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Web-Based Data Access and Analysis Workbench to Support Environmental Restoration Decision-Making

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Seminar Overview

Objective: Discuss web-based software for accessing and analyzing data in support of environmental decisions

Take-aways from today's seminar:

Challenge: Tools for environmental data access and analysis are required to meet needs for consistency, quality, communication, and decision-making.

Approach: Web-based software provides rapid access and analysis capabilities for disparate data from multiple sources.

Impact: Web-based tools effectively provide consistent analyses to support quality requirements and remedy decisions for complex sites.

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Outline of Discussion

- What is the nature of environmental data?
- Approaches to software tools for analysis
- Web-based applications using cloud computing infrastructure
- Analysis as support for decision making
- Web-based approaches for data visualization
- Web-based approaches for data analytics
- Conclusions, benefits, broader perspective

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Disparate Data Sources

- Data inherently comes in different forms and format
- Data access varies among organizations
- Common when multiple agency and organizational projects are participating
  - Overlapping "authoritative" data sources

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Environmental Data Types/Sources

- Electronic Tabulated data
  - Analytical chemistry
  - Well or waste site information
- Information from reports
  - Tables, figures
- Well log or geophysical data
- Sensor data
- Spatial data
  - Points, polygons
- 3D model information
- Satellite/remote sensing
  - Images, datasets

3.6.3 Proposed Input Parameters

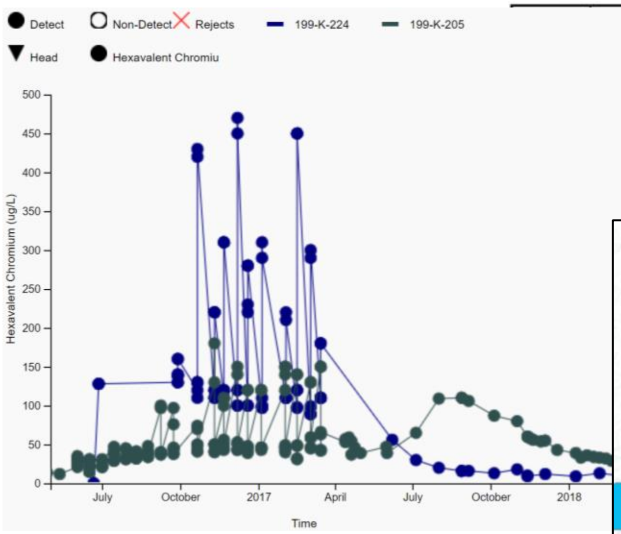
The nominal values in the governing concentration equation for the analytes used in the Composite Analysis are provided in Table 1. The values in Table 1 have been modified to have units of Ci/m³. The modification is performed by multiplying the original data in pCi/L by 10^{-9}.

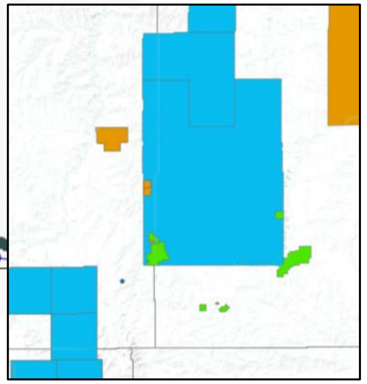
The stochastic distributions associated with the nonzero coefficients defined in Table 1 are defined using the following rules:

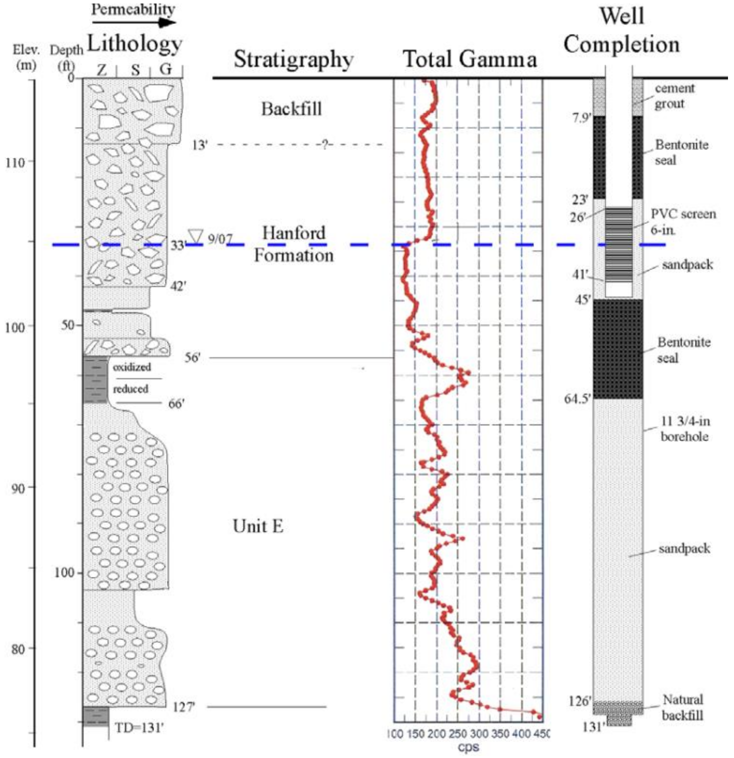
- **Variable C_B.** The triangular distribution will be used for all values of C_B. The distribution will be symmetric about the midpoint, and the half-range will be 50% of the mid-point. The variable tag will be CB.

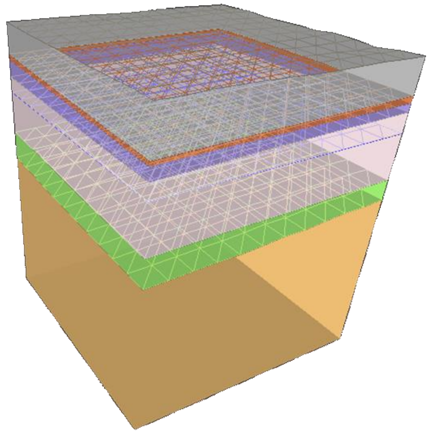
Table 1. Nominal Coefficient Values for Background Concentrations in the Columbia River

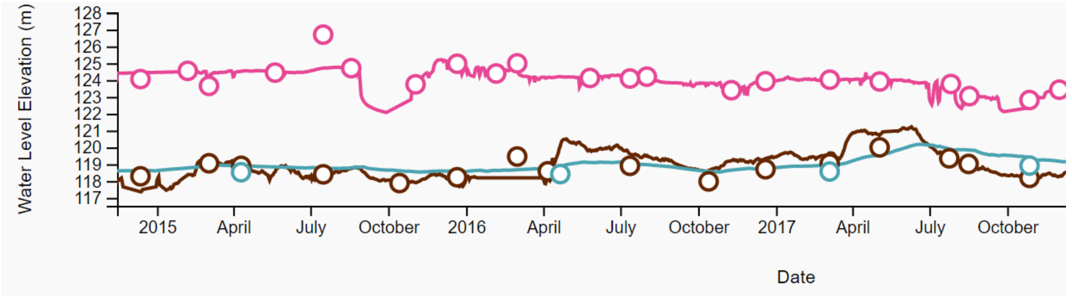
λ_B	Fallout?
0	No
0	No
0.223	Yes
0	Very small
0.0562	Yes
4.41×10^{-4}	Very small
0	Very small
0	No
Not modeled	No
0	Very small
0.0241	Yes











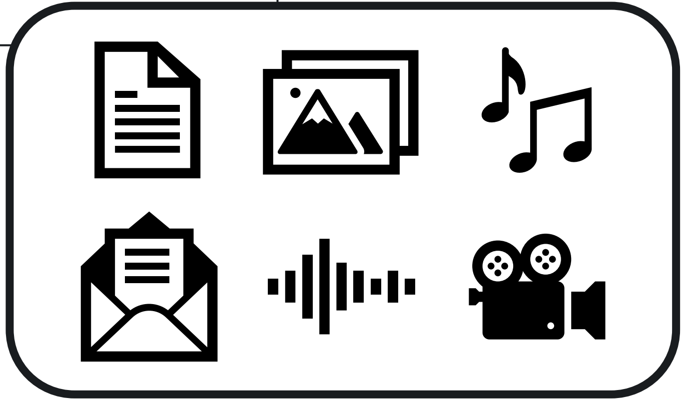
Nature of Data

- Impacts storage, access, and manipulation
- Structured data
  - Data fields in a record
  - Tabular data
  - Typically stored in a relational database
- Semi-structured
  - Non-tabular
  - Uses markers to separate semantic elements and enforce record/field hierarchies
  - e.g., JSON
- Unstructured
  - No pre-defined model/organization
  - e.g., text documents, audio, sensor data, etc.

Date	AvgVa	StdDe	MaxVa	MinVa	NumVa
12/18/2019	101.1904	10.34665	124.566	82.68952	90
12/18/2019	47.39977	0.98256	48.8643	44.81337	90
12/18/2019	28.8651	27.91818	69.87847	0	90
12/18/2019	407.5266	1.755548	411.603	403.2118	85
12/18/2019	404.7679	1.518011	408.2755	399.7396	86
12/18/2019	163.6203	0.416473	164.3519	162.2685	78
12/18/2019	166.1039	0.432044	166.8981	165.0463	87
12/18/2019	100.6407	0.102121	100.8391	100.4051	72
12/18/2019	61.09903	0.126984	61.34259	60.65538	79
12/18/2019	89.84978	0.101705	90.09694	89.62674	78

```
{
    "scenarioTitle": "Inga Site 3",
    "analysisConfigurationAlgorithms": [
    "aquiferPorosity": {
        "title": "Aquifer Porosity",
        "value": 0.3
    },
    "aquiferThickness": {
        "title": "Aquifer Thickness",
        "value": 100,
        "units": "ft"
    },
```

JSON (JavaScript Object Notation)



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Quality Assurance – Data and Software

- Data provenance
  - How, where, when, why, and by whom was the data was produced
  - Key information for trust, credibility, and reproducibility of data and results using that data
- NQA-1
  - ASME Nuclear Quality Assurance standard
  - Structured program of procedures
    - Evaluating, reviewing, and documenting data and calculations
- Key quality concepts:
  - Traceability
  - Reviewing the work
  - Software requirements and testing

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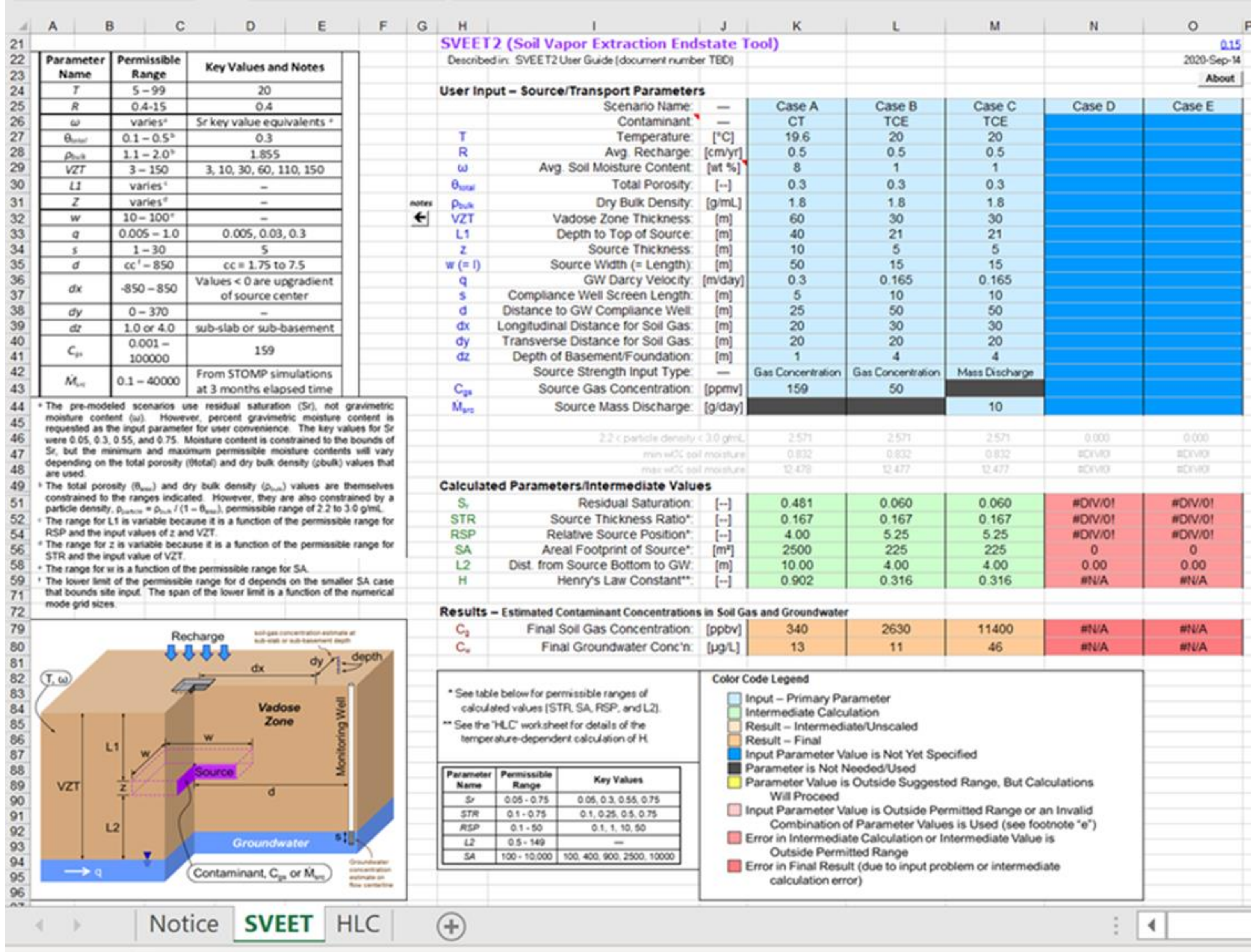
Traditional Approaches to Software Tools

- Traditional
  - Compiled executable for desktop
  - Microsoft Excel-based tool
- Issues
  - Installation on desktop/mobile platforms
  - Users need to have specific software (Excel)
  - Potential version issues
  - Less flexible data access
  - Less flexible geospatial functionality
  - Indirect sharing of results



(Truex et al., 2013; Johnson et al., 2021a)

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PNNL Custom Development vs Commercial-off-the-Shelf (COTS) Platforms

- Geospatial based
  - Esri ArcGIS Online
    - Intuitive, programming knowledge not required
    - Free and subscription-based hosted applications
  - Kepler.gl
    - Open-source geospatial analysis tool for large data sets
- Analytical – with some geospatial
  - Power BI
  - Tableau

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Use the Approach that Fits the Need

- Spreadsheet tools are suitable when
  - Users have the spreadsheet software
  - Quick development is needed
  - Familiar interface is useful
  - External data and geospatial needs are minimal
- Use exploratory data analysis when
  - Very little is known about the data
  - Objectives are vague – mainly about data capture and discovery
- Power user type tools used when
  - Analytics are independent and fragmented
  - Expertise in the tool already exists
- But…web-based applications have advantages

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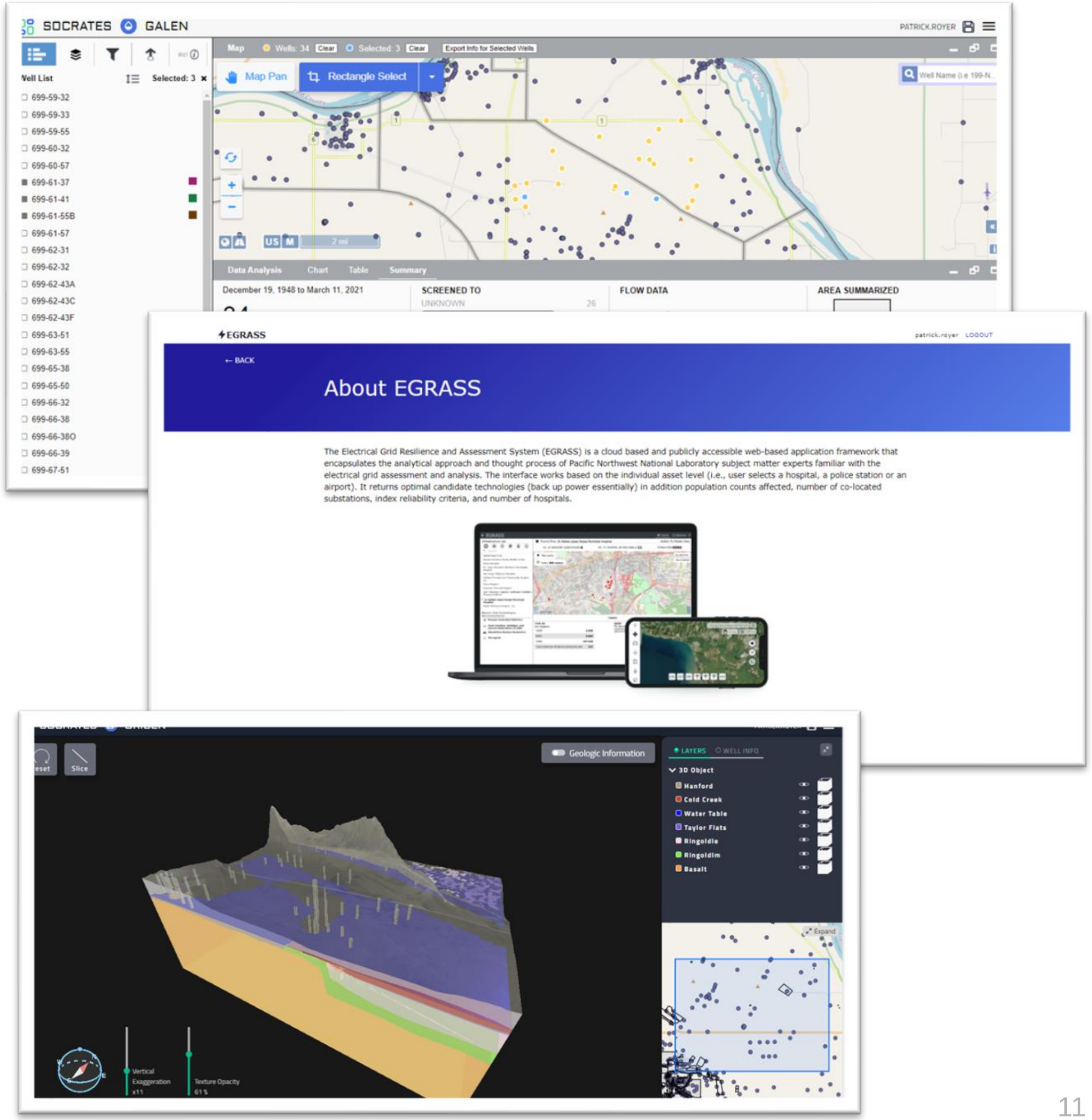
Web-based Applications that Leverage a Modern Cloud Approach

- Domain knowledge coupled with computational and development expertise
- Custom web applications with emphasis on cloud-based architecture
- Managed cloud services
  - AZURE, AWS, and Google Cloud
    - Government, Gov Cloud
  - Support from internal cloud team to guide application developers
- Modular and extensible platform translated to different domains
  - Environmental management
  - Electrical grid – emergency and response
  - Chemicals of mass destruction throughout Asia



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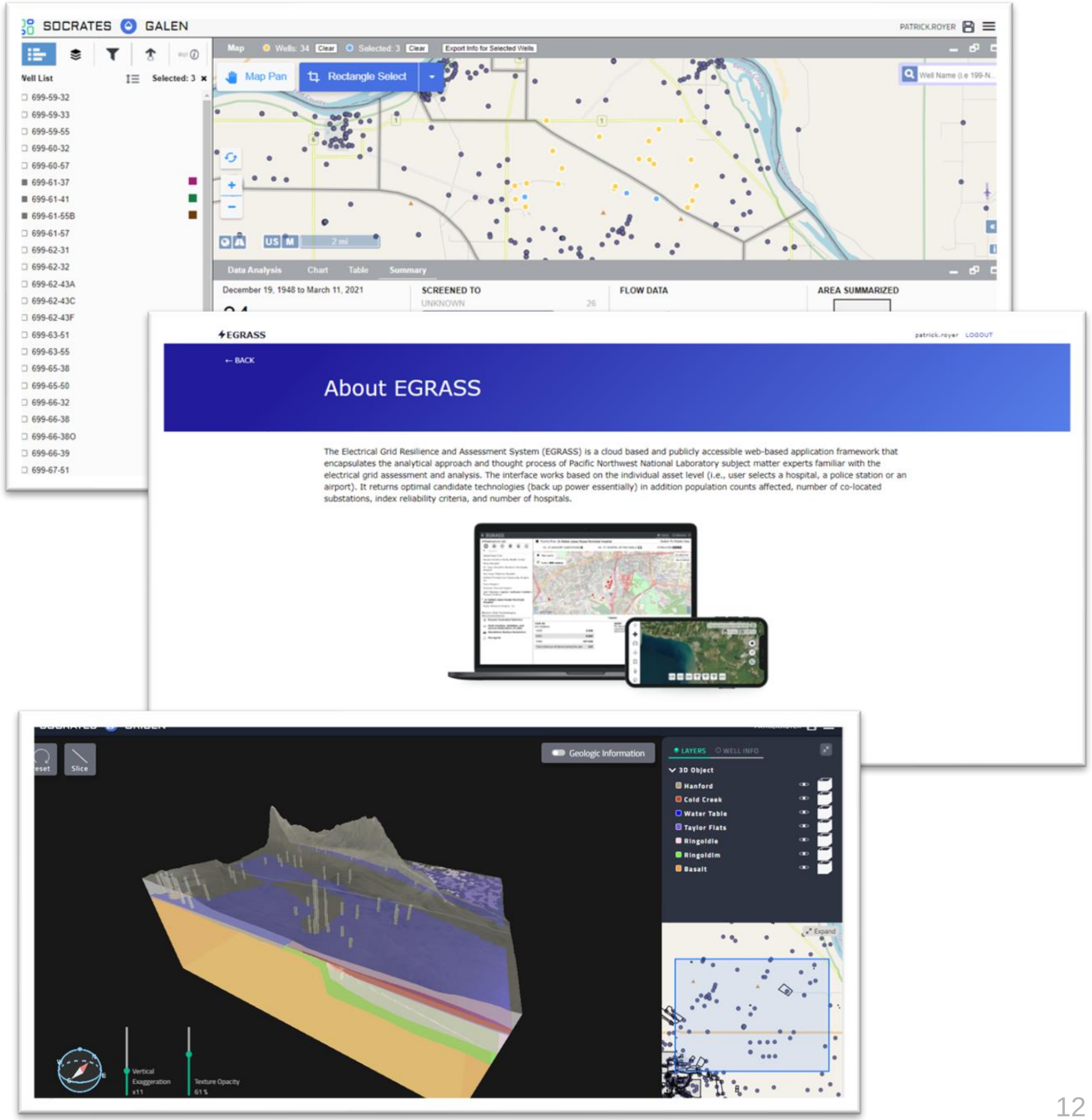
Web-based Applications Leveraging Modern Cloud Approach

- Targeted ***vertical*** applications
  - Meet enterprise-scale analytic objectives
  - Extensive user experience (UX) and user elicitation outreach
  - Tightly coupled with regulatory requirements
  - Transferable to different cloud accounts
- Build and deploy modern, focused analytic and data services
  - Analysis as a Service (AaaS)
  - Data as a Service (DaaS)
- Role based access and profile management



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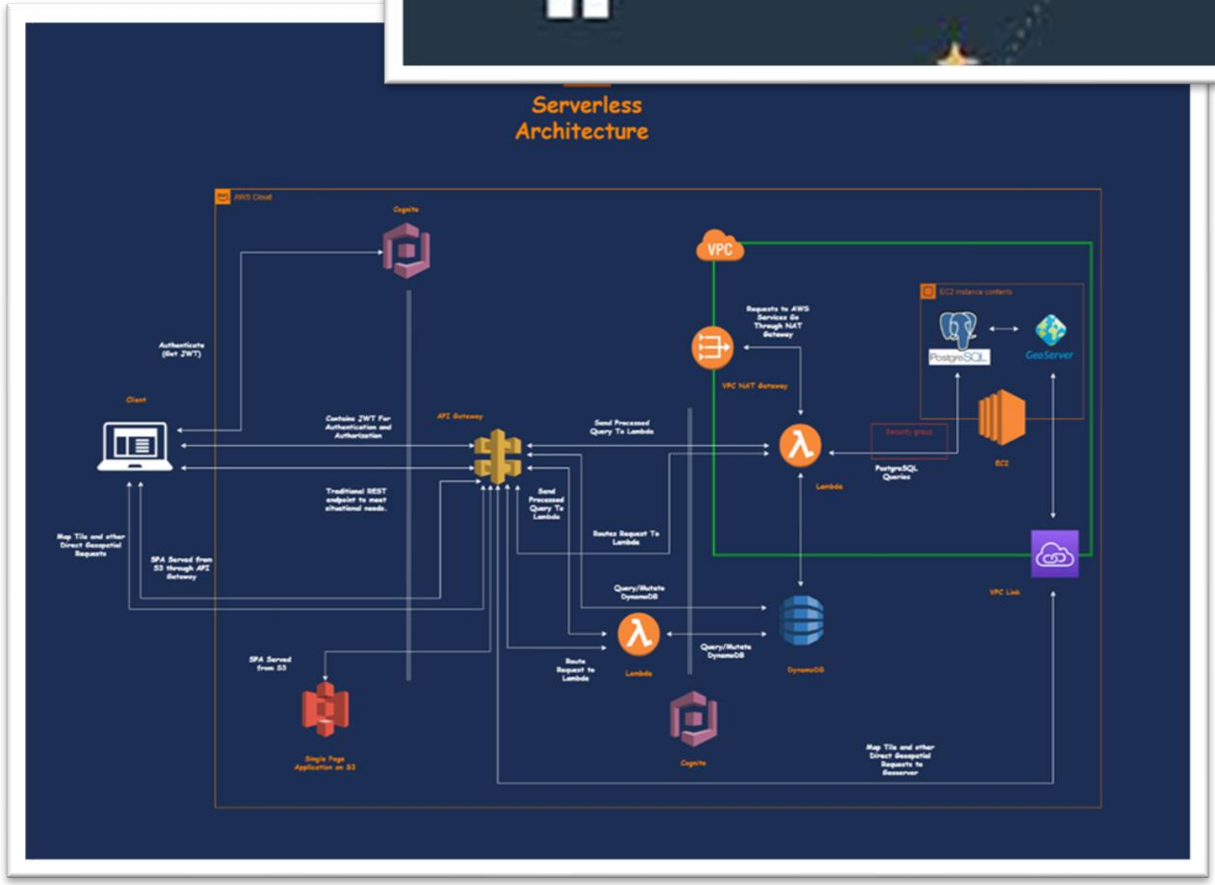
Migration to Cloud? Shifting to Cloud Architecture with emphasis on Serverless

- Serverless computing
  - Machine resources allocated on-demand opposed to virtual machine paradigm
  - Cost-effective
  - Maintenance assumed by cloud provider and customer
  - Elastic scalability
  - Improved productivity
- When to use virtual machines
- Implications for migrating from an on-premise server to the cloud
  - Legacy to modern –“lift and shift”



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Amazon Web Services (AWS) Components

- S3 – Simple Storage Solutions
  - File storage "bucket"; shared access, like FTP
- EC2 – Elastic Cloud Computing
  - Virtual machine; can be used for automated processing
- Lambda – serverless compute service; automated processing
- RDS – Relational Database Service
  - e.g., SQL Server
- DynamoDB unstructured/noSQL key-value data
- Cloudwatch – monitoring services & applications
- Cognito – authentication and user management

aws

Amazon S3

Amazon Lambda

Amazon EC2

Amazon RDS

Amazon DynamoDB

Amazon CloudWatch

Amazon Cognito

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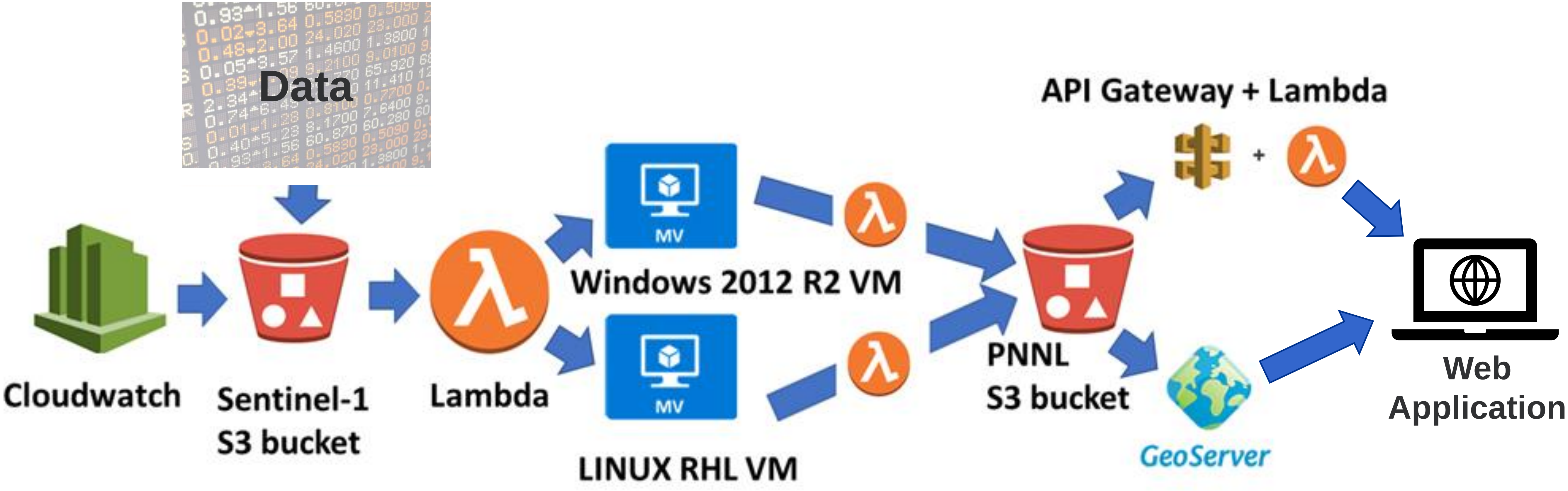
Automated Workflow Example

- AWS and cloud architecture for automating complex, multistep workflow



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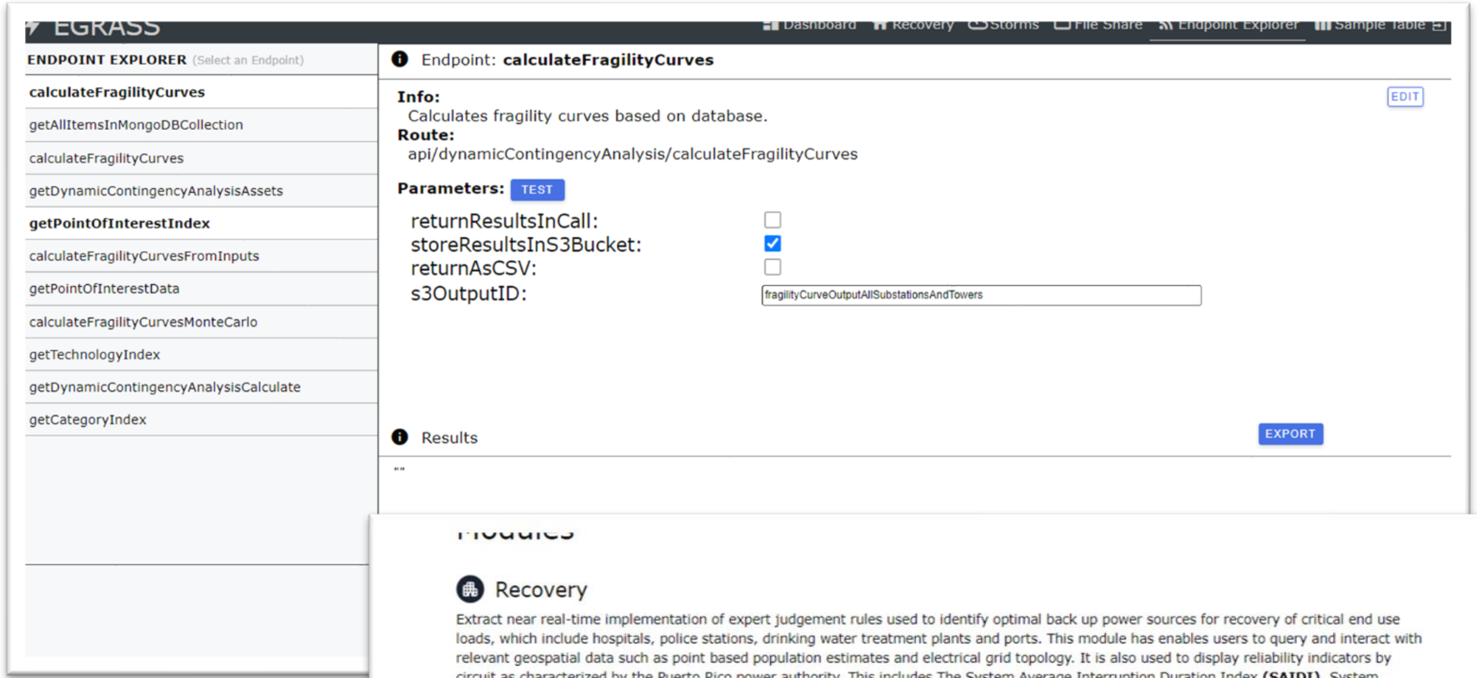
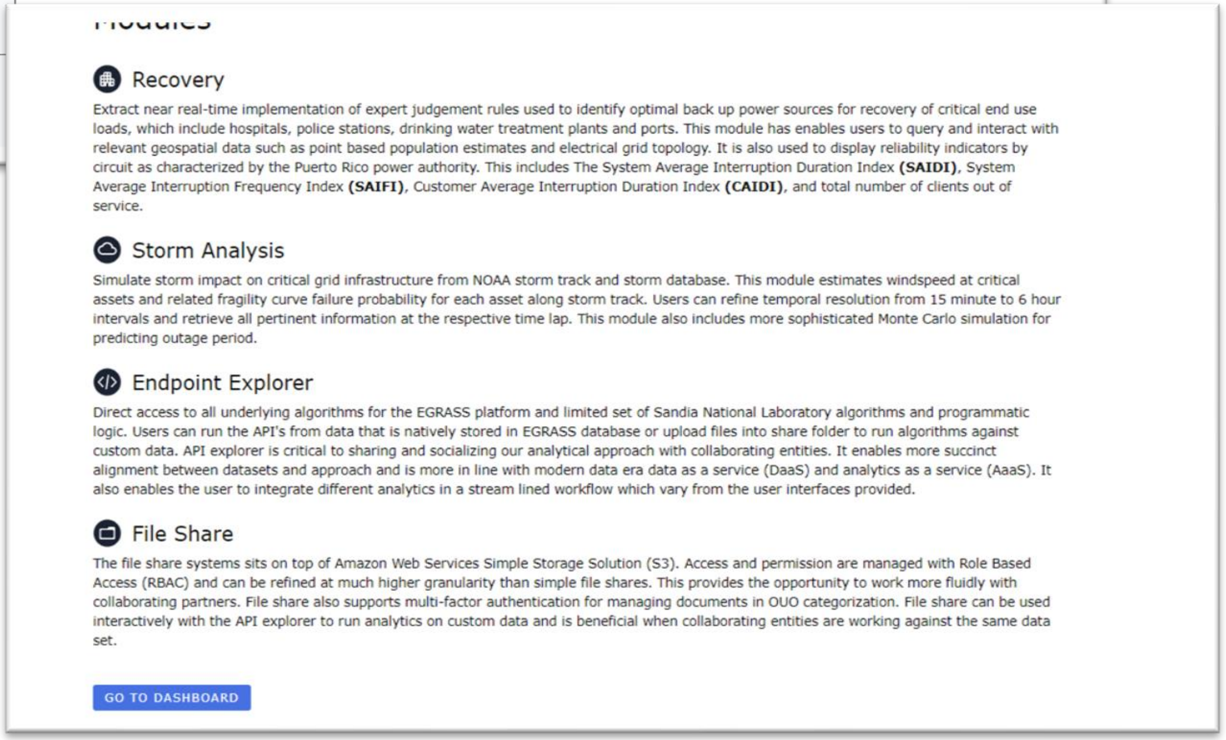
Exposing the Application Programming Interface (API) Directly for Power Users

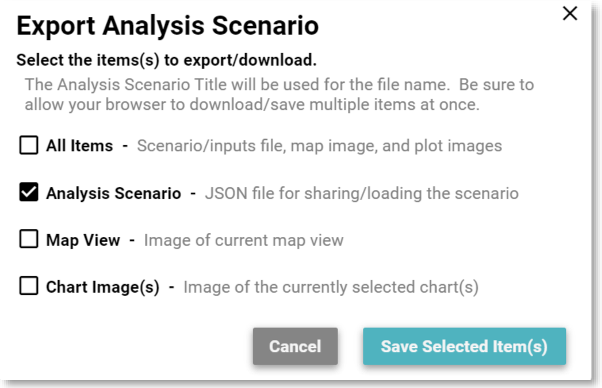
- Combining role-based access with varying data solutions and direct API access
- Data integration and assimilation
- Custom, input-driven API
- Facilitates collaboration between organizations

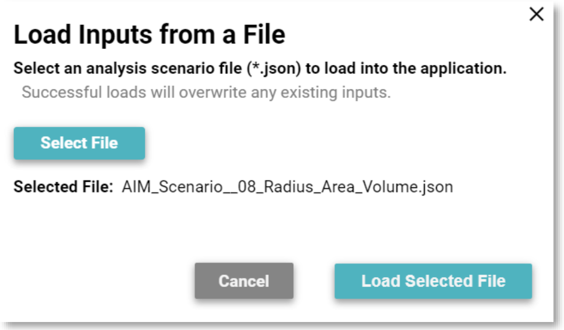


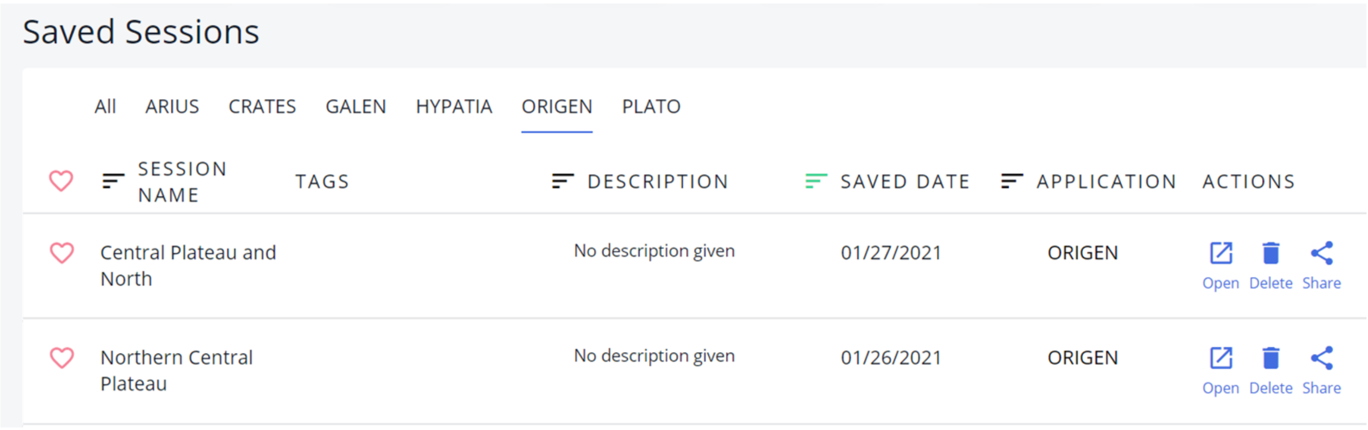


Profile Management

- User login allows user-specific customization
- Control user access based on role, organization, etc.
  - Data access
  - Functionality
  - Pre-defined styles
- Define and maintain user-specific options
  - Favorite contaminants, waste sites, etc.
  - Colors, styles, analysis options, etc.
- Save scenarios
  - Record of work, reproducibility
  - For sharing with colleagues







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Analytics for Environmental Decision Making

- Web-based applications provide
  - Availability, convenience, rapid assessment
  - Consistency and reproducibility in analyses
  - Inter-operability of tools and data
  - Vehicle for communication with technical, management, and regulatory personnel
    - Sharing, reporting
  - Basis for supporting environmental decisions
    - Feeds into approaches such as adaptive management of complex sites
- Examples of tools to support decision making
  - Analysis based on published guidance (e.g., EPA) and standard statistical methods
  - Data access and visualization
  - Rapid data analytics

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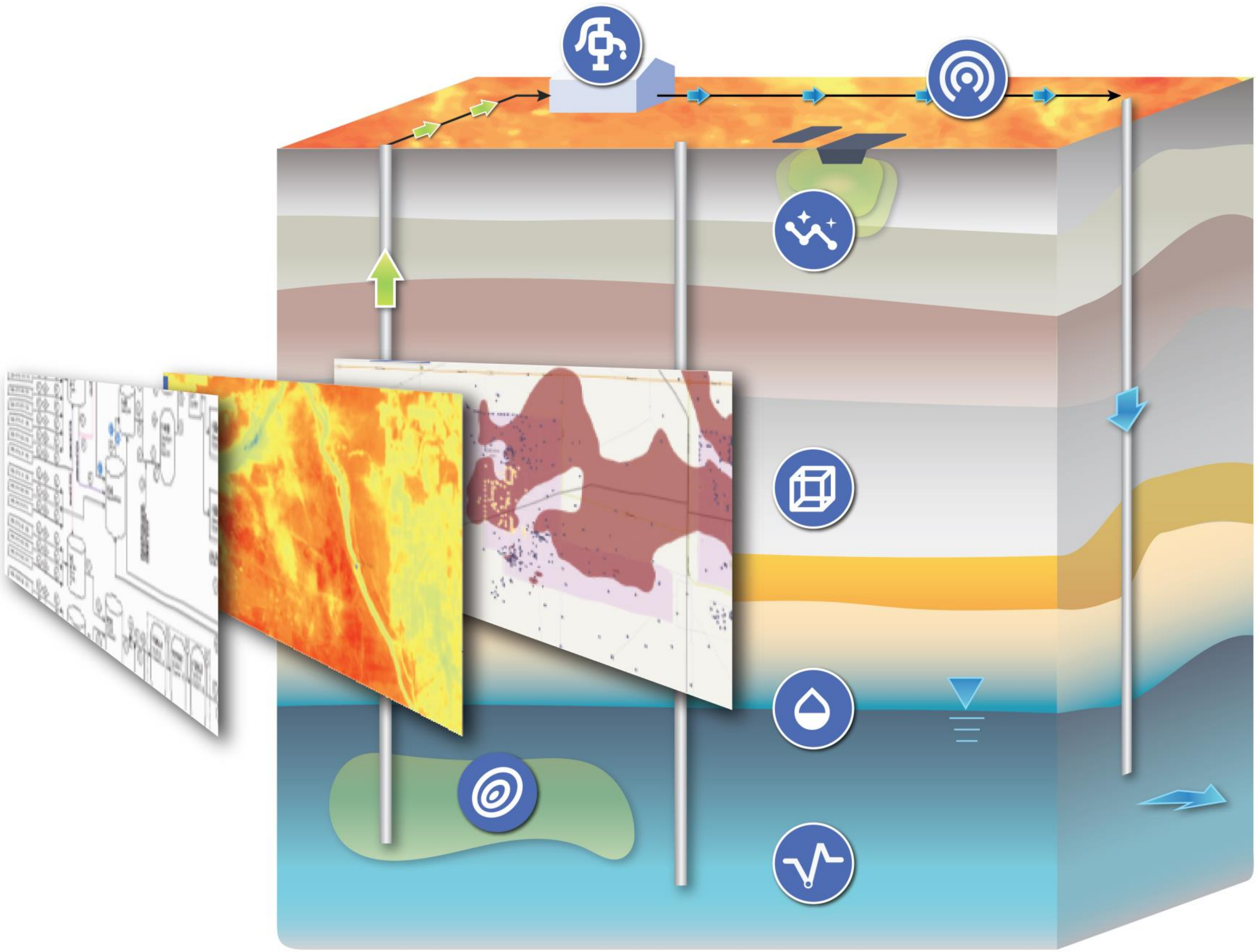
EPA = U.S. Environmental Protection Agency

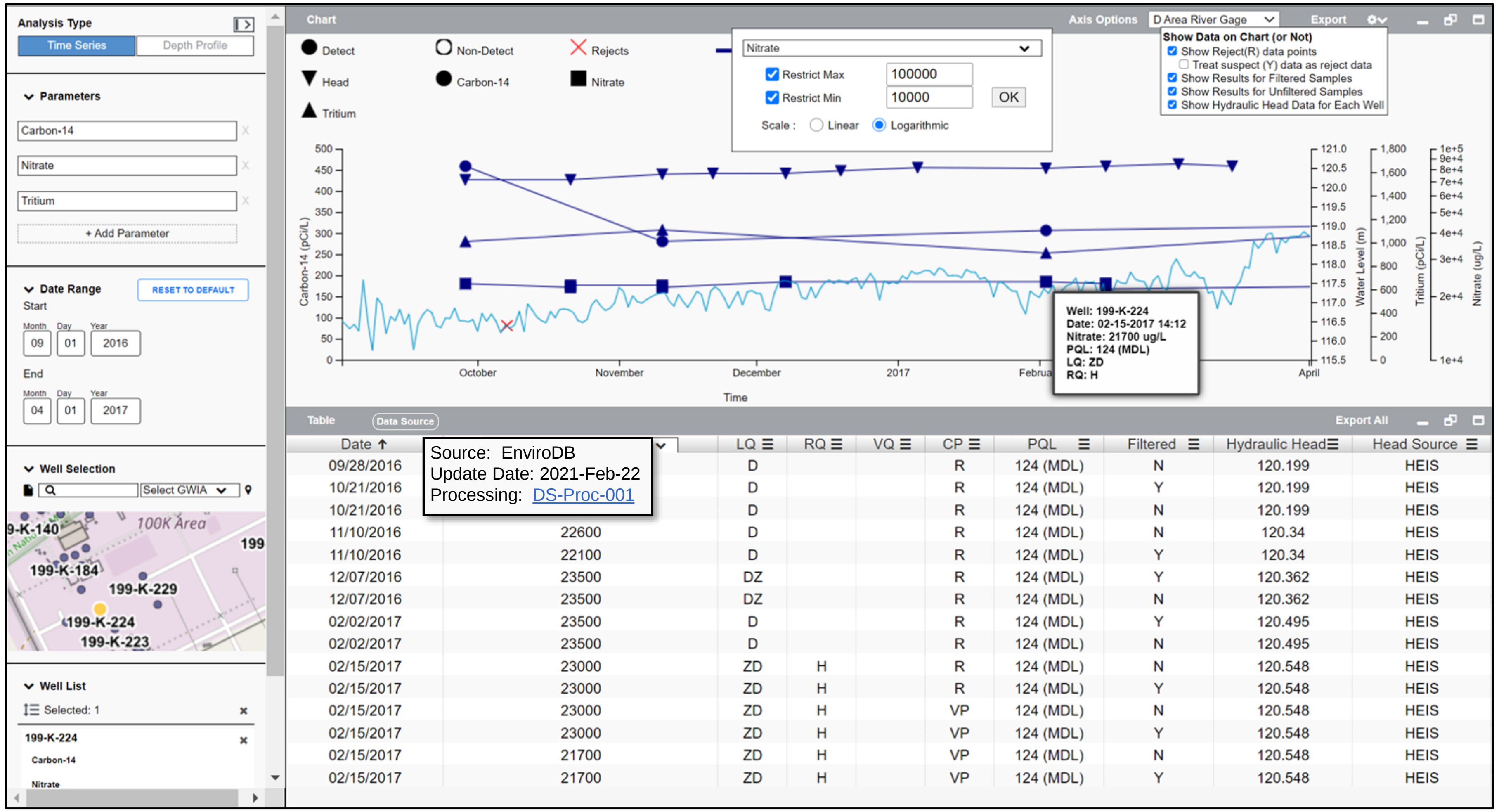
Web-based Tools for Environmental Decision-Making

- Environmental aspects
  - Groundwater
  - Wells
  - Waste sites
  - Remedies
  - Remote sensing
- Supports
  - Exit strategies/endpoints
  - Optimization
  - Adaptive remedy decisions
  - Decisions related to protecting human health and the environment



Access and Visualization of Groundwater Data

- Time series and depth profile visualizations
- Show data in chart and table
  - Multiple measured parameters
  - Specified time frame
  - Filtering based on attributes
- Water table/river levels
- Export figures/data for reporting
- Used in context of remedy and guidance (e.g., EPA, 2013)



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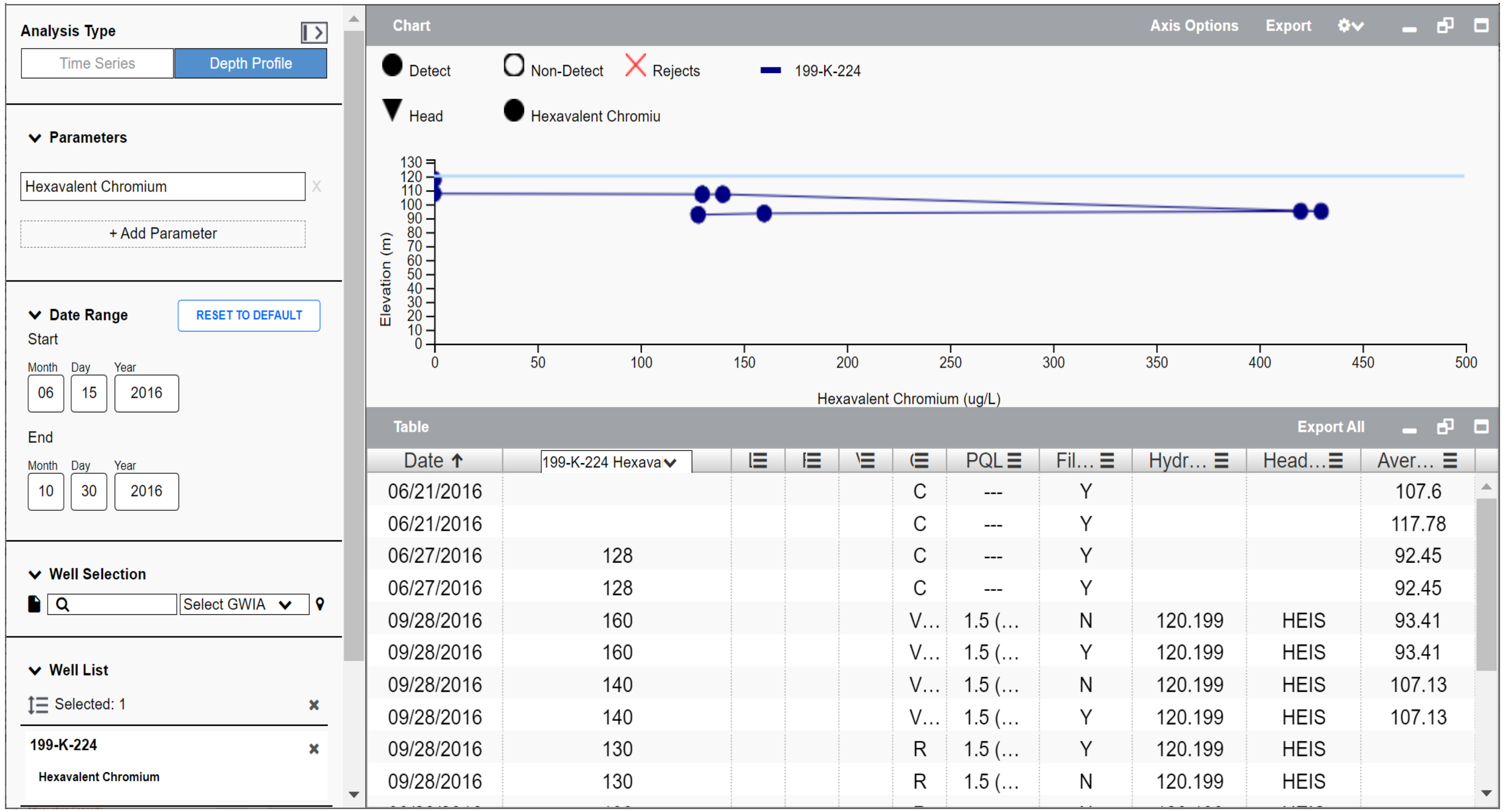

Depth profile information – can help target optimization or adaptive remedy approach

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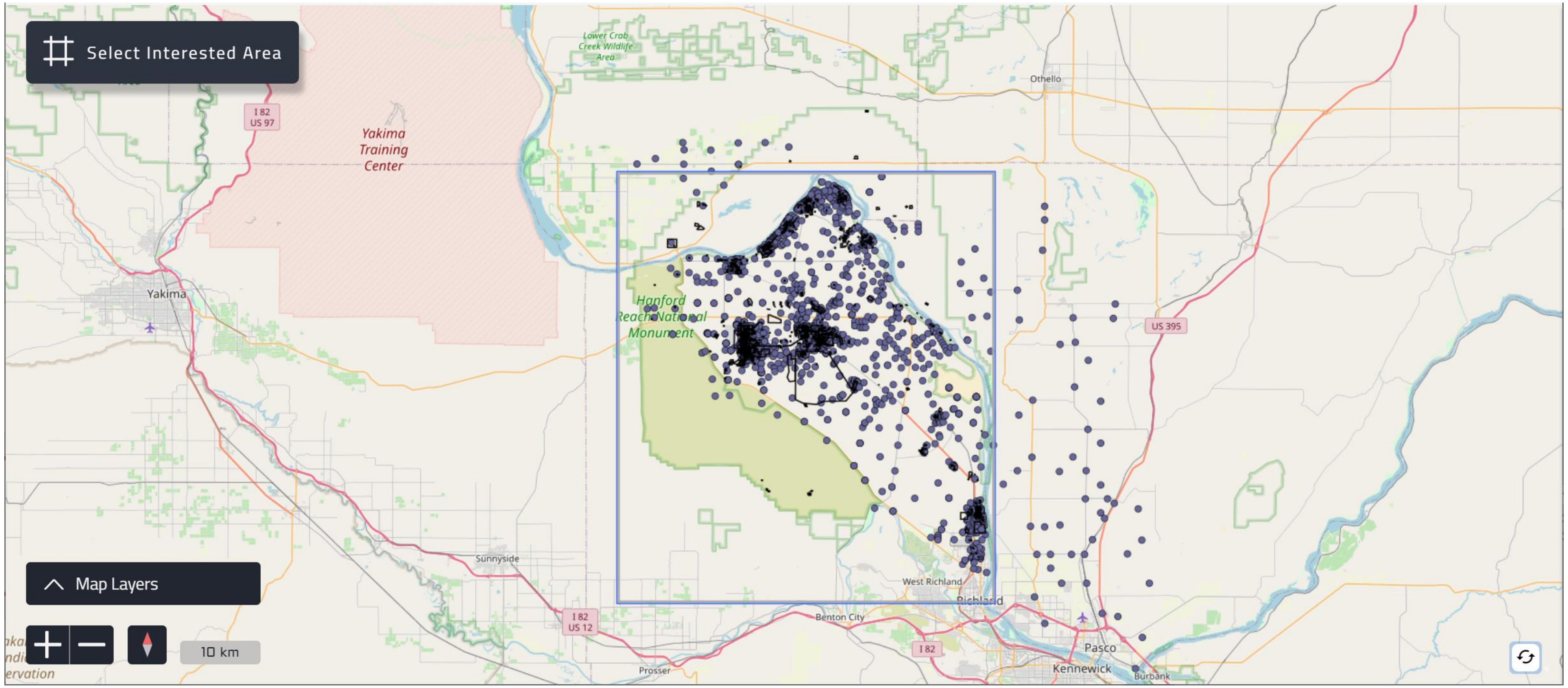
Access and Visualization of 3D Geology

- Hydrogeological units
- Point elevations
- Cross section viewer
- Well construction information
- Link to other tools
  - Provides relevant context



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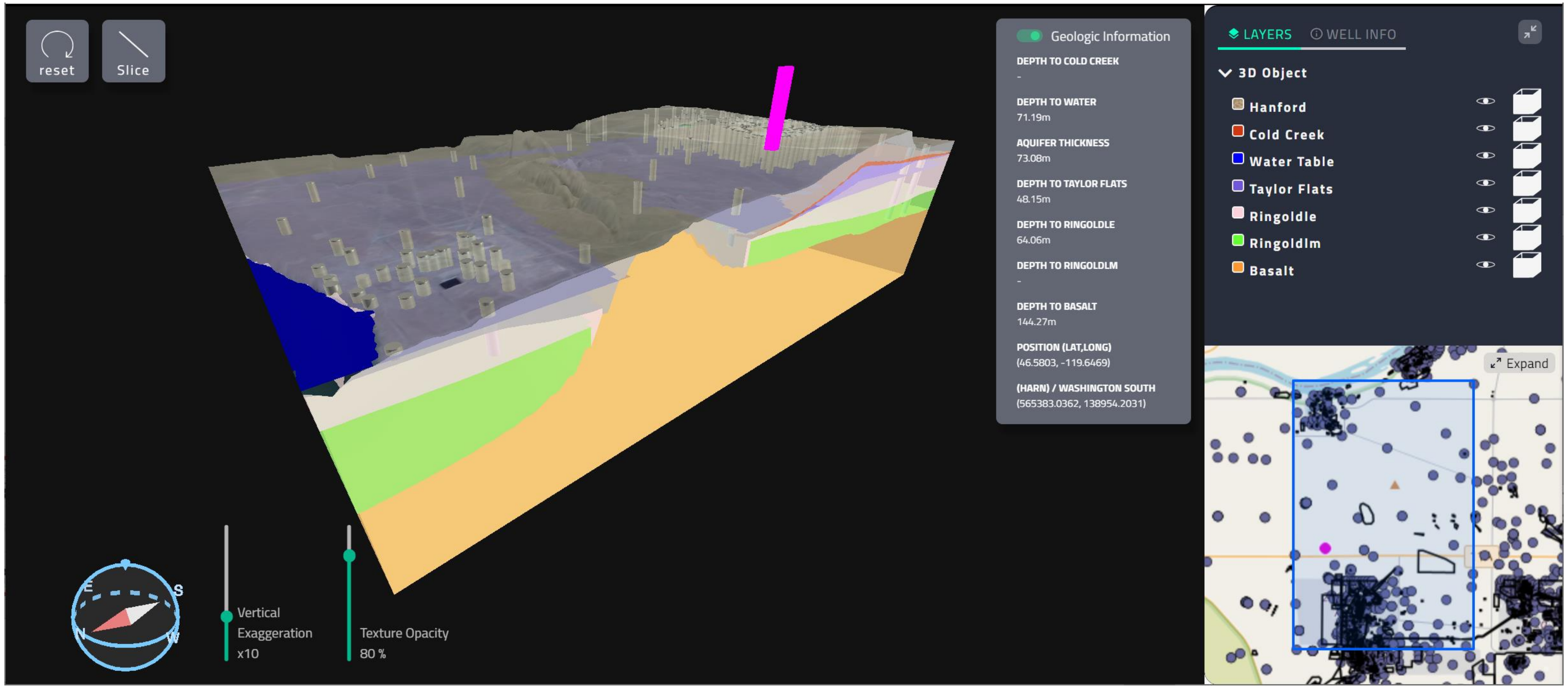

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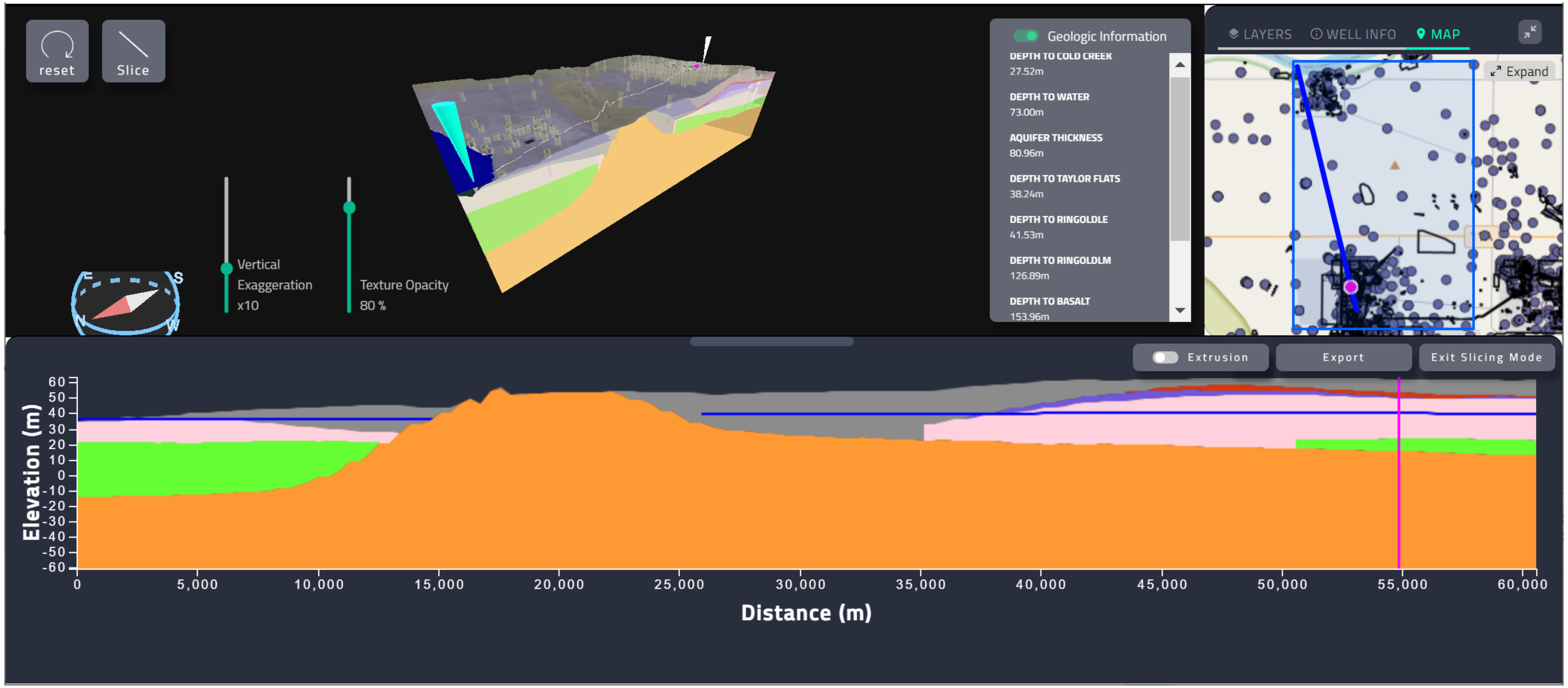

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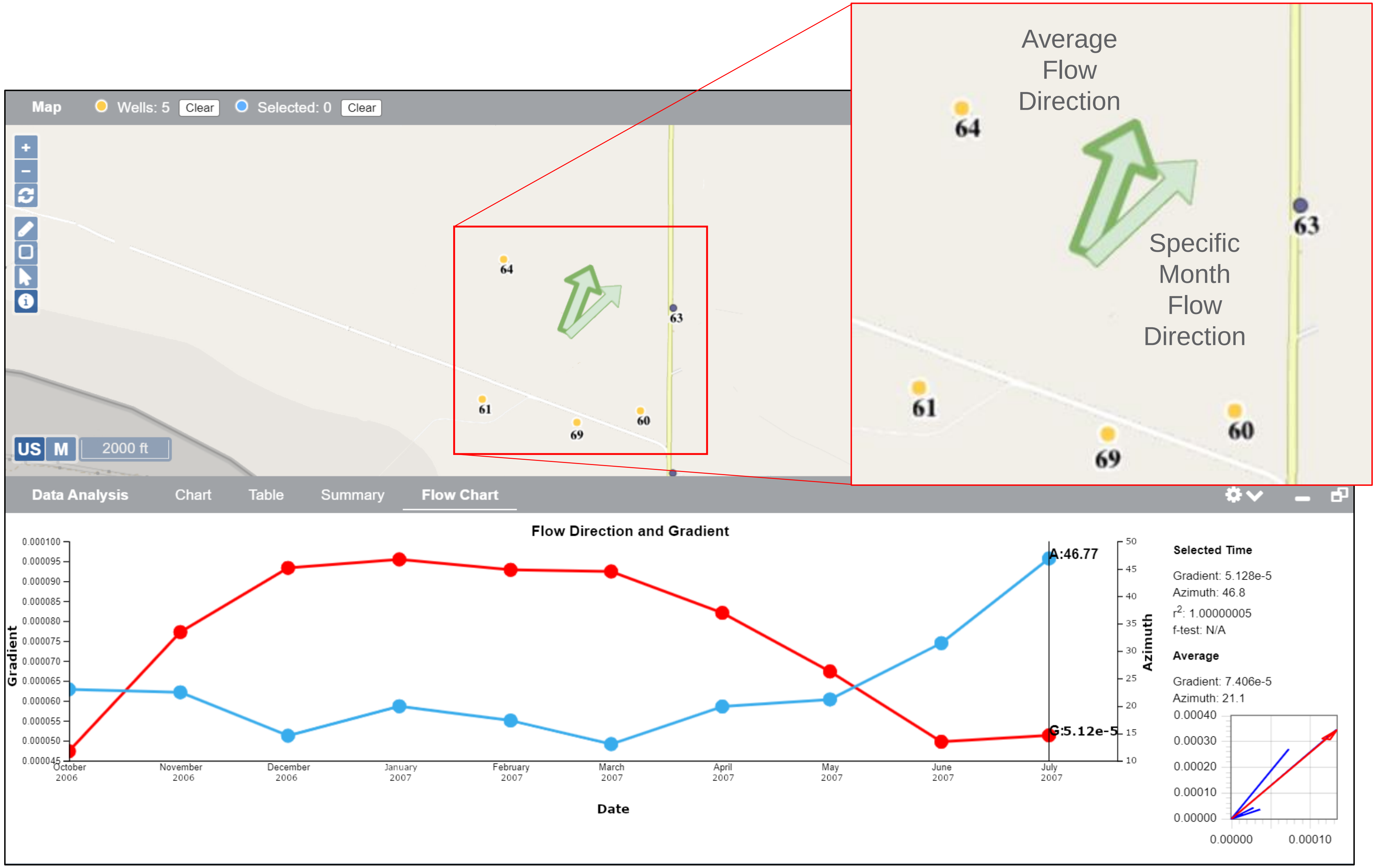
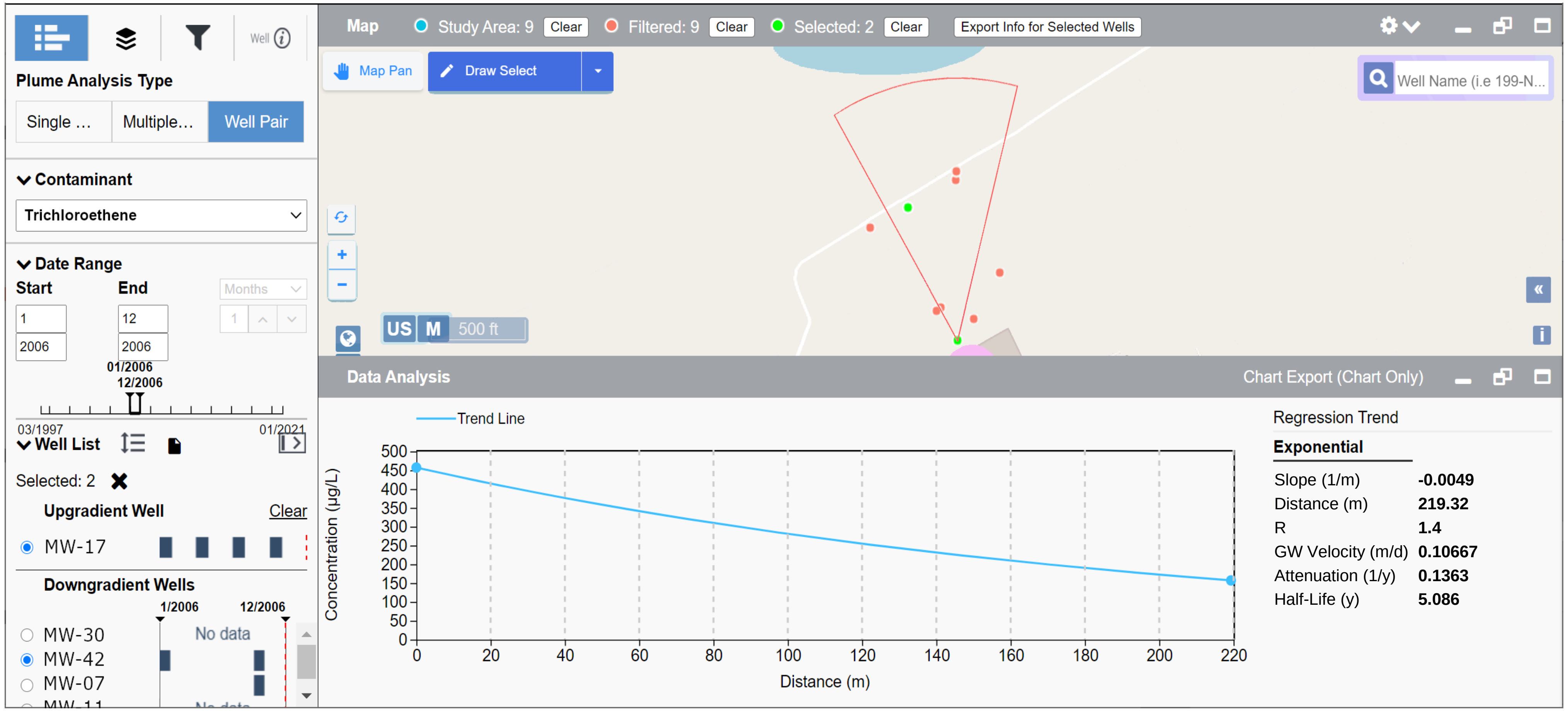
Analysis of Water Level and Flow Direction

- Groundwater elevation data
  - Key for plume understanding
- Where is contamination going?
- What seasonal effects exist?
- How fast is water and contaminant migrating?



Attenuation Capacity Analysis

- Contaminant attenuation capacity?
  - Attenuation zone between source and compliance point
  - Distance/time and attenuation
  - Under natural conditions
- Threshold source concentration
  - Or max. mass flux
- Based on guidance
  - EPA, 2002; Truex et al. 2015



Compliance point is about twice the distance, say 400 m
Compliance point target concentration = 5 µg/L
Thus, attenuation capacity → source concentration must be 35.5 µg/L to meet target

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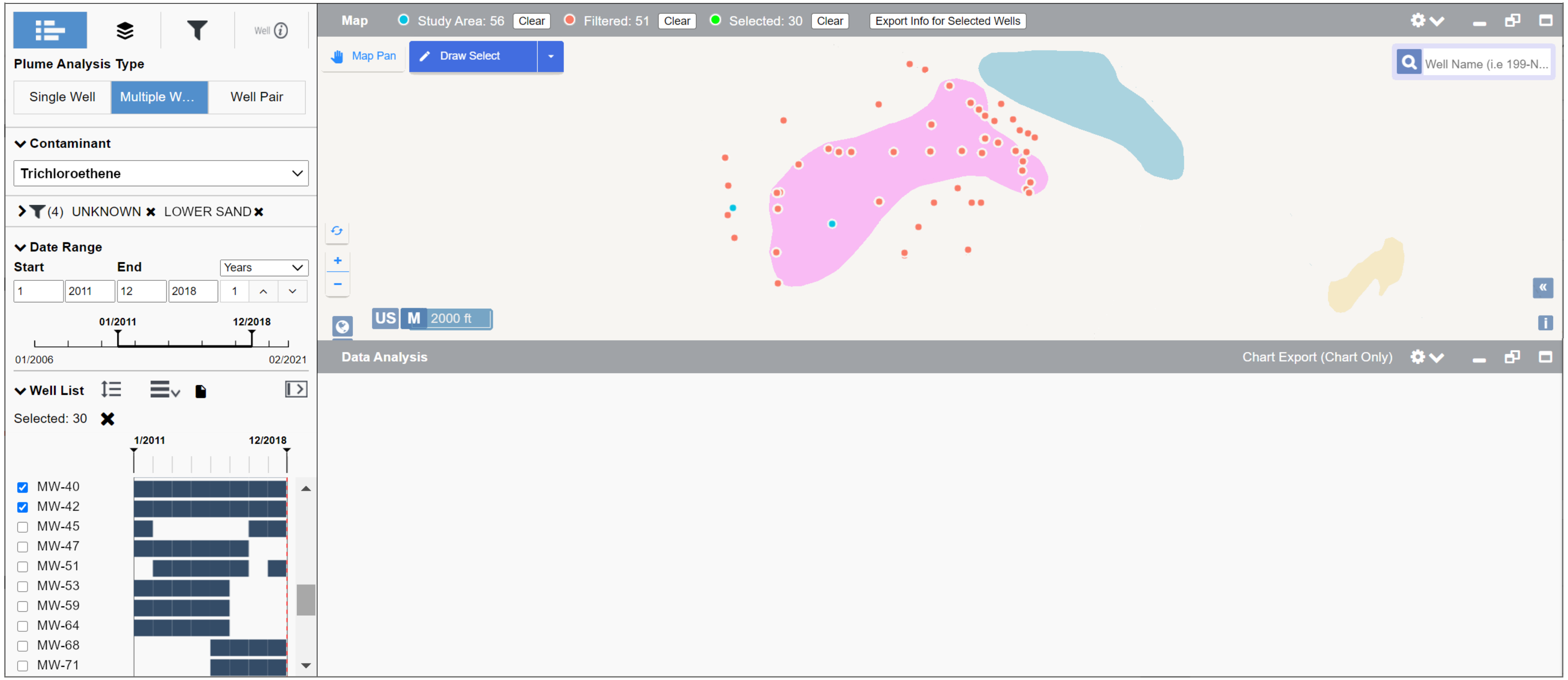
Plume Analysis

- Plume behavior over time
- Temporally consistent well set
- Trend/ attenuation
- Is remedy working?
  - Optimize? Done?
- Based on guidance
  - EPA, 2002; Truex et al. 2015



Wells sampled at different times (different temporal patterns)

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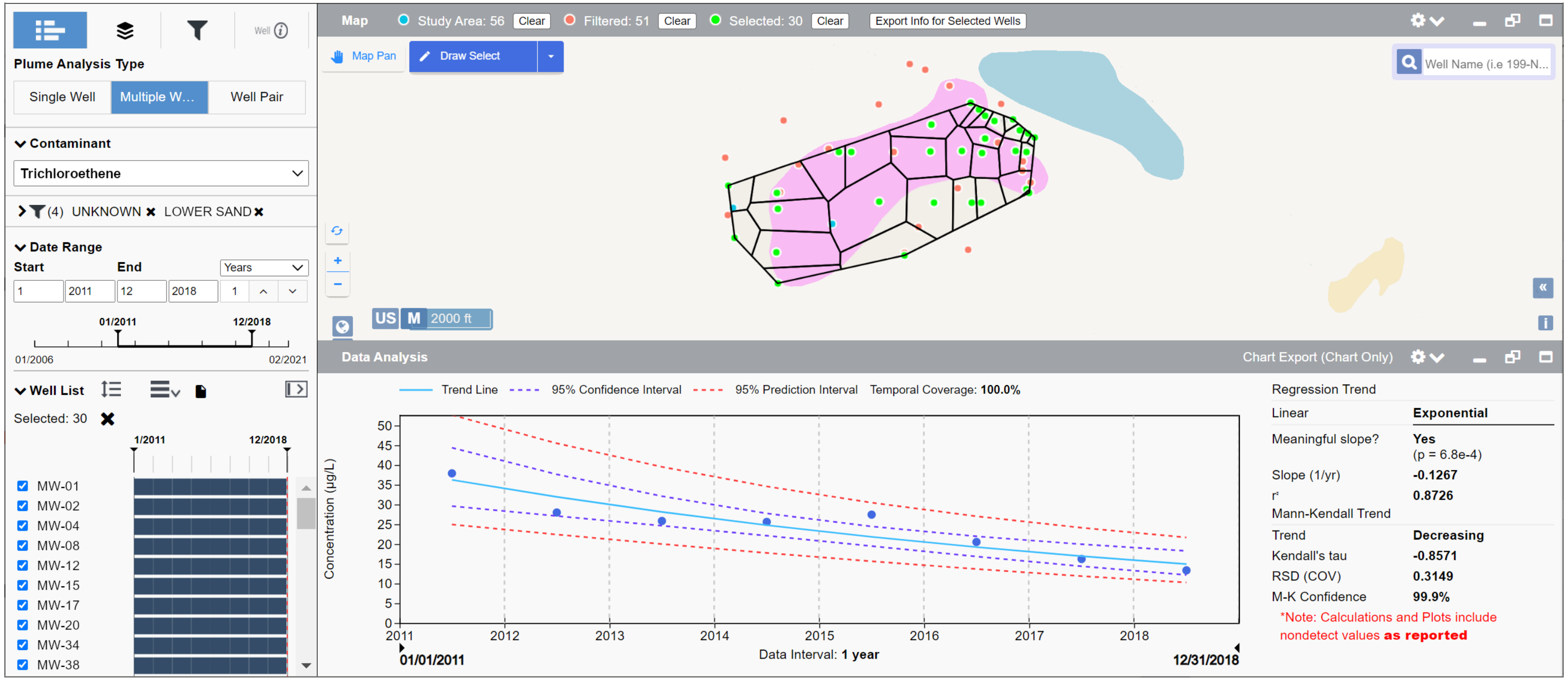

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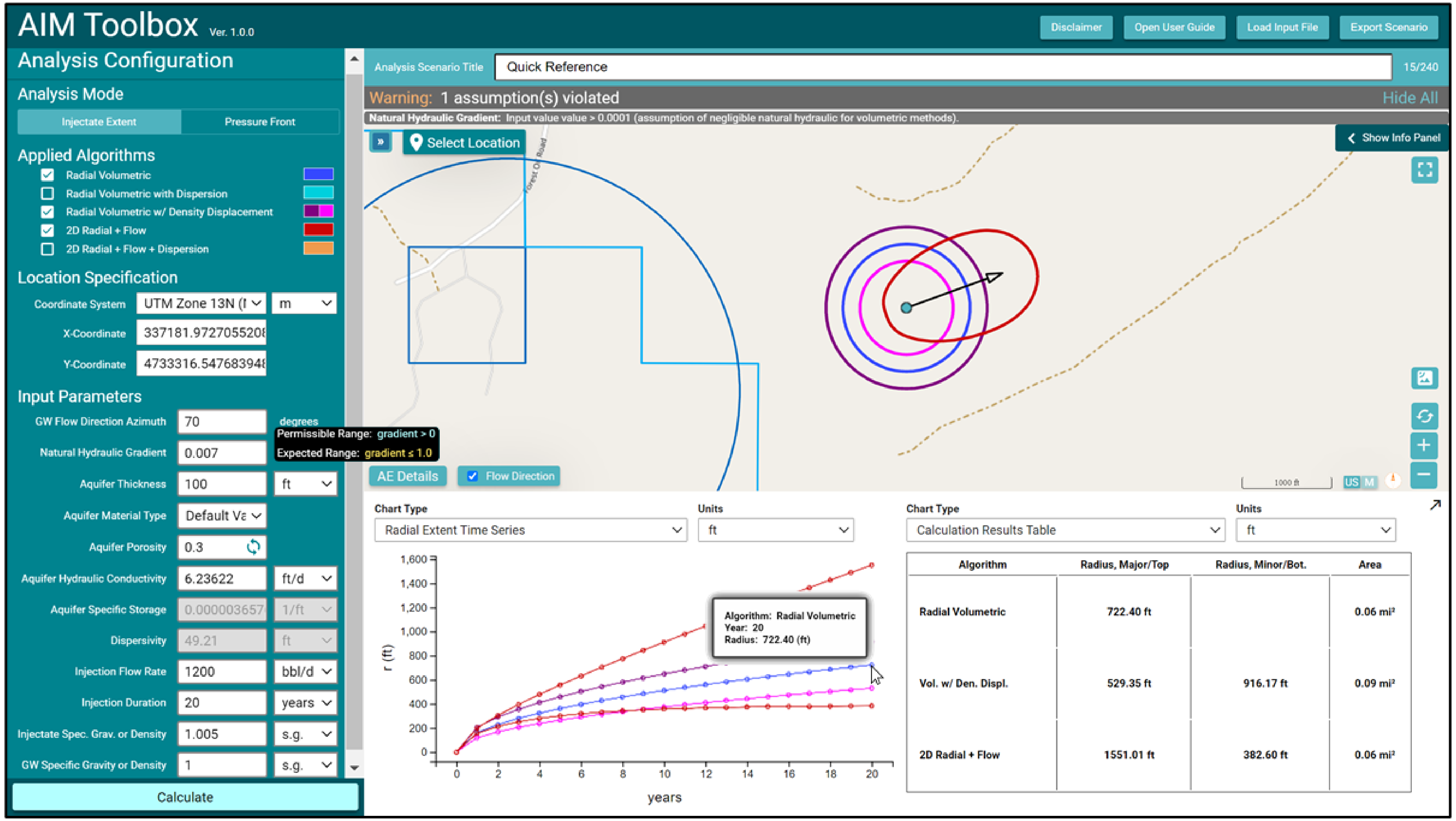
Aquifer Injection Evaluation

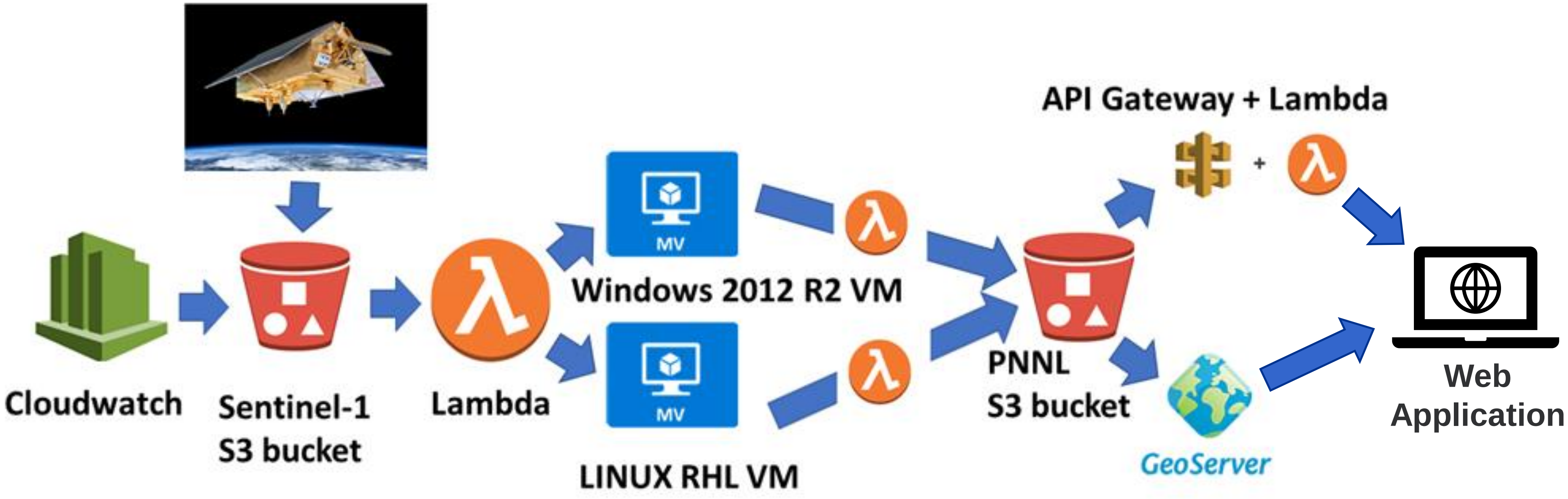
- Injection of produced water (typically a brine)
- What is the radius or area of impact?
  - Displacement
  - Dispersion
  - Groundwater flow
  - Density differences
- Used for assessing aquifer exemption applications



Aquifer Injection Modeling Toolbox – set of analytical models (Johnson et al., 2021b)

Remote Sensing Analyses

- Satellite, airborne data
  - Automated processing
- Thermal data to assess groundwater flow into river
- Subsidence detection
  - Automated alerts



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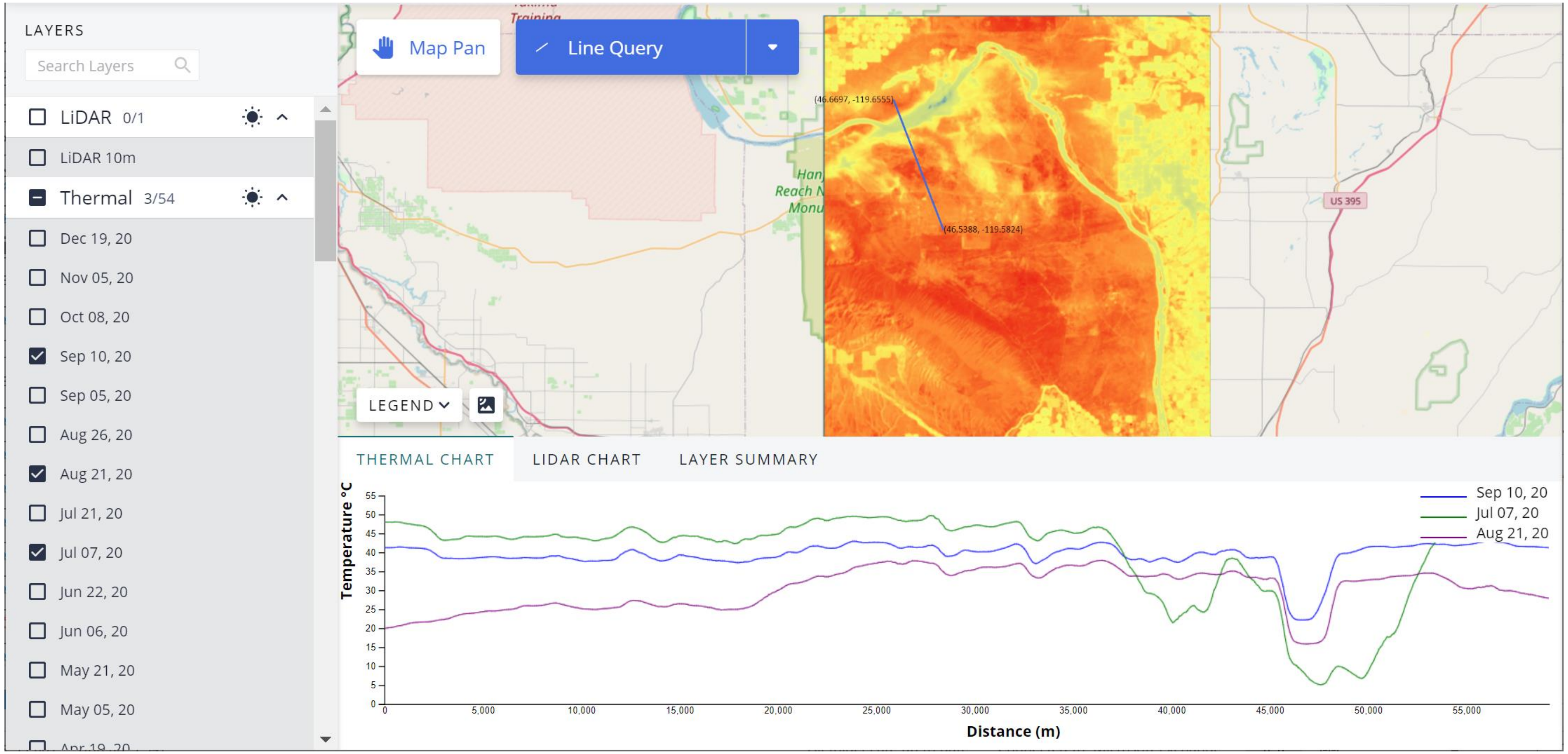

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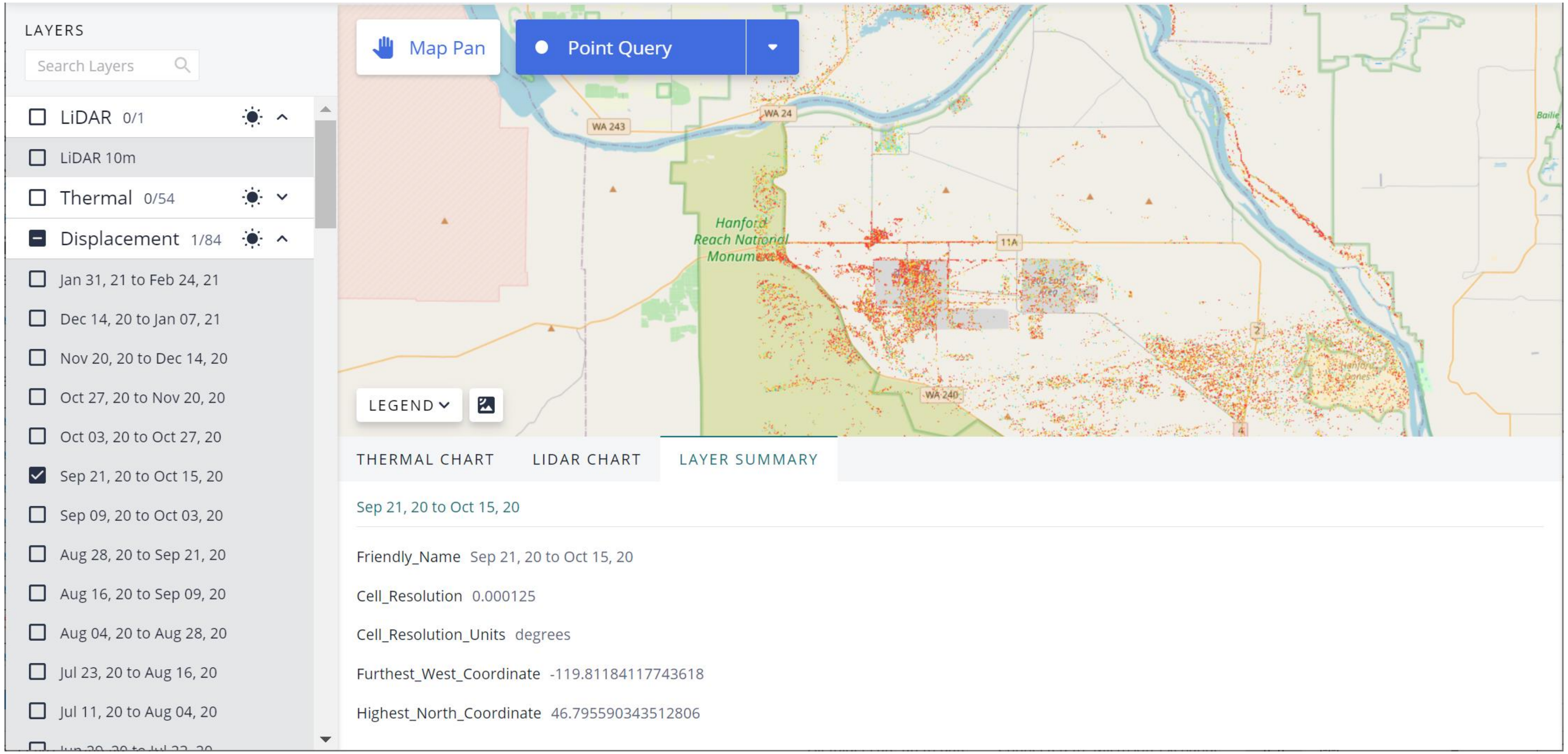

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Conclusions and Benefits

- Environmental professionals and managers need tools
  - Access to environmental/remedy data
  - Consistent and quality-approved approaches for analysis
  - Communication with other technical, management, and regulatory personnel
  - Supporting remedial decisions
- Web-based applications for subsurface remediation and long-term management
  - Minimize complexity associated with large data sets and analytics
  - Maximize consistency and productivity
  - Promote technical communication through sharing, reproducibility, and availability
  - Provide robust and reliable performance
  - Provide a technical basis for environmental decision-making

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Impact and Broader Application

- Data management resilience/adaptability
  - Large volumes of data (e.g., satellite, sensor, climate)
  - Variety of analytics
  - User experience – adapting to changing human interaction patterns
- Cloud computing/serverless architecture
  - Robust and rapid analytics – from analytical methods to complicated machine learning
  - Big data processing
  - Integrating disparate data types, relational and unstructured data
- Web-based tools can support decision making in a range of contexts
  - Water and other natural resources
  - Climate resilience
  - Disaster response

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Thank you

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