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Arcana: THE NATIONAL NUCLEAR MATERIALS AND SIGNATURES DATABASE

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ABSTRACT

The National Nuclear Material Archive (NNMA) collects, characterizes, and preserves nuclear material samples of US origin. The NNMA function is to support attribution of materials discovered out of regulatory control. The program includes a physical archive of relevant materials; a robust materials characterization program; compilation of information about the samples in a database and data repository; and an assessment and query response process including statistical tools and subject matter expertise. The NNMA sample characterization work will produce a large quantity analytical data which must be captured and stored in such a way as to make it appropriately protected, accessible to stakeholders, and available for use for assessments and query response. Another important aspect of the NNMA dataset will be its richness and usefulness for identifying nuclear forensic signatures for archive materials. In support of this goal, we are currently developing Arcana: The National Nuclear Materials and Signatures Database. Arcana is a custom relational database specifically designed for efficient upload, storage, retrieval, and queries of NNMA data. Arcana employs a relational database structure implemented with the Oracle Application Express (APEX) development platform, and includes a web-browser interface for database administration and queries. Arcana is designed to facilitate streamlined data upload from multiple NNMA sites, as well as a straightforward query process. As in all relational databases, data are stored in a series of tables linked by a common data field.
Central to the structure are two principal tables: the Sample Table and the Results Table. These tables are supported by a number of supplementary tables including metadata about the sample, material, process history, facility information and analytical details including QA/QC information, units, uncertainties, and a link to a source document archive. The flexible structure can accommodate detailed processing and signature information about each sample, as well as associations between samples representing similar processes. Finally, Arcana will incorporate a subject matter expertise capability that is able to provide a timely response to queries from across the NNMA stakeholder community, and help to evaluate the NNMA data in Arcana to guide the NNMA analytical program. The NNMA is led and managed by the Office of Nuclear Forensics, located in the Counterterrorism and Counterproliferation Office of the National Nuclear Security Administration.

INTRODUCTION

Operated by the National Nuclear Security Administration Office of Nuclear Forensics (NA-83), The National Nuclear Materials Archive (NNMA) program collects, characterizes, and preserves nuclear material specimens to support material provenance assessments. When nuclear material is found outside of regulatory control, the NNMA will help to determine if the material is consistent with materials that originate with the U.S. Department of Energy (DOE). Lawrence Livermore National Laboratory (LLNL) is one of four analytical laboratories within the U.S. national laboratory system that perform material analyses for the NNMA.

In addition to performing materials characterization work supporting nuclear forensics and the development of the NNMA, LLNL also has significant experience developing and building data management systems supporting safeguards verification and nuclear forensics programs. Based on our role as one of four NNMA supporting laboratories, and our experience in developing and implementing database systems for other programs, LLNL was tasked with developing a data management structure for the NNMA.

Here we present an overview of the development, architecture, and details of Arcana: The National Nuclear Materials and Signatures Database.

OVERVIEW OF ARCANA

The NNMA sample characterization work will produce a large quantity analytical data which must be captured and stored in such a way as to make it appropriately protected, accessible to stakeholders, and available for use for assessments and query response. Arcana: The National Nuclear Materials and Signatures Database is designed to capture the analytical data produced by the NNMA laboratories as well as supporting contextual information for each sample analyzed as part of the NNMA effort. Arcana is a purpose-built relational database designed to facilitate upload, storage, and retrieval of NNMA data. Arcana is also designed to leverage the richness and usefulness of NNMA data for identifying nuclear forensic signatures for archive materials.

Figure 1 Arcana logo

Within the Arcana structure, each sample is comprehensively documented and includes elemental and isotopic compositions, morphological and radiochemical data, and supporting analytical metadata, such as sampling processes, analytical procedures, and quality control. Supporting contextual information including details about the provenance of each material as well area also captured within the Arcana database.

ARCHITECTURE AND TECHNICAL DETAILS

The Arcana database structure is based on the relational database model of the National Nuclear Security Administration's Office of Nuclear Compliance Verification (NA-243)-sponsored Uranium Sourcing Database. Oracle SQL Developer and the Oracle Application Express (APEX) development environment are used to build, update, and administer the database. Oracle APEX is a low-code development platform that enables the development of scalable, secure, enterprise apps, and has proved to be a reliable platform for developing data-driven visualizations and intuitive forms and interfaces. Arcana can be accessed through a secure web interface, and data can be uploaded through either a web form or through direct upload of .csv templates.

Tables are the essential elements of a relational database, they are the database objects that hold data. The Arcana database consists of two primary tables (The Samples Table and the Results Table) which are supported by an additional 15 tables of supporting information. The inter-connectivity of these tables is depicted in Figures 2 and 3 with tables linked via their respective primary keys. A description of key tables is included in Table 1.

Table 1 Brief table content information for key tables

Table Name	Table Description
SAMPLE	Lists all samples, where SAMPLE_ID uniquely describes each row. Contains foreign keys linking to other tables including: Provider, Site, Material, Process, Nom_Package and Analysis Lab
RESULT	Unique result values where RESULT_ID uniquely describes each row. Contains foreign keys linking to other tables including: Unit, Technique, Sample, Instrument, Batch, and Parameter
ANALYSIS_LAB	Lists all labs doing NNMA analytical work, where Analysis_Lab_ID uniquely describes each row.
BATCH	Lists unique Batch identities, with BATCH_ID uniquely describing each row. A Batch identity is formed as a concatenation of the analytical reference date and technique; e.g. "2021-04-17 UID"
DEMAND_TABLE	Lists all Demand Tables for the NNMA including supporting contextual information
INSTRUMENT	Lists all instruments used for NNMA analyses, including unique instrument IDs for each relevant analytical instrument
LOCATION	Lists all locations where NNMA samples are stored or analyzed
MATERIAL	Lists DOE Nuclear Material Control and Accountability Types and details
NOM_PACKAGE	Lists nomination packages with which samples are associated
PARAMETER	lists all analytical parameters (e.g. U assay, Fe concentration, etc.)
SITE	Lists NNMA sample provenances
STANDARD	Lists all standard reference materials used for the NNMA program
TECHNIQUE	Lists all analytical techniques used for the NNMA program; e.g. Pu isotope dilution, Trace Elemental Analysis, etc.
UNIT	Lists standardized units for reporting NNMA data

The Sample table captures metadata about each sample as well as key information about the storage location, nomination package, and other relevant supporting contextual information (Figure 2).

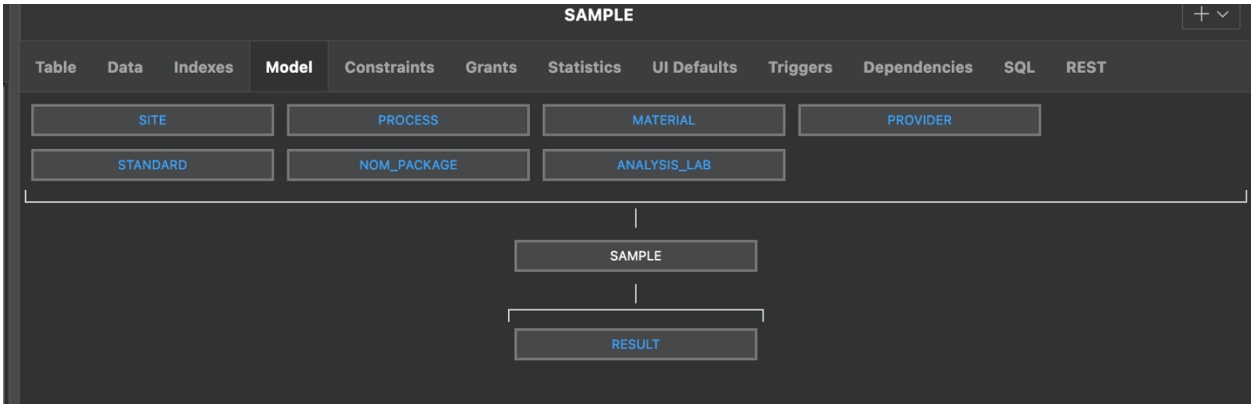

Figure 2. Sample table and supporting tables for the Arcana database. Supporting tables include Site, Process, Material, Provider, Standard, Nom(ination)_Package, and Analysis_Lab. The Sample table tracks both NNMA and quality control (QC) samples, and is linked to the Result table through the Sample ID foreign key.

The Results table captures all results including those in numeric, non-numeric, and date-formatted results, as well as information about linked quality control samples. The Results table is supported by information about analytical techniques, instruments, laboratory, and information about associated quality control data (Figure 3).

Figure 3 The Result table and supporting tables for the Arcana database. Supporting tables include Unit, Technique, Parameter, Instrument, and Batch. The Results table tracks results from both NNMA and quality control (QC) samples, and is linked to the sample table through the Sample ID foreign key.

In order to maintain allow long-term tracking of quality control results over the life of the NNMA project, Arcana has been designed to capture quality control results and maintain their association with specific samples and aliquots. This is achieved by assigning each aliquot of NNMA material and each associated set of quality control samples to a specific batch linked on the basis of a unique Batch ID. Batch IDs are based on the reference date for the analysis as well as by the analytical technique. This approach will allow for long-term QC control charting and also will maintain the association between specific samples and analytical campaigns with the appropriate quality control data.

NNMA data stakeholders will be able to access the data through various *database views*, queries, and purpose-built visualization applications. A *database view* is a subset of a database based on a query that runs on one or more database tables. We have created preliminary views for Arcana including dynamic views that allow stakeholders to search for specific material characteristics, sample types or other data of interest (Figure 4). Development of views and visualization applications will continue as the Arcana database expands and responds to stakeholder requirements.

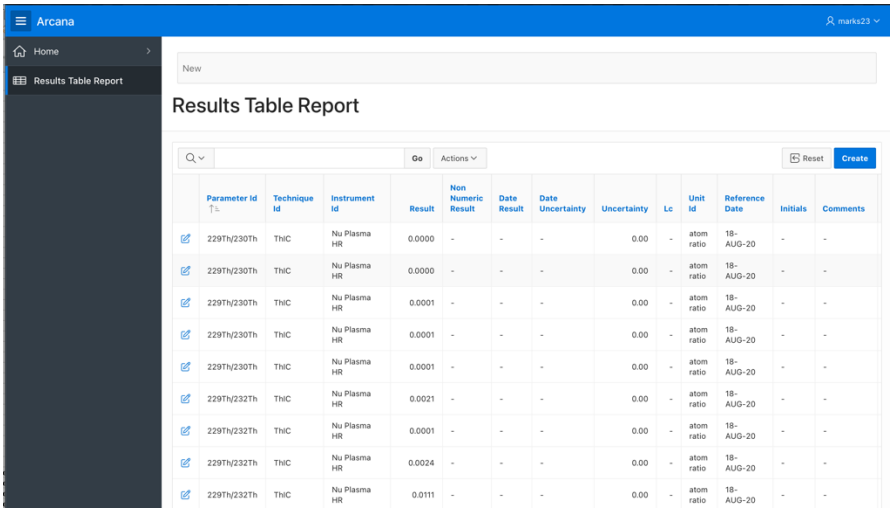

Figure 4 Example of dynamic view of Results from Arcana.

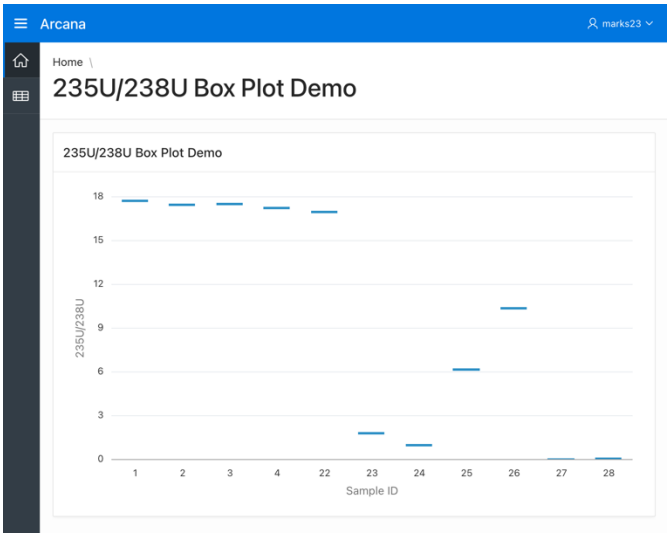

Figure 5 Example Dynamic Box Plot Demonstration App for Arcana showing $^{235}U/^{238}U$ ratios for selected samples.

Arcana is also designed to manage the many images of NNMA materials, ranging from photographs to NanoSIMS ion maps to SEM photomicrographs. As Arcana is developed and grows, it will be able to store and display linked image files in a separate Images table that is currently under development.

PROGRAMATIC MILESTONES

The Arcana database was conceived in the spring and summer of 2020, and was initially funded in the fall of 2020. In this first full year of funding for the Arcana project, we have followed a fairly standard waterfall process for development of the data management system (Figure 6). We began by Establishing Requirements for the database, consulting with stakeholders, contributors, and analysts. This included consultation with stakeholders about what they want from the system, and from these interactions we were able to articulate a statement of requirements. Part of this work included identifying an RDMS software package that we could use for Arcana, that would be compatable across all relevant computing environments.

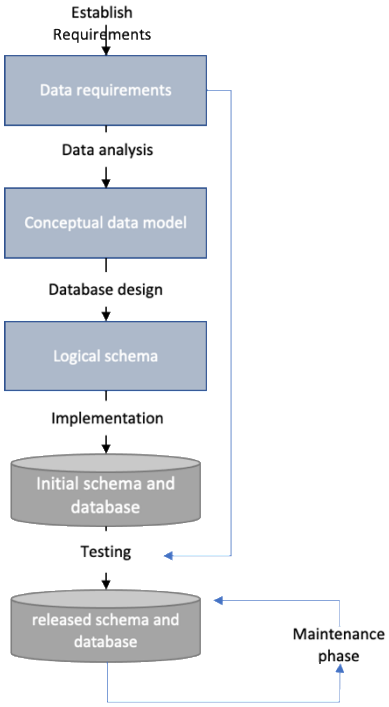

Figure 6 Waterfall model of activities and outputs for database development

This was followed by a Data Analysis phase in which we created a conceptual data model for NNMA data, first using surrogate data and later using real NNMA data. Once actual NNMA data had been produced for the first set of samples at LLNL, we were able to refine our data model and design a database system that would accommodate the NNMA data.

Based on our analysis we specified a logical schema that specified the relational model of Arcana. In order to create a database with the desirable properties of completeness, integrity, flexibility, efficiency and usability, we applied our conceptual data model and embarked on the iterative process of defining the desired tables and attributes and then flexing the model to identify areas for improvement.

In the spring of 2021 we began the implementation phase and had a working initial schema and prototype database populated with surrogate data available for testing and improvement. Throughout the spring and summer of 2021 we have created updates and improvements and begun populating Arcana with NNMA data as it is produced. At the same time, we have created (and flexed) data templates for the NNMA laboratories. At this time Arcana is currently accepting data from NNMA laboratories and we are working to improve the user experience and develop apps that will support signatures research on NNMA data.

Throughout this first year of Arcana development, the Arcana team has also supported the creation of several nuclear materials signatures data analytics products. These include work on U materials produced by DOE, non-power reactor fuels, and a statistically grounded comparative assessment of baseline v.s. full forensics analysis for the NNMA program.

CONCLUSIONS

The National Nuclear Materials Archive (NNMA) program collects, characterizes, and preserves nuclear material specimens to assess whether nuclear material found outside of regulatory control is consistent with materials that originate with the U.S. Department of Energy (DOE).

Lawrence Livermore National Laboratory (LLNL) has developed the data management system for the NNMA. Arcana: The National Nuclear Materials and Signatures Database will be the data storage solution and resource for the NNMA and future nuclear materials signatures research. Over the past year, despite restrictions imposed by the COVID-19 pandemic, LLNL developed, built, and began populating Arcana, while, at the same time, undertaking several data analytics tasks related to nuclear materials signatures development. The achievements over this first year of Arcana development have been substantial, and we look forward to continued growth and buildout of user-oriented features and nuclear materials signatures research possibilities as the program continues to grow.

Acknowledgements

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