Current Status of Predictive Transition Capability in Fuel Cycle Simulation

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Abstract – *This study has identified flexible, general, and performant algorithms available for application to simulating demand-driven deployment of nuclear fuel cycle facility capacity in a fuel cycle simulator. Accordingly, a review of current Nuclear Fuel Cycle (NFC) simulation tools was conducted to determine their current capabilities for demand-driven and transition scenarios. Additionally, the authors investigated promising algorithmic innovations that have been successful for similar applications in other domains such as economics and industrial engineering Finally, the applicability of such algorithms in the context of challenging nuclear fuel cycle simulation questions has been described.*

I. INTRODUCTION

Nuclear fuel cycle simulation scenarios may be described as constrained objective functions. The objectives are often systemic demands such as "achieve 1% growth for total electricity production and reach 10% uranium utilization." The constraints take the form of nuclear fuel cycle technology availability ("reprocessing begins after 2025 and fast reactors first become available in 2050"). To match the naturally constrained objective form of the scenario definition, NFC simulators must bring demand responsive deployment decisions into the dynamics of the simulation logic.

In particular, a NFC simulator should have the capability to deploy supporting fuel cycle facilities which enable a demand to be met. Take, for instance, the standard once through fuel cycle. Reactors may be deployed to meet an objective power demand. However, new mines, mills, and enrichment facilities will also need to be deployed to ensure that reactors have sufficient fuel to produce power. In many simulators, the unrealistic solution to this problem is to simply have infinite capacity support facilities. Alternatively, detailing the deployment timeline of all facilities becomes the responsibility of the user.

II. METHODS

A meta-review of previous NFC gap analyses helped to identify the high level capabilities of existing simulators. Among these, [1], [2] and [3] compared the capabilities of international NFC simulators via systematic transition scenario benchmarks. In [4] and [5], the ability of individual simulators to conduct transition scenarios is addressed, however the flexibility and performance of their varying facility deployment algorithms were not.

Primary references for an array of fuel cycle simulators were consulted to categorize facility deployment logic present in existing NFC simulators. Where the details of dynamic demand-driven simulation were unknown, this review individually investigated available tools. Fuel cycle simulators were categorized as having (1) no automated deployment at all, (2) deployment based on deterministic forecasting, or (3) an alternative method. The vast majority of existing simulators fall into the first two categories. The modeling limitations of both strategies will be discussed. Finally, this study will focus on alternative methods in existing simulators and promising potential methods which might be implemented in future simulators.

We reviewed existing public literature regarding 15 fuel cycle simulators to determine the extent to which those simulators (1) automatically deploy reactors to meet power demand and (2) automatically deploy supporting fuel cycle facilities to meet support demands. The fuel cycle simulation tools reviewed included:

- CAFCA (MIT) [6]
- CLASS (CNRS/IRSN) [7]
- COSI (CEA) [8, 1]
- Cyclus (UW) [9]
- DANESS (ANL) [10]
- DESAE (Rosatom) [1]
- DYMOND (ANL) [1]
- Evolcode (CIEMAT) [1]
- FAMILY (IAEA) [1]
- MARKAL (BNL) [11]

- NFCSim (LANL) [12]
- NGSAM (ORNL) [13]
- NUWASTE (NWTRB) [14]
- ORION (NNL) [11]
- VISION (INL) [11, 1]
- VISTA (IAEA) [15]

We found that automated deployment of supportive fuel cycle facilities is naïve or non-existent in most simulators, including Cyclus, the simulator under development by the authors. Additional details of this review and categorization will appear in the poster and upcoming full length article associated with this abstract.

For the majority of simulators, automated deployment is limited to deploying reactors based on changes in power demand. For example, as the simulation progresses, additional reactors are deployed to meet a power demand projection (e.g. 2% growth over 100 years). However, supportive fuel cycle facilities must also be deployed in response to (or, more realistically, in preparation for) reactor deployment. Typically, current simulators rely on manual deployment of fuel cycle facilities. To reduce effort and the likelihood of a failed simulation, the user often deploys all potentially necessary fuel cycle facilities at the start of the simulation with excess or infinite throughput capacities.

Current strategies can be categorized into four genres:

- **manual**: The user 'guesses' the future required fuel cycle facility deployments needed to support simulated reactors.
- **proportional**: Deployment of fuel cycle facilities is in direct proportion with reactor deployments (e.g. for every 10 new fast reactors, deploy a new reprocessing plant).
- **constrained reactor deployment:** Deployment of reactors is constrained by the existing and projected feedstock amounts.
- **predictive:** The simulator projects the feedstock needs of current and future deployed reactors based on other heuristics and look-ahead predictors.

The focus of this paper will be to improve on the current state of the art implementations of the fourth category above, predictive methods.

III. PROMISING ALGORITHMS

Various algorithms can be implemented in a NFC simulator to predict demand in future commodity markets. These can be divided into three major branches, Non-optimizing, Deterministic Optimizing, and Stochastic Optimizing. These vary in applicability, complexity, compute time, and accuracy. Examples of each of the three categories are explained in detail below.

III.A. Non-Optimizing (NO)
Non-optimizing algorithms predict future deployment schedules based on historical supply-demand data from the simulator. These algorithms do not attempt to meet demand optimally, thus the name 'non-optimizing'. The simple nature of this class of algorithms allows fast execution time, but only limited precision. The two non-optimizing algorithms explored in this paper are autoregressive moving average (ARMA) and autoregressive conditional heteroskedastic (ARCH) methods.

III.A.1 Autoregressive Moving Average (ARMA)
ARMA is a combination of two models, the Autoregressive and the Moving Average model. The Autoregressive model predicts future values with a linear curve fit of the latest datasets, and the Moving Average method does so by fitting the errors [16].

The model is referred to as ARMA(p,q), where the p and q represent the order (number of previous time step values fitted) of the autoregressive, and the moving average parts, respectively.

ARMA is applicable for 'well behaved' time series data, where there is little volatility. This makes ARMA a suitable candidate for demand prediction in the case of slowly changing power demand and corresponding reactor deployment.

III.A.2. Autoregressive Conditional Heteroskedastic (ARCH)
The ARCH model is similar to the ARMA model, except that it uses previous variance terms to calculate current error terms, instead of the value itself. This allows the model to be used in highly volatile time series (e.g. prediction of inflation or stock prices over time [17]).

A comprehensive fuel cycle simulator must have predictive capabilities which can deploy fuel cycle support facilities intelligently even in the face of volatile dynamics. Such volatility may arise during transitions between technologies, from upsets related to unexpected facility shutdowns, due to the variability of an increasingly renewable electric grid, or other nonlinear economic drivers. In these cases, the ARCH model is more generically applicable and should therefore be preferred over the ARMA model.

III.B. Deterministic-Optimizing (DO)
Deterministic-Optimizing algorithms seek to minimize or maximize an objective function with respect to a set of constraints. Compared to stochastic optimizing algorithms, deterministic-optimizing algorithms require less computing power, and are replicable. The most widely used class of deterministic optimizing algorithm is the linear program (LP) model. Simply put, this model optimizes a linear objective function where the variables are constrained by multiple constraints.

Two major models that utilize deterministic-optimizing algorithms are the Global Change Assessment Model (GCAM) and the MARKet and ALlocation (MARKAL) model. GCAM explores consequences to global change by representing various aspects of economy, energy and the environment [18]. MARKAL is a energy demand driven model that assesses the value of new energy technologies [19].

III.B.1. GCAM

GCAM is a dynamic-recursive model that connects various social, economical, political decisions to climate change. It determines the price vector that satisfies all markets by utilizing the GCAM solver, which finds the root of $\vec{y} = F(\vec{p})$, where $F(\vec{p}) = 0$. It does so by using two solver algorithms, the Bisection Method, and Broyden's Method [20].

The Bisection Method has the advantage that it requires little computing time to 'get close' to a solution. However, in a system of equations with multiple dimensions, it is sometimes not possible to even have rigorous bounds around a solution. Thus, in GCAM, the Bisection Method is used to get the solver only 'near' the solution, then the solution is found using Broyden's Method.

Broyden's Method is similar to Newton's method, but it saves computing time by updating the Jacobian rather than computing it at every iteration.

III.B.2. MARKAL

MARKAL uses a general linear-programming algorithm to optimize multiple objective functions, namely cost, security and other environmental functions, given a collection of constraints. The variables and the functions are listed in detail in the reference [19] [21].

The optimization algorithm in MARKAL is a collection of objective functions, subject to a collection of constraints. Multi-objective linear programming is used in various applications, such as economics, finance, engineering design, and power systems [22]. It is used in cases where there are competing objectives that need an optimal decision. For example, a central bank may decide a monetary policy to optimize its objectives to lower inflation, unemployment, or interest rates.

III.C. Stochastic-Optimizing (SO)

Stochastic optimization refers to optimization methods that incorporate probablistic search into either the objective function or the constraints [23]. It aims to find the roots for the objective function by sweeping over random variables. Some SO algorithms operate by directly modeling uncertainty, in addition to the mean. This capability is desirable for many real world problems where uncertainties are known or should be computed. Mathematically, the method attempts to find properties of

an objective f without evaluating f directly, but by using random samples of a model $F(\theta, \xi)$. The stochastic parameters driving the solution are typically sampled from probability distributions.

The Markov Switching Model and the Gaussian Process Regression method are key examples of the Stochastic- Optimizing category of methods.

III.C.1. Markov Switching Model

The Markov Switching Model depends on the idea that the future is independent of the past and only dependent on the present. It utilizes Markov Chains, which characterize the probability of a system transitioning between states.

The Markov Model is used in a wide variety of applications, such as predicting exchange rates [24], labor markets [25] and search trends [26].

III.C.2 Gaussian Process Regression

Gaussian Process Regression distributes a function as a Gaussian Process characterized by a mean function and a covariance function [27]. The mean value denotes the most probable output, and the covariance is the measure of confidence.

IV. SUCCESSFUL APPLICATIONS

The concept of dynamic demand-driven deployment has been used in myriad domains, from lumber mills [28] to coupling building efficiency with weather [29, 30].

To maximize fleet utilization and minimize operating costs, airlines predict future demands and optimize their flight schedules and aircraft types using In the airline industry, linear programming methods are used [31] including a linear optimization method called "Demand Driven Dispatch" [32], a type of deterministic optimization method.

The success of these algorithms in other domains for similar classes of problems is promising for their potential in nuclear fuel cycle analysis.

V. CONCLUSIONS

The review concludes that fuel cycle simulation tools approach scenario objective functions in various ways. Some wrap realizations of the simulator in an external optimizer, while others employ look-ahead methods to predict malformed simulation inputs. These methods fail to realistically model the process by which utilities, governments, and other stakeholders actually make facility deployment decisions.

Dynamic, demand-driven facility deployment may be enabled by algorithms in use in other fields. Deployment models were categorized into into three categories: non-optimizing (NO), deterministic-optimizing (DO), and stochastic-optimizing (SO). Among these, characteristic

performance was addressed (in terms of both compute speed and human effort), flexibility (in terms of the range of scenarios capably simulated), and robustness (in terms of consistent fidelity of the modeling results).

Finally, current NFC simulators may more flexibly support demand-driven deployment through incorporation of non-optimizing algorithms such as ARMA [33] and ARCH [34], deterministically optimizing methods such as those collected in GCAM [18] and MARKAL [19], or stochastic optimization techniques such as Markov Switching Models [35].

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