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Integration of facility modeling capabilities for nuclear nonproliferation analysis

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Abstract

Developing automated methods for data collection and analysis that can facilitate nuclear nonproliferation assessment is an important research area with significant consequences for the effective global deployment of nuclear energy. Facility modeling that can integrate and interpret observations collected from monitored facilities in order to ascertain their functional details will be a critical element of these methods. Although improvements are continually sought, existing facility modeling tools can characterize all aspects of reactor operations and the majority of nuclear fuel cycle processing steps, and include algorithms for data processing and interpretation. Assessing nonproliferation status is challenging because observations can come from many sources, including local and remote sensors that monitor facility operations, as well as open sources that provide specific business information about the monitored facilities, and can be of many different types. Although many current facility models are capable of analyzing large amounts of information, they have not been integrated in an analyst-friendly manner. This paper addresses some of these facility modeling capabilities and illustrates how they could be integrated and utilized for nonproliferation analysis. The inverse problem of inferring facility conditions based on collected observations is described, along with a proposed architecture and computer framework for utilizing facility modeling tools. After considering a representative sampling of key facility modeling capabilities, the proposed integration framework is illustrated with several examples.

Keywords: Nuclear Nonproliferation; Facility Modeling; Integrated Model; Inverse Problem

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Highlights:

- We consider integration of facility modeling into a tool for proliferation analysis.
- We describe the inverse problem of inferring the facility based on observables.
- We propose architecture for integrating facility models into a suitable framework.
- We illustrate the proposed integration framework with several examples.

Acronyms

AMUSE	Argonne's Model for Universal Solvent Extraction (chemical separations model)
BI	Business information
BIGDOT	"Big" (large scale) Design Optimization Tools software library
CANDU	CANada Deuterium Uranium (reactor facility)
CEMO	Continuous enrichment monitor
COBRA	Constant Boiling and Rod Arrays (thermal-hydraulic model)
COTS	Commercial off-the-shelf
CPLEX	C (programming language) simPLEX method
CUSEP	Clemson University Solvent Extraction Program
CUSUM	Cumulative sum
DEDS	Discrete event dynamical systems
DOE	U.S. Department of Energy
DOE-EM	DOE Office of Environmental Management
DOE-NE	DOE Office of Nuclear Energy
DOE-SC	DOE Office of Science
DOT	Design Optimization Tools
DSTA	Distributed source term analysis
ENDF/B	Evaluated Nuclear Data File/B
EM	Expectation maximization
EP	Evolutionary programming
FM	Facility modeling
FORTRAN	FORmula TRANslation
GEANT	GEometry ANd Tracking
GML	Geography Markup Language
gPROMS	general PROcess Modeling System
HEU	Highly enriched uranium
HLA	High Level Architecture
IAEA	International Atomic Energy Agency
IBM	International Business Machines Corporation
ID	Inventory difference
IMSL	International Mathematical Subroutines Library
JEFF	Joint Evaluated Fission and Fusion library
JENDL	Japanese Evaluated Nuclear Data Library
LEU	Low enriched uranium
LINDO	Linear, INteractive, and Discrete Optimizer
LWR	Light water reactor
MCMC	Markov Chain Monte Carlo

MCNP	Monte Carlo Neutral Particle
MCODE	MCNP-ORIGEN DEpletion program
MC-REBUS	MCNP-REBUS (REactor BUrnup System) coupled code
MINPACK	Least squares MINimization PACKage
MIXSET-X	MIXer-SETtler-X (Roman numeral 10)
MOCUP	MCNP-ORIGEN Coupling Utility Program
MONTEBURNS	MONTE Carlo BURNup System (MCNP-ORIGEN coupled code)
MTHM/yr	Metric tons of heavy metal per year
MW-hr	Megawatt-hours
NEA	Nuclear Energy Agency
NEWT	NEW Transport algorithm
NMA	Nuclear materials accounting
NNSA	National Nuclear Security Administration
NPT	Nuclear Nonproliferation Treaty
OECD	Organization for Economic Co-operation and Development
ORIGEN	Oak Ridge Isotope GENeration and depletion code
ORIGEN-ARP	ORIGEN-Automatic Rapid Processing
OTTO	Once through then out
PEBBED	PEBble BED (reactor physics model)
PLTEMP	PLate TEMPerature code[1]
PM	Process monitoring
PUREX	Plutonium URanium EXtraction
PWR	Pressurized water reactor
RTI	Run-Time Infrastructure
SALOME	Simulation numérique par Architecture Logicielle en Open source et à MÉthodologie d'évolution[2]
SAM	Simulations, Algorithms, and Modeling (NNSA program office)
SCALE	Standard Computer Analysis for Licensing Evaluation
SEPHIS	Solvent Extraction Process Having Interacting Solvents
SIMS	Secondary ion mass spectrometry
SNM	Special nuclear materials
SYNTH	Spectrum SYNTHesizer
TIMS	Thermal ionization mass spectrometry
V&V	Verification and validation
VR&D	Vanderplaats Research & Development, Inc.
WIMS	Winfrith Improved Multi-group Scheme
XML	eXtensible Markup Language
XSDRNPM	X(cross)-Section Dynamics for Reactor Nucleonics – Petrie Modified[3]

[1] Acronym explanation provided by Olson A.P., (2011). First created to model plate-type fuel assemblies in low-powered research reactors, the code capabilities have greatly expanded over time and it can model nested round tubes as well.
[2] Acronym explanation provided by Sandler V., (2011). English translation is "Numerical simulation by means of open source software architecture and evolution methodology".
[3] Acronym explanation provided by Parks C.V., (2011). Pronounced "Excedrin-PM."

1. Introduction

The specter of nuclear weapons being used to inflict catastrophic damage on a massive scale has been with us since the detonation of the first "atomic bomb" by the United States in 1945. Over the following decades, at least 22 other nations have pursued the development of nuclear weapons to varying extents. Fourteen eventually discontinued their efforts, leaving nine countries that are known or are widely believed to possess nuclear weapons as of this writing (Li et al., 2010).

More nations have used nuclear energy for peaceful purposes, primarily for electric power generation. At the beginning of 2011, 442 nuclear power reactors were operating in 30 different countries, and another 17 countries had nuclear power plants under construction, planned, or proposed (–, 2011k). Of these 47 nations, all but four have agreed to abide by the Nuclear Nonproliferation Treaty (NPT), which bans signatories (with the exception of China, France, Russia, the United Kingdom, and the United States, known as the "nuclear-weapon States" of the NPT) from having nuclear weapons and commits the five nuclear-weapon States to the ultimate goal of eliminating nuclear weapons altogether (–, 2010b), (UNODA, 2011).

Aside from some notable exceptions, non-nuclear-weapon States have developed civilian nuclear power programs without any direct connection to weapons development, thanks to the NPT and the oversight of the International Atomic Energy Agency (IAEA). Unfortunately, access to special nuclear materials (SNM) and the presence of nuclear scientists implicit in civilian nuclear energy applications makes proliferation a very real possibility. Since the 1990s (and earlier), when the hidden proliferation activities and enrichment facilities were discovered in Iraq, nuclear nonproliferation assessments include monitoring for undeclared facilities as well as monitoring known facilities either in full- or denied-access mode (Goldschmidt, 2004). Recent actions by North Korea and Iran underscore the need for better oversight of nuclear activities worldwide, and for the ability to detect and accurately characterize those actions that suspect proliferators try to conceal. The potential for nuclear proliferation will only increase as the use of nuclear power, and associated technologies, expands to developing countries.

This paper addresses integration of facility modeling (FM) codes and algorithms and their utilization in an inverse problem framework that could ultimately enable the user to infer specific details (in a potential sea of uncertainties) about the nature of monitored facilities and their operations based on available observations and data. Such a tool would improve current capabilities to detect and identify proliferation activities. To avoid sensitive topics, the discussions to follow focus on known facilities with full access allowed (which is the venue of nuclear safeguards and security applications) with some mention of known but denied access facilities.

2. Background/Motivation

The ability to assess accurately whether proliferation activities have occurred or are ongoing at a monitored facility is a crucial element of a successful nuclear safeguards and security program. Effective nonproliferation assessments can help deter or prevent nuclear weapons proliferation, or detect proliferation if it occurs, thereby promoting the peaceful use of nuclear energy. One strategy is to design in proliferation-resistant features such as containment vessels having sealed and monitored access points. However, analyses are typically also conducted to verify nonproliferation compliance, even at monitored facilities that allow access. Analysis of a time series of observations from known facilities allows one to characterize the background and monitor for patterns and anomalies that indicate departures from normal operations. This may sound rather trivial, but data based backgrounds are generally challenging to characterize, and observables from proliferation activities require modeling. Such observations could be falsified to mask facility misuse or material diversion, modified through deception, or simply incomplete or otherwise unreliable. One goal for the analyst is to reduce ambiguity regarding the nonproliferation status of monitored facilities in the presence of partial and/or unreliable observations. Therefore, the analyst needs a set of problem-solving capabilities that allow for incremental refinement in the assessment task. This incremental refinement approach facilitates not only the timely identification of which data and data analysis needs are important, but also the incremental assimilation of findings and the formulation of intermediate analyst conclusions.

In short, the analyst's task is difficult and complex as illustrated in **Figure 1**. It must not only be conducted objectively, through comprehensive evaluation of the available information, but it must also be completed in a timely fashion so that it is useful to decision-makers.

Typical items that an analyst may consider include:

- Type of facility, e.g. whether a nuclear reactor, enrichment plant, reprocessing plant, etc.;
- Production levels, e.g. megawatt-hours (MW-hr), metric tons of heavy metal per year (MTHM/yr), etc.;
- Facility nonproliferation operational status, e.g. within the authorized nonproliferation regime or engaging in facility misuse;
- Objectives, strengths, and vulnerabilities regarding nuclear capabilities.

To characterize the above items, the following questions may need to be answered:

- What kind of work could be done given the current plant and resource configuration?
- What labor, equipment, and facility resources are needed to support both the declared and hypothetical missions?
- What is the impact of changing specific assumptions?
- How does a changing resource base (personnel, equipment, facilities) affect the observables?
- What types of facility operation or misuse are of nonproliferation concern, and what observable indicators are or potentially could be available to recognize facility misuse? The answer varies greatly depending on whether the task is to monitor for an undeclared or declared facility, with full or denied access.

Information about a facility or network of facilities can come in many different forms, at different degrees of reliability and completeness. For example, while time series of high-fidelity data may be available, the data may often arrive as a seemingly random sequence of disconnected elements. In addition, while some information may be usable without processing, other data may require the use of physics, chemistry, social, or economic models to produce higher level indicators before they can be useful to analysts. Because no individual piece of information is likely to characterize, qualify, and quantify definitively a facility's activities, the various data streams must be processed and appropriately combined and utilized in a complete assessment that synthesizes and interprets the data.

To facilitate data processing, the available information can be organized into five types: 1) facts, 2) direct information, 3) indirect information, 4) direct data, and 5) indirect data. Facts are verified items of information, such as the confirmed inventory of SNM at a given nuclear site. Direct information is data that can be considered factual due to the source's high reliability and direct access to the information, such as the number of nuclear reactors at a monitored site obtained by analysis of satellite imagery. Indirect information is data that cannot be considered factual due to the source's questionable reliability and lack of direct access, such as the number of centrifuges installed at an enrichment plant as reported in an open source like a newspaper. Finally, direct and indirect data are collections of organized information gleaned from observations and reports, respectively, used to evaluate the likelihood that a hypothesis under examination is factual, e.g. that a given site is producing nuclear material that could be used in a weapon. (Whether a given nuclear material can be forged into a weapon or used at all is not necessarily a clear-cut question as Bathke et al. (2009) have shown.)

While the process of organizing raw data is essential to manage complexity, the volume of data that is potentially of use to an analyst is now so large that significant parts of the nonproliferation analysis must be automated through the use of a systematic methodology for autonomous intelligent information collection and processing.

Unfortunately, the current state-of-the-art for nonproliferation analysis of monitored facilities is far from automated and exhibits a significant imbalance between the use of manual and machine-assisted methods. This makes for tedious work on the part of analysts. Even if considerable effort is devoted to the manual analysis of collected information, it is possible that proliferation activities could pass undetected due to insufficient utilization of available data and ineffective exploitation of resources. Quantitative methods such as algorithms, modeling, and simulation, can be applied to assist nonproliferation analyses. Use of analytical tools like these can promote higher levels of critical thinking that can significantly improve nonproliferation assessment of facilities for which information may be incomplete, ambiguous, or deliberately distorted.

This paper proposes an analytical framework for effectively and efficiently integrating FM capabilities to process information collected from monitored facilities and to infer whether proliferation activities may be taking place. Anticipated FM capabilities include facility models that simulate components and processes typically found in nuclear installations, and also algorithms for data processing and interpretation. The proposed framework is anticipated to be run in two different modes, constrained and unconstrained. Performing the analysis in the constrained mode would enable the analyst to determine what kind and quantity of production could be sustained given the assumed set of resources, while the unconstrained mode would allow the analyst to determine what level of resources would be needed to sustain the declared or assumed operations.

To the extent possible, the facility models and associated analyses should autonomously ingest a wide range of data streams, run component models (both time-driven as well as event-driven analyses in conjunction), flag significant anomalies, and generate specific information with quantified confidence and uncertainty limits. The models will need to operate within this unified framework in a “plug and play” fashion, seamlessly retrieving and transmitting data in self-defining formats. In the near term, considerable iteration between analysts and modelers will be required as the computational framework matures. The analytical tool proposed in this paper will always require human interaction, but the focus will be on optimizing FM analysis by reducing the need for routine human interaction while simultaneously improving the quality of the analysis. Semantic data structures and domain ontology will be used to create a unified framework that automates communication between different components of the facility model, enabling analysts to focus more on overall objectives and less on the details of information collection, processing, and utilization.

This paper is organized as follows. Section 3 formulates the problem of assessing the proliferation status of a monitored facility. Section 4 proposes a systematic architecture for integrating FM capabilities for effectively conducting nonproliferation analyses. Key capabilities for FM integration and utilization are addressed in Section 5. To illustrate the potential benefits for the analyst, the proposed framework for nonproliferation analysis is then illustrated in five examples in Section 6. Section 7 concludes this paper with a brief description of anticipated challenges and future work.

3. Problem formulation

Consider an analyst interested in determining the operating conditions of a given monitored facility, including, for example, assessing whether proliferation activities have occurred. In this context, a facility is defined as one or more structures in which people use feed materials, production hardware and support equipment (such as heating and ventilation and generators) to create a product and waste material (including contaminated water, heat and gaseous effluents) along with process control procedures and software, and production documentation and communications related to that production effort. As mentioned, the facility (or group of facilities) might grant or deny the analyst full access. While full-access facilities can be monitored either remotely or by physical inspection, denied-access facilities generally must be monitored remotely.

As full observability (i.e. access to all process variables) of a monitored facility is often not feasible, partial observability, in which only a subset of possible observations may actually be available, is more common. An FM-oriented strategy to address this partial observability issue could be for the analyst to assume a given characterization or model for the facility under study and determine for which conditions (i.e. values of process parameters) this model best predicts the available observations. The estimated conditions could subsequently be used to infer the actual operations at the plant, allowing assessment of its nonproliferation status. Therefore, under this proposed FM-assisted strategy, the analyst would need two key elements: observations (data or judgments) and characterizations (models) of the monitored facility.

Required information may be of different types, including process data and expert judgments. For example, process data may consist of observations (e.g. temperature profiles, imagery time series, etc.) collected from deployed sensors (e.g. remote infrared detectors, satellite cameras, etc.), while expert judgments may correspond to suggestions regarding the best characterizations/models for describing the target facility, which will depend on the type of nuclear installation (nuclear reactor power plant, isotope enrichment facility, nuclear reprocessing facility) being considered.

A facility model is here defined to be an algorithm or a set of coupled algorithms, along with their respective input parameter files, that simulates some or all of the components of a facility, as described above. These forward models are typically derived from empirical or first principles knowledge of the physical systems of interest, and they compute values for process outputs from process input data via mathematical relations. Thus, facility models can either be scaled physical models or mathematical models that use computational methods to simulate the facility. Facility models may also include algorithms used to collect, integrate, and interpret synthetic and/or actual data (i.e. working in a hybrid fashion).

A complete facility model typically incorporates physics and chemistry-based models that simulate the production process and the waste streams it creates, including those that can be monitored either through direct sampling outside the facility or by remote sensing systems. A complete facility model also must simulate the intermittent nature of production (e.g. batch processing), human factors, support systems, and the transport processes that disperse or transform the waste streams after they are discharged to the environment. These parts of the simulation may require the use of discrete-event models and a computational ontology that links together qualitative, verbal information in an archive of documents. Semantic structures that use keywords and precise technical definitions specific to the production process allow a user to search the document archive more successfully and find objects and relationships between them that would otherwise be difficult to identify.

The FM strategy suggested above, which is commonly referred to as an inverse problem, consists of estimating the values of some model parameters (traditional model inputs) from the observed data (traditional model outputs). This problem can be formulated as follows:

$$\text{Data} \Rightarrow \text{Model parameters}, \tag{1}$$

which informally denotes that the data informs us about model parameters. For example, the inputs could be measurements of shielding between source nuclear material and detector, and the outputs could be detected gamma counts, C which are assumed to be well-modeled by a Poisson distribution, denoted $C \sim \text{Poisson}(\theta)$. Here, θ is a scalar function of $\{\lambda, \mu\}$ which includes a parameter, λ for shielding and a parameter, μ for source strength. Typically the goal is to infer source strength μ in the presence of shielding effects λ.

The collected data typically consist of paired inputs and corresponding outputs. As mentioned, an objective of an inverse problem formulation may be to estimate some parameters of a forward model (linking model inputs to model outputs) based on observations, assuming that the model structure is provided. In some applications, an inverse problem may also require discovering unknown structural relationships (e.g. unknown dynamics) of the forward model. Furthermore, an inverse problem may require that values of model parameters be estimated first, assuming different model candidates G_i, and then selecting the model candidate G^* that best explains the observed data.

Regardless of the specific details of the inverse problem, the initial step of the process is to establish a forward model or a set of forward models whose outputs for various inputs can be compared with corresponding collected data. Given collected data d and the forward model or operator G characterizing the system under consideration, the inverse problem is to find the model parameters θ such that

$$d \approx G(\theta) \ , \tag{2}$$

where G describes the relationship between θ and d, and θ is a p-dimensional vector of the parameters that are being adjusted. Note that G can be a linear or nonlinear operator, correspondingly leading to linear or nonlinear inverse problems. In general, the inverse problem is solved by comparing the observed data to data predicted using the forward model and a given set of model parameters. The set of parameters giving the minimum residual is chosen as the estimated model characteristics. In the above example, measurements and a model inform us about shielding effects λ, and the estimate of μ is chosen to give a good fit to the counts C as in Equation (2) (or more specifically as in Equation (4) below) with θ a scalar function of $\{\lambda, \mu\}$ and data d including C and shielding measurements.

This procedure can be mathematically formulated by first introducing a loss function, $L(\theta)$, defined as,

$$L(\theta) = \left\| d - G(\theta) \right\|, \quad (3)$$

which is then minimized with respect to θ as follows,

$$\theta^* = \arg\min_{\theta \in \Theta} \left\| d - G(\theta) \right\|. \quad (4)$$

Often, the loss function L is squared error and denotes the average squared error.

In the equation above, it is assumed that a unique characterization G for the monitored facility is considered. However, it is possible that an exact characterization for the monitored plant is not known but is assumed to be one G_i from a finite set G of possible characterizations instead. In this case, the optimization problem can be expressed as follows,

$$G^* = \arg\min_{G_i \in \mathrm{G}} \left\{ \left\| d - G_i(\theta_i^*) \right\| : \theta_i^* = \arg\min_{\theta \in \Theta_i} \left\| d - G_i(\theta) \right\| \right\}. \quad (5)$$

Note that the outcome of solving the equation above is identification of a particular model, $G_i = G^*$, with its corresponding parameters, $\theta_i = \theta^*$, that best explains the observations. While G^* can be used to suggest which type of process(es) the monitored facility may consist of, θ^* can be used to infer its operating conditions, including the existence of any proliferation activities. An iterative, inverse problem algorithm is then needed that searches for the solution that produces the best overall fit to the observable facility data. Model averaging is an extension of this strategy that might also be considered (Burr et al., 2008). In the example above, perhaps the shielding is known to be either iron or lead with a measured thickness, so the gamma attenuation correction would be applied for either iron or lead. Provided there were counts in multiple energy bins and the attenuation behavior of iron and lead were known as functions of gamma energy, either model averaging or model selection could be successful.

As expressed above, the loss function, $L(\theta)$, can be minimized by standard optimization algorithms formulated in infinite dimensional spaces, although, in practice, it could also be recast in discrete form to address a finite number of observations and unknown parameters instead. The latter may lead to an ill-conditioned problem. In that case, the introduction of heuristic, experience-based assumptions concerning acceptable solutions may help resolve this issue. In addition, since facility model inputs are often incomplete and/or contain errors, the facility model must perform error propagation analyses to estimate the overall uncertainty of the model predictions such as types of material being produced and production rates.

4. Overall architecture

The nonproliferation analysis tool proposed in this paper is expected to require input data that describe the facility of interest, process simulation models, and methods that can predict observable indicators created by the facility that can be related to the type and amount of production. **Figure 2** shows the relationships between different facility components and the software system that comprises the FM-based nonproliferation analysis. The software system has seven major components:

- Ontology/semantic constructs that identify objects and relationships most relevant for addressing specific queries;
- Input databases/process knowledge that provide information needed to identify and build the model and drive it toward the best estimate of expected observable indicators;
- Process models and simulation codes, including components, processes, activities, and facility inputs and outputs that characterize the primary production process;

- FM integration environment for integrating FM components;
- Activity indicators to be collected and estimated for determining the best model(s) and parameter(s) to explain the observations;
- Anomaly detection algorithms for detecting and isolating anomalies that cause deviations from expected conditions;
- Control software and optimization algorithms that solve the inverse problem, including statistical and sensitivity analysis methods for hypothesis assessment and uncertainty quantification.

Figure 2 depicts aspects of a complete facility model. Fragments of facility models can also be constructed and used to simulate parts of a facility. For example, the heat dissipation systems of a facility, such as cooling towers or chillers, can be modeled to determine the rate at which waste heat is being discharged to the environment. Other models would then have to be applied to estimate production rates from the rate of thermal energy dissipation. A complete facility model gathers all available information about the facility (or facilities) and uses the necessary combination of codes, possibly selected following semantic, context-related knowledge, to simulate what may be going on in the facility, including the various external indicators of activity (gaseous and particulate emissions, waste heat, acoustic and RF signals, vibrations, movement of materials and people into and out of the facility, financial transactions, etc.). Given that databases for these activities exist, the complete facility model simulation will produce predictions of the external indicators, which can be combined into a higher confidence statement about what may be going on in the facility (relative to a partial simulation that uses only one or two indicators). If contradictory information is contained in the input databases, the complete facility model will not be able to produce high-confidence predictions but rather many low probability solutions that are far from unique. A complete facility model can also assist in isolating potential conflicting data.

In summary, a complete facility model simulates aspects of the facility operations that produce some measurable indicator of activity. If there is no measurable indicator, then that aspect of facility operations does not need to be modeled unless it is necessary for continuity of the simulation, e.g. step B is modeled because it is necessary to predict the indicator associated with step C.

5. Facility modeling system components

As shown above in **Figure 2**, seven key capabilities are needed for successful FM integration, utilization, and interpretation. Brief descriptions of each capability are provided in the subsections that follow.

5.1. Ontology/semantic constructs

The proposed analytical tool will utilize a semantic module to identify efficiently those models, methods, and observations that are expected to be best for answering analysts' queries, in addition to their interrelationships. As illustrated in **Figure 3**, these relationships identify how these objects should be interconnected and used for consistent data exchange, execution, and exploitation. In particular, an ontology is defined to be "a formal specification of a conceptualization" (Gruber, 1993). Furthermore, an ontology is "a common vocabulary for researchers who need to share information in a domain," including "machine-interpretable definitions of basic concepts in the domain and relations among them," which is important for integrating various computational components, especially when they are remotely coupled across the Internet.

An important concept for modern data representation is Extensible Markup Language, which is a set of rules for encoding documents (or data) in machine-readable form (Wikipedia, 2010). XML is commonly used on the Web to facilitate document display. It is also widely used to represent arbitrary data structures for computational codes, both stand-alone and those connected via the Internet. Associated with an XML document is a schema, which defines the structure of the document. An XML schema is a "means for defining constraints on well formed XML documents. It provides basic vocabulary and predefined structuring mechanisms for providing information" in the XML document (Klein et al., 2001). XML has become the dominant standard for exchanging information on the Web, and is widely used in computational codes which require interoperability with other codes for consistent data exchange.

Computational systems utilize ontologies in a multitude of ways, but the following is a common approach for integrated modeling (Klein et al., 2001), (Quix et al., 2007). First is a forward process that creates an XML schema of a particular type from the ontology and other data; for example, if one is doing structures on the surface of the earth, one might choose Geography Markup Language (GML). Once this schema is created to one's liking, the reverse process is used to construct "data" in the form of the XML schema (based on GML in this case), for input into facilities modeling codes. This reverse process uses the ontology to provide "annotations" to query the geodatabases (and other data sources) for data of importance to the specific model one is working with. The items found are then encoded into GML to produce a "data" structure that is usable by the modeling codes. This approach is quite general and used across a number of different fields. The ontology becomes the terminology standard by which all software conforms, either by using the "standard" terms or by using mappings to the "standard" terms. This allows for maximum conformity for software interoperability across multiple applications. The use of XML-based schema allows for operational ease within the programming languages, most of which will have XML-parsers. In this manner, a high degree of interoperability can be created across multiple programming paradigms for support of integrated facilities modeling.

5.2. Database/process knowledge

A database of information/knowledge describing the processes that are pertinent to potential proliferation activities will be an essential component of a facility model that is intended for use by an analyst. The data residing in the database will come from a variety of sources including existing databases, written archives, sensors, satellites, other agencies, computer models, news media resources, as well as experiments. The data will be in many different formats ranging from text and written information, to numerical data, to image data (of various formats not restricted to visual), and others. Personnel or intelligent systems building and utilizing facility models will need to access the data in order to construct models, design experiments, analyze results, form relationships, make decisions, and expand the database. Many results may be obtained simply by visualizing the data, comparing values to each other, considering various data streams together, or comparing data values to know constraints. An extensive database may become as useful as a model to a nonproliferation analyst.

The information that may be important to an analyst will encompass all aspects of nuclear weapons production. This would include the broad categories of product data, resource data, and process data. Product data would include information on part and components for all types and forms of potential nuclear devices. Product data would also include materials data, and descriptions of possible assemblies and subassemblies including assembly directions, instructions, or relationships if known. Resource data would include all of the resources that might be associated with production of nuclear weapons. Resources should include personnel, for example security, scientific, labor, administrative, and support staff and could be highly detailed covering skills, training capability, pay rate, age and retirement/attrition information, shift, schedule, and attendance knowledge, and cross training/job sharing capabilities. Complete data at this level of detail is unlikely; however, partial information at any level needs to be included in the data sets because it may still be useful to an analyst. Resource data would also include equipment information. Equipment is needed for manufacturing, for example, machining, shaping, forming, etc., for chemical processing, for metallurgical processes, and certainly for computing systems not limited to scientific computing alone but including administrative and other support information processing. Equipment data may be highly detailed as well, covering equipment type, capability, capacity, and even possibly maintenance information. Resource data encompasses a broad set of ancillary resources that could be critical to the determination of a facility's actual use. These resource data might include financial data, descriptions of transportation methods including equipment, paths, and timing, facility infrastructure such as buildings, and utilities (electrical, water, process gases, etc). They might also include descriptions of less tangible resources such as communications with vendors, consultants, or decision makers. Process data would cover traditional manufacturing knowledge such as assembly steps, supply chains, and waste streams as well as weapon specific processes such as enrichment and special materials processing.

Data visualization coupled with the process knowledge resident in the database may be very useful for analysis and identification of candidate proliferation sites. Consider an analyst trying to make a decision about which of many sites deserve closer attention given data from numerous sources (sensors, observation, news media, model runs, etc.). Perhaps visualizing the data in a parallel coordinates format (Inselberg, 1985) and through a filtered plot that shows only those sites that meet specific criteria determined from the database would enable the analyst to quickly (and visually) select possible sites. See **Figure 4** for an illustration of this approach.

In this example, there are four sites each with information from ten data sources. The example shows the data visualized in parallel coordinates and also illustrates the application of the process knowledge filter. Using parallel coordinates for exploratory data analysis was first suggested by Wegman (1990). In the example, we are looking for sites with the value from data stream 5 to be greater than 0.95. Only site 2 meets this criterion; therefore it is highlighted in the visualization. This is a simplified example made to illustrate the approach. In an actual application, multiple criteria can be applied and multiple sites can meet the criteria. Parallel coordinates is one simple example of data visualization with multiple criteria. There are many other types of visualizations and many more ways in which to analyze the data. Data and information visualization is a very active research area and has many potential applications besides nonproliferation analysis. See, for example, Tufte (1997), Spence (2007), Pabian (2008), and (2010a).

Because of the richness of the data and the numerous ways to view, analyze, and utilize the data, the database itself will be a principal tool for the proliferation analyst. Just as fragments of models may be developed and used to simulate portions of a facility, fragments of the database will be used to model and analyze smaller portions of a facility or complex.

Finally, a fully populated database will not only provide data for input into models and for comparison with collected data but it will also hold data, both real and synthetic, that will be used for facility model verification and validation (V&V). V&V data will allow analysts to construct new models, simplified models, meta models, trends, and other analytical comparisons to use in proliferation analysis.

5.3. Process models/simulation codes

A wide variety of process models and codes is available, with some having overlapping purposes. For example, in full-access facilities, nuclear material accounting (NMA) requires accountability measurements, each having a σ_S (standard deviation of the "systematic error," which is the standard deviation of the instrument bias) and σ_R (standard deviation of the random error), and commensurate detector design. Therefore, detector and source models are available and are continually being improved. Models of material flows and related measurements are becoming even more important with process monitoring (Burr et al., 2003; Burr et al., 2011) being included as a safeguards component to complement NMA. In denied access facility modeling, models of production processes and corresponding effluents that might provide observable indicators for illicit SNM production include physics-based first principles models having varying model fidelity (Heasler et al., 2006). These models could be used, for example, to infer recovery of weapons-grade plutonium from spent fuel based on burn-up indicators (Burr et al., 2005).

Component/process models can be classified as either steady-state or dynamic depending on their temporal characteristics. Steady-state process models provide material and energy balance information, which can be used to estimate parameters such as material flow and waste heat discharge rates, equipment size, and capital and operating costs. Those process parameters that have observables that can be remotely detected (e.g. mass and energy flows and equipment size) should then be considered when conducting nonproliferation analyses. On the other hand, dynamic models can predict the response of the process to changes in operating conditions and the impact of upsets such as equipment failure. This type of capability is needed to investigate possible indicators of temporary facility misuse, perhaps misdirecting SNM into waste streams for later recovery. However, they typically require more effort and specialized skill to construct, and the additional information they provide may not be worthwhile from the standpoint of observable indicator interpretation or correlation. One obvious exception would be catastrophic equipment failure or other observable dynamic event for which a dynamic model would be needed to correlate an observable for that event.

Component/process models can also be grouped according to their general purpose. For nonproliferation analyses, model classifications by purpose would primarily include fission reactor models, chemical process models (for facilities such as isotope enrichment and aqueous reprocessing plants), and detector response models. Instances within each classification are briefly discussed next to illustrate their possible integration and utilization within the proposed analytical framework.

5.3.1. Reactor models

Reactor physics simulation codes can be further divided between two different code classifications, based on methodology: deterministic and Monte Carlo. Both types require input data from evaluated nuclear data libraries, and the first step in the performance of any reactor simulation is the processing of such data into a form that can be used in the reactor physics code.

As an example of input nuclear data, the ENDF/B library contains recommended data on cross-sections, spectra, angular distributions, fission product yields, thermal neutron scattering, photo-atomic and other nuclear phenomena, with an emphasis on neutron induced reactions. ENDF/B-VII.0 (Chadwick et al., 2006) is the latest version of the ENDF/B library. The JEFF Nuclear Data Library series contains different versions of the Joint Evaluated Fission and Fusion Library. The most recent version is JEFF-3.1-1 (Santamarina et al., 2009) , which contains evaluated neutron reaction, incident proton, radioactive decay, activation, fission yield, and thermal neutron scattering data. The JEFF series is maintained by the Nuclear Energy Agency (NEA) of the Organization for Economic Co-operation and Development (OECD). Similar nuclear data are provided by the Japanese Evaluated Nuclear Data Library (JENDL) (Shibata et al., 2011).

Among deterministic methods, material temperatures can be calculated with a thermal hydraulics code like COBRA (Rowe, 1973) or PLTEMP (Olson and Kalimullah, 2010). COBRA is a subchannel code for calculating heat transfer in Light Water Reactor (LWR) cores in rod bundle geometries and PLTEMP is a code for steady-state heat transfer calculations in cores having plate or tube type fuel elements (e.g. research and plutonium production reactors). For point depletion simulations, the code ORIGEN (Gauld et al., 2002) is widely used. ORIGEN computes the time-dependent concentrations and source terms (radiation, heat) for over 1600 nuclides that are simultaneously generated or depleted through interactions of materials with neutrons and radioactive decay. ORIGEN has been subjected to numerous verification checks through intercode comparisons and validation tests by comparing code predictions with measured radionuclide concentrations in irradiated LWR and CANDU (CANada Deuterium Uranium) fuel (Tait et al., 1989), (Hermann et al., 1981), (Tait et al., 1995). Similarly, one- and two-dimensional depletion simulations can be performed with SCALE (–, 2009). SCALE 6 is a system of coupled codes which includes the basic physics codes XSDRNPM (one-dimensional discrete ordinates), NEWT (two-dimensional arbitrary geometry discrete ordinates), and ORIGEN-S (point depletion and decay). SCALE 6 includes continuous energy and multigroup transport cross-section libraries based on ENDF/B-VII data. A number of studies have been performed to validate SCALE for Pressurized Water Reactor (PWR) fuel (Hermann et al., 1995), (Hermann, 2000), (Ilas and Gauld, 2009). As reported in (Ilas and Gauld, 2009), the maximum relative discrepancy between code predictions and measurements for the major isotopes is: ^{239}Pu - 9%, ^{240}Pu - 4%, ^{241}Pu - 4%, ^{235}U - 2.5%, and ^{238}U - 1%. The average relative discrepancies are smaller. For example, for ^{239}Pu the mean relative discrepancy is 5%, and for ^{235}U it is 0.5%.

A number of codes have also been developed for particle transport and Monte Carlo depletion simulation. For example, MCNP (Brown et al., 2002) is a general purpose Monte Carlo neutral particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. It treats an arbitrary three-dimensional system geometry, using continuous energy nuclear and atomic data, so there is no need to generate multigroup cross sections. MCNP accounts for all neutron reactions given in cross-section evaluation data libraries (e.g. ENDF/B-VI). Other Monte Carlo based depletion codes include MOCUP (Moore et al., 1995), Monteburns (Poston and Trellue, 1999), MCODE (Xu and Hejzlar, 2008), MC-REBUS (Hanan et al., 1998) and VESTA[4] (Haeck, 2009). These provide a coupling of MCNP with a version of the depletion code ORIGEN, or with the depletion code REBUS (MC-

[4] VESTA is not an acronym, but a reference to the Roman goddess of the hearth and her sacred fire instead, considered by its developers to be appropriate for a depletion code used to “burn” materials under irradiation (per Haeck W., (2011)).

REBUS). In this coupling, MCNP provides the neutron flux and the cross-sections and the depletion code performs the depletion calculation. The Monte Carlo method allows accurate modeling of complex heterogeneous geometries and detailed simulation of the energy dependence of the nuclear data (no need for energy and spatial homogenization of neutron cross sections). Although MCNP provides high accuracy to these depletion codes, it is also responsible for their very long computation times.

5.3.2. Chemical process models

Chemical process unit operation (component) or process (facility) models can be simulated using a variety of open-source and commercial off-the-shelf (COTS) tools. For example, Aspen Plus® (Aspen Technology, Inc., Burlington, MA) (–, 2011b) is arguably one of the most widely used COTS tool for modeling chemical processes. This tool includes rigorous models for numerous unit operations and provisions for creating custom Fortran- or Microsoft Excel-based models of those that are not included. A broad range of sophisticated activity coefficient- and equation-of-state-based physical property models is provided, along with pure component and interaction parameters for most common systems. Custom properties models and property parameter databanks can also be easily set up. Data regression capability allows the fitting of custom physical property parameters to pure component and mixture data. Property parameter estimation methods are also available in the absence of data. Time-dependent, semi-batch, or cyclic operations can also be modeled using time-averaging. Steady-state Aspen Plus® models can be converted into time-dependent dynamic models using Aspen Dynamics® (–, 2011b) and customized using Aspen Custom Modeler® (–, 2011c). Other process simulators include, but are not limited to, CHEMCAD (Chemstations, Inc., Houston, TX), (–, 2011a), ProSimPlus (ProSim SA, France) (–, 2011d), PRO/II™ (Invensys/SimSci-Esscor) (–, 2011h), Plano, TX), and gPROMS (Process Systems Enterprise Ltd., London, UK) (–, 2011g).

Several of the unit operations typically found in reprocessing plants have been modeled independently. Krebs et al. (2010) recently reviewed models for both the dissolver and solvent extraction unit operations. They found that several sets of differential equations have been developed by various authors to describe the dissolution rates of unirradiated UO_2 pellets and powders. Far fewer such models have been developed specifically for the dissolution of actual spent fuel. Only a few dissolver models have been implemented using common computer languages like FORTRAN.

Over six decades of research have gone into the development of various models for the three primary types of solvent extraction units: mixer-settlers, centrifugal contactors, and pulse columns. The Krebs review noted over thirty models and codes that have resulted from this work. Of these, SEPHIS (U.S.), AMUSE (U.S.), and MIXSET-X (Japan) have seen more continuous use. All three codes were developed for mixer-settlers; AMUSE is also regularly used for centrifugal contactors. The AMUSE and MIXSET-X codes have separation factor (D-value) models for a number of the fission products and TRU elements and have been kept current. For pulse column models, the most notable codes are CUSEP, developed by Beyerlein and Geldard at Clemson University, and PULCO from Japan. Both of these pulse column models track UO_2^{2+}, Pu^{4+}, and Pu^{3+} with no evidence that they have been kept current.

Independent models for post-solvent extraction unit operations are harder to find. Models for evaporation, denitration, and calcination unit operations specific to spent fuel reprocessing are rare in the open literature.

5.3.3. *Detector response models*

Detector response modeling is typically used during planning stages to evaluate the potential for exploiting candidate misuse indicators. Because the effects of facility misuse are often superimposed onto synthetic or real background (no misuse) facility data to create hybrid data, detector response modeling is also crucial for generating realistic hybrid data suitable for comparing misuse detection algorithms. MCNP is used for gamma and neutron detector models, as are GEANT and others (LaFleur et al., 2010).

5.4. Facility modeling integration environments

Implementation of the concept illustrated in **Figure 2** will require integration of multiple codes and databases, which will probably reside on different platforms. An adequate and complete facility model could probably be constructed for some purposes, largely from pieces of software that already exist in other large integrated models. The challenging aspect of a complete facility model will be the different types of sub-models that may have to be linked together and possibly synchronized in time. These sub-models will include, for example, not only physics and chemistry-based models but also discrete event models for simulating the start-and-stop aspects of process control, including human factors such as work day length, shift schedules and 24-7 work schedules versus schedules where facilities only run part of the time. Other discrete event model inputs include material delivery schedules, types of transport to facility (rail, truck) and waste tank storage capacity.

COTS software packages exist that may have some applicability to the problem of creating a facility model that integrates many sub-models and databases. For example, SALOME (–, 2011j) has been used in the nuclear power industry for design and simulation of coupled reactor physics, waste processing, waste storage and waste disposal steps in the nuclear cycle. SALOME could serve as a starting point for constructing the physics and chemistry based components of a nuclear facility model. Likewise, ModelCenter® 9.0 (–, 2011j) by Phoenix Integration is a graphical environment for process integration that allows quick creation of engineering processes. Processes can involve diverse modeling and simulation tools that were not necessarily designed to communicate with each other, which make them particularly difficult to automate. Integration of models is performed using a visual environment, without involving tedious programming. Once created, these integrated processes can be used to answer what-if questions and standardize and share common processes across models and organizations. This tool allows users to perform detailed optimization and validation studies efficiently and effectively, including parametric studies, design of experiments, response surface modeling, and gradient and non-gradient based optimization. However, the Phoenix Integration tool is not suited for time-synchronized integration of disparate models. At the other end of the spectrum of potential integration solutions, SAS® Enterprise BI Server (–, 2011f) by SAS Institute, Inc. is an enterprise business information (BI) software product consisting of a suite of applications that facilitate the integration of data from across an enterprise. This product can be used for understanding the past, monitoring the present, predicting outcomes, and reporting conclusions. Its relevance for FM integration, as well as for other BI products, is for metadata management from a repository, where metadata from multiple sources (e.g. models) can be accessed, integrated, combined, managed, and shared across the enterprise.

Simulation standards and languages also exist that have been specifically developed for integrating simulation codes. For example, High Level Architecture (HLA) is a general-purpose architecture for distributed computer simulation systems (Kuhl et al., 1999). Using HLA, multiple computer simulations can communicate with each other regardless of the computing platforms they may reside on. Communication between simulations is managed by a Run-Time Infrastructure (RTI). Two key terms are federate and federation. A federate is an HLA-compliant simulation. On the other hand, a federation is a collection of multiple simulations or federates connected via the RTI. Using HLA, facility models developed and running on different platforms can be integrated and closely synchronized in time.

5.5. Indicators of facility activity

As illustrated in **Figure 2**, indicators of facility activity are not only collected from observations, but also estimated as part of the process through which facility models and parameters are matched to the observations. To this end, the goal of monitoring capabilities is to collect and make use of data for decision making. For nuclear nonproliferation, decision making could imply declaring the existence of proliferation activities at a monitored facility. Consequently, data on the monitored facility are needed, (e.g. indicators or observations.) These data may come not only from physical, cyber, and business observations (i.e. actual data) but also from estimations derived from predictive models (i.e. synthetic data) characterizing aspects of the monitored facility. Regardless whether the data is real or synthetic, data generation capabilities or sensors are deployed and utilized. Sensors, which receive and react to stimulus, may thus come in all forms. For example, a physical sensor may measure a physical quantity (e.g. temperature, pressure, light, motion, sound, radiation, electric field, magnetic field, etc.) and convert it into a signal for further processing. On the other hand, an electronic sensor may collect electronic communications occurring over networks. A sensor may also be biological (a biosensor) or even a human individual collecting information about the monitored facility. Sensor types typically used for nuclear nonproliferation purposes include process monitoring (e.g. temperature, pressure, flow, volume, density, material concentration, etc.), spectroscopy, passive/active interrogation (e.g. alpha/gamma/neutron detectors), geospatial, and surveillance and containment (e.g. cameras and seal/portal indicators).

Regardless of the data processing methods being considered, finding an optimized sensor configuration for a particular application is computationally difficult unless the problem is structured in a way to allow practical solutions. Stochastic search and optimization techniques (e.g. gradient-based algorithms, simulated annealing, genetic algorithms, etc.), along with the incorporation of heuristics, may be used to help solve the sensor selection problem.

5.6. Algorithms for anomaly detection and indicator generation

Given raw, unprocessed observations, data processing algorithms can be used to collect, integrate, and interpret actual and synthetic data to generate high-level indicators characterizing facility activities. Observations and indicators may then both be used to solve the inverse problem and thus infer the operating conditions at the monitored facility. In doing so, data are translated, at different levels of abstraction, into information and then into knowledge for decision making through the use of integration, analysis, and interpretation capabilities. These data-driven methods may be loosely grouped into three broad categories: reasoning-without-time, reasoning-over-time, and hybrid methods. **Figure 5** illustrates the differences between these broad categories. Overall, however, all three methods seek to understand past data, interpret present observations, and then predict future outcomes. Useful methods have been developed by various technical communities, including physical scientists, computer scientists, statisticians, and mathematicians.

Reasoning-without-time methods interpret data without the explicit incorporation of time. If there is a natural division of the data into "responses" and "predictors," then many "regression" methods have been developed to relate the response, y, to predictors, x, via a fitted function, $y = f(x)$ + error.

Methods differ according to what is assumed or known about f, whether x has appreciable or negligible error, whether all components of x are continuous-valued or some components are categorical, and the possible values for y. If y is discrete-valued (such as "proliferation is occurring" or "proliferation is not occurring") then "regression" is referred to as classification, pattern recognition, or supervised learning, for which there are many analysis options (Hastie et al., 2009). The distribution of the predictors, x, will change as the value of y changes, so the inverse problem can be addressed. If y is continuous-valued, then parametric fitting options include ordinary linear least squares and variations thereof, and nonparametric fitting options include kernel regression.

Semi-parametric options include both parametric and nonparametric components. In the context of the $d = G(\theta)$ model in Section 2, x could be the observed data, and θ could include both the y value and other model parameters. The function G could be learned from archived data or based on FM predictions, or a combination of both.

Reasoning-over-time methods interpret data with explicit incorporation of time and include capabilities such as discrete event dynamical systems (DEDS)-based methods (e.g. discrete stochastic models/automata, Petri nets, etc.), Markov models and hypothesis testing methods (e.g. CUSUM, sequential likelihood testing, dynamic belief networks, Kalman filters, etc.), statistical learning methods (e.g. reinforcement learning, learning automata, etc.), temporal methods, and multi agent-based methods (including game theory-based methods).

Finally, hybrid methods can be loosely characterized as exhibiting features from both previous categories. A hybrid method may thus integrate, for example, dynamic knowledge derived from physical modeling with measured input-output characterizations derived from data-driven techniques, such as neural processing, to produce an acceptable and often accurate model of the dynamical process being observed.

Although the various technical communities tend to favor certain methods, all invoke some type of statistical reasoning (even if only at the most rudimentary level of division into training and testing data and estimating performance). Methods that have already been used in FM applications include: CUSUM, parametric regression, kernel-regression, Gaussian process modeling, data mining (clustering is a key tool), nonparametric analysis, belief networks, Bayesian networks, support vector machines for pattern recognition and regression, statistical expectation-maximization (EM) algorithms, adaptive dynamic programming, expert systems, Markov models, and many signal processing tools including filters, smoothers, and spectral analysis, typically via Fourier or wavelet transforms.

Many COTS software systems are available to support development of anomaly detection and indicator generation algorithms. For example, general packages such as R (–, 2011i) and Matlab (–, 2011e) can be used to prototype, develop, and possibly implement these methods. These software packages are routinely used to develop models of complex industrial facilities. They typically include libraries of code implementing standard statistical tests as well as the capability to build customized tests to monitor specialized activities. If implementation requires fast computer run times, then compiled executables in C, Java, or C++ are common.

5.7. Algorithms for solving inverse problems

Many algorithms can be used to solve the minimization problem formulated in Section 3 once the corresponding forward models have been constructed and the available observations collected. These are typically classified as either gradient-based or gradient-free algorithms. Examples include simplex, steepest descent, Newton-Raphson search, evolutionary computation (e.g. genetic algorithms), reinforcement learning, numerical Bayesian via Markov Chain Monte Carlo (MCMC), and annealing-type algorithms. For instance, the Nelder–Mead gradient-free simplex method can be used wherever a simplex defined by $p + 1$ vertices in p-dimensional space defines a convex hull or volume in search space, with p equal to the number of parameters being estimated. The loss function is evaluated at each of these points, one is replaced, and the process repeated until a local minimum is contained within a small simplex volume. It is customary to make the initial simplex large enough to encompass all reasonable values of the model parameters.

To find a solution, it is important that the inverse problem be well-posed, even though it may likely be ill-posed as initially formulated. Well-posed problems exhibit three desirable characteristics: existence, uniqueness, and stability of the solution. While ill-posed inverse problems can arise from a loss of dimensionality, their typical fallout is violation of the stability condition. The effects of ill-posedness may be mitigated by the inclusion of any prior knowledge of constraints on the parameter statistic. Alternatively, additional observations may allow the estimation of incomplete but meaningful statistical metrics.

Given the richness of available stochastic search and optimization methods, a large number of software packages are available for solving the inverse problem. The following list of techniques and software packages covers capabilities that may be relevant for the proposed analytical tool.

Techniques – Newton's, steepest descent, conjugate gradient, stochastic gradient-based, least-mean-squares, recursive-least-squares, finite-difference, interior point, hill climbing, sample path, simulation-based and MCMC, particle swarm optimization, ant colony optimization, simulated annealing, Robbins-Monro stochastic approximation, Kiefer-Wolfowitz stochastic approximation, simultaneous perturbation stochastic approximation, direct search, Tabu search, and nonlinear dynamic reconstruction methods; linear (e.g. simplex), quadratic, and nonlinear programming (e.g. Nelder-Mead and trust-region), firefly, and genetic algorithms.

Packages – Mathematica/Optimization, Knitro, IBM CPLEX, IMSL numerical libraries, Matlab/Optimization and Global optimization toolboxes, MINPACK, LINDO Systems/Optimization, VR&D/Design Optimization Tools (DOT), and Large Scale Optimization Software Library (BIGDOT)

The list of stochastic search and optimization techniques above is too extensive for individual detailed descriptions. However for the purpose of illustration and completeness, more detailed descriptions are given below of the MCMC and evolutionary programming (EP) methods for solving general inverse problems.

The MCMC method begins with an educated “guess” posed as the solution to a difficult inverse problem. A forward model of the process is then run to predict the output data. The algorithm compares the predicted data (e.g. activity indicator estimates) against actual data (e.g. activity indicator observations) to decide whether to accept the current proposal as a better approximation, or to back up to the most recently accepted model and guess again. Rather than a single “best” structure, the MCMC engine generates a range of plausible structures and the corresponding probabilities that they are correct, which is known as the Bayesian “posterior” distribution. This facilitates decision analysis and needs-based experimental planning. As an important aside, if the forward model is expensive or slow to run, then code emulation (Conlin et al., 2011) provides an effective shortcut that substitutes model approximations via the emulator for actual code runs inside the MCMC loop.

The Stochastic Engine (Aines et al., 2004) is an efficient implementation of MCMC methodology. In particular, it allows the analyst to construct a reasonable estimate of the state of nature that is consistent with observed data and modeling assumptions. The key engine output is an estimate of the posterior distribution, which is the conditional probability distribution of the state of nature, given the data. In applications, the state of nature may refer to a complicated, multi-attributed feature like the lithology map of a volume of earth, or to a particular related parameter of interest, e.g. the centroid of the largest contiguous sub-region of specified lithology type. The posterior distribution can be thought of as the best stochastic description of the state of nature that incorporates all pertinent physical and theoretical models as well as observed data. Characterization of the posterior distribution is the primary goal in the Bayesian statistical paradigm. In applications of the Stochastic Engine, however, analytical calculation of the posterior distribution is typically precluded, and only a sample drawn from the distribution is feasible. The engine's MCMC technique, which employs the Metropolis-Hastings algorithm, provides a sample in the form of a sequence (chain) of possible states of nature. The sequencing is motivated by consideration of comparative likelihoods of the data. Multiple chains are often generated, to demonstrate convergence.

On the other hand, EP is attractive because it can be applied to highly non-linear forward models with discontinuous functions. EP is based on biological evolution, in which many offspring are created by randomizing guesses at input variables, which are then used to produce model predictions of facility indicators. The most successful offspring are defined to be those that produce the best agreement with facility indicators according to some skill or fitness score. Those offspring are re-randomized to produce another generation, from which the most successful offspring are re-randomized. This process continues until the skill score does not get sufficiently smaller with successive generations.

6. Illustrative examples

To illustrate how FM capabilities could be integrated and utilized under the proposed framework for nonproliferation analysis, five facility examples are discussed next. Although still of practical value, these examples have been deliberately formulated so as to remove any possibility of revealing sensitive information. The examples include enrichment, fuel fabrication, nuclear power generation, and fuel reprocessing. For brevity, we consider only declared facilities with full access allowed. All five facility examples describe: (1) proliferation concern(s); (2) available data; (3) forward model(s) used in the inverse problem(s); (4) the inverse problem(s), and (5) how estimated model parameters can be used by the analyst.

6.1. Example 1: LEU enrichment facility misuse

The concerns are overproduction of low enriched uranium (LEU) or illicit production of highly enriched uranium (HEU) (Carchon et al., 2011). Overproduction of LEU could suggest intent to enrich to HEU at another facility/state. Because of IAEA inspection resource limitations, the desired "continuity of knowledge" regarding facility operations contains gaps. For example, some UF_6 cylinders could be loaded into the plant and never declared.

Available data include both traditional NMA and process monitoring (PM). Gaps in data to support NMA are described in Carchon et al. (2011). To address these gaps, PM is being explored, for example, by monitoring load cells which probably cannot be bypassed during cylinder loading (Carchon et al., 2011). Such load cell monitoring could provide continuity of knowledge regarding facility operation. PM is also used to detect illicit production of HEU including both periodic environmental sampling and the continuous enrichment monitor (CEMO) using a gamma detector to detect high ^{235}U enrichments.

Forward models always include mass balances used in NMA, and models of detector quality as summarized by σ_S and σ_R (Section 5.3). This allows the inventory difference (ID), also known as the material balance, to be evaluated statistically using an estimate of the standard deviation of the ID, σ_{ID}, for agreement with the null hypothesis, that no SNM has been lost during the balance period. Forward models for PM include material balances for the load cells and modeling of associated facility misuse behavior. Gamma detectors can monitor header pipes outside the inaccessible cascade hall that houses gas centrifuges. The CEMO outputs a go/no-go signal intended to detect HEU. However, various measurement challenges exist, including deposits on the pipe walls, very low pipe pressures, and heterogeneous hold-up in the pipes. These challenges add noise to the signal and hinder the ability of CEMO to detect HEU in the pipes. Forward models for CEMO include the source terms, transport through the pipes/containers, and the detector response. Appropriate forward models include MCNP applications which can be used to evaluate these measurement challenges and develop noise mitigation strategies. A complementary approach (Dixon et al., 2007) to detect HEU involves neutron monitoring of a vacuum system cold trap that is also accessible and outside the cascade. Again, MCNP can predict the impact of resident ^{235}U in the trap at the time HEU production begins, thereby facilitating the ability of neutron monitoring (of neutrons produced by ^{234}U) which provides an indirect measurement of ^{235}U.

The inverse problem for NMA is to use the measured ID to estimate the true SNM loss, or to test the hypothesis that the true loss is 0 (except for nominal process losses). For continuous load cell monitoring, the inverse problem is to infer whether the facility is operated as declared (or whether, for example, undeclared feed material was introduced). For CEMO, MCNP is the main forward model in conjunction with measured gamma counts at various energies to infer whether HEU is present in the pipes. Carchon et al. (2011) describe another role for forward modeling to address the inverse problem of whether the cascade hall is being improperly used as follows. Inspector access to the centrifuge cascade halls is extremely limited or denied. However, improper operation of the cascade hall could lead to excess LEU or HEU production. A physical model of the centrifuge cascade hall (Delbeke, 2009) can be used in conjunction with frequent measurements of the feed, product, and tails cylinders to help assess whether the facility is operating as declared. A cascade hall model can help confirm whether unusual cylinder measurements, particularly of tails cylinder enrichments, are indicators of a possible diversion scenario.

Estimated parameter values include the estimated true ID (using the measured ID and forward models of the assay methods' capabilities to estimate σ_{ID}), the true material enrichment at various facility locations (using a gamma-based CEMO or neutron-based cold trap monitoring, which is the key source term in MCNP for CEMO or for the neutron-based detector), and the true material throughput as estimated using continuous load cell monitoring and periodic enrichment measurements. All these model parameter values are estimated periodically and provide the analyst a data- and model-driven basis for assessing whether the facility is operating as declared.

6.2. Example 2: LEU and/or mixed oxide fuel fabrication facility misuse

The material form is LEU and the major concerns are overproduction or removal of LEU for use in producing Pu in a hidden reactor. Because there should be no capability to produce HEU and because Pu production requires a hidden reactor, LEU fuel fabrication is not considered a high proliferation threat activity; nevertheless, illicit misdirection of LEU is possible, so verification and inspection are required. At a mixed oxide facility, both LEU and Pu are present so diversion of Pu and/or U is a concern.

Available data include traditional NMA and PM, with PM being particularly important in estimating the Pu held up in processing glove boxes. Estimates of the amount of Pu held up in glove boxes can be used to support NMA and to monitor for SNM diversion from the glove boxes.

Forward models always include mass balances used in NMA, and models of detector quality as summarized by σ_S and σ_R (Section 5.3) so that the ID can be statistically evaluated using an estimate of σ_{ID} for agreement with the null hypothesis that no SNM has been lost during the balance period. In one example of PM used to support NMA (Shimizu et al., 2006), a method is described using MCNP to relate Pu distributed in complicated geometries in a glove box to neutrons detected in surrounding detectors. This forward model involves an application of MCNP that simulates generation, transport, and detection of neutrons. The observed neutron counts can then be used with the forward model to inject Pu amounts in small volume elements ("voxels") contained within the glove box. In a second example, extensions to multiple glove boxes and/or other large volume elements is described (Nahamura et al., 2010), again using an application of MCNP as the forward model to simulate generation, transport, and detection of neutrons. The corresponding distributed source term analysis (DSTA) approach is an interesting application of "errors in variables," in which errors in the forward model play the role of errors in predictors. In both examples, the forward model is used to interpret detected neutron count rates so that Pu inventory within each voxel can be inferred.

As in any facility that uses NMA, the inverse problem for NMA is to use the measured ID to estimate the true SNM loss, or to test the hypothesis that the true loss is 0 (except for innocent process losses).

Estimated parameter values include the estimated true ID (using the measured ID and forward models of the assay methods' capabilities to estimate σ_{ID}). The ID is estimated periodically and provides the analyst a data- and model-driven basis for assessing whether the facility is operating as declared. The neutron-based glove box monitoring also provides a direct capability to detect undeclared removals of Pu from glove boxes, which could be beneath the lower limit of Pu loss detection capability of the NMA system.

6.3. Examples 3 and 4: Power production reactor misuse

Two different power production reactor misuse examples are considered below. One, motivated by Heasler et al. (2006), involves graphite moderated reactors, while the other, motivated by Ougouag et al. (2002a), Ougouag and Gougar (2001), and Ougouag et al. (2002b), entails reactors with on-line refueling capability (e.g. pebble bed modular reactors).

6.3.1. Graphite-moderated reactor example

The concern is overproduction of Pu or verification of declared total Pu produced at a given reactor. Because Pu is controlled under non-proliferation agreements, an estimate of total Pu production is often required and declaration of total Pu may need to be verified.

Available data include samples extracted from the graphite moderator of the reactor under consideration, and reactor information. Isotopic ratios of trace elements from the extracted samples are measured with mass spectrometry – thermal ionization mass spectrometry (TIMS) for U or Pu isotopic ratio determinations, and secondary ion mass spectrometry (SIMS) for boron isotopic ratios. Thus, at a given location, the TIMS mass spectrograph provides isotopic ratios of key U and Pu isotopes. Reactor information, on the other hand, may include reactor core dimensions, fuel rod specifications, and operating history. The availability and accuracy of reactor information generally determines the number of samples that need to be extracted and the uncertainty of the resulting Pu production estimate.

Two forward models are used sequentially to estimate the total Pu production from isotopic ratio measurements. The first step is a statistical analysis, in which local Pu fluence is estimated from isotopic ratios measured in the extracted samples by mass spectrometry, using a lattice physics code such as Winfrith Improved Multi-group Scheme (WIMS) (Newton et al., 2008). The second step is also a statistical analysis in which a global three-dimensional (3-D) linear regression model is used to fit a 3-D Pu fluence field for the entire reactor to the local Pu fluence estimates. A 3-D stochastic reactor physics code like KENO[5] (Bowman, 2008) is used to compute the basis functions utilized by the 3-D regression model.

The inverse problem in the first step is to use the measured isotopic ratios to estimate the Pu fluence value. Isotopic ratio curves generated by WIMS for specific Pu fluence values are related to the ratios measured with mass spectrometry. Solution of the first inverse problem finds the Pu fluence value that minimizes a quadratic loss function based on the sum of the squared errors calculated by subtracting measured isotopic ratios from the estimated isotopic curves. Pu fluence estimates provide the local Pu production rate at each sample location. In the second step, the inverse problem is to use the local Pu fluence values determined in the first step to estimate a set of unknown parameters that determine the shape of the global fluence field. The unknown parameters in the fluence field model, which is formulated using basis functions calculated by a 3-D reactor physics code like KENO, are fitted to the local Pu fluence estimates from the first step using a global linear weighted regression model. Thus, solution of the second inverse problem finds values of the shaping field parameters that result in a fluence field as close as possible to the local fluence estimates. The adequacy of this global linear regression model depends upon the set of basis functions or reactor fluence profiles selected, which are computed using 3-D reactor physics models and reactor operating history.

Estimated parameter values include an estimate of the total Pu production determined by integrating the fitted 3-D Pu fluence field for the reactor over all of the fuel channels. This total Pu production estimate gives the analyst a data- and model-driven basis for assessing whether the reactor under consideration was operated as declared. Other estimated parameters include the shaping field parameters for the global Pu fluence field as well as the local Pu fluence values.

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[5] KENO is not an acronym, but a reference to the well-known game of chance (per Parks C.V., (2011)).

6.3.2. <u>On-line refueled reactor example</u>

The concern is clandestine dual use of a power reactor to produce Pu. In particular, the online defueling and refueling capabilities of certain reactor designs (e.g. pebble bed reactors) facilitate their potential use as production facilities for weapons materials. One possible covert dual use scenario would involve illicitly feeding natural U-graphite target pebbles, optimized to minimize the decrease in reactivity, into the inner reactor reflector. It could include deliberately keeping the feed rate sufficiently small to minimize the impact on reactor neutronics and power plant operations. In addition, the target natural U pebbles could be circulated once and then removed in a "once through then out" (OTTO) operation for optimum plutonium isotopic quality. This scenario implies the retrieval and extraction of targets from the reactor prior to their detection by monitoring systems.

Available data may include measurements of power production, rate of fresh fuel usage, refueling needs, and discharge burn-up and isotopics. Power production and periodic fuel needs are usually highly predictable. Consequently, Pu production can be estimated from these measurements. In particular, introduction of U targets for Pu production will result in a reduction in core reactivity as well as energy production, and in an increase in the fresh fuel requirement to maintain criticality and reactivity. Lower burn-up at discharge is likewise expected. Departures from anticipated patterns for these parameters could be viewed as suspicious and possibly indicative of attempts at fuel diversion for dual use. An effective monitoring system would keep track of these parameters for the purpose of detecting illicit operations with dual use intent.

Forward models include reactor physics codes tailored for specific reactor designs, such as PEBBED (Terry et al., 2002), which is intended for use with pebble bed reactors. These codes include empirical data and typically can compute with high accuracy a variety of operating parameters, including power production, refueling needs, and the spatial distribution of burn-up and principal nuclides throughout the reactor core and in the discharged fuels.

One conceivable inverse problem is to estimate the total Pu production in the reactor by calculating the number of targets containing natural uranium that might have been illicitly inserted into the core for Pu production based on the measured energy production rate. The number of targets that need to be inserted into a reactor can be related to the measured power production with a forward model. Thus, the inverse problem finds the total number of inserted targets that minimizes a loss function that depends on the difference between the measured energy production rate and the rate estimated by assuming the given number of targets. Similar inverse problem approaches can be envisioned using, and possibly combining other measurable parameters, e.g. the rate of fresh fuel consumption, fuel needs, and discharge burn-up and isotopics. This total Pu production estimate then gives the analyst a basis for assessing whether the target reactor is being operated as declared or illicit production may be in progress.

Estimated parameter values include the number of targets containing natural uranium that were inserted into the core for illicit Pu production as well as an estimate of the total Pu production rate.

6.4. Example 5: Fuel reprocessing facility misuse

The principal concern with fuel reprocessing is the potential for separation and diversion of SNM, specifically Pu, for weaponization. This is what drove the decision to stop reprocessing in the United States in the 1970s (Andrews, 2008). Making detection of covert diversion easier and more definitive would help overcome the single biggest obstacle to closing the fuel cycle and minimizing the volume of high level wastes that need to be isolated and stored in waste repositories. The example considered here is from a recent paper by Orton et al. (2011), which focuses on the monitoring of process variables solely within a declared facility. Not considered here is the more challenging problem of assessing the processing intent of hidden or denied facilities based on limited, discontinuous external observations or indicators. However, in principle, the approach would be identical.

Fuel reprocessing facilities separate dissolved irradiated fuel elements into separate U and Pu product streams, along with fission product waste stream(s). Widely used and accepted reprocessing methods like PUREX rely on solvent extraction between two immiscible phases (aqueous and organic) to achieve separation between the elemental constituents of the dissolved spent fuel elements (Godfrey et al., 2000). In the situation described by Orton et al. (2011), the available data include, in addition to traditional NMA and PM, gamma emission spectra of the aqueous and organic phases in the reprocessing plant as well. Of particular importance in the NMA is the history of the spent fuel inventory. In addition to current, real-time measurements, a historical database of archived measurements is also required.

The forward models should allow the analyst to predict the U and Pu product streams given the feed stream and the process operating conditions. A gamma spectrum would then be available for each process stream. Forward models include point depletion codes like ORIGEN-ARP, chemical process models like AMUSE , and detector models like SYNTH (Hensley et al., 1995). ORIGEN-ARP would be used to compute detailed isotopic feed stream compositions based on the available spent fuel history. Given a range of process scenarios, U and Pu product streams could be predicted using AMUSE. The range considered should include both nominal and off-nominal conditions. Finally, synthetic gamma spectra for each process stream prediction could be computed using SYNTH.

The inverse problem would be: estimating whether normal or off-normal operation is indicated, given process stream gamma spectra (and traditional NMA and PM data). Variations in stream composition can be expected during normal and off-normal operations. Furthermore, on-line gamma ray monitors will have limited resolution and inherent measurement uncertainty and noise. An approach can be envisioned combining gamma spectra data with other NMA or PM measurements such as waste stream flow or indicators of off-normal container or material movement. There generally will not be a unique solution to the inverse problem, but through statistical analysis the most probable scenario should be discernible.

Estimated parameter values would include the probability whether a given event is normal or off-normal. Furthermore, a material balance would be provided that could be used to determine the likelihood that an off-normal event is either an unintended process upset or an undeclared diversion.

7. Summary, challenges, and future work

The problem of modeling facilities engaged in some aspect of nuclear weapons production is a subset of the more general problem of modeling any facility that produces something of interest but which cannot be directly accessed. Information about such a facility may be disparate, intermittent, erroneous, deliberately misleading, and may have hard-to-estimate uncertainties associated with it. Indicators of facility activity can be used to identify and quantify facility production via models, which may combine physics-based, empirical/statistical, economic, cultural/human factor, event-driven (discrete event), and time-driven (continuous) components. An essential component of a facility model is the method used to estimate uncertainties in the input data and in the model itself, and to track those uncertainties through the model calculations to determine their cumulative impact on the reliability and accuracy of the model predictions.

The software and other analytical methods described in this paper cover many aspects of FM. For illustrative purposes, this paper discussed only a few specific codes and data that can be applied to nuclear proliferation analysis, as well as more general algorithms and analytical methods that can be applied to other types of facilities. The problems required general purpose techniques, such as inverse problem methods and integrated modeling.

A basic conclusion is that the analytical tools needed to build a comprehensive model of a facility possibly engaged in some aspect of nuclear proliferation already exist. However, the effort to combine existing integrated modeling software with nuclear proliferation-specific codes would be a significant undertaking. For decades, the main quantitative figure of merit for inspected facilities has been σ_{ID}. The proposed integration of multiple data sources from process monitoring and materials accounting extends the system figure of merit to system alarm probabilities for a range of misuse or diversion scenarios. Such an approach requires comprehensive modeling of the effects of diversion scenarios and multivariate data analyses to combine data from various subsystems. Despite the associated technical challenges, we anticipate moving in the direction of using more data streams, modeling, and analyses, particularly when safety and safeguards concerns are considered simultaneously. Two benefits from such an effort would be:

The combination of disparate, uncorrelated information sources should produce higher-confidence model predictions, provided that appropriate statistical methods are used to quantify the combined impact of the different uncertainties.

Construction of a comprehensive facility model for nuclear proliferation will require application of advanced methods to search through, assimilate, evaluate and visualize the often large amounts of data that must be examined to create inputs for the model. Representative examples of these methods are described in this paper. Newer, relatively untested methods which have been applied to related problems, such as detection of terrorist networks, should also be considered.

This paper does not address the particular problems posed by data sources that are largely classified. Combination of a wide variety of data sources may entail acquisition of classified data from multiple government organizations. Although some development work could be done in an unclassified environment, much of it would have to be done in secure areas.

Finally, although most, if not all, of the software needed to construct a comprehensive nuclear proliferation facility model exists, there would be opportunities to conduct some basic research. The following passage is from a recent Science article: “Drawing on approaches from artificial intelligence, computer programs increasingly are able to integrate published knowledge with experimental data, search for patterns and logical relations, and enable new hypotheses to emerge with little human intervention” (Evans and Rzhetsky, 2010). If actually feasible, automated hypothesis generation would be an important tool for the busy analyst who has to try to track and understand activities at many (possibly denied) sites at the same time.

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References

–, (2009), SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation. Oak Ridge National Laboratory, Oak Ridge, TN.
–, (2010a), STARLIGHT Visual Information System (VIS). Pacific Northwest National Laboratory, Richland, WA.
–, (2010b), Treaty on the Non-Proliferation of Nuclear Weapons. U.S. Department of State.
–, (2011a), Aspen Custom Modeler, V7.2 ed. Aspen Technology, Inc., Burlington, MA.
–, (2011b), Aspen Plus, V7.2 ed. Aspen Technology, Inc., Burlington, MA.
–, (2011c), Aspen Plus Dynamics, V7.2 ed. Aspen Technology, Inc., Burlington, MA.
–, (2011d), CHEMCAD, 6.2 ed. Chemstations, Inc., Houston, TX.
–, (2011e), MATLAB® 2010b ed. The MathWorks, Inc., Natick, MA.
–, (2011f), ModelCenter, 9.0 ed. Phoenix Integration, Inc., Wayne, PA.
–, (2011g), PRO/II™, 9.0 ed. Invensys PLC, Invensys Operations Management/SimSci-Esscor, Plano, TX.
–, (2011h), ProSimPlus. ProSim SA, Labege, France.
–, (2011i), R, 2.12.2 ed. The R Foundation for Statistical Computing, Vienna, Austria.
–, (2011j), SALOME, 5.1.5 ed. Open Cascade S.A.S., Guyancourt, France.
–, (2011k), World Nuclear Power Reactors & Uranium Requirements, 6 January 2011. World Nuclear Association.
Aines R.D., Nitao J.J., Hanley W.G., Carle S., Ramirez A.L., Newmark R.L., Johnson V.M., Glaser R.E., Sengupta S., Kosovic B., Dyer K.M., Henderson K.A., Sugiyama G.A., Hickling T.L., Franz G.A., Pasyanos M.E., Jones D.A., Grimm R.J., Johannesson G., Levine R.A., (2004), Stochastic Engine Final Report: Applying Markov Chain Monte Carlo Methods with Importance Sampling to Large-Scale Data-Driven Simulation. Lawrence Livermore National Laboratory, Livermore, CA.
Andrews A., (2008), Nuclear Fuel Reprocessing: U.S. Policy Development. The Library of Congress, Congressional Research Service, Washington, DC.
Bathke C.G., Ebbinghaus B.B., Sleaford B.W., Wallace R.K., Collins B.A., Hase K.R., Jarvinen G.D., Bradley K.S., Ireland J.R., Johnson M.W., Prichard A.W., Smith B.W., (2009), The Attractiveness of Materials in Advanced Nuclear Fuel Cycles for Various Proliferation and Theft Scenarios, Global 2009, Paris, France, Paper 9543.
Bowman S.M., (2008), KENO-VI Primer: A Primer for Criticality Calculations with SCALE/KENO-VI Using GeeWiz, p. Medium: ED.
Brown F.B., Barrett R.F., Booth T.E., Bull J.S., Cox L.J., Forster R.A., Goorley T.J., Mosteller R.D., Post S.E., Prael R.E., Selcow E.C., Sood A., Sweezy J., (2002), MCNP Version 5. Los Alamos National Laboratory, Los Alamos, NM.
Burr T., Fry H., McVey B., Sander E., Cavanaugh J., Neath A., (2008), Performance of Variable Selection Methods in Regression Using Variations of the Bayesian Information Criterion. Communications in Statistics - Simulation and Computation 37, 507 - 520.
Burr T.L., Charlton W.S., Nakhleh C.W., (2005), Assessing confidence in inferring reactor type and fuel burnup: A Markov chain Monte Carlo approach. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 555, 426-434.

Burr T.L., Coulter C.A., Howell J., Wangen L.E., (2003), Solution Monitoring: Quantitative and Qualitative Benefits to Nuclear Safeguards. Journal of Nuclear Science and Technology 40, 256-263.
Burr T.L., Suzuki M., Howell J., M.S. Hamada, Longo C., (2011), Signal Estimation and Change detection in Tank Data for Nuclear Safeguards. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment to be published.
Carchon R., Dechamp L., Eklund L.G., Janssens W., Mercurio G., Peerani P., Richir P., (2011), Load cell monitoring in Gas Centrifuge Enrichment Plants: Potentialities for improved safeguard verifications. Nuclear Engineering and Design 241, 349-356.
Chadwick M.B., Oblozinský P., Herman M., Greene N.M., McKnight R.D., Smith D.L., Young P.G., MacFarlane R.E., Hale G.M., Frankle S.C., Kahler A.C., Kawano T., Little R.C., Madland D.G., Moller P., Mosteller R.D., Page P.R., Talou P., Trellue H., White M.C., Wilson W.B., Arcilla R., Dunford C.L., Mughabghab S.F., Pritychenko B., Rochman D., Sonzogni A.A., Lubitz C.R., Trumbull T.H., Weinman J.P., Brown D.A., Cullen D.E., Heinrichs D.P., McNabb D.P., Derrien H., Dunn M.E., Larson N.M., Leal L.C., Carlson A.D., Block R.C., Briggs J.B., Cheng E.T., Huria H.C., Zerkle M.L., Kozier K.S., Courcelle A., Pronyaev V., van der Marck S.C., (2006), ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology. Nuclear Data Sheets 107, 2931-3060.
Conlin J.L., Tobin S.J., LaFleur A.M., Hu J., Lee T., Sandoval N.P., Schear M.A., (2011), On Using Code Emulators and Monte Carlo Estimation to Predict Assembly Attributes of Spent Fuel Assemblies for Safeguards Applications. to appear in Nuclear Science and Engineering.
Delbeke J.F.A., (2009), Theoretical Analysis To Assess the Separative Power of Reconfigured Cascades of Predesigned Gas Centrifuges. Industrial & Engineering Chemistry Research 48, 4960-4965.
Dixon E.T., Pickrell M.M., Geist W.H., Boyer B.B., Burr T.L., Beddingfield D.H., (2007), Neutron Monitoring of Vacuum System Cold Traps to Detect Undeclared HEU Production at Gas Centrifuge Enrichment Plants, 48th Institute of Nuclear Materials Management Annual Meeting, J. W. Marriott Starr Pass Resort, Tucson, AZ.
Evans J., Rzhetsky A., (2010), Machine Science. Science 329, 399-400.
Gauld I.C., Hermann O.W., Westfall R.M., (2002), ORIGENS-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms. Oak Ridge National Laboratory, Oak Ridge, TN.
Godfrey W.L., Hall J.C., Townes G.A., (2000), Nuclear Reactors, Chemical Reprocessing. John Wiley & Sons, Inc.
Goldschmidt P., (2004), The Additional Protocol and the Road to Integrated Safeguards. Journal of Nuclear Materials Management 32, 4-5.
Gruber T.R., (1993), A Translation Approach to Portable Ontology Specifications. Knowledge Acquisition 5, 199-220.
Haeck W., (2009), VESTA User's Manual, Version 2.0.0. Institut de Radioprotection et de Surete Nucleaire.
Haeck W., (2011), personal communication. Institut de Radioprotection et de Surete Nucleaire.
Hanan N.A., Olson A.P., Pond R.B., Mates J.E., (1998), A Monte Carlo Burnup Code Linking MCNP and REBUS. Argonne National Laboratory, Argonne, IL.
Hastie T., Tibshirani R., Friedman J., (2009), The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition. Springer, Newe York.

Heasler P.G., Burr T., Reid B., Gesh C., Bayne C., (2006), Estimation procedures and error analysis for inferring the total plutonium (Pu) produced by a graphite-moderated reactor. Reliability Engineering & System Safety 91, 1406-1413.
Hensley W., McKinnon A., Miley H., Panisko M., Savard R., (1995), SYNTH: A spectrum synthesizer. Journal of Radioanalytical and Nuclear Chemistry 193, 229-237.
Hermann O.W., (2000), San Onofre PWR Data for Code Validation of MOX Fuel Depletion Analyses - Revision 1. Oak Ridge National Laboratory, Oak Ridge, TN.
Hermann O.W., Bowman S.M., Brady M.C., Parks C.V., (1995), Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses. Oak Ridge National Laboratory, Oak Ridge, TN.
Hermann O.W., Parks C.V., Renier J.P., Roddy J.W., Ashline R.C., Wilson W.B., LaBauve R.J., (1981), Multicode Comparison of Selected Source-Term Computer Codes. Oak Ridge National Laboratory, Oak Ridge, TN.
Ilas G., Gauld I.C., (2009), SCALE 6 Analysis of Isotopic Assay Benchmarks for PWR Spent Fuel. Transactions of the American Nuclear Society 101, 691-693.
Inselberg A., (1985), The plane with parallel coordinates. The Visual Computer 1, 69-91.
Klein M., Fensel D., Harmelen F.v., Horrocks I., (2001), The relation between ontologies and XML schemas. Linköping Electronic Articles in Computer and Information Science 6.
Krebs J.F., Pereira C., Frey K.P., Wardle K.E., (2010), Implementation of time-dependency into a spent fuel reprocessing plant model, AIChE Annual Meeting, Salt Lake City, UT.
Kuhl F., Weatherly R., Dahmann J., (1999), Creating Computer Simulation Systems: An Introduction to the High Level Architecture. Prentice Hall PTR, Upper Saddle River, NJ.
LaFleur A.M., Charlton W.S., Menlove H.O., Swinhoe M.T., Lee S.Y., Tobin S.J., (2010), Experimental Benchmark of MCNPX Calculations Against Self-Interrogation Neutron Resonance Densitometry Fresh Fuel Measurements, 51st Annual Meeting, Institute of Nuclear Materials Management, Baltimore, MD.
Li J., Yim M.-S., McNelis D.N., (2010), Model-based calculations of the probability of a country's nuclear proliferation decisions. Progress in Nuclear Energy 52, 789-808.
Moore R.L., Schnitzler B.G., Wemple C.A., Babcock R.S., Wessol D.E., (1995), MOCUP: MCNP-ORIGEN2 Coupled Utility Program. Idaho National Engineering Laboratory, Idaho Falls, ID.
Nahamura H., Beddingfield D.H., Hakamichi H., Kurita T., (2010), Concept of a New Glove Box Cleanout Assistance Tool (BCAT) by using Distributed Source-Term Analysis (DSTA), 51st Institute of Nuclear Materials Management Annual Meeting, Baltimore Marriott Waterfront, Baltimore, MD.
Newton T., Hosking G., Hutton L., Powney D., Turland B., Shuttleworth T., (2008), Developments within WIMS10, International Conference on the Physics of Reactors, "Nuclear Power: A Sustainable Resource", Casino-Kursaal Conference Center, Interlaken, Switzerland.
Olson A.P., (2011), personal communication. Argonne National Laboratory.
Olson P., Kalimullah M., (2010), A Users Guide to the PLTEMP/ANL V3.9 Code. Argonne National Laboratory, Argonne, IL.
Orton C.R., Fraga C.G., Christensen R.N., Schwantes J.M., (2011), Proof of concept simulations of the Multi-Isotope Process monitor: An online, nondestructive, near-real-time safeguards monitor for nuclear fuel reprocessing facilities. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 629, 209-219.

Ougouag A.M., Gougar H.D., (2001), Preliminary Assessment of the Ease of Detection of Attempts at Dual Use of a Pebble-Bed Reactor. Transactions of the American Nuclear Society 85, 115-117.
Ougouag A.M., Modro S.M., Terry W.K., Gougar H.D., (2002a), Rational Basis for a Systematic Identification of Critical Components and Safeguards Measures for a Pebble-Bed Reactor. Transactions of the American Nuclear Society 87, 367-368.
Ougouag A.M., Terry W.K., Gougar H.D., (2002b), Examination of the Potential for Diversion or Clandestine Dual Use of a Pebble-Bed Reactor to Produce Plutonium, 1st International Topical Meeting on High-Temperature Reactor Technology, HTR2002, Petten, Netherlands.
Pabian F., (2008), Commercial Satellite Imagery: Another Tool in the Nonproliferation Verification and Monitoring Tool-Kit, in: Doyle J.E. (Ed.), Nuclear Safeguards, Security, and NonProliferation: Achieving Security with Technology and Policy. Elsevier, Inc., Burlington, MA, pp. 239-244.
Parks C.V., (2011), personal communication. Oak Ridge National Laboratory.
Poston D.I., Trellue H.R., (1999), User's Manual, Version 2.0, for Monteburns, Version 1.0. Los Alamos National Laboratory, Los Alamos, NM.
Quix C., Kensche D., Li X., (2007), Matching of Ontologies with XML Schemas Using a Generic Metamodel, in: Meersman R., Tari Z. (Eds.), On the Move to Meaningful Internet Systems 2007: CoopIS, DOA, ODBASE, GADA, and IS. Springer Berlin / Heidelberg, pp. 1081-1098.
Rowe D.S., (1973), COBRA-IIIC: a digital computer program for steady state and transient thermal hydraulic analysis of rod bundle nuclear fuel elements. Battelle Pacific Northwest Laboratories, Richland, WA.
Sandler V., (2011), personal communication. Open CASCADE S.A.S.
Santamarina A., Bernard D., Blaise P., Coste M., Courcelle A., Huynh T.D., Jouanne C., Leconte P., Litaize O., Mengelle S., Noguère G., Ruggiéri J.-M., Sérot O., Tommasi J., Vaglio C., Vidal J.-F., (2009), The JEFF-3.1.1 Nuclear Data Library, JEFF Report 22, Validation Results from JEF-2.2 to JEFF-3.1.1. Nuclear Energy Agency, Organization for Economic Co-operation and Development.
Shibata K., Iwamoto O., Nakagawa T., Iwamoto N., Ichihara A., Kunieda S., Chiba S., Furutaka K., Otuka N., Ohsawa T., Murata T., Matsunobu H., Zukeran A., Kamada S., Katakura J.-i., (2011), JENDL-4.0: A New Library for Nuclear Science and Engineering. Journal of Nuclear Science and Technology 48, 1-30.
Shimizu J., Yamay K., Hiruta K., Fujimaki K., Menlove H., Swinhoe M.T., Miller M.M., Rael C.D., Marlow J.B., (2006), Development of Non- Destructive Assay System to Measure Pu Inventory in Glove Boxes, 47th Institute of Nuclear Materials Management Annual Meeting, Nashville Convention Center and Renaissance Hotel, Nashville, TN.
Spence R., (2007), Information Visualization: Design for Interaction, 2nd Edition ed. Pearson Education Limited, Harlow, England.
Tait J.C., Gauld I., Kerr A.H., (1995), Validation of the ORIGEN-S code for predicting radionuclide inventories in used CANDU fuel. Journal of Nuclear Materials 223, 109-121.
Tait J.C., Gauld I.C., Wilkin G.B., (1989), Derivation of Initial Radionuclide Inventories for the Safety Assessment of the Disposal of Used CANDU Fuel. Atomic Energy of Canada Limited.
Terry W.K., Gougar H.D., Ougouag A.M., (2002), Direct deterministic method for neutronics analysis and computation of asymptotic burnup distribution in a recirculating pebble-bed reactor. Annals of Nuclear Energy 29, 1345-1364.

Tufte E.R., (1997), Visual Explanations: Images and Quantities, Evidence and Narrative. Graphics Press, Cheshire, CT.
UNODA, (2011), NPT(in alphabetical order). United Nations Office for Disarmament Affairs.
Wegman E.J., (1990), Hyper-dimensional data analysis using parallel coordinates. Journal of the American Statistical Association 85, 664-675.
Wikipedia, (2010), XML. Wikipedia.
Xu Z., Hejzlar P., (2008), MCODE, Version 2.2: An MCNP-ORIGEN DEpletion Program. Massachusetts Institute of Technology, Cambridge, MA.

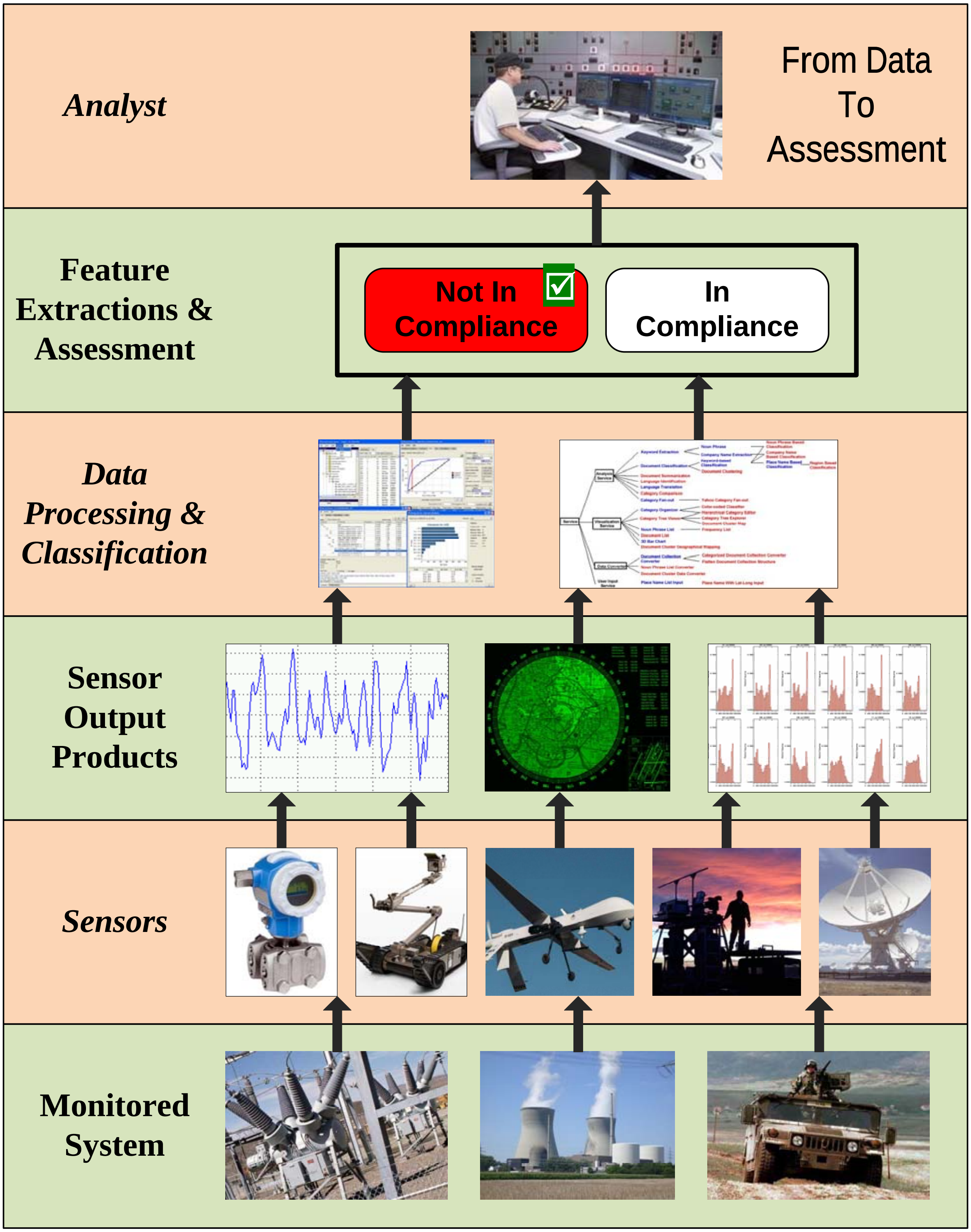

Figure 1 The task of the nonproliferation assessment analyst

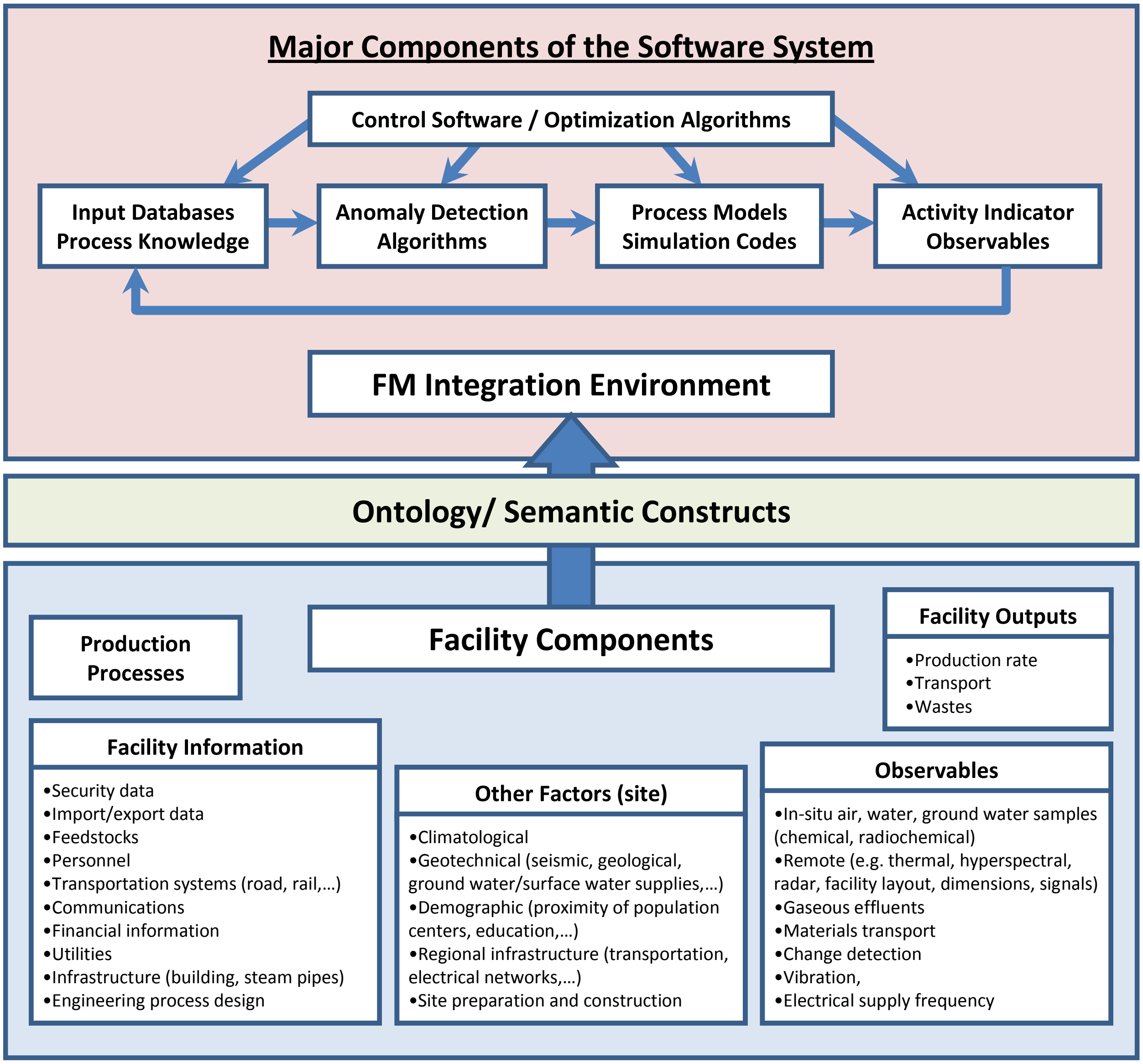

Figure 2 Schematic of complete facility model that relates different components of facility information to simulation code structure

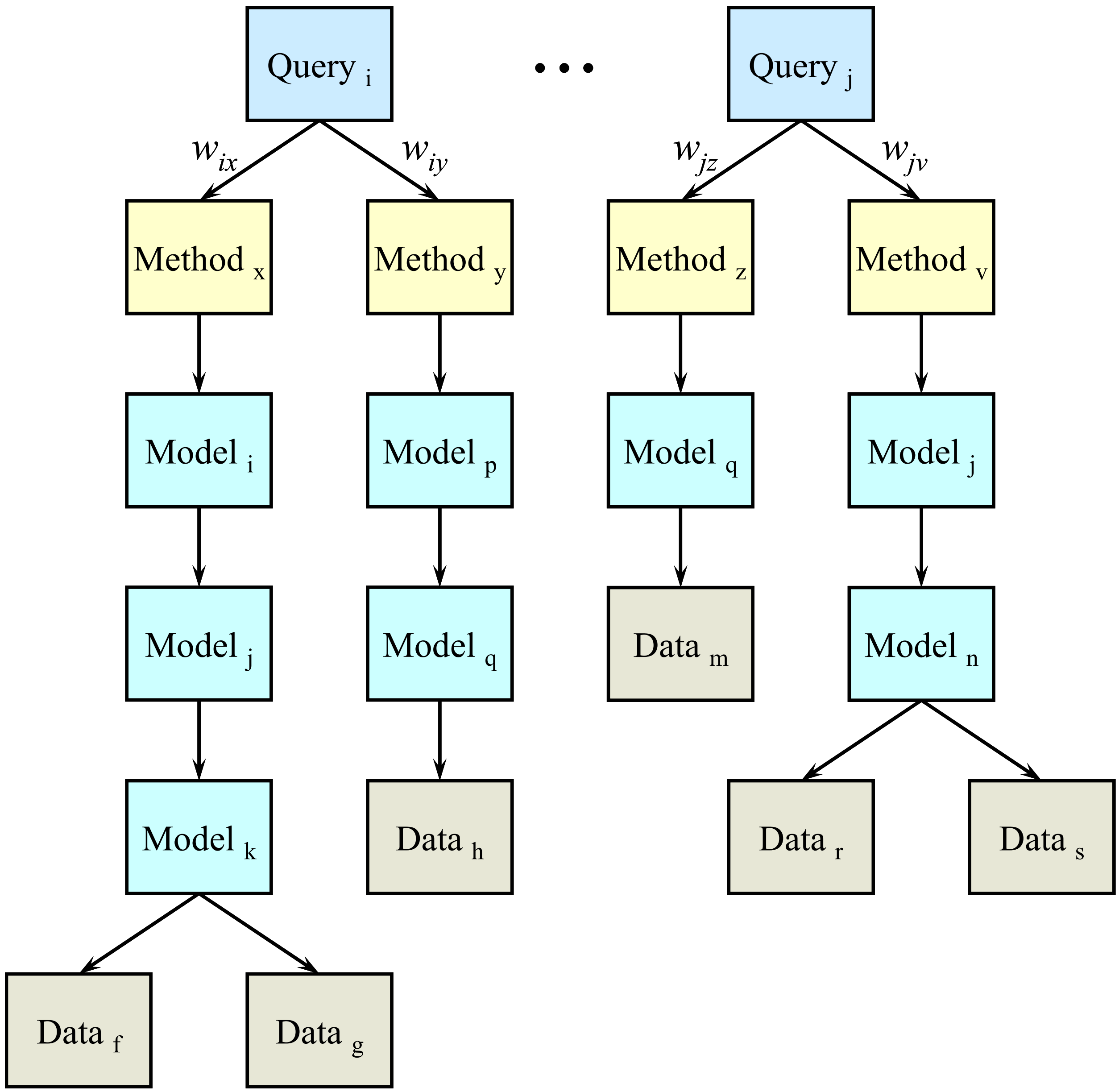

Figure 3 Semantic network relating queries to methods, models, and data

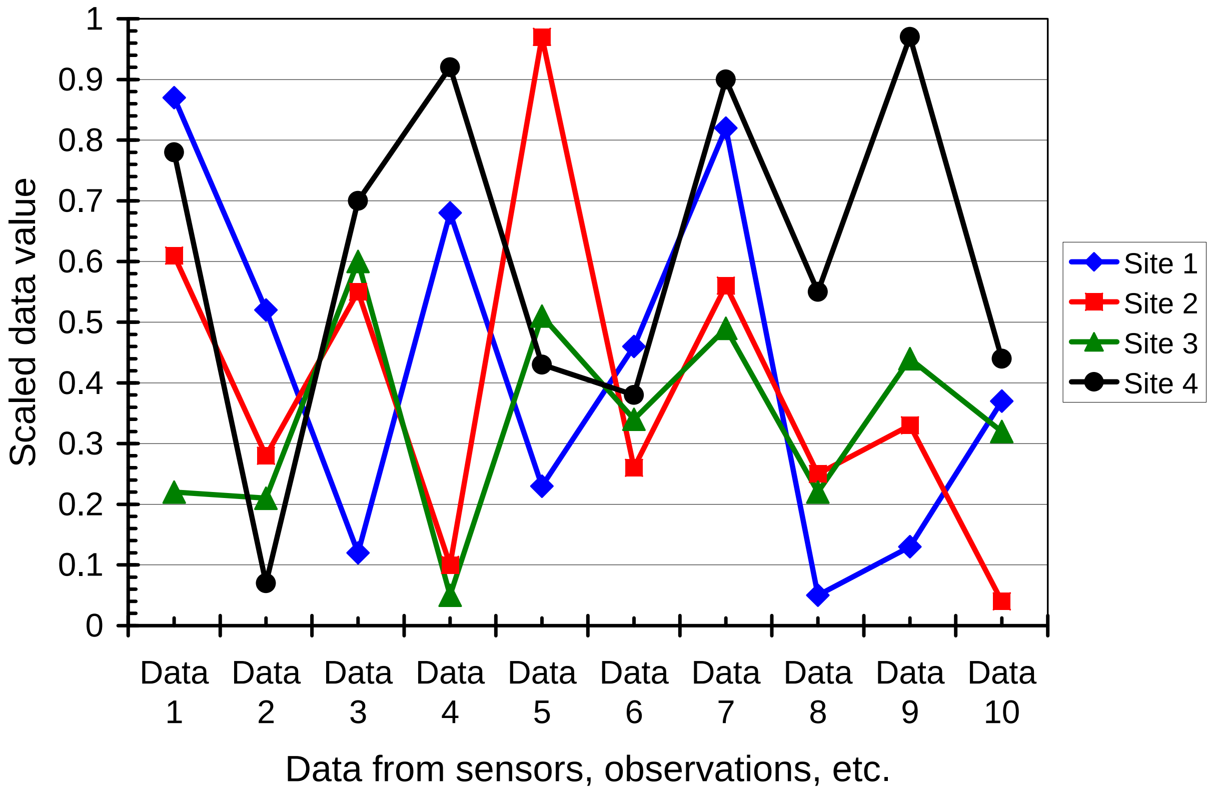

Figure 4 Parallel coordinates example for data visualization

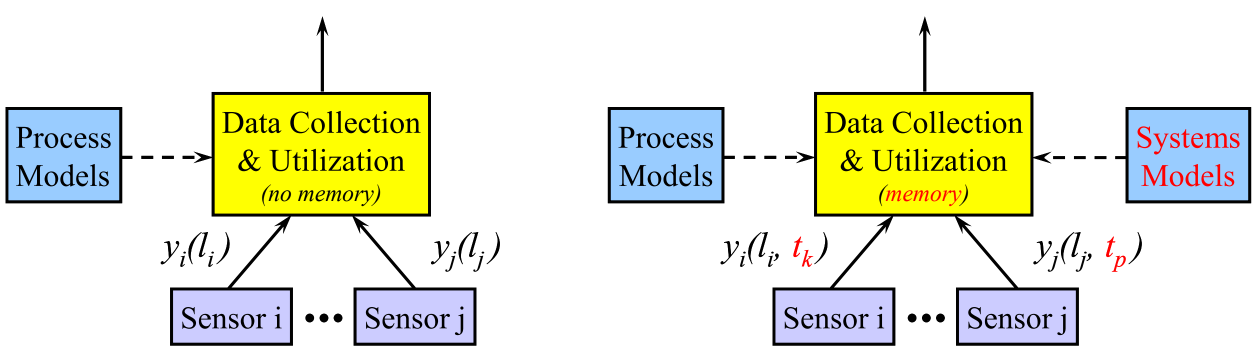

Figure 5 Differences among data-driven methods