Data Science Methodology Transfer: Space Science to Biomedicine

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Data Lifecycle Model for NASA Missions

From Onboard Computing to Scalable Data Analytics

Emerging Solutions

- Next-Generation
 Flight Computing
- Onboard Data
 Analytics



Observational Platforms and Flight Computing

Scaling Pressures Expose the Need for an Integrated End-to-End Data and Computational Architecture

Emerging Solutions

- Intelligent Ground Stations
- Agile Mission Operations



Ground-based Mission Systems

Emerging Solutions

- Data-Driven Discovery
 from Archives
- Scalable Computation and Storage



Interactive Analytics and Visualization and Decision Support



NASA Data Archives

- NASA captures robust scientific archives of data to support long-term analysis
 - A requirement on every mission
 - Adheres to specific standards (both in terms of structure + description/metadata)
 - Mandates public access after a specified time period
- The capture of well-curated, organized data collections is the basis for enabling data analysis
 - This is a critical precursor step to analysis
 - The scientific community uses these collections as the basis for studies (often grant funded)
 - The development of robust architectures and systems to support data management and data analysis services are emerging
- Evolving from research preservation and stewardship towards driving analysis from these archives...

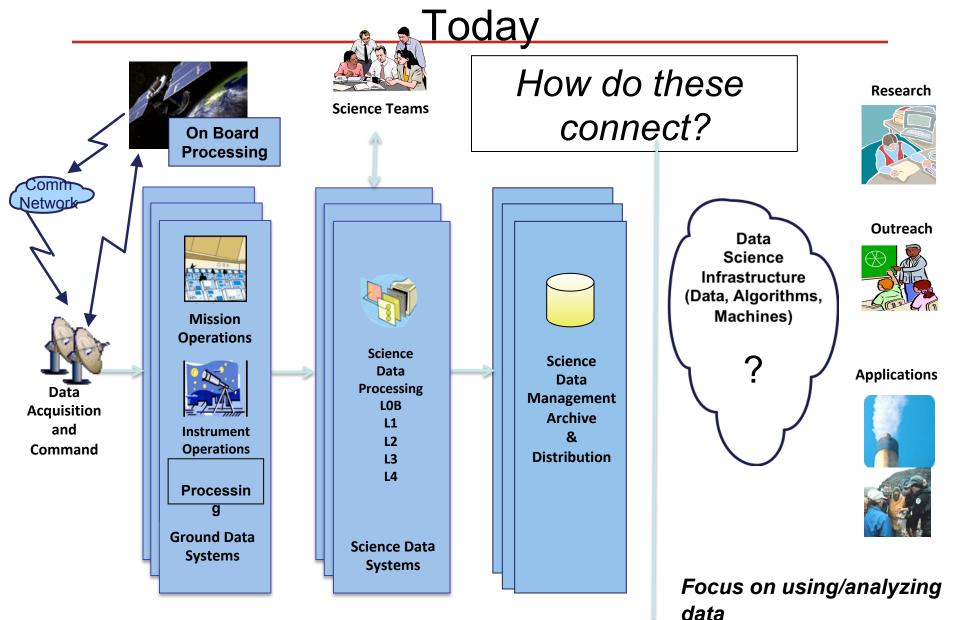


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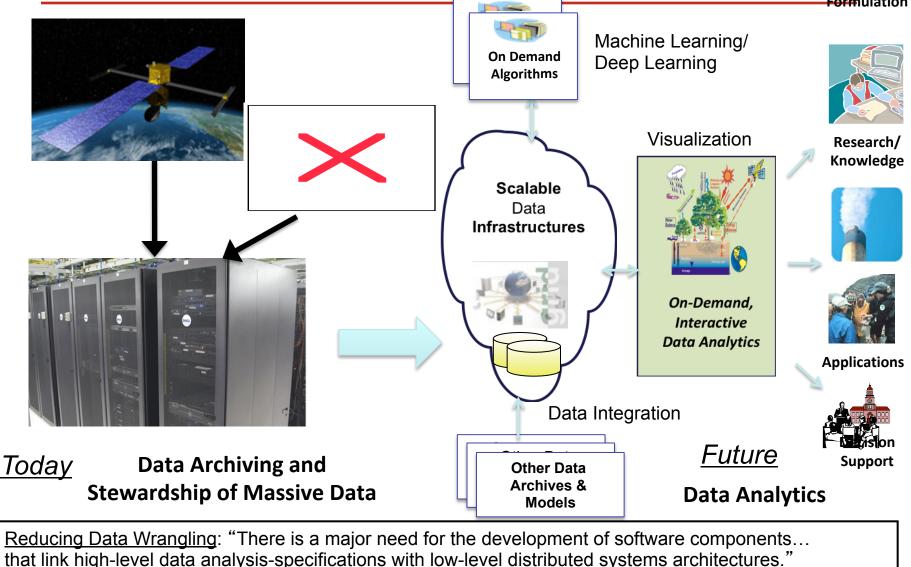
Planetary Science Data Analytics Support



Focus on generating, capturing, managing data

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Expanding to Data-Driven Analytics

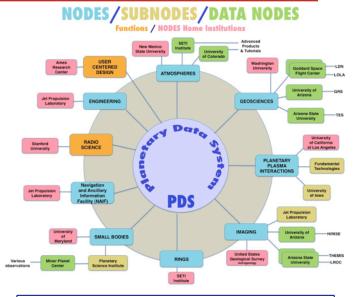


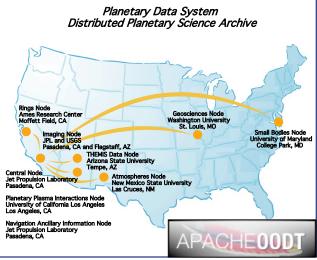
Frontiers in the Analysis of Massive Data, National Research Council, 2013.



Planetary Data System

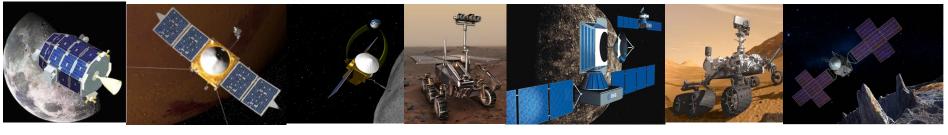
- <u>Purpose</u>: To collect, archive and make accessible digital data and documentation produced from NASA's exploration of the solar system from the 1960s to the present.
- Infrastructure: A highly distributed infrastructure with planetary science data repositories implemented at major government labs and academic institutions
 - System driven by a well defined planetary science ontology
 - Approximately 1.7 PB of data
 - About 4000 different types of data and 40M data products
 - International adoption
 - NASA's de facto archive for all planetary data



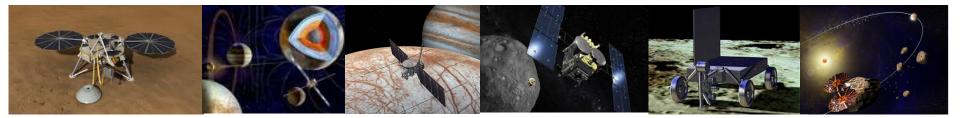




International Collaboration on PDS4 Through IPDA



LADEEMAVENOsiris-RExExoMarsBepiColomboMars 2020Psyche(NASA)(NASA)(NASA)(ESA/Russia)(ESA/JAXA)(NASA)(NASA)



InSight (NASA)

JUICE (ESA)

Europa (NASA) Hyabussa-2 (JAXA) Chandrayaan-2 (ISRO)

Lucy NASA

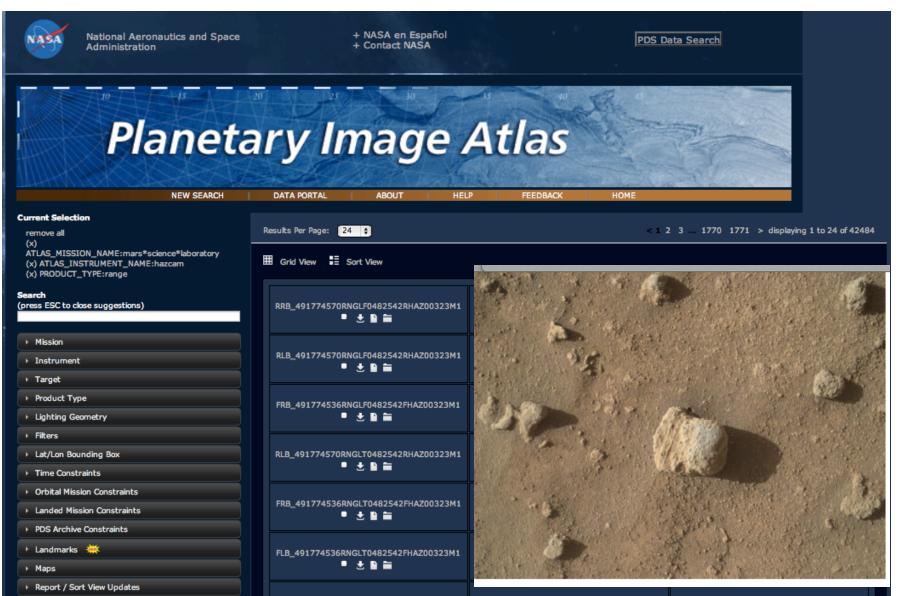
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Endorsed by the International Planetary Data Alliance in July 2012 –

https://planetarydata.org/documents/steering-committee/ipda-endorsements-recommendations-and-actions



Planetary Image Archiving



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Mars Trek: The Google Earth of Mars



sedimentary minerals including clays, sulfates, and salts that

require water to form.

Curiosity Landing Site

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Curiosity landed in Gale Crater on Mars on August 6th, 2012. With a diameter of 154 km and a central peak 5.5 km tail, Gale Crater was chosen as the landing site for the Mars

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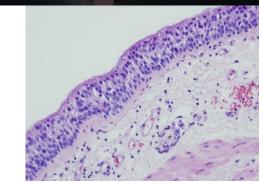
Science Laboratory Curiosity rover. The choice was based on evidence from orbiting spacecraft that indicate that the crater may have once contained large amounts of liquid water. The central peak, Mount Sharp, exhibits layered rock deposits rich in sedimentary minerals including clays, sulfates, and salts that require water to form.

Region Information Download for 3D Printer

NCI/JPL Informatics Collaboration: Crossing Disciplines to Support Scientific Research

- Development of an advanced Knowledge System to *capture*, process, *share* and support *reproducible analysis* for biomarker research
 - Genomics, Proteomics, Imaging, etc data types of data
- NASA-NCI partnership, leveraging informatics and data science technologies from planetary and Earth science
 - Reproducible, Big Data Systems for exploring the universe
 - Software and data science methodology transfer based on JPL open source technologies and architectures





APACHE



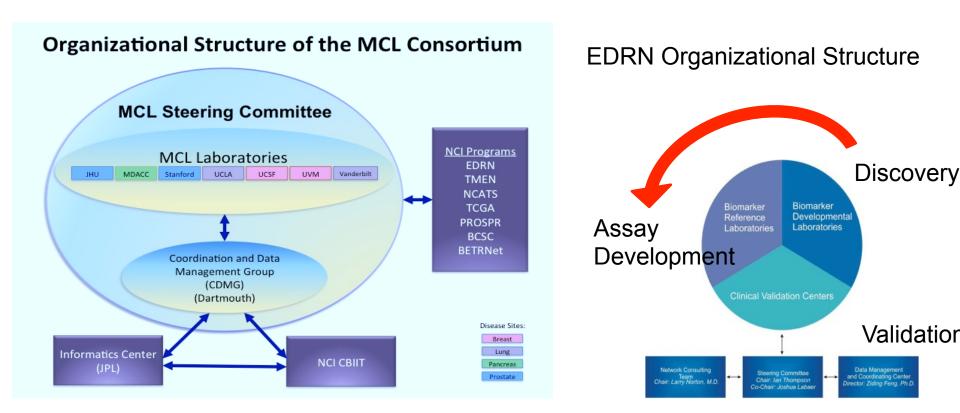


Biomarkers Knowledge Environment

- Integrate diverse research into an online data environment
 - Integrate data as opposed to re-managing data
 - Be agnostic to data formats and structure
- Provide a well architected data management environment that captures, integrates, and shares data for biomarker research including:
 - Biomarkers
 - Biospecimens
 - Validation Study Information
 - Protocol Information
 - Study Results and Data Sets
 - Publications
 - Artifacts supporting collaboration
 - Curated metadata
- Support diverse community needs



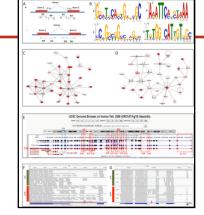
Two Key Programs



Develop cross-cutting informatics capabilities to support the capture, curation, management, distribution, and analysis of diverse data and results

Capture – Process – Search – Access – Analyze - Visualize

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CBIS-DDSM	Rebecca Sawyer Lee	Breast
MD Anderson Pancreas IPMN Images	Anirban Maitra	Pancreas
RNA Sequencing	Chris Arnos	Lung
Team 37 CTIIP Animal Models	Robert D. Cardiff	Breast
O Manage LabCAS		

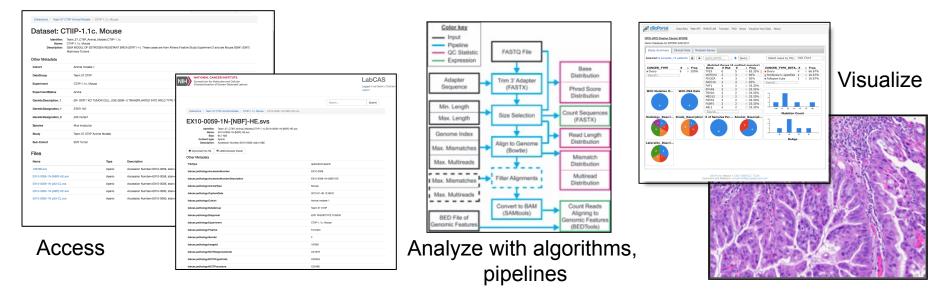


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Capture data and metadata

Process reproducibly

Search Metadata





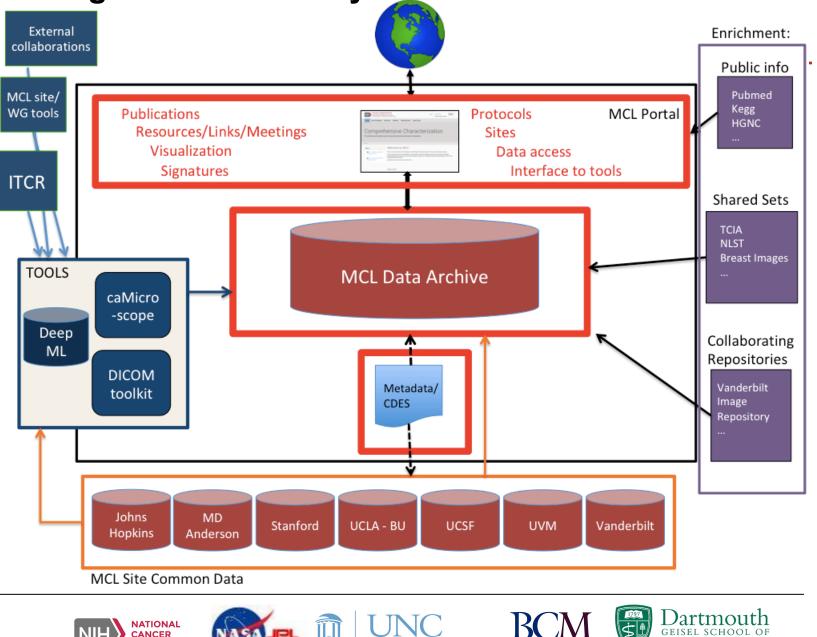


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MCL Integrated Data Ecosystem Overview



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Baylor College of Medicine

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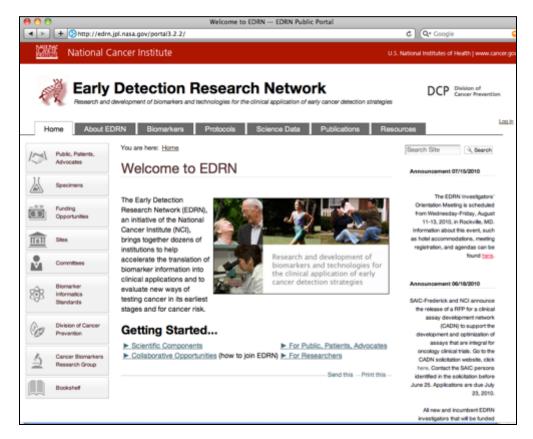
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Portal: Dissemination and Access to Biomarker Data



- Gateway to information
- Information managed both within and outside the knowledge system
- Initial starting point for community to get to research data
- Google-like search to access the wealth of data
- Multi-level Security

http://cancer.gov/edrn http://mcl.jpl.nasa.gov

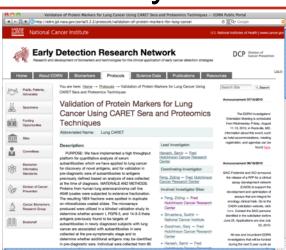


Navigating the Knowledge System: Data Semantically Linked



Biomarker Annotations

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Protocols

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Public Portal

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Early Detection Research Network

Welcome to EDRN

Getting Started...

Entered Strength

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à là	Early Detection Research Network	DCP Division of Cancer Preven
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Home	About EDRN Biomarkers Protocols Science Data Publications F	
new P	You are here: Home → Science Data	Search Site
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Specime	**	
	Captured scientific data results from biomarker studies	The EDRN investigato Orientation Meeting is schedul
ER Opportu	rites The EDRN is involved in researching hundreds of biomarkers. The following is a partial list of associated results from biomarker research that are currently available	from Wednesday-Friday, Aug 11-13, 2010, in Rockville, M
	for access and viewing. The bioinformatics team at EDRN is currently working with	information about this event, su
Tell Dies	EDRN collaborative groups to capture, curate, review and post additional data as it available. EDRN also provides secure access to additional biomarker information no	
Converte	available to the public that is currently under review by EDRN research groups. If yo	
_	have access to this information, please ensure that you are logged in. If you are unsure or would like access, please contact the operator for more information.	Announcement 06/16/2010
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Science Data — EDRN Public Portal

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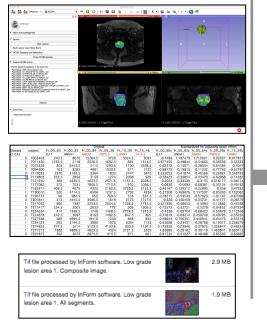
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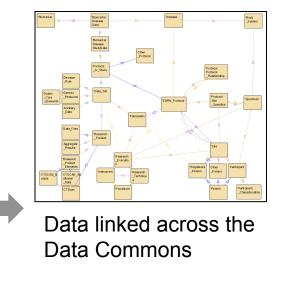
Access to download data

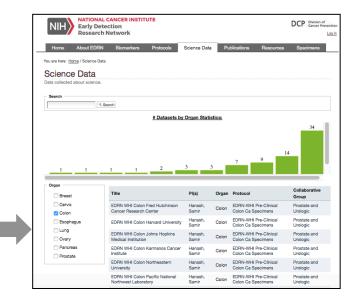


Data Models and Elements

Data generated in the course of research from any source







Data is linked and available for integration of different analytical methods and tools to drive data-driven discovery.

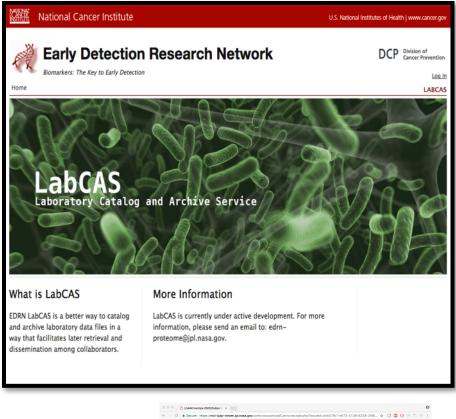
Instruments, etc.

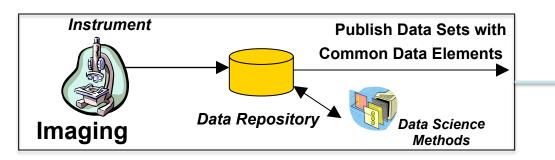
Addition of data sets over time - any data type generated

Drives a consistent data architecture across the consortium.

LabCAS: Capturing and Sharing Science Data Analysis Data and Pipelines

- A secure, reliable means to capture, process and manage data
- Plug in analytical methods
 - Repeatable data processing pipelines
- Integrate visualization

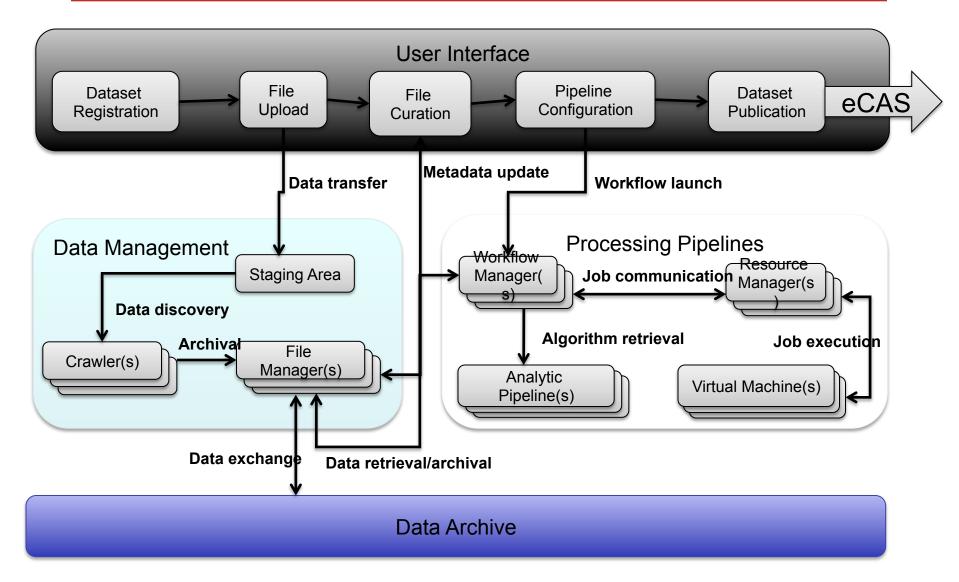






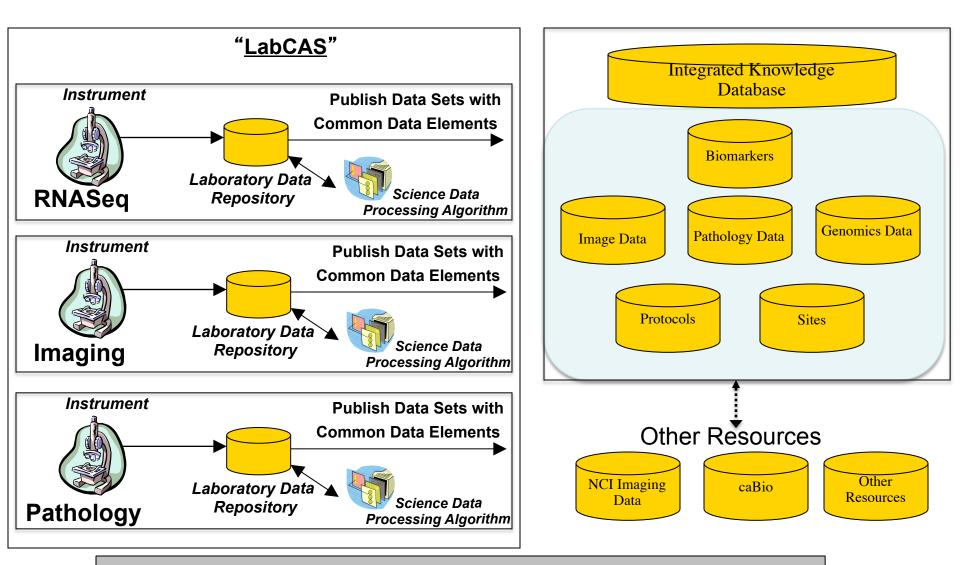


Data Capture, Processing and Ingestion





Data Pipelines and the Knowledge Environment

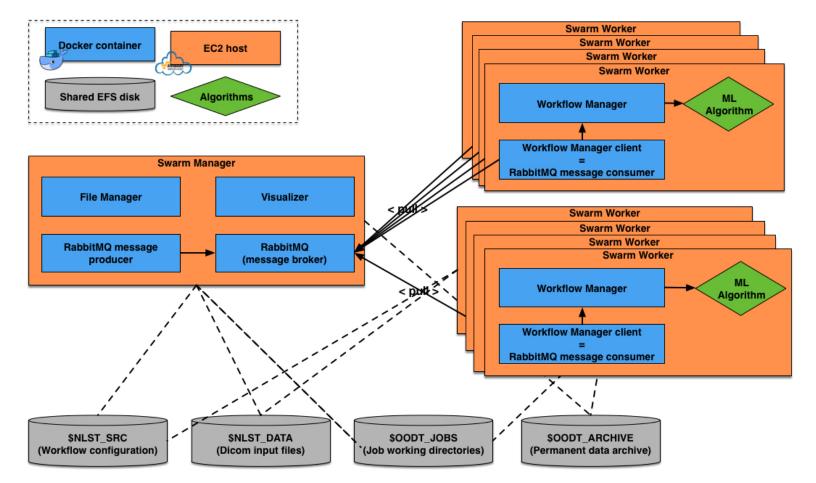


Scalable computing, common data elements, computational methods





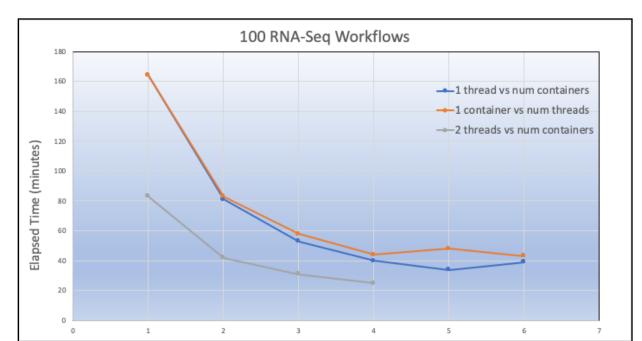
- Uses Docker Swarm, Apache OODT workflows (from NASA/JPL), RabbitMQ messaging
- Can scale/auto-scale to any number of EC2 nodes







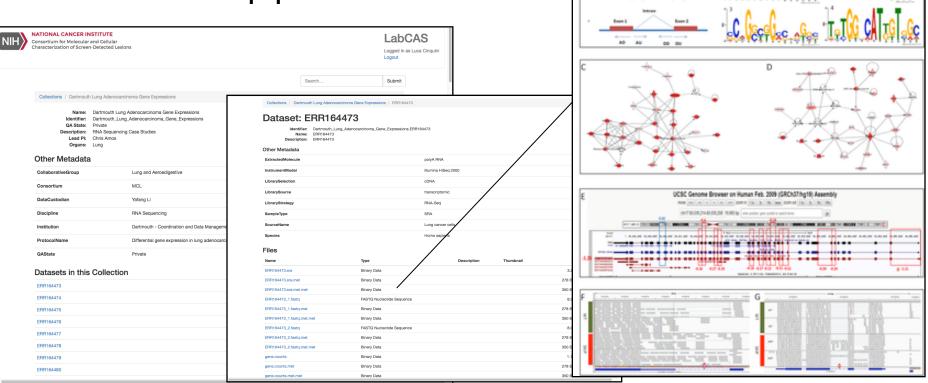
- Executing genomics workflow on single EC2 server (r5.2xlarge, 8 CPUs, 64 GB memory)
- Measuring time to execute 100 workflows vs # of containers, # of processes/container
- Can scale horizontally until processes start to compete for resources







- In collaboration with Dr. Chris Amos, Yafang Lee (Dartmouth)
- 10 TB of data for full study comparing gene expression profiles between smoking and non-smoking patients.
- Integrated Dartmouth analysis tools with 99% accuracy into LabCAS pipelines







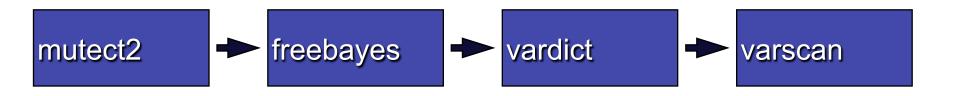
- In collaboration with Robert West, Joseph Foley, Sujen Vennam @ Stanford School of Medicine
- Smart-3SEQ: new method for quantifying gene expressions in small RNA samples including single cells (see: <u>https://github.com/jwfoley/3SEQtools</u>)
- Smart-3SEQ pipeline is composed of 3 steps:
 - FastQ generation and alteration (w/ Illumina bcl2fastq)
 - Gene alignment (w/ Samtools, STAR, UMI-dedup)
 - Read counting (w/ Bioconductors







- In collaboration with Olivier Harismendy at UCSD
 - See https://github.com/bcbio, http://bcbio.io
- Using bcbio ("Bue Collar Bioinformatics"): Python framework and community tools for analysis of biological data (variant calling, RNA-SEQ and small RNA pipelines)
- Experimented with running sample pipelines (big and small)

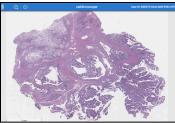




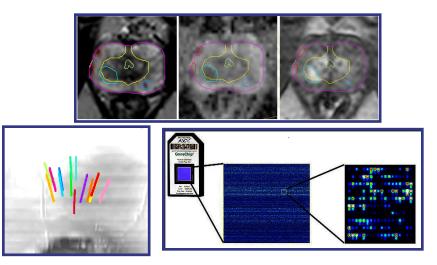
Multi-dimensional Integrated Data

- Collaboration with Sandy Borowsky/UC Davis and Anirban Maitra/ MD Anderson
- Developed a pathology archive for MCL
- Dr. Maitra goal: multi-dimensional data IPMN ppts
 Collaboration with Radka Stoyanova and Alan Pollack
 MAST (Mapped Active Surveillance Trial). Longitudinal
- multivariate data (mpMRI, pathology and gene expression) is
- obtained from patients on Active Surveillance for prostate cancer.

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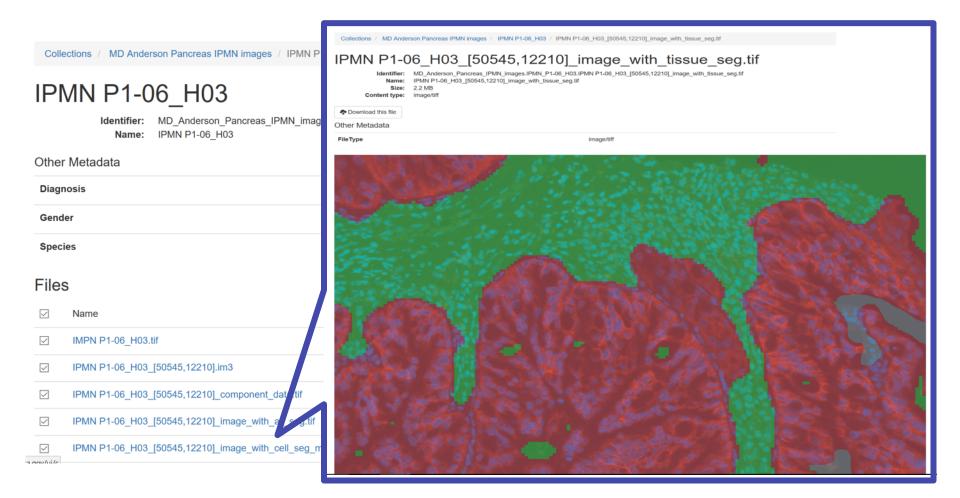


Path Viz Tool Credit: aMicroscope - Dr. Joel Saltz Lab TCR Program





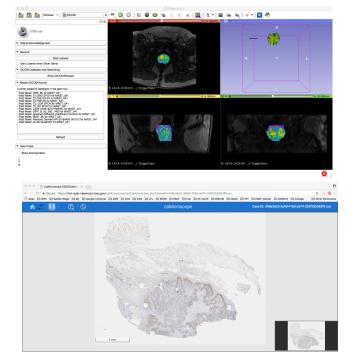


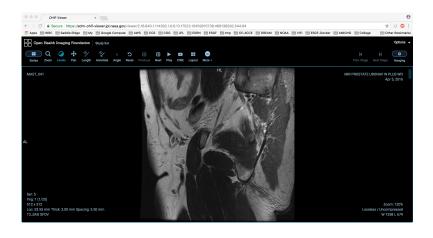




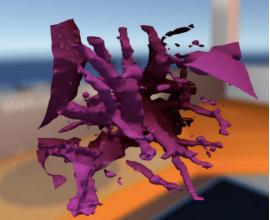


- Framework to plug-in many open-source viewers (client and server side)
 - caMicroscope
 - OHIF DICOM Viewer
 - 3D Slicer
- Capture additional metadata
- User specified organization of data
- Explore VR and other approaches for multii-dimensional imaging





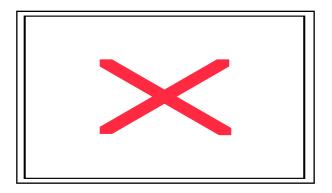
3D rendered isosurfaces: section of lung tissue

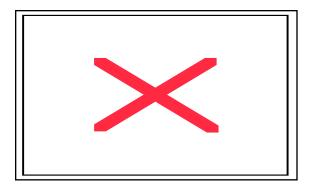






- Remote desktops running on the AWS Cloud
- Support analysis tools that must be installed on client machines, to access local data:
 - QuPath for use by Sandy Borowsky's group (UC Davis)
 - 3D Slicer for use by Radka Stoyanava's group (Univ. Of Miami)







AWS Workspaces: QuPath



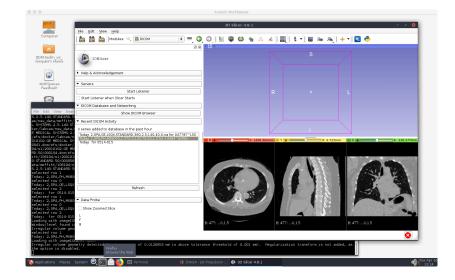
UC Davis Pathology data

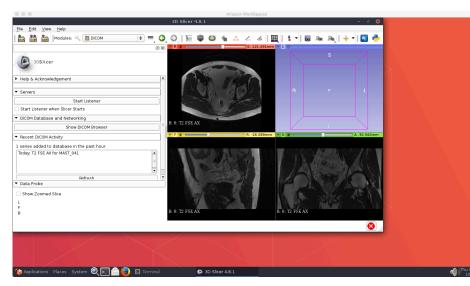






Moffitt lung data

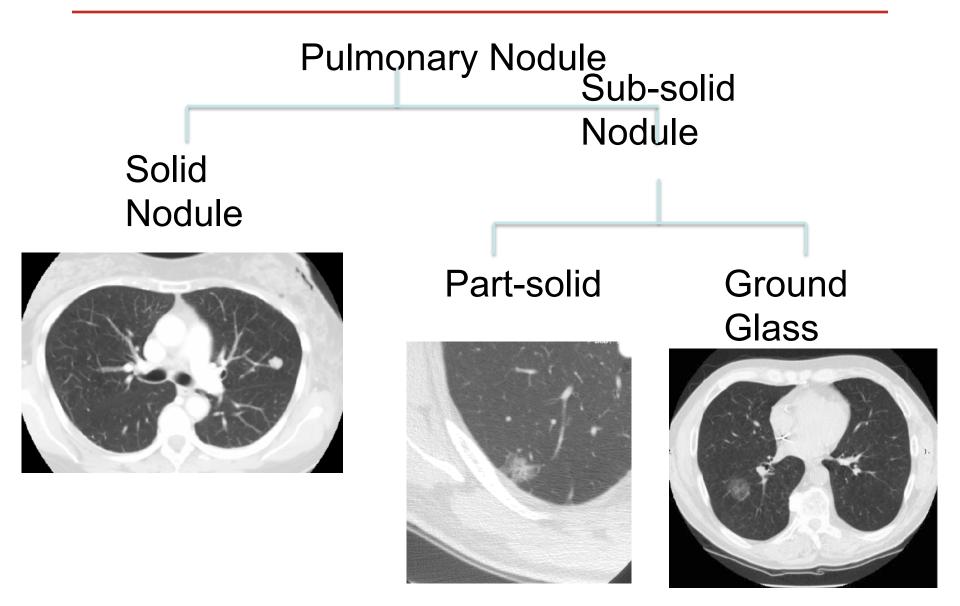




Univ. of Miami prostate data



Feature classification in images





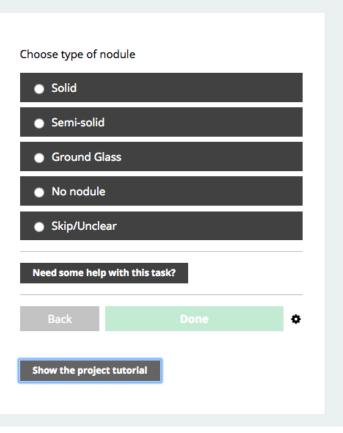
Crowd Sourcing Image Analysis

Lung cancer

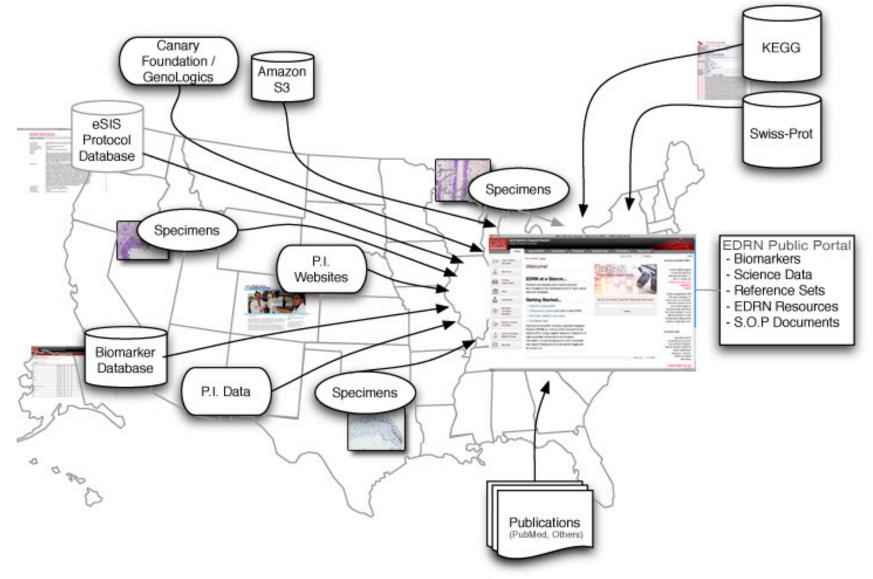
ABOUT CLASSIFY TALK COLLECT



Adaptation of Zoonverse Reduce False Positives from traditional ML Enable radiologists seed unsupervised clusters Drive towards ML pipelines



What's Emerged: A Virtual, National Integration Biomarkers Knowledge System



UNC



What's in Place Today

- A national, biomarker knowledge system serving multiple programs
- A biomarker data infrastructure consisting of ~1000 biomarkers, ~200 protocols, 1500 publications, 100 TB data
- Tools for laboratories to support the processing, capture, curation and sharing of data before publications
- Pilot projects in imaging, scalable workflows, data integration, etc
- Support for data-driven approaches for data discovery and analysis
- Common portals to access the knowledge environment



NIH Data Science Strategic Plan*

Workforce Modernized Data Data Management, Stewardship and Data Infrastructure Ecosystem Analytics, and Tools Development Sustainability Modernize data Enhance the NIH Optimize data Support useful. Develop policies generalizable, and data-science for a FAIR data storage and repository accessible tools security workforce ecosystem ecosystem and workflows Connect NIH data Support storage Expand the Enhance and sharing of Broaden utility of national research stewardship systems individual datasets and access to workforce specialized tools Engage a broader Better integrate clinical and Improve discovery community observational data and cataloging into biomedical resources data science

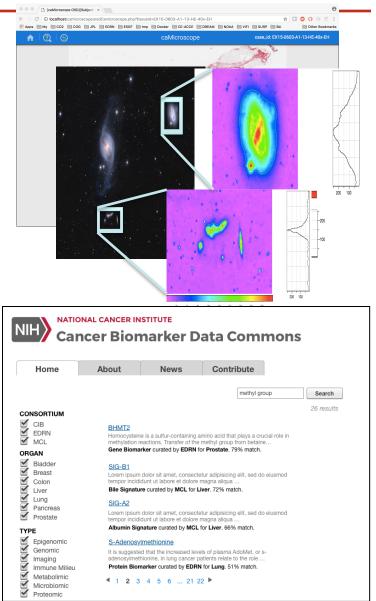
Figure 2. NIH Strategic Plan for Data Science: Overview of Goals and Objectives

* By 2025, the total amount of genomics data alone is expected to equal or exceed totals from the three other major producers of large amounts of data: astronomy, YouTube, and Twitter.



Future Directions

- Systematize the capture of data endto-end into a knowledge environment
- Integrate data-driven techniques and tools such as machine learning as part of the end-to-end knowledge environment
- Enable collaborative analysis that scales
- Unify consortium enterprises and data
- Enable science through an explicit and well architected data science strategy and platform



JPL Informatics Center Data Science Team





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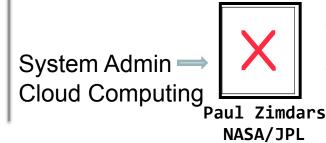


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