FIU Applied Research Center

DOE-FIU Cooperative Agreement Annual Research Review – FIU Year 1

September 14, 2021		
9:00 - 9:05 am EDT	Kick-Off	Kurt Gerdes (Director, Technology Development) – DOE EM-3.2
9:05 - 9:10 am EDT	Welcoming Remarks (DOE-EM)	Nicole Nelson-Jean (Assoc. Principal Deputy Asst. Secretary for Field Ops) – DOE EM-3
9:10 - 9:15 am EDT	Welcoming Remarks (DOE-LM)	Carmelo Melendez (Director, Office of Legacy Management) – DOE LM-1
9:15 - 10:30 am EDT	Projects 4 & 5: STEM Workforce Development and Training	FIU, DOE HQ (EM & LM), SRNL, PNNL, WIPP, SRS, ORP, LBNL, WRPS, INL, Grand Junction
10:30 am - 12:00 pm EDT	Project 1: Chemical Process Alternatives for Radioactive Waste	FIU, DOE HQ, PNNL, WRPS, SRNL, SRS
1:30 - 3:00 pm EDT	Project 3: Waste and D&D Engineering & Technology Development	FIU, DOE HQ, SRNL, PNNL, LBNL, INL, ANL
3:00 - 4:30 pm EDT	Project 2: Environmental Remediation Science & Technology	FIU, DOE HQ, SRNL, PNNL, LANL, ORNL
September 15, 2021		
9:30 - 11:00 am EDT	Wrap Up (FIU Projects 1, 2, 3, 4 & 5)	FIU, DOE HQ (EM & LM)

PROJECT 3

Waste and D&D Engineering & Technology Development

FIU Applied Research Center

FIU Personnel and Collaborators

Project Manager: Leonel Lagos

Faculty/Researcher: Himanshu Upadhyay, Joseph Sinicrope, Walter Quintero, Clint Miller, Santosh Joshi, Tushar Bhardwaj, Suresh Peddoju, Masudur Siddiquee, John Dickson, Mellissa Komninakis, Kexin Jiao

DOE Fellows/Students: Roger Boza, Aurelien Meray, David Mareno, Christian Gonzalez, Christian Dau, Rohan Shanbhag, Derek Gabaldon, Philip Moore

DOE-EM: Dinesh Gupta, Genia McKinley, Jean Pabon, Jonathan Kang, Douglas Tonkay, Jennifer McCloskey

SRNL: Jennifer Wohlwend, Connor Nicholson, Nick Groden, Aaron Washington, *Tristan Simoes-Ponce, Carol Eddy-Dilek

PNNL: Vicky Freedman, Rob Mackley

INL: Rick Demmer

LBNL: Haruko Wainwright

*Former staff/student contributors

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Project Tasks and Scope

TASK 1: WASTE INFORMATION MANAGEMENT SYSTEM (WIMS) (HQ)	
Subtask 1.1	WIMS System Administration - Database Management, Application Maintenance & Performance Tuning
Subtask 1.2	Waste Stream Annual Data Integration
Subtask 1.3	Upgrade GIS module with Google Map API
Subtask 1.4	Deploy Power BI Reporting Server for Waste Stream Reports
Subtask 1.5	Cyber Security of WIMS Infrastructure
TASK 2: D&D SUPPORT TO DOE EM FOR TECHNOLOGY INNOVATION, DEVELOPMENT, EVALUATION AND DEPLOYMENT	
Subtask 2.1	Development of Uniform Testing Protocols and Standard Specifications for D&D Technologies
Subtask 2.2	Applications of Intumescent Foams and Other Fire-Retardant Materials to Mitigate Contaminate Release during Nuclear Pipe Dismantling and other D&D Activities
Subtask 2.3	Support to SRNL and SRS 235-F to Complete Final Data Collection and Technical Report for Onsite Hot Demonstration of Intumescent Fixative at SRS 235-F
Subtask 2.4	Certifying Fixative Technology Performance when Exposed to a Variety of Stressors Postulated in Contingency Scenarios Highlighted in Safety Basis Document
Subtask 2.5	Multi-functional 3D Polymer Framework for Mercury Abatement **(NEW)**

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Project Tasks and Scope

TASK 3: D&D KNOWLEDGE MANAGEMENT INFORMATION TOOL (KM-IT) (HQ, SRNL, INL, ANL)	
Subtask 3.1	D&D KM-IT Enhancements
Subtask 3.2	KM-IT Development – Enhance D&D Research Module for Multiple DOE EM Sites and National Laboratories
Subtask 3.3	Software Upgrades (Database and .NET Framework)
Subtask 3.4	Content Management
Subtask 3.5	Marketing and Outreach
Subtask 3.6	D&D KM-IT System Administration
Subtask 3.7	Cyber Security of D&D KM-IT Infrastructure
TASK 6: AI FOR EM PROBLEM SET (D&D): STRUCTURAL HEALTH MONITORING OF D&D FACILITY TO IDENTIFY CRACKS AND STRUCTURAL DEFECTS FOR SURVEILLANCE AND MAINTENANCE (SRNL)	
Subtask 6.1	Design & Development of Convolutional AutoEncoder Algorithm to Identify Cracks in D&D Mockup Facility
Subtask 6.2	Use LiDAR technology to scan the walls of the hot cell testbed to establish a baseline model using AI/deep learning technologies
Subtask 6.3	Object Detection (2D Space) (NEW)
Subtask 6.4	Object Detection (3D Space) (NEW)

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Project Tasks and Scope

TASK 7: AI FOR EM PROBLEM SET (SOIL AND GROUNDWATER) - EXPLORATORY DATA ANALYSIS AND MACHINE LEARNING MODEL FOR HEXAVALENT CHROMIUM (CR [VI]) CONCENTRATION IN 100-H AREA (PNNL) (NEW)	
Subtask 7.1	Identification of Data Sources and Datasets from the Soil and Ground Water Repositories
Subtask 7.2	Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples
Subtask 7.3	Machine-Learning and Deep-Learning Model Development for Anomaly Detection
TASK 8: AI FOR EM PROBLEM SET (SOIL AND GROUNDWATER) - DATA ANALYSIS AND VISUALIZATION OF SENSOR DATA FROM WELLS AT THE SRS F-AREA USING MACHINE LEARNING (LBNL, SRNL) (NEW)	
Subtask 8.1	Exploratory Data Analysis
Subtask 8.2	Identify the Master/Proxy Variables
Subtask 8.3	Machine Learning Model Development & Optimization for Sensor Placement in Groundwater Wells

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Task 1

Waste Information Management System (WIMS)

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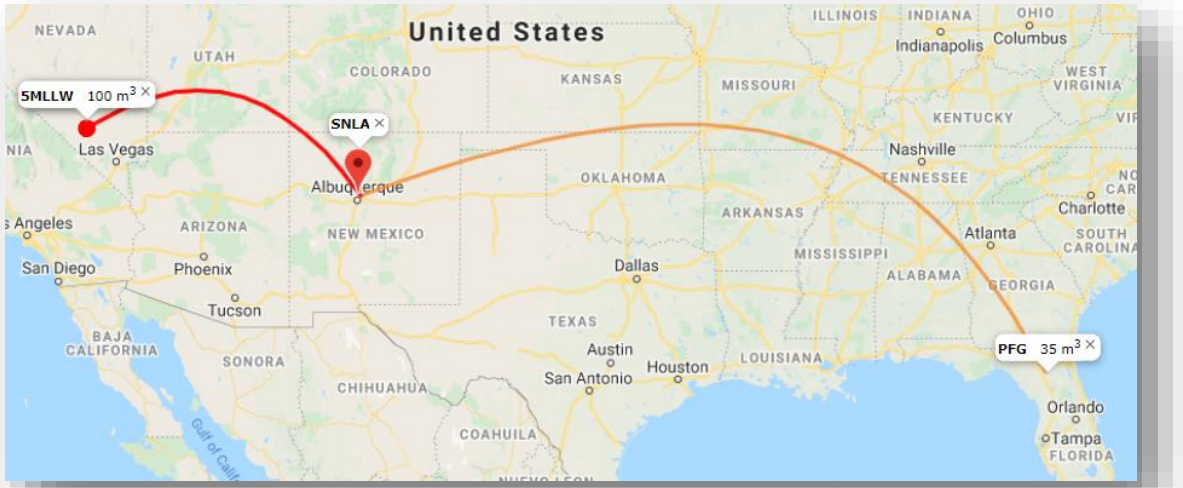
Waste Information Management System (WIMS)

Subtask 1.1	WIMS System Administration - Database Management, Application Maintenance & Performance Tuning
Subtask 1.2	Waste Stream Annual Data Integration
Subtask 1.3	Upgrade GIS module with Google Map API
Subtask 1.4	Deploy Power BI Reporting Server for Waste Stream Reports
Subtask 1.5	Cyber Security of WIMS Infrastructure



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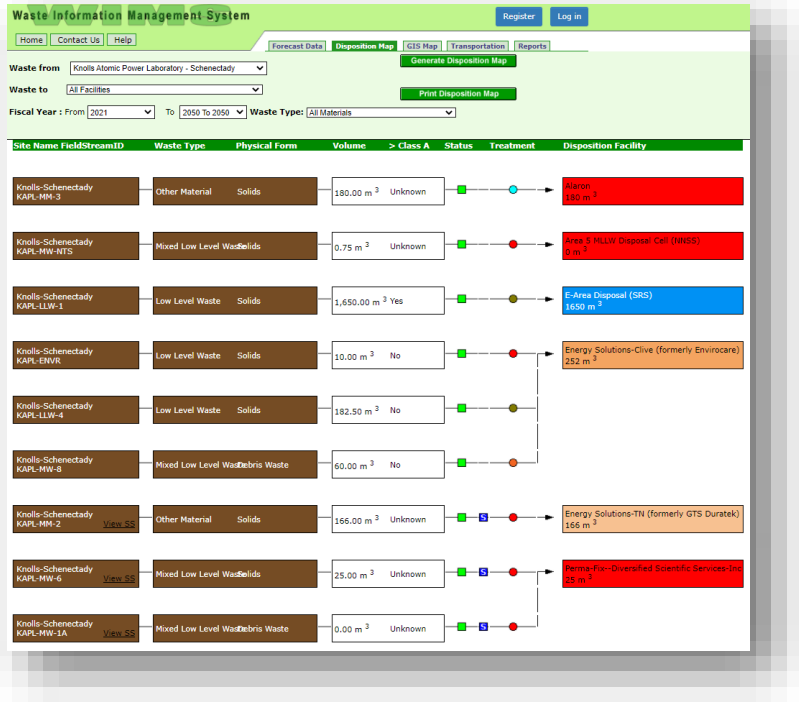
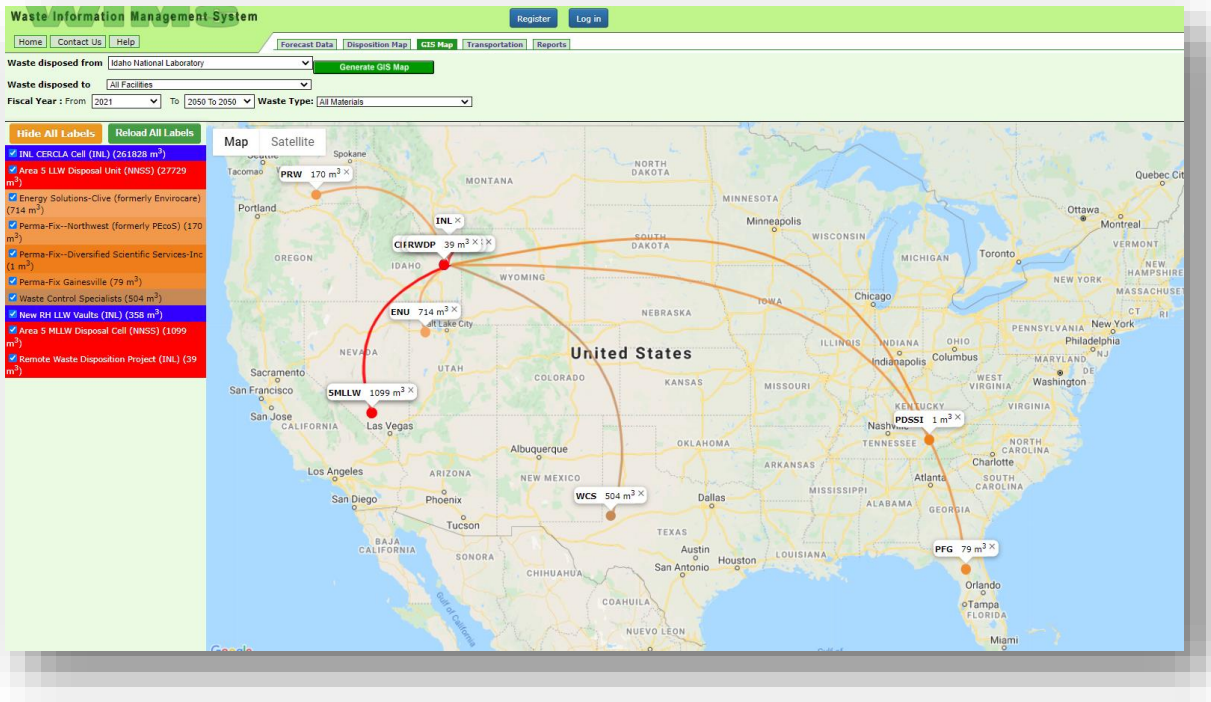
Waste Information Management System (WIMS)

- Easy-to-use system to visualize and understand the forecasted DOE-EM waste streams & transportation information.
- Various modules of WIMS are Forecast Data, Disposition Map, Successor Stream Map, GIS Map, Transportation, Reports and Help.
- WIMS is deployed and available at https://www.emwims.org





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Subtask 1.1: WIMS System Administration - Database Management, Application Maintenance & Performance Tuning

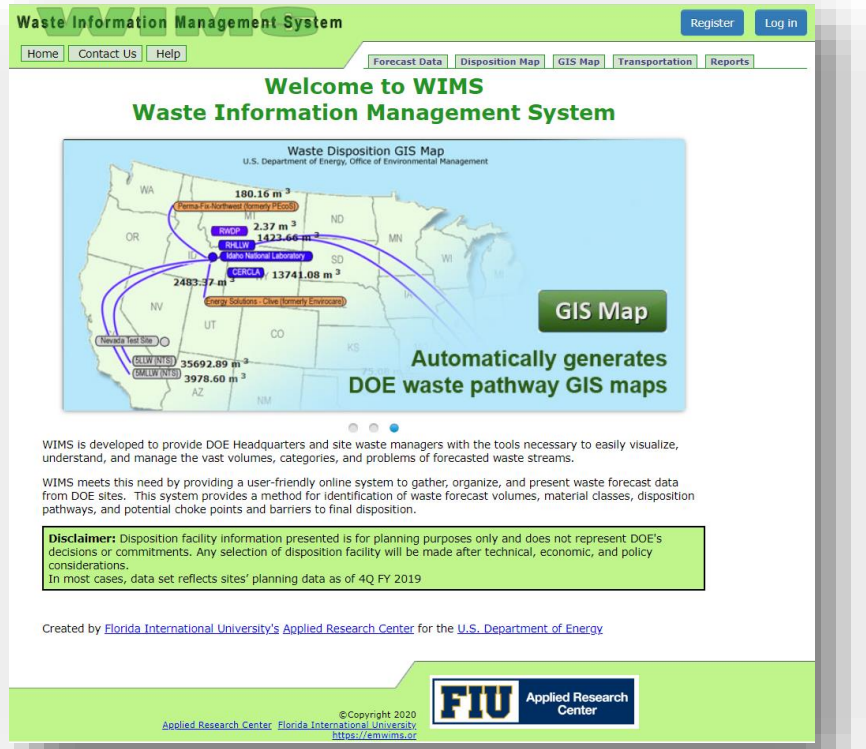
Accomplishments:

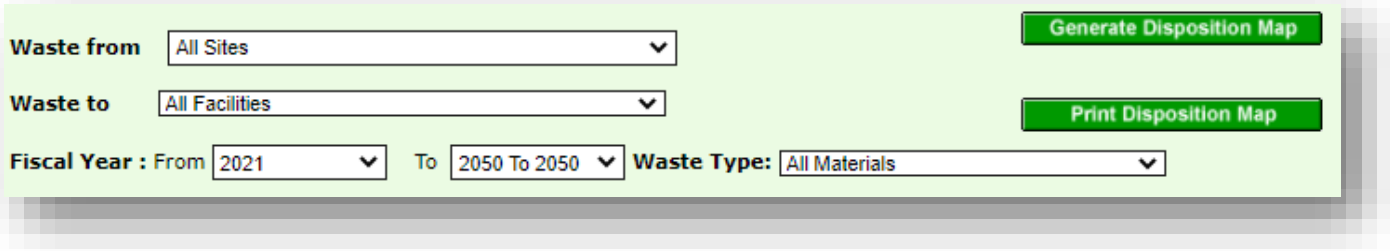
- Continue to perform day-to-day maintenance and administration to ensure consistent high level of performance of WIMS application
- Updating patches and OS fixes, updating antivirus engines and definitions, updating drivers and assuring that the network is working properly.
- Hardware upgrades (memory, hard drives, video cards, routers, firewall, etc)
- Created development environment to support Subtask 1.3 (Upgrade GIS Module with Google Map API).
    - This included backing up of production environment application and database

Subtask 1.2: Waste Stream Annual Data Integration

Accomplishments:

- FIU received and incorporated the revised waste forecast data files into the system
- Completed integration of 2021 waste forecast and transportation data into WIMS system.
- Published 2021 Forecast Waste stream information in May 2021.
- FIU presented WIMS research in 2021 Waste Management Symposia.





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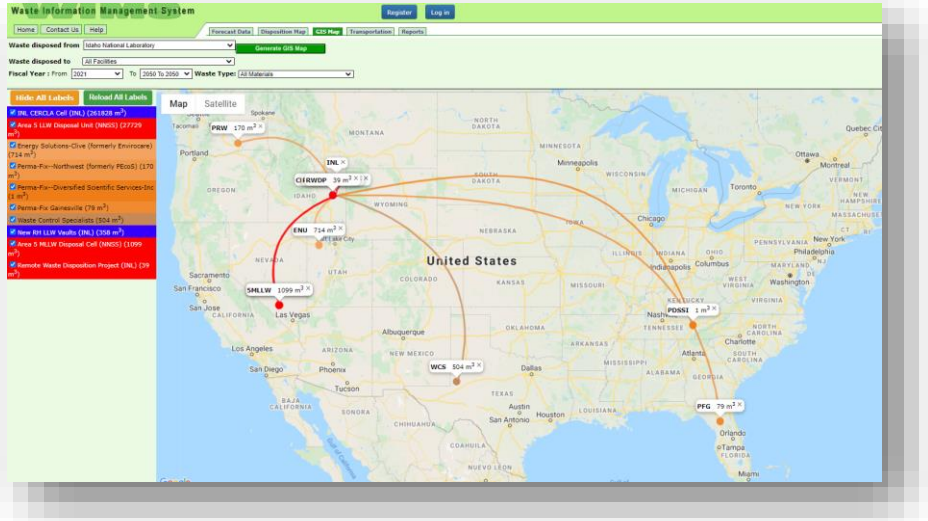
Subtask 1.3: Upgrade GIS module with Google Map API

Accomplishments:

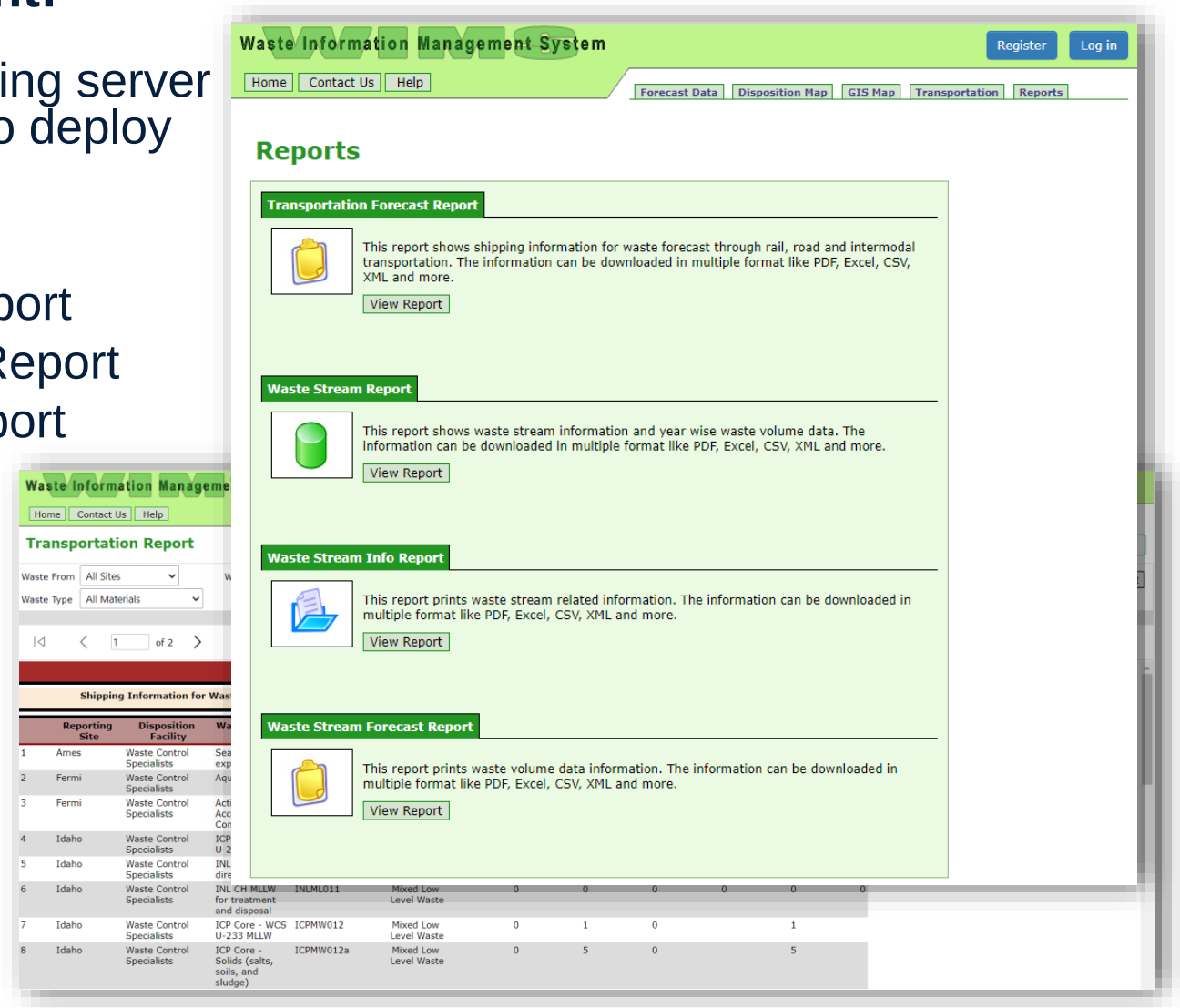
- The objective of this task is to upgrade the GIS module to use the Google Map API in order to improve the performance, stability, and user experience of the GIS module.
- Created development environment
- DOE Fellows assisted with collecting GIS coordinates (latitude and longitude) for each site and disposition location
- Imported Google GIS MAP API into WIMS solution
- Modified backend code and database to accommodate new functionality
- Disposition paths are dynamically generated based on coordinates
- Users can filter their results and hide/show labels using the new sidebar capability
- Deliverable completed on April 29, 2021.
- The updated module is available at https://emwims.org/GoogleGISMap



Subtask 1.4: Deploy Power BI Reporting Server for Waste Stream Reports

Description and Accomplishment:

- Replace the existing SQL reporting server with Power BI reporting server to deploy SQL reports
- Four types of reports supported
  - Transportation Forecast Report
  - Waste Stream Information Report
  - Waste Stream Forecast Report
  - Waste Stream Report
- The information can be downloaded in multiple format like PDF, Excel, CSV, XML and more.
- Successfully deployed Power BI reporting server with SQL server 2019 in DOE-EM infrastructure.



Subtask 1.5: Cyber Security of WIMS Infrastructure

Description and Accomplishments:

- Cyber security of WIMS involves securing the network infrastructure that is deployed, secured and maintained in the FIU facility.
- This involves coordination between the FIU security team and DOE Fellows who learn cyber security skills while assisting staff do penetration testing and other tasks to test the overall security of the system at the application, database and infrastructure levels.
- Example of this task include:
  - Updating the DOE server room network switch from 24-port unmanaged switch to 50-port to managed switch. This switch supports the network connectivity of the server running the emwims application.
  - Updating security patches and applications for the servers and firewall of the DOE server room. This includes the server hosting the emwims application.

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Task 1: Waste Information Management System (WIMS)

FIU Year 2 Projected Scope

- **Subtask 1.1: WIMS System Administration - Database Management, Application Maintenance & Performance Tuning**
  - This subtask includes the day-to-day maintenance and administration of the application and the database servers.
  - Administrator will monitor the network and server traffic and performs updates necessary to optimize the application performance.
  - FIU will provide application and database security as well as help desk support to DOE site managers, HQ managers and other users who need assistance with WIMS.
- **Subtask 1.2: Waste Stream Annual Data Integration**
  - Update WIMS modules – Forecast Data , Waste Stream and GIS map
  - Update and publish reports
  - Update and publish transportation module
- **Subtask 1.3: Cyber Security of WIMS Infrastructure**
  - Provide cyber security to WIMS infrastructure, application, database server and reporting server.
  - Cybersecurity training and support of DOE Fellows while working with pen testing & forensics tools used with WIMS system.

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Task 3

D&D Knowledge Management Information Tool (KM-IT)

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Subtask 3.1	D&D KM-IT Enhancements
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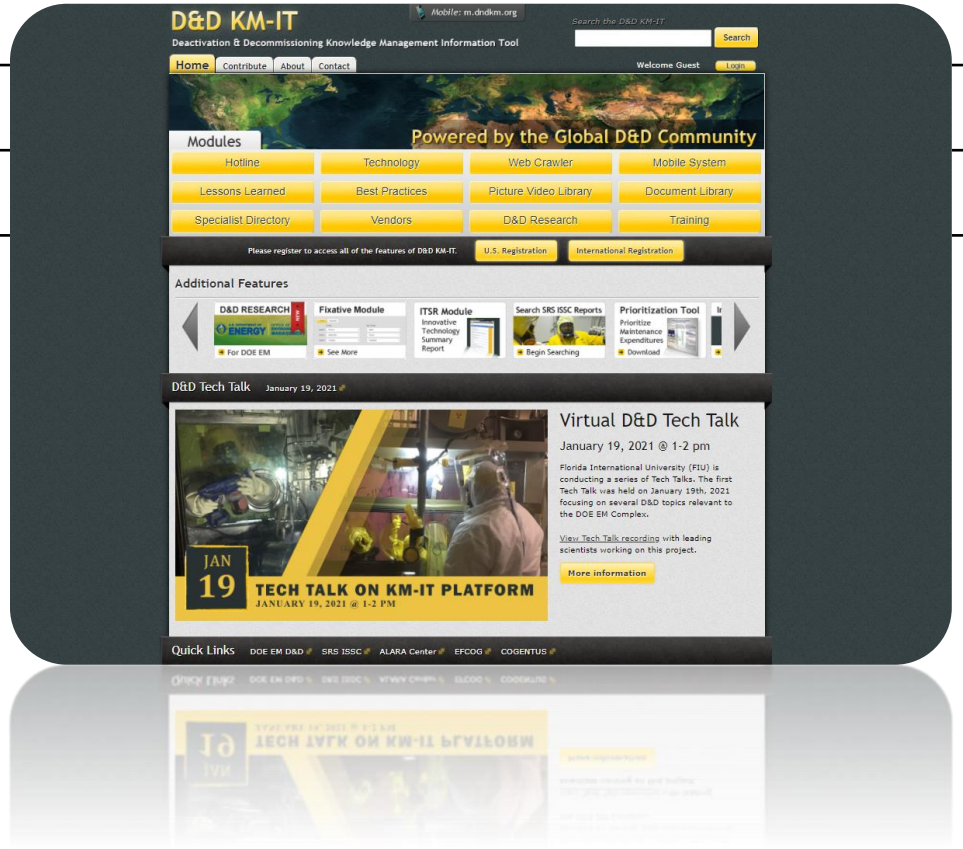
Subtask 3.7	Cyber Security of D&D KM-IT Infrastructure



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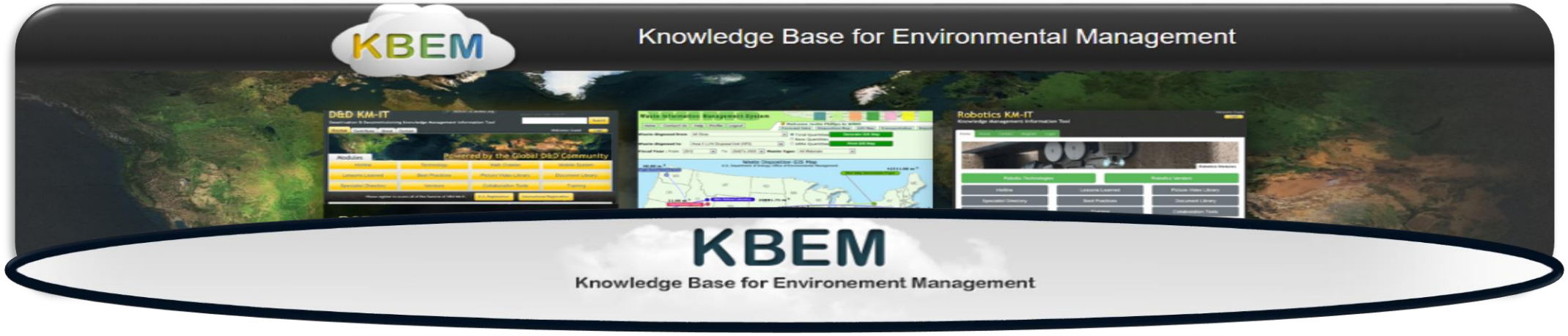
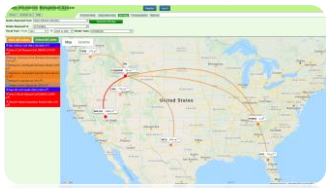
Knowledge Base for Environmental Management



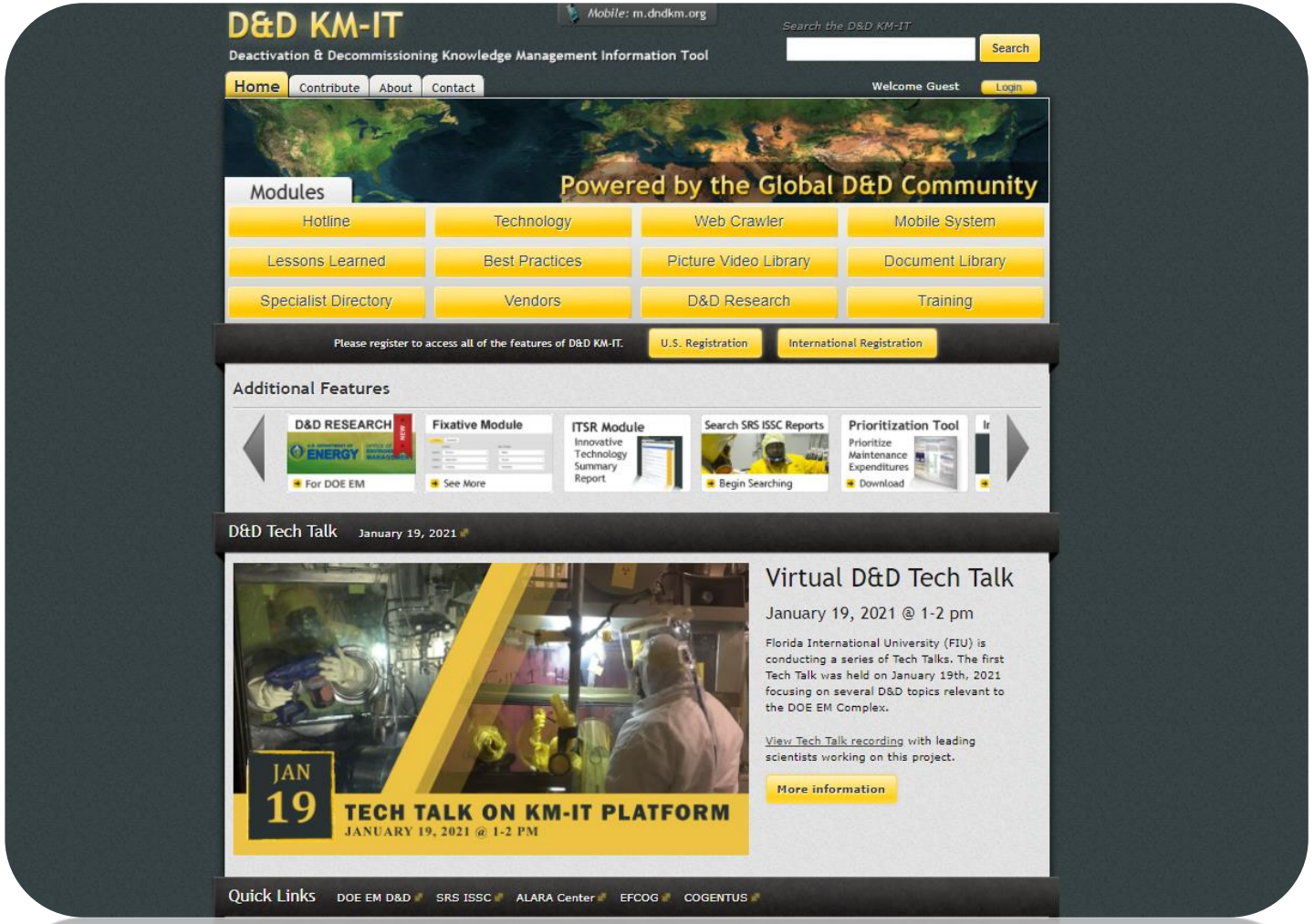
DND KM-IT dndkm.org	WIMS emwims.org	DOE FELLOWS fellows.fiu.edu	DOE RESEARCH doeresearch.fiu.edu	Robotics KM-IT rkmit.org



KM-IT Modules

- D&D Hotline
- Technology Module
- Vendor Module
- D&D Research
- Mobile applications
- Lessons Learned
- Documents
- Pictures/videos
- Search tools
- Training
- Specialists
- Best Practices

https://www.dndkm.org/



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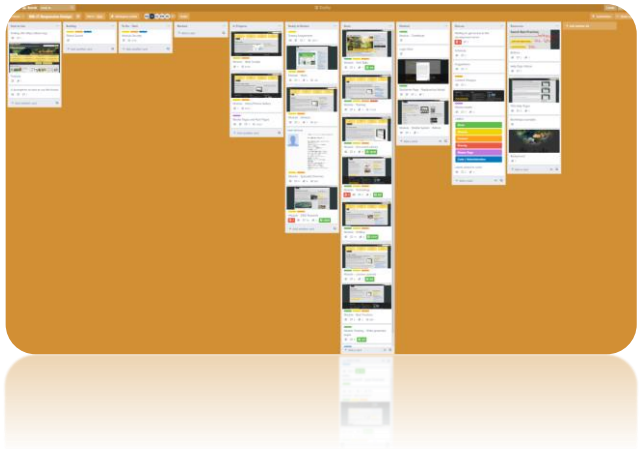
Subtask 3.1: D&D KM-IT Enhancements

Accomplishments:

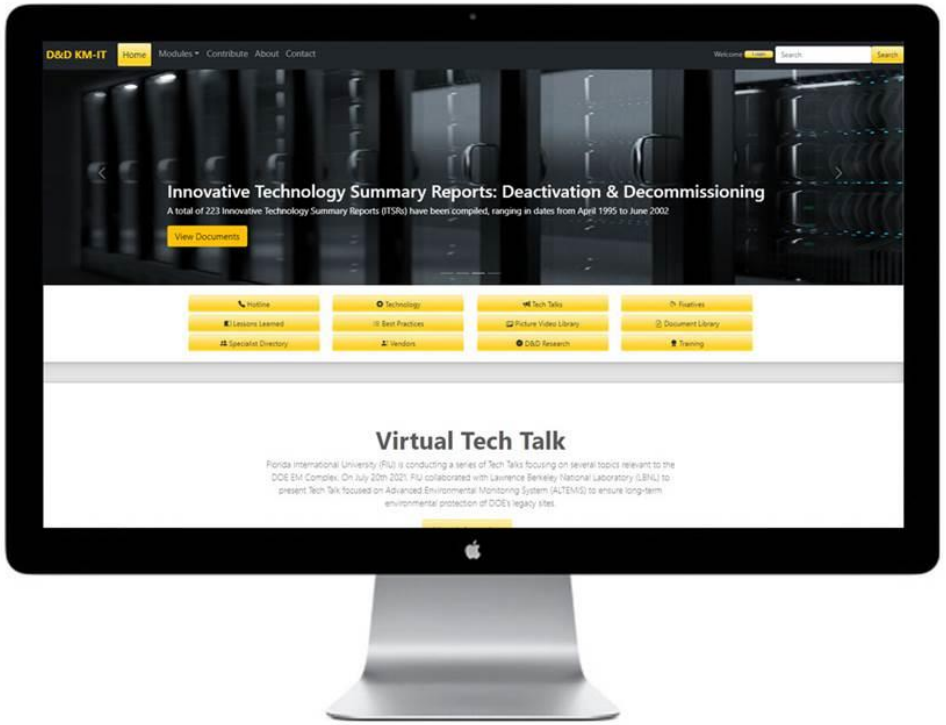
- Focused on user interface responsive design and development
- Updated D&D KM-IT front-end to be mobile device friendly
- All landing pages, templates and modules were updated with Bootstrap framework
- Create Trello board so that staff and DOE Fellows could collaborate
- Imported Bootstrap framework to solution
- Updated landing page theme, main master theme, module themes (12), and individual pages for each theme (over 100 pages)
- Updated back-end code where necessary (security module, login, administration)
- Deployed application to staging server for testing
- Published to production server



Subtask 3.1: D&D KM-IT Enhancements

Accomplishment:

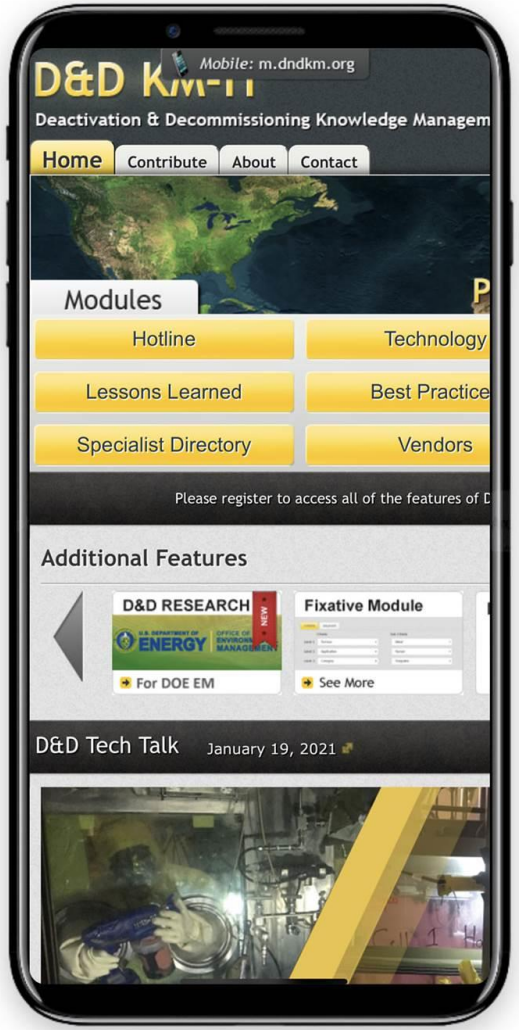
- FIU completed deliverable (2020-P3-D6) on August 20, 2021
- Image below shows screenshot of homepage

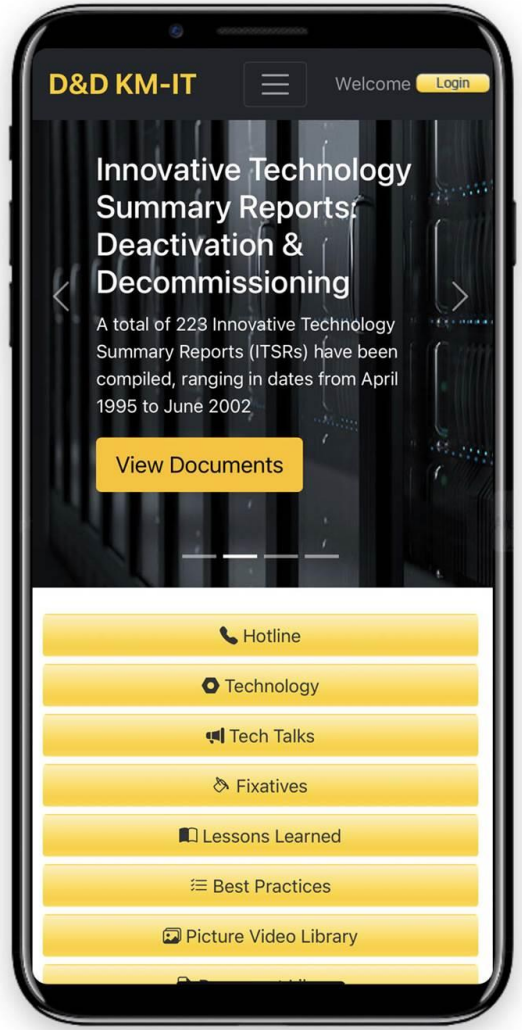


Subtask 3.1: D&D KM-IT Enhancements

Accomplishment:

- Accomplished objective to make KM-IT application mobile friendly
- New design provides a better user experience
- Updated framework encourage search crawlers to properly index the site to improve better search result rankings

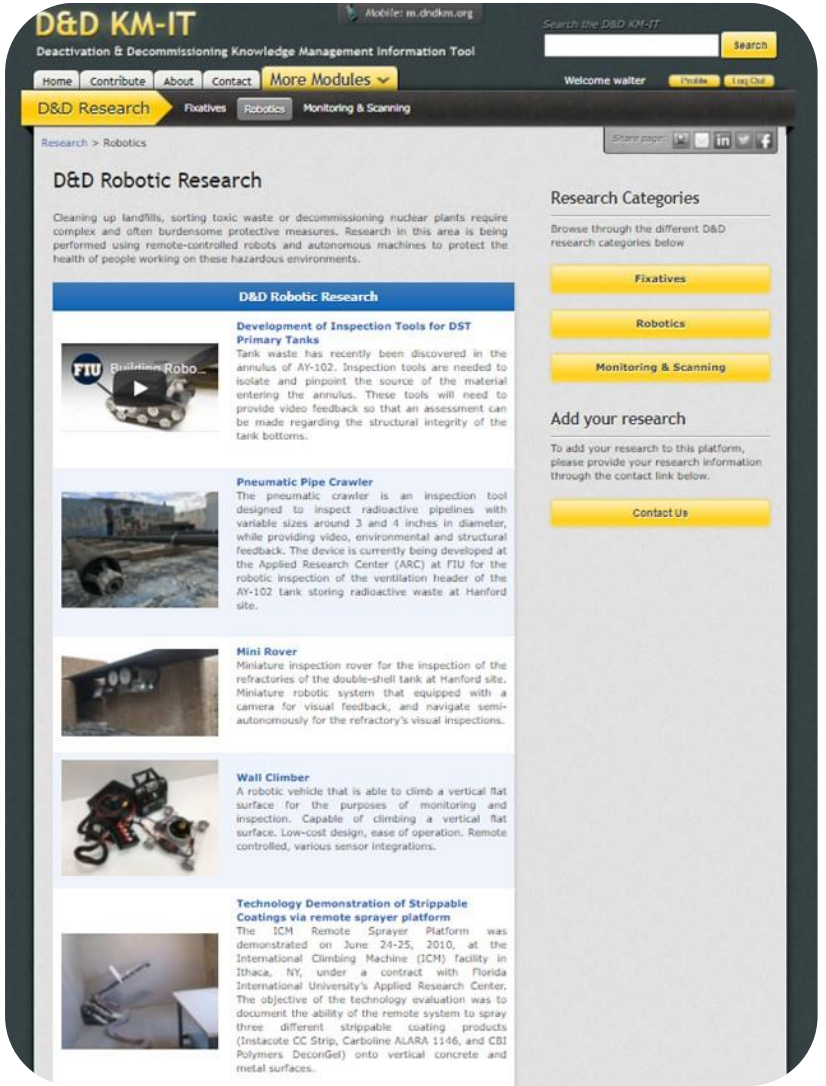




Subtask 3.2: KM-IT Development – Enhance D&D Research Module for Multiple DOE EM Sites and National Laboratories

Accomplishments:

- FIU team continued to expand the research module to publish current D&D research being performed across multiple DOE EM sites, national labs and universities
- In January 2021, FIU successfully completed the deliverable (2020-P3-D3)
- Research framework integrated various D&D areas like Fixatives, Robotics and Monitoring & Scanning.
- Research details captured in this framework include: Title, description (or abstract), factsheet (or paper/presentation), contact information, images and in some cases videos.
- The research module can be accessed using the link https://www.dndkm.org/Research/



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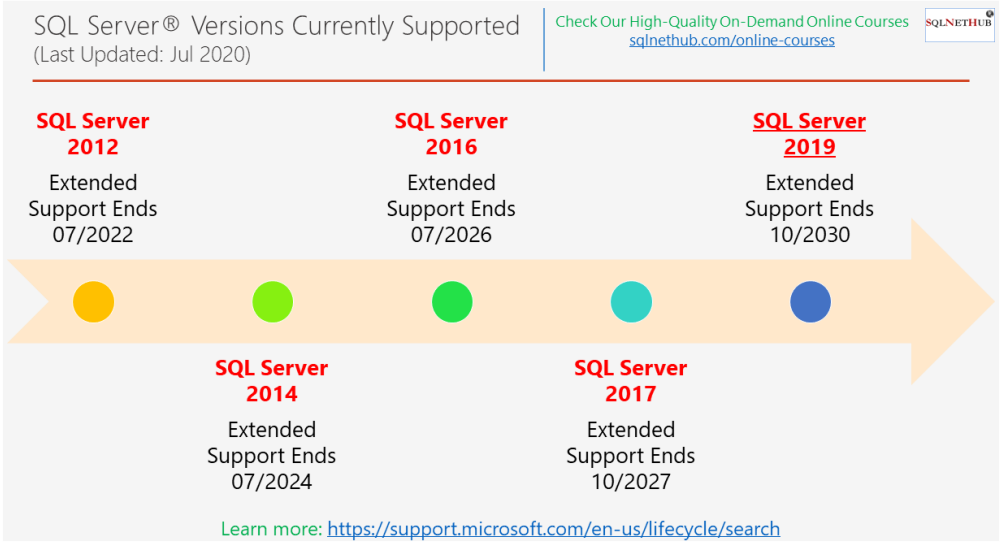
Subtask 3.3: Software Upgrades (Database and .NET Framework)

Description, Process and Accomplishment:

- This task involves migration of the existing database to SQL Server 2019 and KM-IT modules to the .NET Framework 4.2.
- Created a development environment for the application and database server
- Installed SQL Server 2019 on new server and use migration tool on Microsoft Visual Studio to upgrade the D&D KM-IT application to new .NET Framework 4.2
- Tested application before moving to production
- FIU completed milestone 2020-P3-M4 in February 2021
- This upgrade improves performance, security, stability and long term support of the system

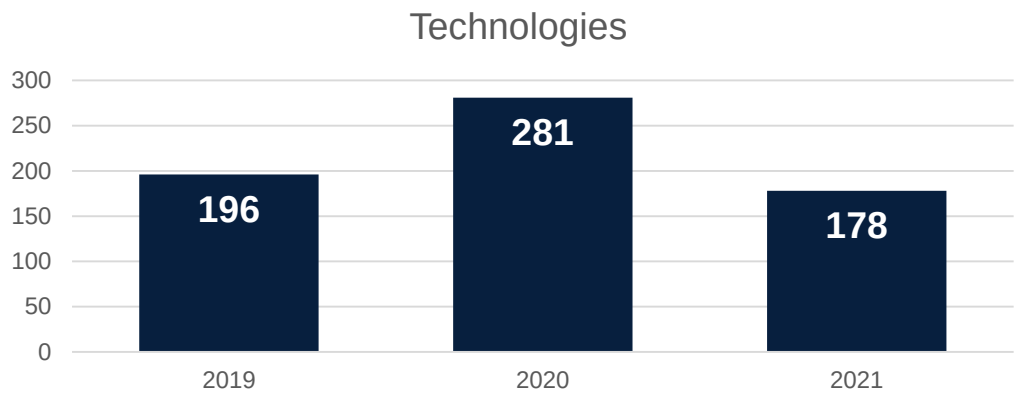


Microsoft® .NET Framework

Subtask 3.4: Content Management

Accomplishments:

- Publishing D&D technologies, vendors, D&D technologies, lessons learned, best practices, D&D news, conferences and other content to KM-IT
- Perform QA/QC of existing content in the system with assistance of DOE Fellows
- 178 technologies were published on this platform in this fiscal year, bringing the total technologies published to 1437
- 655 technologies published in the last 3 years



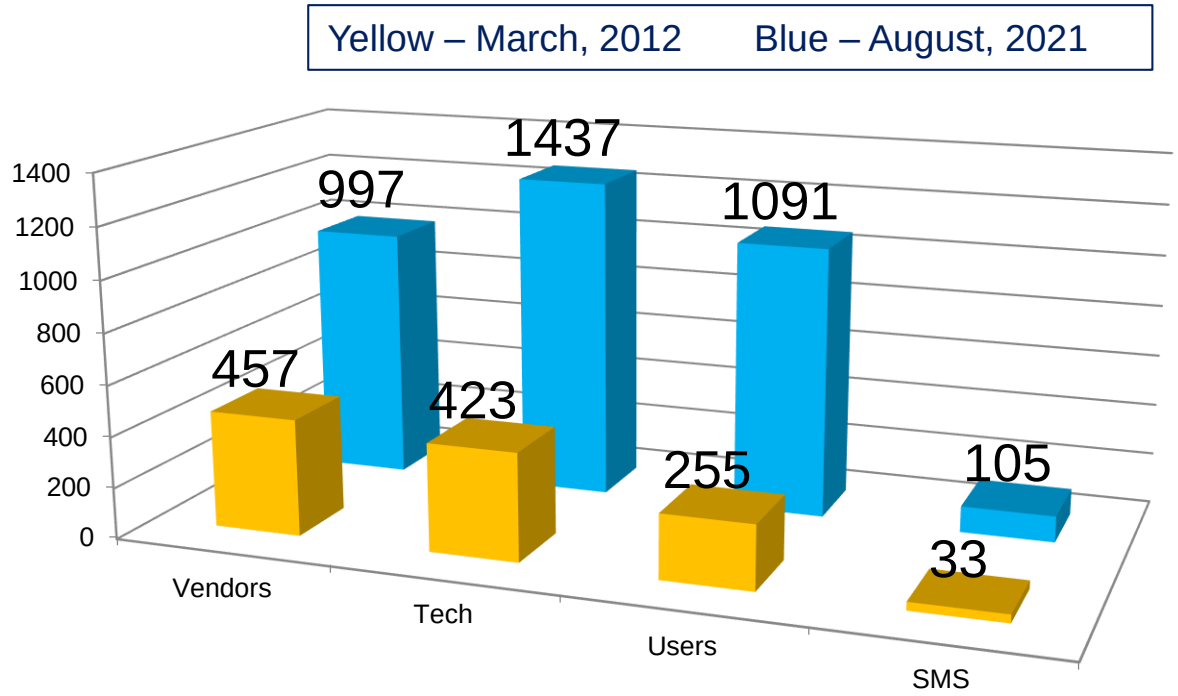
Brokk 400

Anti-Contamination "BLU" Suit

Subtask 3.4: Content Management

Accomplishments:

- D&D KM-IT web analytics to track usage metrics.
- 1437 D&D technologies
- 1091 registered users
- 997 D&D vendors
- 105 subject matter specialists
- Since last year, the D&D KM-IT has added 523 files (html, pdf and doc)
- Content increased from 7,911 documents on 8/19/2020 to 8,434 8/19/2020



Growth from March 2012 to Aug 2021

<u>Fully searchable resources – Original sources no longer available</u>

- 169 ALARA Center reports archived (Hanford and SRS)
- 231 Innovative Technology Summary Reports archived

Subtask 3.4: Content Management

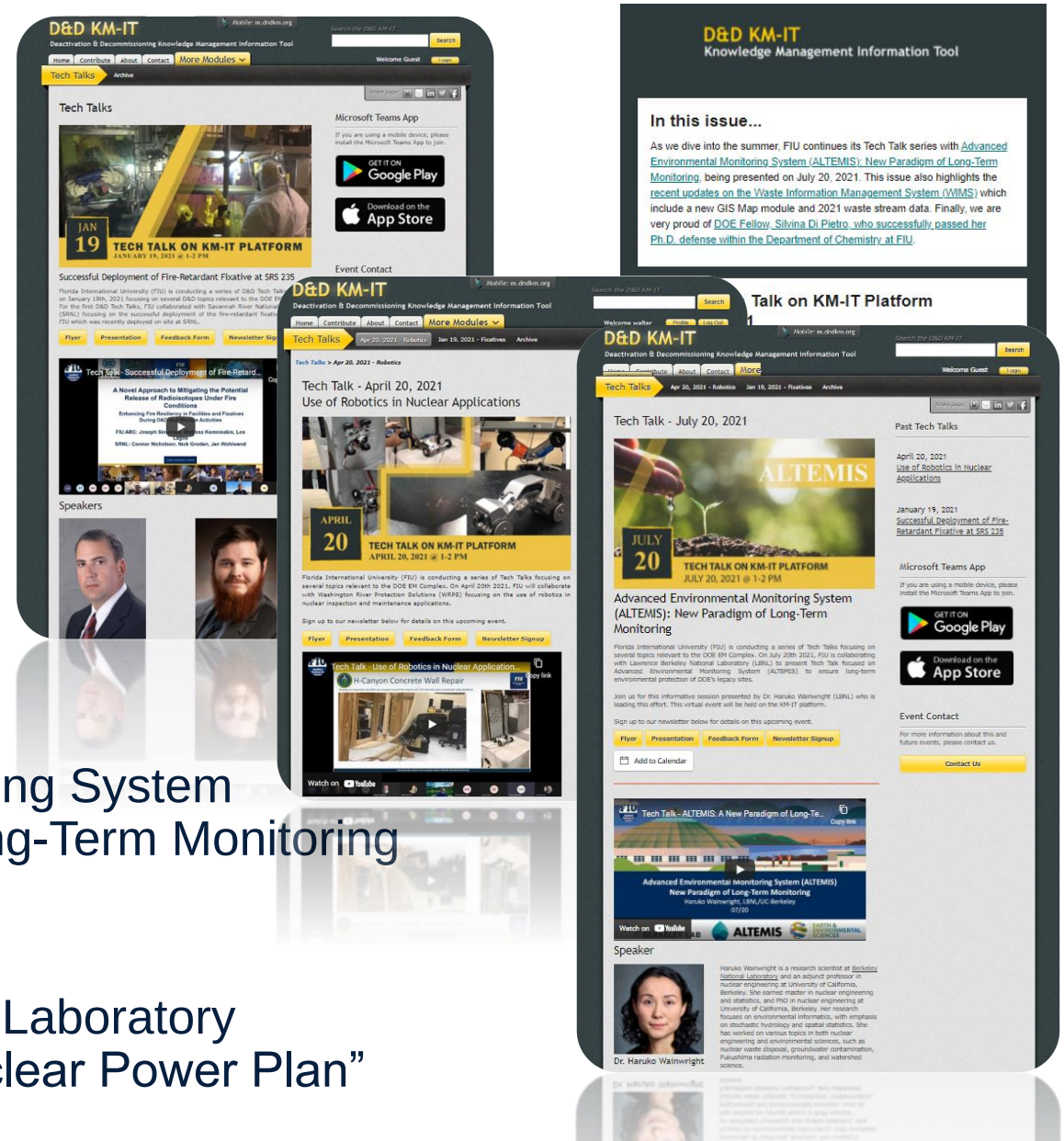
Accomplishments:

- KM-IT visited by every state of the union in the last 12 months
- 9 of the top 10 states showed double digit increased
- Top 10 states include:
  - Illinois – 230%
  - California – 26%
  - Virginia – 20%
  - Texas – 32%
  - Florida – 14%
  - New York – 16%
  - Washington – 28%
  - Pennsylvania – 17%
  - Tennessee – 39%
  - Ohio – 12%

Subtask 3.5: Marketing and Outreach

Accomplishments:

- Reached to the community to increase KM-IT user involvement
- Presented poster at WM2021
- Conducted 3 Tech Talks
  - January 19, 2021
    Successful Deployment of Fire-Retardant Fixative at SRS 235
  - April 20, 2021
    Use of Robotics in Nuclear Applications
  - July 20, 2021
    Advanced Environmental Monitoring System (ALTEMIS): New Paradigm of Long-Term Monitoring
  - Next Tech Talk
    October 19, 2021
    Collaborating with Idaho National Laboratory
    “Industrial Control System for Nuclear Power Plan”



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Subtask 3.6: D&D KM-IT System Administration

Description and Accomplishments:

- D&D KM-IT System Administration is an ongoing task, which involves day-to-day administration of servers that house the KM-IT databases and web applications.
- This task includes updating patches and OS fixes, updating antivirus engines and definitions, updating drivers and assuring that the network is working properly.
- Under this task, hardware upgrades are also conducted (memory, hard drives, video cards, routers, firewall, etc)
- Other administrative task consist of network access control of staff and DOE Fellows (including remote network access)
- This task also support creating development environments for other subtasks, data and application backups

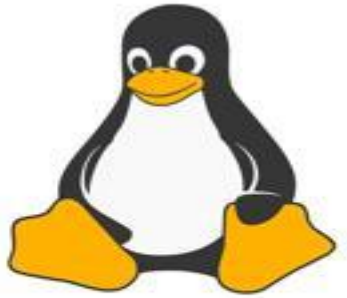
Virtualized Server Architecture

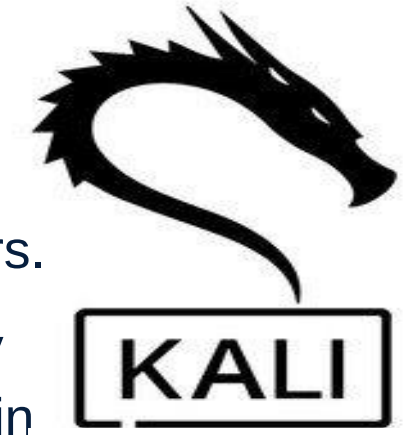
FIU Applied Research Center

Subtask 3.7: Cyber Security of D&D KM-IT Infrastructure

Description and Accomplishments:

- Cyber security of D&D KM-IT involves securing the network infrastructure maintained in the FIU facility.
- Updating of Secure Socket Layer (SSL) for dndkm.org domain
- Maintaining and optimizing firewall rules
- Regularly performed penetration testing on network, KM-IT database and application servers.
- Trained DOE Fellows in DOE-EM Cybersecurity lab on advanced security tools commonly used in the industry.
    - ISO OSI seven-layer network model, hacking tools to simulate cybersecurity attack, Kali Linux which contains a suite of cybersecurity tools and nMap





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Task 3: D&D Knowledge Management Information Tool (KM-IT)

FIU Year 2 Projected Scope

- **Subtask 3.1: KM-IT Tech Talks**
  - Conduct D&D related Tech Talk every quarter on the D&D KM-IT platform.
  - Collaborate with National Laboratories and/or DOE sites to identify and present technical topics of interest to the community.
  - Tech Talks will be performed virtually using an online meeting platform (KM-IT)
  - Promote Tech Talks via newsletters, website, emails and flyers developed by FIU.
- **Subtask 3.2: Content Management**
  - Publishing D&D technologies, vendors, D&D technologies, lessons learned, best practices, D&D news, conferences and other content to KM-IT
  - Perform QA/QC of existing content in the system with assistance of DOE Fellows
- **Subtask 3.3: Marketing and Outreach**
  - Reaching out to sites/national labs to increase KM-IT user involvement
  - Participation at workshops and conferences such as Waste Management and collaboration with the IAEA.
  - Other marketing and outreach to introduce the system to SME who may not be aware of its features and capabilities (newsletters, post cards, factsheets)

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Task 3: D&D Knowledge Management Information Tool (KM-IT)

FIU Year 2 Projected Scope

- **Subtask 3.4: D&D KM-IT System Administration**
  - D&D KM-IT System Administration is an ongoing task which involves day-to-day administration of servers that house the KM-IT databases and web applications.
  - This task includes updating patches and OS fixes, updating antivirus engines and definitions, updating drivers and assuring that the network (firewall, routers and switches) is working properly.
- **Subtask 3.5: Cyber Security of D&D KM-IT Infrastructure**
  - Cyber Security of D&D KM-IT Infrastructure involves securing the network not only by system administration tasks mentioned above, but also by conducting routine cyber security tasks to test the network's vulnerability.
  - This involves coordination between the FIU security team and DOE Fellows who learn cybersecurity skills while assisting staff do penetration testing and other tasks to test the overall security of the system at the application, database and infrastructure levels.

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Task 6

AI for EM Problem Set (D&D):

Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

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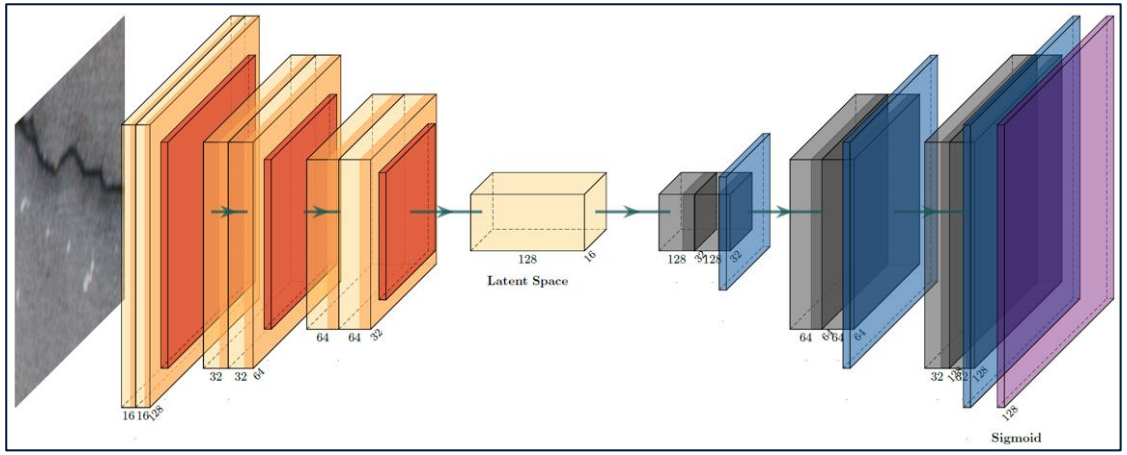
Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

Subtask 6.1	Design & Development of Convolutional AutoEncoder Algorithm to Identify Cracks in D&D Mockup Facility
Subtask 6.2	Use LiDAR technology to scan the walls of the hot cell testbed to establish a baseline model using AI/deep learning technologies
Subtask 6.3	Object Detection (2D Space) (NEW)
Subtask 6.4	Object Detection (3D Space) (NEW)

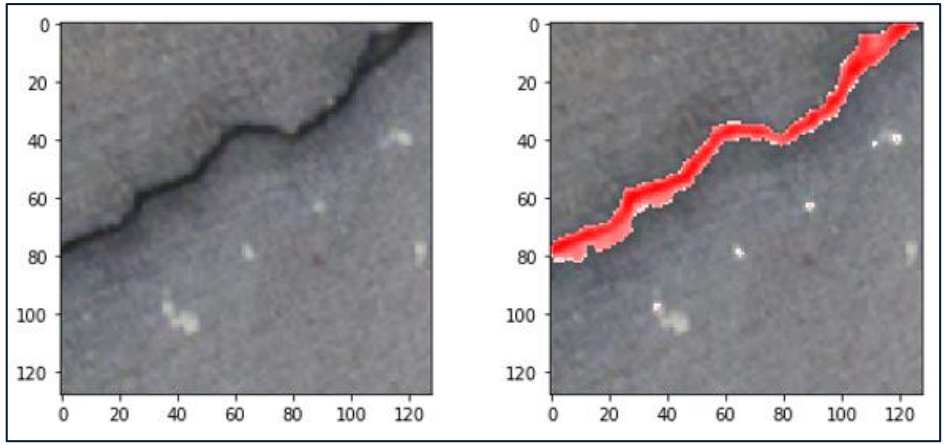
Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

FIU Year 1 Research Highlights:

- Implemented a Convolutional AutoEncoder (CAE) deep learning architecture for the crack detection.
- The CAE was able to learn an encoding representation of the training set successfully.
- This led to high reconstruction rates for images that contained anomalies.
- The reconstruction error was used as the criterion for the anomaly heat map.



Crack Detection and Heat map



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Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

FIU Year 1 Research Highlights:

- Implemented deep learning algorithms for object detection in 2-dimensional space.
- Collected 51 images with different types of cracks and environments from an open-source repository.
- Implemented YOLOv3 (You Only Look Once) algorithm to make detections through the Convolutional Neural Network (CNN).
- Performed knowledge transfer using pre-trained neural network weights for the detection of cracks.
- Optimize the model for a low false-negatives detection rate.
- Implemented deep learning algorithms for object detection in 3 -dimensional space (point clouds, LiDAR data).
- DOE Fellow Roger Boza contributed in a peer review journal titled “A RELAP5-3D/LSTM model for the analysis of drywell cooling fan failure” (Idaho National Laboratory)

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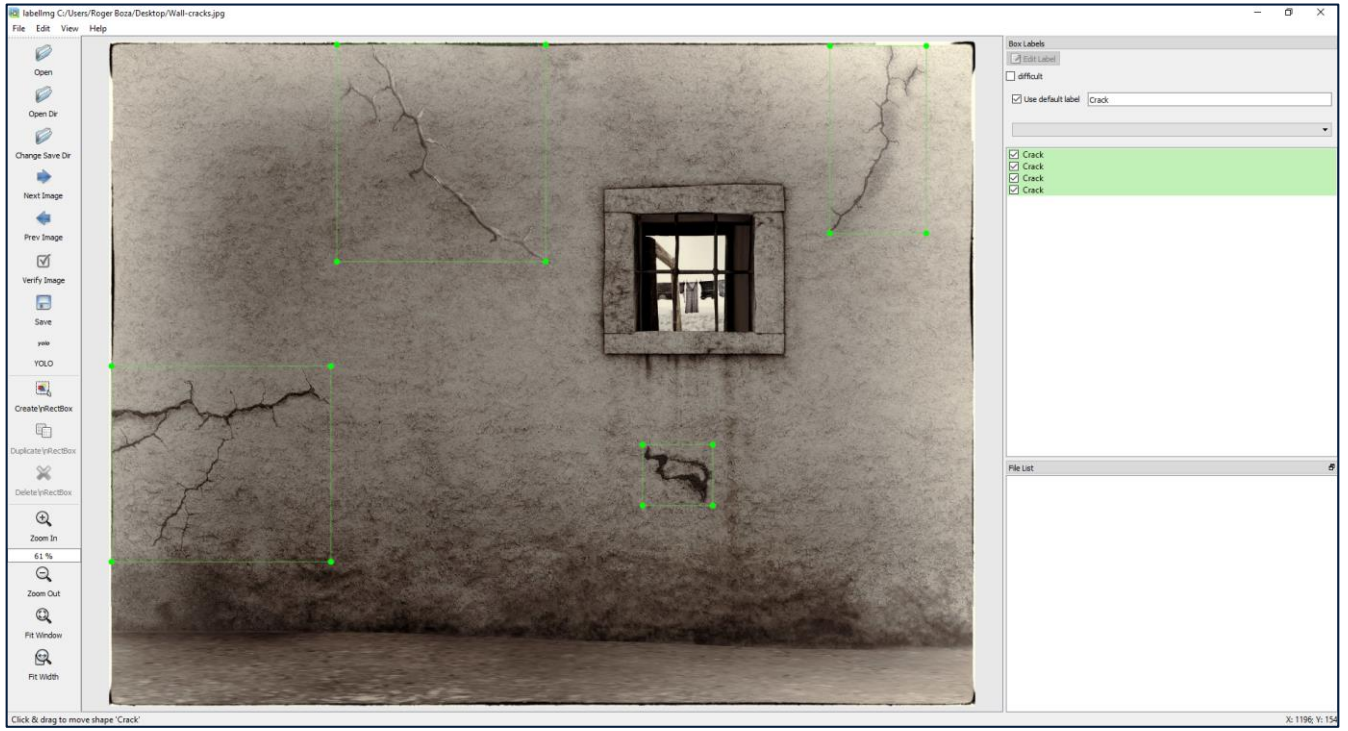
Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

FIU Year 1 Research Highlights:

Sample Images with Cracks:

LabelIMG Annotation Tool



Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

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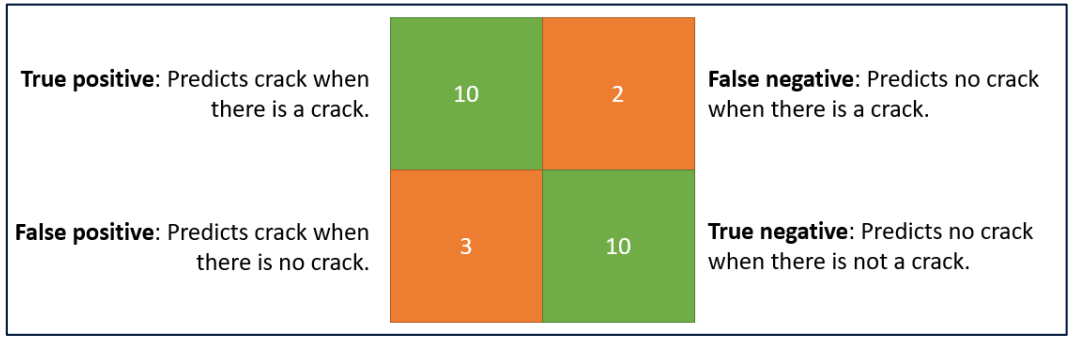
FIU Year 1 Research Highlights:

- Achieved low false negatives.
- Cracks are detected and tightly bounded by the model.

Confusion Matrix



Before Augmentation

After Augmentation

Hyperparameters

Parameter	Values
Batch size (frozen)	4, 8
Epoch count (frozen)	25, 50
Batch size (unfrozen)	4
Epoch count (unfrozen)	15
Confidence score	0.01, 0.1, 0.2
Intersection over union	0.01, 0.1, 0.2

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Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance

FIU Year 2 Projected Scope

Subtask 6.1: Design and development of Machine Learning and Deep Learning algorithms to identify and locate cracks in D&D mockup facility.

- Under the continuation scope of work from Year 1, the FIU team will improve the accuracy and detection rate of the current models that specialize in detection of structural defects such as cracks.
- Some of the models will be tailored for anomaly detection which can detect abnormalities in the datasets of interest. The objective is to identify outliers with high accuracy when compared to classical mathematical models.
- Other models will target the localization problem which focus on locating (spatially) the defects of interest in the data set.

Subtask 6.2: Deploy trained Machine Learning and Deep learning models in iOS devices on site.

- The goal of this task is for the trained models on subtask 6.1 to be deployed in a mobile environment such as smart phones and tablets running the Apple operating system iOS.
- A Graphical User Interface (GUI) will be developed to interact with the neural network backend libraries and run the models.
- Predictions results will be displayed adequality in the GUI on the hand held device.

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Task 7

AI for EM Problem Set (Soil & GW):

Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area (NEW)

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Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

Subtask 7.1	Identification of Data Sources and Datasets from the Soil and Ground Water Repositories
Subtask 7.2	Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples
Subtask 7.3	Machine-Learning and Deep-Learning Model Development for Anomaly Detection

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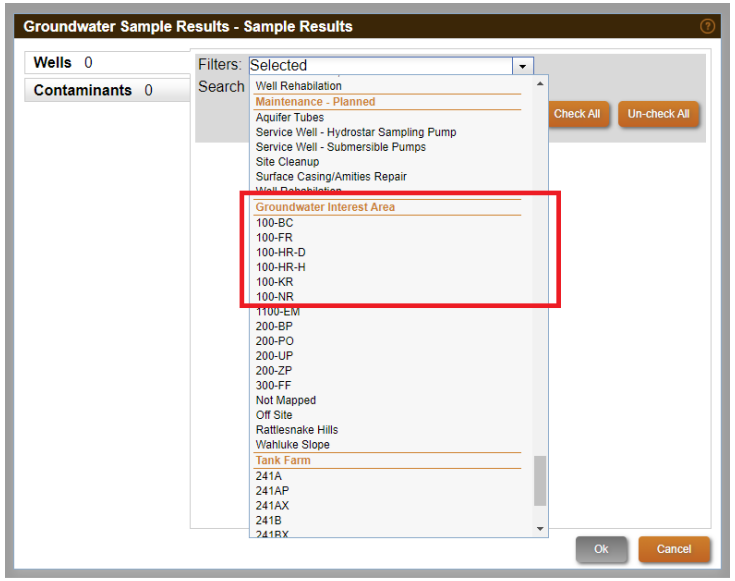
Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

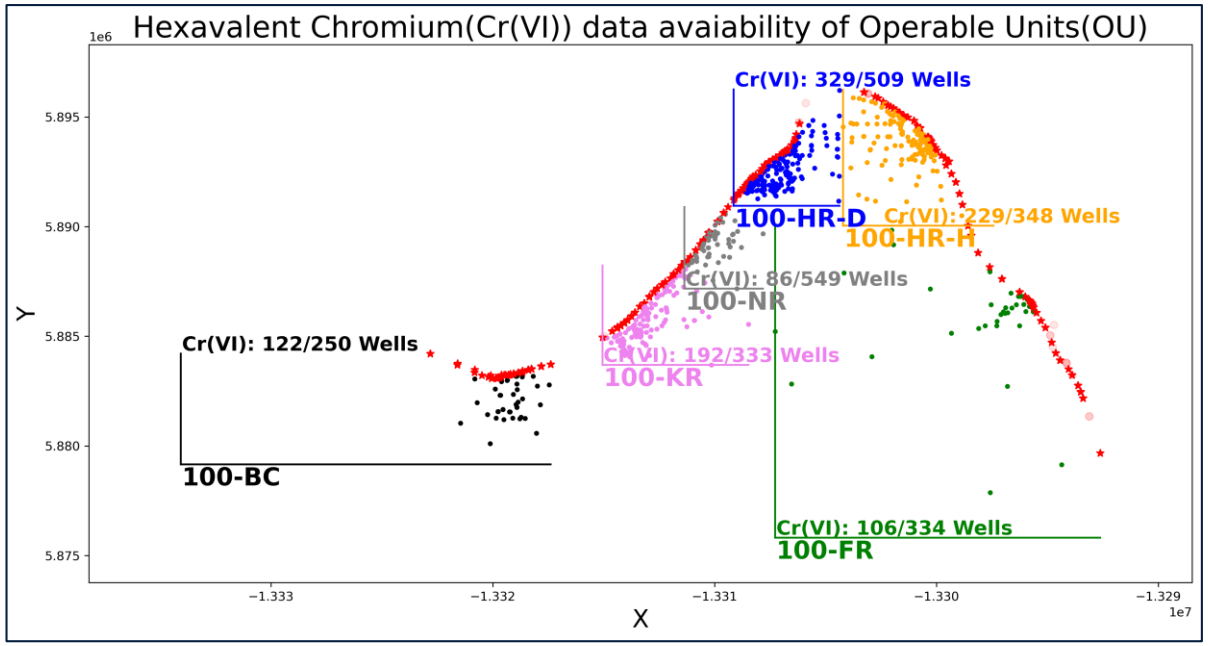
FIU Year 1 Research Highlights:

Identification of Data Sources and Datasets :

- Data source PHOENIX from PNNL was explored and C(VI) datasets were gathered for operable units 100-BC, 100-FR, 100-KR, 100-HRD, 100-HRH and 100-NR. The collected datasets of 100 Areas of the Hanford site contain 2323 wells.
- The collected datasets of 100 Areas of the Hanford site contain 2323 wells. The identified dataset was segregated by well types such as groundwater wells and aquifer tubes, data availability and operable units.

Data source PHOENIX





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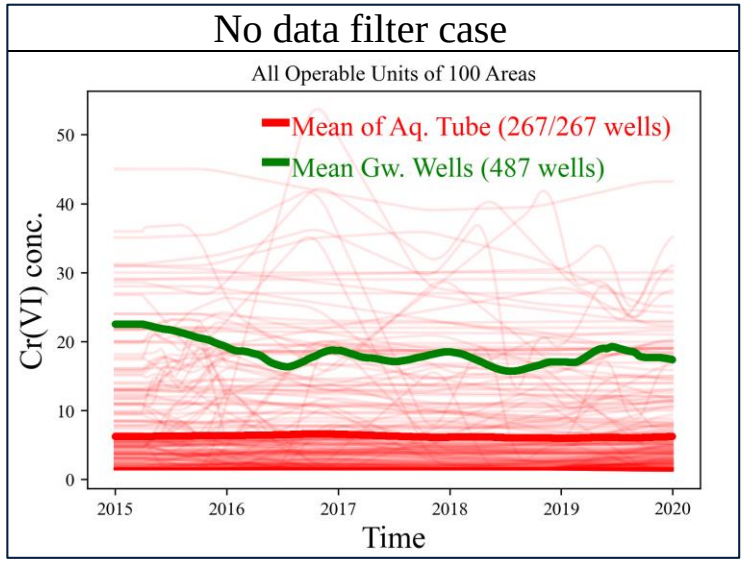
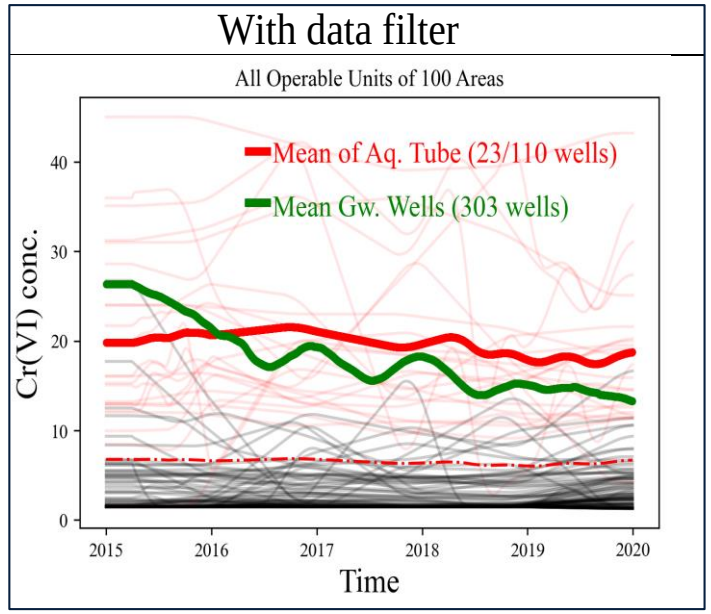
Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

FIU Year 1 Research Highlights:

Data Filtering and Similarity Analysis:

- Two data filters were implemented in the similarity analysis pipeline
- Filter 1: filter wells with at least 1 data points in each year
- Filter 2: filter Aquifer tube with time-series mean >10 µg/L
- The subjective and quantitative analysis reveals some degree of similarity between groundwater and surface water Cr(VI) concentration time series which may not be apparent without data filters.





OU name	AQT (No filter)	GW and AQT similarity measures		AQT (filter 1)	GW and AQT similarity measures		AQT>=10µg/L (filter 1 & 2)	GW and AQT similarity measures	
		Pearson	cosine		Pearson	cosine		Pearson	cosine
100BC	59	-0.0466	0.9923	19	**0.0276**	0.9918	14	**0.2886**	**0.9929**
100KR	55	-0.7135	0.9731	44	**0.1514**	0.9889	4	-0.2636	0.9723
100NR	16	0.5409	0.9990	9	0.3903	0.9947	0	-	-
100HRD	67	0.7879	0.9705	15	0.0127	0.9215	3	**0.2419**	**0.9308**
100HRH	58	0.3221	0.9902	18	-0.0230	0.9808	2	**0.4417**	**0.9847**
100FR	12	0.1916	0.9951	5	**0.2639**	0.9824	0	-	-
ALL 100 Areas	267	0.1323	0.9953	110	**0.6909**	0.9833	23	0.6044	**0.9846**

FIU Applied Research Center

Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

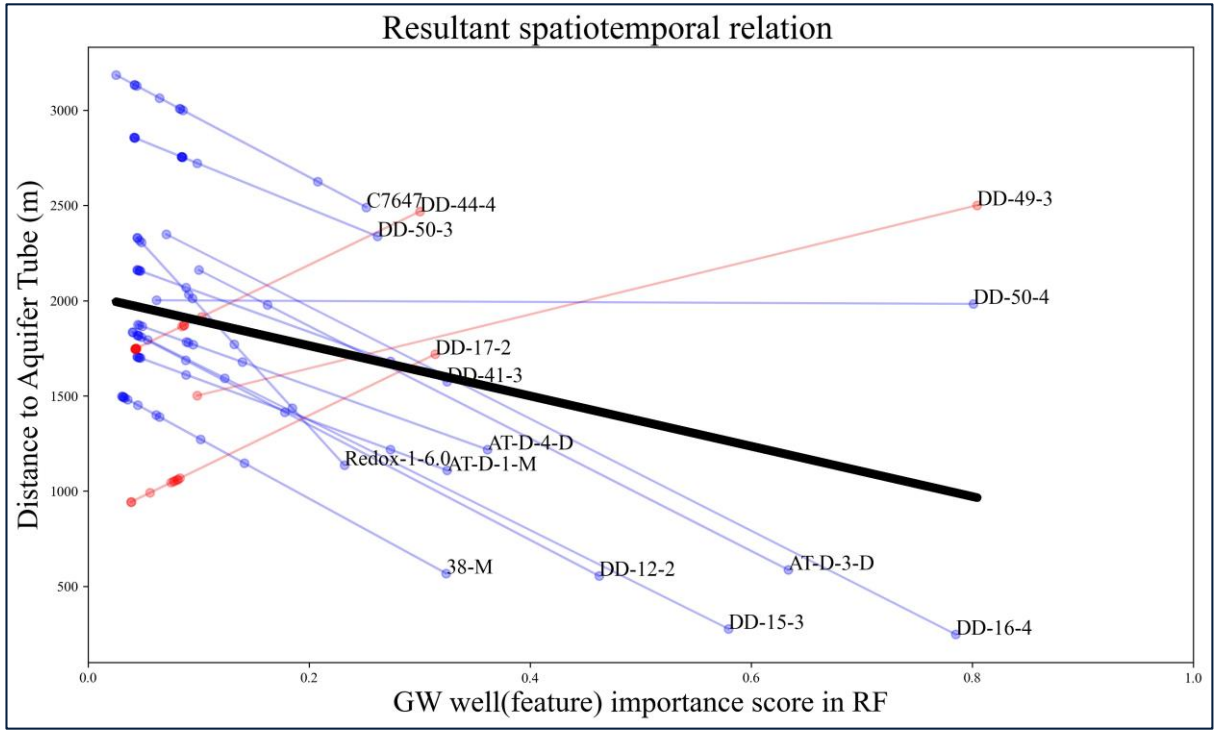
FIU Year 1 Research Highlights:

Spatiotemporal Temporal Relationship Using AI/ML:

- Spatiotemporal relationships between inland monitoring wells and shoreline Hexavalent Chromium (Cr(VI)) concentrations was researched using machine learning (ML) algorithm on the soil and groundwater dataset on the Hanford site 100 Areas.

- Based on all the regression models for individual aquifer tubes, a grand regression line was fitted to get an overall picture of the spatiotemporal relationship in respective operable units.
- For the representative operable unit presented here, an overall decreasing trend in feature score vs distance to target aquifer was observed.

Spatiotemporal Relation



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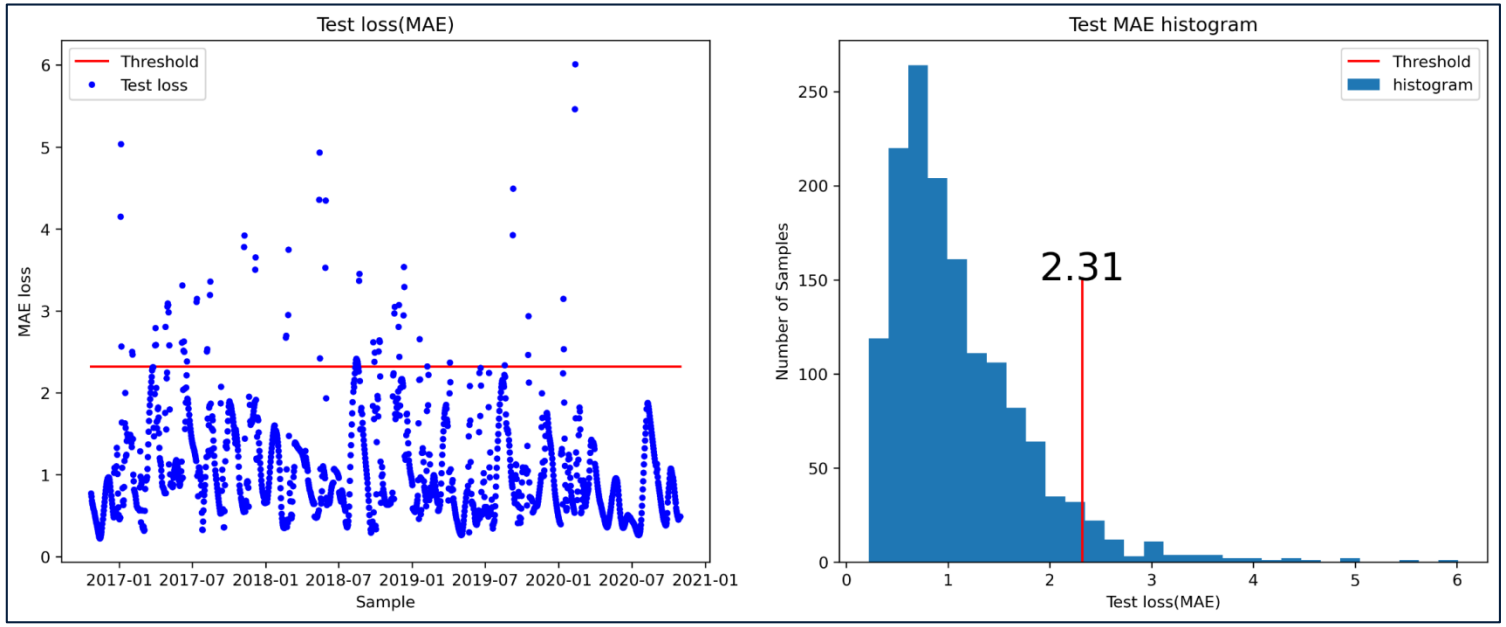
Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

FIU Year 1 Research Highlights:

LSTM Autoencoder/Decoder Based Anomaly Detection

- Developed a deep learning-based anomaly detection system using 100-H Area Cr (IV) concentration dataset.
- Based on the test MAE distribution and the MAE threshold selected in the training phase, certain data points are marked as anomalous data points by the anomaly detection system.



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Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

FIU Year 2 Projected Scope

Subtask 7.1: Groundwater and surface water spatiotemporal relationship identification:

- Machine learning and deep learning-based exploratory research will be conducted to explore the relationship between the groundwater and surface water hexavalent chromium (Cr(VI)) concentration.
- This effort expect to surface the presence of any spatiotemporal relationship which might not be apparent in the subtle temporal and spatial features of the Cr(VI) dataset.

Subtask 7.2: Cr(VI) spatiotemporal relation influencing variables exploration:

- Research will be conducted to find and incorporate Cr(VI) dynamics influencing variables dataset in the spatiotemporal relationship exploration machine learning models.
- This effort expects to fine-tune the quantification of the spatiotemporal relationship and may enhance the causality of the relationship.

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Task 8

AI for EM Problem Set (Soil & GW):

Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

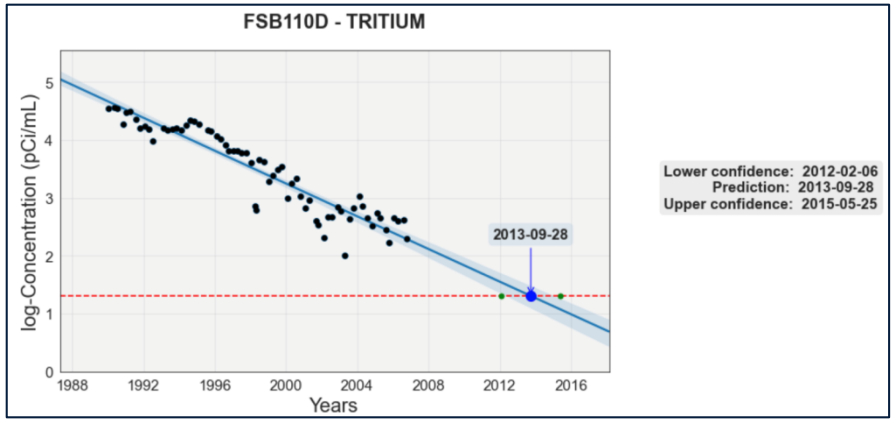
Subtask 8.1	Exploratory Data Analysis
Subtask 8.2	Identify the Master/Proxy Variables
Subtask 8.3	Machine Learning Model Development & Optimization for Sensor Placement in Groundwater Wells

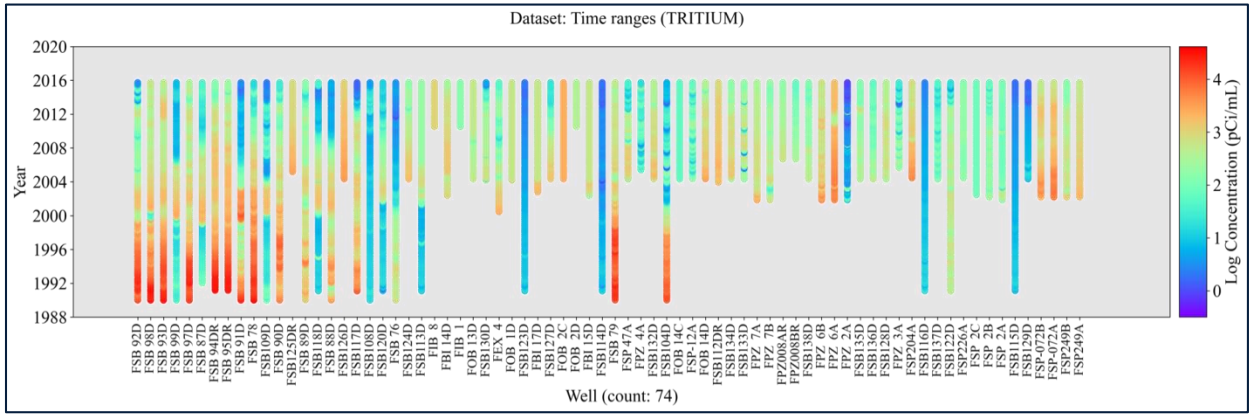
FIU Applied Research Center

Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

FIU Year 1 Research Highlights:

- Developed data exploration tools to understand the spatial and temporal distribution of the F-Area dataset.
- Performed Trend analysis, Correlation analysis, and implemented Preprocessing / Transformation functions (interpolation etc.)
- Developed a Python package for Long-term Environmental Monitoring - pyLEnM
- Developed insightful visualizations for spatial estimation
- DOE Fellow Aurelien Meray won graduate poster competition at WM2021 with his poster titled “pyLEnM: Machine Learning and Analytics Toolkit for Long-term Water Quality Monitoring Using a Remote Sensing Network”





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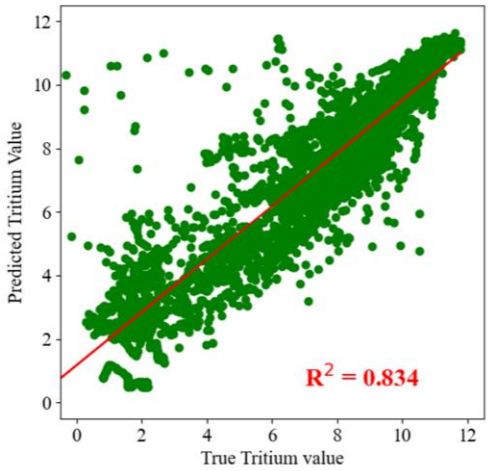
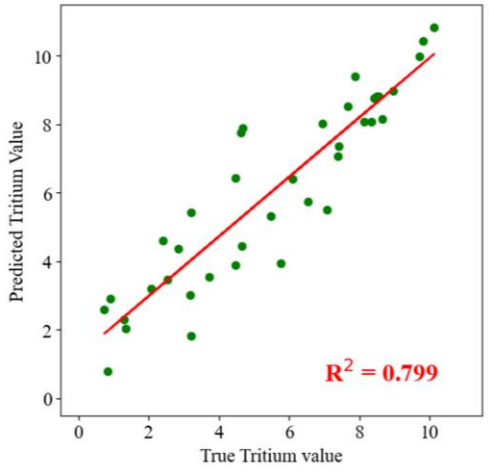
Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

FIU Year 1 Research Highlights:

- Explored proxy variable relationships.
- Observed a consistent correlation between Specific Conductance (SC) and Tritium (R^2 above 0.8).
- Spatially estimated Tritium by using the in-situ parameter SC.

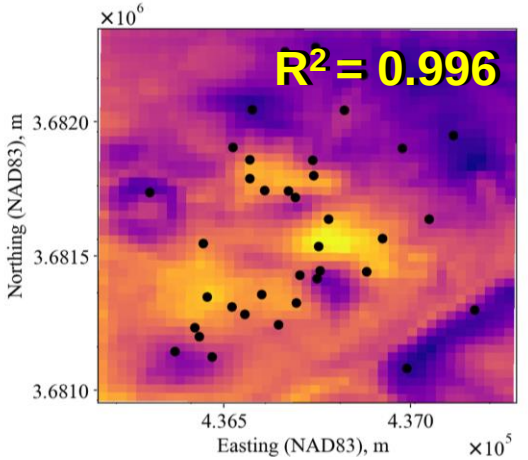


Test set (20% of data) prediction

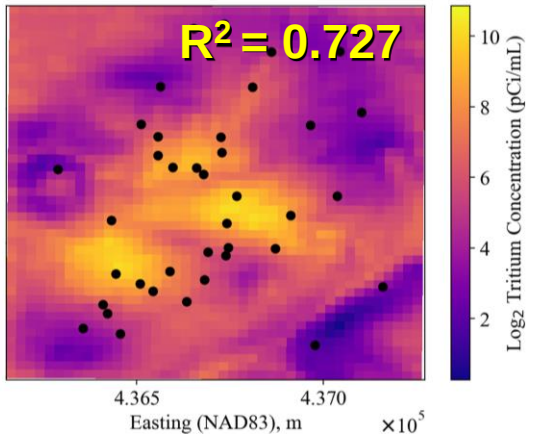


Average $\log_2$ 2015 prediction

Average $\log_2$ 2015 **True** Tritium Estimation (Lasso Regression)



Average $\log_2$ 2015 SC~Tritium **Prediction** Estimation (Lasso Regression)

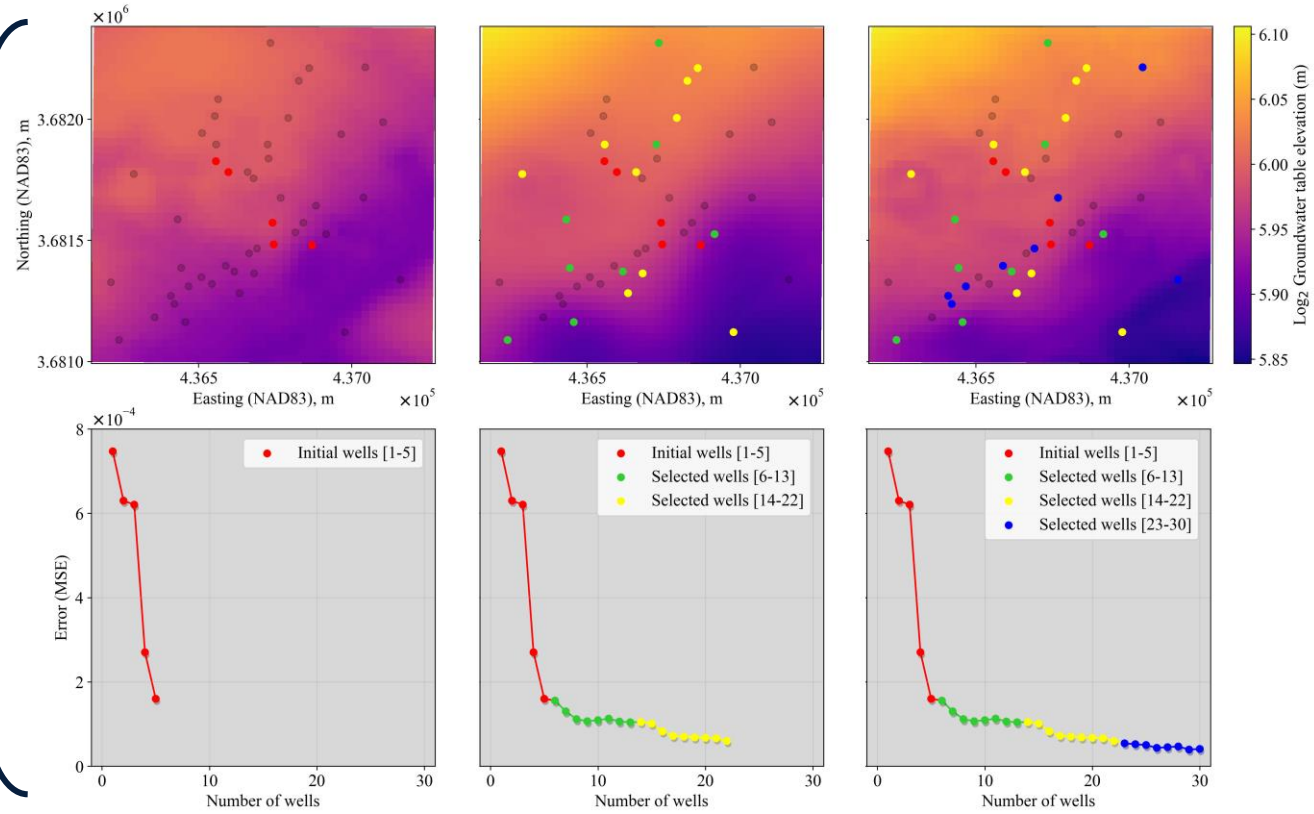


Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

FIU Year 1 Research Highlights:

- The main idea of the optimization is to minimize the overall error (MSE) between the high-quality reference field and the spatial interpolated map with the 15-20 subset wells.

Water Table optimization (single timestep)



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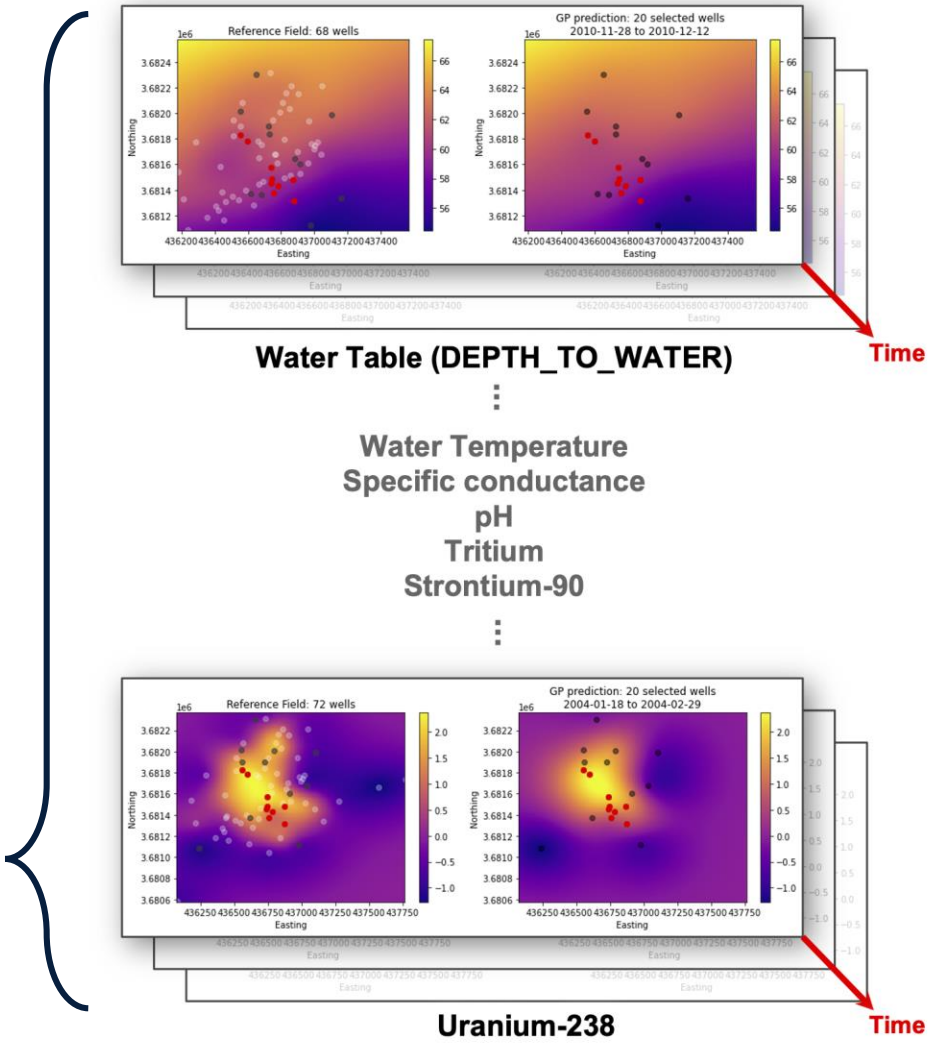
Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

FIU Year 1 Research Highlights:

- Majority voting approach to capture multiple parameters (8 analytes) and multiple time steps.
- **Results:**
  - 'FSB 97D', 'FSB 95DR', 'FSB 78', 'FSB126D', 'FSB130D', 'FSB 79', 'FEX 4', 'FSB 99D', 'FSB 91D', 'FSB118D', 'FSB124D', 'FSB128D', 'FSB135D', 'FSB132D', 'FSB138D'
  - ALTEMIS Team chose:
    - 13/15 within top 20
    - 2/15 within top 22

Multi-analyte optimization
(Multiple timesteps)



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Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

FIU Year 2 Projected Scope

Subtask 8.1: AI System interface:

- The AI system interface will be developed in order to ingest sensor data for long-term storage and provide analysis. The data analysis will include informative statistics and visualizations.

Subtask 8.2: AI development for QA/QC and predictive analysis:

- Machine learning based models will be used to achieve pattern identification, anomaly detection and prediction of the sensed groundwater well variables. The developed algorithms/solutions will be produced for future integration with the main system interface.

DOE EM IT/AI Deployment Roadmap

	Technology	2020	2021	2022	2023	2024
HQ All Sites	WIMS	Site Deployment				
HQ, SRNL, ANL, PNNL	KM-IT	Site Deployment				
HQ SRNL	AI D & D	Algorithm Development	AI System Development	In-house Deployment	Site Deployment	
PNNL	AI Soil & Ground Water	Data Exploration /Visualization	Algorithm Development	AI System Development & Integration	In-house Deployment	Site Deployment
LBNL, SRNL	AI Soil & Ground Water	Data Exploration & Visualization	Algorithm Development	AI System Development & Integration	In-house Deployment	Site Deployment

Thank You. Questions?