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California Institute of Technology
Pasadena, California

Lessons Learned in Creating Big Science Data Analysis Solution for the Cloud

Thomas Huang
thomas.huang@jpl.nasa.gov

Group Supervisor, Computer Science for Data Intensive Applications
Instrument Software and Science Data Systems

Strategic Lead for Interactive Analytics
National Space Technology Applications Program Office

[CL # 18-xxxx]

Background

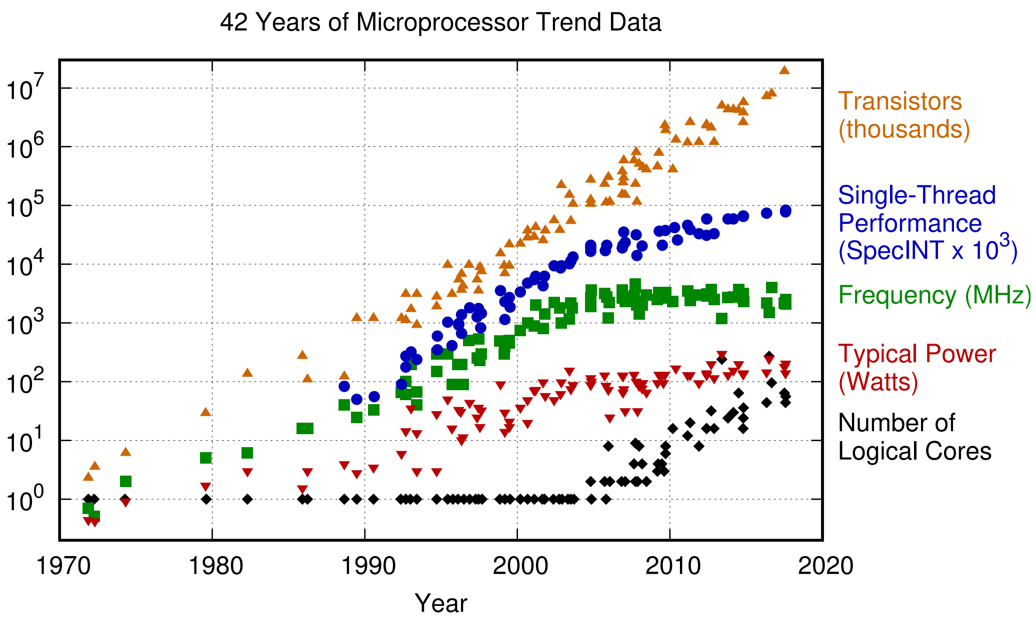
- **NASA has historically focused on systematic capture and stewardship of data for observational Systems**
- **With large amount of observational and modeling data, finding and downloading is becoming inefficient**
- **Reality with large amount of observational and modeling data**
  - Downloading to local machine is becoming inefficient
  - Search has gotten a lot faster. Too many matches.
  - Finding the relevant measurement has becoming a very time consuming process "*Which SST dataset I should use?*"
  - Analyze decades of regional measurement is labor-intensive and costly
- **Increasing "big data" era is driving needs to**
  - Scale computational and data infrastructures
  - Support new methods for deriving scientific inferences
  - Shift towards integrated data analytics
  - Apply computational and data science across the lifecycle
- **Scalable Data Management**
  - Capture well-architected and curated data repositories based on well-defined data/information architectures
  - Architecting automated pipelines for data capture
- **Scalable Data Analytics**
  - Access and integration of highly distributed, heterogeneous data
  - Novel statistical approaches for data integration and fusion
  - Computation applied at the data sources
  - Algorithms for identifying and extracting interesting features and patterns

Processors are not Getting Faster

2004: First Pentium 4 processor with 3.0GHz clock speed

2018: Apple's MacBook Pro has clock speed of 2.7GHz

14 years later, not much has gain in raw processing power



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

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Data Centers

- **Mainly focus on archives and distributions**
- **With additional services**
  - Better searches – faceted, spatial, keyword, ranking, etc.
  - Data subsetting – home grown, OPeNDAP, etc.
  - Visualization – visual discovery, PO.DAAC’s SOTO, NASA Worldview, etc.
- **Limitations**
  - Little to no interoperability between tools and services: metadata standard, keyword, spatial coverage (0-360 or -180..180), temporal representation, etc.
  - Making sure the most relevant measurements return first
  - Visualization is nice, but it doesn’t provide enough information about the event/phenomenon captured in the image.
  - With large amount of observational data, data centers need to do more than just storing bits
    - “Is the red blob in the middle of Pacific normal this time of the year?”
    - “Any relevant news and publications relate to what I am looking at?”
    - ”What other measurements, phenomena, news, publications relate to the period and location I am looking at?”
    - “I can see the observation from satellite, are there any relevant in situ data I can look at?”

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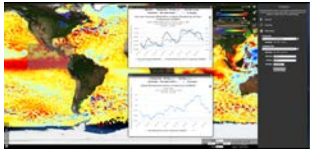
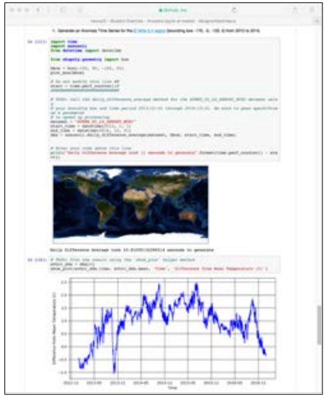
Enabling Next Generation of Ocean Science Tools and Services

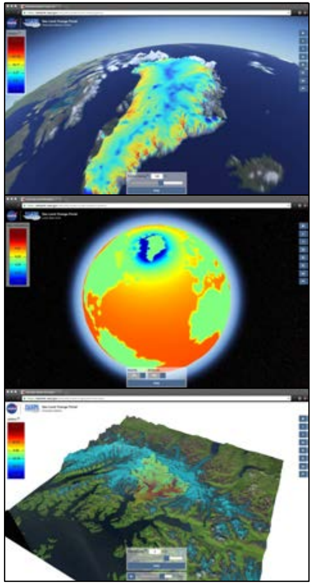
NASA Sea Level Change Portal



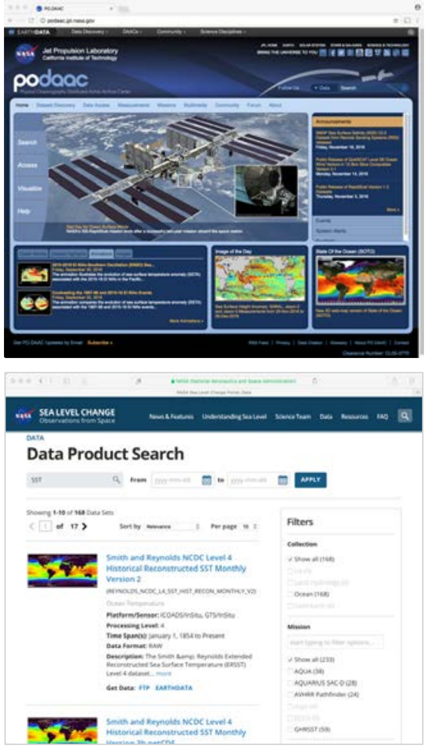
Jupyter Notebook - Interactive Workbench



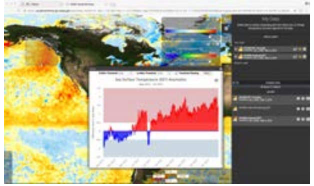
Model Simulations



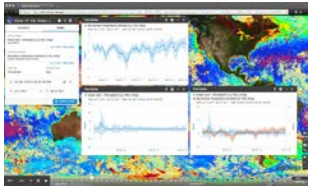
Integrated Search and Discovery



Oceanographic Anomaly Detection

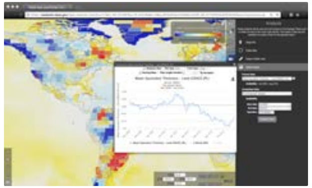


PO.DAAC State Of The Ocean

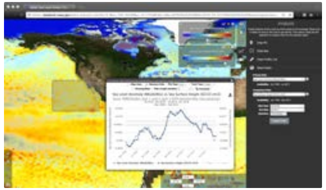


Mobile Analysis

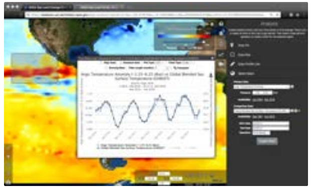
Hydrological Basin Analysis



In Situ Data Analysis



Model - Observation Comparison



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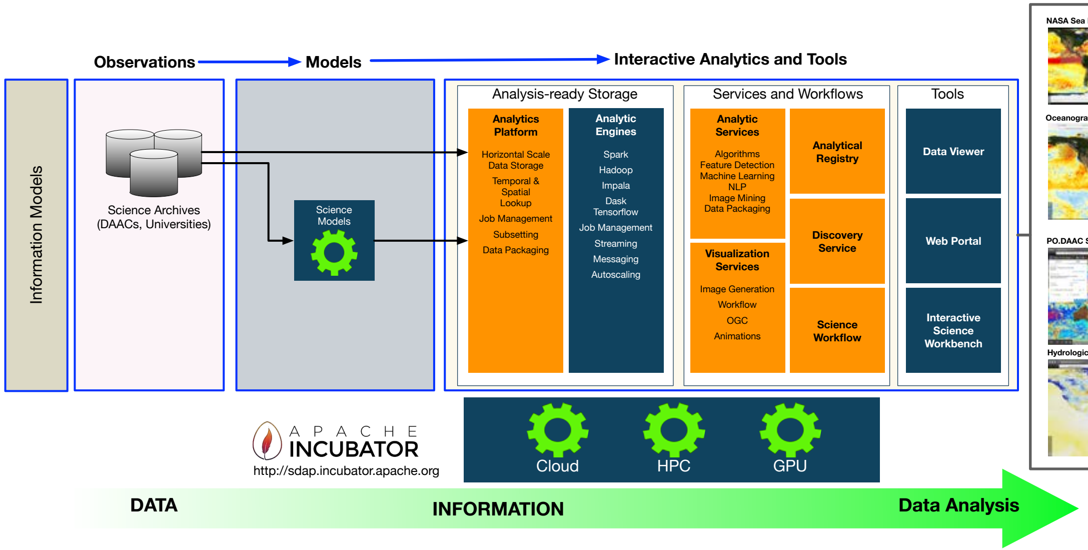
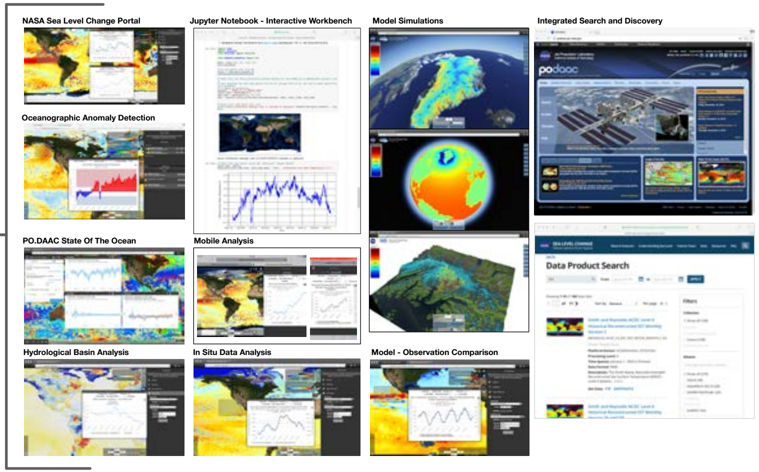
Integrated Ocean Science Data Analytics Platform





Systematic analysis of massive data

- **Integrated Ocean Science Data Analytics Platform**: an environment for conducting a Ocean Science investigation
  - Enables the confluence of resources for that investigation
  - Tailored to the individual study area (physical ocean, sea level, etc.)
- Harmonizes data, tools and computational resources to permit the ocean research community to focus on the investigation
- Scale computational and data infrastructures
- Shift towards integrated data analytics
- Algorithms for identifying and extracting interesting features and patterns

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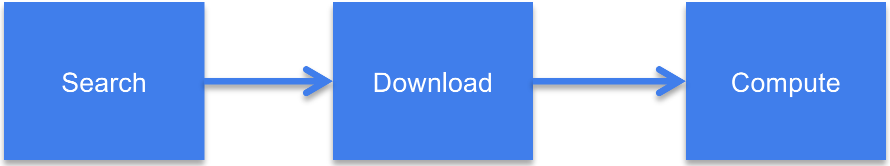
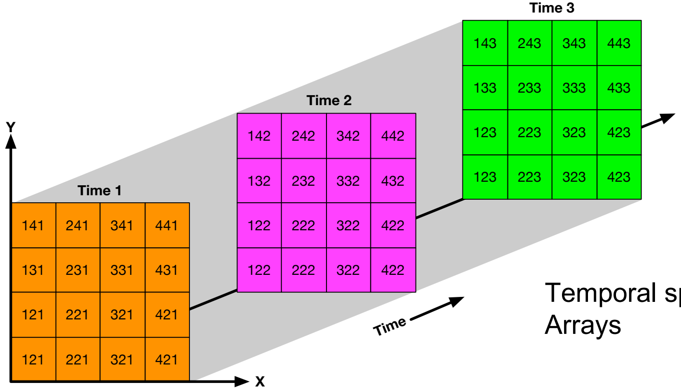
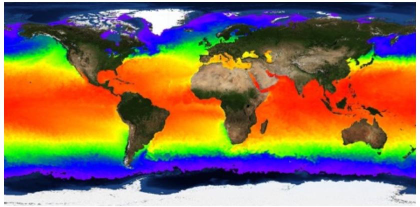
Traditional Method for Analyze Satellite Measurements

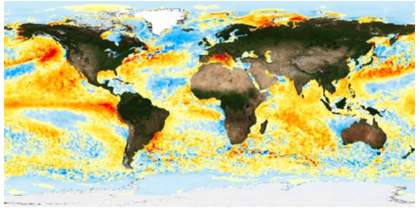


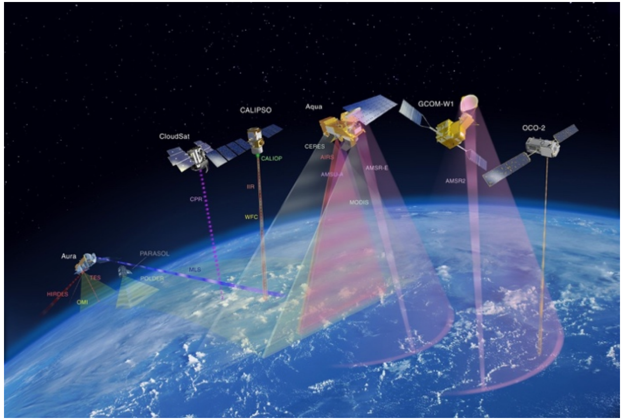


Temporal spatial Arrays

- Depending on the data volume (size and number of files)
- It could take many hours of download – (e.g. 10yr of observational data could yield thousands of files)
- It could take many hours of computation
- It requires expensive local computing resource (CPU + RAM + Storage)
- After result is produced, purge downloaded files





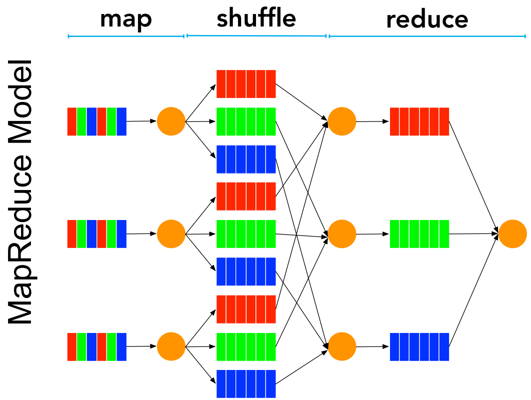


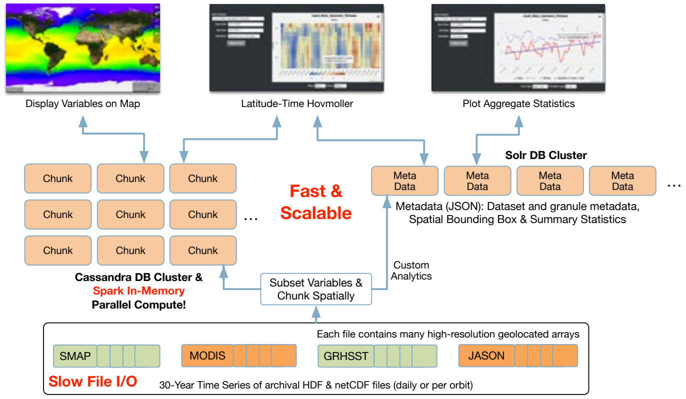
Observation

- Traditional methods for data analysis (time-series, distribution, climatology generation) can't scale to handle large volume, high-resolution data. They perform poorly
- Performance suffers when involve large files and/or large collection of files
- A high-performance data analysis solution must be free from file I/O bottleneck

NEXUS: Scalable Data Analytic Solution

- **MapReduce**: A programming model for expressing distributed computations on massive amount of data and an execution framework for large-scale data processing on clusters of commodity servers. - J. Lin and C. Dyer, "*Data-Intensive Text Processing with MapReduce*"
  - **Map**: splits processing across cluster of machines in parallel, each is responsible for a record of data
  - **Reduce**: combines the results from Map processes
- **NEXUS** is a data-intensive analysis solution using a new approach for handling science data to enable large-scale data analysis
  - Streaming architecture for horizontal scale data ingestion
  - Scales horizontally to handle massive amount of data in parallel
  - Provides high-performance geospatial and indexed search solution
  - Provides tiled data storage architecture to eliminate file I/O overhead
  - A growing collection of science analysis webservices





Two-Database Architecture

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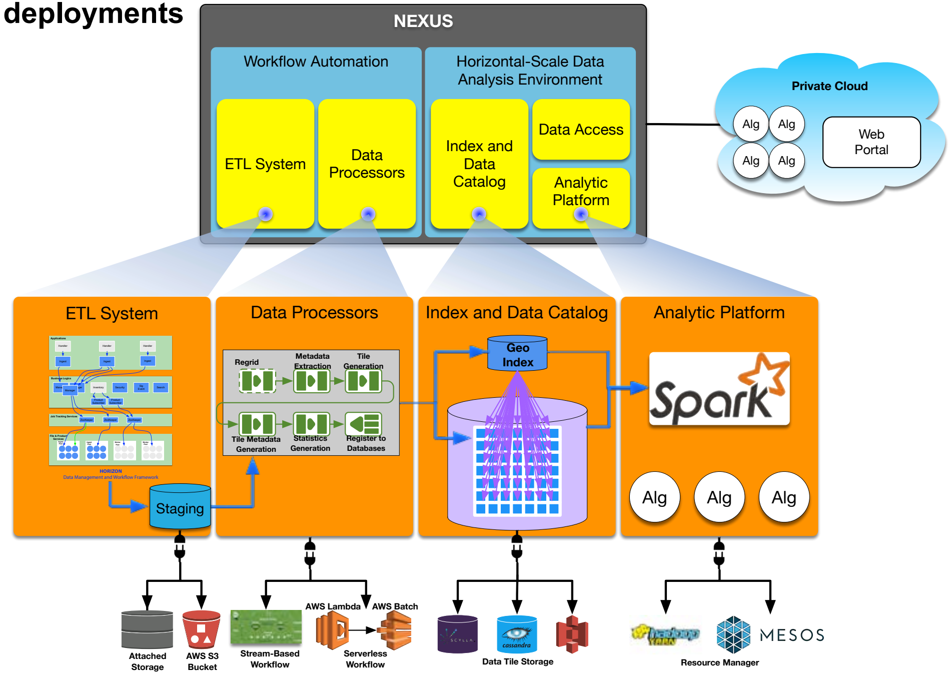
NEXUS' Pluggable Architecture for different Operation Needs

- **NEXUS supports public/private Cloud and local cluster deployments**
- **Several container-based deployment options**
  - Local on-premise cluster
  - Private Cloud
  - Amazon Web Service
- **Automate Data Ingestion with Image Generation**
  - Cluster based
  - Serverless (Amazon Lambda and Batch)
- **Data Store Options**
  - Apache Cassandra
  - ScyllaDB
  - Amazon Simple Storage Service (S3)
- **Resource Management Options**
  - Apache YARN
  - Apache MESOS
- **Analytic Engine Options**
  - Custom Apache Spark Cluster
  - Amazon Elastic MapReduce (EMR)
  - Amazon Athena (work-in-progress)



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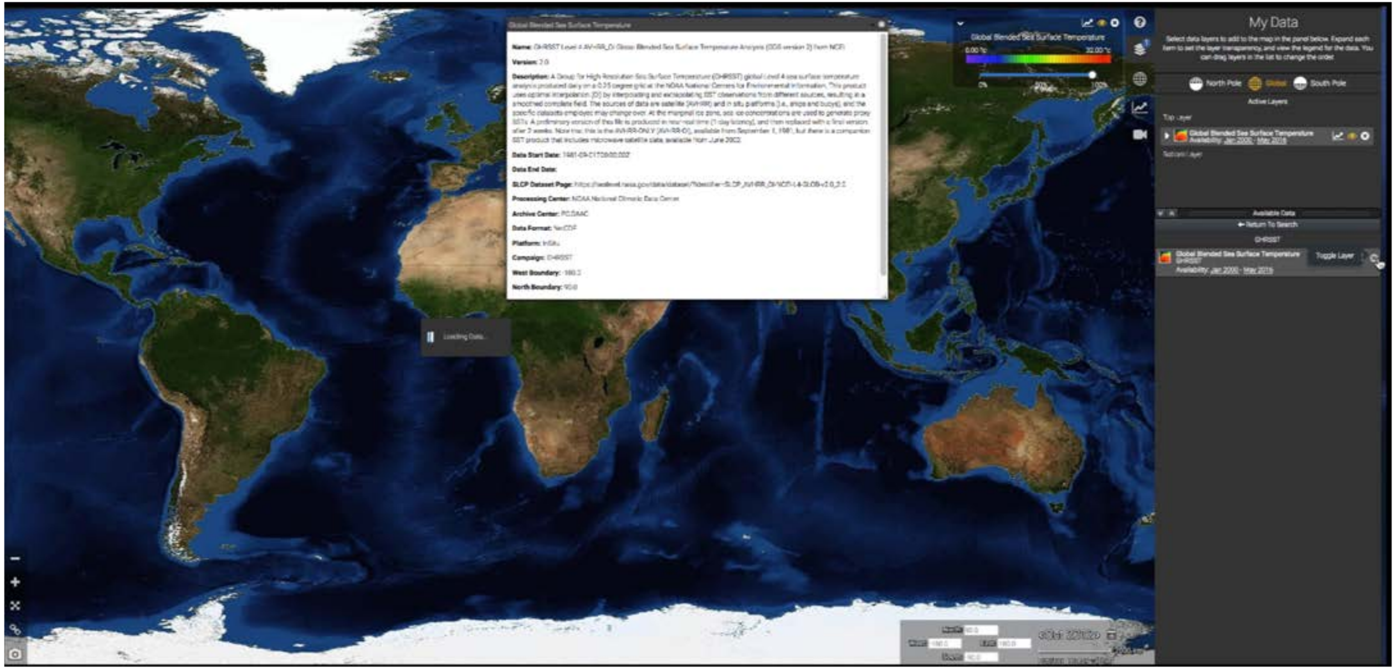
Analyze Sea Level On-The-Fly *https://sealevel.nasa.gov*



Sea Level Change - Data Analysis Tool

Visualizations | Hydrological Basins | Time Series | Deseason | Data Comparison | Scatter Plot | Latitude/Time Hovmöller | Etc.

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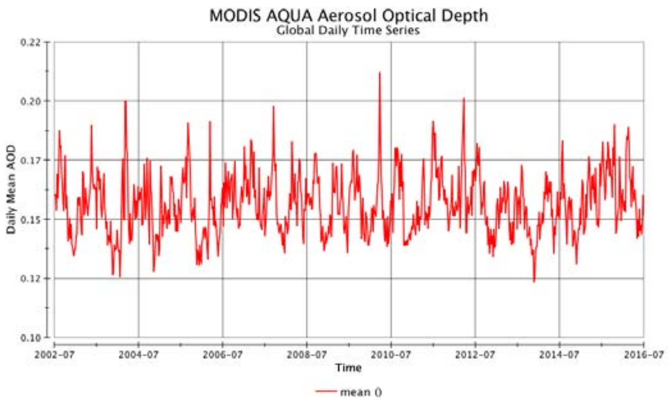
NEXUS Performance: GIOVANNI vs. Custom Spark vs. AWS EMR

Dataset: MODIS AQUA Daily
Name: Aerosol Optical Depth 550 nm (Dark Target) (MYD08_D3v6)
File Count: 5106
Volume: 2.6GB
Time Coverage: July 4, 2002 – July 3, 2016

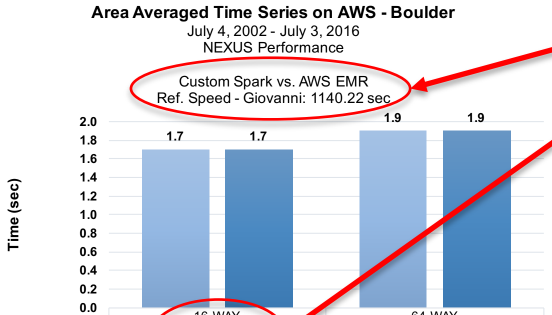
Giovanni: A web-based application for visualize, analyze, and access vast amounts of Earth science remote sensing data without having to download the data.

- Represents current state of data analysis technology, by processing one file at a time
- Backed by the popular NCO library. Highly optimized C/C++ library

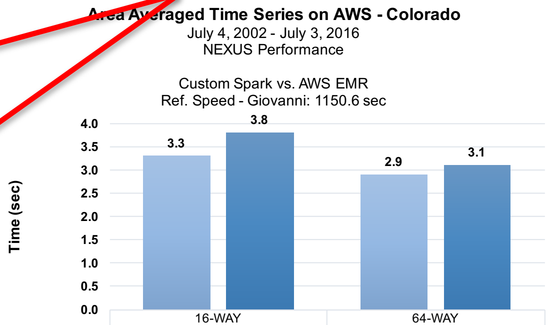
AWS EMR: Amazon's provisioned MapReduce cluster



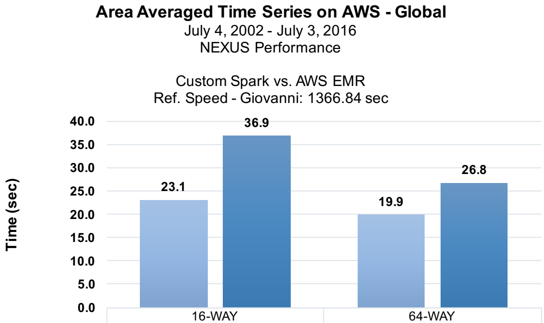
Giovanni: 20 min
NEXUS: 1.7 sec



	16-WAY	64-WAY
Custom Spark	1.7	1.9
AWS EMR	1.7	1.9



	16-WAY	64-WAY
Custom Spark	3.3	2.9
AWS EMR	3.8	3.1



	16-WAY	64-WAY
Custom Spark	23.1	19.9
AWS EMR	36.9	26.8

Algorithm execution time. Excludes Giovanni's data scrubbing processing time

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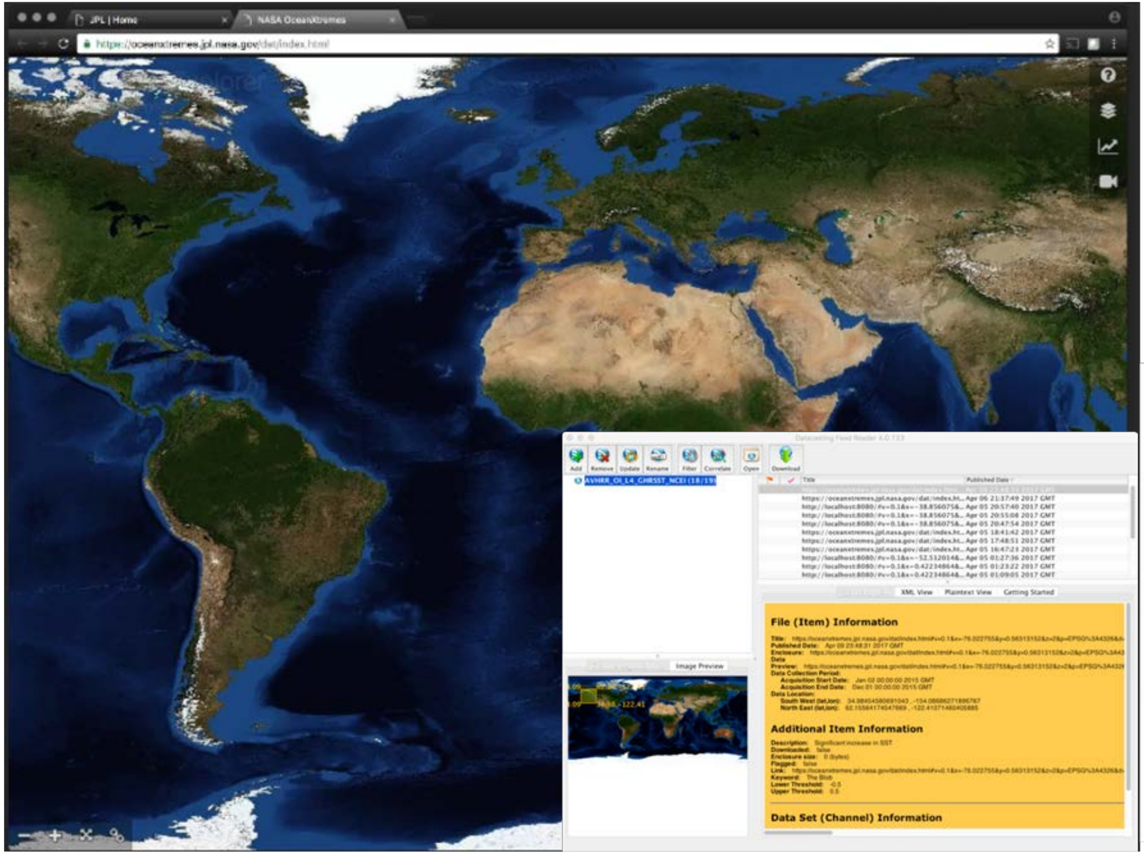
Analyze Ocean Anomaly – “The Blob”



- **Visualize** parameter
- **Compute** daily differences against climatology
- **Analyze** time series area averaged differences
- **Replay** the anomaly and visualize with other measurements
- **Document** the anomaly
- **Publish** the anomaly

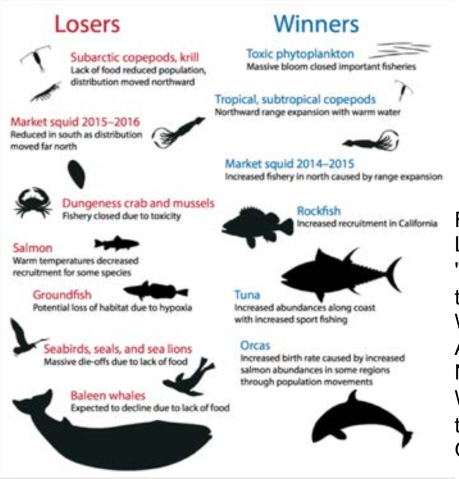


Figure from Cavole, L. M., et al. (2016). "Biological Impacts of the 2013–2015 Warm-Water Anomaly in the Northeast Pacific: Winners, Losers, and the Future." Oceanography 29.

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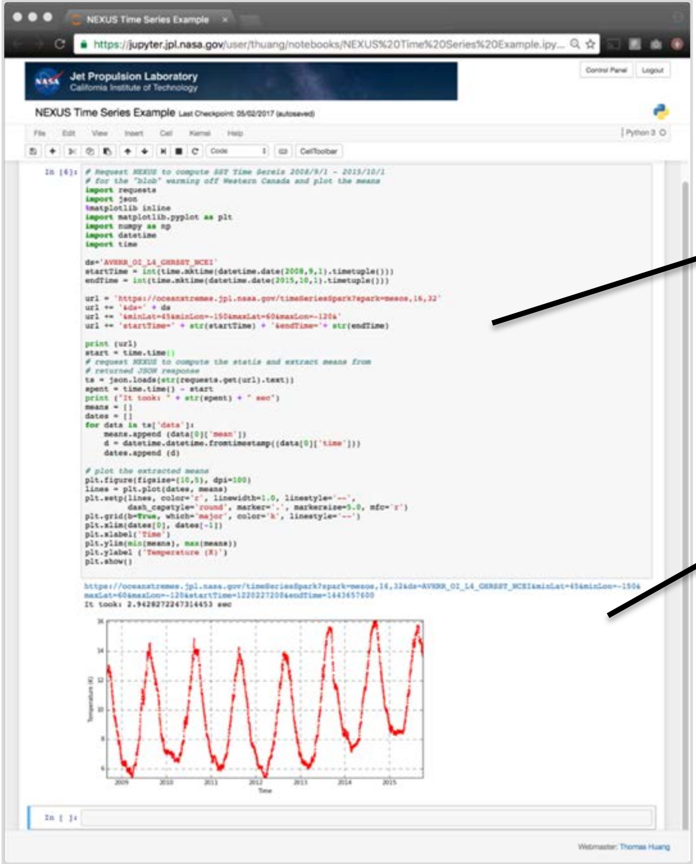
Enable Science without File Download




```
# Request NEXUS to compute SST Time Series 2008/9/1 - 2015/10/1
# for the "blob" warming off Western Canada and plot the means
…
ds='AVHRR_OI_L4_GHRSST_NCEI'

url = … # construct the webservice URL request


# make request to NEXUS using URL request
# save JSON response in local variable
ts = json.loads(str(requests.get(url).text))

# extract dates and means from the response
means = []
dates = []
for data in ts['data']:
    means.append (data[0]['mean'])
    d = datetime.datetime.fromtimestamp((data[0]['time']))
    dates.append (d)

# plot the result
…
```

```
https://oceanxtremes.jpl.nasa.gov/timeSeriesSpark?spark=mesos,16,32&ds=AVHRR_OI_L4_GHRSST_NCEI&minLat=45&minLon=-150&maxLat=60&maxLon=-120&startTime=1220227200&endTime=1443657600

It took: 2.9428272247314453 sec
```

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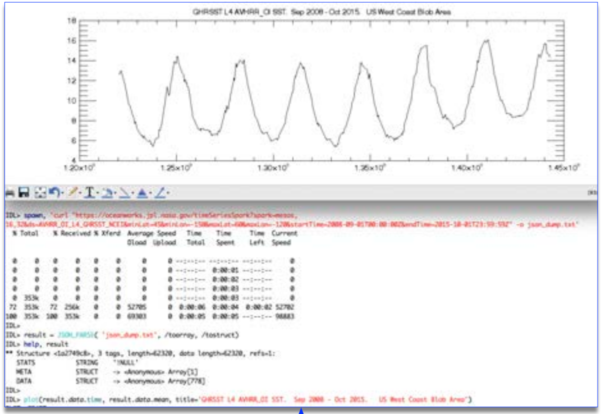
Using IDL with NEXUS

```
IDL> spawn, 'curl
"https://oceanworks.jpl.nasa.gov/timeSeriesSpark?spark=mesos,16,32&ds=AVHRR_OI_L4_GHRSST_NCEI&minLat=45&minLon=-150&maxLat=60&maxLon=-120&startTime=2008-09-01T00:00:00Z&endTime=2015-10-01T23:59:59Z" -o json_dump.txt'
  % Total    % Received % Xferd  Average Speed   Time    Time     Time  Current
                                 Dload  Upload   Total   Spent    Left  Speed

  0      0    0      0    0     0      0      0 --:--:-- --:--:-- --:--:--     0
  0      0    0      0    0     0      0      0 --:--:--  0:00:01 --:--:--     0
  0      0    0      0    0     0      0      0 --:--:--  0:00:02 --:--:--     0
  0      0    0      0    0     0      0      0 --:--:--  0:00:03 --:--:--     0
  0   353k    0      0    0     0      0      0 --:--:--  0:00:03 --:--:--     0
 72   353k   72   256k    0     0  52705      0  0:00:06  0:00:04  0:00:02 52702
100   353k  100   353k    0     0  69303      0  0:00:05  0:00:05 --:--:-- 98883
IDL>
IDL> result = JSON_PARSE( 'json_dump.txt', /toarray, /tostruct)
IDL> help, result
** Structure <1a2749c8>, 3 tags, length=62320, data length=62320, refs=1:
   STATS            STRING    '!NULL'
   META             STRUCT    -> <Anonymous> Array[1]
   DATA             STRUCT    -> <Anonymous> Array[778]
IDL>
IDL> plot(result.data.time, result.data.mean, title='GHRSST L4 AVHRR_OI SST.  Sep 2008
- Oct 2015.   US West Coast Blob Area')
PLOT <29457>
```



Credit: Ed Armstrong

Jun. 05, 2018

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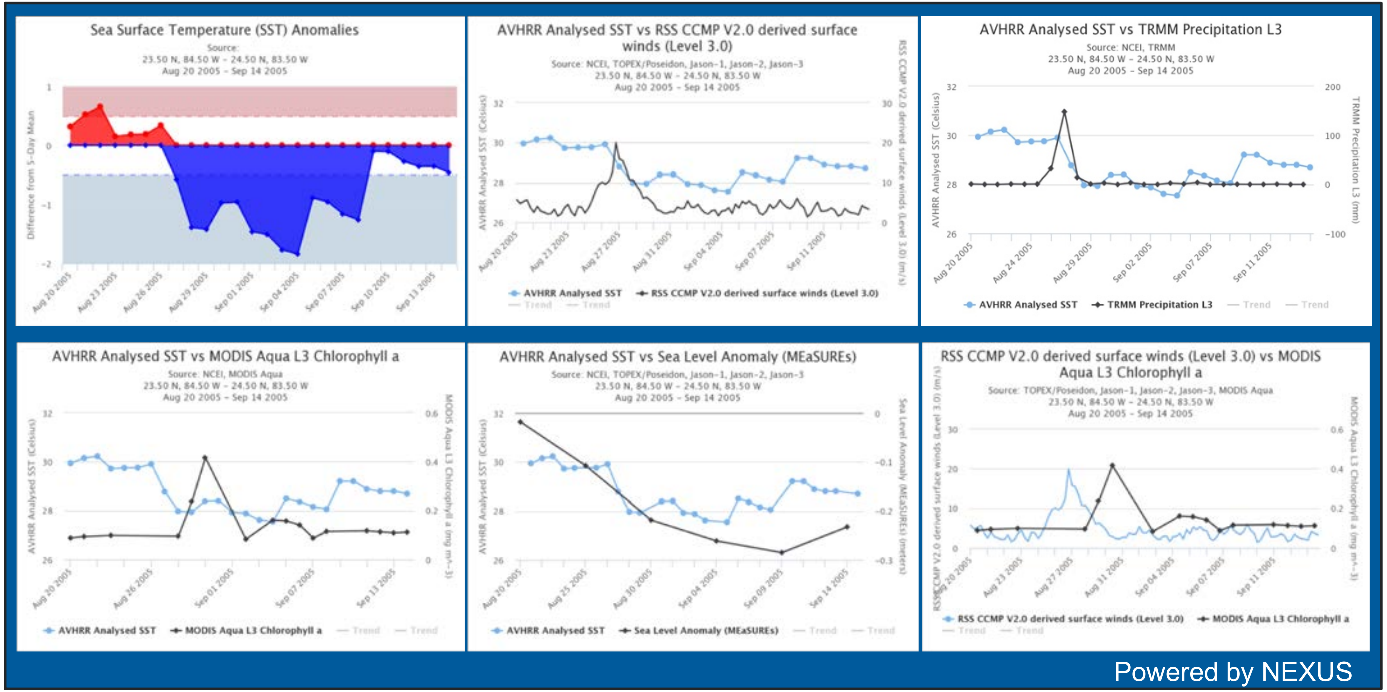
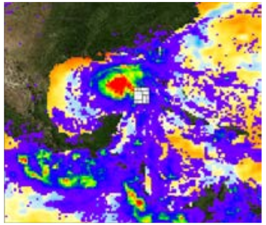
Hurricane Katrina Study



Hurricane Katrina passed to the southwest of Florida on Aug 27, 2005. The ocean response in a 1 x 1 deg region is captured by a number of satellites. The initial ocean response was an immediate cooling of the surface waters by 2 ℃ that lingers for several days. Following this was a short intense ocean chlorophyll bloom a few days later. The ocean may have been “preconditioned’ by a cool core eddy and low sea surface height.

The SST drop is correlated to both wind and precipitation data. The Chl-A data is lagged by about 3 days to the other observations like SST, wind and precipitation.



Hurricane Katrina TRMM overlay SST Anomaly

A study of a Hurricane Katrina–induced phytoplankton bloom using satellite observations and model simulations
Xiaoming Liu, Menghua Wang, and Wei Shi
JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 114, C03023, doi:10.1029/2008JC004934, 2009

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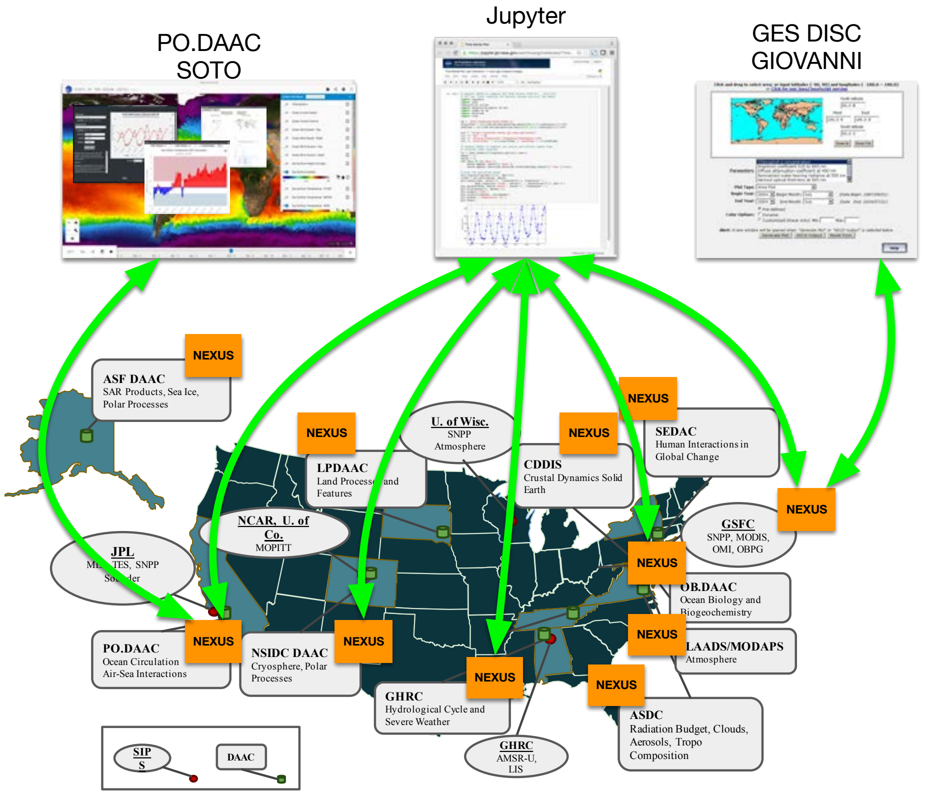
Multi-Variable Analysis

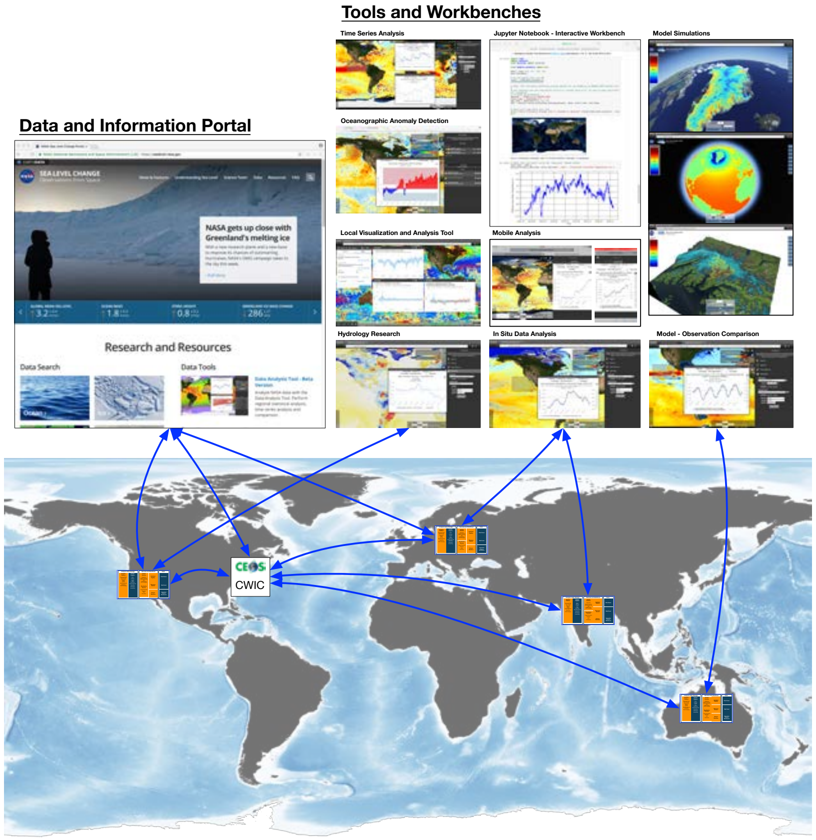
- Public accessible RESTful analytic APIs where computation is next to the data
- NEXUS as the analytic engine infused and managed by the DAACs on the Cloud
- Researchers can perform multi-variable analysis using any web-enabled devices without having to download files
- Reduce unnecessary egress charges
- An architecture to enable next generation of scientific applications



Architecture for Distributed Data System and Analysis

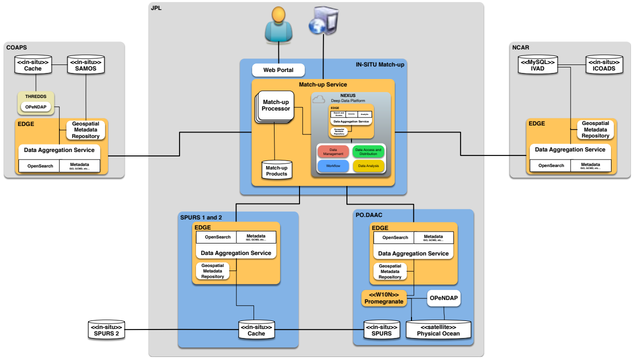
Committee on Earth Observation Satellites (CEOS)

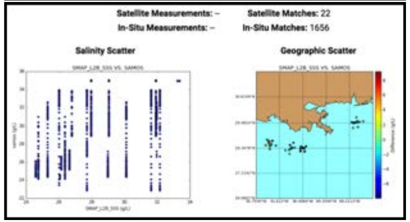
- A common service registry
- Putting value-added services next to the data to eliminate unnecessary data movement
- Avoid data replication
- Public accessible RESTful analytic APIs where computation is next to the data
- Analytic engine infused and managed by the data centers perhaps on the Cloud
- Researchers can perform multi-variable analysis using any web-enabled devices without having to download files
- Reduce unnecessary data movement and egress charges
- An architecture to enable next generation of scientific applications



In Situ to Satellite Matchup

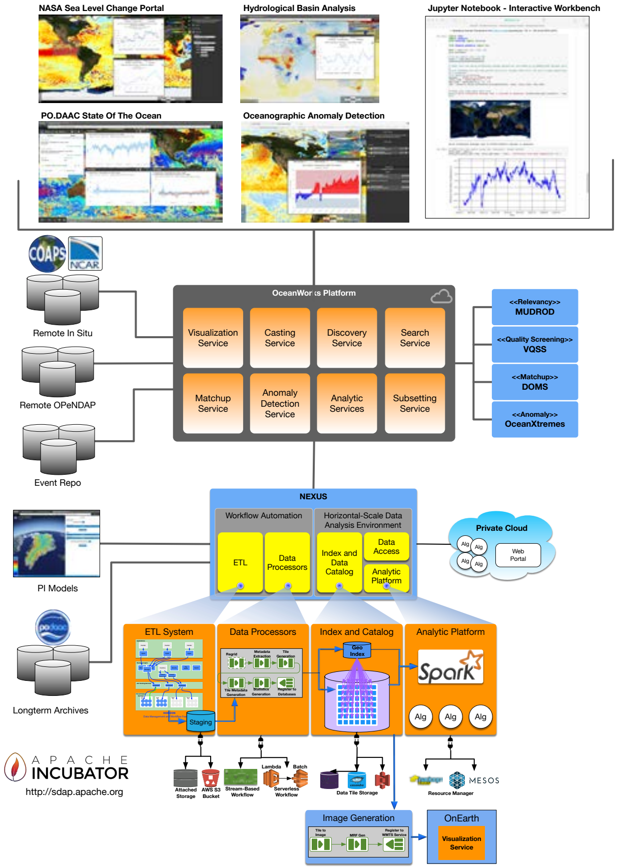
- Distributed Oceanographic Matchup Service (DOMS)
- Typically data matching is done using one-off programs developed at multiple institutions
- A primary advantage of DOMS is the reduction in duplicate development and man hours required to match satellite/in situ data
  - Removes the need for satellite and in situ data to be collocated on a single server
  - Systematically recreate matchups if either in situ or satellite products are re-processed (new versions), i.e., matchup archives are always up-to-date.
- In situ data nodes at JPL, NCAR, and FSU operational.
- Provides data querying, subset creation, match-up services, and file delivery operational.
- Plugin architecture for in situ data source using EDGE, a open source implementation of Open Search





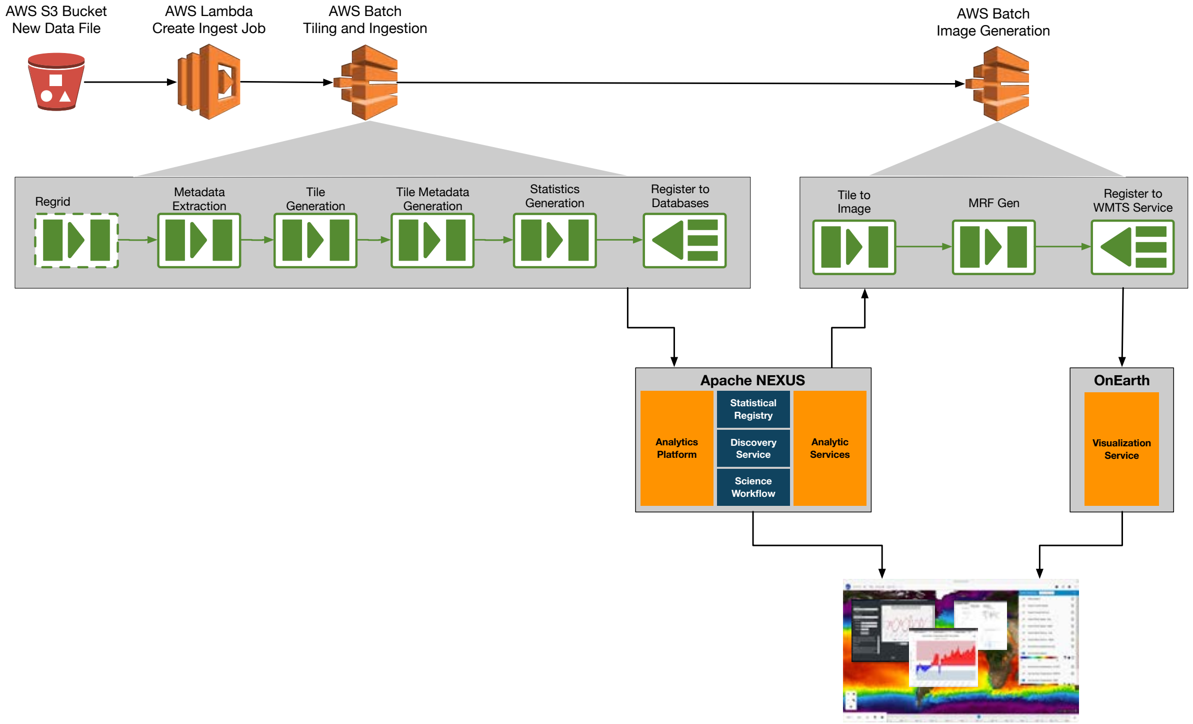
NASA AIST OceanWorks: Ocean Sciences Platform

- **OceanWorks** is to establish an **Integrated Data Analytic Center** at the NASA Physical Oceanography Distributed Active Archive Center (PO.DAAC) for Big Ocean Science
- Focuses on technology integration, advancement and maturity
- Collaboration between JPL, FSU, NCAR, and GMU
- Bringing together PO.DAAC-related big data technologies
    - Anomaly detection and ocean science
    - Big data analytic platform
    - Distributed in-situ to satellite matchup
    - Search relevancy and discovery – linking datasets, services, and anomalies through recommendations
    - Metadata translation and services aggregation
    - Fast data subsetting
    - Virtualized Quality Screening Service



Severless Ingestion Workflow Architecture

- The cluster ingestion workflow requires several EC2 instances and attached EBS storage. Amazon bills active EC2 and storage even there is no data to be processed
- Cost-saving serverless architecture using AWS S3 Bucket trigging AWS Lambda job to create AWS Batch jobs



Analytic Storage

Blocked Storage (EBS)

v.s.

Object Storage (S3)

$0.045/GB-month
$47,186/PB-month

$0.021/GB-month
$22,020/PB-month

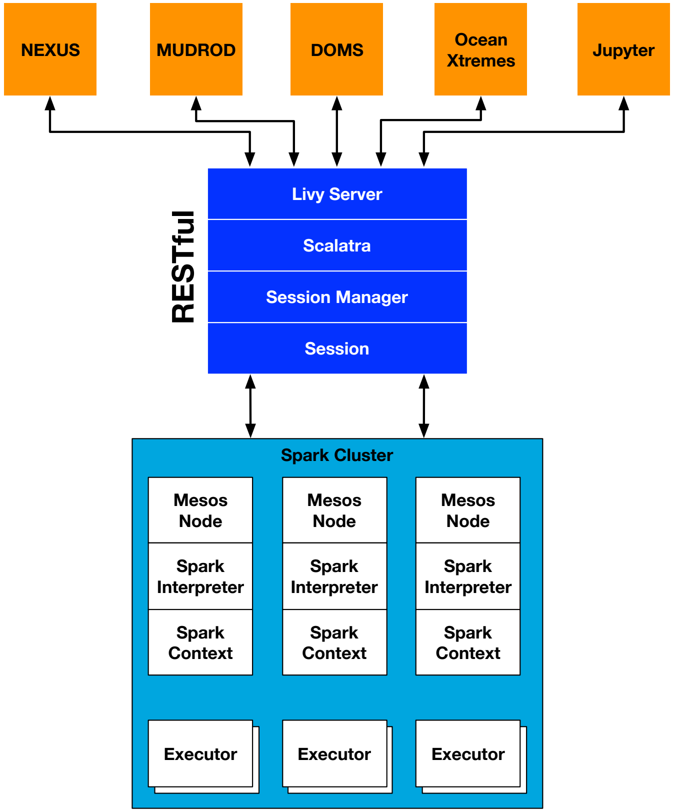
NEXUS supports 2 types of cloud storage

- Blocked storage (e.g. Amazon EBS), Attach to computing node. Generally faster
  - Cassandra and ScyllaDB
- Object storage (e.g. Amazon S3), Independent storage service. Highly scalable

For a data center, not all data need to be served on fast storage, Object storage provides a better, scalable alternative

Architecture for Custom Algorithms and Cluster Sharing

- Developed independently, all the major services in OceanWorks require Apache Spark cluster.
- If OceanWorks simply deploy these services to Amazon, it will require dedicated Apache Spark cluster for each.
- Too many clusters and very costly, especially for high memory machine instances.
- Looking at the Amazon's EMR model. It is designed to be a job execution solution, and the jobs could from different applications.
- Apache Livy provides a RESTful interface to Apache Spark cluster.
- We built upon the Livy solution and extended the NEXUS Command Line interface to enable "push" of custom code for execution on OceanWorks' remote Spark cluster.
- Scientists can use the Jupyter environment to design their analytic algorithms that will be executed in the OceanWorks' Spark cluster.



Push Python/Scala Code to Spark Cluster

- Users can now push their own custom map-reduce algorithms in Python/scala to OceanWorks for execution in the cloud.
- For our Python users, this is part of the NEXUSCLI library. It is Jupyter friendly and standalone python applications
- Enables services to share Apache Spark computing cluster.
- **New REST endpoints:**
  - https://oceanworks.jpl.nasa.gov/run_str
  - Run custom code in a (multi-line) string.
  - https://oceanworks.jpl.nasa.gov/run_file
  - Run custom code in a local file.
  - These new endpoints are not public.
  - For trusted (authenticated) users.

New NEXUS CLI Python library methods:

```
from nexuscli import nexuscli_ow
nexuscli_ow.set_target('https://oceanworks.jpl.nasa.gov’)
code = '[x*x for x in range(11)]’
ans = nexuscli_ow.run_str(code)
fname = ’custom_code.py'
ans = nexuscli_ow.run_file(fname)
```

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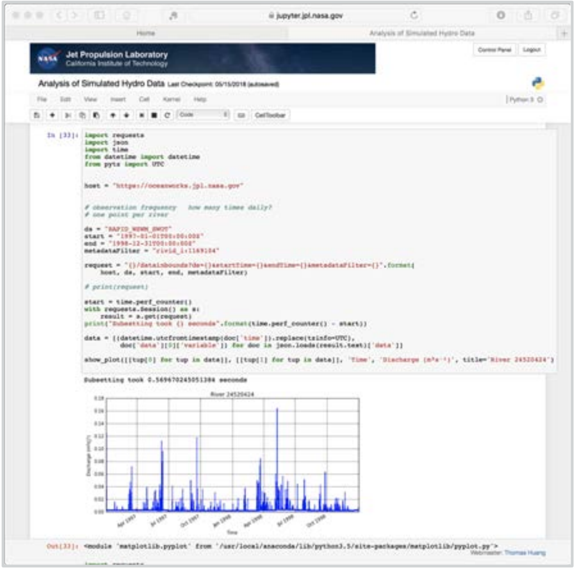
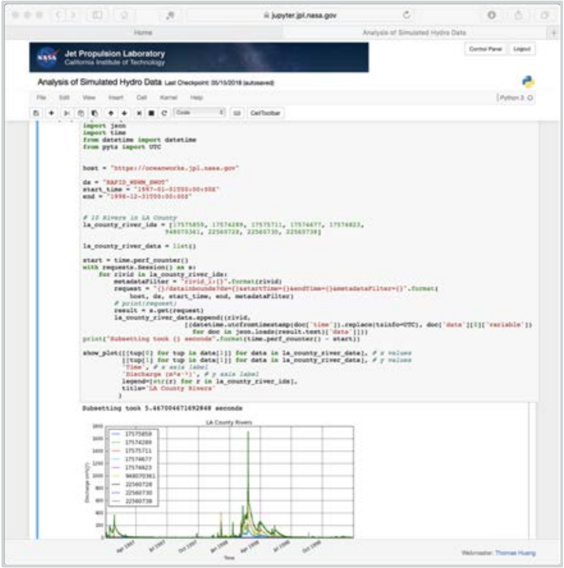
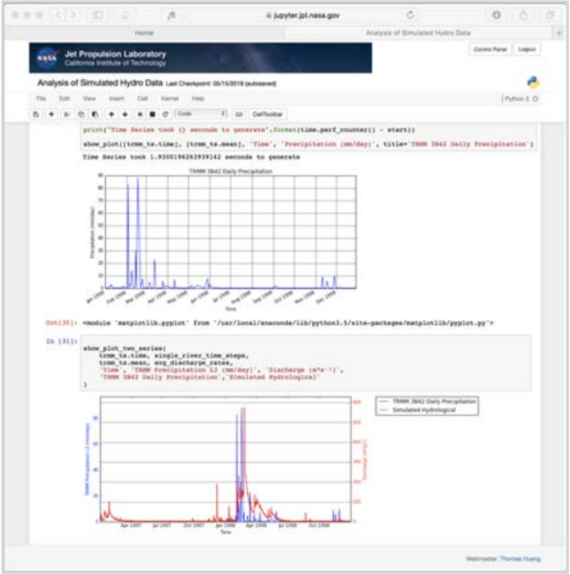
Support for Hydrology



Retrieval of a single river time series



Retrieval of time series from 9 rivers



Time series coordination between TRMM and river

- Simulated hydrology data in preparation for SWOT hydrology
- **River data**: ~3.6 billion data points. 3-hour sample rate. Consists of measurements from ~600,000 rivers
- **TRMM data**: 17 years, .25deg, 1.5 billion data points
- Sub-second retrieval of river measurements
- On-the-fly computation of time series and generate coordination plot

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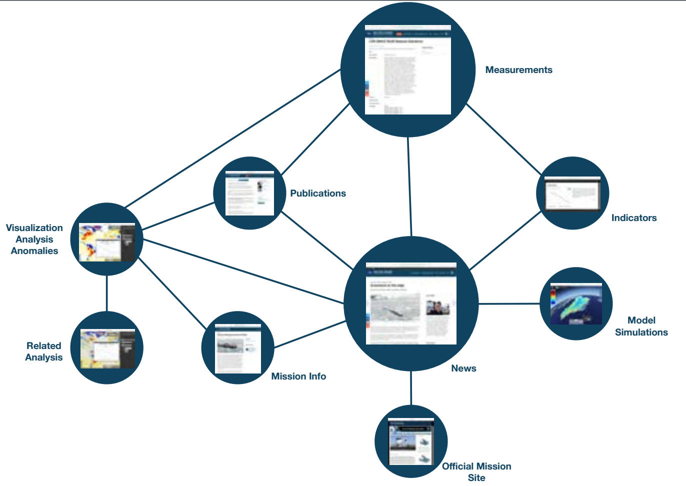
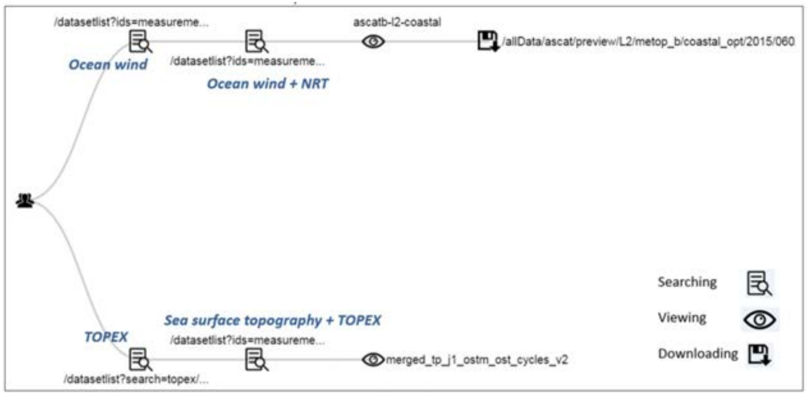
Tackling Information Discovery

- Adjust search result according how user search and retrieval
- Use Machine Learning approach to adjust search ranking by taking a number of features into consideration – version, processing level, release date, all-time popularity, monthly-popularity, and user popularity
- Semantically mind dataset metadata to identify relationship
- **Relevancy** is
  - Domain-specific
  - Personal
  - Temporal
  - Dynamic

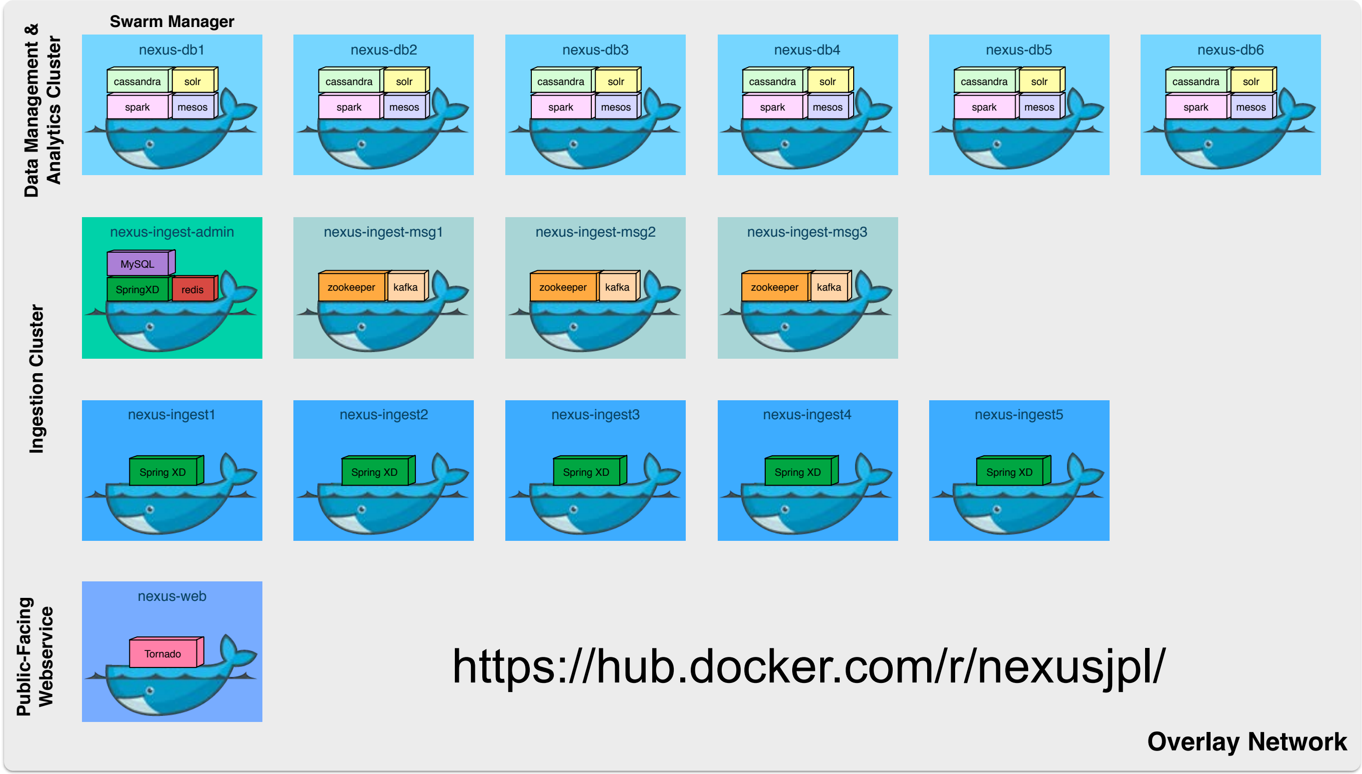


Dynamic Ranking and Recommendation



Container-based deployment using Docker

- Dockerized all service components
- Register with DockerHub
- Integration with Continuous Integration (CI) solutions (e.g. Jenkins or Atlassian Bamboo)
- Same container deployment process for on-premise hardware or commercial Cloud environment



Example Container Deployment of our Open Source Analytic Engine, NEXUS

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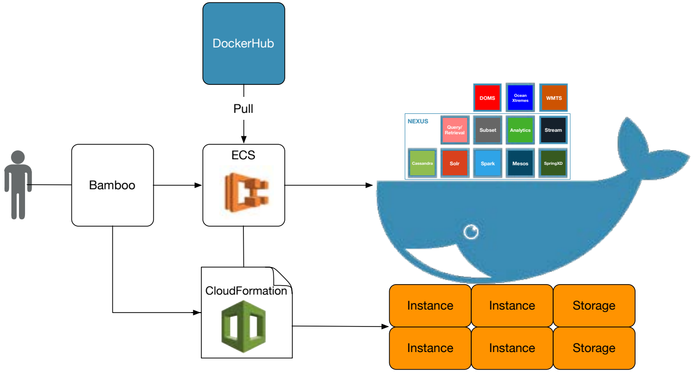
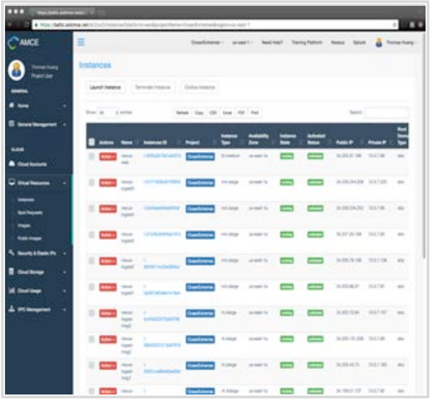
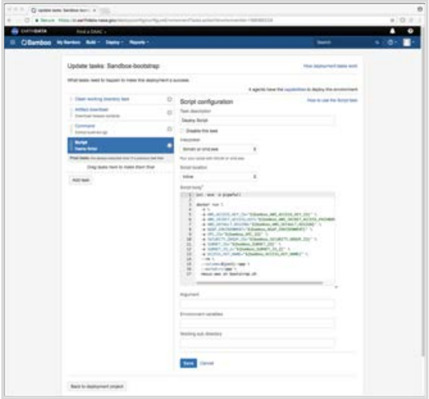
Deployment Automation

- Cloud Deployment is nontrivial
- Infrastructure Definition
  - Various machine instances
  - Storage and buckets
- Software Deployment.. manually
  - Build
  - Package
  - Install
  - Configure
  - Shell login (security issues)
- Best Practice: Deployment Automation
  - Script Infrastructure Definition (e.g. Amazon CloudFormation)
  - Container-based Deployment (e.g. Amazon ECS and DockerHub)





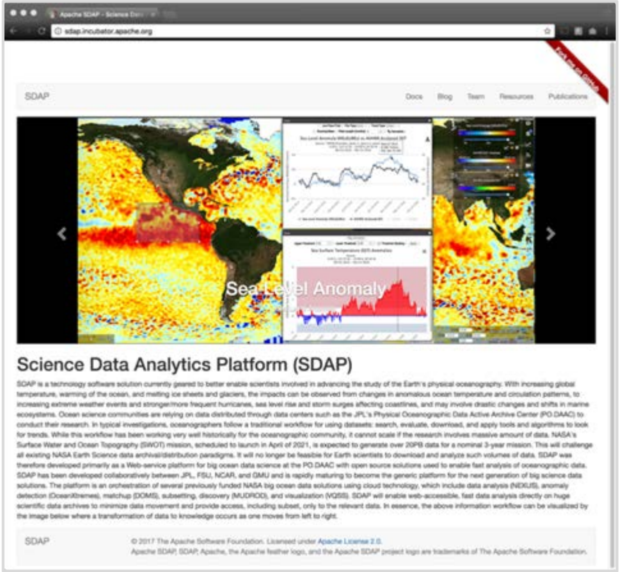
AIST Managed Cloud Environment



ESDIS NGAP

Free and Open Open Source Software (FOSS)

- October 2017, the OceanWorks project released all of its source code to Apache Software Foundation and established the **Science Data Analytics Platform (SDAP)** in the **Apache Incubator**
- Technology sharing through Free and Open Source Software (FOSS)
- Why? Further technology evolution that is restricted by projects / missions
- It is more than GitHub
  - Quarterly reporting
  - Reports are open for community review by over 6000 committers
  - SDAP has a group of appointed international Mentors: Jörn Rottmann, Raphael Bircher, and Suneel Marthi
- OceanWorks is now being developed in the open
  - For local cluster and cloud computing platform
  - Fully containerized using Docker (multiple containers)
  - Infrastructure orchestration using Amazon CloudFormation
  - Analyzing satellite and model data
  - In situ data analysis and colocation with satellite measurements
  - Fast data subsetting
  - Data services integration architecture
  - OpenSearch and dynamic metadata translation
  - Mining of user interactions and data to enable discovery and recommendations
  - Streamline deployment through container technology



http://sdap.apache.org

APACHE INCUBATOR

Notable Public Engagements

- Host hands-on cloud analytics workshops using Amazon Web Services (AWS)
- Invited to speak at the **Space Studies Board of The National Academy of Sciences**
- Invited to present to the **NASA Advisory Council's Ad-Hoc Big Data Task Force (BDTF)**
- Invited to present to the **JPL Deputy Lab Director and Chief Technologist**
- Invited to present to **CNES Chief Technologist and Delegations**

In Summary

- Traditional method for scientific research (search, download, local number crunching) is unable to keep up
- Let’s think beyond archive and file downloads
- Connected information enables discovery
- Community developed solution through open sourcing
- Investment in data and computational sciences
- Data Centers might want to be in the business of Enabling Science!
- OceanWorks infusion 2018 – 2019
    - Turnkey AMCE deployment
    - Solution for large job management
    - Integration with Amazon Athena
    - Integration with Pangeo
    - Watch for changes to the NASA’s Sea Level Change Portal
        - Even faster analysis capabilities
        - More variety of measurements – satellites, in situ, and models
        - Event more relevant recommendations
    - NASA’s Physical Oceanography Distributed Active Archive Center (PO.DAAC)
        - More than just pretty pictures. SOTO will have new analytic capabilities.
- Coming Soon: 2018 Wiley Book on **Big Earth Data Analytics in Earth, Atmospheric and Ocean Sciences**

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Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

Thomas Huang
Thomas.huang@jpl.nasa.gov
Jet Propulsion Laboratory
California Institute of Technology