An Agent-Based Modeling Framework and Application for the Generic Nuclear Fuel Cycle

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Outline

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1. Introduction
2. Methodology
3. Experimentation and Results
4. Conclusions

What's the Point?

- $P \propto N\sigma_f \Phi V_{\text{core}}$
  - Power, P
  - Isotope Density, N
  - Probability of Fission, σ_f
  - Neutron Flux, Φ
  - Core Volume, V_{core}
- $$
- National energy policy
- Waste management
- Proliferation

Producing Fission Power, σ_f

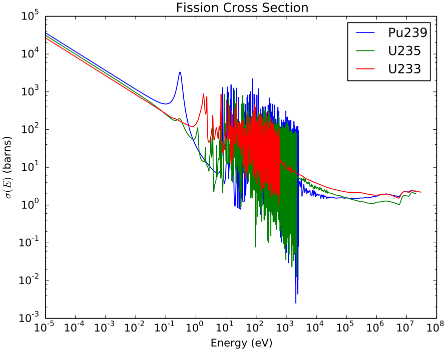


Figure : Fission cross section as a function of energy.

The Nuclear Fuel Cycle (NFC)

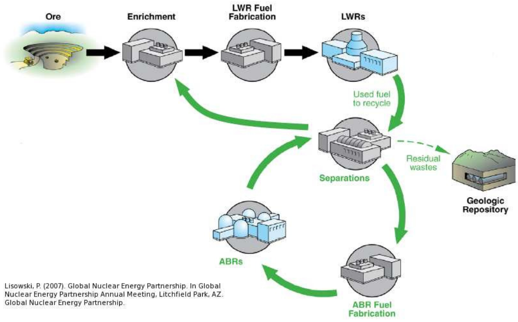
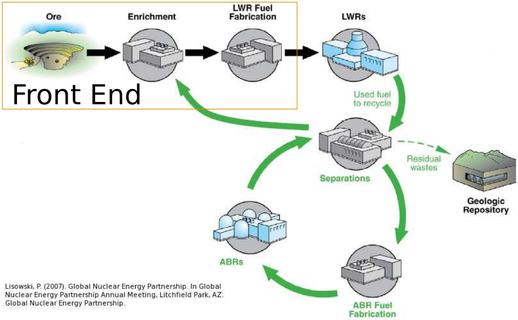


Figure : A fuel cycle with recycling. [3].

The Nuclear Fuel Cycle (NFC)



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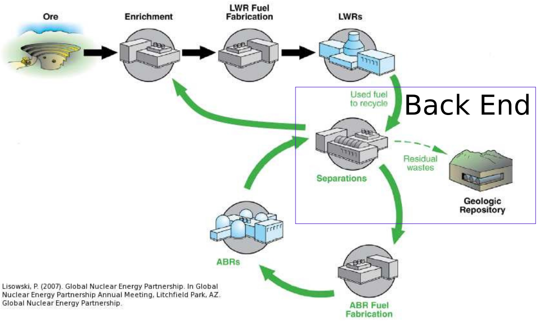


Figure : A fuel cycle with recycling. [3].

Table : LWR Spent Fuel

Element Group	wt %
Uranium	$\sim$ 95
Plutonium	$\sim$1
Minor Actinides	$\sim$0.1
Fission Products	$\sim$4

Simulation

It's hard.

- resource fungibility
- recycling
- constrained supply
- modeling individual fuel assemblies
- *in situ*, *ex situ*
  - physics
  - economics
  - *et cetera*
- arbitrary numbers, types of facilities
- geo-political effects
- "endless" possible fuel cycles [4]
- an "art" and a science [1]

"Old School"

- no physics or "too much" physics
- fleets of facilities
- aggregate material flows
- hard-coded connections between facility types
- little or no *in situ* decision making
- no regional information
- no idle facilities

Motivation

A tool is needed that can determine isotope-specific, quantized resource flows for arbitrary numbers and types of facilities where demand can be met by fungible resources and supply is constrained both by resource quantity and quality.

And supporting social (e.g., geopolitical) models is plus!

Outline

Dynamic Resource Exchange (DRE) Goals

- complex definitions of resource quality (e.g., arbitrary isotopic vectors)
- communication between suppliers and consumers
- constrained supply
- fungible demand
- arbitrary numbers and types of facilities
- enable geopolitical models

DRE Phases & Layers

Phases

1. Information Gathering
2. Solution
3. Trade Execution

Layers

- Resource Layer
- Exchange Layer
- Formulation Layer

Constructs

- Bids/Requests
- Exchange Graph
- NFC Transportation Problem

DRE Phases & Layers

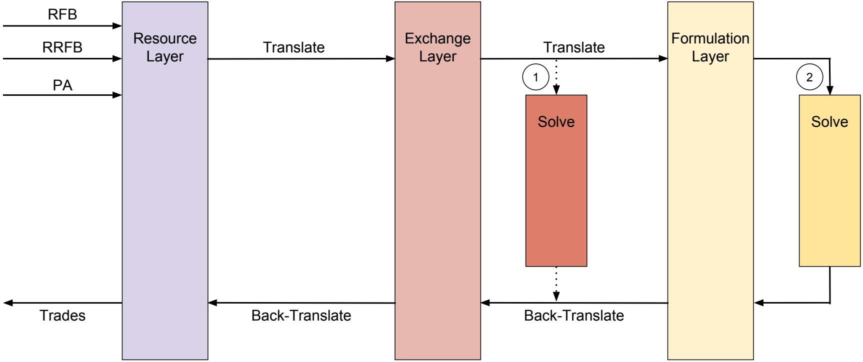
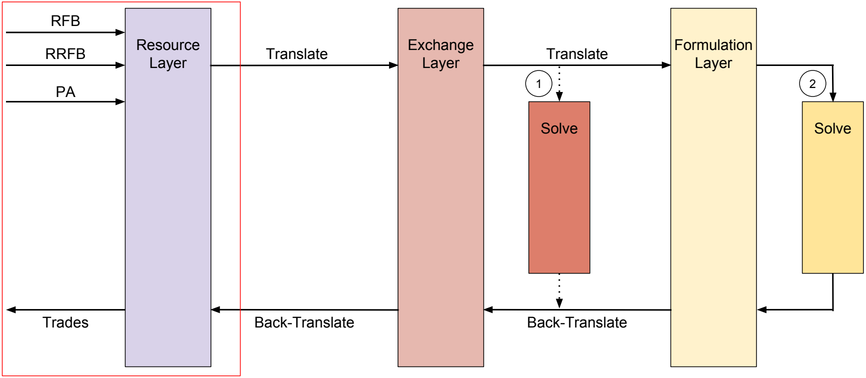


Figure : DRE logical flow through layers resulting in trades.

DRE Phases & Layers



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Entity Interaction

Agent-Based Modeling (ABM)

- agents interact with an environment
- facility agents manage inventory
- institution agents can build facility agents
- region agents inform system demand for facility types

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Supply-Chain Management (SCM)

- couples with ABM [2]
- facilities inform the system of resource-specific supply and demand
- institutions and regions can inform resource flows

Information Gathering Phase

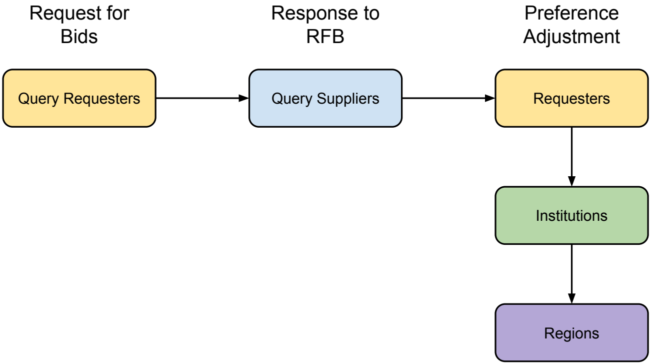


Figure : Information gathering logic flow.

Information Gathering Phase

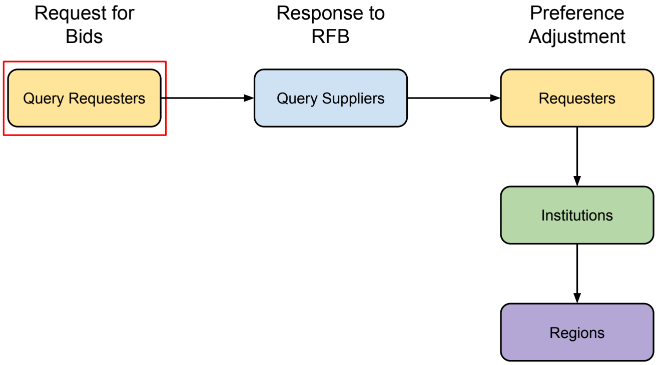
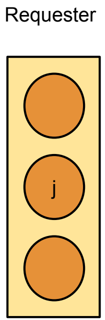


Figure : Information gathering logic flow.

Request For Bids (RFB)

- ask for a quantity, $\tilde{x}$, of a (complex) resource
- collection of `Requests` in `RequestPortfolios`
- mutual requests
- exclusive requests
- cardinal preferences



Information Gathering Phase

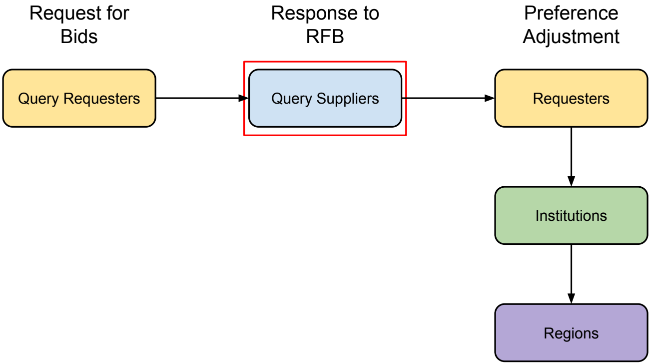


Figure : Information gathering logic flow.

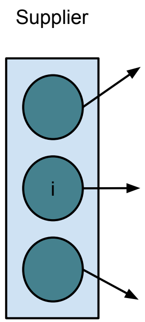
Response to Request For Bids (RRFB)

- respond with (complex) resource
- collection of `Bids` in `BidPortfolios`
- mutual and/or exclusive
- constraint values and translation functions

Constraint Example

$$\sum_{j \in J} f_{SWU}(\varepsilon_j) x_{i,j}^{EU} \leq s_{i,SWU}$$

$$\sum_{j \in J} f_{NU}(\varepsilon_j) x_{i,j}^{EU} \leq s_{i,NU}$$



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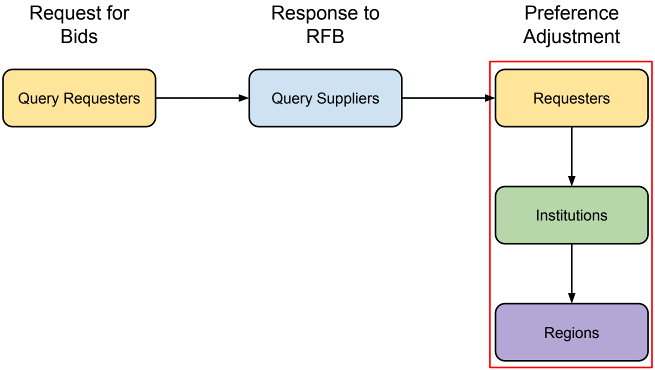
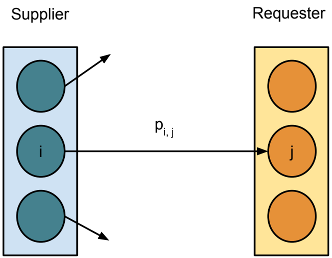


Figure : Information gathering logic flow.

Preference Adjustment (PA)

- Requesters adjust preferences given known bids
- Institutions adjust preferences given known bids & entities
- Regions adjust preferences given known bids & entities



DRE Phases & Layers

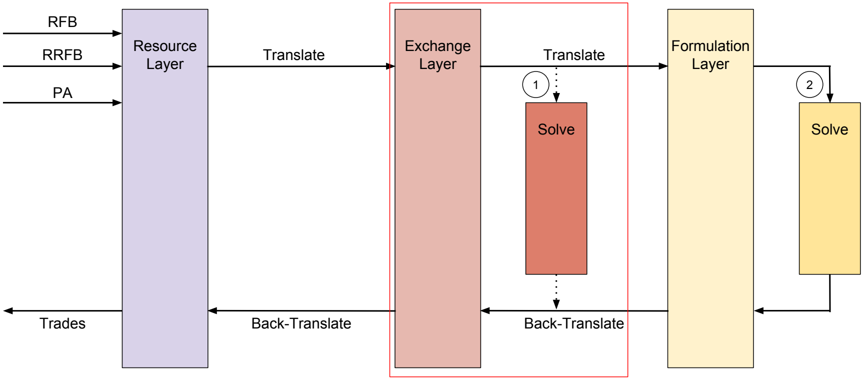


Figure : DRE logical flow through layers resulting in trades.

Translation to Exchange Layer

Properties

- Abstract away complex resource
- `Requests` and `Bids` to `Nodes`
- Possible trades and preferences known
- Constrained-graph representation of exchange via an `ExchangeGraph`

Constraint Example

$$\sum_{j \in J} f_{SWU}(\varepsilon_j) x_{i,j}^{EU} \leq s_{i,SWU} \rightarrow \sum_{j \in J} a_{i,j}^1 x_{i,j} \leq s_i^1$$

$$\sum_{j \in J} f_{NU}(\varepsilon_j) x_{i,j}^{EU} \leq s_{i,NU} \rightarrow \sum_{j \in J} a_{i,j}^2 x_{i,j} \leq s_i^2$$

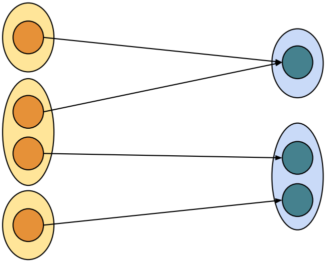


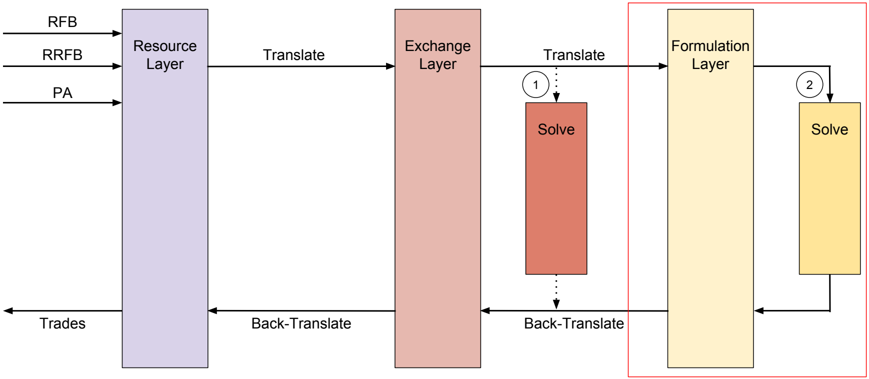
Figure : An ExchangeGraph.

Solution in Exchange Layer

Algorithm 1: Greedy Heuristic, $\mathcal{O}(n \log n)$

```
order request portfolios by average preference;
forall the request portfolios do
    order requests by average preference;
    matched ← 0;
    while matched ≤ q_J and ∃ a request do
        get next request;
        order arcs by preference;
        while matched ≤ q_J and ∃ an arc do
            get next arc;
            remaining ← q_J - matched;
            to_match ← min{remaining, Capacity(arc)};
            matched ← matched + to_match;
        end
    end
end
```

DRE Phases & Layers



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Transportation Problem

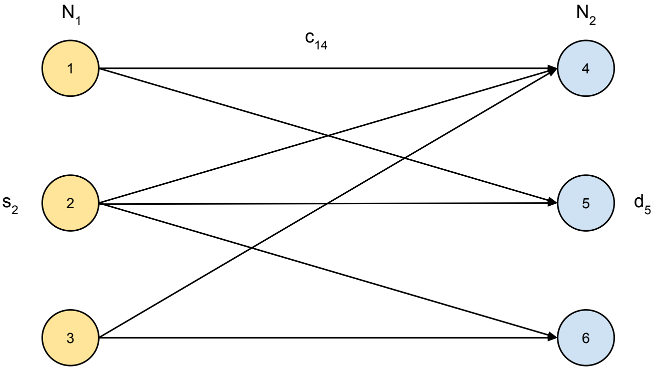

Figure : A bipartite graph with attributes.

Minimum Cost Transportation Problem

$$\min_{x} \sum_{(i,j) \in A} c_{i,j} x_{i,j} \tag{1a}$$

$$\text{s.t.} \sum_{j \in N_2} x_{i,j} \leq s_i \qquad \forall i \in N_1 \tag{1b}$$

$$\sum_{i \in N_1} x_{i,j} \geq d_j \qquad \forall j \in N_2 \tag{1c}$$

$$x_{i,j} \geq 0 \qquad \forall (i,j) \in A \tag{1d}$$

Translation to Formulation Layer

- Cost translation function
  $f : p_{i,j} \rightarrow c_{i,j}$
- $f(x) = \frac{1}{x}$
- False arcs have "large" cost
  $c_F > \max c \in C$

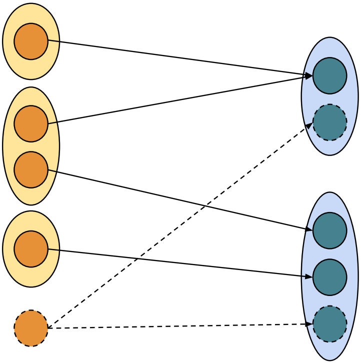

Figure : An ExchangeGraph with false arcs.

Nuclear Fuel Cycle Transportation Problem (NFCTP)

Linear Program (LP) without exclusive trades.

$$\min_{x} \ z = \sum_{i \in I} \sum_{j \in J} c_{i,j} x_{i,j} \tag{2a}$$

$$\text{s.t.} \ \sum_{i \in I_s} \sum_{j \in J} a_{i,j}^k x_{i,j} \leq b_s^k \qquad \forall\, k \in K_s, \forall\, s \in S \tag{2b}$$

$$\sum_{j \in J_r} \sum_{i \in I} a_{i,j}^k x_{i,j} \geq b_r^k \qquad \forall\, k \in K_r, \forall\, r \in R \tag{2c}$$

$$x_{i,j} \in [0, \tilde{x}_j] \qquad \forall\, i \in I, \forall\, j \in J \tag{2d}$$

Nuclear Fuel Cycle Transportation Problem (NFCTP)

Mixed Integer-Linear Program (MILP) with exclusive trades.

$$
\begin{aligned}
\min_{x,y} \; z \; &= \sum_{(i,j)\in A_p} c_{i,j} x_{i,j} + \sum_{(i,j)\in A_e} c_{i,j} \tilde{x}_j y_{i,j} && && \text{(3a)} \\
\text{s.t.} \quad & \sum_{(i,j)\in A_{p_s}} a^k_{i,j} x_{i,j} + \sum_{(i,j)\in A_{e_s}} a^k_{i,j} \tilde{x}_j y_{i,j} \le b^k_s && \forall\, k \in K_s, \forall\, s \in S && \text{(3b)} \\
& \sum_{(i,j)\in M_s} y_{i,j} \le 1 && \forall\, s \in S && \text{(3c)} \\
& \sum_{(i,j)\in A_{p_r}} a^k_{i,j} x_{i,j} + \sum_{(i,j)\in A_{e_r}} a^k_{i,j} \tilde{x}_j y_{i,j} \ge b^k_r && \forall\, k \in K_r, \forall\, r \in R && \text{(3d)} \\
& \sum_{(i,j)\in M_r} y_{i,j} \le 1 && \forall\, r \in R && \text{(3e)} \\
& x_{i,j} \in [0, \tilde{x}_j] && \forall\, (i,j) \in A_p && \text{(3f)} \\
& y_{i,j} \in \{0, 1\} && \forall\, (i,j) \in A_e && \text{(3g)}
\end{aligned}
$$

Outline

Strategy

Explore DRE performance in a High-Throughput Computing (HTC) setting

- Generate front and back-end exchanges
- Test problem-size scaling
- Test sensitivity to instance stochasticity
- Investigate formulation effects
    - Preference and cost
    - False arc cost

Overview

Process:

- Read parameter vector
- Instantiate entity surrogates
- Simulate Information Gathering Phase
- Translate to Exchange Layer
- Solve

Overview

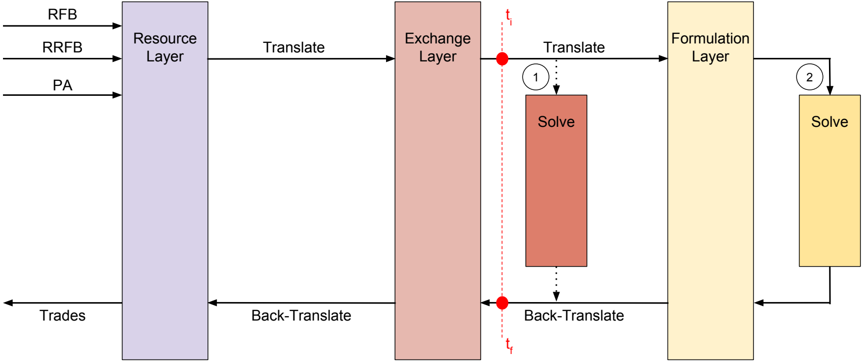

Figure : The time points for comparing different solutions.

Splitting Exchanges

Fails when

- Reactors directly connected to other reactors
- Reactors and repositories compete for resources

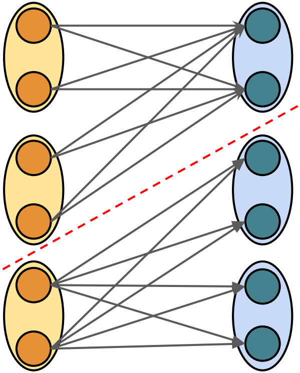

Figure : A separable Exchange Graph with nodes grouped by portfolio and the separating partition shown as a red dashed line.

Fuel Cycles (f_{fc})

Once-through

- Commodities: UOX
- Reactor Types: Thermal

Fuel Cycles (f_{fc})

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MOX

- Commodities: UOX, Thermal MOX, Fast MOX
- Reactor Types: Thermal, MOX-based Fast

Fuel Cycles (f_{fc})

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MOX

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MOX/ThOX

- Commodities: UOX, Thermal MOX, Fast MOX, ThOX
- Reactor Types: Thermal, MOX-based Fast, ThOX-based Fast

Reactors

Modeled as either Thermal (AP-1000) or Fast (BN-600) reactors

Properties

- core volume
- assemblies per batch (39 vs. 92)
- consumable commodities
- preferred enrichment range
- enrichment chosen randomly

Fidelity (f_{rx})

- Single batch
- N_a assemblies

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Commodity Preferences

Reactor type	Commodity Preference Order
Thermal	$p_{\text{TMOX}} > p_{\text{UOX}} > p_{\text{FMOX}}$
Fast MOX	$p_{\text{FMOX}} > p_{\text{TMOX}} > p_{\text{FThOX}} > p_{\text{UOX}}$
Fast ThOX	$p_{\text{FThOX}} > p_{\text{FMOX}} > p_{\text{TMOX}} > p_{\text{UOX}}$

Location Effects

$$p_l(i,j) = \delta_{\text{reg}} \frac{\exp(-|\text{reg}_i - \text{reg}_j|) + \delta_{\text{loc}} \exp(-|\text{loc}_i - \text{loc}_j|)}{1 + \delta_{\text{loc}}} \tag{4}$$

Fidelity (f_{loc})

- None ($\delta_{\text{reg}} = 0, \delta_{\text{loc}} = 0$)
- Regional ($\delta_{\text{reg}} = 1, \delta_{\text{loc}} = 0$)
- Regional + Distance ($\delta_{\text{reg}} = 1, \delta_{\text{loc}} = 1$)

Parameter Vector

Scaled by number of reactors in the system.

Table : Front-End Exchange Parameters.

Parameter	Reference Value	Related To
$r_{rx,\mathrm{Th}}$	0.75	Number of Thermal and Fast Reactors
$r_{rx,\mathrm{FThOX}}$	0.25	Number of Thorium Fast Reactors
$r_{s,\mathrm{Th}}$	0.08	Number of Thermal (UOX/TMOX) Suppliers
$r_{s,\mathrm{TMOX,UOX}}$	1.	Number of TMOX Suppliers
$r_{s,\mathrm{FMOX}}$	0.2	Number of FMOX Suppliers
$r_{s,\mathrm{FThOX}}$	0.2	Number of FThOX Suppliers

Information Gathering Simulation

Requests/Bids

- Reactors make N requests per commodity

Portfolio Constraints

- Support facilities have process and inventory constraints, function of resource quality (enrichment)
- Reactors have mass-based, mutually-exclusive constraints.

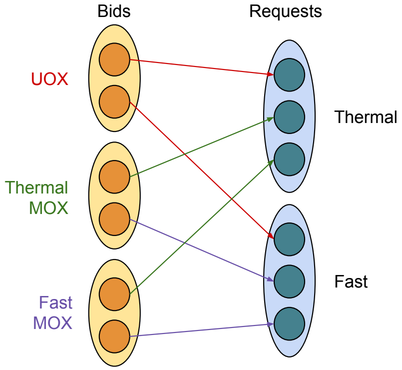
Preferences

- Facility locations chosen randomly
- $p(i,j) = p_c(i,j) + p_l(i,j)$

Example

A front-end MOX fuel cycle with one entity of each type:

- thermal reactor
- fast reactor
- UOX supplier
- thermal-spec MOX supplier
- fast-spec MOX supplier



Setup

Solvers

1. Greedy Heuristic with Exclusive Trades
2. Coin Branch-and-Cut (CBC) with Exclusive Trades
   - 1% convergence criteria
   - $\frac{z_U - z_L}{z_U} \leq 0.01$
   - 3-hour maximum time limit

Setup

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Metrics

- Time $t_f - t_i$
- Objective $z = \sum c_i x_i + \sum c_j \tilde{x}_j y_j$
  - z vs. z^*
- Simulation Objective $z_{\text{sim}} = \sum p_i x_i + \sum p_j \tilde{x}_j y_j$

Scaling Behavior

Problem Size: Arcs

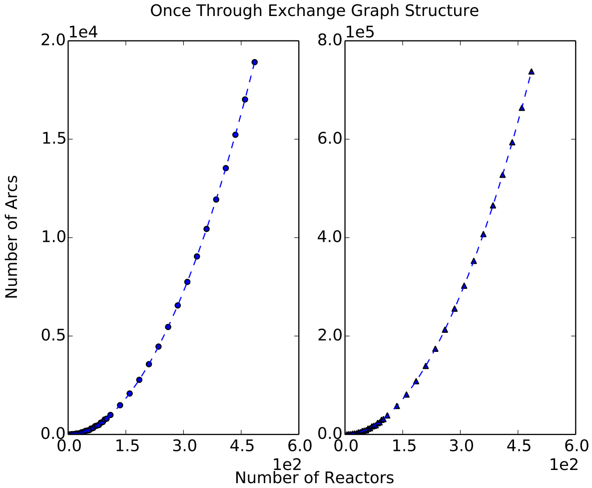


Figure : Arc Population Scaling, low-fidelity reactor model on left, high-fidelity on right.

Problem Size: Constraints

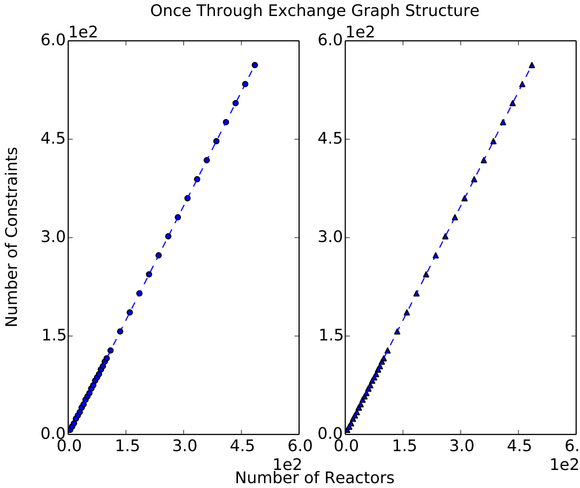


Figure : Constraint Population Scaling.

Greedy Solver

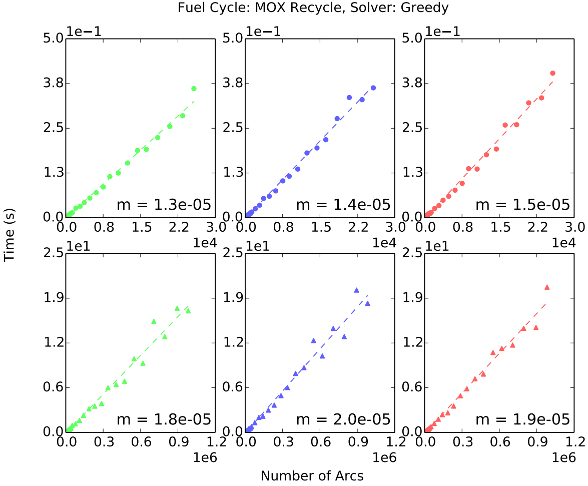


Figure : Greedy Solution Times for a MOX Fuel Cycle.

Cbc Solver

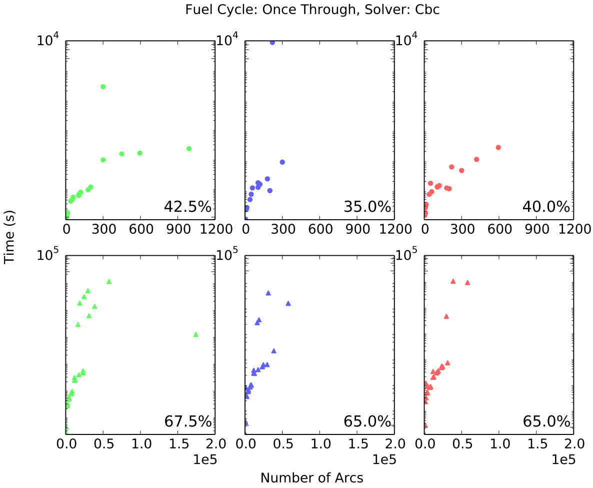
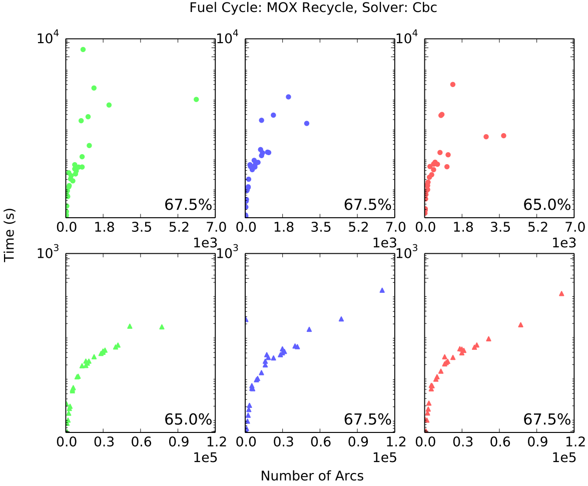


Figure : Cbc Solution Times for a Once-Through Fuel Cycle.

Cbc Solver



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Comparing Solutions

Comparing simulation objective solutions via:

$$\frac{z^*_{\text{sim}} - z_{\text{sim,Greedy}}}{z^*_{\text{sim}}}$$

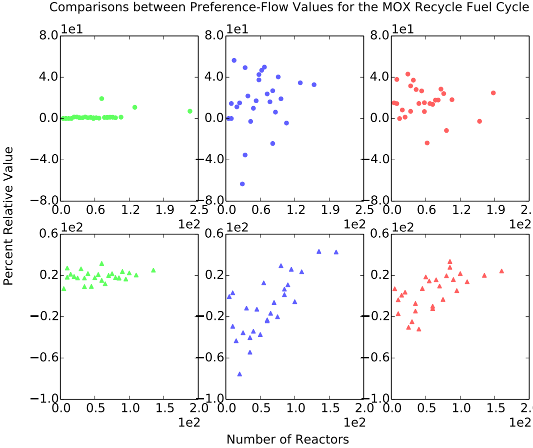


Figure : Solution Time Comparison.

Comparing Solutions

- c_F and convergence criteria can cause Cbc to perform poorly in preference-space.
- $c_{F,\text{new}} = c_{\max} + 1$

Table : Results from Reducing False-Arc Cost Coefficients.

Sim ID	**Greedy**		**Cbc, Large Cost**		**Cbc, Small Cost**	
	z (large/small)	z_{sim}	z^*	z^*_{sim}	z^*	z^*_{sim}
54a5a	5.2e8/1.9e6	1.41e5	5.0e8	1.38e5	1.8e6	1.98e5
938d8	3.97e8/1.40e6	1.08e5	3.81e8	8.8e4	1.38e6	1.12e5

Stochastic Behavior

Stochastic Experiment Methodology

- Choose a problem size (65 reactors)
- Generate and execute N observations
- Stochasticity from
  - location (objective coefficients)
  - enrichment (constraint coefficients)
- N measurements of a value x reported as

$$f(x_n) = \frac{1}{n} \sum_i^n x_i \;\; \forall \; n \in N$$

Greedy Solver

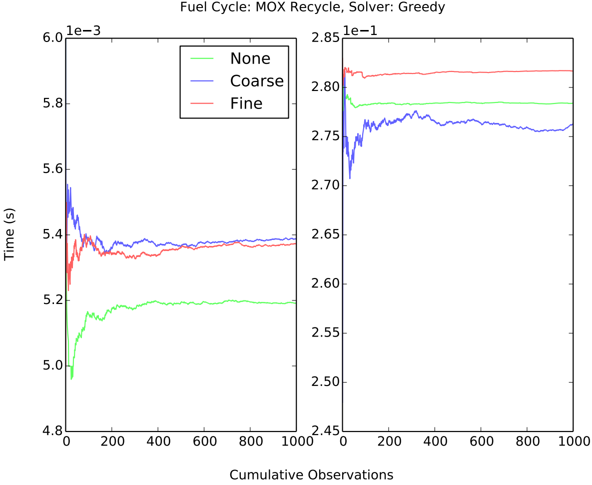


Figure : Greedy Average Solution Time for a MOX Fuel Cycle.

Cbc Solver

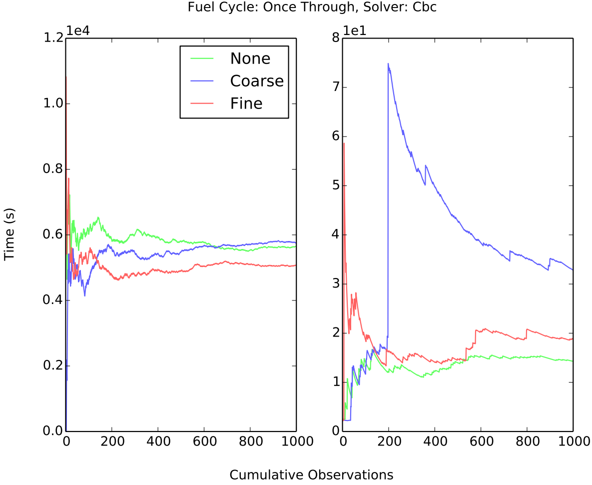
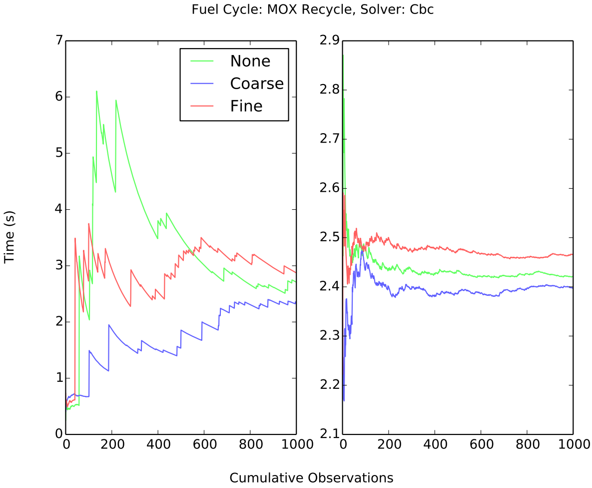


Figure : Cbc Average Solution Time for a Once-Through Fuel Cycle.

Cbc Solver



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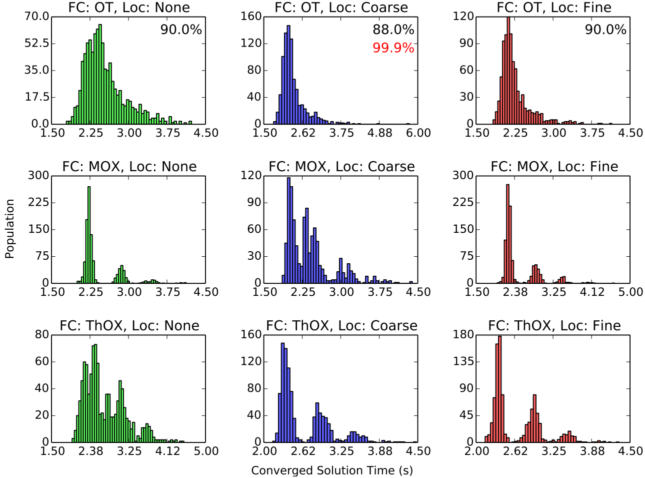

Figure : Cbc Solution Time Distribution For Assembly-Based Reactors.

Arc Cost Effects

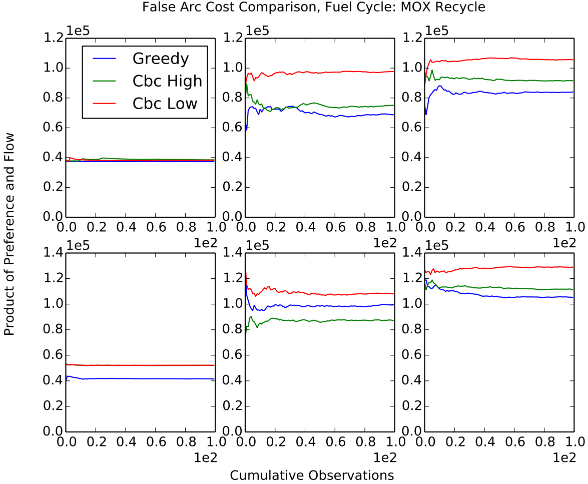

Figure : Greedy Solutions vs. Cbc solutions with high and low false-arc costs.

Outline

ABM in NFCS

Dynamic Resource Exchange

- communication of supply and demand of complex resources
- arbitrary supply and demand constraints
- arbitrary number and types of facilities
- enables agent-specified preferences/costs
    - support for geopolitical models
    - provides interface for other cost models
- heuristic or optimization solvers supported

Already providing novel capability to multiple users!

Exploring DRE Behavior

- Framework developed to rapidly generate and execute exchange instances
- Using HTC,
  - thousands of instances can run simultaneously (w/o reliable timing)
  - $\sim$100 can be run with timing support
- Inevitable trade off between performance and solution fidelity

Utilizing the DRE

- selecting a solver
  - reliability of input data
  - requirements of model
- tradeoffs between ease of archetype development and formulation
- large performance hit for full optimization for medium-large problem
- importance of cost translation function
- importance of false arc cost in practice

Future Work: Cyclus Incorporation

- COIN-Based DRE solver support
- generalizing supply and demand constraints
- cost function selection
- preference-based formulation
- advanced fuel fabrication models

Future Work: Publications

- DRE theory paper
  - archetype development
- DRE performance paper
  - in tandem

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Questions?

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