Final Technical Report for Project DE-NE0000673

Market-Based and System-Wide Fuel Cycle Optimization

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Executive Summary

Alternatives nuclear cycles offer a number of possible advantages over the current once-through fuel cycle, but there are lingering uncertainties in how to assess those advantages and unclear transition paths to arrive at those alternatives. The field of nuclear fuel cycle simulation provides tools for investigating these transitions, studying their technical challenges and identifying their broad societal benefits. Most fuel cycle simulation relies on the analyst to propose a specific deployment plan for different technologies in the future, and then use the simulation tools to measure the consequences. Any attempt to optimize has generally relied on manual iteration to revise the deployment plan and reassess the transition.

This work seeks to introduce automated optimization into fuel cycle simulation, specifically using the Cyclus fuel cycle simulation platform. At the system-level, this consists of implementing an optimization driver that can automatically assess the performance of a single deployment plan and adapt it to seek a better alternative. In addition to identifying a preferred optimization algorithm, some consideration must also be given to the structure of the decision space and the formulation of the objective function. While there is too much uncertainty in many nuclear fuel cycle performance metrics for a complete single objective function to be defined, it is possible to define some useful functions.

In order to support the flexibility of Cyclus in responding to the needs of system-level optimization, a form of optimization must also be introduced at the market-level. Individual facilities trade in nuclear materials using a market paradigm in which requests for material are matched with offers of material. The consumers of material have the freedom to determine the best offers based on algorithms that meet their individual needs, whether physics, economics or otherwise. Such a market mechanism allows each facility to respond freely, and possibly with nuance and richness, to perturbations introduced to the simulation by the system-level optimization process. This mechanism also preserves the ability for individual facility models to operate without any special knowledge of the internal state or decisions of other facilities. Their only interaction is in the form of requests and offers.

Although the consumers retain the agency to make the final preference decisions, it is important for the supplier to have some input to those decisions. It is also valuable for suppliers to have a mechanism to assess how any given offer will be received by the potential consumers. Tailored offers will help maximize the performance of the market as a whole. Both of these capabilities have been introduced as part of the otherwise consumer-centric market model.

Finally, the system-level optimization has been extended to perform nested optimization under postulated disruptions to the deployment plan, thus identifying deployment strategies that hedge against the impact of those disruptions.

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1 Introduction

The goal of this project is to introduce optimization capabilities into the Cyclus fuel cycle simulator at two different levels of the simulation capability.

1.1 Cyclus Fundamentals

Cyclus is a nuclear fuel cycle simulation platform with a primary design goal of flexibility to accommodate future innovations in nuclear fuel cycles. This flexibility is achieved, primarily, through an agent-based paradigm in which different models for agent behavior can be introduced through runtime plugin modules. The most important outcome of this paradigm is that new behaviors can be introduced without having to change the fundamental platform, thus allowing for better understanding of the impacts of those new behaviors. Such new behaviors can represent different levels of fidelity for modeling similar facilities, or entirely novel facilities that require different modeling options.

A Cyclus simulation consists of a deployment plan for a series of facilities, possibly over many decades, with each facility represented by a particular behavior model. Each facility has a set of commodities that it consumes and/or supplies, and a market for each commodity exists to facilitate their exchange. Commodities are traded in discrete quanta, each of which has a specific quantity (often measured in mass) and a specific quality (e.g. isotopic composition). At each time step, consumers issue requests for resources while suppliers issue offers of resources. A market model uses some mechanism to determine which requests will be matched with which offers, and resources are exchanged among facilities. A more complete description of the Cyclus platform, including some of the work described here, can be found in Ref. [1].

1.2 Optimization Needs

The first target of optimization is at the level of individual commodity markets during each time step. Fundamental to the design of Cyclus is the ability for different facilities (often referred to as agents) to trade discrete quanta of resources in the nuclear fuel cycle. Initial implementations of Cyclus relied on an omniscient market agent that would collect all the offers and requests and use some algorithm to determine which trades would take place. While this did allow for market like behavior, it did not allow for different agents to value the same discrete quantum of material differently. Market-level optimization was implemented in the form of the Dynamic Resource Exchange (DRE) with the primary purpose of supporting agent-based valuation of individual resource bids, accounting for flexibility in the behavior of the facility, and fungibility among isotopes within a particular commodity. As will be seen, this encapsulation of the resource bid valuation entirely within each agent promotes the fundamental flexibility of Cyclus.

By itself, the consumer-centric DRE left one gap in the efficient implementation of commodity markets: suppliers had no knowledge of how the consumers would value their bids and therefore no ability to customize their bids to the consumer. This was remedied by extending the contents of a request for resources to also include a mechanism for suppliers to query the consumers for the value of a particular offer, so-called objective function callbacks. One original aim that proved unrealistic was the introduction of realistic economic value functions in the context of these callback functions. The ability to define the value of a resource offer in purely economic terms is an appealing notion. However, there remains too much uncertainty in the various components of the costs of most fuel cycle facilities and processes to provide credible estimates of the economic value of any single resource offer. As will be discussed, the implementation of the objective function callbacks does not preclude the introduction of purely economic valuation, but none were explicitly provided as part of this work.

The second target of optimization is at the level of an entire simulation. A single Cyclus instance can simulate the deployment, interaction and decommissioning of a set of facilities over time, and provide metrics for the performance of those facilities as well as for the overall fuel cycle. It is frequently interesting, however, to find a particular set of deployment, interaction and decommissioning characteristics that will optimize some combination of those metrics. Given the emergent behavior that can arise from an agent-based simulation, stochastic optimization techniques are the best choice. A swarm-based algorithm was implemented and demonstrated on representative nuclear fuel cycle transition scenarios. This same algorithm was then also used to explore the limitations of different modeling paradigms in achieving the same optimum solution[2]. Finally, a nested optimization was carried out to identify best hedging scenarios given the likelihood of disruption in the fuel cycle during transition.

While economic valuation of individual resource offers at the market level was not implemented, there is also interest in determining an economic/financial metric for the performance of an entire fuel cycle, particularly during transition. Such a metric would permit system-level optimization that focused entirely/primarily on the economic performance over time. Some work was done to consider the economic metrics for complete nuclear fuel cycles, particularly during transition.

1.3 About this Report

This report documents the implementation, testing, characterization and demonstration of each of these features. Section 2 describes the DRE and the addition of objective function callbacks. Section 3 describes the fundamental optimization capability and two advanced demonstrations of its use in fuel cycle simulations.

2 Market-level Optimization

The original design of Cyclus included a notion of markets that presumed a universal objective function for ascribing a value to resources offered for a trade. All consumers would submit their requests and all suppliers would declare what resources they were able to offer, and the market would apply some algorithm to match offers with requests. While it did provide a capability of swapping market models, it quickly became apparent that this solution presumes a universal function for ascribing value to individual quanta of material, while different facilities would generally have very different ways of assessing the relative value of different resource offers.

This section describes the capability that allows Cyclus to match consumer requests with supplier offers while remaining consistent with the fundamental goals of the Cyclus framework. In particular, this capability must support the following.

Flexibility: In order to support a maximum level of flexibility in Cyclus, each agent must operate as a *black box*, with no assumed knowledge of the capabilities or current state of other agents. This permits individual facilities to be represented by plugins that can be swapped without imposing restrictions on other agents in the system. The market clearing mechanism must be able to accept any request for resources, regardless of its ability to be satisfied by the system.

Fungibility: Since different fissile nuclides can fill similar roles in the fuel cycle, resource offers may differ in composition but still satisfy the needs of the consumer. The market clearing mechanism must be able to accept any offer of resources, without judgment on whether or not it meets the goals of the corresponding request.

Agency: Given the prior two characteristics, the final ability to determine the details of a specific request, a specific offer, or which offer is the most suitable match to a specific request must rest solely in the hands of the facilities making those requests and offers. The market clearing mechanism may not impose any problem-wide value judgment on the transactions.

A market clearing mechanism that satisfies these high level requirements, known as the DRE, was designed and implemented. Section 2.1 first discusses the conceptual design of the DRE, followed by a formal definition of this system as a mixed-integer linear program to solve a modified network flow problem. Different solvers were studied to assess the trade-off between accuracy and efficiency. A number of sample problems are presented to demonstrate the capability of the DRE. A more comprehensive treatment of the DRE can be found in Refs. [3] and [4]. Although the DRE provides the necessary components for market clearing in Cyclus, it does not lead to the most computationally efficient results. In particular, the DRE does not provide a mechanism for suppliers to tailor their offers to the specific interests of the consumers, even if their behavior models would allow them to do so. Section 2.2 introduces just such a mechanism, also allowing suppliers to ascribe differing values to different offers for use in resolving the DRE.

2.1 Dynamic Resource Exchange

2.1.1 Conceptual Design

At the conceptual level, the DRE implements the following communication cycle at each time step in a CYCLUS simulation:

1. All consumers broadcast their requests to all suppliers. Each request describes the desired quantity and quality (isotopic composition).

2. Suppliers respond to each consumer request with an offer to supply material. Each supplier has the agency to decide whether or not to respond, and if so, how to respond. Each offer describes an available quantity and quality.

3. Consumers use their own valuation process to rank the offers using the notion of preference.

4. All preferences are collected to be solved by an algorithm that maximizes the total preference in the system.

5. The solution identifies specific resource trades that are then carried out among the facilities/agents.

At the heart of the DRE is a the Multi-commodity Transportation Problem (MTP) [11] which belongs to the network flow family of optimization problems. A network flow problem is represented by a graph, $G(N, A)$, that comprises nodes N and arcs A. If flow can occur between some node i and some other node j, then it flows along arc (i, j). Given a graph instance, optimal flow between nodes can be found subject to *objective coefficients* and *constraints*. *Decision variables* for this optimization problem comprise the optimal *flow assignment*. If all decision variables are linear, then the resulting formulation is termed a linear program (LP). If some decision variables are integer (e.g., binary), the formulation is termed a mixed-integer linear program (MILP).

Transportation problems model the flow of a commodity between source nodes and sink nodes which can have supply and demand constraints. A more complex transportation-problem formulation can support systems in which supply or demand can be met by multiple commodities. There is a unit cost $c^h_{i,j}$ for commodity h to traverse arc (i, j). A supplier of commodity h has a certain supply capacity s^h_i which cannot be surpassed and consumers of commodity h have a certain demand level which must be met, d^h_i.

In the simplest extension from the single-commodity to multi-commodity transportation problem, arc constraints for all commodities are combined, i.e., there is a single capacity $u_{i,j}$ for a given arc (i, j). A classic application of this enhanced complexity deals with data networks. Multiple classifications of data exist, but they all must traverse the same network infrastructure. Accordingly, the infrastructure can only accommodate a certain quantity of total flow among all communication types.

2.1.2 Mathematical Formulation

The formulation of the multi-commodity flow problem is shown in Equation 1, in which the solutions are the set of flows of each commodity between each request-bid pair, $\{x_{i,j}^h\}$. Note the commodity coupling in Equation 1d.

$$
\begin{aligned}
\min_x \quad & \sum_{i \in I} \sum_{j \in J} \sum_{h \in H} c_{i,j}^h x_{i,j}^h & & \text{(1a)} \\
\text{s.t.} \quad & \sum_{i \in I} x_{i,j}^h \geq d_j^h & \forall\, j \in J, \forall\, h \in H & \quad \text{(1b)} \\
& \sum_{j \in J} x_{i,j}^h \leq s_i^h & \forall\, i \in I, \forall\, h \in H & \quad \text{(1c)} \\
& \sum_{h \in H} x_{i,j}^h \leq u_{i,j} & \forall\, (i,j) \in A & \quad \text{(1d)} \\
& x_{i,j}^k \geq 0 & \forall\, (i,j) \in A, \forall\, h \in H & \quad \text{(1e)}
\end{aligned}
$$

A number of adjustments are made to a canonical MTP to accommodate specific features of a nuclear fuel cycle, transforming it into a so-called Nuclear Fuel Cycle Transportation Problem (NFCTP):

- portfolios of requests, R, and offers, S, that represent the fungibility of resources,
- partitioning of the graph into individual commodities,
- multiple constraints, $k \in K_{\{s,r\}}$, on individual suppliers or consumers,
- constraints that depend on the quality of the individual trade (e.g. SWU constraints), $a_{i,j}^k$, and
- mutually exclusive requests, $\tilde{x}_j$, that must be fulfilled by a single supplier such that $x_{i,j} = \tilde{x}_j y_{i,j}$ (e.g all fuel assemblies should come from the same fuel fabrication facility).

This allows the MTP to be redefined into a more problem specific NFCTP as shown in Equation 2. A more detailed discussion of these details is available in Ref. [3].

$$
\begin{aligned}
\min_{x,y} \; z \; &= \sum_{(i,j)\in A_p} c_{i,j} x_{i,j} \; + \sum_{(i,j)\in A_e} c'_{i,j} y_{i,j} && && \text{(2a)}\\
\text{s.t.} \; & \sum_{(i,j)\in A_{p_r}} a^k_{i,j} x_{i,j} \; + \sum_{(i,j)\in A_{e_r}} a^{k\prime}_{i,j} y_{i,j} \geq b^k_r && \forall\, k \in K_r, \forall\, r \in R && \text{(2b)}\\
& \sum_{(i,j)\in M_r} y_{i,j} \leq 1 && \forall\, r \in R && \text{(2c)}\\
& \sum_{(i,j)\in A_{p_s}} a^k_{i,j} x_{i,j} \; + \sum_{(i,j)\in A_{e_s}} a^{k\prime}_{i,j} y_{i,j} \leq b^k_s && \forall\, k \in K_s, \forall\, s \in S && \text{(2d)}\\
& \sum_{(i,j)\in M_s} y_{i,j} \leq 1 && \forall\, s \in S && \text{(2e)}\\
& x_{i,j} \in [0, \tilde{x_j}] && \forall\, (i,j) \in A_p && \text{(2f)}\\
& y_{i,j} \in \{0, 1\} && \forall\, (i,j) \in A_e && \text{(2g)}
\end{aligned}
$$

With the introduction of mutually exclusive requests, this problem becomes a MILP, requiring more complex methods for a rigorous solution.

Another important feature of the NFCTP is the introduction of false consumers and suppliers to ensure a feasible solution. If the total requests of any single commodity exceed the supply, the network flow problem will match one consumer with the false supplier, and vice versa. No resources are traded along such arcs. Instead, consumers matched with false suppliers simple receive no response to their request during that time step.

2.1.3 Solution Engines

The formulation of this problem in a classical linear programming representation enables Cyclus to draw on both the literature for this field and the various software libraries that exist to solve such problems. The leading open source solution is the Computational Infrastructure for Operations Research (COIN-OR) project [12] that provides robust implementation of standard algorithms for solving both linear programs and mixed integer linear programs.

Cyclus includes layers of abstraction to translate from an agent-centered resource exchange formulation that will be most natural to fuel cycle modelers into a network-centered linear program formulation that facilitates the use of standard algorithms for solution. These abstraction layers also enable developers to connect alternative solver algorithms and libraries.

Testing was carried out with a simple, so-called *greedy* solver, in addition to the COIN-OR linear programming (Clp) solver and the COIN-OR branch and cut (Cbc) mixed integer linear programming solver. The greedy solver guarantees a feasible solution but not necessarily an optimal solution, by using a heuristic of matching the highest preference request with its highest preference bid, and so on until everything is matched, including matches with false consumers/suppliers. These different solvers were tested to develop an understanding of their behavior in a number of configurations.[4] In addition to the overall computational performance of the different solvers, there was also interest in understanding under what circumstances the solvers achieved similar solutions. These results were measured as a function of the total number of requests and/or offers in the system. In some cases, calculated preference for individual trades included stochastic components to introduce variability into the simulations. In these cases, large numbers of distinct realizations were performed to study the mean behavior of the DRE.

A sample of the results in shown in Figure 1. This problem has many reactors, each requesting fresh fuel for periodic reloads. In the reference case, the reactors are requesting individual assemblies rather than batches of assemblies and trade preferences are adjusted based on a model for relative facility location that allows for fine adjustment. Three different fuel cycle configurations were tested. In each case, the x-axis shows the deviation in the achieved value of the objective function being optimized by the DRE while the y-axis shows the deviation in simulation time. The greedy solver is generally much faster, but does not achieve the same level of optimization. It is noteworthy, however, that the difference in value of the objective function is not a perfect indicator of the differences in the flows achieved by this solution. Very similar flows may have different objective function values. A richer and more comprehensive analysis is offered in Ref. [4].

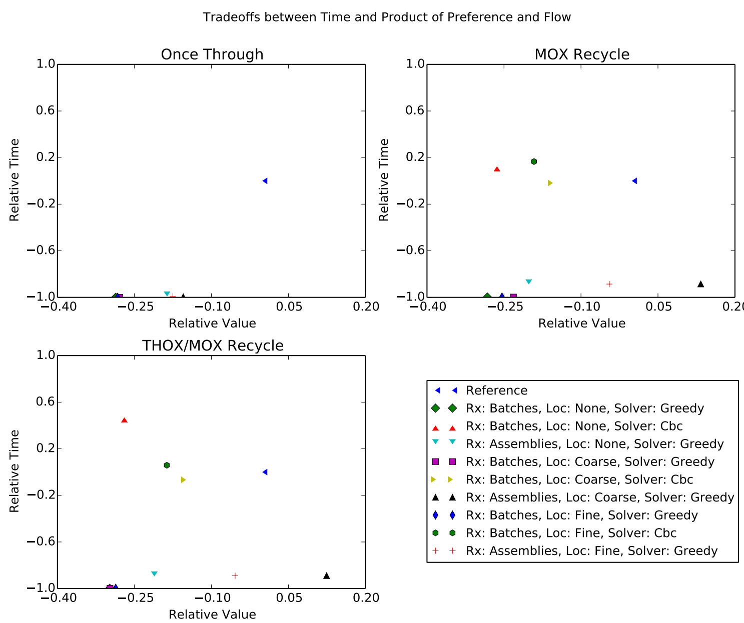


Figure 1: A comparison of simulation-objective values and solution times between instances solved with Greedy and CBC solvers. Reference values are comprised of high-fidelity reactor instances solved with CBC. Each other combination of fundamental parameter and solvers are then compared against the reference. Note that the once-through fuel cycle pane does not include other CBC solvers, because their solution times were very long.

Table 1: Short Descriptions of Scenarios

Scenario Name	**Scenario Handle**	**Primary Departure from Base Case**	**Capability Highlighted**
Separations Outage	outage	Separations facility halts operation mid-simulation	System flexibility to recycling facilities operation
External MOX Supplier	external	An additional supplier of MOX enters mid-simulation	System flexibility to entry and exit of commodity suppliers
Regional Tariffs	tariff	Two regions are modeled with dynamic trade relationships	Ability to model nontrivial international relationships

2.1.4 Demonstration Problems

A number of computational experiments are conducted to highlight unique features enabled by the DRE in Cyclus. Each experiment is performed by solving instances of the DRE using both the greedy heuristic solver and optimally with the branch-and-bound solver COIN-OR Cbc solver. A UOX-MOX one-pass recycle system with all required fuel cycle facilities is taken as the base case scenario in order to reduce the complexity of the fuel cycle and highlight departures from available simulators. For simplicity of demonstration, reactors are assumed to refuel completely with a single commodity rather than a combination of fuel types as is done in practice. A simulation time frame of 50 years is chosen with one-month time-steps (totaling 600 simulation time steps), sufficient to display all relevant effects. The nominal parameters of all common facilities in the simulation are shown in Ref. [3].

The base case scenario is not process constrained (i.e., it is constrained only by the dynamics of Pu availability in the recycling stream). Reactors are allowed to be fueled by either UOX or MOX, with a preference for MOX over UOX, and refuel one-third of their total core mass every 18 months. Spent UOX fuel is allowed to be recycled, whereas spent MOX fuel is sent directly to a repository. In order to involve dynamism in the simulation, the population of reactors grows linearly over time at a rate of 1 reactor every 5 years. An initial population of 20 reactors are deployed individually in each of the first 20 time-steps of the simulation as shown in Figure 2. Note that deployments are staggered in the initial period in order to avoid supply/demand clustering effect. A diagram of the full base case fuel cycle is shown in Figure 3.

Three perturbations from the base case scenario are used to provide examples of modeling capability enabled through the use of the DRE. The scenarios are summarized in Table 1 below and described in more detail in the Ref. [3].

The first perturbation shows how the DRE allows the system to respond to arbitrary changes in the state of any facility. In this case, the separations facility shown in Figure 3 suffers an outage from $250 \leq t \leq 300$, during which all other facilities continue to engage in trade, adapting their trades for the available material. The second perturbation demonstrates how the DRE can easily adapt to new facilities entering the scenario. An external source of MOX enters the simulation at $t = 250$ and continues until it is exhausted. The last perturbation demonstrates the ability of agents to change their preference assignment algorithm dynamically within the simulation. In this case, it also engages the

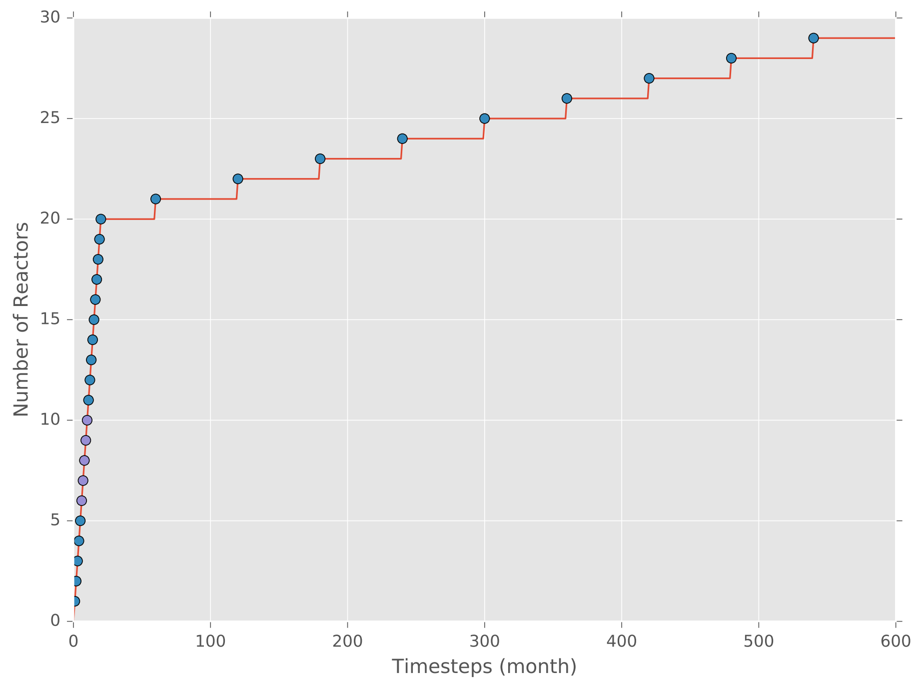


Figure 2: Reactor deployment in each simulation as a function of simulation time steps. Each point in the graph is a reactor being deployed in the simulation. Deployments for the tariff scenario are distinguished by color: blue represents deployments in Region A and purple represents deployments in Region B.

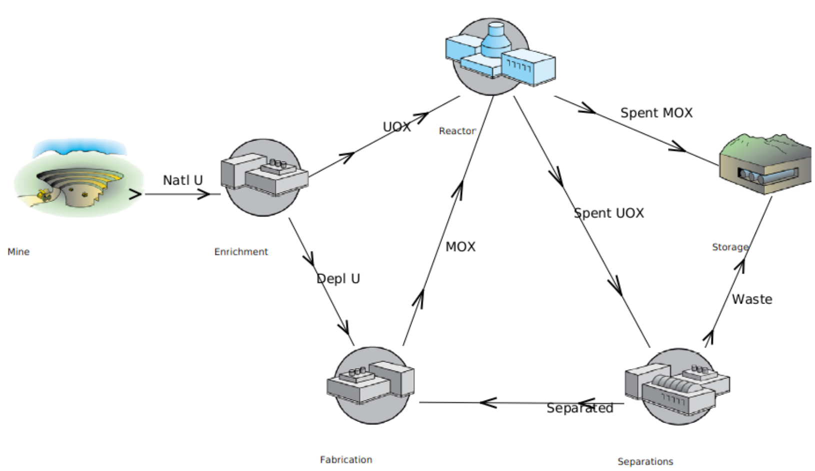
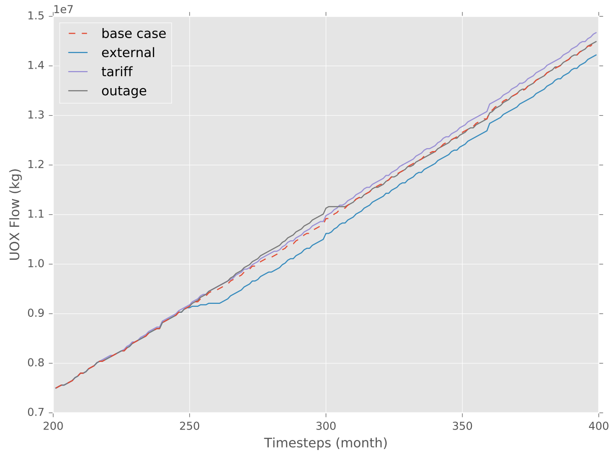
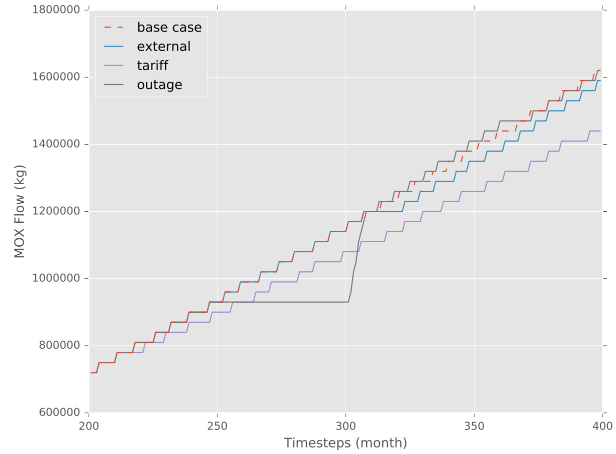


Figure 3: Material routing between in the base case scenario, single-pass MOX fuel cycle. Possible arc flows are labeled with commodity names.



(a) UOX flow.



(b) MOX flow

Figure 4: Cumulative flow of fuel in all Scenarios. The timestep period between 200 and 400 is chosen to highlight all relevant transients.

Region-Institution-Facility (RIF) hierarchy built into CYCLUS that allows for facilities to be owned by an *institution* that operates in a geopolitical *region*, each of which can influence how preferences are determined[1]. In this case, a second region is added and a tariff is imposed on trade between the regions at $150 \leq t \leq 300$.

Importantly, in all cases, the only changes necessary to perturb the system are local to the facility experiencing the perturbation. All other facilities, if properly configured to take advantage of flexibilities in the base case, will automatically respond. As such, these perturbations represent much larger potential changes that can be introduced, either dynamically or by user input into a fuel cycle.

A summary of the results is shown in Figures 4a and 4b. Figure 4b showcases the cumulative flow of MOX fuel into all reactors as a function of simulation time step. Because reactors can be fueled only with UOX or MOX, it represents the inverse of Figure 4a. For example, whereas the tariff scenario utilizes the most UOX, it utilizes the least MOX for the same reasons. A number of additional features can be observed in Figure 4b dealing with departures from dynamic equilibrium of the base case scenario. The undershooting and then overshooting of MOX consumption in the outage scenario is visible. During the outage, less MOX is consumed, but immediately after the outage, excess MOX is consumed until there is a return to dynamic equilibrium. Additionally, a reduction in the total amount of MOX (sourced from recycled UOX) consumed is observed in the external scenario. This is due to a reduction in the available recycled UOX supply during periods of external MOX consumption. In short, for each reload of external MOX, the system loses a future amount of recyclable UOX. A more complete discussion can be found in Ref [3].

2.2 Objective Function Callbacks

2.2.1 Motivation

As previously discussed, the basic implementation of the DRE provides the ability for consumers to evaluate different resource offers, but does not provide the suppliers with any mechanism to judge how well those offers will be received. For suppliers that are unable to match the request exactly, but otherwise have flexibility in the quantity and/or quality of the offers that they issue, this leaves them essentially guessing which offers will be best received by the consumer. If the suppliers offers are poor matches, the consumers may operate below their ideal performance or even experience supply disruptions. Three major types of remedy exist:

1. encourage supplier facilities to make many offers with different qualities/quantities,
2. increase the information included in a request to enable the supplier to make informed choices, or
3. provide a mechanism for the supplier to query the consumer.

The first of these was ruled out because of the burden it would place of the DRE optimization algorithms. Suppliers with continuously varying parameter spaces might need to issue 1 or 2 orders of magnitude more offers for each request in order to ensure that they were well-matched to the consumers preference. Since the performance of the DRE scales with the number of request-offer pairs, this would increase the time to resolve the market even though the number of material flows would not change.

The second of these was ruled out because it would violate the Cyclus principle that each agent should operate as a black box to ensure flexibility. As each new piece of information is added to the request, all agents would need to implement algorithms that could use that information to guide their responses.

This leaves the preferred solution of extending the request once to include a function pointer that can be used by the supplier to query the consumer, in which each consumer is free to respond to this query with as much complexity as they require.

2.2.2 Implementation

Two small changes were made to give suppliers more control over the nature of their offers and their interaction with the DRE. First, the contents of a bid were expanded to include the supplier's preference for each bid. This information can then be used by consumers to impact their algorithm for determining the ultimate request-bid preference. As with the consumer's ability to establish preference, the supplier is free to use any algorithm to establish this preference.

The objective function callbacks have also been implemented, simply by extending the contents of a request to include a pointer to a function with a single argument of a single bid, and extending the interface with a function that will return that pointer. Suppliers are free to query the callback function (or not) and implement any algorithm to use that information to amend their bids.

Both of these changes require no changes to existing agent archetypes, unless they want to take advantage of the new functionality. A default bid preference of 0 is assigned for all bids where it is not assigned explicitly, so that all methods to generate bids will continue to function with no changes. Similarly, the callback functions are only queried if a supplier archetype chooses to do so.

2.2.3 Demonstration Problem

This capability was demonstrated with a storage facility archetype that determined its preference based on the specific decay heat of the offered resource. When added to the simulation, the archetype was configured with a maximum specific decay heat and will never accept a material with a specific decay heat above that threshold. In addition, it will prefer materials with a preference as high as possible below that threshold.

This archetype was used to fill multiple storage roles in a simulation that also included a standard recipe reactor: wet storage with no maximum allowable specific decay heat, dry storage with a modest maximum allowable specific decay heat, and a geologic repository with a low maximum allowable specific decay heat. In such a simulation, the reactor, wet storage and dry storage always offer their material to be taken by one of the other facilities.

There are a number of more subtle benefits of this approach. These materials can be offered in a single commodity market with no need to constrain the possible flows *a priori*. If material happens to remain in wet storage long enough that its decay heat drops sufficiently, its material can be sent directly to the geologic repository. All storage facilities participate in the same market and only accept material that is suitable for their characteristics. In addition, intermediate storage facilities can trade material based on its actual decay heat rather than its residence time. Many fuel cycle models rely on storage facilities with minimum residence times to approximate the notion that spent-fuel transport and acceptance is typically limited by its decay heat (among other related characteristics). In this case, the archetype can make decisions based on the operational characteristic that matters rather than an approximate surrogate.

The preference function of the consumer always ensures that material only flowed when the decay heat is sufficiently low. In the absence of objective function callbacks, however, the intermediate storage facilities would offer all the resources in their inventory during every time step. This would result in many superfluous offers that exceeded the decay heat limits of the consumers. By using a callback function to probe the preference of the receiving facility for each possible offer, it can avoid making offers that are not going to be accepted by the receiving facility.

2.3 Summary

The implementation of the DRE satisfied the goals of allowing for a flexible market mechanism to match requests for resources with offers for resources. A detailed study of different solution algorithms was completed[4] and the flexibility was demonstrated on a series of specific problems[3].

3 System-level Optimization

The majority of fuel cycle analysis effort involves users running single simulations defined primarily by the deployment history of various facilities over time. In some cases, users may manually alter those deployment histories to meet some objective, iterating until they find the best possible outcome. In fewer instances, that iteration has been automated to seek optimal solutions (e.g. [13]). By modeling discrete facilities over 1 month time steps, Cyclus offers many degrees of freedom for defining the deployment history of its facilities, underscoring the value in an automated optimization system.

This task focuses on the design, implementation and testing of a system that uses Cyclus to find optimal deployment histories within the bounds of specific fuel cycle scenarios. The first section defines a reference fuel cycle scenario to be used when developing a system for fuel cycle optimization. The following section discusses the development of the basic optimization system, including the choice of optimization algorithm and the structure of the decision space.

This capability was then extended to seek an optimum deployment strategy under the possibility of disruption of the fuel cycle at some future time. The methodology employed for this work used the same optimization algorithm, but added nested layers of optimization to identify a hedging strategy that minimizes the impact of a disruption during the transition.

3.1 Reference Problem Description

The EG23 transition defined by the Fuel Cycle Options campaign provided a convenient problem for studying the optimization of fuel cycle scenarios. This scenario starts with 100 light water reactor (LWR)s and follows an exponential growth of 1% per year for 200 years, while transitioning to a fuel cycle based entirely on sodium fast reactor (SFR)s. Plutonium from the separations of LWR fuel is used to start the SFR fleet, transitioning to recycling of their own fuel in the long term. The deployment history of LWR separations capacity is fixed, and reactor deployment history is to be optimized. The goal is to complete the transition, defined by the decommissioning of the last LWR, as quickly as possible. More details of this transition are available in Ref. [5].

3.2 Optimization Design, Implementation and Demonstration

3.2.1 Requirements and Algorithm Options

Using a fuel cycle simulator as part of an optimization objective is a challenging problem for several reasons:

- The objective function is generally not a linear function of input parameters.
- No derivative information for the objective is available.
- The objective function may be discontinuous.
- Input variables to the objective function may be discrete.

- The input parameter space could be large necessitating constraints for reasonable performance.
- The objective function may be stochastic - i.e. different runs with the same inputs may produce different outputs.
- The objective function is expensive to evaluate - seconds to minutes for a single iteration.

This kind of problem is often referred to as black-box[1] optimization. Another challenge is desirability of the optimization process to be effective over many different simulation scenarios. There is no single, well-defined objective to be optimized.

There are several classes of algorithms for addressing block-box optimization of this nature:

- **Pattern Search** algorithms expand and contract their search over a discretized decision space, with convergence governed by the rates of expansion and contraction.
- **Swarm** algorithms follow the trajectories of a set of search points through the decision space, with the velocities of those points determined by the location and magnitude of the objective function at each evaluation.
- **Evolutionary** algorithms evaluate the objective function across a population of points sampled from the decision space, and then look at "genetic" combinations of the best available points to identify better possible points. Mutations can be used to modify the search process.
- **Surrogate** algorithms form an approximate model of the objective function over the decision space, often of a form that can be optimized with algorithms that rely on information note available from the black-box approach.

In order to test these algorithms with the reference EG23 problem, it is necessary to define the decision space and objective function.

3.2.2 Decision Space Formulation

Conceptually, the decision space is defined by the number of reactors of each variety being deployed at each time step, with the total capacity constrained to match the total electricity growth rate. A naive implementation based on this conceptual problem results in unbounded decision variables in a space bounded by explicit constraints. Many black-box algorithms are challenged by such a decision space, resulting in evaluations of infeasible solutions (those outside the constraint) that are then penalized in the evaluation of the objective function because of they are outside the constraint. It is therefore preferable to develop a formulation with a bounded decision space, in which the constraints are represented by the bounds of the decision variables.

[1]While this use of "black box" is functionally different than the usage in Section 2, it is based on the same notion that there is no ability to have internal knowledge of the system.

The decision space for one such formulation is defined by the fraction of capacity additions at each time step that will composed of each reactor type. Each decision variable is then bounded on the interval $[0, 1]$. Furthermore, by selecting the fraction of each reactor type in succession, and updating the bounds for the next reactor type after each selection, the entire search space is accessible without violating the constraint.

These fractions can be converted to the number of reactors as shown in Equation 3.

$$N(t,r) = \begin{cases} floor\left(\dfrac{V_{fac}(t,r) \cdot \left[P_{new}(t) - \sum\limits_{r'=1}^{r-1} N(t,r') \cdot C(r')\right]}{C(r)} + 0.5\right) & : r > 0 \\ floor\left(\dfrac{P_{new}(t) - \sum\limits_{r'=1}^{r_{last}} N(t,r') \cdot C(r')}{C(r)} + 0.5\right) & : r = 0 \end{cases} \tag{3}$$

$N(t, r)$ is the number of reactors of type r to deploy at time t, $floor(x)$ is the closest integer to x that is less than or equal to x, $V_{fac}(t, r)$ is the decision variable value for facility r at time t, $P_{new}(t)$ is new capacity to be deployed at time t, and $C(r)$ is the power capacity for a single reactor of type r (e.g. 1000 MWe). The $N(t, r = 0)$ deployments must be computed after all $N(t, r > 0)$ deployments. Reactor type $r = 0$ is used to deploy any remaining new power capacity that is not satisfied by the other reactor types.

3.2.3 Objective Function

Many possible objective functions can be used to assess fuel cycle transitions, and selecting objective functions is an area of study in its own right (in addition to defining them with sufficient certainty to be useful). The objective function was designed to drive toward a fast-reactor-only fuel cycle as quickly as possible while simultaneously discouraging/penalizing unfueled reactors. Because fast reactors are fueled only with recycled fissile material, it is possible for some deployment schedules to cause fast reactors to idle without fuel. The objective function used is shown in Equation 4.

$$O_{sim} = \frac{\sum\limits_{t \in sim} E_{t,\,LWR}}{\sum\limits_{t \in sim} E_{t,\,tot}} \tag{4}$$

O_{sim} is the objective function value for an entire simulation, $E_{t,\,LWR}$ is the energy produced by all LWRs in time step t, and $E_{t,\,tot}$ is the energy produced by all reactors in time step t. Because the optimizer is trying to minimize the objective value, more LWRs results in a larger numerator (a worse objective value), and unfueled fast reactors shrinks the denominator (also a worse value). It is notable that this objective function does not penalize unfueled reactors very heavily relative to the penalty for LWR energy. This is intentional and allows the optimization to explore potentially interesting trade-offs related to expediting the transition.

3.2.4 Master-worker implementation

As black box techniques, all of the optimization algorithm classes explored here rely on a large number of independent evaluations of the objective function. After the optimization algorithm selects the set of decision variables for each evaluation, an objective function evaluation consists of a CYCLUS simulation followed by some post-processing of the results. Depending on the algorithm there were $O(200)$ evaluations per iteration, with $O(300)$ iterations, for a total of $O(60,000)$ evaluations.

The optimization system for CYCLUS was developed using a master-worker paradigm in a high-throughput computing environment. For each iteration, the optimization algorithm "master" would assign work, in the form of a CYCLUS input file, to a set of independent "workers", each of which would run CYCLUS and evaluate the objective function based on the output. Such a system is flexible to the number of available workers at any time, and multiple masters can share the same pool of workers. Such a system allowed a thorough exploration of the different algorithms, with over 700,000 CYCLUS evaluations used for the final comparison. Development and testing relied on about 1 million additional CYCLUS evaluations, consuming about 30,000 CPU hours over 7 days.

3.2.5 Algorithm Selection and Sample Results

A variety of open source libraries, each implementing algorithms in one or more of the classes of optimization algorithms, were tested for their performance using the reference problem described above.

The overhead and time involved in dispatching and running CYCLUS simulations is much larger than the time and computational resources required to run the each optimizer itself. Because of this, the optimizers are compared by primarily looking at the best objective function value achieved as a function of the total number of objective function evaluations. Table 2 summarizes the results for all runs done with each optimizer. Only a single run was performed with the DIRECT algorithm because it is deterministic and multiple runs on the same problem will always give the same result. The optimizers are listed in order of performance/effectiveness with PSwarm being the best performer and DIRECT being the least effective.

The PSwarm and JEGA solvers were the strongest performers, with PSwarm beating out JEGA slightly in both convergence rate and best solution found. The other solvers performed unsatisfactorily. Figure 5 provides a good picture for roughly evaluating how each optimizer performed with respect to the following criteria:

1. How good was the best objective value found?
2. How quickly did the optimizer converge toward a good solution?
3. How consistently does the optimizer perform on criteria 1 and 2 over multiple runs and/or problems?

In addition to the runs for each optimizer described above, Table 2 and Figure 5 contain data from one additional run using the PSwarm optimizer with bi-annual deployments instead of annual deployments. More detailed discussion of each result is available in Ref. [6].

	Run	# evaluations	# iterations	Best objective
PSwarm	1	60,046	356	0.1704
PSwarm	2	60,062	349	0.1670
PSwarm	3	60,153	349	0.1671
PSwarm-biannual	3	62,022	368	0.1423
JEGA	1	28,029	246	0.1884
JEGA	2	59,203	518	0.1848
JEGA	3	26,821	236	0.1889
HOPSPACK	1	60,012	310*	0.2816
HOPSPACK	2	59,840	310*	0.2637
HOPSPACK	3	59,956	310*	0.2900
SCOLIB EA	1	60,048	402	0.4742
SCOLIB EA	2	60,048	402	0.4871
SCOLIB EA	3	60,048	402	0.4871
SCOLIB DIRECT	1	58,260	16	0.5531

Table 2:
Summary results for all optimizer runs. The additional *PSwarm-biannual* run is identical to the other PSwarm runs except it had bi-annual instead of annual deployments resulting in only 200 optimization variables.

* The HOPSPACK optimizer did not have well-defined iteration boundaries.

The PSwarm optimizer was selected as the primary optimization algorithm for the Cyclus optimization system.

Figure 6 shows both the total power and LWR power generated over time for the best deployment schedule found among all runs. Figure 7 shows both the total power and LWR power generated over time for the best deployment schedule found by the PSwarm optimizer using smaller ±5% bounds instead of ±10% bounds around the growth curve. This deployment schedule results in an objective value of 0.1557. This is noticeably better than the best result by other 400-variable optimizer runs which was 0.1671 from the PSwarm optimizer. The larger 10% power curve bounds effectively result in a solution space containing $[\frac{\text{new range}}{\text{prev. range}}]^n$ times as many possible solutions as the 5% bounds where range refers to the difference between upper and lower bounds and n is the number of variables in the problem. So doubling the size of the bounds for this 400-variable problem results in a solution space with 2^{400} times as many possible solutions – much larger than before.

Figure 6 shows that the optimizer found a solution near a corner of the parameter space, building along the upper power bound and only building fast reactors as soon as they become available. The solution shown in Figure 7 is similar in that it rides the +5% upper bound for nearly all of the 200 years. The only significant exception is a short period in the 10 years leading up to fast reactor availability in year 35. This makes sense - LWR deployments are stopped and the optimizer utilizes its 5% flexibility to achieve a jump start in year 35 with a larger number of SFR deployments than would otherwise have been possible. This allows the LWRs to be phased out more quickly over all.

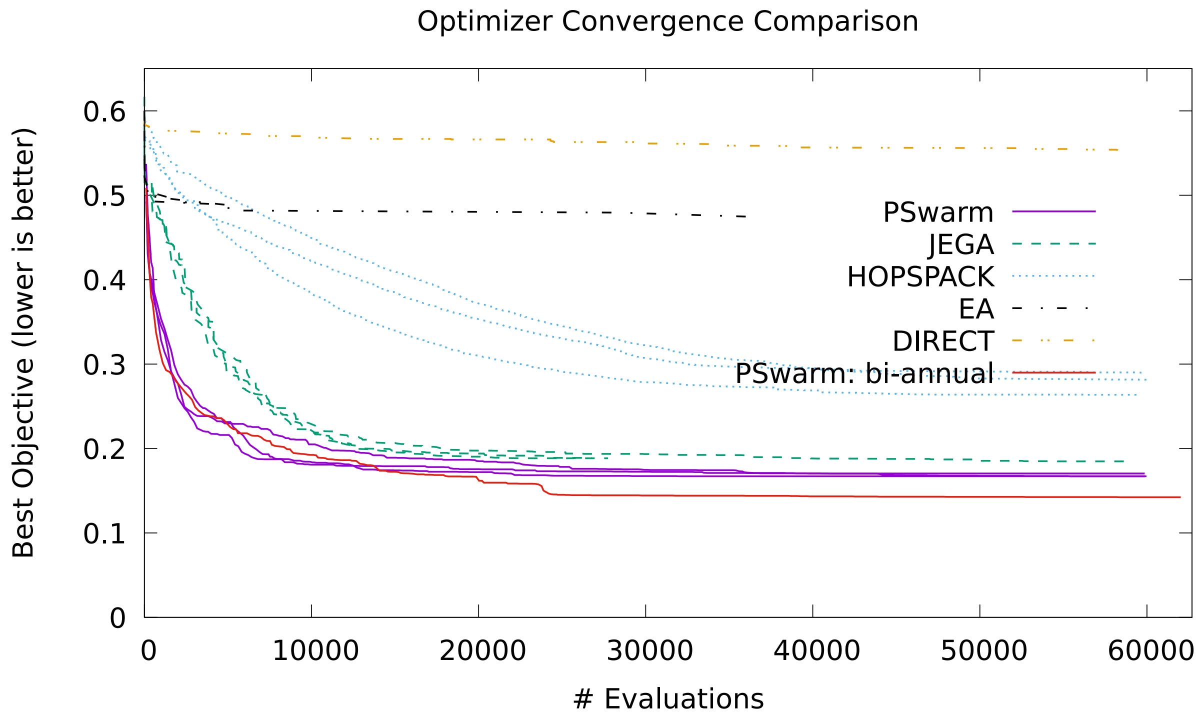


Figure 5: Objective value convergence curves for all optimizer runs.

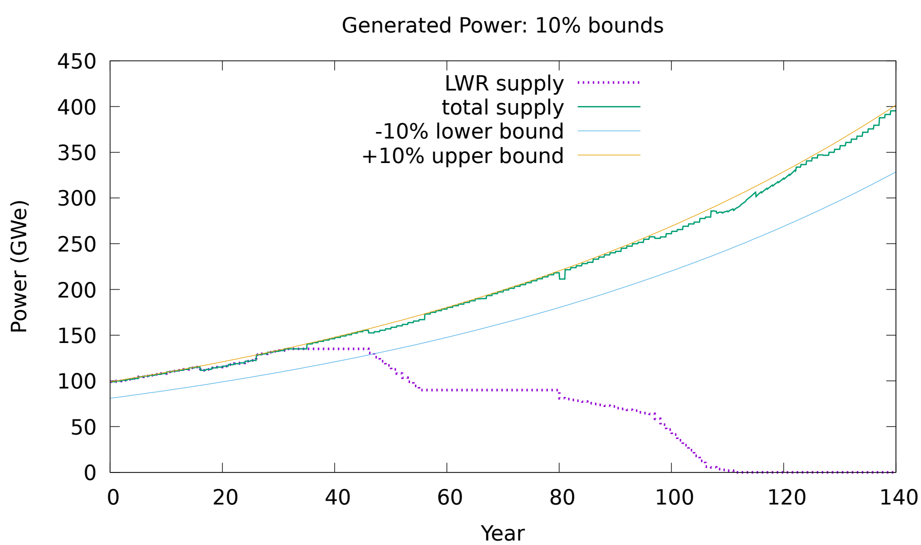


Figure 6: Both LWR and total (SFR and LWR) generated power over time for the best deployment schedule found among all the primary optimization runs using the ±10% bounds around the 1% power growth curve and annual deployments.

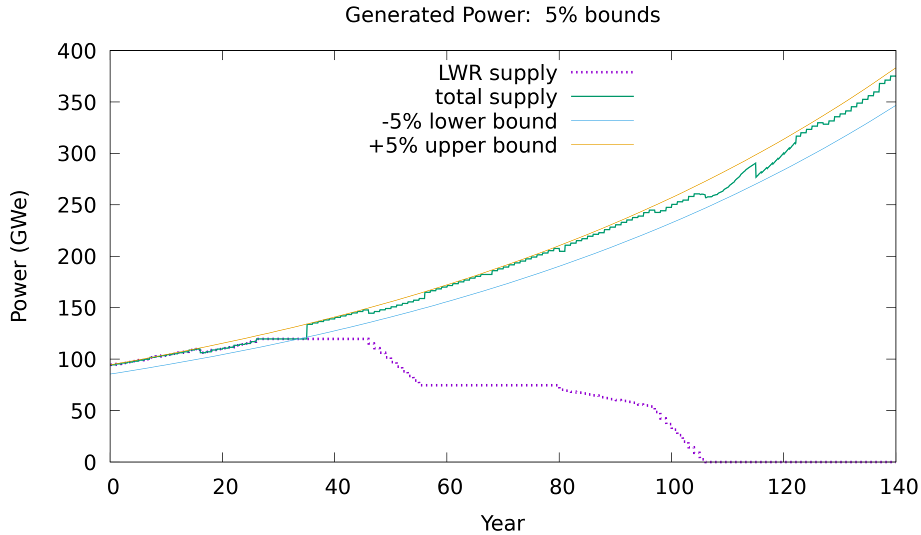


Figure 7: Both LWR and total (SFR and LWR) generated power over time for the best deployment schedule found by the PSwarm optimizer using smaller ±5% bounds around the 1% power growth curve and annual deployments.

3.3 Disruption Analysis and Hedging Strategies

3.3.1 Motivation

When conducting transition analysis for nuclear fuel cycles, a fundamental assumption is that the transition will proceed in an orderly fashion from the current configuration until it is complete. Transitions typically take over 100 years to become complete, and often longer. Societal motivations and needs are very likely to change over such time scale, probably leading to changes in course for nuclear fuel cycle transitions, calling into question this fundamental assumption.

The work under this task builds upon the system-level optimization to study the response of the system to a disruption in the trajectory to a new fuel cycle concept. Many types of disruption are possible, from small changes in the configuration of the systems being deployed during the transition, to large changes in policy that render some key systems no longer usable. Over the time scales of interest, it is possible that there may be multiple disruptions. It is not generally possible to predict when such disruptions will occur.

Nuclear fuel cycle transitions are often assessed according to a set of performance metrics, where the best transition is determined by optimizing against one or more of these metrics. In the face of disruption, it may be more valuable to identify a transition that will be impacted the least by such a disruption. Such a transition may not be optimal in the event that no disruption occurs, but can have the highest likelihood of a near optimal performance under the presumption of disruption. The optimization system for Cyclus can be nested to identify such transitions, known as hedging strategies since they hedge against the risk of disruptions.

3.3.2 Methodology

The previous section showed how to determine the optimum deployment history for a given objective function and given scenario description. While the addition of a disruption changes the scenario, it is still possible to identify an optimum for this new scenario. However, the decision space of such an optimization problem must be slightly different. First, consider a candidate deployment history, D, that will be subject to a disruption. All histories must start on this path as they have no *a priori* knowledge if or when a disruption will occur. After the introduction of a disruption at time, t_d, an optimization analysis can occur to find the optimal deployment history, D', that must only differ from D in the time period after the disruption. That is, the decision space for this optimization problem does not include the decisions made prior to t_d. We define $R^*(D, t_d)$ as the optimum deployment history that begins as history D but suffers a disruption at time t_d, and $S^*(D, t_d) = O[R^*(D, t_d), t_d]$ as the value of the objective function, $O(D)$, when deployment history $R^*(D, t_d)$ is evaluated in a scenario in which a disruption occurs at time t_d.

Since the actual time of disruption is not known, we must assume a probability distribution, $p(t_d)$, so that is finally possible to determine the hedging score for a given initial deployment history, D, as:

$$H(D) \equiv \int_0^\infty S^*(D, t_d) \cdot p(t_d) dt_d,$$

which can be approximated as:

$$H(D) \approx \sum_{i=0}^{m} S^*(D, t_i) \cdot p(t_i) \Delta t. \tag{5}$$

Finally, this can be used as an objective function itself, to seek the initial deployment strategy, D, that results in the optimum value of $H(D)$.

3.3.3 Implementation

Using this conceptual methodology directly requires many levels of optimization:

1. $O(10^5)$ evaluations of objective function $H(D)$
2. For each evaluation of $H(D)$, $O(10)$ evaluations of $S^*(D, t_d)$, and
3. For each evaluation of $S^*(D, t_d)$, $O(10^5)$ evaluations of objective function $O(D)$ in order to find $R^*(D, t_d)$.

Given the limited ability to parallelize across the PSwarm algorithm (or any black-box algorithm), this results in a currently unrealistic amount of computational effort, even using the high throughput master-worker paradigm. One way to reduce the effort is to introduce an approximation for $S^*(D, t_d)$. While the choice of such an approximation is an interesting research topic itself, for the purpose of demonstrating the overall capability, we chose the approximation:

$$S^*(D,t_d) \approx \frac{t_d}{t_{end}} O(D,t_d) + \frac{t_{end}-t_d}{t_{end}} O^*(t_d),$$

where $O^*(t_d)$ is the value of the objective function for the deployment history that is optimum for a disruption at time t_d. For a discrete set of disruption times identified in Eqn 5, each $O^*(t_d)$ can be evaluated once *a priori*. Each subsequent approximation of $S^*(D,t_d)$ requires only a single evaluation of the objective function, $O(D)$.

3.3.4 Problem Definition

A variation of the EG23 transition analysis was used to demonstrate this capability. The presence of disruptions is likely to increase the chance that reactors are idle after their deployment, so the objective function is modified to introduce a penalty for such circumstances.

$$O_{sim} = \frac{\sum\limits_{t \in sim} E_{t,\, LWR}}{\sum\limits_{t \in sim} E_{t,\, tot}} \cdot \frac{\sum\limits_{t \in sim} C_{t,\, tot}}{\sum\limits_{t \in sim} E_{t,\, tot}} \tag{6}$$

In this case, $C_{t,tot}$ is the total installed capacity; the lower the capacity factor, the higher the objective function.

3.3.5 Disruption Details

In order to focus on the methodology, a simple disruption was introduced in the form of a 33% reduction in the Pu available for fabrication of SFR fuel. This could be interpreted as an approximation to a number of different realistic scenarios, including a policy decision to shift away from breeders and towards burners.

It is also necessary to introduce a probability distribution for the when the disruption occurs. In this case, a gamma distribution is chosen, and shown in Figure 8.

$$p(t_d) = \frac{600}{\Gamma(1.5) \cdot 2^{1.5}} \left(\frac{t}{600}\right)^{0.5} e^{\frac{-t}{600 \cdot 2}} \tag{7}$$

3.3.6 Results

This problem was used to demonstrate the hedging strategy analysis. Intermediate results were used to assess the impact of the assumptions inherent in this analysis and are analyzed more comprehensively in Ref. x[6]. To assess the quality of the best hedging deployment history identified by this methodology, it is useful to compare its performance to other possible deployment histories. In addition to comparing the value of $H(D)$ for different deployment histories, it is valuable to consider the probability distribution functions (PDFs) of objective function values, over a large set of randomly sampled disruption times.

Figure 9 shows the PDFs for the hedging strategy compared to 6 other deployment histories, specifically the best deployment strategies for 6 different fixed/known disruption times. It is apparent that a number of deployment histories have lower objective function values in their best case than the best case for the hedging strategy, but may also have a higher prevalence of higher objective function values.

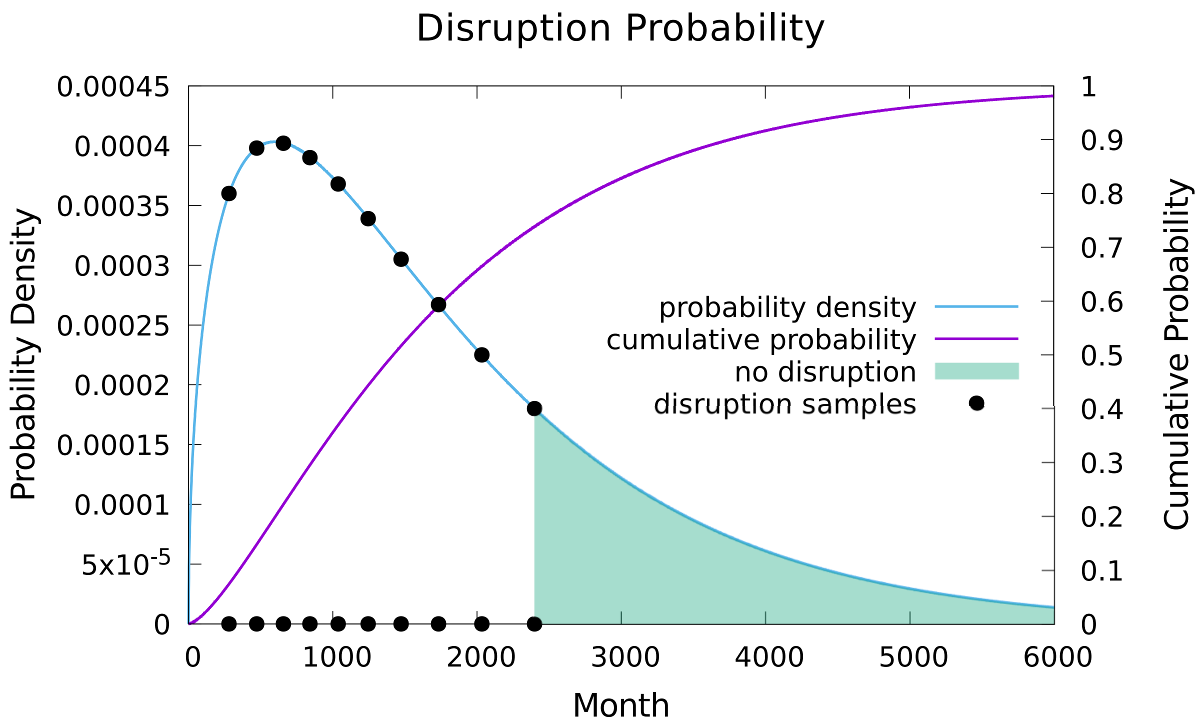


Figure 8: The disruption probability density function is a scaled gamma distribution (i.e. Equation 7). Note that the simulation duration is 2,400 months; times after month 2,400 are beyond the planning horizon and represent no disruption occurring.

3.3.7 Summary

Because of the black-box nature of the Cyclus optimization system, it was possible to extend it to a nested optimization system by changing the mechanism for evaluating the objective function. In a typical scenario optimization, a single objective function evaluation is a single Cyclus simulation with some post processing. For the hedging analysis, using an approximation at one layer of the nested optimization, a single objective function evaluation is $O(10)$ Cyclus simulations that are combined into a single value. This methodology was demonstrated using a posited disruption to the EG23 transition scenario, identifying a the best deployment history for minimizing the exposure to that disruption.

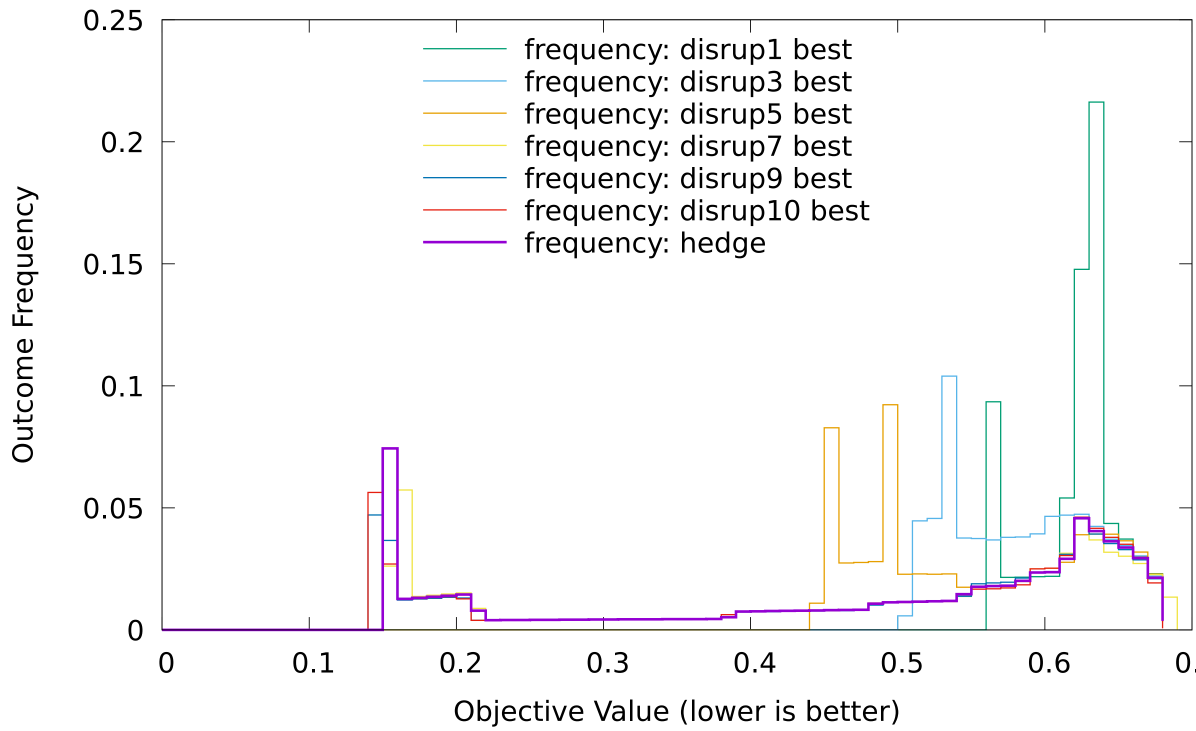


Figure 9: The best deployment schedules from select disruption times and the hedging schedule were used in to sample disruption times from the PDF. Best achievable objectives were then collected and the outcome frequency for each is shown. Better hedging strategies shift more outcomes to the left toward better values (e.g. hedge, disruption 10, etc.). The 26.1% no-disruption probability causes a spike of outcomes all at the left/lower edge of each distribution curve. Because this obscures other data, the no-disruption outcomes are omitted from the plot.

4 Summary

This project identified two primary goals related to the introduction of optimization capability into the Cyclus fuel cycle simulation ecosystem:

1. optimization at the market-level for individual commodity trades at each time step, and
2. optimization at the system-level to identify the best deployment histories over a fuel cycle transition.

Both of these goals were successfully accomplished with minor variations from originally proposed research plan.

4.1 Market-level Optimization

The mechanism for matching resource requests made by some facilities with resource offers made by other facilities was finalized and implemented as a variation of a classic network transportation problem. Specific additions were made to account for the fungibility of some nuclear materials, the desire for exclusive supply arrangements, and the possibility for constraints that are functions of both resource quality and quantity. This approach also preserves the important feature of retaining full agency within each facility for determining its preference among the offers that can satisfy its requests.

The specific task of assessing different optimization algorithms was completed with a comprehensive comparison of a fast heuristic market matching algorithm with more rigorous linear programming algorithms provided by COIN-OR. The heuristic matching algorithm was found to be sufficient in many cases, although it is not yet clear how to determine that it will be sufficient for any particular problem. Although the total objective function value of different material flow solutions may vary, such variations do not always represent substantially different flows.

The specific task of introducing objective function callbacks to allow suppliers to determine what preference each consumer will assess for its offers, and therefore tailor the offers to maximize the likelihood of matching. This feature both adds efficiency to the market mechanisms by improving the quality of individual offers and/or reducing the total number of offers necessary to reach an optimal solution.

The single deviation from the original research plan was that realistic economic value functions were not implemented in place of preference. While it is possible for each facility archetype to rely on realistic economic values to assess its preference for individual trades in the current implementation of Cyclus, insufficient certainty in economic models exists to justify incorporating this in specific facility archetypes being delivered formally as part of the standard software.

4.2 System-level Optimization

A system for seeking and identifying optimal deployment histories was developed based on black-box optimization techniques. A PSwarm algorithm was found to be the most effective at converging on optimal deployment histories, following comparison with a variety of open source algorithms that satisfied the requirements for optimization of this kind of problem. The formulation of the decision space was found to be important to improve the rate of convergence. A master-worker paradigm was implemented to take advantage of high throughout and/or cloud computing resources necessary to accomplish the $O(10^5)$ Cyclus simulations necessary in this kind of optimization.

The optimization system was demonstrated using the EG23 fuel cycle transition defined by the Fuel Cycle Options campaign. While the FCO campaign relied on manual iteration to identify an optimum deployment history, the optimization system was able to automatically arrive at an equivalent deployment history. Allowing for some flexibility in the overall power constraint allowed the system to find a more optimal solution that completes the transition more quickly.

One contribution beyond the original research plan was to use this optimization system to compare the impacts of different modeling choices, namely the difference between modeling individual facilities and fleets of facilities, and the difference between 1 month and 3 month time steps[2].

One substantial contribution beyond the original research plan was the adaptation of the optimization system for identifying hedging strategies in the face of possible disruptions to the planned fuel cycle transition. A conceptual methodology was designed that relies on nested optimization, and implemented with an approximation to one level of optimization to reduce the overall computational burden to a reasonable level.

Products

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