 - Near data knowledge and curation
- · Each Archive publishes a (web) service
 - Schema: documents the data
 - Methods on objects (queries)
- · Scientists get "personalized" extracts
- · Uniform access to multiple Archives
 - A common global schema

Federation

What's X-info Needs from us (cs)



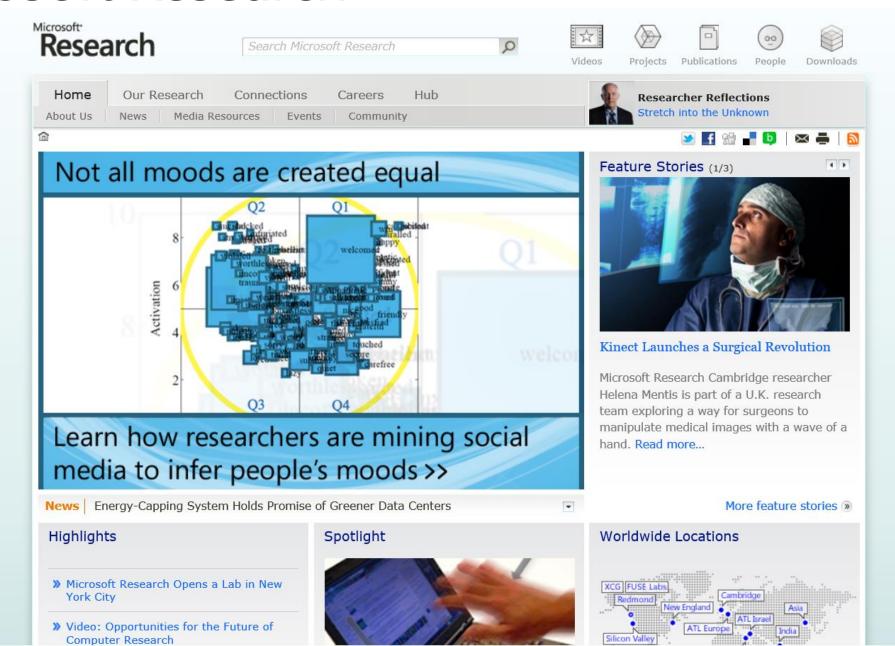
How to Help?

- Can't learn the discipline before you start (takes 4 years.)
- Can't go native you are a CS person not a bio,... person
- Have to learn how to communicate Have to learn the language
- Have to form a working relationship with domain expert(s)
- · Have to find problems that leverage your skills

Call to Action

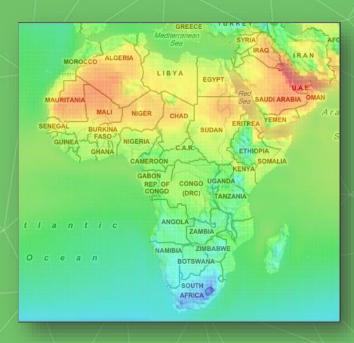
- X-info is emerging.
- · Computer Scientists can help in many ways.
 - Tools
 - Concepts
 - Provide technology consulting to the commuity
- · There are great CS research problems here
 - Modeling
 - Analysis
 - Visualization
 - Architecture

Microsoft Research



Earth, Energy & Environment



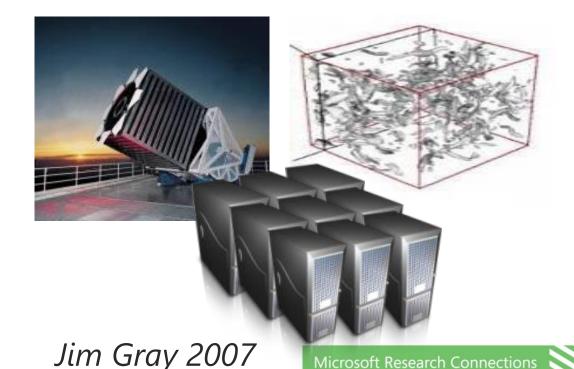


- Visualizing and Experiencing E³ Data + Information: Provide a unique experience to reduce time to insight and knowledge through visualizing data and information
- Accessible Data: Ensure \mathcal{E}^3 data (remote and local sensing) is easily discoverable, accessible and consumable in the scientists domain
- Enabling Scientific Collaboration: Look at new ways to enable collaboration in scientific virtual organizations

Emergence of a Fourth Paradigm

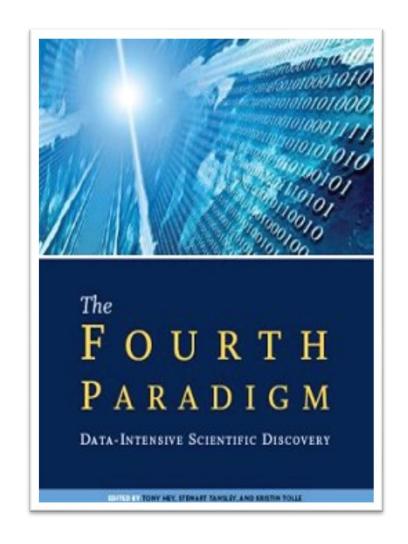
- Thousand years ago Experimental Science
 - Description of natural phenomena
- Last few hundred years Theoretical Science
 - Newton's Laws, Maxwell's Equations...
- Last few decades Computational Science
 - Simulation of complex phenomena
- Today Data-Intensive Science
 Scientists overwhelmed with data sets
 from many different sources
 - Data captured by instruments
 - Data generated by simulations
 - Data generated by sensor networks
 - eScience is the set of tools and technologies to support data federation and collaboration
 - For analysis and data mining
 - For data visualization and exploration
 - For scholarly communication and dissemination

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - K\frac{c^2}{a^2}$$



Changing Nature of Discovery

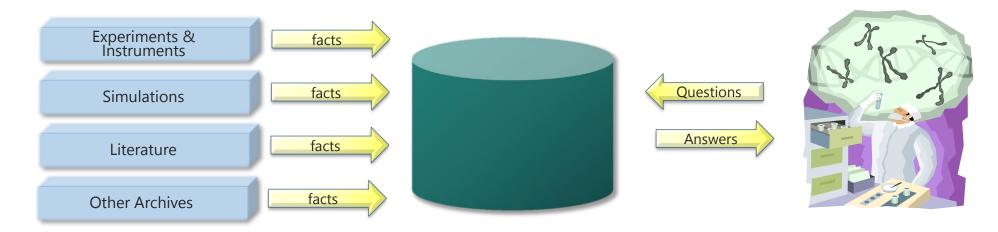
- Complex models
 - Multidisciplinary interactions
 - Wide temporal and spatial scales
- Large multidisciplinary data
 - Real-time steams
 - Structured and unstructured
- Distributed communities
 - Virtual organizations
 - Socialization and management
- Diverse expectations
 - Client-centric and infrastructure-centric



http://fourthparadigm.org

The Problem for the e-Scientist

How to codify and represent our knowledge



The Generic Problems

- Data ingest
- Managing a petabyte
- Common schema
- How to organize it
- How to reorganize it
- How to share with others

- Query and Vis tools
- Building and executing models
- Integrating data and Literature
- Documenting experiments
- Curation and long-term preservation

EOS Article: Mountain Hydrology, Snow Color, and the Fourth Paradigm by Jeff Dozier

Eos, Vol. 92, No. 43, 25 October 2011



VOLUME 92 NUMBER 43 25 OCTOBER 2011 PAGES 373–384

hard-won, long-term data do show trends

Mountain Hydrology, Snow Color, and the Fourth Paradigm

PAGES 373-37

The world's mountain ranges accumulate substantial snow, whose melt produces the bulk of runoff and often combines with rain to cause floods. Worldwide, inadequate understanding and a reliance on sparsely distributed observations limit our ability to predict seasonal and paroxysmal runoff as climate changes, ecosystems adapt, populations grow, land use evolves, and societies make choices.

To improve assessments of snow accumulation, melt, and runoff, scientists and community planners can take advantage of two emerging trends: (1) an ability to remotely sense snow properties from satellites at a spatial scale appropriate for mountain regions (10- to 100-meter resolution, coverage of the order of 100,000 square kilometers) and a daily temporal scale appropriate for the dynamic nature of snow and (2) The Fourth Paradigm [Hey et al., 2009], which posits a new scientific approach in which insight is discovered through the manipulation of large data sets as the evolutionary step in scientific thinking beyond the first three paradigms: empiricism, analyses, and simulation. The inspiration for the book's title comes from pioneering computer scientist Jim Gray, based on a lecture he gave at the National Academy of Sciences 3 weeks before he disappeared at sea.

Water From the Mountain Snowpack

Of the seasonal changes that occur on Earth's land surface, the most profound are accumulation and melt of snow, filling rivers and recharging aquifers that support downstream ecosystems and supply water for 20% of Earth's population. These high, miditalitude snowpacks are at risk because a warming climate would change some snowfall to rainfall and deliver runoff months before demand. Management of this water for competing requirements (flood control, irrigation, hydropower, recreation, and habitat) now uses assessments of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow storage and the plausible rate of melt. Even in one that the control of the snow stor-

By J. Dozer

well-instrumented basins, seasonal forecasts are sometimes wrong, in the Sierra Nevada's American River, for example, the median error of the 1 April forecast of the April-luly runoff is 18%; 1 year out of every 5 exhibits an error that reaches nearly 40%. Comparison between forecasts and river flows shows that the maximum error from 1990 to 2011 was 129% (Figure 1). Worldwide, mountain ranges like the flindu Kush, Iren Shan, Karakoram, Himalayas, and Andes pose formidable difficulties even for rough estimates.

Manual and automated ground measurements of snow water equivalent—all on nearly flat ground and many in forest clearings—do not represent snow on the landscape. Historically, water managers assumed that ground measurements provide some index to the actual volume of water, but established forecasting methods depend on statistical relations developed while land use and climate have been changing. Rich, already, but statistical uncertainty will get worse as the past becomes less represent tive of the present [Milly et al., 2008]. Thus scientists and water managers need physi cally based approaches that account for topographic heterogeneity and estimate th volume of water in basin-wide snow, relative to historical trends and extremes. Some mountain regions where snow falls contain austere infrastructure, meager gaug ing, challenges of accessibility, and emer ing or enduring insecurity related to water resources, Remote sensing, models, and data-intensive analyses offer opportunities to address this need. Similar methods can be applied to Earth's polar and subpolar

The Significance of the Color of Snow

If human eyes were sensitive to radiation through the whole solar spectrum, snow would be one of nature's most "colorful" surface covers, whose spectral reflectivity varies as snow crystals change size and shape and gather dust or soot [Dozier et al., 2009]. Satellike borne sensors such as the Landsat

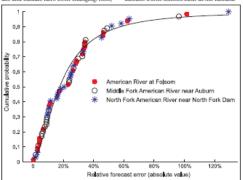
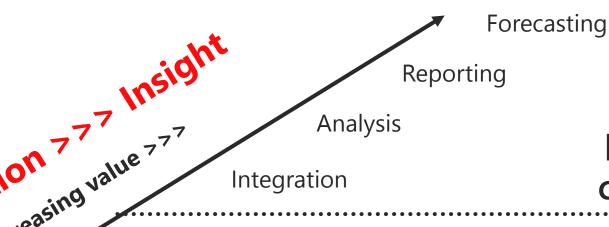


Fig. J. Errons in the 1 April Forecast for April-July rumol in the American Rices, 1900–2011, based on gauges at Aubum and Folsom, in California. Note that the median error is 18% and the 80th percentile (1 year in 5) error is 39%. The plot was generated from information from the California

Snow is one of nature's most colorful materials (Landsat Thematic Mapper snow & cloud) Spatially distributed snow water equivalent SWE, mm 4500 2500 1900 1300 600 (N. Molotch) 04/10/05 wiicroson: Research Connections Information about water is more useful as we climb the value ladder





Done poorly, but a few notable counter-examples

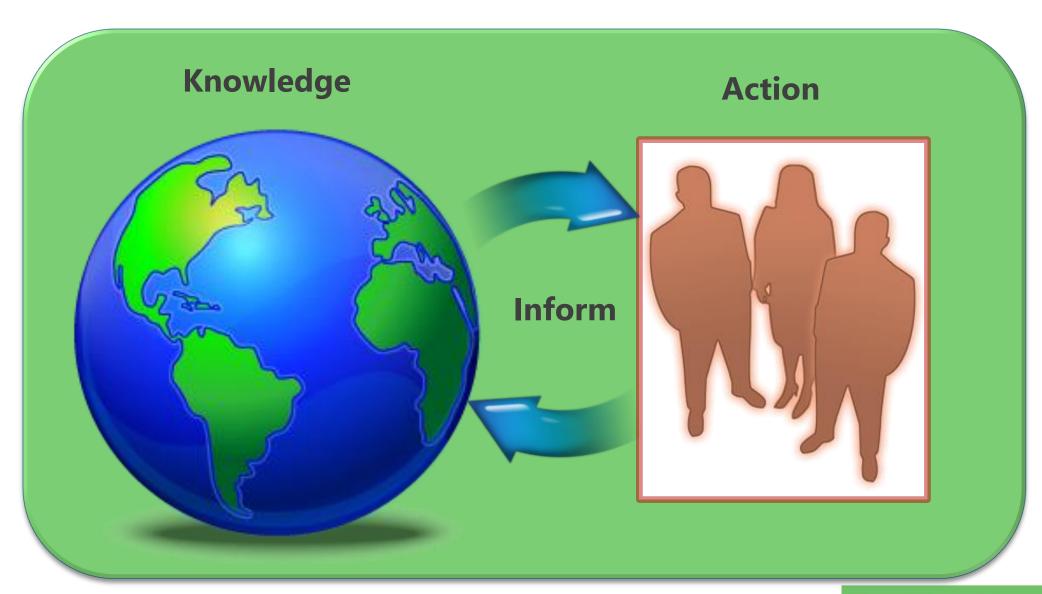
Data 777 Information 777 In. Distribution Collation Monitoring

Done poorly to moderately, not easy to find

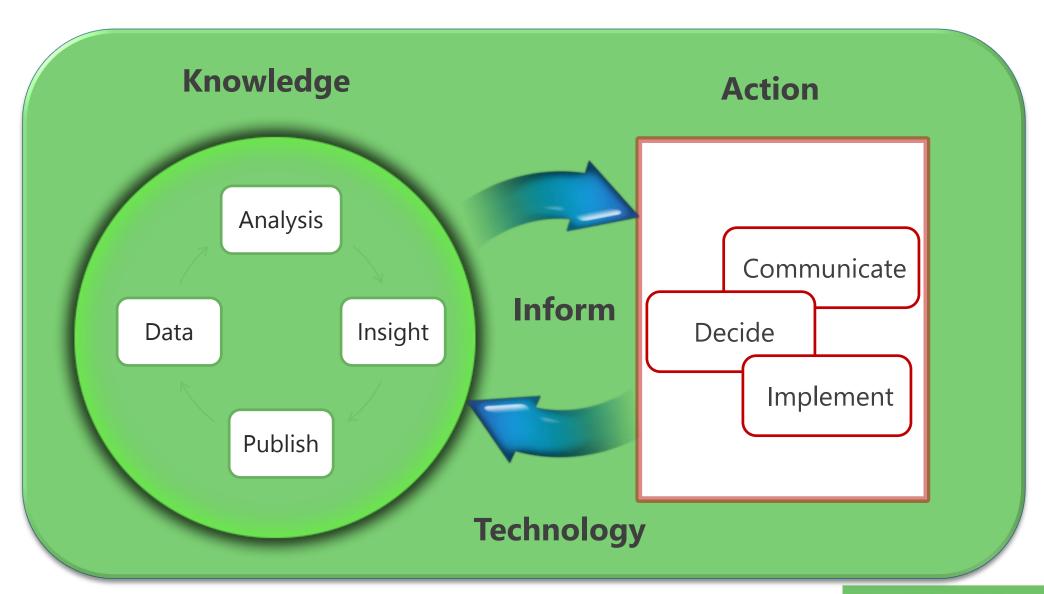
Sometimes done well, generally discoverable and available, but could be improved

(I. Zaslavsky & CSIRO, BOM, WMO)

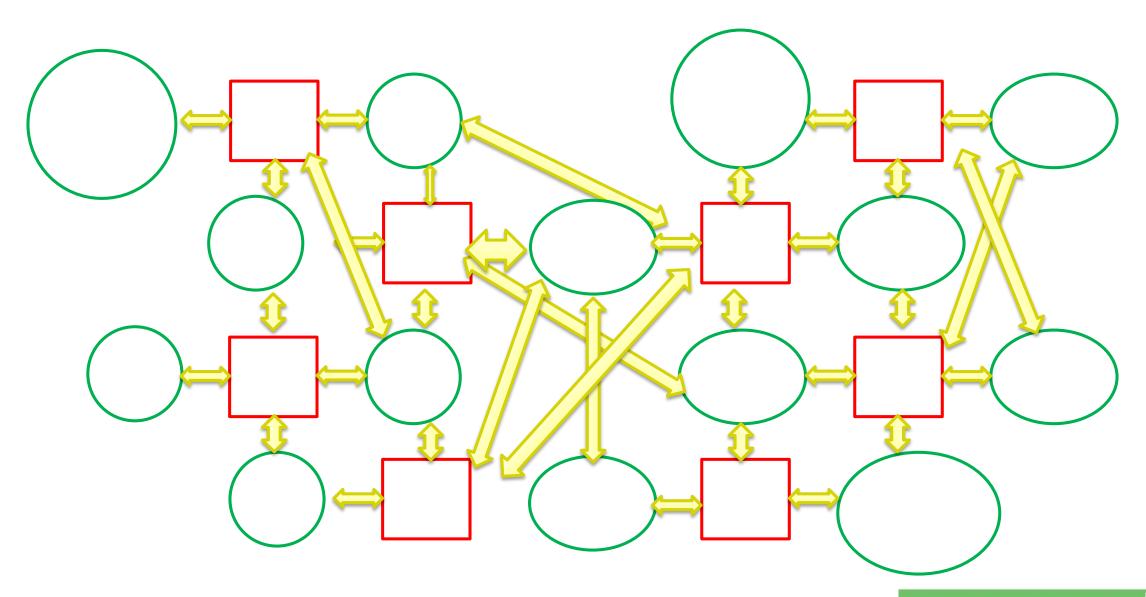
Environmental Ecosystem



Environmental Ecosystem

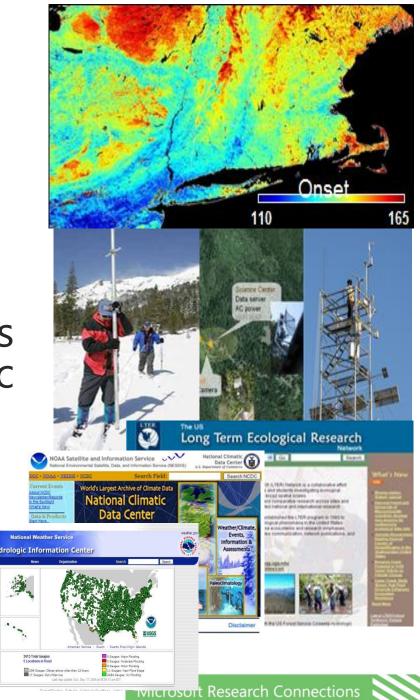


Information ecosystem: It is chaotic, unstructured and ad hoc



The Ecological Data Flood

- We're living in a perfect storm of remote sensing, cheap ground-based sensors, internet data access, and commodity computing
- Yet deriving and extracting the variables needed for science remains problematic
 - Specialized knowledge for algorithms, internal file formats, data cleaning, etc, etc
 - Finding the right needle across the distributed heterogeneous and very rap growing haystacks



Data Variety – The Spice of Life



Manual Measurement



Automated Measurement



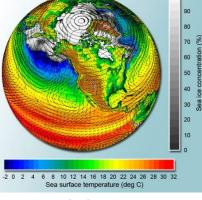
Sample Collection



Typing



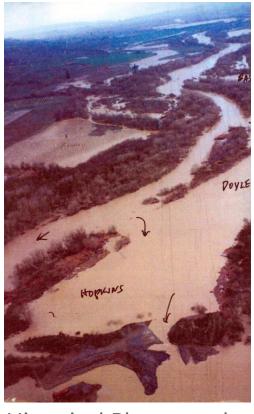
Aircraft Surveys



Model Output



Counting



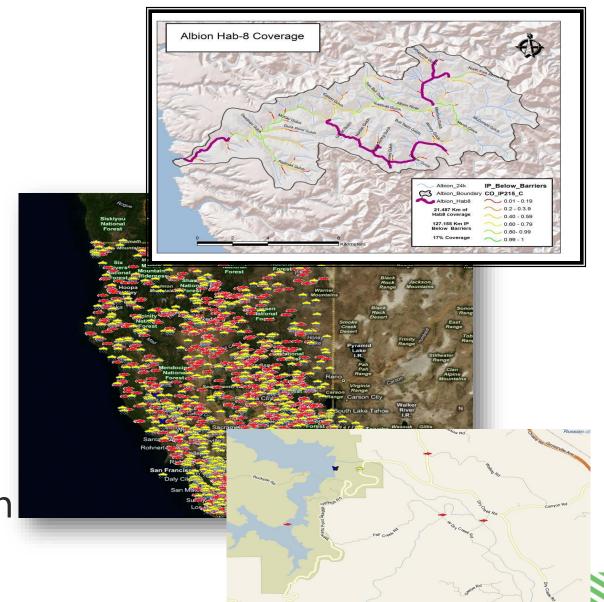
Historical Photographs



Satellite

Data Integration Challenges

- Regular rasters, points, and spatial features
- Time series and intermittent
- Vocabulary meanings (ontology)
- Sparse in time, duration, or location
- Science variable derivation
- Gaps
- Spatial/temporal harmonization



Why Make this Distinction?

Provenance and trust widely varies

Data acquisition, early processing, and reporting ranges from a large government agency to individual scientists.

Smaller data often passed around in email; big data downloads can take days (if at all)

Data sharing concerns and patterns vary

Open access followed by (non-repeatable and tedious) pre-processing

True science ready data set but concerns about misuse, misunderstanding particularly for hard won data.

Computational tools differ.

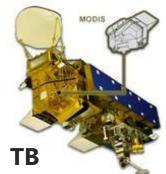
Not everyone can get an account at a supercomputer center

Very large computations require engineering (error handling)

Space and time aren't always simple dimensions









Complex shared detector

Simple instrument (if any)

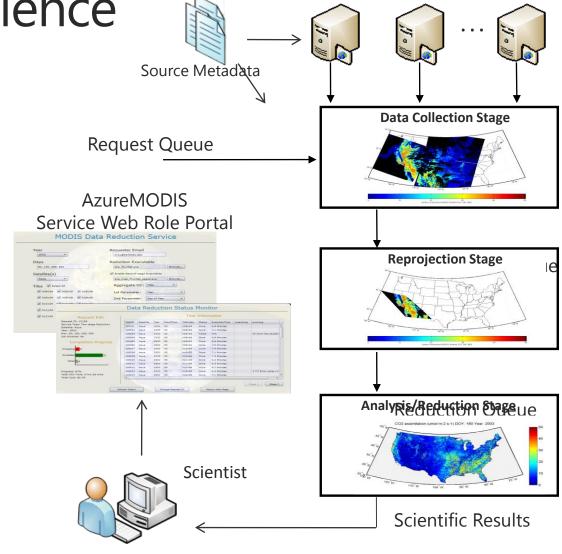
Science happens when PBs, TBs, GBs, and KBs can be mashed up simply

Complex and Heavy process by experts

Ad hoc observations and models

AzureMODIS – Azure Service for Remote Sensing Geoscience

- Science pipeline for download, initial processing, and reduction of satellite imagery. Developed by MSR, UVa, UCB.
- Dramatically lowers resource and complexity barriers to use satellite imagery for terrestrial hydrology and geoscience.
 - Common imagery location determination and upload from diverse sources
 - Optional scientist-provided reduction algorithm (.NET, Java, or MatLab)
 - On-demand scalability beyond local desktop or cluster
- In use now to compute 10 year continental scale water balance for North America. Per year:
 - 500 GB (~60K files) upload of 9 different source imagery products from 15 different locations
 - 400 GB reprojected harmonized imagery consuming ~3500 cpu hours
 - 5 GB reduced science result leveraging reported field data aggregates consuming ~60 cpu hour



Source Imagery Download Sites



Microsoft Codename "Cloud Numerics"

numerical and data analytics library for data scientists, quantitative analysts, and others



Microsoft Codename "Data Explorer"

organize, manage, mash up and gain new insights from your data.



Microsoft Codename "Data Hub'

Organizationsto curate and publish its data on a private data marketplace



Microsoft Codename "Trust Services"

data encryption services for cloud applications so that they can roam encryption keys in a secure way.







Fetch Climate

Tools

new tools for new science Tools home

Computat

FetchClimate

Inspiration | Features | Try online | Download | Case studies | People | Acknowledgements

Retrieve climatic and environmental information with the click of a button or a few lines of code

FetchClimate is a fast, free, intelligent climate information service that operates over the cloud to return exactly the information you need. FetchClimate can be accessed either through a simple web interface, or via a few lines of code inside any .NET program. FetchClimate is intended to make it easy for you to retrieve information for any geographical region, at any grid resolution: from global, through continental, to a few kilometres, and for any range of years (1900 – 2010), days within the year, and / or hours within the day. FetchClimate can also report the uncertainty associated with the values it returns and list data sources used to fulfil the request. When multiple sources could potentially provide information on the same environmental variable, FetchClimate automatically selects the most appropriate data source. Finally, the entire query you ran can be shared as a single URL, enabling others to retrieve the identical information.

Inspiration

Many environmental science research and applications require information about climate and

Service of the forms of the for

Documentation

- [] Manual & examples for web version []
- Manual & examples for programmatic [pdf]

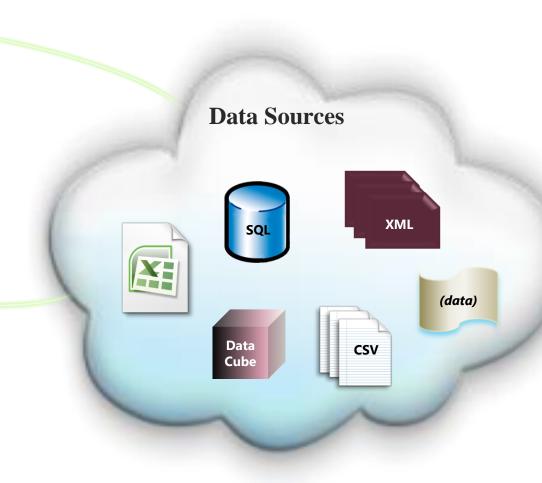


http://fetchclimate.cloudapp.net/

Environmental Informatics Framework (EIF)

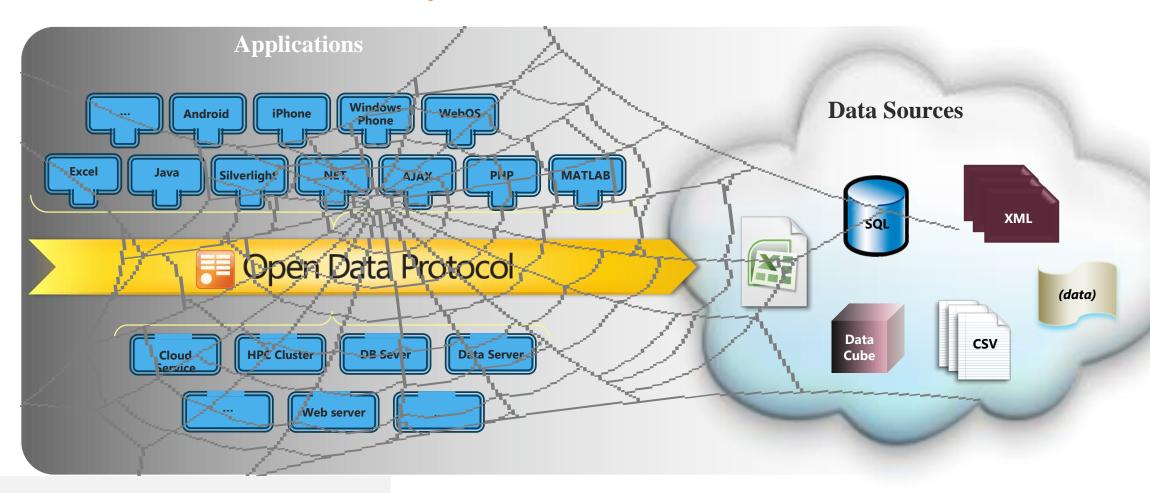
Common Problems with Data

- > To use data from different sources
 - Non-standard formats, scales, and units
 - Lack of data quality control
 - Lack of metadata
 - Difficult to repurpose data for different (my) tools
- > To share data
 - Lack of incentive (no credit)
 - Need extra resources and toois
- > Hidden problems, seldom addressed
 - Versioning
 - Provenance
 - Curation



Environmental Informatics Framework (EIF)

Current State of Data Ecosystem



Environmental Informatics Framework (EIF)

Advance data discoverability, accessibility, and consumability



Open Data Protocol (OData)

http://www.odata.org

It allows you to form URLs based on what you know about the underlying data

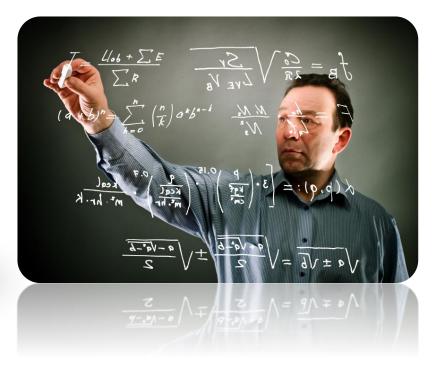
- > A Web protocol for querying and updating data
 - provides a way to unlock your data and free it from data silos
 - does this by building upon Web technologies such as <u>HTTP</u>, <u>Atom Publishing Protocol</u> (AtomPub) and <u>JSON</u> to provide access to information from a variety of applications, services, and stores.
- ➤ In Open Source/Specifications Promise being submitted to OASIS
- > An application of a set of internet standards:
 - □ HTTP.
 - □ Atom (RFC 4287),
 - □ AtomPub (RFC 5023),
 - REST semantics
- Existing standards + easy data access API
- > Added Geospatial data support -
 - □ Feedback from the Community encouraged www.odata.org



New ways to analyze and communicate data







The 'Cosmic Genome' Project

- The Sloan Digital Sky Survey is the first major astronomical survey project:
 - 5 color images of ¼ of the sky
 - Pictures of 300 million celestial objects
 - Distances to the closest 1 million galaxies
- Jim Gray from Microsoft Research worked with astronomer Alex Szalay to build the public 'SkyServer' archive for the survey
- New model of scientific publishing
 - Have to publish the data <u>before</u> astronomers publish their analysis





Public Use of the SkyServer

Posterchild in 21st century data publishing

- 380 million web hits in 6 years
- 930,000 distinct users vs 10,000 astronomers
- 1600 scientific papers
- Delivered 50,000 hours of lectures to high schools
- Delivered 100B rows of data

Citizen Science: GalaxyZoo

- Goal of 1 million visual galaxy classifications by the public
- Allows general public to search for photographs and classify different types of galaxies





World Wide Telescope

Seamless Rich Social Media Virtual Sky and I Web application for science and education

Goals

- Integra
- e Easy ac
- Tours f

Spatial

Updat

A

⊜ Ex

Not ju Being

We in







www.layerscape.org

Powered by WorldWide Telescope

 Community Site for WWT Tours and Layers (Data)

Top Categories

Rating: ***** (2)

Rating: ***** (1)

III Cold Regions

Tags: climate change proxy data, cascades, C

*** Solid Earth

Community: Climate

General Interest

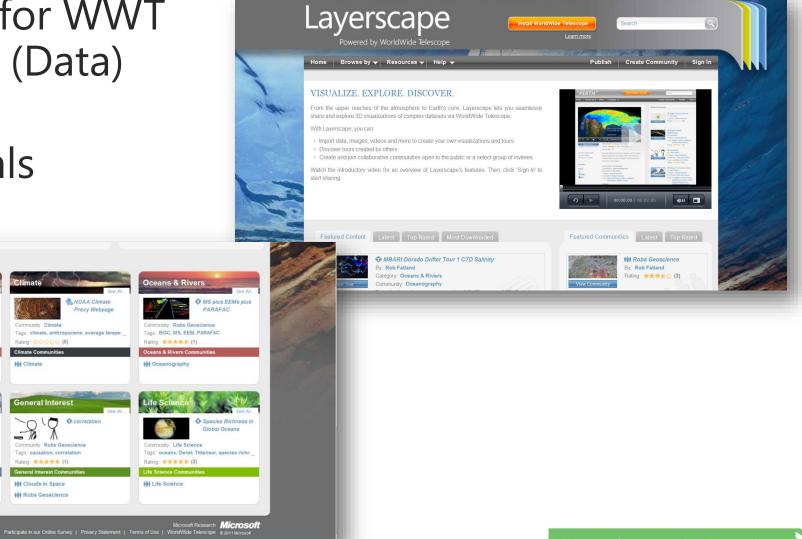
Tags: causation, correlation

Rating ***** (2)

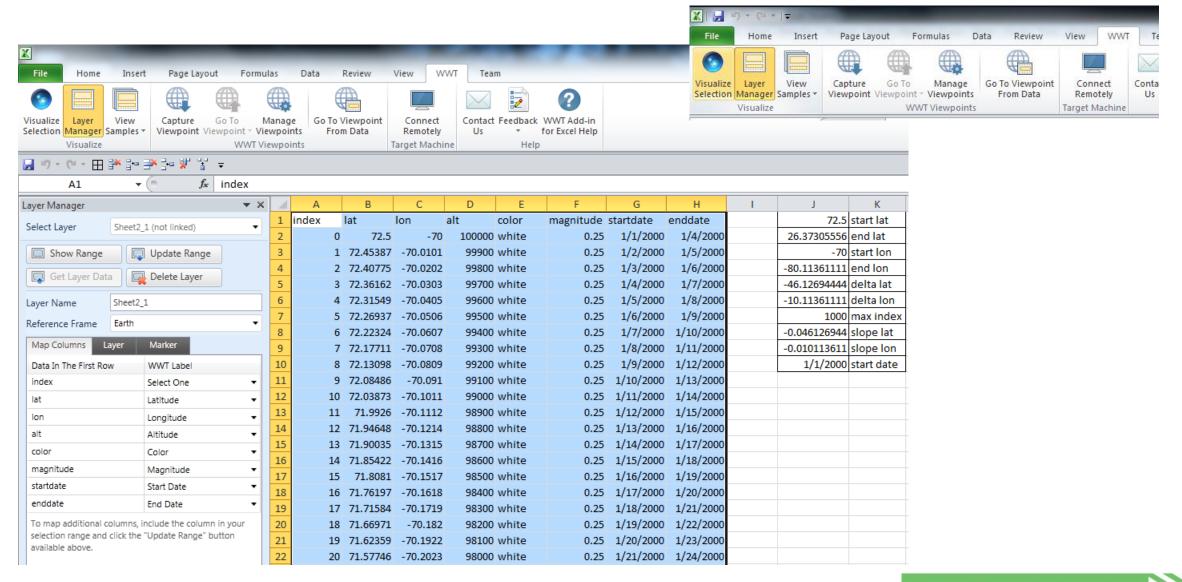
Rating: ***** (1)

††† Clouds in Space (iii) Robs Geoscience

 Sharing by groups/individuals



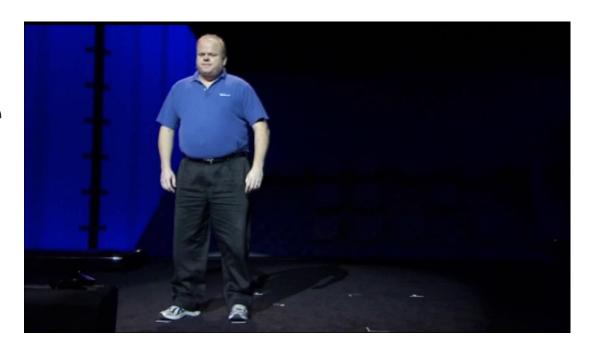
Excel to Visualize in seconds



Natural User Interfaces (NUI) Kinect SDK and WWT

- Rethinking ways in which people will interact with computers/technologies of the future
- Re-evaluating everything from their (non-) physical design to the human needs and interaction models
- Revolutionize the way we think about technology and what it can do on our behalf





Our Next Steps

- Continue to work with Scientists
 - Implement features from feedback
 - le. Netcdf support
 - New clients and User Interface
 - Make it easier to use/create tours
- Cloud: Windows Azure integration Write, Run, or Use Software
 - Write: Platform as a Service
 - Web Sites
 - Storage
 - Languages .Net, Java, Python, PHP, Ruby, NodeJS, C++
 - Run: <u>Infrastructure as a Service</u>
 - Virtual Machines Windows Servers & Linux
 - Connect to on-premises
 - Use: <u>Software as a Service</u>
 - Azure Media Services
 - HPC and Big Data Hadoop, etc
 - Windows Azure Marketplace



October 8–9, 2012 | Chicago, Illinois http://research.microsoft.com/events/escience2012

Data Storage Sustainability?

- Digital Data can be open who should pay the cost?
- Spinning Disks, Bandwidth, Cooling, etc.



No Silver Bullet - What is needed?

- Algorithms that scale
- Data Management from the Start
- Automatic Ancillary Data capture
- Thinking about the Data, and retention
- Data sharing is natural from the start
- Visualization for everyone
- Best practices insights and challenges shared amongst domains
 - le. eScience Workshop, etc

Challenges

- Balancing
 Data Acquisition | Bandwidth | Storage/Processing
- Cross Discipline Collaboration Knowledge sharing
- The data deluge How to manage and analyze information?
- New types of Scientists:
 - Data Collectors & Data Analysis
- Riding the commodity curve
- Technology/Computing in support of Science

