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Data Catalog Selection and Implementation

21 August 2024

Rebecka Bence

Aaron Moreno

Kenneth Ham

Chris Johnson

U.S. DEPARTMENT OF ENERGY BATTELLE

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Agenda

1. Need for data catalogs
2. Function of a data catalog
   a) Metadata overview
   b) Required functionality in practice
3. Evaluating data catalog tools
4. Data catalog requirements
   a) Defining requirements
   b) Implementation considerations
5. Example of data catalog prototype and features

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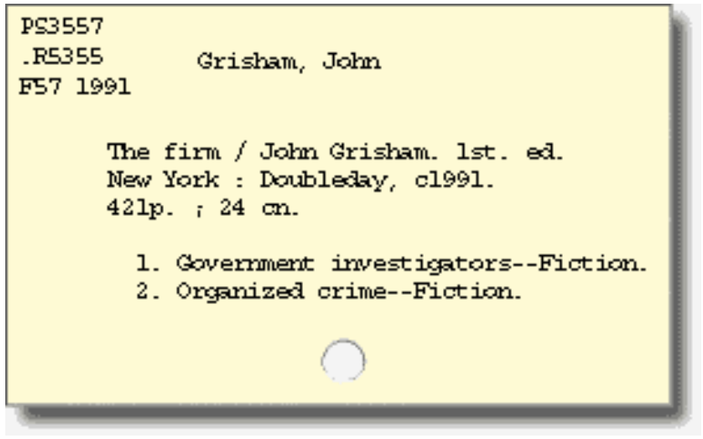
Background and Need

- What is a data catalog?
  - Consider a library card catalog
    - Why did you need the catalog?
    - What would have happened if you didn't have the card catalog?

- Definition
  - **From IBM**: An inventory of all data assets in an organization, designed to help professionals quickly find the most appropriate data for any analytical or business purpose



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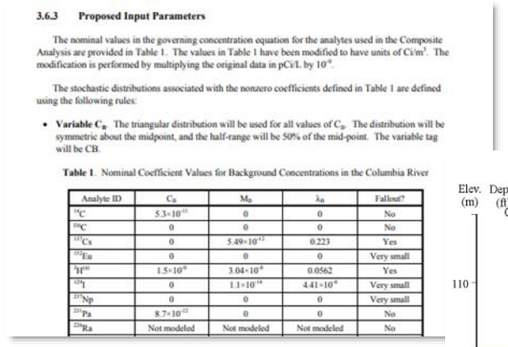
Background and Need

- What need is there for a data catalog?
  - Multiple environmental databases and data assets
    - Data inherently comes in different forms and formats
      - Models
      - Electronic tabulated data
      - Geospatial data
      - Report narratives
      - Tables and figures
      - Images
  - Need a means to find these data resources across multiple systems
  - Multiple agencies/contractors
    - Overlapping "authoritative" data sources


3.6.3 Proposed Input Parameters

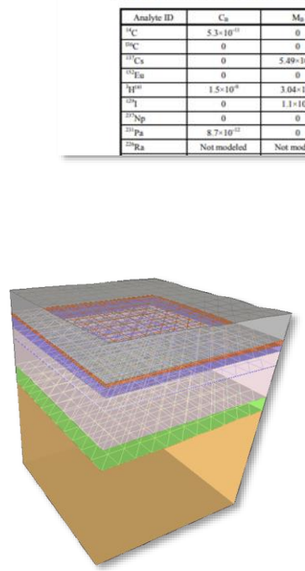
The nominal values in the governing concentration equation for the analytes used in the Composite Analysis are provided in Table 1. The values in Table 1 have been modified to have units of Ci/m³. The modification is performed by multiplying the original data in pCi/L by 10⁻⁹.

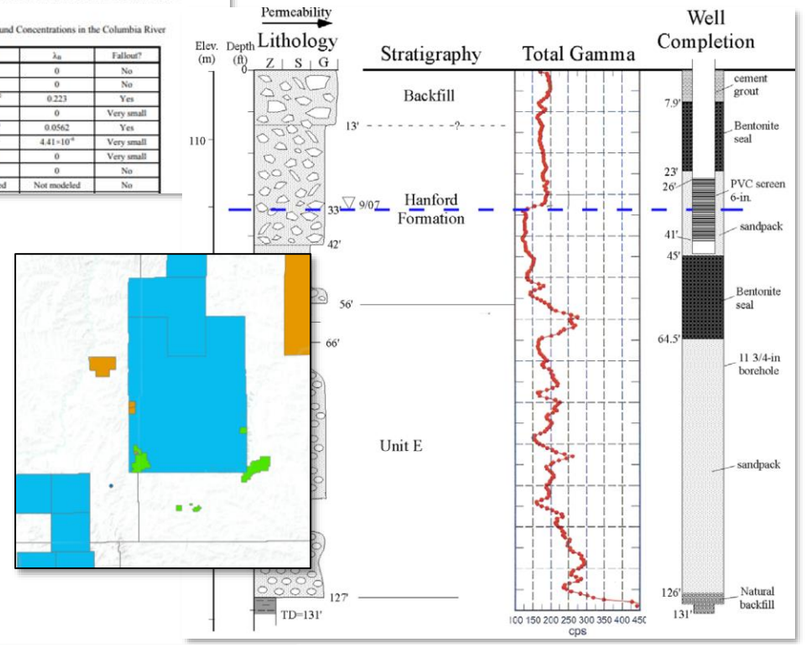
The stochastic distributions associated with the nonzero coefficients defined in Table 1 are defined using the following rules:

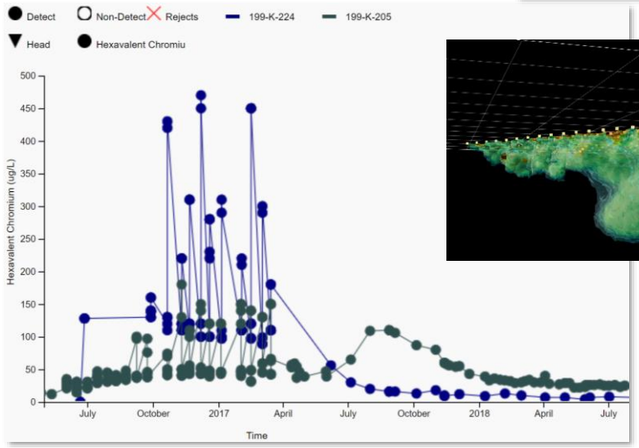
- **Variable C_B.** The triangular distribution will be used for all values of C_B. The distribution will be symmetric about the midpoint, and the half-range will be 50% of the mid-point. The variable tag will be CB.

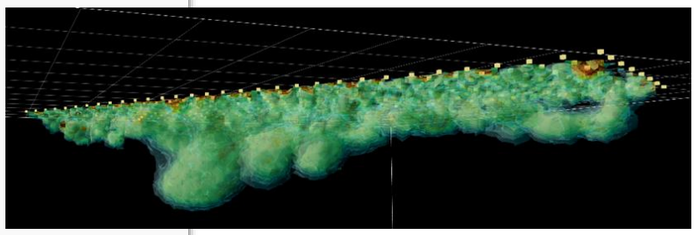
Table 1. Nominal Coefficient Values for Background Concentrations in the Columbia River

Analyte ID	C_B	M_B	λ_B	Fallout?
^{14}C	5.3×10^{-11}	0	0	No
^{36}Cl	0	0	0	No
^{137}Cs	0	5.49×10^{-12}	0.223	Yes
^{152}Eu	0	0	0	Very small
$^{3}H^{HO}$	1.5×10^{-8}	3.04×10^{-8}	0.0562	Yes
^{129}I	0	1.1×10^{-14}	4.41×10^{-8}	Very small
^{237}Np	0	0	0	Very small
^{231}Pa	8.7×10^{-12}	0	0	No
^{226}Ra	Not modeled	Not modeled	Not modeled	No









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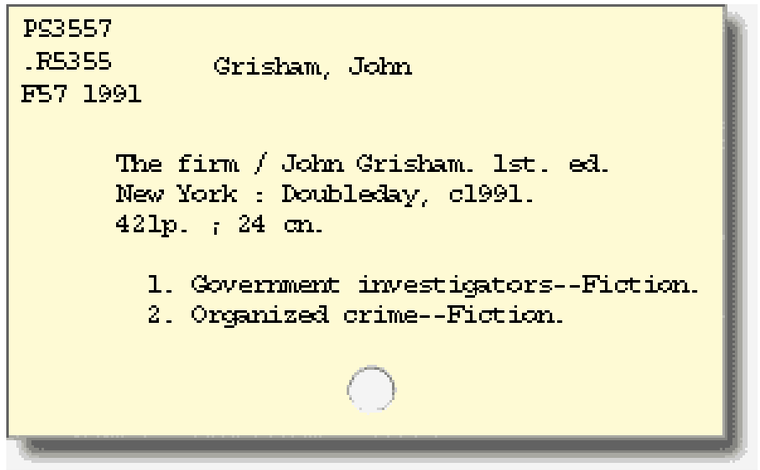
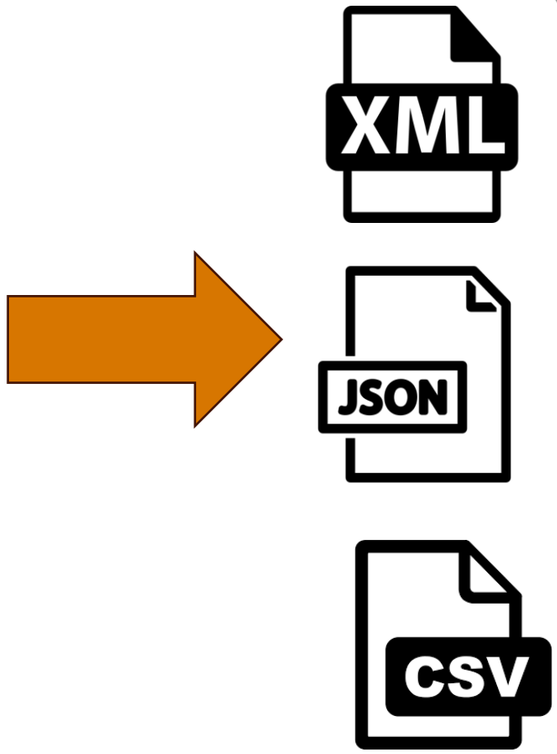
Basic Functionality

- Catalogs are a key aspect to making data FAIR (findable, accessible, interoperable, and reusable)
- To make data FAIR, catalogs store **metadata**



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Metadata Standards

- How information is organized in a metadata file matters for readability and interoperability

09/06/2022 Rev. 0

RJ LEE GROUP

Heather Medley
Central Plateau Cleanup Company, LLC (Env)
PO Box 1464
Richland, WA 99352
Client Project: Anions

Laboratory Report

RJ Lee Group No.: W208169
SDG No: RJLG22C0529
Samples Received: 08/18/22 09:10
Analysis/Prep Date: 08/19/22 04:23
Report Date: 08/31/22 07:34

Sample Name: B45NF7 **Batch No:** BH20086 **Date Sampled:** 08/17/22 12:06
RJ Lee Grp. ID: W208169-01 **Matrix:** Water **Date Analyzed:** 08/19/22 04:23

Analyte	Method	Result µg/mL	PQL µg/mL	MDL µg/mL	Dilution Factors	Qualifiers
Bromide	EPA 300.0	0.29	0.20	0.10	2	D
Chloride	EPA 300.0	19.7	1.50	0.75	50	D
Fluoride	EPA 300.0	0.28	0.04	0.02	2	D
Nitrate as NO3-N	EPA 300.0	41.9	1.15	0.60	50	D
Nitrite as NO2-N	EPA 300.0	< 0.03	0.06	0.03	2	U, D
Sulfate	EPA 300.0	46.5	7.50	3.75	50	D

```
▼<gmd:MD_Metadata xmlns:gmd="http://www.isotc211.org/2005/gmd" xmlns:gco="http:
 xmlns:gml="http://www.opengis.net/gml" xmlns:xlink="http://www.w3.org/1999/xli
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Metadata Standards and Schema

- There are many types of metadata standards – generic to domain-specific
  - Dublin Core
  - International Organization for Standardization (ISO) 19XXX series
  - Federal Geographic Data Committee (FGDC)
  - Darwin Core
  - NASA's Standards
- *Schema* is the part of the standard that outlines the overall structure of the metadata and addresses how to handle common components like dates, names, and places
- Adopting vs. adapting metadata schema
- Encoding schemes to further standardization

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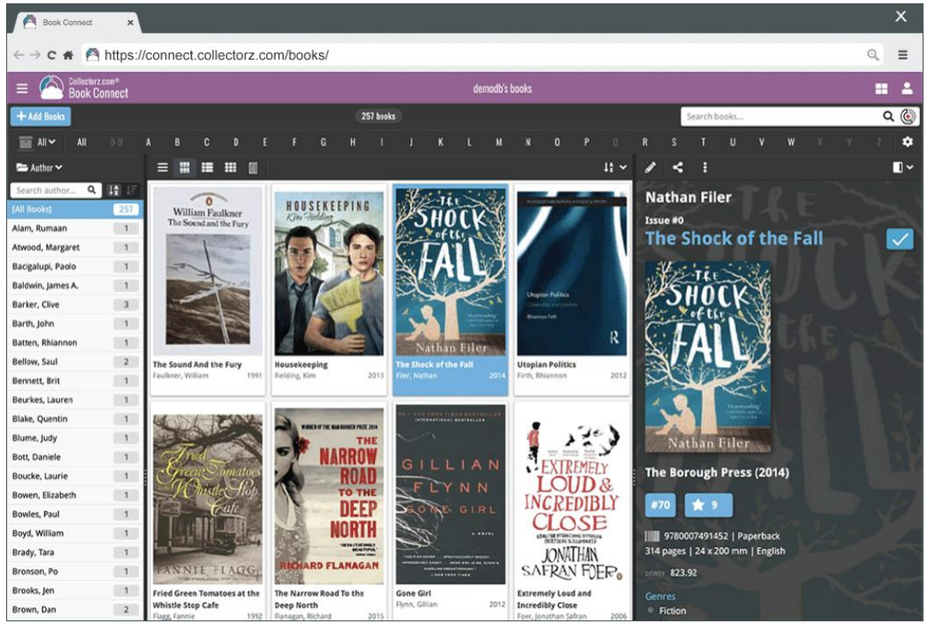
Catalog Functions



- To provide access to datasets, a data catalog must:
  - Manage records
  - Enable users to find datasets of interest
  - Provide a way to retrieve the dataset of a selected catalog record
  - Be able to manage/store large numbers of catalog records

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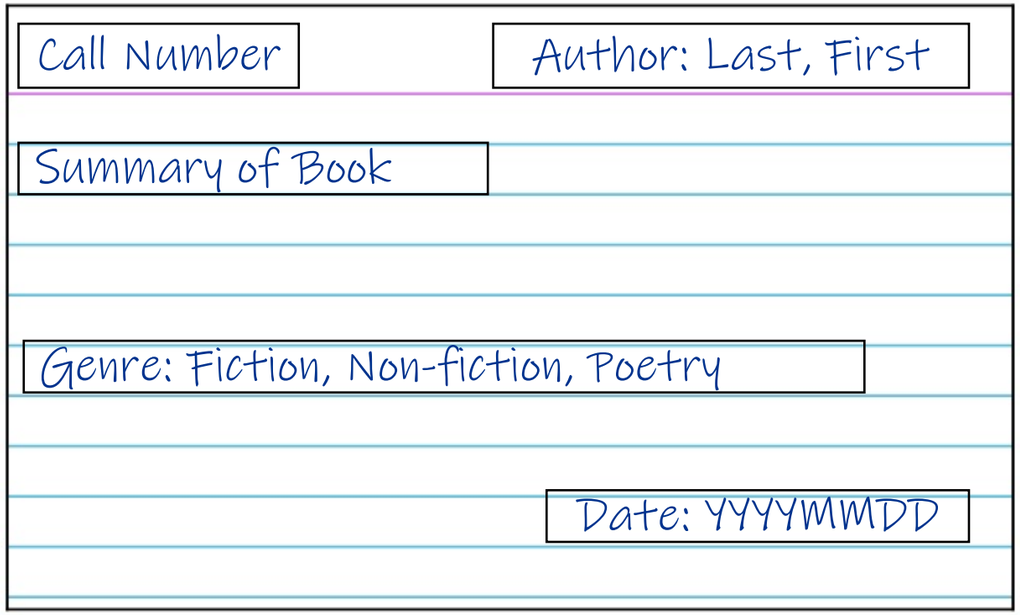
Catalog Functions: Cataloging

- A record is created by compiling descriptive and well-organized metadata
- A record usually includes a link to the dataset/asset
  - Assisting features:
    - ✓ A well documented metadata standard/schema
    - ✓ Ability to validate incoming metadata
    - ✓ A metadata creation wizard or tool



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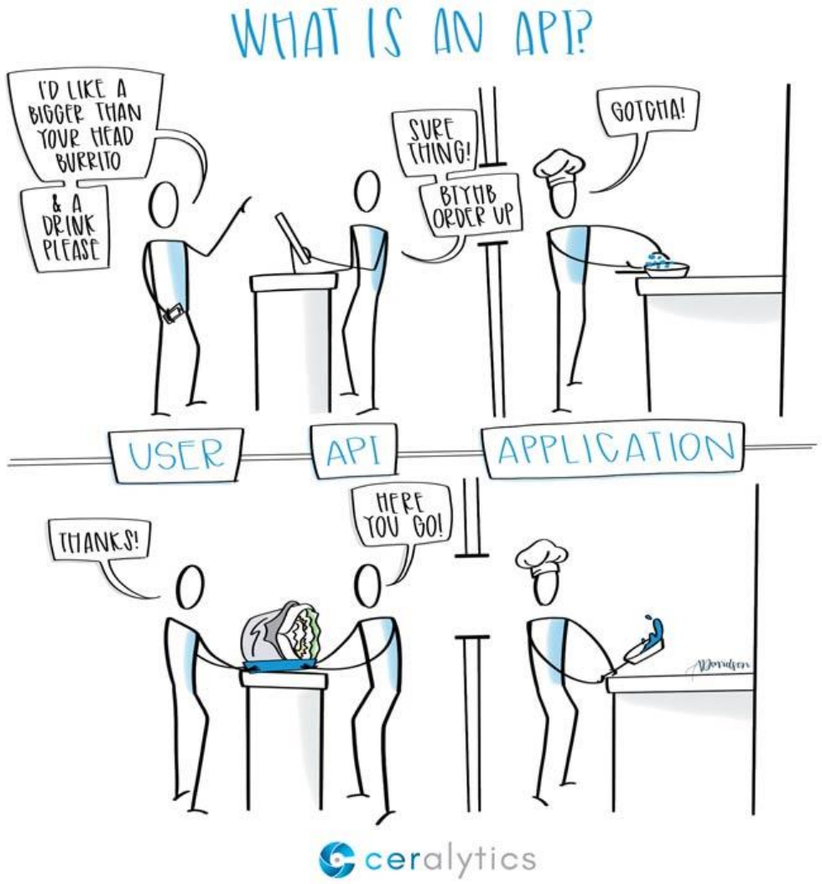
Catalog Functions: Cataloging

- The number of records to catalog will continue to grow
- The ability to easily import and export data is a key function of the catalog
  - Minimize manual data entry and transformation
  - Minimize the need to transform metadata (i.e., import and export metadata in common standard schemas)
  - Possible Solutions
    - **Application Programming Interfaces** (APIs)
    - **REpresentational State Transfer** (REST) **API**s



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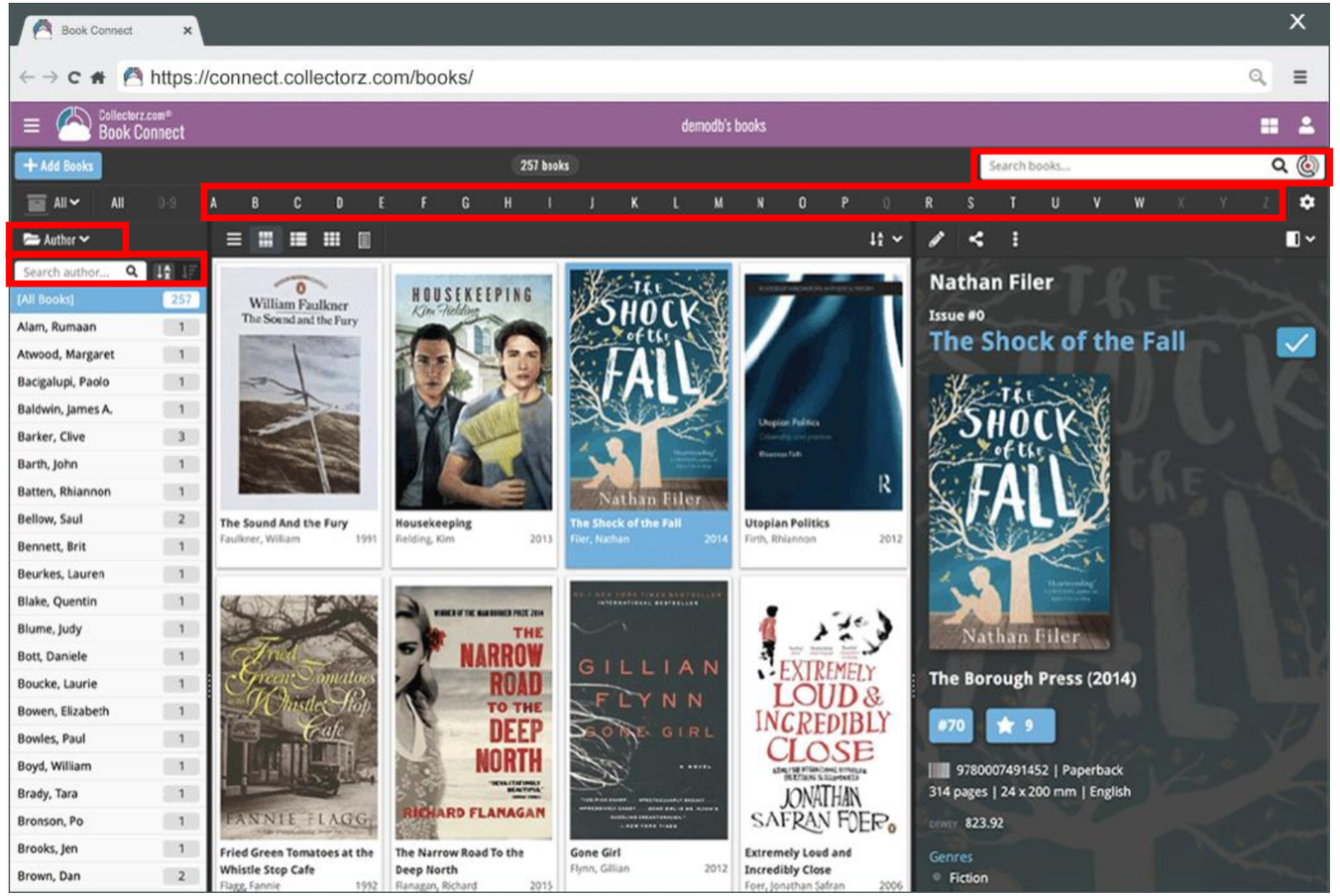
Catalog Functions: Find and Retrieve

- Finding a record relies on imposing selection criteria on the metadata fields
  - Filter – words or spatial data
- Retrieve the record directly
  - Inspect the resource
  - Access the resource (if role-based restrictions allow it)
    - ✓ Links to the resource allows for cataloging large datasets
    - ✗ This can limit the ability to map, plot, or filter data within the catalog interface



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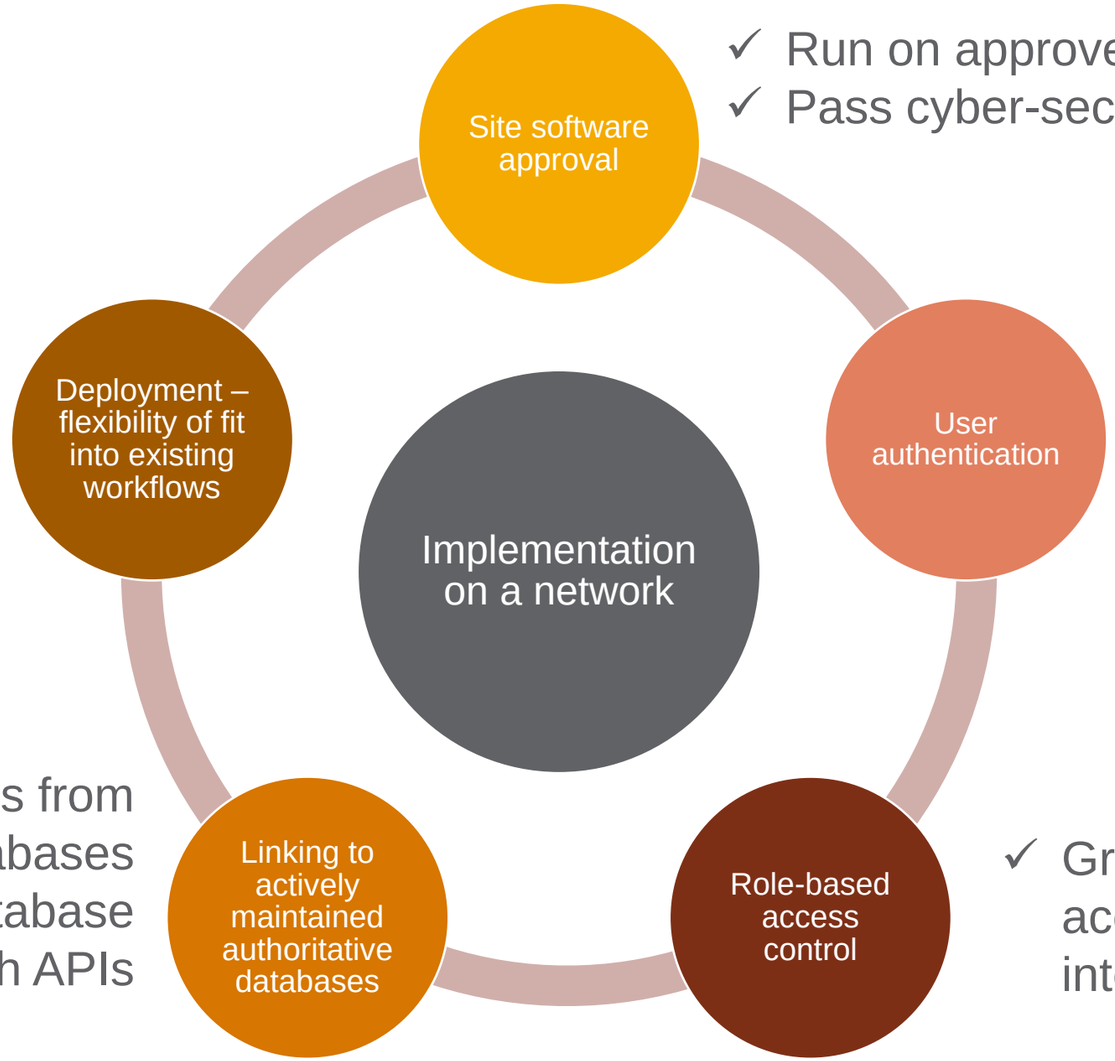
Catalog Functions: Practical Implementation Considerations at Hanford



✓ Run on approved operating system
✓ Pass cyber-security checks

✓ Supports authentication using credentials already created for users (Single Sign-On)

✓ Grants permissions to users according to their need to interact with the catalog

✓ Mirror resources from HLAN databases
✓ Link HLAN database through APIs

✓ Limit custom coding
✓ Similar to other applications used on the HLAN

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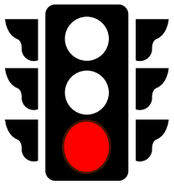
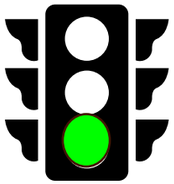
HLAN = Hanford Local Area Network

Review Questions



1. What does FAIR stand for?
2. Name two common minimum requirements for metadata.
3. True or False – I should upload Word documents, PDF files, and Excel files to a catalog

Review Questions



1. What does FAIR stand for?

   Findable, Accessible, Interoperable, Reusable

2. Name two common minimum requirements for metadata
   a. **Title**
   b. **Description**
   c. **Date**
   d. **File format**
   e. **Metadata Standard**
   f. **Unique identifier**
   g. **Contact information**

3. True or False – I should upload Word documents, PDF files, and Excel workbooks to a catalog

   False

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Catalog Software Evaluation

- Compared leading commercial and open-source data catalog platforms
  - Criteria to assess functionality
  - Capabilities supporting data discoverability, retrieval, and archiving
  - Metadata standard compatibility
  - Integration into chosen network: Hanford network (HLAN)

Proprietary Platforms	Non-proprietary Platforms
• ArcGIS Enterprise Sites • Junar • OpenDataSoft • Socrata	• Energy Data eXchange (EDX) • Comprehensive Knowledge Archive Network (CKAN) • DKAN (Drupal-based open data portal based on CKAN)

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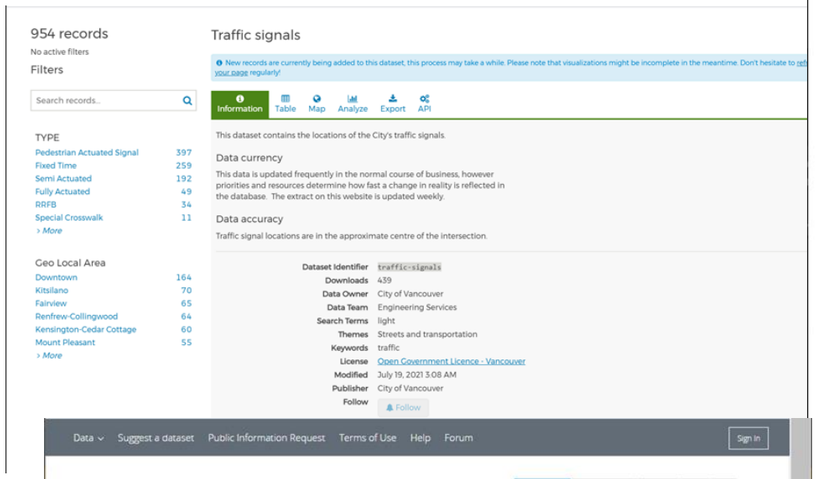
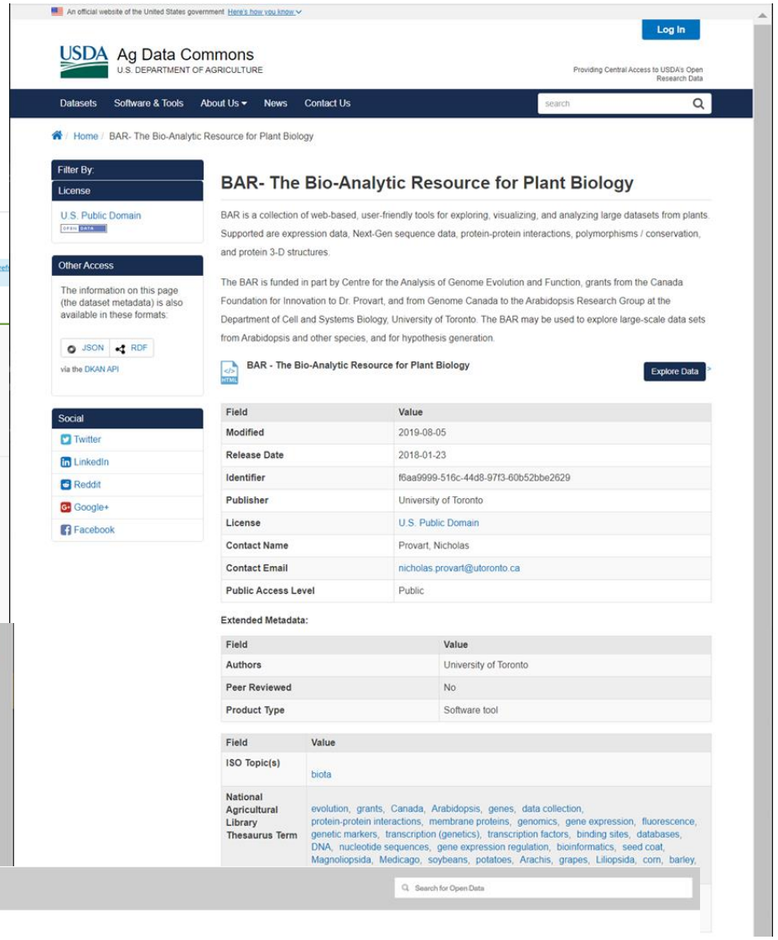
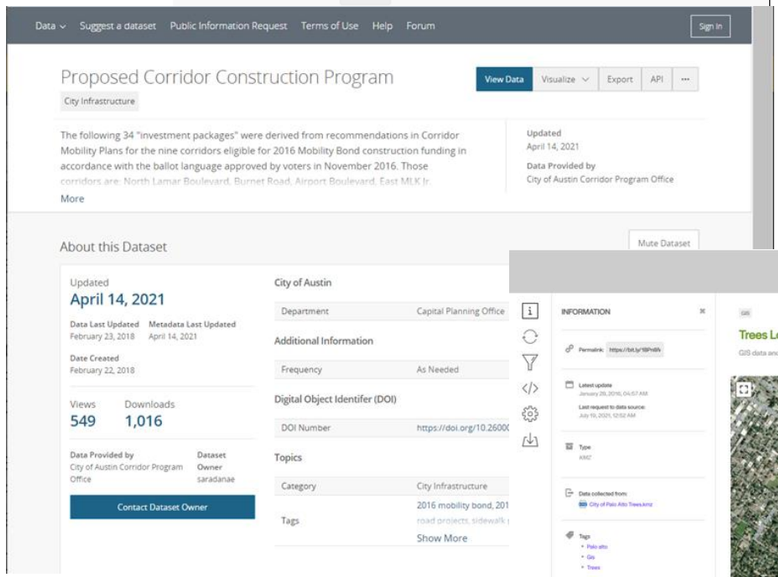
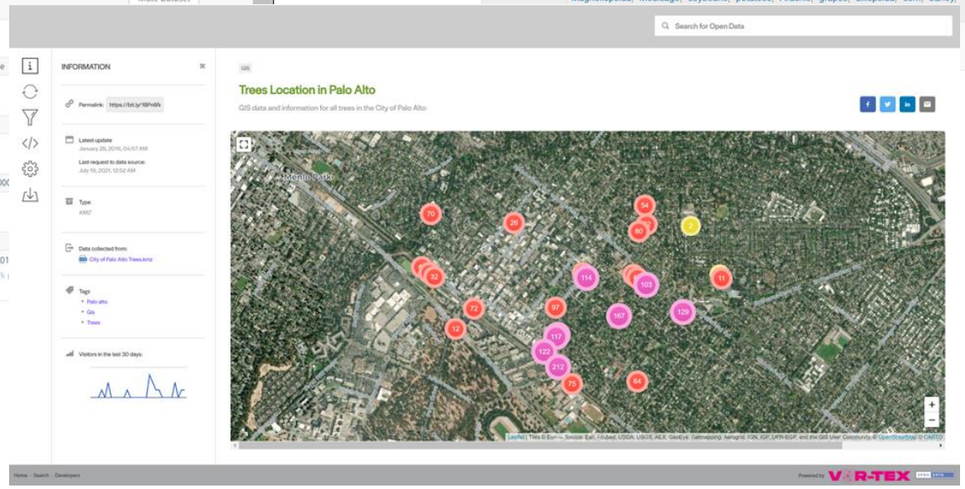
Example Deployments

- Existing deployments were helpful to under-stand capabilities
- Clockwise from top left:
  - OpenDataSoft – City of Vancouver Open Data Portal
  - DKAN – USDA Ag Data Commons
  - Junar – City of Palo Alto Open Data Portal
  - Socrata – City of Austin, Texas, Open Data Portal









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Assessment of Data Catalog Software Tools

- F = fails to meet requirements
- M = meets requirements
- E = exceeds requirements (i.e., meets requirements and delivers additional desired features)
- Lowest rating for any capability area was assigned as the overall rating

Capability	ArcGIS	CKAN	DKAN	EDX	Junar	OpenDataSoft	Socrata
Catalog	E	E	E	M	F	E	E
Find	E	E	E	M	E	M	E
Retrieve	E	E	E	E	M	E	E
Large dataset storage	E	E	E	M	F	F	E
Hanford Site software approval	E	E	E	E	M	M	E
Single sign-on	E	E	E	F	F	E	E
Role-based access	E	E	E	M	F	M	E
Linking/federation	E	E	E	E	E	E	E
Deployment	E	M	M	M	F	F	M
Overall rating	**E**	**M**	**M**	**F**	**F**	**F**	**M**

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Key Assessment Findings

- Propriety software-as-a-service (SaaS) model of delivering a data catalog
  - E.g., Junar, OpenDataSoft
  - Favors consistency across customers at expense of customization/configurable roles
  - Limits size of dataset hosted on the shared commercial platform
  - Socrata, however, provided custom roles and gateways allowing local datasets to be incorporated into an online catalog
- Inability to incorporate authentication from site network (e.g., HLAN) was an issue
  - EDX and Junar couldn't meet that capability
- Initial evaluation found strong candidates ("M" or "E" ratings)
  - ArcGIS Enterprise Sites, Socrata, CKAN, and DKAN
  - Provide fully self-hosted options, allowing for greater control and flexibility
- Explored ArcGIS Hub (non-enterprise version of ArcGIS Enterprise Sites)
  - Straightforward to use for cataloging datasets and managing metadata
  - Difficult to implement some requirements (e.g., custom keyword lists and other limitations)

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Catalog Requirements

- Cataloging data so it can be discovered, retrieved, interpreted, and reused usually requires context-specific requirements to be met to be functional
- Requirements can be implemented in different aspects of the catalog:

Requirement Implementation Area	Description
Metadata Schema*	Defines the structure of catalog entries and what is available for searching and organizing the catalog
Metadata Editor	Controls how catalog entries are created, requiring certain fields, limiting field contents, etc.
Data Catalog Interface	Defines how users interact with the catalog, how searches are built, and what fields are available to be searched
Network Setting	Defines and controls user authorization and roles, and facilitates interaction among data systems

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*For the following requirements, assuming an FGDC approved schema, including ISO19115

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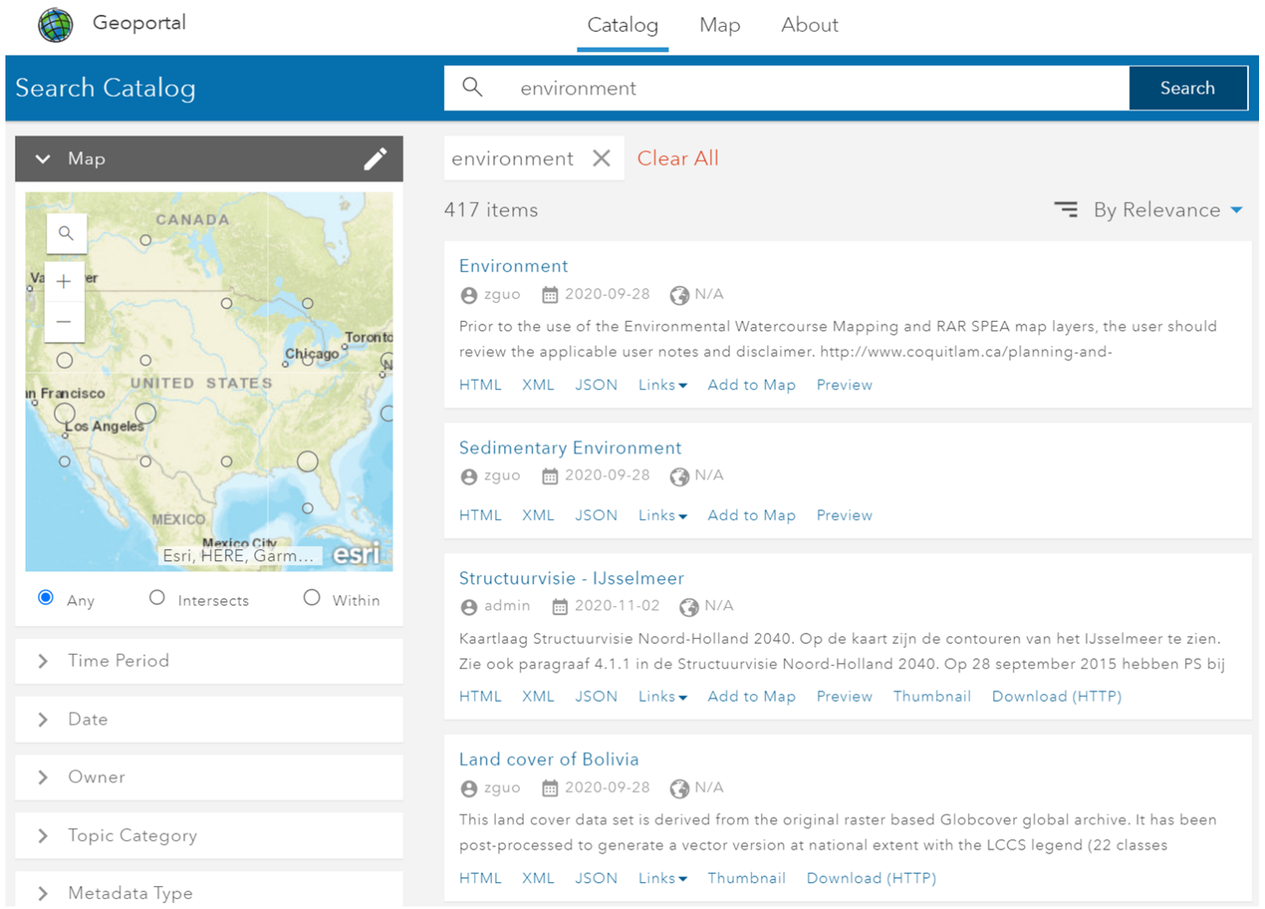
Esri Geoportal Server

- Free, open-source tool with web interface and broad functionality
  - Flexible, customizable, and compatible with ArcGIS tools
  - Supports enterprise authentication
- Catalog
  - Inventories the metadata
  - Find & view resources
  - OGC catalog service compliant
  - Multiple interfaces to resources
    - ✓ E.g., RESTful endpoint for data transfer
- Metadata editor
  - Metadata creation/editing
  - Supports ISO 19000-series standards
    - ✓ ISO 19115 North American Profile (NAP)
- Harvester
  - To incorporate existing data catalog entries



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OGC = Open Geospatial Consortium

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Catalog Requirements: Theming and Authoritative Naming

- Keywords categorize data, usually by theme, place, stratum, or temporal aspect
- Topic keywords should be able to be translated or adapted to site-specific theme keywords

ISO Topic Keywords	Hanford Environmental Data Theme
Farming	Atmospheric
Biota	Biota
Boundaries	External Radiation
Climatology	Groundwater
Meteorology/ atmosphere	Miscellaneous Material
Economy	Pore Water
Elevation	Sediment
Environment	Soil Gas
Geoscientific information	Soil
Health	Surface Water
Imagery/ basemap/ earth cover	Waste Solid
Intelligence	Waste Water
Military	
Inland waters	
Location	
Oceans	
Planning/ cadaster	
Society	
Structure	
Transportation	
Utilities/ communication	

Requirement Implementation Area	Requirement
Metadata Schema	Support custom lists for keywords, including multiple types of place keywords to reflect differing “uses” of a site
Metadata Editor	Enforce custom lists for keywords
Data Catalog Interface	Make custom keywords accessible in search criteria
Network Setting	Consistent use of theming nomenclature across environmental data information systems

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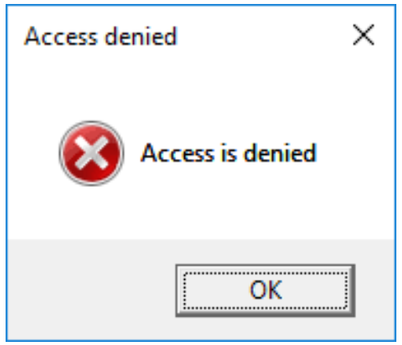
Catalog Requirements: Resource Access Limitations

- There may be a need to limit access to catalog record for security purposes
- Access limitation can be both to the catalog record and to actual resource
- Can be difficult to enforce – federation with existing network settings/authentication is usually key



Requirement Implementation Area	Requirement
Metadata Schema	Support differentiating classes of records by access limitation
Metadata Editor	Require access limitation entry into appropriate metadata field
Data Catalog Interface	Enforce limitation on access to catalog record based on network identity or role
Network Setting	Maintain lists of identities with similar roles and access

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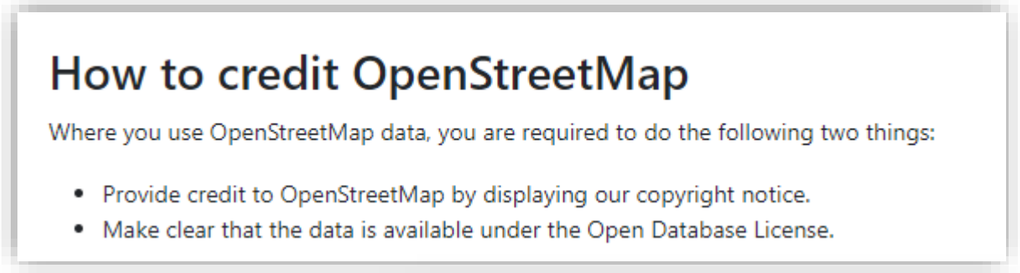
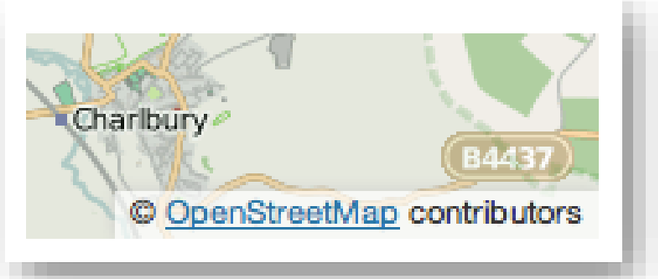
Catalog Requirements: Resource Use Limitations

- Related to but different from access restriction
- Use limitations drive what a user should or should not do with the resource
- Can be difficult to enforce





Requirement Implementation Area	Requirement
Metadata Schema	Support specifying constraints on use of the resource
Metadata Editor	Support or require use limitation entry in appropriate metadata field
Data Catalog Interface	Prominently display constraints on use of the resource
Network Setting	Not Applicable. (Limiting how data is used outside of the catalog involves voluntary compliance with terms of use or external controls)

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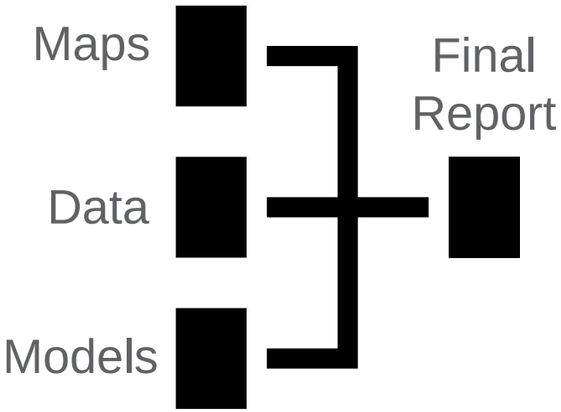
Catalog Requirements: Link Data to Deliverable

- Accessing the source data for a final report or output is a key part of data transparency and reproducibility
- Can produce more robust analyses by contextualizing new data with historical data
- Spectrum of complexity – site specific need drives the requirement within constraint of implementation areas



Requirement Implementation Area	Requirement	Alternative Requirement
Metadata Schema	Support aggregate datasets	Support a deliverable as a resource
Metadata Editor	Link aggregate datasets to a deliverable	Use lineage fields to identify data sources
Data Catalog Interface	Make aggregate datasets findable based on a deliverable	Handle deliverables as a resource in a catalog entry
Network Setting	Enable linking to deliverables to deliverable database	Enable linking to deliverables in IDMS

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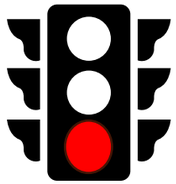
Catalog Requirements: Testing Results for Esri Geoportal

Requirement	Schema	Editor	Catalog Interface	Network	Notes
Theming	✓	✓	✓	✗	Consistent use of theming nomenclature across environmental data systems not in use
Access Limitations	✓	✓	✗	✓	Continuing to test if role-based permission can be applied to a metadata field
Use Limitations	✓	✓	✓	N/A	
Link to Deliverable	✓	✓	✓	✗	Alternative requirements only. Linking to document deliverable system unable to be tested due to security constraints.

Review Question



1. What are the four requirement areas you could consider when determining and testing requirements for a catalog?

Review Question

1. What are the four requirement areas you could consider when determining and testing requirements for a catalog?
    a. Metadata schema – does the selected schema fulfill your site-specific requirements?
    b. Metadata editor – can site-specific metadata requirements be easily applied in the catalog's metadata editor ‘wizard’ or in an automated way?
    c. Catalog interface – does the chosen software meet the usability needs of your target users? Will it find, retrieve, and display catalog entries in a way that fulfills site-specific requirements?
    d. Network – what network requirements does the catalog software need to meet to be functional when deployed?

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Hanford Case Study

- Defined a use case
  - ✓Hanford-specific requirements and HLAN enterprise data system implementation
- Tested available software
  - ✓Selected Esri Geoportal Server
- Selected metadata standard
  - ✓ISO 19115
- Defined catalog requirements
  - ✓Geophysical data as a use case
- Began prototype testing
  - ✓Protype catalog built using local environment, hosting metadata from the Hanford Administrative Record and other open sources
  - ✓Customization and Hanford-specific requirements (e.g., Hanford-specific theming, catalog entry restriction) were demonstrated

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Collaboration and User Stories...

- Meet as a “Hanford Working Group” every two weeks with site contractor and sponsor representatives
  - Refines requirements
  - Functional testing

- User stories developed

A scientist needs data on all waste sites including location.

A geophysicist need seismic data, magnetic and gravity for the suprabasalt sediments in the 600 area.

A hydrologist needs to locate hourly historic barometric pressure to normalize aquifer tests in the 1960’s in 200E.

How do I…?

Environmental Dashboard Application

Hanford Maps

Hanford GIS

Hanford Waste Information Data System

Hanford Well Information System

SOCRATES

PHOENIX

Contractor Datasets

Future Datasets

Hanford Environmental Information System

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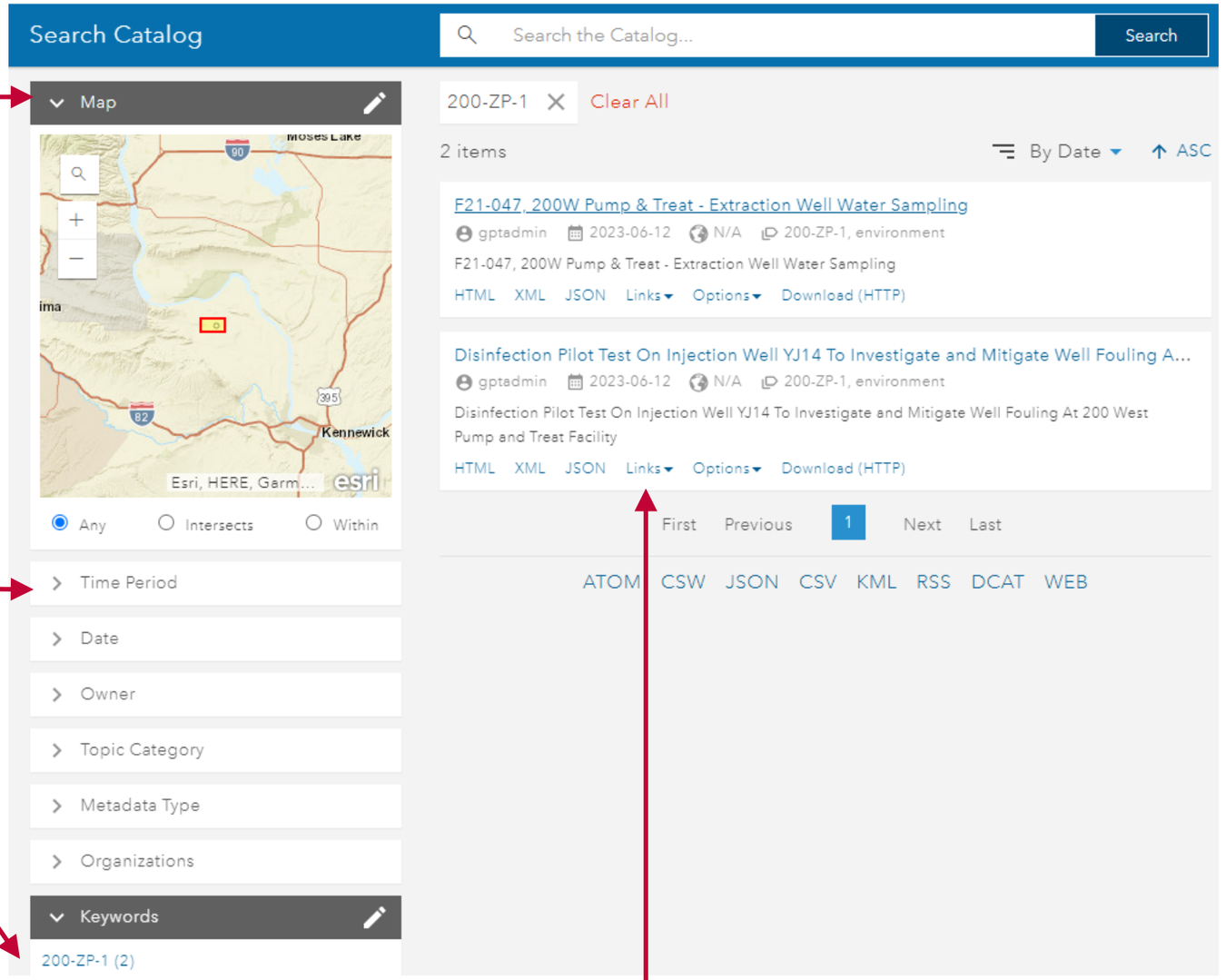
Prototype in Esri Geoportal Server

Search using map feature

Sort and filter (customizable)

Hanford themed keywords

Metadata ‘tiles’ to view, edit, add to map, etc.



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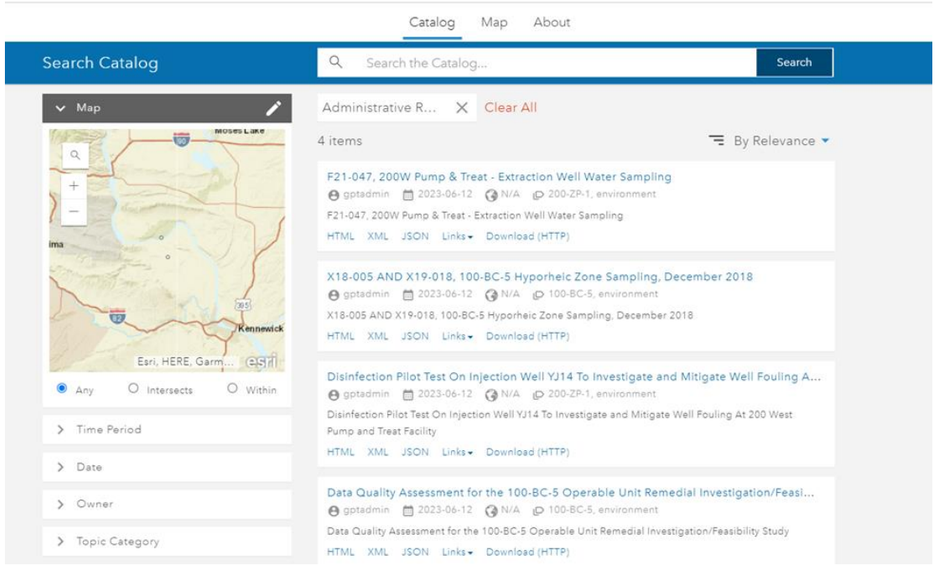
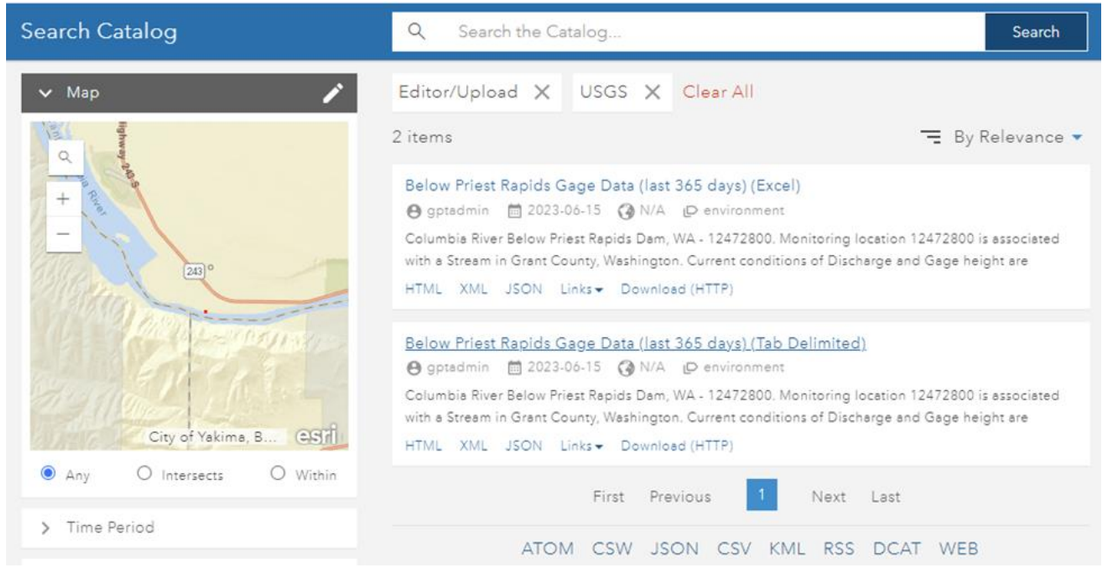
Geoportal Server – Example Data Records

- Hanford Administrative Record entries
  - Via web scraping
  - Geospatial context (operable unit) was added



- Records for Columbia River stage gage data
  - Station 12472800, below Priest Rapids Dam
  - Retrieved from USGS Daily Values Web Service



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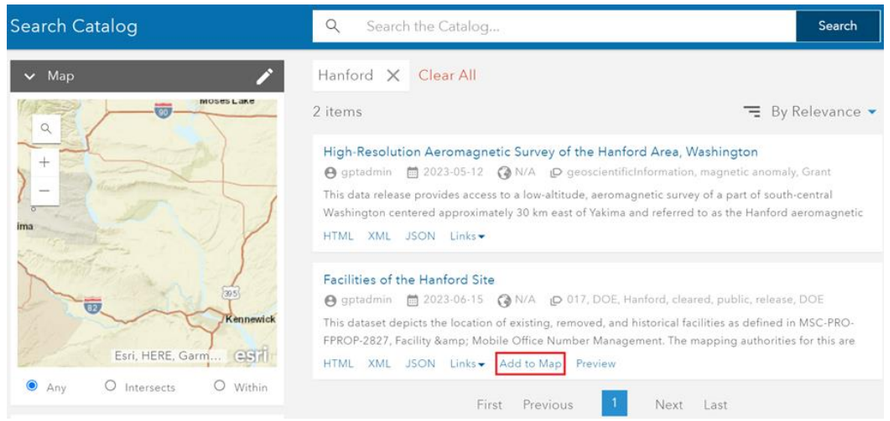
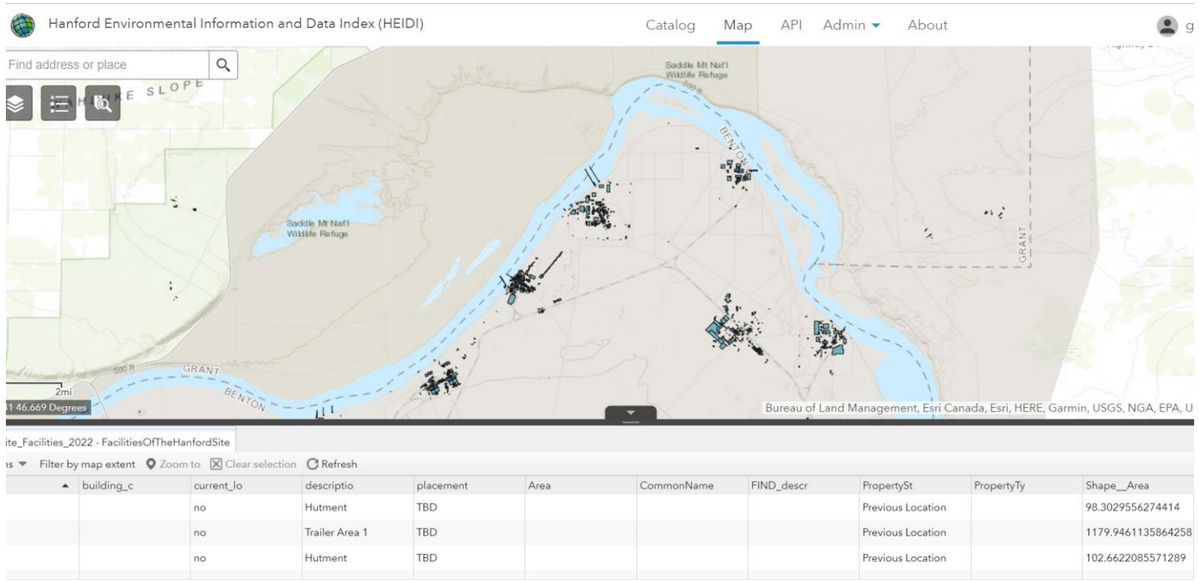
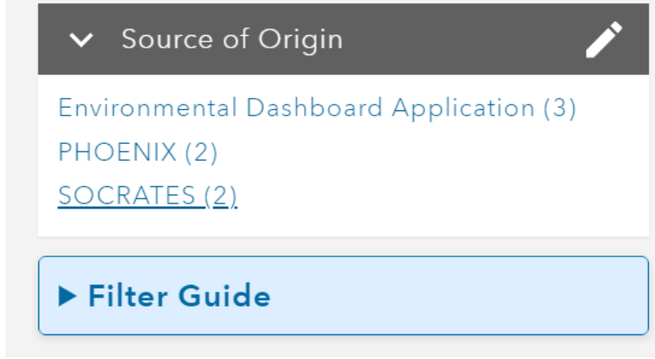
Geoportal Server – Add to Map Feature

- Example: “Facilities of the Hanford Site” added to map





- Custom filter fields, linking databases to resources, and helpful navigation tips



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Benefits of a Prototype and Full-Scale HEIDI

Short Term

- A catalog implementation plan at the ready
- Metadata files for cataloging and template use
- Cyber security approval confirmation

Long Term

- Refinement of geological framework models
- Capitalize on existing data to inform sampling plans and other environmental studies
- Effective, data-driven, strategic decisions to meet long term remediation goals

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Summary

- Findable, accessible, interoperable, and reusable (FAIR) data resources are critical
  - Cost effective use / re-use of data
- Metadata based on standards is the backbone of a data catalog
  - May need some customization for site-specific requirements
  - Describes data lineage/quality, resource location, access restrictions
  - Used to facilitate needs such as theming and consistent place/entity naming
- Catalog requirements should be developed for each implementation area and should be tested before full-scale deployment
  - Catalog requirements are generally site/case specific

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Summary

- Evaluated data catalog tools and found potential candidates
  - ArcGIS Enterprise Sites, Socrata, CKAN, and DKAN
  - Further testing led to Esri Geoportal Server
- Have built a prototype HEIDI with Hanford and external data resources
- Next: Complete the prototype with additional data and federated user authentication

Hanford Environmental Information and Data Index (HEIDI)

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Thank You

Rebecka Bence
rebecka.bence@pnnl.gov