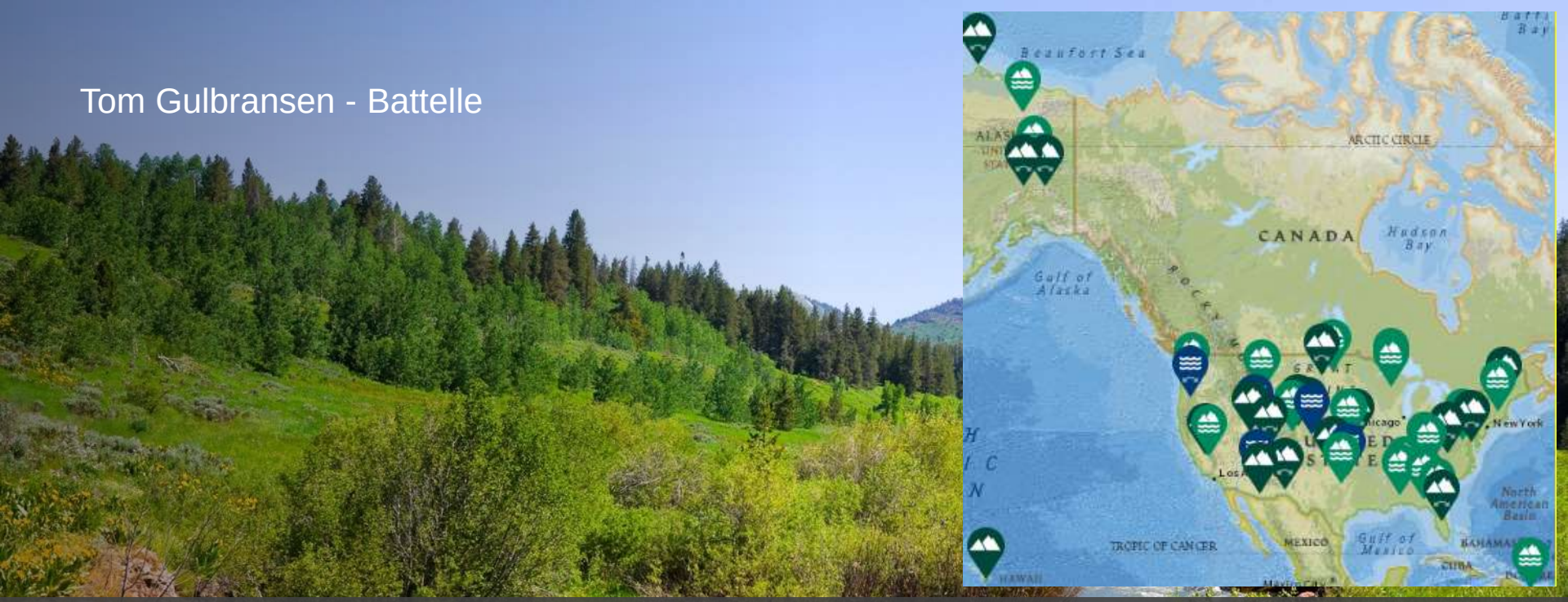
Tom Gulbransen - Battelle



NEON Data Delivery & Cyberinfrastructure

(mission, data products, data delivery, processing, architecture, interoperability, improvement plans)

This material is based upon work supported by NSF's National Ecological Observatory Network, a major facility fully funded by the National Science Foundation.

Why is NEON important?

NEON provides a coordinated national system for monitoring a number of critical ecological and environmental properties at multiple spatial and temporal scales.

…transformative science …workforce development





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NEON's 176 Data Products Overlap Multiple Themes

Atmospheric 58	Organismal 51	Ecohydrology 47	Biogeochemistry 85	Land Related 47
				
+11 from AmeriFlux	+1 from PhenoCam +3 from MG-RAST	+2 from AeroNet		
H_2O, CO_2 Heat Isotopes Turbulence Storage Fluxes	Abundance Composition Pathogens Phenology DNA Barcodes Marker Genes Metagenomics	Water quality Precipitation Levels Discharge Radiation Geomorphology	Soil conditions Chemistry Particulates Foliar characteristics	Spectrometry Hi-Res imagery LiDAR

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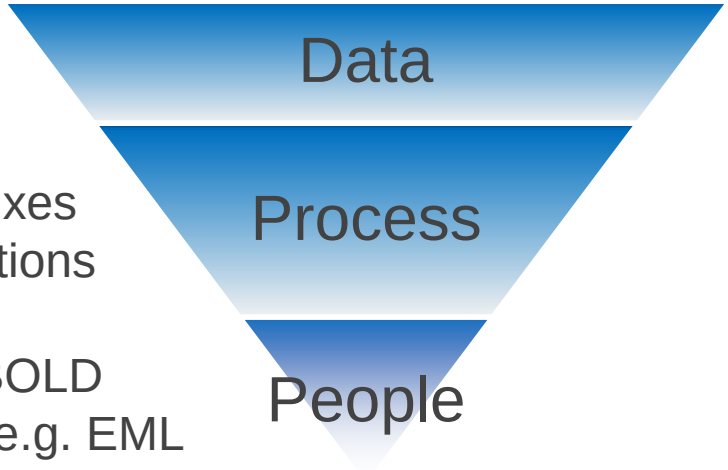
NEON CI & Data Science Offerings

National
Ecological
Observatory
Network

Cyberinfrastructure = resources, tools & services, observation to delivery



- of **field observational results**
- of **sampling protocols**
- of **algorithms**
  - surface atmospheric exchange/fluxes
  - meteorological temporal interpolations
- of **data science methods**
  - APIs @ PhenoCam, MG-RAST, BOLD
  - Ecological semantic conventions e.g. EML
  - Dictionary-driven generic observational pipeline
  - Data integration via workflow models
- of **practitioners**
  - ***21 Working Groups; ~1,500 unique users & 75k API hits/month***
  - Carpentry workshops & interns
  - Digital identifiers for data use/provenance
  - Large data facilities coalitions, e.g. RDA, CDF, ESIP

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NEON CI Data Delivery

Data Product Type	General Latency from Sampling to Portal	Primary Influence on General Latency	Existing Backlog	Estimated Complete Publication of Backlog
AOP	2 months	Staff during flights	2018 ongoing	Nov2018
AOP legacy		Reprocessing with new algorithms	2013-2016	Dec2018
Land, Water, Soil, Meteorology	15th of next month	5 day communications completion buffer	2018 ongoing	Monthly
Land, Water, Soil, Meteorology legacy		Volume of prior site-months	2013-2017	Nov2018
Eddy Covariance	15th of next month	5 day communications completion buffer	2018 ongoing	Monthly
Eddy Covariance legacy		Volume of prior site-months & configurations	2013-2017	Nov2018
OS – field observations	1-4 months (~9-13 for fish & veg structure)	Reviews as season progresses. HQ staff.		Oct2018
OS – domain lab results	1-3 months (6 & 13 for morphospp. & bathy)	Reviews as season progresses. HQ staff.		Sep2018
OS – external lab rolling batches	1-9 months	Reviews as season progresses. Lab deliveries.		Dec2018
OS – one time samples (megapits, soil)		external lab processing - MBL		Dec2018

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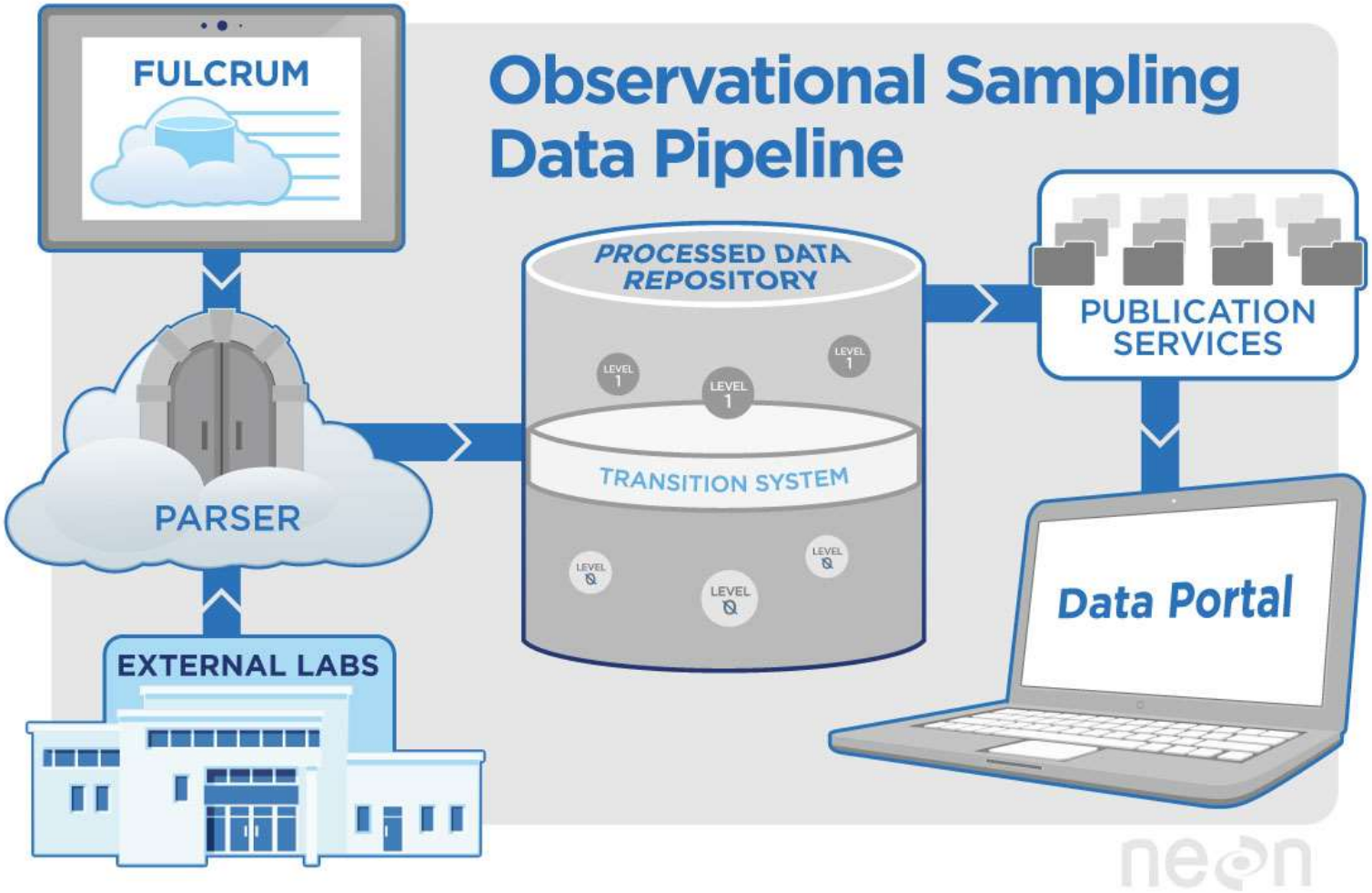

- 47 terrestrial & 34 aquatic sites, 100s protocols, dozens of labs
- Latencies from 5 to 365+ days

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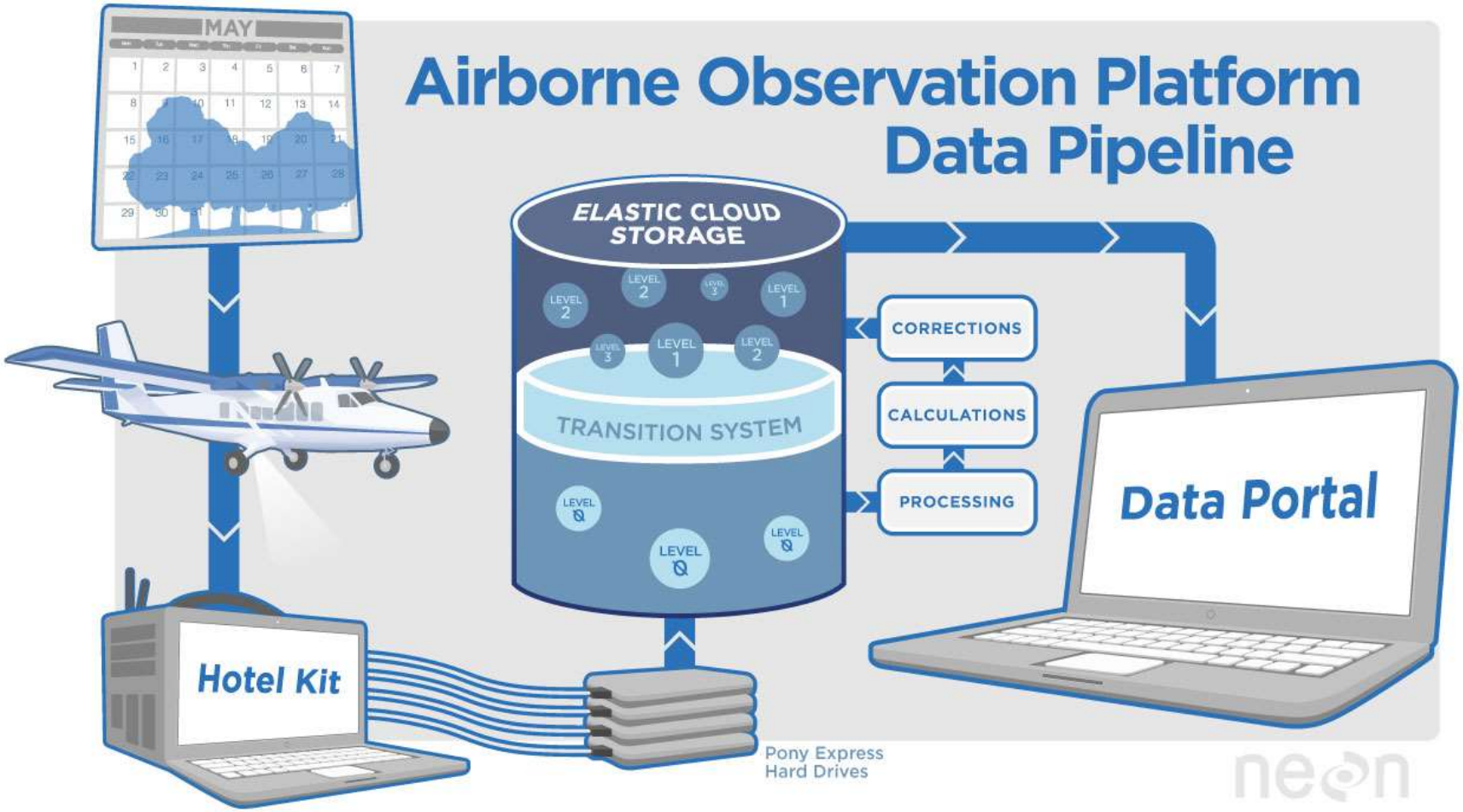

- 19 domains, 100-300km^2 flown annually at peak greenness
- Images, Spectroscopy (380 to 2500 nm), LiDAR
- 1-500GB/data product, ~2PB/yr

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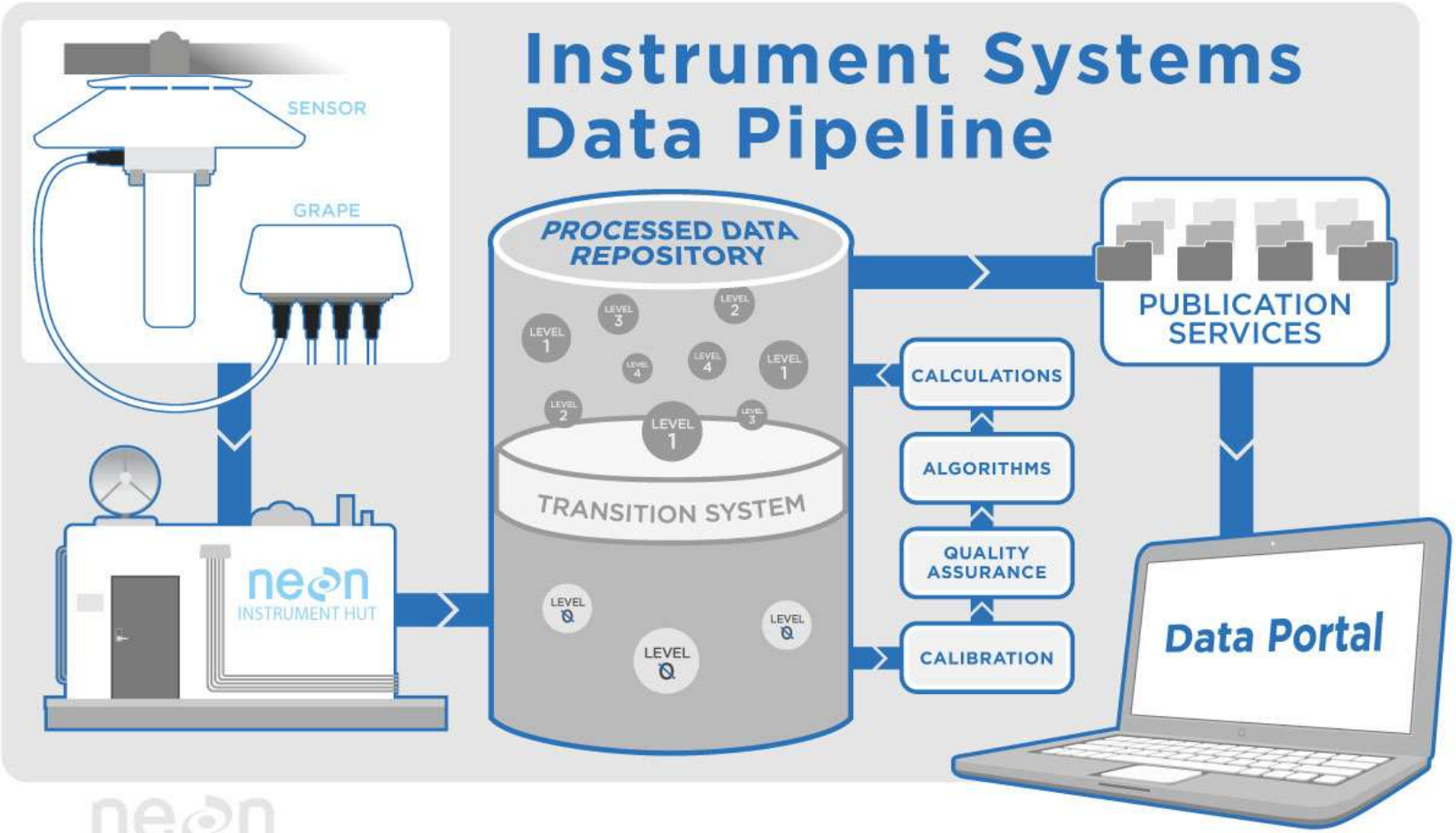

- 81 sites, 100s sensors per site, up to 40Hz
- Sensor→GRAPE→LC→HQ 5day lag, ~5TB/month

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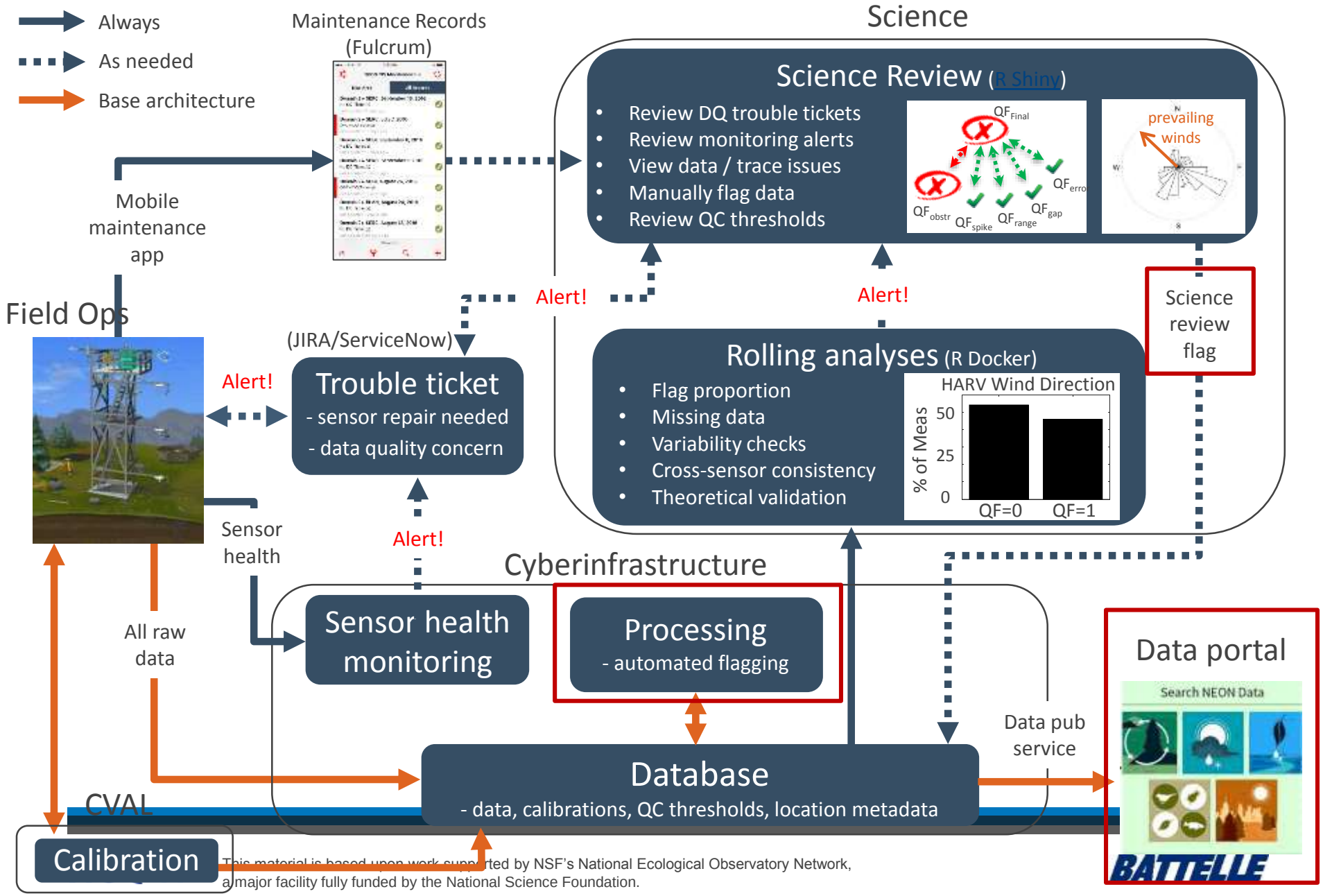
Instrumented Systems Data QA/QC Framework



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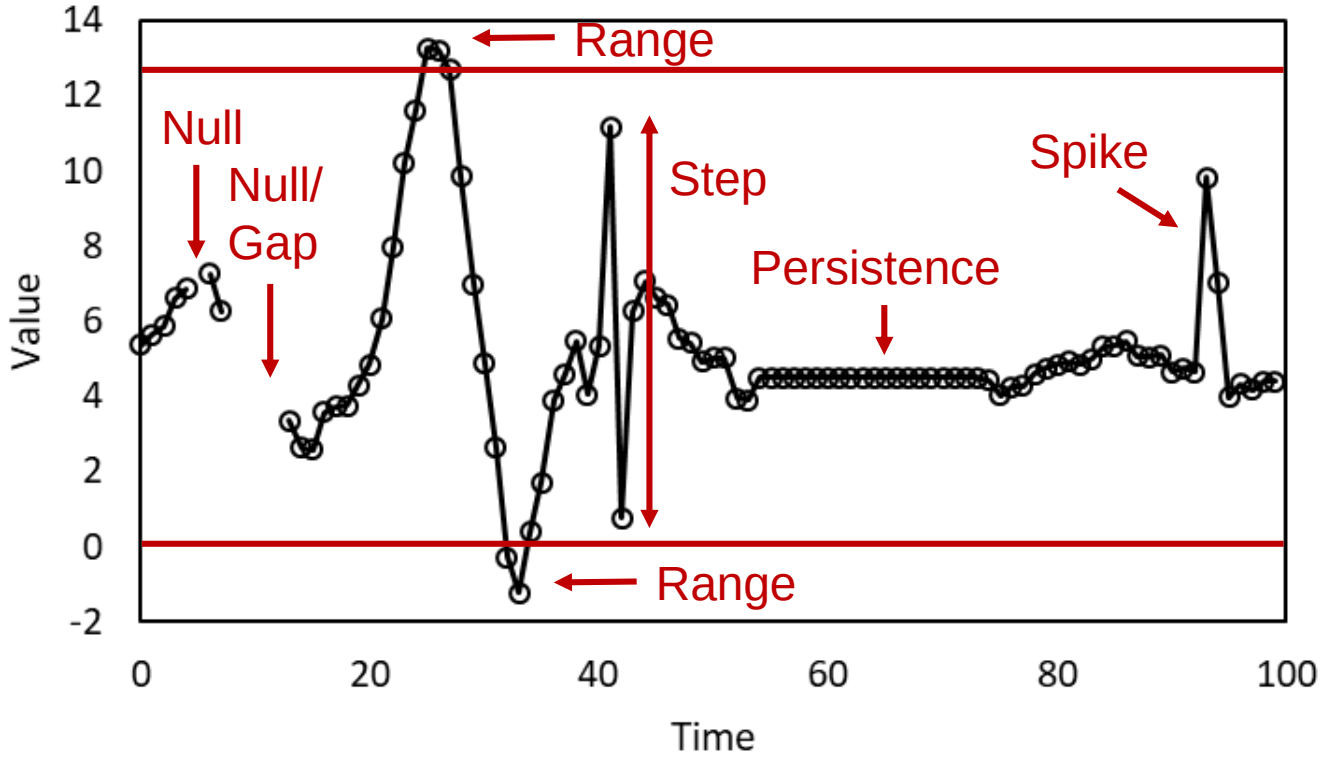
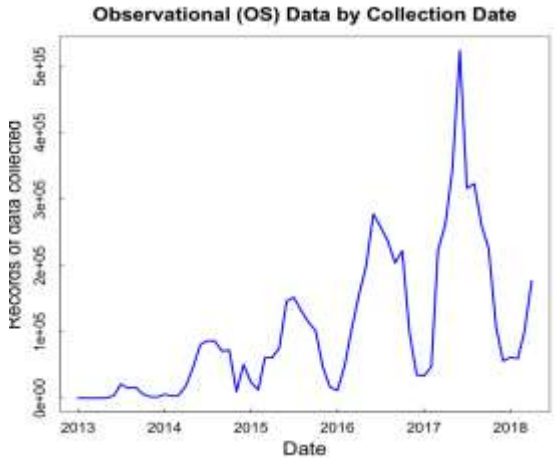
Automated flagging

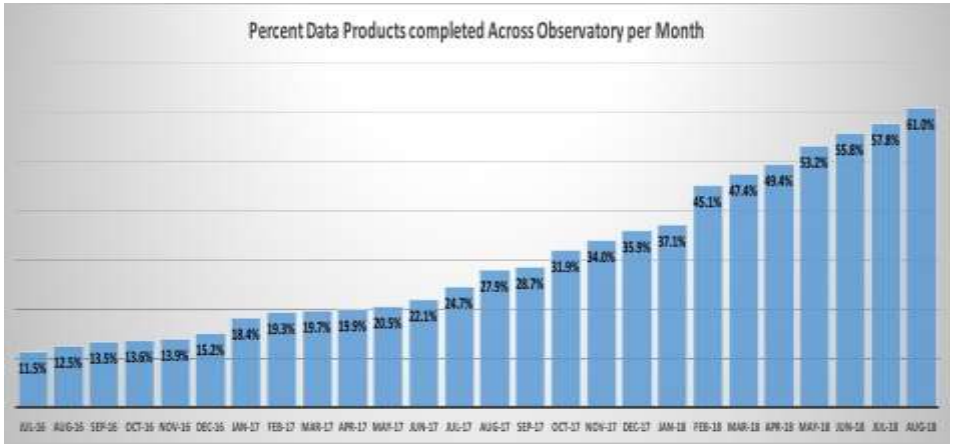
- Applied on each calibrated data value (native resolution)
- Basic tests: Null, Gap, Range, Step, Spike, Persistence
- Sensor-specific tests: e.g. sensor diagnostic
- If chosen, can remove any data point that fails a test



What's in a data package?

- Monthly or Annual data files with all basic data and quality flags
- CSV (IS, OS), HDF5 (EC, AOP), TIF (AOP), LAS (AOP), FASTA (metagenomics)
- Readme text file – general info about the data product
- Additional quality metrics, external lab data
- User guides & protocols; algorithm & sensor configuration documents
- Variable definitions, validation rules, and sensor positions
- Machine-readable metadata (EML)





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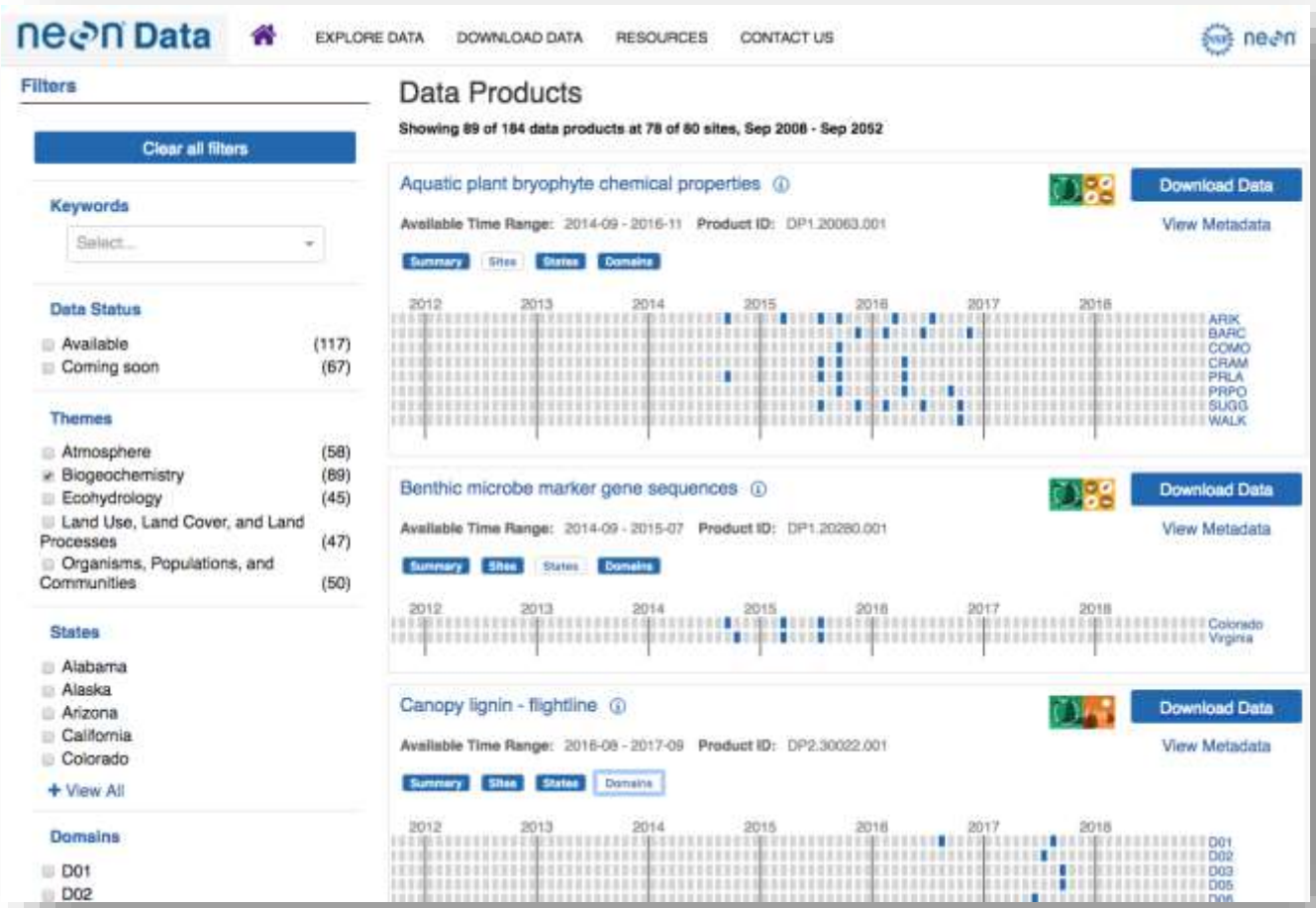
Interactive Browse



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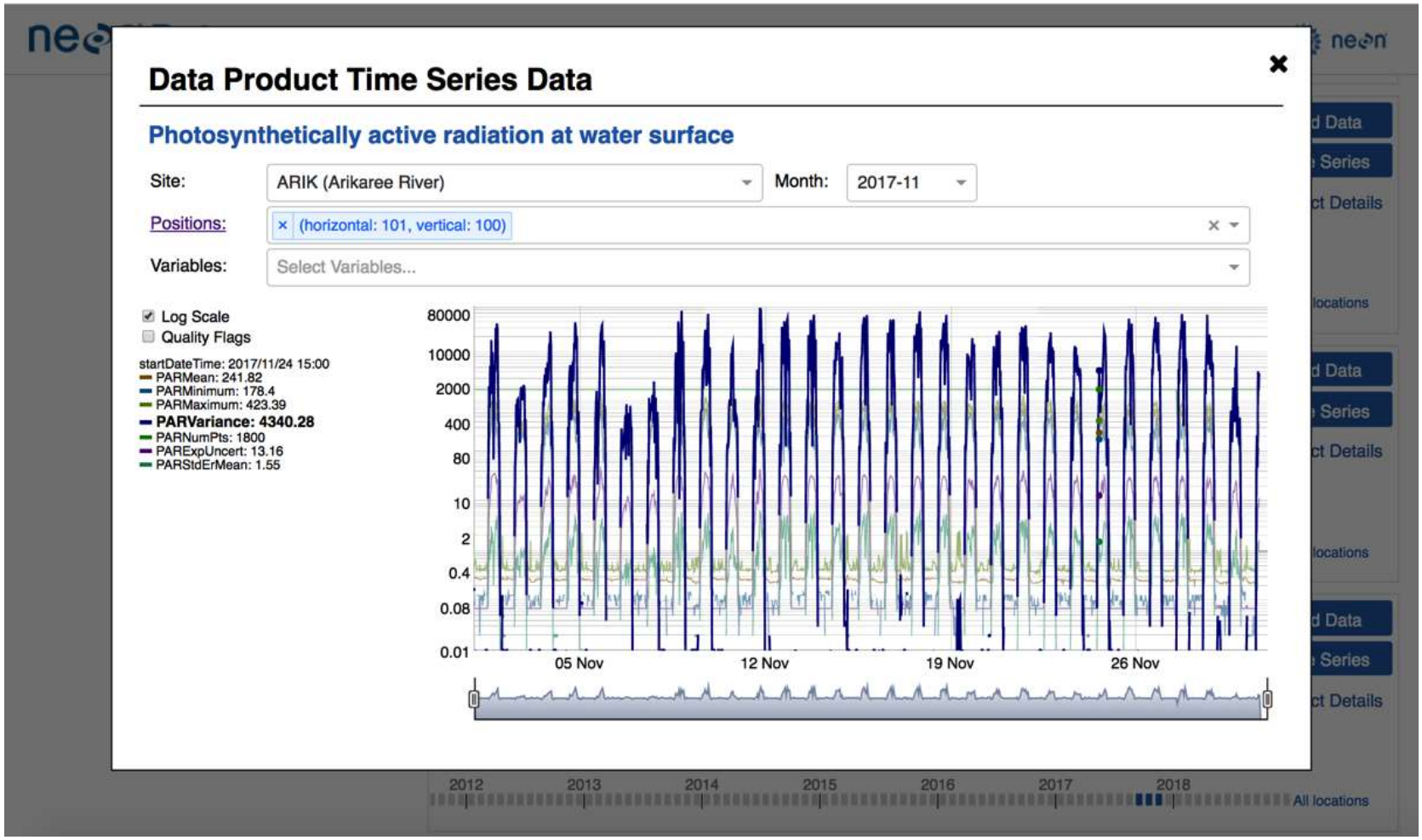
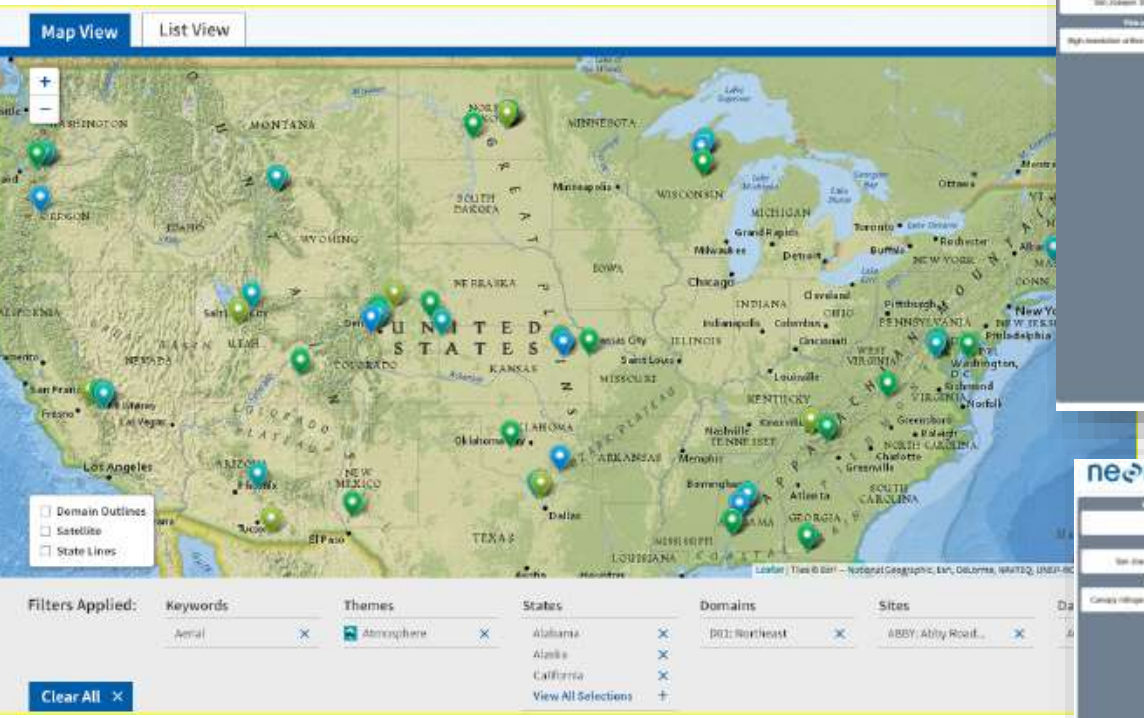
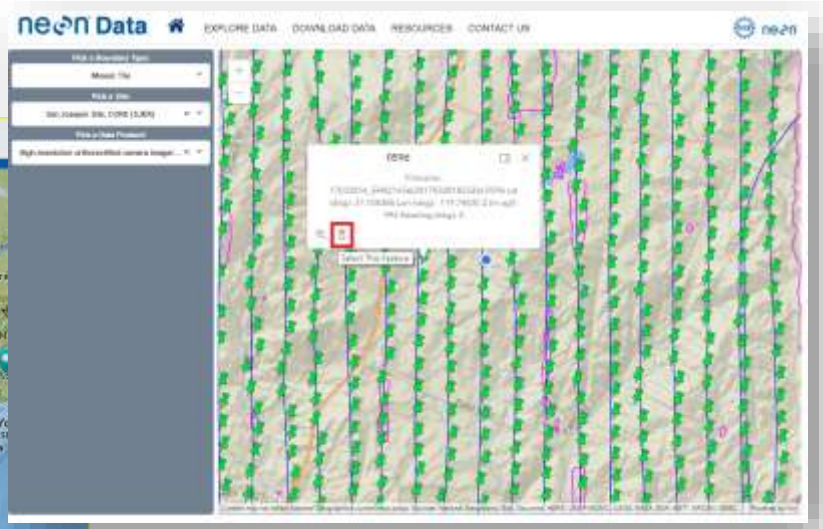
Interactive Time Series



Spatial Viewer (prototypes)





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Partner Repositories

- Work with specialized repositories for domain-specific data
- Use their APIs to keep NEON caches in sync
- Field data on portal; specialized data hosted

Current

MG-RAST metagenomics analysis server

AERONET AEROSOL ROBOTIC NETWORK

BOLDSYSTEMS

PhenoCam Gallery

DataONE Data Observation Network for Earth

Future

AMERIFLUX

OpenTopography High-Resolution Topography Data and Tools

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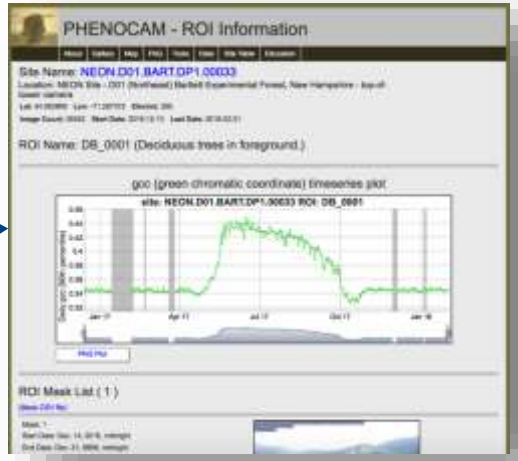
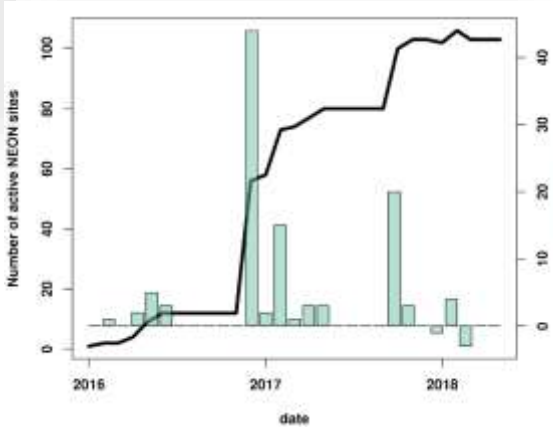
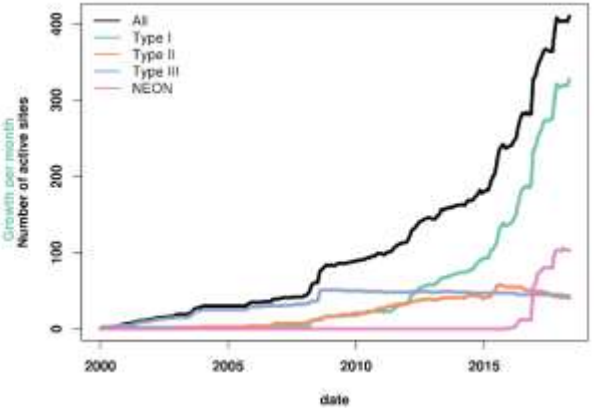
Data Portal & Phenocam Gallery



Collaborative work between 2 NSF programs – co-located sites and API modeled on NEON's.





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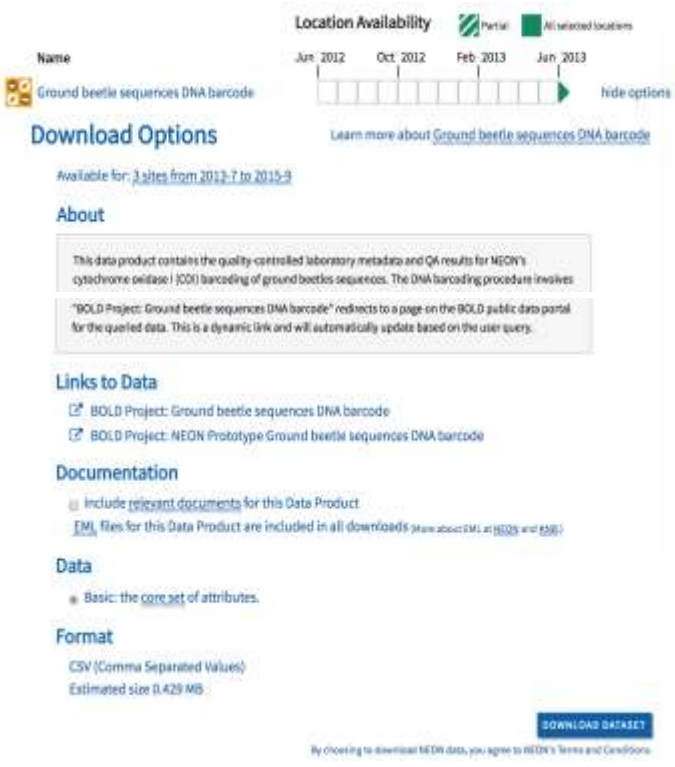
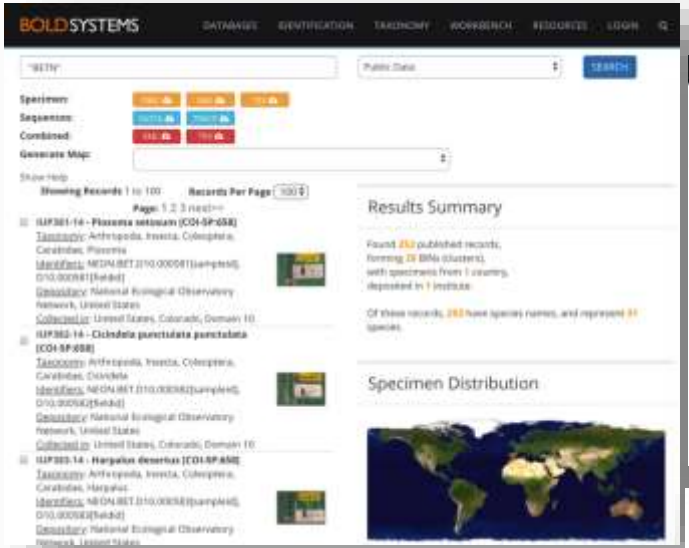
Data Portal & BOLD





MG-RAST is similar in functionality

Access to thousands of beetle, mosquito, small mammal, and fish records, from current protocols as well as prototype protocols and sites.

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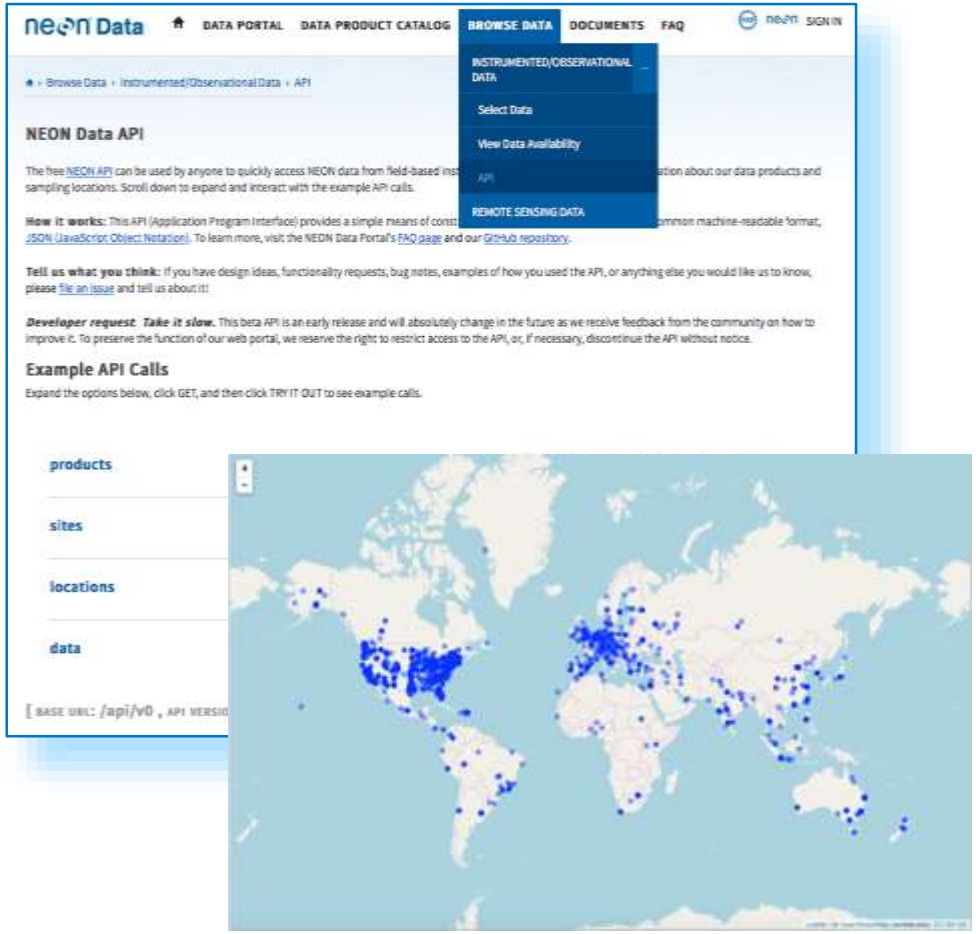
REST API: Programmatic Access

http://data.neonscience.org/data-api

- Open access
- Provides product information, site and within-site information, documents, and data
- Returns information in JSON format
- Returns both zipped data packages and individual data files
- Recently added endpoints for access to taxonomic lists and sample custody histories



NEON CI Software Architecture - Layers

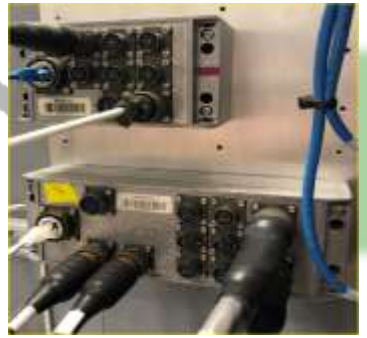
Publish

Process

Store

Acquire

data services, transport, queuing



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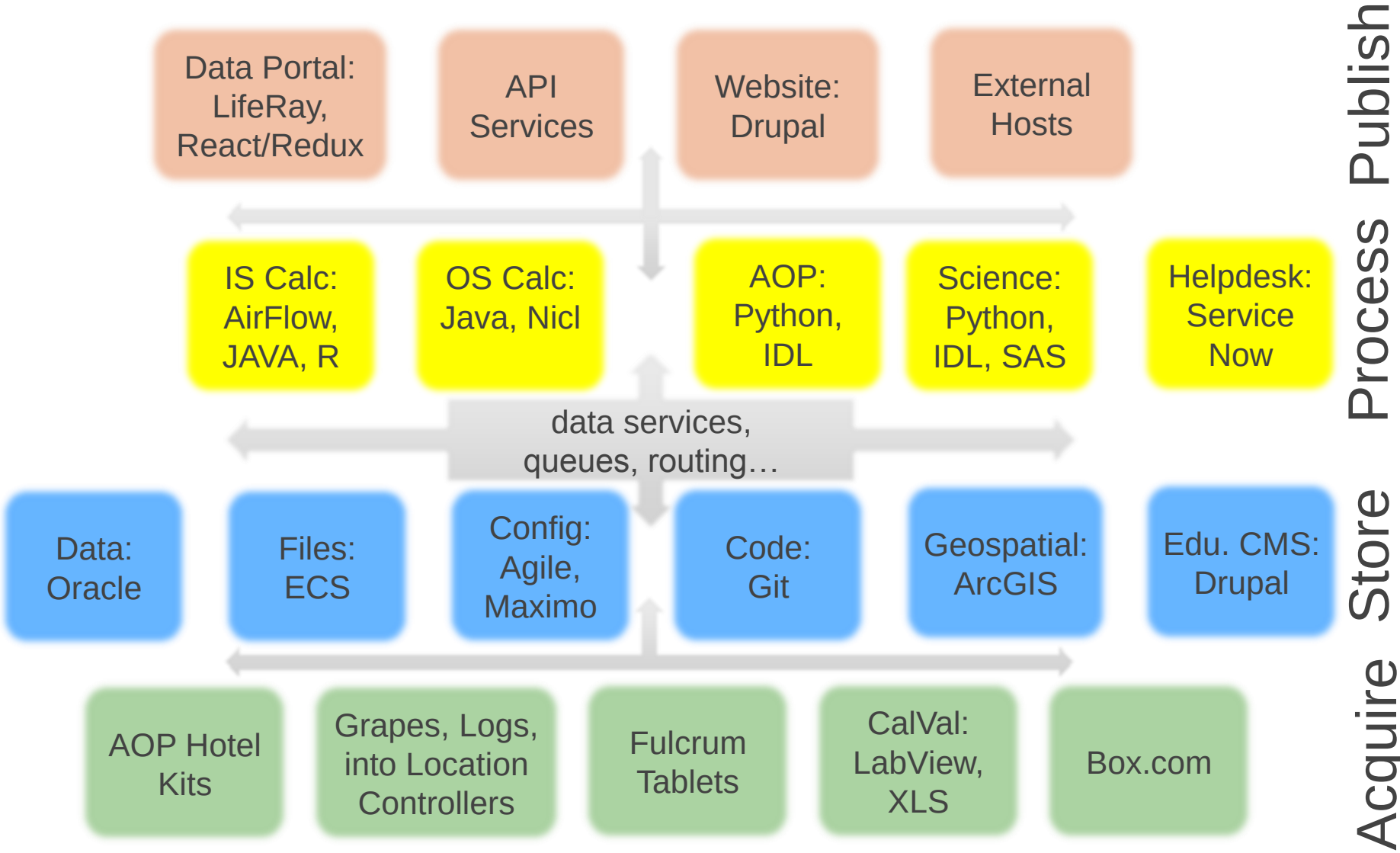
NEON CI Software Architecture - Elements



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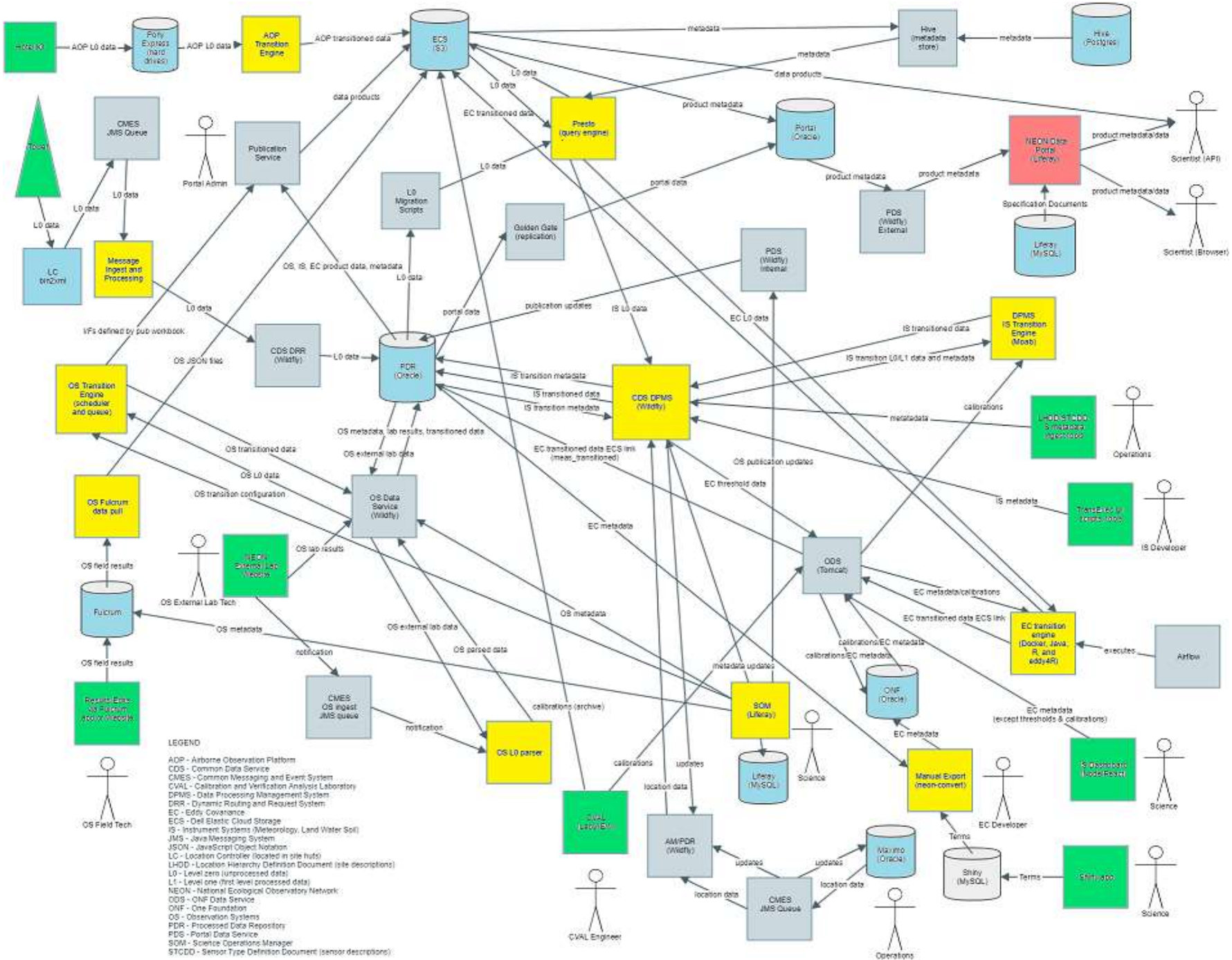
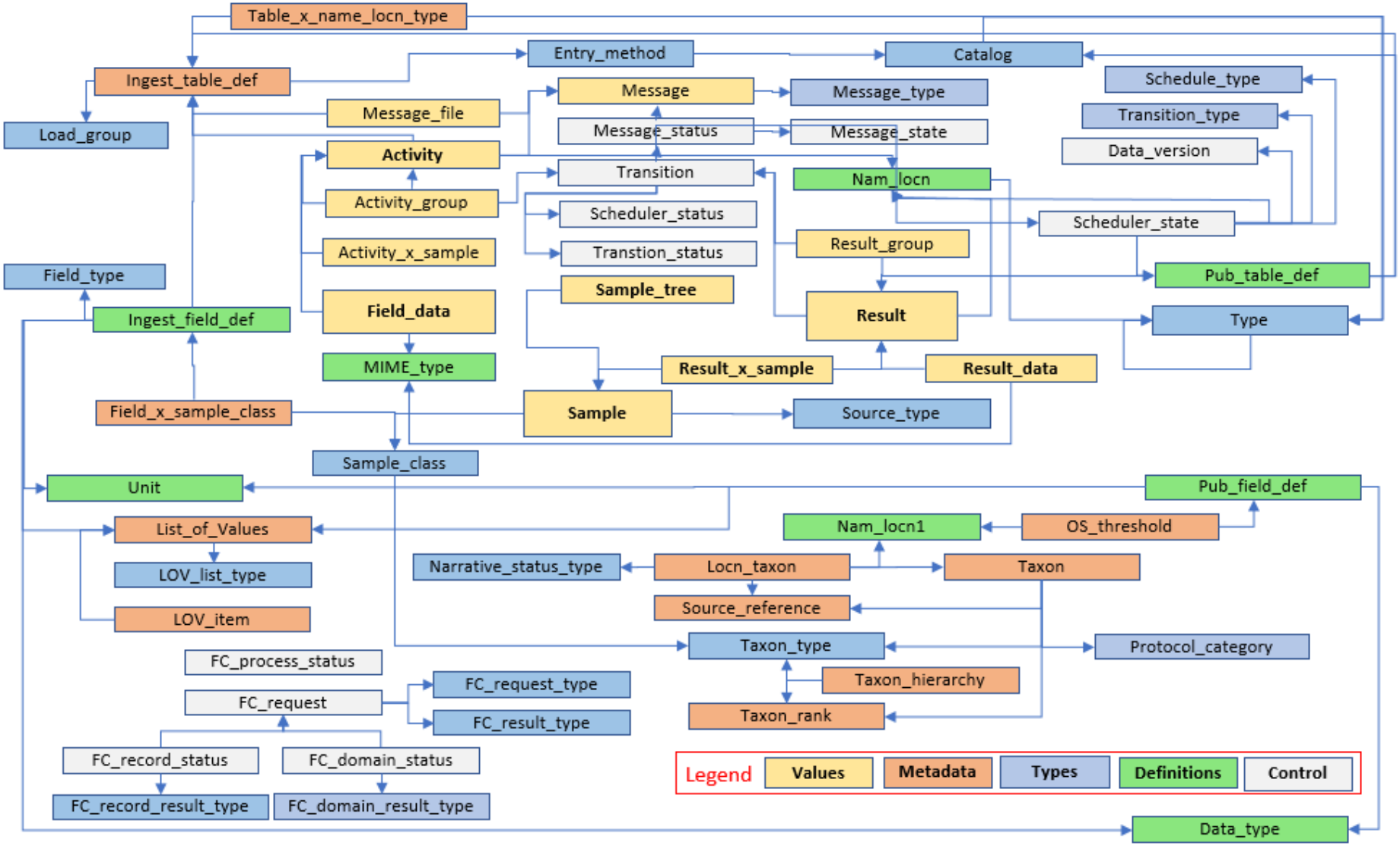
NEON Data Flow in CI Architecture



PDR Database – Observations Logical Model



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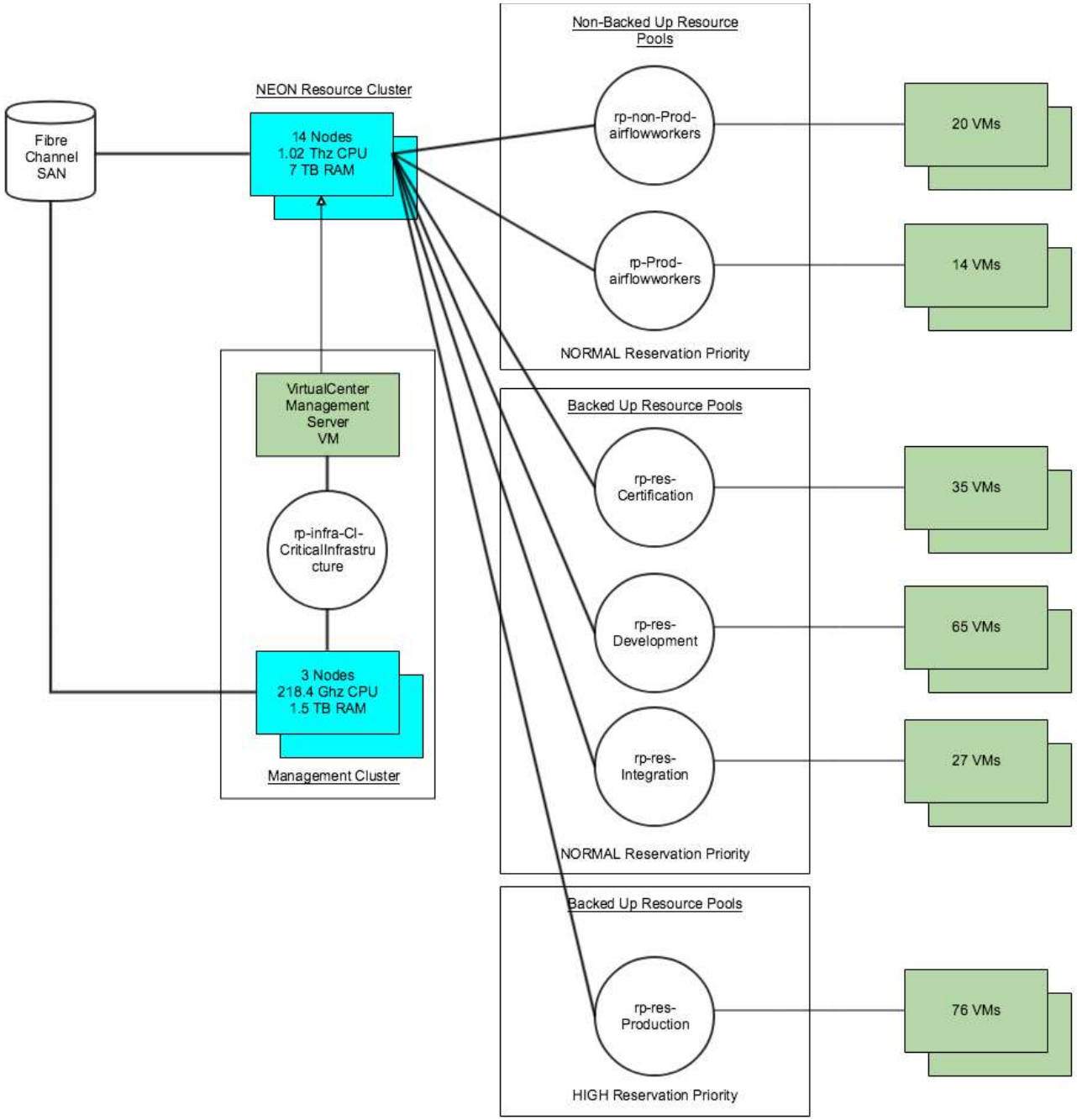
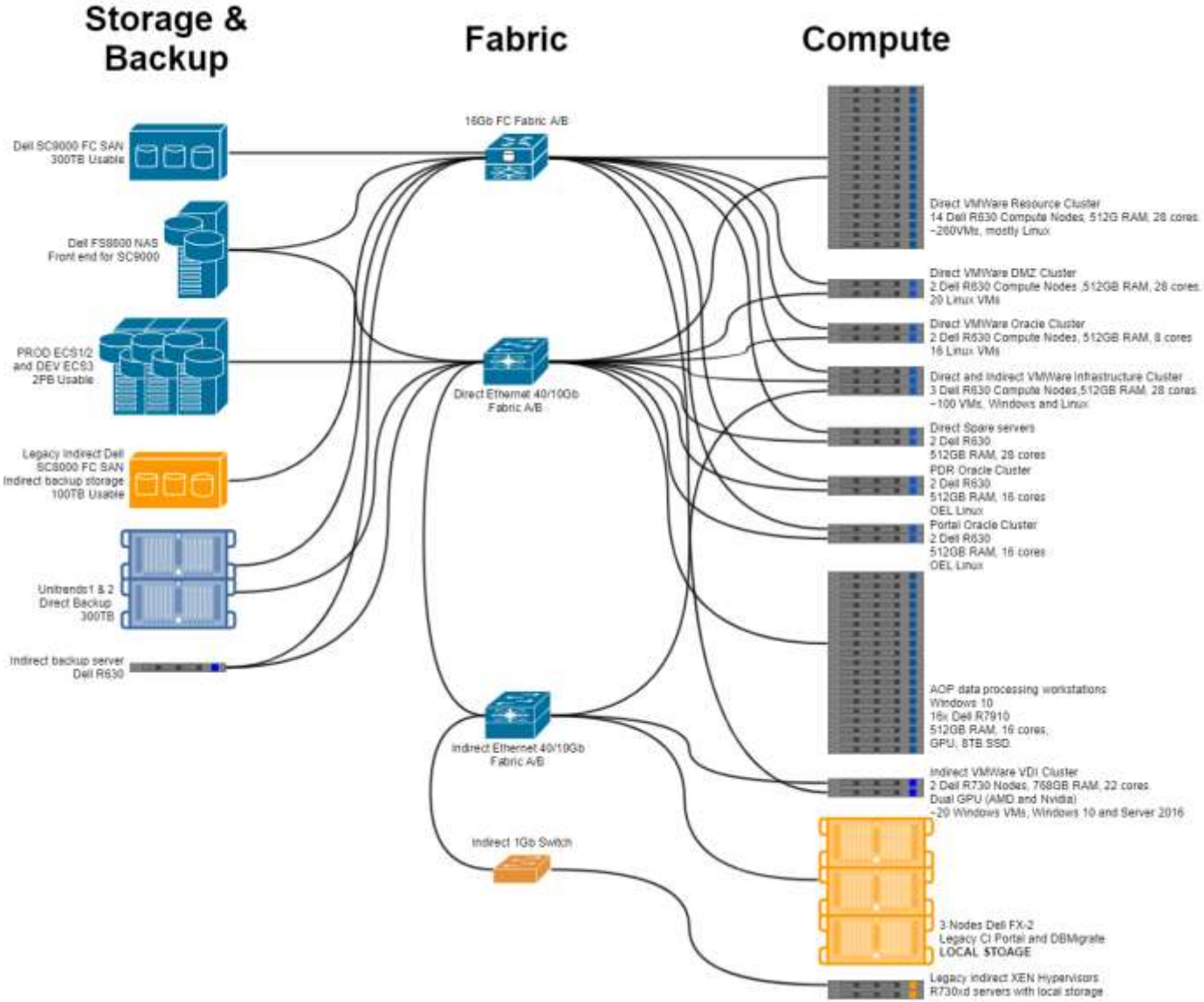
NEON CI Virtual Machine Resource Pools



Denver Datacenter – Configuration Schema



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Cyber Security Overview

1. Security Strategy – NIST Cyber Security Framework: Identify, Protect, Detect, Respond, Recover
2. NIST CSF Timeframe – Program in progress – Goal is to address all categories by mid 2019
3. Perimeter Security – All Ingress / Egress Points are Firewall protected
4. Cloud Security – Encrypted Connections (TLS 1.0+) to Cloud Apps
5. Endpoint Security – Anti-malware / Endpoint Controls
6. Vulnerability Remediation – Constant patching schedule
7. Email Security – Microsoft Advanced Threat Protection – Phishing, Malware, Safelink protection
8. User Awareness – All employees are required to complete annual cyber security training

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NEON CI & Data Interoperability

1. Across the community of researchers
   - Data collection, QA, standardized encoding and uncertainty handling protocols
   - Data exchange I/O formats & metadata
   - Data processing algorithms, code libraries

2. Between research facilities
   - NEON, AmeriFlux and Fluxnet common methods
   - Fully compliant metadata provisioning of NEON results to 6 partner host systems
   - Participation in meta-analyses of international CI methods, e.g. workflow objects

3. In active collaboration with aggregators
   - DataOne partner and metadata practitioner
   - EarthCube, CDF, ESIP, RDA coalition participants

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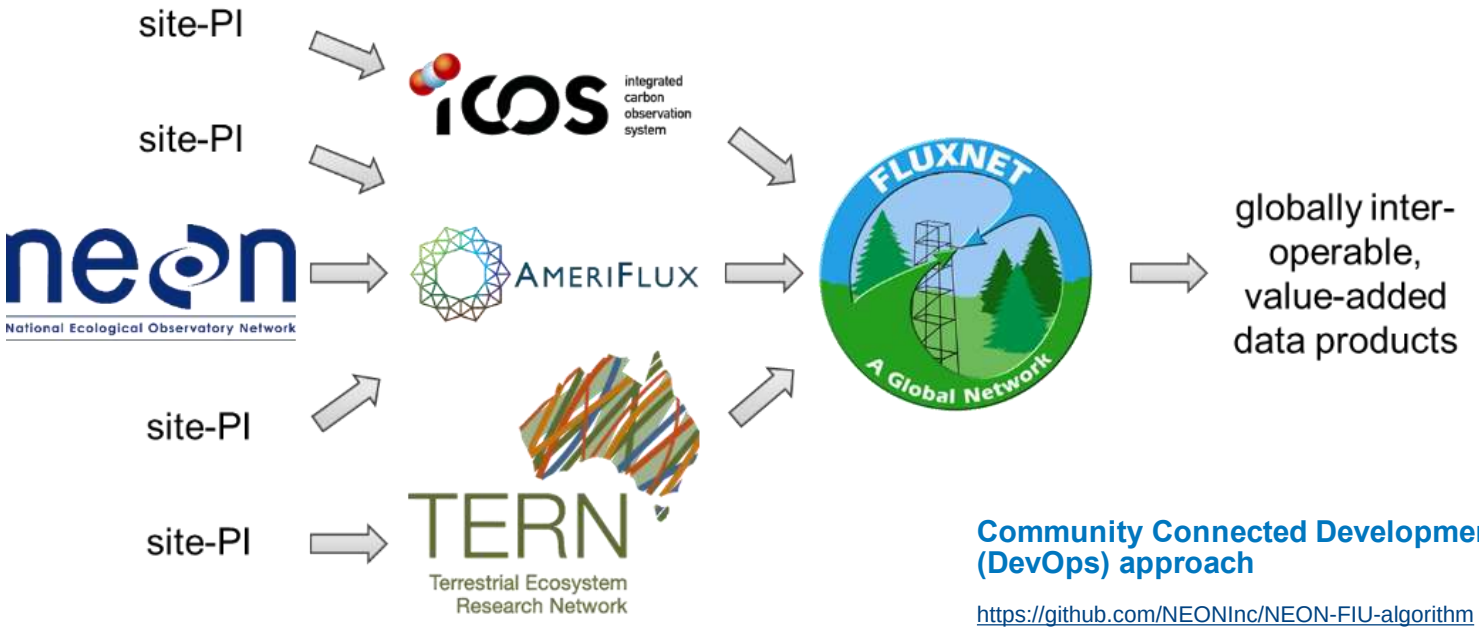
Data Product Collaboration (example)



Community Connected Development and Operations (DevOps) approach

https://github.com/NEONInc/NEON-FIU-algorithm

https://hub.docker.com/u/stefanmet/

Metzger, et.al. 2017. eddy4R 0.2.0: a DevOps model for community-extensible processing and analysis of eddy-covariance data based on R, Git, Docker, and HDF5. Geosci. Model Dev., 10, 3189–3206.

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Data Science Tools and Training: NEONScience on GitHub

- Open-source code packages to facilitate NEON data access and use
- Access to code used to generate NEON data products

```
Console   Terminal
~/
downloaded 29 KB

85 files downloaded to /Users/clunch/Desktop/filesToStack10003
> stackByTable("/Users/clunch/Desktop/filesToStack10003/", folder=T)
Unpacking zip files
  |=================================================================================================| 100%
Stacking table brd_countdata
  |=================================================================================================| 100%
Stacking table brd_perpoint
  |=================================================================================================| 100%
Finished: All of the data are stacked into  2  tables!
Copied the first available variable definition file to /stackedFiles and renamed as variables.csv
Copied the first available validation file to /stackedFiles and renamed as validation.csv
Stacked brd_countdata which has 74604 out of the expected 74604 rows (100%).
Stacked brd_perpoint which has 5506 out of the expected 5506 rows (100%).
Stacking took 4.126218 secs
All unzipped monthly data folders have been removed.
>
```

neonUtilities R package:

- Download data from NEON API
- Merge data files from Portal or API
- Convert file format for interoperability

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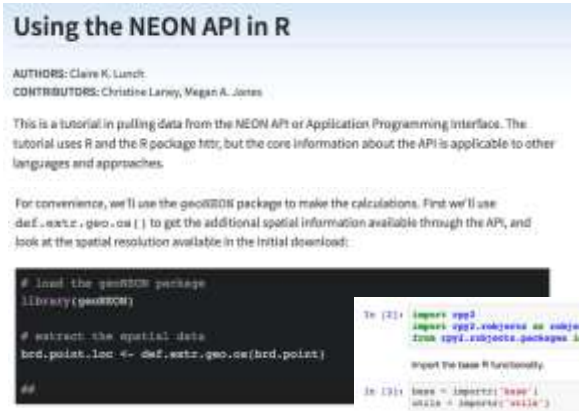
Data Science Tools and Training: Tutorials & Workshops

- Advance users' data analysis skill levels
- Online tutorials for self-directed training
- Data Institute on-site at NEON HQ
- Workshops at meetings and conferences
- Includes training in using the GitHub.com/NEONScience packages



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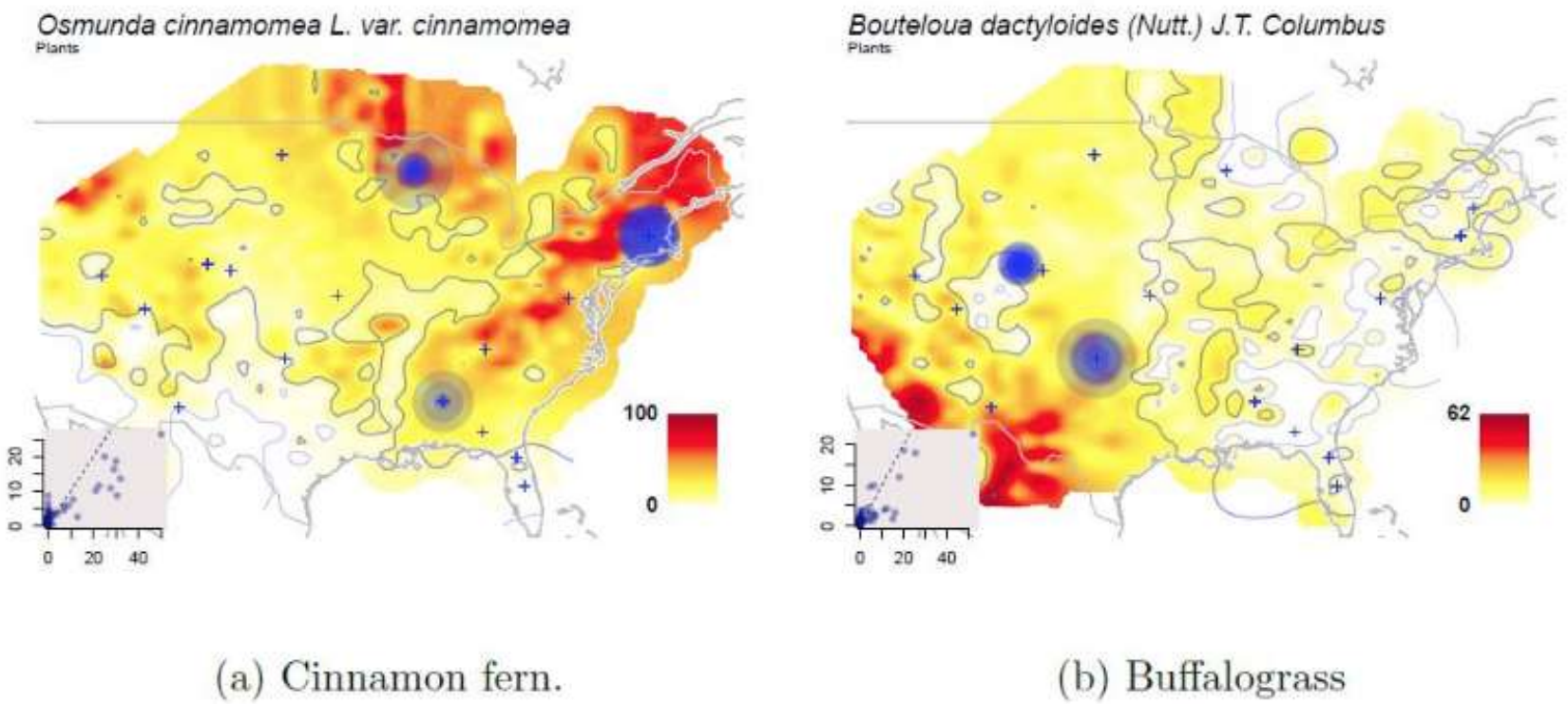
User Community Projects: Predictive Distributions



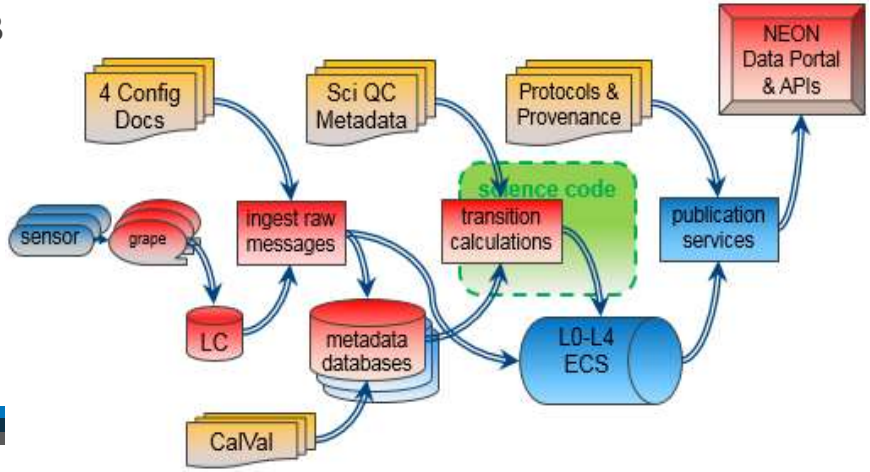
(a) Cinnamon fern. (b) Buffalograss

Figure 10: Predictive distributions for plant cover. Symbolism follows Figure 4.

Clark lab: sites.duke.edu/neon/prediction

NEON CI Improvement Plans

1. Ongoing cyberengineering support
   - e.g. better interface to manage sensor metadata; unexpected data gap checks…
2. Prioritized queue of CI or Data Product enhancements
   - e.g. improve minimum viable products; address tech debt; better algorithms…
3. Service Management continued expansion/integration
   - e.g. more workflow delegation; closer linkage with SOM & monitoring…
4. Asset management tools & methods assessment
   - e.g. mitigate risks of vulnerable sensor installation metadata addressing…
5. Proposed research & development towards VI version2
   - Redesign data acquisition hw&sw (i.e. “GRAPE” data streams)
   - Pilot optimized transition engine & DB
   - Upgrade Data Portal platform & tools
   - Evaluate CI capacity, connectivity & offsite disaster recovery options



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