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Integration of Data Systems and Technology Improves Research and Collaboration for a Superfund Research Center

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Abstract

Large collaborative centers are a common model for accomplishing integrated environmental health research. These centers often include various types of scientific domains (e.g., chemistry, biology, bioinformatics) that are integrated to solve some of the nation's key economic or public health concerns. The Superfund Research Center (SRP) at Oregon State University (OSU) is one such center established in 2008 to study the emerging health risks of polycyclic aromatic hydrocarbons while using new technologies both in the field and laboratory. With outside collaboration at remote institutions, success for the center as a whole depends on the ability to effectively integrate data across all research projects and support cores. Therefore, the OSU SRP center developed a system that integrates environmental monitoring data with analytical chemistry data and downstream bioinformatics and statistics to enable complete "source-to-outcome" data modeling and information management. This article describes the development of this integrated information management system that includes commercial software for operational laboratory management and sample management in addition to open-source custom-built software for bioinformatics and experimental data management.

Keywords

informatics and software, system integration, Laboratory Information Management Systems (LIMS)

Introduction

Large scientific research centers can be effective in using many facets of science to tackle a key problem, although integration between these scientific modalities is needed. In the age of scientific computing, integration usually happens at the data level, and due to the volume and heterogeneity of data, this can be a daunting task. Add in the complexities of collaborating across organizations, and a real need for data integration and collaborative solutions develops to make these science centers efficient and prolific.

There are many software systems available that manage laboratory data such as Laboratory Information Management Systems (LIMS), Electronic Laboratory Notebooks (ELN), sample management solutions, and hybrids attempting to coordinate all three. In addition, most laboratories have instruments that are controlled by computers that produce data in various formats. Open-source and commercial solutions are often tailored for a particular scientific modality, although some general solutions do exist. There are two key problems with these solutions: They do not work well together due to proprietary data formats, and they lack interconnectivity to other systems short of reporting entire result sets.

Many vendors attempt to sell end-to-end solutions, but these are costly to implement in time, money, and infrastructure. Most commercial systems are developed for large service and production laboratories that perform fully developed and validated assays with defined parameters, quality control measures, and data quality objectives as

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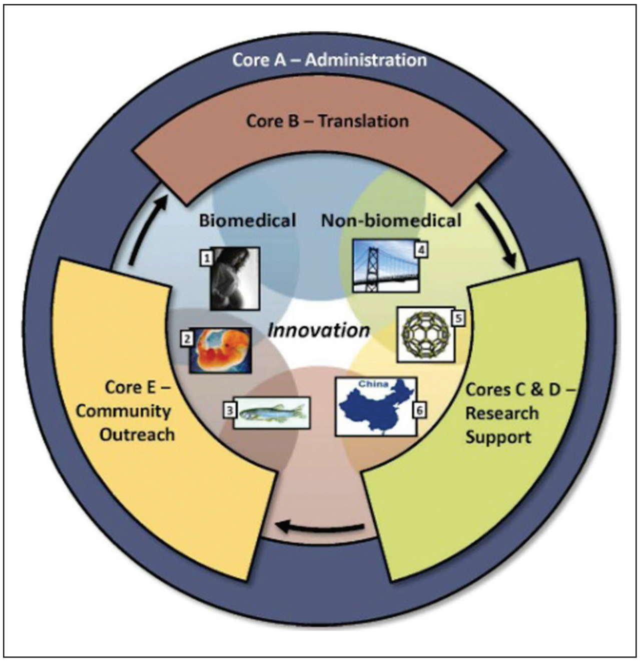

Figure 1. Organization of the Oregon State University (OSU) Superfund Research Program Center. The research support cores are (C) Bioinformatics and (D) Chemistry. Project 1 and Core C reside at Pacific Northwest National Laboratory (PNNL); all other projects and cores reside entirely or in part at OSU with collaborators in many parts of the nation and world.

seen in labs with Quality Assurance Program Plans (QAPPs). In most academic research laboratories, however, the parameters will perpetually change as personnel turn over, different assays are performed, and the observational outcome is reported. In recent years, ELN implementations are adapting better than LIMS to the research and development markets[1] but are not always a complete solution. The data still need to be managed and shared while standardized protocols are in development. Further challenges exist when bioinformatics are being used to help define experimental parameters, and data need to be shared before study results are concluded. In these many areas of research, there is a need for both production-level laboratory management and research-level data management.

The Superfund Research Program (SRP) Center at Oregon State University (OSU) (www.oregonstate.edu/superfund) established by the National Institute of Environmental Health Sciences (NIEHS), outlined in **Figure 1**, uses a high level of integration and collaboration to research the environmental and human health impacts of polycyclic aromatic hydrocarbons. This diagram shows five support cores that support six research projects. These collaborative research projects involve biomedical and non-biomedical disciplines, including environmental and analytical chemistry, molecular biology, bioinformatics, and toxicology. This article focuses on the efforts of the research support cores to develop an extensible and reliable computing infrastructure to improve scientific data management and collaboration in the center. The research support cores include the bioinformatics core housed at Pacific Northwest National Laboratory (PNNL) in Richland, Washington, and the chemistry core housed at OSU in Corvallis, Oregon. The chemistry core was established to provide laboratory technical assistance, analytical services, and a shared standard reference material repository to the center. The bioinformatics core provides study design review, as well as statistical and computational analysis, to all projects. Geographic separation between these two facilities and the research efforts at the project level was an additional challenge to this center.

Determining System Requirements

The keys to determining the right system requirements are to engage the right people early in the process and to think both short and long term. If representation from all aspects of the research does not exist, the possibility of developing short-sighted solutions that lack scalability or do not meet all the needs of the center manifests. For example, software systems engineers often attempt to determine requirements based on the need to store data but miss the needs of collaborating or reporting data. In the early stage of the establishment of the SRP center, representatives of the various scientific and computational areas met to determine requirements. These requirements were then used to define a set of short-term and long-term data management goals for the center. The representatives included lead research scientists, bioinformaticists, software engineers, and lab managers. It was determined that the center was going to need a data management system that would aid in laboratory workflow and regulatory compliance as well as capture and report research data across the center. A mockup of sample processing and data workflow was created to identify the key operators throughout a collaboration shown in **Figure 2**. The workflow helped identify who would be handling the samples and inputting data, as well as the types of data being captured and reported at any given stage. The foundation of the workflow was the sample receipt and laboratory analysis performed by the chemistry core facility. These data are then used to generate new research and supply the bioinformatics core with the required information to create statistical workflows and data visualizations.

Existing software developed at PNNL was identified that would benefit the workflow for reporting data across the center. The Experimental Data Management System (EDMS) captures data tied to laboratory experiments and provides collaborative access to experimental design metadata. Building on the workflow concept, a LIMS or ELN system could be the center of the data production pipeline used by the chemistry core facility. The data collected in a LIMS or ELN could then feed other systems involved and could be collaboratively connected to the rest of the center through the EDMS.

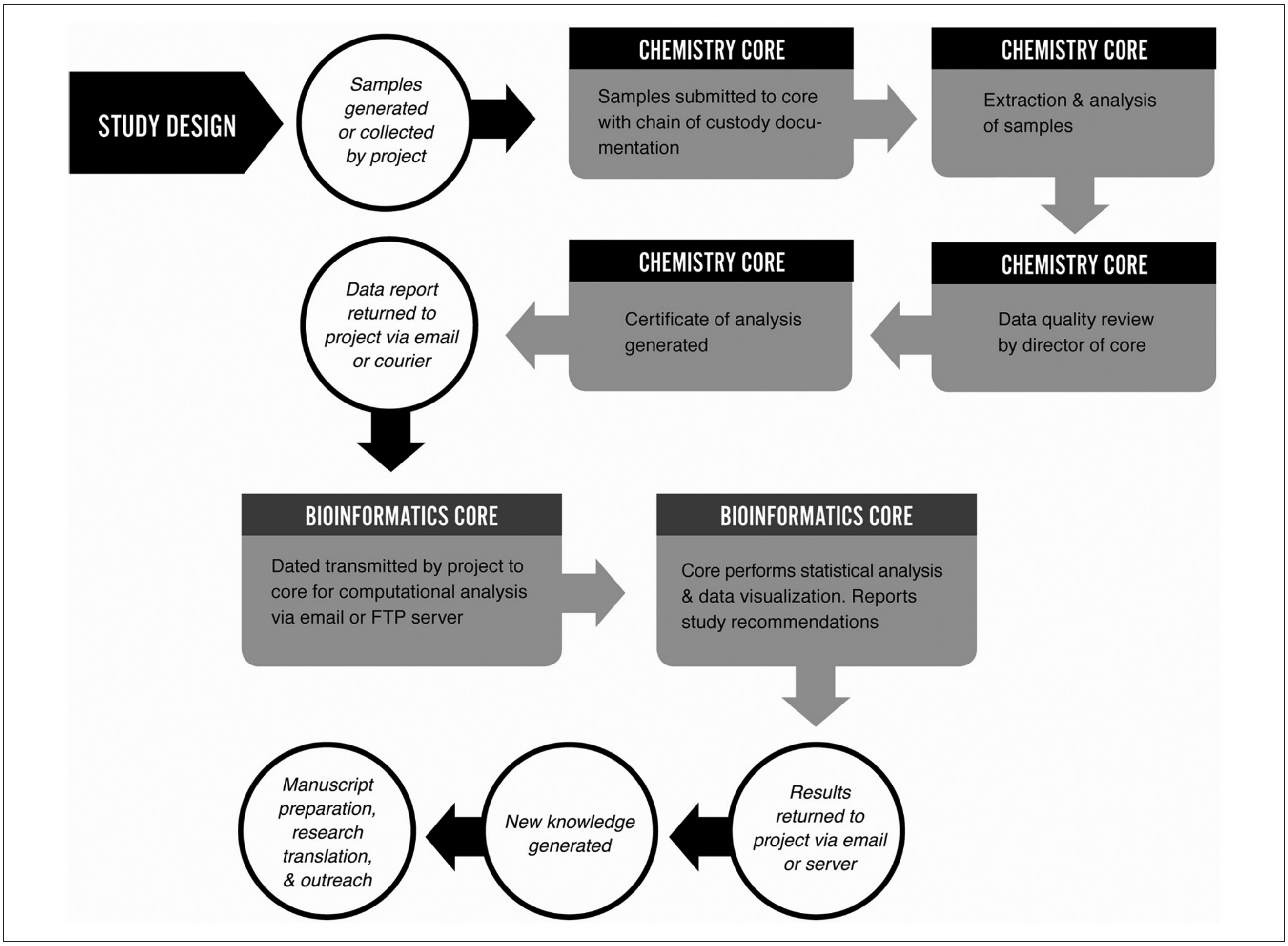

Figure 2. Mockup of sample processing and data workflow used to identify key operators and data migration.

The sample receipt and analysis traceability requirements of the chemistry core suggested that a LIMS would be most beneficial. The next decision was whether to build versus buy a solution for the chemistry core. The solution would have to work in the current laboratory environment and network infrastructure at OSU. It would have to either provide an application programming interface (API) for EDMS connectivity or at a minimum have an accessible database schema that could be accessed by developers without compromising traceability. Last, it needed to be user-friendly as rapid adoption by lab staff was critical to getting this integrated system off the ground. Online research helped determine that there are open-source and commercial solutions that meet these requirements. Other groups working on scientific and human health research have had success developing LIMS in-house using open-source software and database applications such as Microsoft Access[2,3] (Microsoft Corporation, Redmond, WA).

The benefits of developing software internally versus purchasing a commercially available product for implementation in the Superfund center were discussed. Developing software in-house would allow the center to tailor its own product to its needs that would fit into the existing IT infrastructure at OSU. However, this would take a lot of time to launch and would need extensive testing, and the project could fail if key staff left. On the other hand, purchasing a commercial product that was ready to deploy would provide both long-term support and additional training from the vendor if staff turnover became a problem. Although this would come at a larger upfront cost, the center determined that it was advantageous in this situation to go with the option that would have the fastest deployment while still keeping within the budget of the chemistry core. Thus, the decision was made to purchase a commercial product and begin developing the utilities necessary to integrate software systems.

Evaluation of Commercial LIMS

Through experience and a bit of trial and error, an evaluation process was developed that led to an applicable solution in a reasonable time frame. Because the LIMS purchase is a large cost relative to the center's budget, as well as a long-term commitment, it is important to find the best fit for the dollars and environment. However, the evaluation process should not cost more than the purchase or take so long that requirements become obsolete. The four key aspects to finding the best-fit commercial LIMS product for the center are as follows: use the right team of evaluators, evaluate in person, limit options by key criteria, and test potential prospects with real data and workflows.

The right team to evaluate. A small team consisting of a laboratory manager, key end-user, and a lead software engineer worked together to evaluate the current LIMS market. All three were critical in finding a good end solution; the lab manager understood the QAPP compliance desired and the data formats most commonly handled, the end-user could evaluate the user experience, and the lead software engineer could evaluate the vendor's architecture. The first step was to research the current market for potential solutions, then to see these solutions in action.

Evaluate in person. Most key LIMS vendors attend and market themselves at the major conferences and associated trade shows. The evaluation teams attended two of the major conferences, PITTCON and Lab Automation. PITTCON is the largest scientific exposition in the United States and has a large contingent of laboratory automation vendors and speakers. Since the first LIMS implementation was in the chemistry core, this was an excellent place to start. Continuing the search at Lab Automation (now part of the Society for Laboratory Automation and Screening [SLAS]) identified additional vendors supplying general LIMS, ELN, and sample management solutions. Taking teams to both events to evaluate each potential solution in person turned out to be a key element of the purchase. The end-user could see the software in action and evaluate the user experience while two other experts could ask direct questions of the vendors about software and hardware architectures and their ability to support the needed scientific workflows.

Reduce candidates by key criteria. The key criteria used were upfront and maintenance costs, applicability out of the box, scalability, and usability. Keeping initial costs less than \$100k for a small laboratory of 20 scientists substantially reduced the number of options. Identifying products geared toward environmental or analytical chemistry labs but could be easily scaled and adapted to biology labs further narrowed the options. Hosted or cloud solutions, client-server-based software, Web-based software, and several database protocols such as Oracle (Oracle Corporation, Redwood Shores, CA) and Microsoft SQL (Microsoft Corporation) were evaluated. Due to expected maintenance of regulatory and institutional review board compliance, the team ruled out hosted or cloud solutions. The team determined that a Web-based solution was more cost-effective for the center due to the licensing, which typically charges per concurrent users (Web-based) as opposed to per named users (client-server). The final candidates consisted of three different commercial solutions; two of them were LIMS and the third was an ELN.

Use real test use cases from your own laboratory. Semi-weekly Web meetings were established with the three companies, two of which set up hosted instances of their software for the team to implement test use cases and evaluate user experience. These instances allowed evaluation of workflow and dataflow management with the processes and instruments in the core facilities. In addition, the response time needed for each vendor to make specific changes or fixes could be observed. The test instances were the most important tool for deciding which software to purchase, enabling the team to determine which marketed concepts were in development versus fully implemented at the time of purchase.

After an extensive evaluation of the ELN solution, it was determined that this ELN could potentially allow the chemistry core to maintain its QAPP but did not store the analytical results in a manner that was easily queried and reported, so it was eliminated. At the conclusion of the evaluation period, X-LIMS[4] (Ethosoft, Inc., Norcross, GA) was procured due to its ease of operation, open relational database protocol for querying results,[5] integration with Microsoft Excel (Microsoft Corporation), and the company's willingness to provide licensed users with documentation of the database schema.

Accommodating the Research Laboratories

The addition of a LIMS did not fully satisfy the center's needs for data integration between production operation at the core facilities and research operation at the project laboratories, and thus an additional system was needed to aid the operations in the research laboratories. Simply providing a means of tracking samples and their storage locations to the project laboratories was determined to be an initial step in data integration for the center. The addition of this software system allows the cataloging of method development samples or research samples in the project facilities separately from service samples submitted to the core that would be captured in LIMS. Once the center achieves full data integration, this additional indexing system will aid in identifying sample results and observational information recorded in paper laboratory notebooks to samples in the project lab archives. Software such as Laboratory Inventory Network Application (LINA), developed by an academic laboratory for inventory management using Microsoft Access, is offered free to other academic facilities and could be used in this facet.[6] But to accommodate multiple client operating systems encountered in the project facilities throughout the center, it was decided to purchase a reasonably priced Web-based laboratory inventory management application called FreezerPro[7] (RuRo, Inc., Frederick, MD).

Systems Integration Approach

The chemistry core facility deployed X-LIMS onsite, providing workflow management, automation of data collection, approval, and reporting. After implementation of a LIMS, the chemistry core had a data source that could serve the rest of the Superfund center. The LIMS was capable of producing Web-based reports, but specific data were needed to support the statistical analysis, a chemical standard repository, and other management resources. Replicating data in more than one system can jeopardize data integrity and increase labor required to maintain data quality assurance. To keep data replication at a minimum, the solution was to create a layer of abstraction through the use of an API to the LIMS system that could be used by any other system to query needed LIMS information.

The key design aspect of this API is to maintain read-only access directly to the relational database management software (Microsoft SQL Server 2008 R2)[5] to not jeopardize the complete auditability of the database for regulatory compliance, a key reason to purchase the X-LIMS system. Since X-LIMS does not provide an API, other systems could not add data to the LIMS database on the backend but could query database tables directly and then return the results to the requesting program. By isolating access from the underlying structure, the LIMS could be upgraded by the vendor, and the schema could change without breaking the functionality of the API. An API can provide connectivity to new systems in the workflow as seamlessly as possible, which cannot be achieved if the current systems are simply hardwired together. Thus, creating an API that can easily be used by many systems, some of which have not yet been developed or purchased, was desired.

The software developers at PNNL used their experience in this area to develop a Representational State Transfer (REST)–based API for the communication layer between systems. REST is a lightweight protocol that is used most commonly in Web applications. It provides an easy to use communication layer based on standard hypertext transfer protocol (HTTP) that supports extensible markup language (XML) and JavaScript Object Notation (JSON), but it is not limited to these protocols. This RESTful Web service provides versatility and easily handles the data types that are most often managed by the center.

Shown in **Figure 3**, the addition of the REST API provides information from the LIMS database to systems at OSU and PNNL. The API layer is versatile, which will allow future connectivity to additional software systems implemented at any of the core or project facilities. To access the LIMS database, a set of stored procedures queries the LIMS tables directly and creates data views that can be accessed by the API. In addition, a table of stored procedure names and links to the actual stored procedures is maintained for encapsulation. When the LIMS database schema changes, modifications to only one or two stored procedures are required. This structure is highly configurable to new types of relationships as they are added as long as basic query rules are observed, providing ease of maintenance and flexibility throughout the life of the center.

Systems Integrated

Chemical Repository. The chemistry core established a chemical repository to share standard reference materials with all the projects in the Superfund center. To effectively share these resources, an easily managed request system was needed to share the current chemical inventory maintained by the LIMS. Thus, a Web store that uses the LIMS database to keep track of chemical inventory and a separate data store for collaborator requests and order processing were created, as shown in **Figure 3**. This chemical repository Web store is written in Drupal,[8] an open-source-based Web management system that uses a MySQL[9] database to quickly and easily manage content. The Web store notifies chemistry core staff when an order has been placed and tracks chemical transactions while users can view stock levels and certificates of analysis. The first iteration of the Web site required lab staff to manage the chemical inventory via a user input, and although this worked, the long-term goal was to remove as much hand-entered, replicate data as possible since the inventory was already being managed in the LIMS.

The integration of the Web store to the LIMS database was achieved through the REST-based API. The LIMS provided an auditable real-time inventory off all the standards in the chemistry core facility, whereas the Web store would offer a select set of these materials to center researchers. By duplicating the applicable chemical inventory from LIMS in the Web store database and refreshing this inventory through automated nightly updates, the burden on the LIMS system was reduced and laboratory staff input was streamlined while allowing collaborators to view and request materials.

FreezerPro. To fulfill one of the short-term goals of the center, FreezerPro was implemented to allow the research facilities to manage samples. FreezerPro can be rapidly deployed as a virtual appliance and adapts easily to any IT environment, due to its capability to use Oracle, Microsoft SQL, IBM DB2,[10] PostgreSQL,[11] and MySQL[9] database protocols. The center used Microsoft SQL to reduce database server maintenance requirements and ease future system integration. Additional system integration was desired by the chemistry core facility to provide a more complete solution for managing sample storage, thus running FreezerPro in parallel with the LIMS system. These systems did not naturally talk to each other, so there was a gap in the data workflow of the samples. The solution was to have

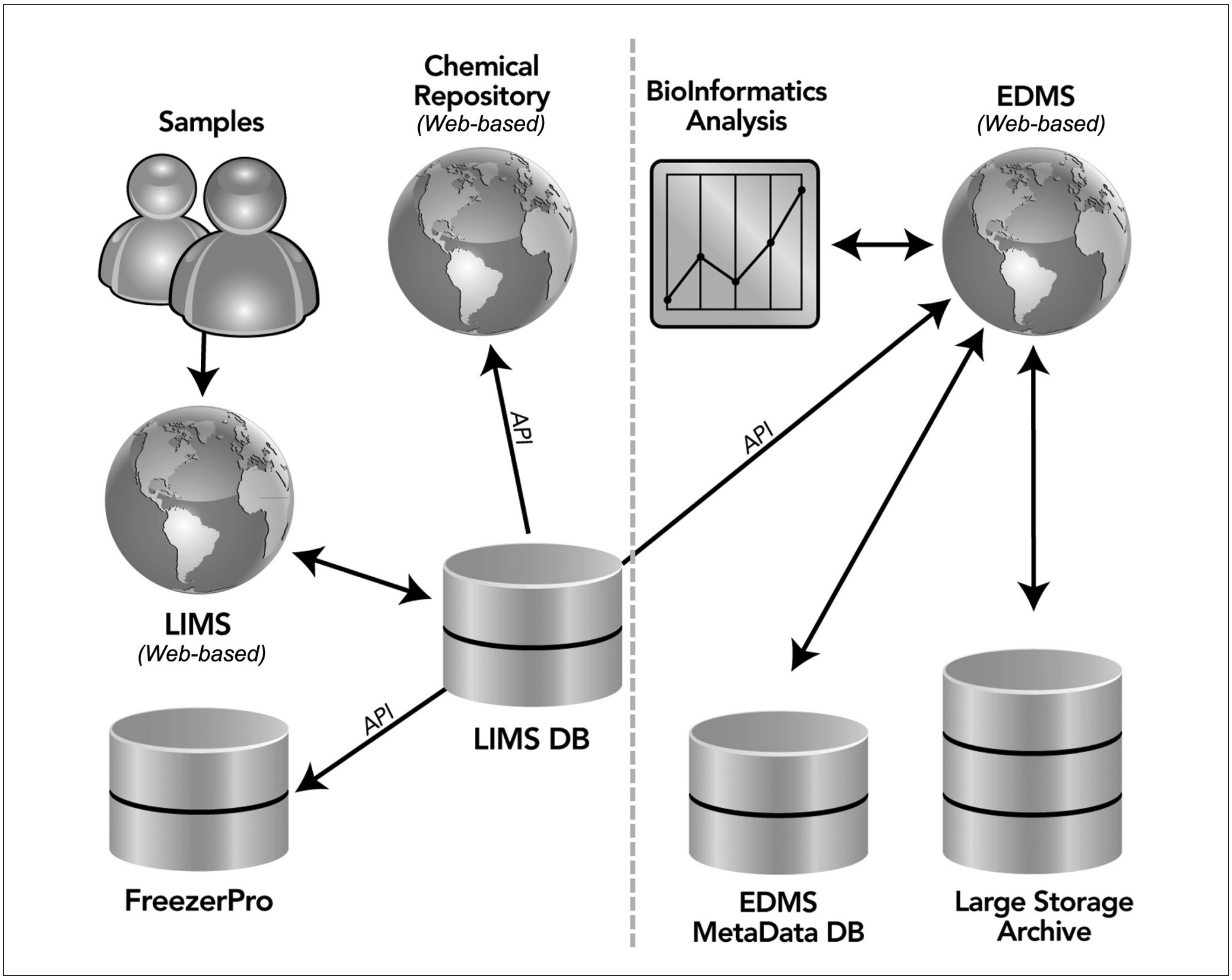

Figure 3. Map of Oregon State University's (OSU's) Superfund Research Center data management systems and the resulting integration. Systems on the left half of the diagram reside at OSU and the right half reside at Pacific Northwest National Laboratory (PNNL). LIMS, Laboratory Information Management Systems; EDMS, Experimental Data Management System.

samples received in the lab entered into LIMS also be entered into FreezerPro. The potential for human error from data replication was alleviated by pushing sample information from X-LIMS to FreezerPro without human intervention. FreezerPro Enterprise Edition included a Ruby API, which was used for entering data in both systems in real time. To maintain the read-only access to the LIMS database, the system was designed to push data from LIMS into FreezerPro but not allow it to flow back in, thus maintaining data integrity. Database triggers in the X-LIMS database execute stored procedures to prepare data for FreezerPro, which then create the entry in FreezerPro automatically through the Ruby API. As metadata are updated in LIMS, they are also updated in FreezerPro through the same process. This allows users to maintain all metadata in LIMS, where changes are audited, and then switch to FreezerPro when making derivatives, labeling, or finding samples in various freezers, shelves, and boxes.

Experimental Data Management System (EDMS). The EDMS is a Web-based portal developed at PNNL to store and manage data associated with biological experiments using MySQL[9] and a large Lustre[12] archive system. Key experimental metadata are captured through a wizard-like Web interface. The metadata are determined by creating a template based on the experimental parameters and other provenance information. The research projects use a number of tools (eg, high-content imaging, miRNA arrays, RNA sequencing, and others) that produce large data sets that are attached to the experimental data and stored in a large archive via EDMS, shown in **Figure 3**. These data sets are often produced from the same samples that are already stored in the chemistry core's LIMS and attached to the workspace in EDMS with the results of statistical and bioinformatics analyses. The rapid accessibility of analytical results is essential for the research projects to write up their outcomes, and therefore connectivity between X-LIMS and EDMS was desired.

The integration was accomplished through the REST API and stored procedures that collect and process the needed sample information and derive some experimental parameters from the test data stored in LIMS. EDMS requests these through the API and populates its data store supporting the Web interface. Using the API to generate the sample entry for the applicable experiment in the EDMS database, double entry of sample and experimental information is eliminated. The results can then be shared as soon as they are available through EDMS access and downloaded for further analysis. Some additional key features of EDMS include a search capability (metadata and data sets) and a notification system. In the end, EDMS contains sample and site information, environmental contaminate data, toxicity data, microarray data, and statistical information and visualizations, allowing for enhanced collaboration thorough ubiquitous sharing of the results.

Discussion

The Oregon State University Superfund Research Center has been able to generate more repeatable and comparable results between projects while maintaining privacy and traceability through deployment and integration of information management systems. Other groups have successfully integrated systems for use in public health surveillance,[13] emergency response,[2] and human health research.[14] Similarly, the OSU SRP center developed a versatile and deployable data infrastructure to improve collaboration and data management in biomedical and non-biomedical research facilities. This was accomplished by purchasing and implementing two commercial products, building in-house Web-based applications, and developing an API to move data between them. This was achieved in approximately 24 months and is currently operational.

After a thorough LIMS evaluation period, involving finding the right team to evaluate, evaluating the products in person, reducing candidates by key criteria, and using real test use cases from our own laboratories, the chemistry core purchased and implemented a commercial LIMS system. The system, X-LIMS, allows for service sample indexing, chemical inventory management, lab workflow management, and data storage and reporting in the chemistry core facility. This system is the heart of the information network and, with the use of APIs, provides data used by other projects and cores via the Chemical Repository Web store, FreezerPro, and EDMS shown in **Figure 3**.

The Chemical Repository Web store interoperability with the LIMS system allows lab staff to maintain one chemical inventory, and only the compounds associated with this project are shared via the Web store. The Web store maintains a transaction history that can be reported as utilization statistics by the chemistry core annually. This streamlined system of sharing resources saves time and money. By using an open-source database-backed Web page system such as Drupal in combination with the REST API, this platform can now be repackaged and deployed in other instances where it is necessary to share resources and manage requests in the center.

X-LIMS and FreezerPro interoperability was achieved using database triggers that create an entry for a sample or standard logged into X-LIMS in the FreezerPro database, allowing the chemistry core to use FreezerPro to monitor sample storage conditions, manage aliquots, and produce container-specific labeling. This enables better inventory control of samples and standards and allows Good Laboratory Practice compliance when a study requires the enhanced protocols. FreezerPro also fulfilled the short-term sample management needs of project laboratories where X-LIMS did not fit the purpose and could be rapidly deployed without the lengthy implementation of laboratory workflow and data storage required with a LIMS deployment. Cataloging the history of research and development samples allows investigators to match a researcher's lab notebook to experimental samples and instrument results stored in the archive. Future integration with an ELN will provide a means to mine past research and method development data to achieve research goals more efficiently. This is important in an academic research lab that regularly cycles through graduate students and requires a robust means of preserving institutional knowledge.

In addition, using FreezerPro and X-LIMS as a paired sample management system offers the center a means to satisfy enhanced regulatory compliance associated with clinical studies. Biomedical facilities can use FreezerPro to store sensitive study subject information and code a sample; then samples are submitted blindly to the chemistry core for analysis and logged into LIMS, and the sensitive information is not carried forward. Once testing is complete, results are combined with the critical information in EDMS securely for the lead researchers to use. If the center has future needs for Health Insurance Portability and Privacy Act compliance, an additional FreezerPro instance could be brought online and isolated with controlled access to store patient data.

The Superfund center uses genomics in combination with other biological and chemical end points to provide a holistic approach to understanding the complex biological interactions of contaminants in the environment. This provides information about mechanism of action from chemical or chemical mixture exposure during development that

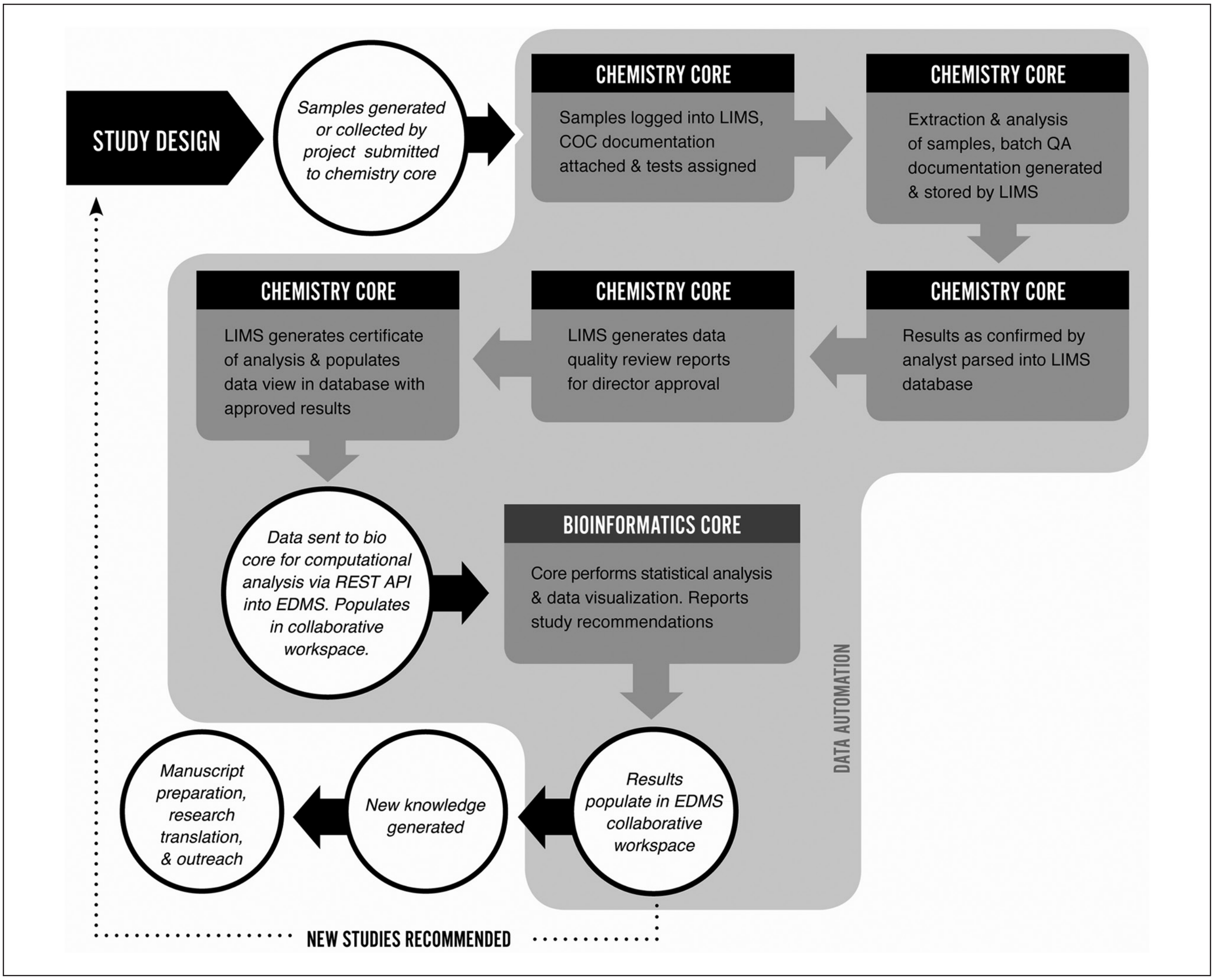

Figure 4. Sample processing and data workflow following system integration. LIMS, Laboratory Information Management Systems; EDMS, Experimental Data Management System; REST, Representational State Transfer; API, application programming interface; COC, chain of custody; QA, quality assurance.

can be used for predictive models and risk assessments. By connecting data systems, the research support cores enabled a complete source-to-outcome chain with minimal data duplication that allows collaboration throughout the center without the need to "send" data from one institution to another through e-mail or external hard drives.

A diagram of this interaction between institutions can be seen in **Figure 4**. Samples are collected or generated by the project laboratories and submitted to the chemistry support core for analysis. At the core lab, samples are logged into LIMS, processed, and analyzed, and then instrument results are compiled for an approval step. Once results pass quality control criteria, the data can flow to the EDMS where the bioinformatics core at PNNL provides computational analysis. Results are returned to the collaborators in the EDMS workspace, and this repeats as an iterative process between the investigator and the cores. Automation of key processes in which samples are received and data are generated, approved, and sent to the next step has saved time versus manual prompts and data handling.

As instrumentation becomes more complex, the amount of data generated can become staggering as seen in many mass spectrometry and nuclear magnetic resonance facilities.[15] The ability to readily access study data, while accommodating large data sets that are becoming larger as instrument technology improves, allows the center to keep pace with the advancement of science. This is achieved through system integration, such as EDMS and its ability to populate information from other core and project data management systems. Future directions of the center will include a laboratory "virtual front door" to inform new center researchers and collaborators of resources and services available at the research support core facilities. This Web application will ease sample submission by producing chain of custody documentation, automate sample login and test assignment in LIMS at the core facilities, and allow users to track the progress of samples during testing and retrieve results. Finally, by leveraging the center's data infrastructure, statistics will be reported to grantors through the Web, and enhancement of outreach efforts to the public will be achieved through live maps and risk predictive tools based on current information. These successes have and will continue to stretch grant dollars by improving center efficiency and enhance collaboration between cores and projects at OSU and PNNL, as well as ease project collaboration with other organizations and governmental agencies.

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Declaration of Conflicting Interests

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