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Acquire and Test IDAES Framework Components

August 2021

Changing the World's Energy Future

Paul W Talbot, Joshua J Cogliati, Andrew Wilkin Foss, Paul Christopher Schuck, Shannon M Bragg-Sitton

Idaho National Laboratory

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ABSTRACT

The cooperation under the Grid Modernization Initiative and the Applied Energy Tri-Laboratory umbrellas requires mutual understanding of capabilities and a common effort to identify gaps existing in the available computational modeling and analysis tools. In this work, we report acquisition and testing of the National Energy Technology Laboratory's Institute for the Design of Advanced Energy Systems (IDAES) framework, particularly including both electric power systems production cost model simulator Prescient as well as system optimization IDAES itself. Further, we consider the methods in which developments in Prescient and IDAES for grid-energy simulation and optimization may be included in the Framework for Optimization of ResourCes and Economics (FORCE) ecosystem that has been under collaborative development by Idaho National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory. We propose two integration methods to introduce Prescient and IDAES into existing FORCE automated workflows. One integration involves using Prescient as a market reduced-order model and IDAES models similar to how existing Modelica models are used. The other integration involves wrapping the Prescient-IDAES dispatch optimization process with the stochastic capacity optimization workflow in FORCE.

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ACRONYMS

AML	Algebraic Modeling Languages
ANL	Argonne National Laboratory
APEA	Aspen Process Economic Analyzer
API	Application Program Interface
CPU	Central Processing Unit
EGRET	Electrical Grid Research and Engineering Tool
FMI	Functional Mock-Up Interface
FMU	Functional Mock-Up Unit
FORCE	Framework for Optimization of ResourCes and Economics
HERON	Holistic Energy Resource Optimization Network
IEEE	Institute of Electrical and Electronics Engineers
IES	Integrated Energy Systems
INL	Idaho National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LMP	Locational Marginal Price
NETL	National Energy Technology Laboratory
NHES	Nuclear Hybrid Energy Systems
NPP	Nuclear Power Plant
NPV	Net Present Value
O&M	Operation and Maintenance
ORNL	Oak Ridge National Laboratory
RAVEN	Risk Analysis and Virtual Environment
ReEDS	Regional Energy Deployment System
ROM	Reduced-order model
SNL	Sandia National Laboratory
SQA	Software Quality Assurance
SVR	Support Vector Regressor
VRE	Variable Renewable Energy

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1. INTRODUCTION

The cooperation under the Grid Modernization Initiative (GMI) [37] and the Applied Energy Tri-Laboratory [17] umbrellas requires mutual understanding of capabilities and a common effort to identify gaps existing in the available computational modeling and analysis tools. In this work, we report acquisition and testing of the National Energy Technology Laboratory (NETL) Institute for the Design of Advanced Energy Systems (IDAES) framework [21], particularly including both electric power systems production cost model simulator, Prescient [32], as well as system optimization, IDAES [21], itself. Further, we consider the methods in which developments in Prescient and IDAES for grid-energy simulation and optimization may be included in the Framework for Optimization of ResourCes and Economics (FORCE) [14] [15] ecosystem that has been under collaborative development by Idaho National Laboratory (INL), Argonne National Laboratory (ANL), and Oak Ridge National Laboratory (ORNL).

Determining the potential synergies in these software ecosystems requires careful consideration of the software design and data flow in both systems. To that point, in this document, we first discuss the existing FORCE ecosystem by way of introduction, including design specifications and data flows used in analyses with that software package in Section 1.1. Next, we discuss the available implementations of the IDAES ecosystem including Prescient and IDAES, occasionally noting similarities and compatibilities with FORCE tools in Section 2. In Section 3, we consider potential applications leveraging tools from both FORCE and IDAES ecosystems, identifying opportunities and work that may be needed to leverage the development of both these systems in modern grid-energy system analysis. Finally, we summarize the findings of this work and identify potential following activities in Section 4.

1.1 FORCE Ecosystem

The FORCE ecosystem is a collection of tools developed at INL, ANL, and ORNL with the focus of identifying potential applications of Integrated Energy Systems (IES) [2] in the changing modern energy market landscape. The significant increase in non-dispatchable variable renewable energy (VRE) sources that has occurred or is projected to occur in U.S. energy markets presents an economic challenge to traditional baseload nuclear energy generation. Introduction of IES configurations allows thermal energy produced in a nuclear reactor to be used for either electricity generation or secondary product generation such as hydrogen [35] or potable water [11]. IES is seen as a potentially economic configuration of existing and future nuclear power plant (NPP) technology in these highly variable energy markets.

FORCE tools are designed to answer gaps in existing toolsets for accurately modeling phenomena of interest to IES configurations. Existing economic analysis toolsets for grid-energy systems have been largely designed with only electricity in mind and are not well-equipped to introduce new co-generation technologies for viability analysis. FORCE tools have been designed with this flexibility as a requirement. Further, considering the dispatchable energy generation in traditional U.S. energy markets, many existing economic analysis tools for grid-energy systems use a “snapshot” approach, allowing a dozen or more instances of time in a year to be representative of electricity needs throughout the year. These snapshots allow a screening curve approach to solving energy needs; however, they are not well suited for considering inertial effects such as energy storage and the ramp rates of dispatchable resources in response to non-dispatchable load variability. The FORCE toolset has therefore been designed to treat inertial phenomena by simulating asset generation during continuous time periods.

The tradeoff for increased focus on co-generation and continuous time is in the homogenous way FORCE treats technology deployment. Within FORCE, Holistic Energy Resource Optimization Network (HERON) performs stochastic technoeconomic analysis workflows of co-generation grid-energy systems. HERON treats technologies as homogeneously extendable; that is, the cost per capacity for generating components is considered to follow a power law and scale continuously rather than treat individual generating units within that technology discretely. Further, HERON does not contain predetermined configurations for markets, generators, electricity demand, or other factors; instead, it provides a framework for the user to add these elements to the simulation.

The current tools in FORCE are:

- HERON, for capacity optimization and stochastic technoeconomic analysis [36]
- HYBRID, for dynamic model simulation and validation [12]
- TEAL, for economic analysis such as net present value determination [3]
- FARM, for process model control feedback [28]
- RAVEN, for synthetic history generation and optimization engine [29].

The interaction of these tools for two example workflows, economic analysis and process model analysis, is shown in Figure 1. HERON uses TEAL and RAVEN as part of its technoeconomic analysis. Process models in HYBRID can be used to inform HERON components as well as FARM control feedback. HYBRID primarily consists of dynamic process models in the Modelica [16] language. HYBRID workflows can also help determine the operational specifications and economics, such as capital costs and operating expenses, for use in HERON.

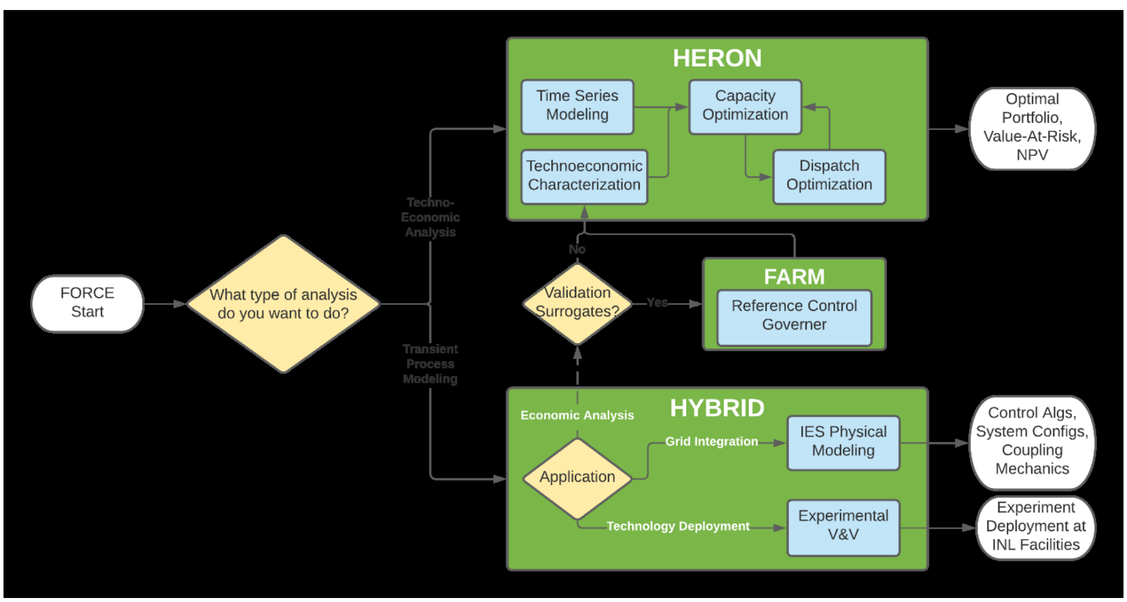

Figure 1. FORCE workflow decision tree.

In Figure 2 the data flow for a capacity optimization in HERON is shown with delineation between the capacity optimization, dispatch optimization, and process model components. In this workflow, HERON generates the capacity and dispatch optimization RAVEN workflows; HERON also provides the dispatch optimization strategy, and a combination of Modelica and

Aspen HYSYS (via the Aspen Process Economic Analyzer (APEA) plugin) provide the physical and economic properties of the components normally from the HYBRID repository. The nominal HERON dispatch optimization strategy uses Pyomo [7], an optimization library interface. In this strategy, Pyomo solves short (e.g., 24 contiguous time steps) analytic dispatch optimization problems and rolls the window forward in time until the required dispatch is solved. The code operation proceeds from left to right, with capacity optimization driving synthetic time series generation and stochastic dispatch, which takes information from the costing and physical models. The capacity optimization then uses the statistical results from the synthetic scenarios and dispatch to inform optimization steps. More information on this workflow can be found in [35] and [36].

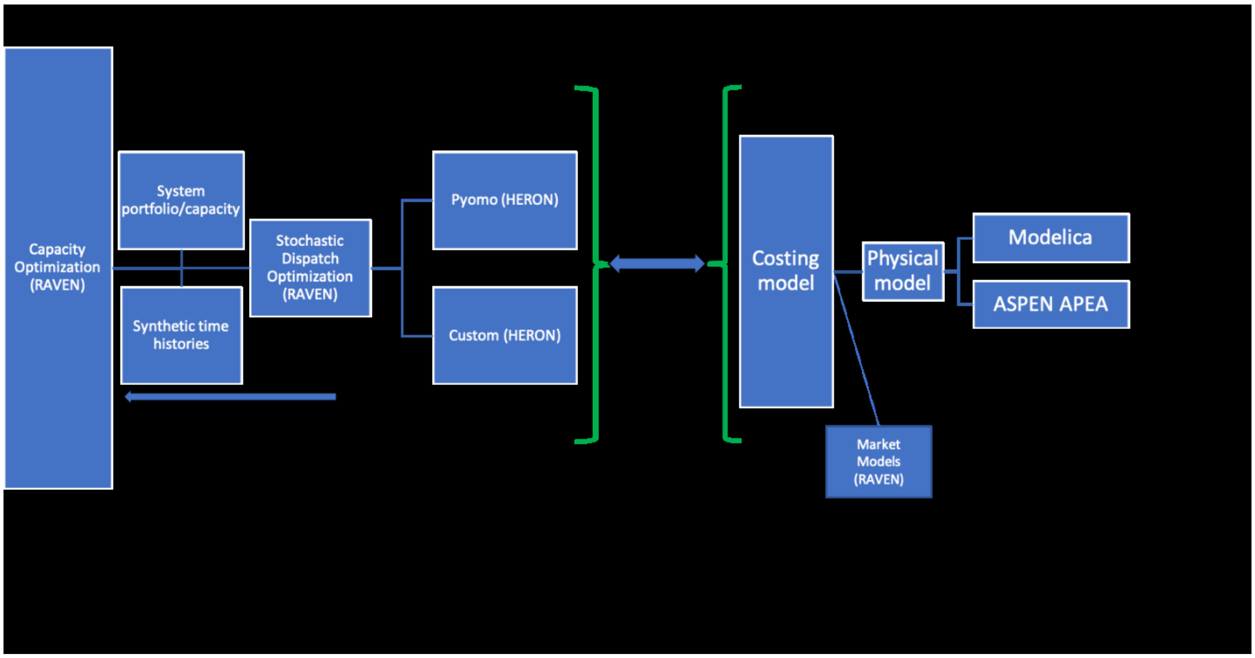

Figure 2. FORCE capacity optimization workflow.

2. IDAES AND PRESCIENT TOOLSETS

In this section, we discuss the IDAES and Prescient tools, and lessons learned in the acquisition and testing of these tools.

2.1 Overview

IDAES [21] and Prescient [32] are useful tools for simulation of electric grids. Both are open source and available on Github.[a] Prescient is a production cost model for simulating electricity production on a grid. IDAES is a toolkit for simulating advanced energy systems with an emphasis on simulating power plants.

2.2 Prescient

Prescient is a production cost model for simulating a regional wholesale electricity market with high fidelity. It was developed in the mid-2010s by researchers at Sandia National Laboratory (SNL) and the University of California Davis to assess the impacts of stochastic

[a] Prescient is at https://github.com/grid-parity-exchange/Prescient; IDEAS is at https://github.com/IDAES/idaes-pse and https://idaes.org/.

demand (load) and renewables generation on thermal power plant dispatch and electricity market prices. Development and applications of Prescient as a stand-alone model are described in [32], [40], [8], and [30]. Prescient code is written in Python, and the unit commitment of thermal power plants is optimized with Pyomo [7]. Prescient's developers have confirmed its results align well with commercial electricity market modeling software (PROMOD and Polaris Systems Optimization), as discussed in [31].

Since the initial development of Prescient, researchers at national laboratories and universities have taken advantage of its availability as an open-source electricity market model to expand its use cases. The most relevant extension for the INL work scope is its subsequent integration into the IDAES framework, as described in [31]. In a separate extension of Prescient, Knueven et al. [22] used it as the foundation for developing the Electrical Grid Research and Engineering Tool (EGRET) as an improvement on Pyomo for unit commitment of thermal power plants.[b] Gao and Dowling [18] express an intention to combine Prescient with IDAES for integrated high-fidelity stochastic analysis of energy resources in regional wholesale electricity markets. This work remains ongoing by Gao, Dowling, and other IDAES partners (including INL) under the DOE Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems (DISPATCHES) project.[c] The INL work scope for this task involved acquiring and testing both Prescient and IDAES for integration into the FORCE ecosystem because both models are highly relevant to evaluating nuclear plant concepts from a holistic perspective that accounts for internal physical processes as well as external market dynamics.

The open-source version of Prescient includes a fictitious data set that builds upon a representative electricity grid created by the Institute of Electrical and Electronics Engineers (IEEE). The version of the data set used in the open-source version of Prescient is called the Reliability Test System – Grid Modernization Lab Consortium (RTS-GMLC).[d] It is described in [5], and examples of national laboratory studies using the RTS-GMLC data set outside of Prescient include [4], [9], and [39]. If analysts have access to real-world grid data comprising demand, thermal power plants, renewables resources, and transmission constraints in a particular region, the analysts can input the real-world data set into Prescient instead of RTS-GMLC.

The remainder of this section is organized as follows. It begins with a general overview of production cost modeling for electricity markets and describes the instantiation of these components in Prescient with the RTS-GMLC fictitious data set. The section then proceeds with summaries of running Prescient through the command line for initial demonstration and testing. Finally, the section describes integration of Prescient into the INL RAVEN framework and presents the results of performing surrogate modeling on Prescient electricity market price outputs.

Production cost modeling of the electricity sector in general and in Prescient

Production cost models provide forecasts of power plant dispatch and electricity market prices based on demand (load), generation capacity, and transmission constraints. The two overarching categories of generation capacity are non-dispatchable renewables and dispatchable thermal power plants. Generation from the first category, which includes solar, wind, and hydro, depends on the availability of natural resources, and the variable production costs in this

[b] EGRET is available at https://github.com/grid-parity-exchange/Egret.

[c] DISPATCHES is described at https://gmlc-dispatches.github.io/, and its GitHub repository is https://github.com/gmlc-dispatches/dispatches. The INL work scope described in this file is part of DISPATCHES, and INL is participating in other parts of DISPATCHES as well.

[d] The RTS-GMLC data set is available at https://github.com/GridMod/RTS-GMLC.

category are essentially zero. The second category comprises the thermal power plants that require fuel to generate electricity, namely coal, natural gas, oil, and nuclear. Their need for fuel, as well as their variable operation and maintenance (O&M) costs, constitute the production costs for electricity generation.[e] Production cost models order available generation capacity from lowest to highest production costs to form the supply stack (i.e., supply curve).

The intersection of the supply stack with demand determines the dispatch of particular power plants to meet demand, as well as electricity market prices, in each time period. More specifically, in light of the near-zero marginal costs of renewable resources, price formation in production cost models reflects the marginal production costs of thermal power plants relative to the remainder of demand after subtracting the portion met by renewable resources (i.e., net demand).

Analysis of dispatch and prices in Prescient and similar production cost models thus proceeds through the following steps for each time period: (1) forecast total demand, (2) forecast natural resource availability and renewable generation, (3) calculate net demand by subtracting renewable generation from total demand, (4) forecast thermal power plant availability and order plants by production cost, (5) determine necessary dispatch of thermal power plants to satisfy net demand, and (6) determine market price from the intersection of net demand and the marginal thermal power plant (i.e., the last plant in the supply stack that must operate to meet demand, whereas other plants in the supply stack with higher production costs do not need to operate). This methodology of shifting both the supply and demand curves inward by the quantity of renewable generation enables analysts to focus on thermal power plants for price formation, assuming total demand exceeds renewable generation. This situation always occurs in Prescient with the RTS-GMLC data set, but increased penetration of renewables in real-world markets has led to increased frequency of time periods with sufficient renewable production to fully satisfy total demand, as discussed in [26], [24], [20], [27], and [34].

Prescient and other production cost models simulate the wholesale markets for electric energy with prices in $/MWh or similar units. Prescient does not address supplemental payments for capacity, ancillary services, or other aspects of grid participation to support reliable operation while providing sufficient revenue to power plants for recovery of capital investments and annual fixed costs. This limitation is not considered significant for present purposes, because electricity sector analysis within the FORCE ecosystem aims to demonstrate surrogate modeling of dynamic market prices based on supply and demand. If supplemental payments are also of interest in a particular application of FORCE, they can be included separately from the market analysis. The size of supplemental payments relative to market revenue differs across electricity systems and changes over time, as discussed in [25] and [19]. Further details on electricity markets, production cost modeling, and supplemental payments are available, for example, in [6], [13], [33], [19], and [34].

The RTS-GMLC fictitious data set for Prescient comprises 73 demand buses (i.e., nodes) grouped into three regions and labeled as A, B, and C. The maximum total demand across the buses and regions is approximately 8,000 MW. Each generator in the model provides power at a bus in a mapping that allows for multiple generators per demand bus (or none at certain demand buses), and transmission lines impose limits on the flow of power across the system. The data set includes approximately 2,900 MW of solar capacity, 2,500 MW of wind capacity, and 1,000 MW of hydro capacity. As noted above, the initial development of Prescient addressed the

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[e] Production cost models typically treat nuclear fuel costs as variable production costs, though nuclear plants purchase fuel on set schedules through long-term contracts, which makes fuel more of a fixed than a variable cost for them.

significance of stochastic demand and renewables generation for electricity market outcomes, but the INL team operated Prescient only in the deterministic mode to maintain consistent input values for demand and renewables generation across simulations and to reduce necessary run times.

The thermal power plants in the RTS-GMLC data set comprise 73 units: 37 natural gas combined cycle and combustion turbine units with collective capacity of approximately 4,900 MW, 16 coal units with collective capacity of 2,300 MW, 19 oil steam and combustion turbine units with collective capacity of 131 MW, and one nuclear unit with capacity of 400 MW. The total installed system capacity of approximately 14,100 MW exceeds maximum total demand by over 6,000 MW.

Each thermal power plant unit has input parameters for capacity, minimum up time when operating and down time when not operating, ramp rates up and down (MW/minute), heat rate reflecting efficiency of fuel consumption for electricity generation (Btu/kWh), fuel price ($/Btu), fixed outage rate, mean time to fix outages, variable O&M, and emissions rates. The marginal fuel cost for thermal units is calculated as the heat rate multiplied by the fuel price, and the production cost for thermal units is calculated as the sum of marginal fuel cost and variable O&M. Prescient uses these input parameters to determine the availability of units and order them by production cost for the supply stack. Note capital costs do not enter into Prescient because plant dispatch and electricity market prices only reflect marginal production costs.

Figure 3 provides an initial illustrative approximation of the Prescient electricity market modeling with the RTS-GMLC data for a representative time period: Friday, July 10, 2020 at 10:00 a.m. The supply curve aggregates the renewable resources with near-zero marginal cost generating at that time (solar in yellow, wind in green, and hydro in blue) and thermal power plants (nuclear in red and fossil in gray). The vertical orange bar represents total demand, and the expectation for market price from the marginal production cost of the marginal thermal power plant unit is $28/MWh. Thermal power plants with low-production costs to the left of the orange demand bar are "in the market" and dispatched; whereas, those with high production costs to the right of demand are "out of the market" and not dispatched.

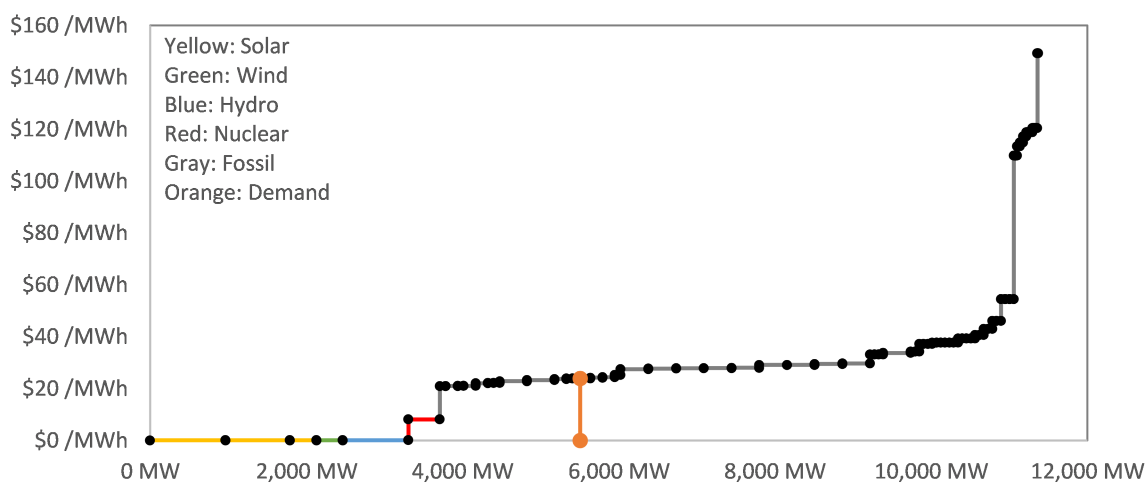

Figure 3. Prescient electricity market approximation with RTS-GMLC input data set for representative time period.

Figure 3 is only an initial illustrative approximation of the Prescient electricity market modeling because it was created using the input parameters for demand, renewables, and dispatchable thermal power plants. The model was not run to produce the figure. The actual market modeling with Prescient is more complicated for two main reasons. First, Prescient must determine whether thermal power plants are available to operate using the Pyomo unit commitment optimization algorithms and the unit-specific parameters on outages, ramp rates, and other timing constraints. The unit commitment algorithms must account for demand, renewable generation, and preliminary estimates of market prices throughout the modeling horizon in order to determine optimal unit commitment for any time period. Second, Prescient divides thermal power plant units into capacity cut points with different heat rates, as shown in Figure 4. In the figure, the output percentages along the horizontal axes relate to the nameplate (maximum) capacity of each thermal power plant unit. The nuclear unit has a constant heat rate of 10,000 Btu/kWh. The initial illustrative approximation of the electricity market in Figure 3, by contrast, used only a single heat rate for the thermal power plant units to assemble the simplified supply stack.

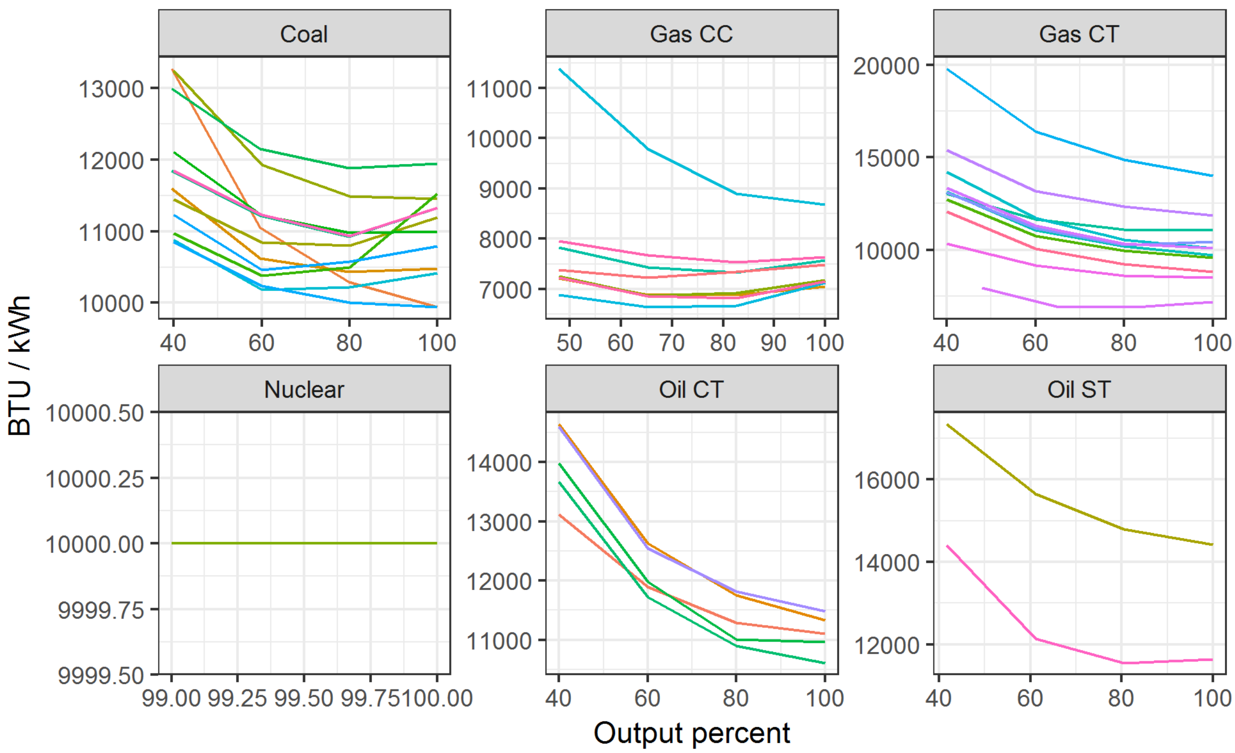

Figure 4. Thermal power plant heat rates varying across output capacity percentages in Prescient.

Marginal production costs to form the supply stack reflect incremental fuel costs at each unit for additional power output beyond its current capacity cut point. The combination of optimized unit commitment over the modeling horizon and unit heat rates that depend on cut points necessitate running Prescient for full functionality of its market modeling capabilities rather than simply comparing aggregate supply to aggregate demand, as in Figure 3. In addition to these two main complications, the division of the electricity system into buses and regions, linked by transmission lines with transfer limits, could in theory lead to separate electricity submarkets with various prices, rather than the simple aggregation of system-wide demand and supply in Figure 3. As discussed below, however, modeling runs with Prescient indicated uniform electricity prices occurred across all buses in nearly all time periods, implying the absence of congestion pricing (i.e., non-binding transmission constraints). In other words, the locational marginal prices (LMPs) from the Prescient runs were typically the same for all locations. Additional observations on unit availability, heat rate cut points, market prices, and supply adequacy relative to demand are provided in the context of Prescient model runs in the following subsection.

Analogously with actual wholesale electricity markets, Prescient simulates electricity markets in two time scales: the day-ahead market in hourly increments and the real-time settlement market in 5-minute increments. The day-ahead market uses expectations of demand and renewable generation 24 hours in advance as an initial step in planning unit commitment by the thermal power plants to meet net demand. The real-time settlement market accounts for differences in actual demand and renewable generation outcomes relative to day-ahead forecasts. Prescient must modify unit commitments by the thermal power plants in the real-time settlement modeling, usually only to a slight degree, in order to meet actual net demand. The day-ahead modeling occurs during Prescient runs as an intermediate step without producing output on electricity prices. Instead, Prescient's run results include real-time electricity prices in 5-minute intervals (288 outputs per day per bus). Prescient does not model electricity imports or exports with other systems. As a result, any supply shortfall relative to demand in the real-time market modeling leads to loss of load and undefined electricity price. Although the total installed capacity in the system exceeds the maximum total demand, such supply shortfalls can occur if the constraints on thermal power plant unit commitment prevent timely response to high-load or low-renewables generation in the real-time modeling. In particular, many of the natural gas and oil combustion turbine units in the data set need too much time to ramp up to meet sudden unexpected increases in load or decreases in renewables generation.

The RTS-GMLC data set for Prescient represents a single year: 2020. Prescient does not perform capacity expansion modeling to identify the optimal path for meeting long-term demand forecasts as existing power plants retire, new generators connect to the grid, and technoeconomic inputs such as fuel prices, plant costs, and performance parameters evolve in the future. As noted above, however, analysts could replace the RTS-GMLC data set with other inputs representing conditions in a region and future time period of interest. Alternative tools to perform capacity expansion modeling include National Renewable Energy Laboratory's (NREL's) Regional Energy Deployment System (ReEDS) and commercial products such as PROMOD and PLEXOS,[f] as discussed in [38].

Prescient runs through the command line

The INL team downloaded the Prescient model with the RTS-GMLC data set from GitHub and performed initial test runs through the command line (before integration with RAVEN) by following the standard setup and operations instructions. The team selected the 7 days from Friday, July 10 to Thursday, July 16, 2020 as modeling horizon for these runs. In addition to capturing the diurnal and weekly patterns of electricity demand and supply, this modeling horizon during summer contains hours with high demand for assessing whether supply shortfalls, congestion prices, or other atypical outcomes occur in such circumstances.

Figure 5 illustrates thermal power plant dispatch from initial runs by INL. The nuclear unit is the 400 MW of capacity in red that operates steadily throughout the modeling horizon. The blue and gray bands represent baseload coal units. The gold and peach bands represent natural gas units. Most of these are combined cycle units, which have better heat rates (shown in Figure 4) and hence lower marginal fuel costs than natural gas combustion turbines. The natural gas

[f] PLEXOS is often used only for production cost modeling, but it is also capable of capacity expansion modeling if users purchase the LT-PLAN module [10].

combined cycle units are dispatched with significant ramping to meet the diurnal pattern of demand; whereas, dozens of natural gas and oil combustion turbines are “out of the market” throughout the modeling horizon.

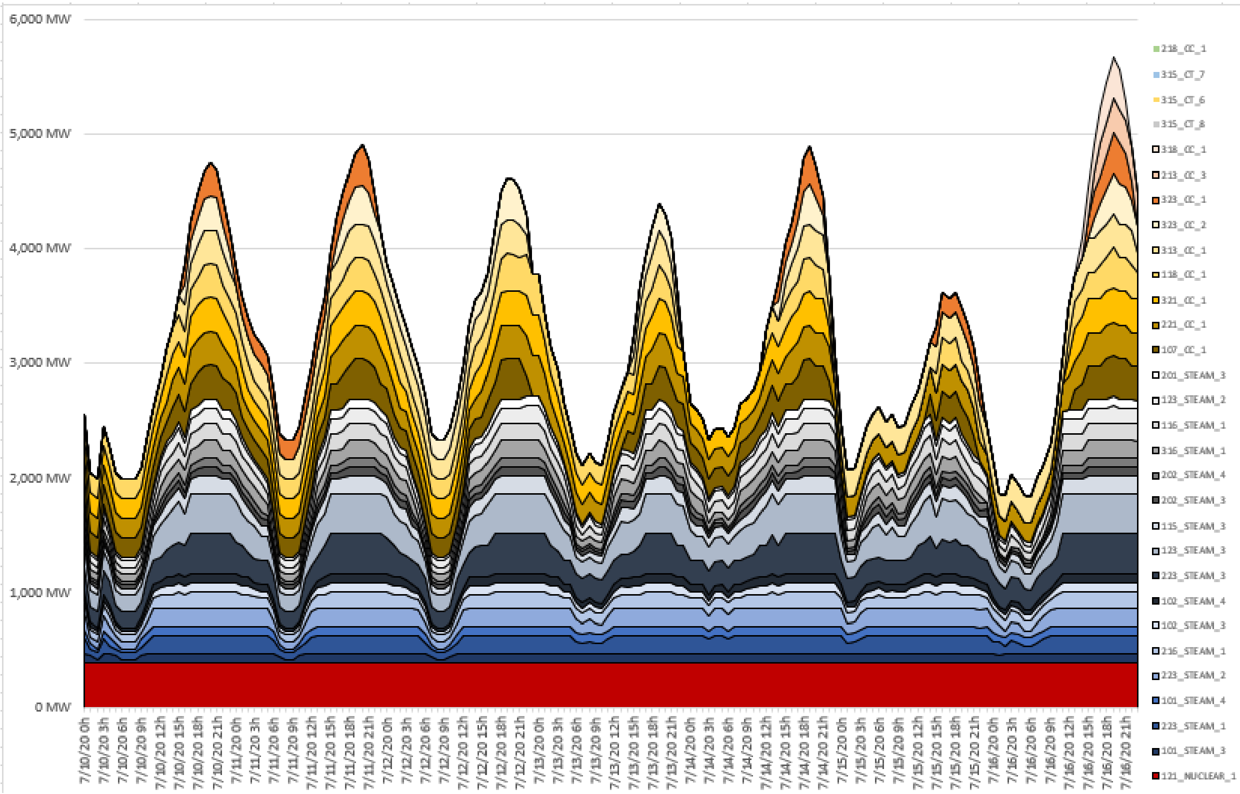

Figure 5. Thermal power plant dispatch from initial Prescient model runs by INL team.

Figure 6 illustrates LMPs from initial runs by INL for one of the buses in Region 3: Clay. For most of the modeling period, prices oscillate between \$20/MWh and \$30/MWh. This aligns well with the input parameters and profile of thermal power plant dispatch because these prices reflect the marginal production costs of natural gas combined cycle units with heat rate around 7,000 Btu/kWh, natural gas fuel price around \$3.80/MMBtu (hence a marginal fuel cost of \$27/MWh), and variable O&M approximated as \$0/MWh in the RTS-GMLC input data set. Figure 6 also shows 2 hours on July 11 when the LMP is \$0/MWh because the marginal thermal power plant unit at the intersection with demand is exactly at its heat rate cut point in terms of output capacity, implying no need for incremental production costs by this marginal unit or any other. Moreover, the figure shows some hours on July 12 when market price is undefined (represented by an arbitrarily high-placeholder price in the modeling input parameters) because supply cannot meet demand according to the unit commitment algorithm and real-time deviations relative to day-ahead expectations. The typical pattern of uniform LMPs across buses ceases to occur around the supply shortfall hours.

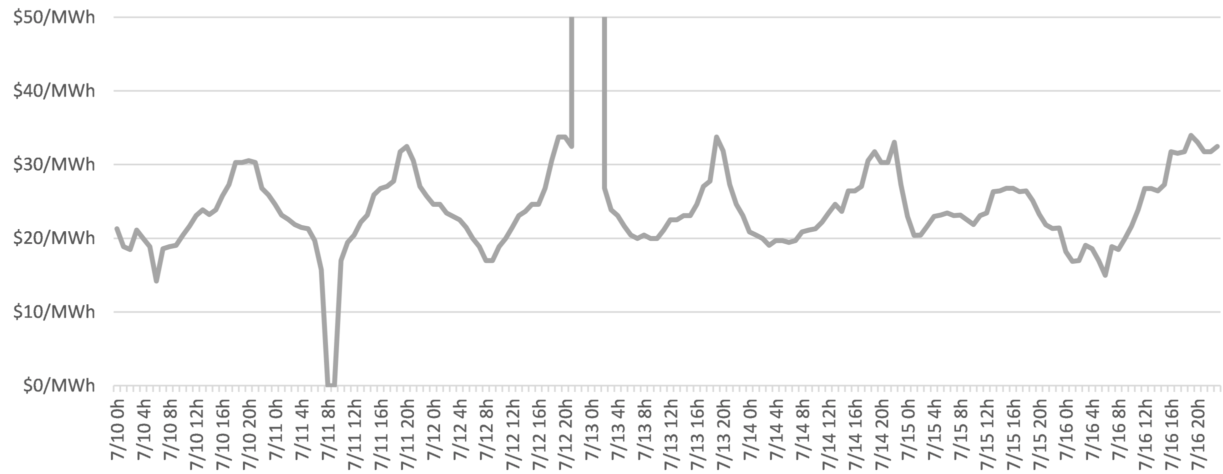

Figure 6. LMP at the Clay bus from initial Prescient model runs by INL team.

As part of the initial Prescient runs from the command line, the INL team perturbed input parameters to assess the impacts on market modeling outcomes. The team confirmed increases or decreases in the input parameters for demand, renewables generation, and thermal power plant unit capacity led to corresponding changes in output variables (e.g., an increase in demand inputs was also evident in demand outputs). The observed price effects were more complex. In general, adjustments to input parameters that raised or lowered net demand (i.e., higher demand inputs and/or lower renewables generation to raise net demand) led to the expected direction of price effects from consideration of demand and supply curve shifts. During some hours of the modeling horizon, however, the direction of price effects would violate expectations, such as an increase in net demand inputs unexpectedly leading to a decrease in price during some hours. Although contrary to simplified economic frameworks of supply and demand, these unexpected price effects and other outcomes effectively illustrate the complexity of electricity market modeling with Prescient and other high-fidelity tools, which account for unit commitment constraints, heat rate cut points, and other realistic complications.

Integration into INL RAVEN framework to add production cost modeling

The RAVEN code allows code interfaces to be created that allow external codes to be used. The RAVEN code interface creates the input for the external code with varying parameters from a RAVEN sampler. The code is then run, and the output from the external code is read in and can be used by RAVEN. The following is the code block of a full RAVEN input.[g]

```
<Models>
 <Code name="TestPrescient" subType="Prescient">
  <executable>
  </executable>
 </Code>

</Models>
```

The amount of time required to model a simulated day of time in Prescient is approximately 5 minutes on 1 CPU core (this of course varies depending on the Prescient input and the

g The full input is included in RAVEN at tests/framework/CodeInterfaceTests/test_Prescient_code_interface.xml.

computer used). Running multiple Prescient runs on separate CPU cores and on INL's High Performance Computing center resources were tested, which can be used to speed up this process via parallelization.

Any of the parameters in the Prescient input can be perturbed by RAVEN. The code interface reads the hourly data and the bus detail data, which gives it access to TotalCosts, FixedCosts, VariableCosts, LoadShedding, OverGeneration, ReserveShortfall, RenewablesUsed, RenewablesCurtailment, Demand, Price, and NetDemand for the grid, and for each individual bus, it reads the LMP, LMP_DA, Shortfall and Overgeneration. Not all variables are output by all Prescient inputs.

Figure 7 shows a surrogate model compared to the original data from first running Prescient (through RAVEN) with different parameters for demand and amount of solar energy (one 24 hour period was simulated multiple times) and then generating a support vector regressor (SVR) surrogate model. The SVR was trained on NetDemand as an input feature and Clay LMP as a target output. The LMP in $/MWh for the Clay bus from Prescient and the SVR surrogate are plotted against net demand across the full modeling region in MW. The SVR generally fits this model, but since it is only taking into account current NetDemand, it cannot satisfy places like around 2000 $/MWh where there are multiple values. In addition, it does not provide useful numbers is places where it has to extrapolate beyond the inputted data.

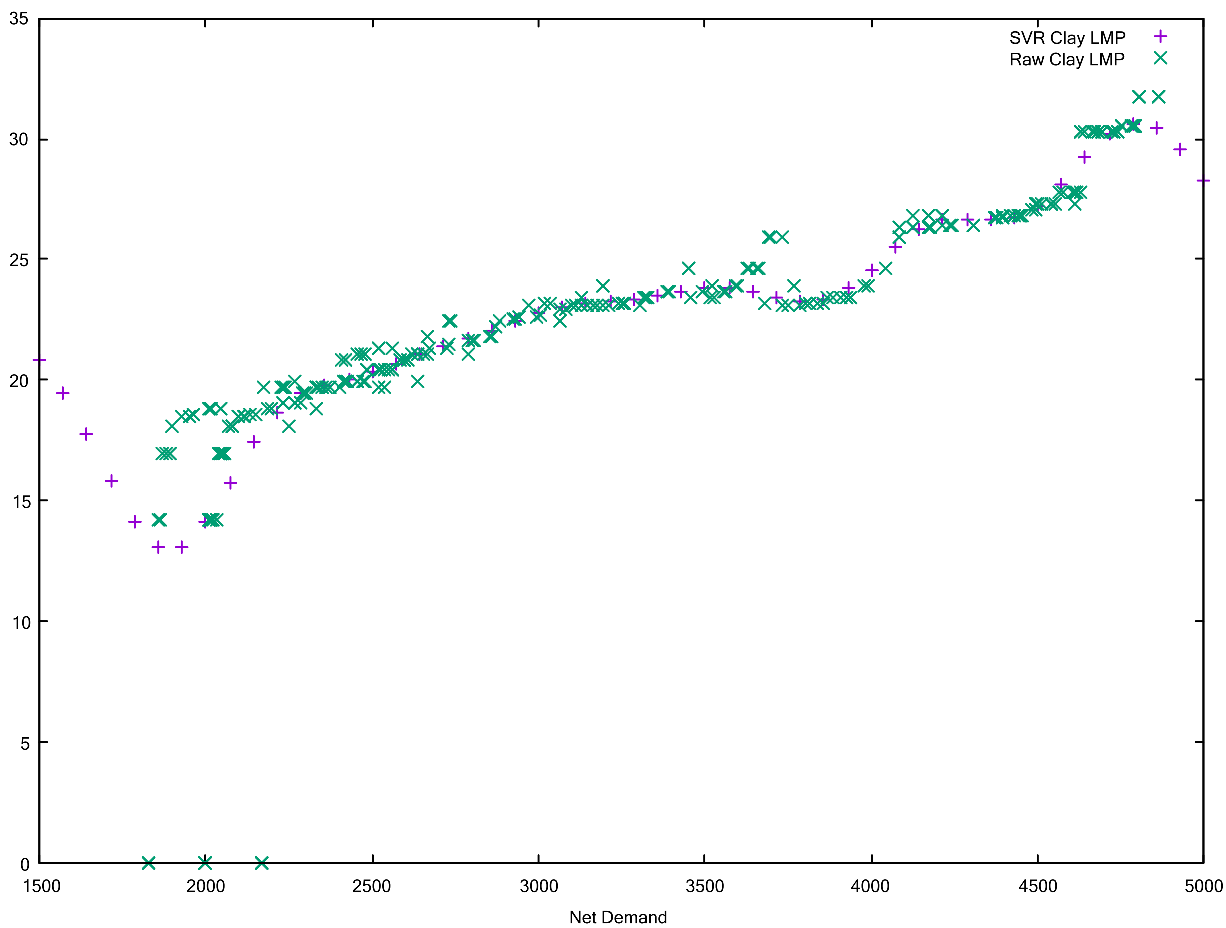

Figure 7. Example surrogate model from RAVEN and Prescient.

2.3 IDAES

NETL created the IDAES[h] platform in 2016 to utilize next-generation engineering capabilities for optimizing the design and operation of chemical processes and energy systems beyond current constraints on complexity, uncertainty, and scales ranging from materials to process to market. In addition to NETL, the IDAES consortium includes SNL, Lawrence Berkeley National Laboratory (LBNL), Carnegie Mellon University, West Virginia University, and the University of Notre Dame. IDAES is used in the GMLC Hybrids initiative to model and optimize hybrid systems in energy markets [38].

IDAES aims to bridge the gap between commercial chemical plant simulation packages and algebraic modeling languages (AML). Commercial packages are excellent at their unit model libraries and thermophysical property databases. However, they have difficulty optimizing flowsheets and have limited support for non-standard units (solids handling) and uncertainty quantification. AMLs are incredibly flexible and support large-scale optimization, but considerable work is needed to construct process models. The IDAES Integrated Platform bridges the gap by integrating an extensive equation-oriented process model library with Pyomo (a Python-based AML). The platform includes capabilities for conceptual design, optimization, parameter estimation, and uncertainty quantification.

A visual overview of an IDAES simulation is shown in Figure 8 and described as follows. An IDAES simulation is centered around a process flowsheet. Each process contains a network of unit operations. Unit operations represent physical components (reactors, turbines, pumps, etc.) in the process. Unit operations are connected by mass or energy flows through the components. Each unit operation is comprised of a unit model, thermophysical property package, and reaction package (if applicable). Unit models describe the behavior and performance of the component. They contain material, energy, and momentum balance equations which explain how material flows through the component. In addition, unit models have performance equations which explain heat and mass transfer. Thermophysical property packages contain a set of ideal, pure component properties for each chemical component, and a set of mixing rules. Reaction packages contain chemical reaction data. A completed chemical process flowsheet can perform optimizations, dynamics and control, conceptual design, parameter estimation, and data reconciliation.

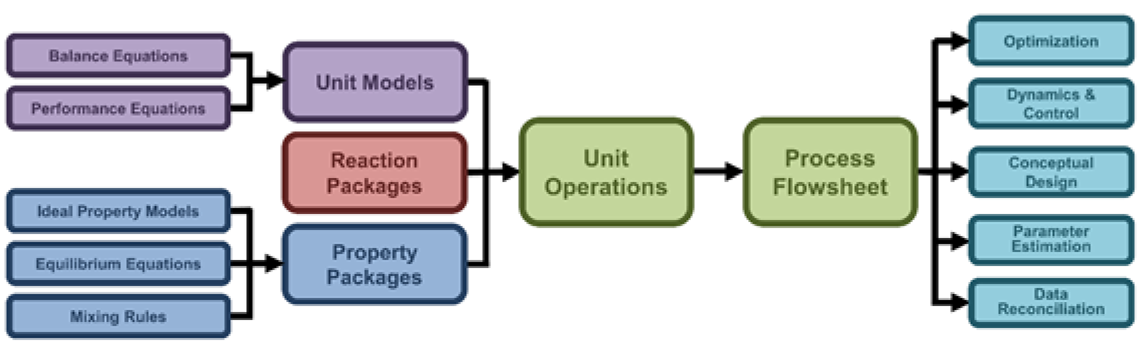

Figure 8. Overview of an IDAES simulation.

An IDAES simulation is coded in Python and follows object-oriented programming. The object-oriented programming follows a similar logic to Figure 8. IDAES is built on Pyomo, the

[h] This section draws on the IDAES user guide [21] and [23].

object-oriented Python-based package for algebraic modeling and optimization discussed above. The first step is to create a Pyomo model object. A flowsheet object is attached to the model object. Multiple objects (properties, unit operations, and connections) are created from the flowsheet object. The properties object defines the thermodynamic properties. Components are attached as unit operation objects. The user defines known parameters like inlet/outlet flows, temperature, pressure, composition, and thermodynamic parameters and associates those values to the unit operation as variables. If multiple unit operations exist, inlet and outlet feeds are identified, and connections are defined as objects associated with the flowsheet.

With the flowsheet, unit operations, connections, and properties defined, the simulation is prepared for solving the desired analysis. Sufficient initial conditions must be set to meet the required degrees of freedom. IDAES has a built-in function to determine the degrees of freedom to aid the user. Solver objects are created, objective functions are defined, and the simulation is executed. Pyomo models have built-in functions to visualize the results.

The object-oriented nature of IDAES allows flexibility in problem solving. If the included features of IDAES are insufficient for the desired task, capabilities (Python code) can be added to satisfy the need. For example, if a desired component is not included in IDAES, a class can be written that describes the physical phenomenon and constraints. The new component can then be added to the flowsheet just like other components. This flexibility extends to property packages as well. In addition, new variables can be added for optimization. For example, IDAES contains formulas for purchase price of components based on size and materials. However, operation costs are not included in IDAES by default. With the flexibility of Pyomo and the algebraic modeling language, expressions can be incorporated into the unit operations to define operation costs. Then, the system can be optimized for total costs (purchase and operation).

According the IDAES website, over the past 5 years, 50+ conference papers and presentations have been given. The focus of these contributions has been on optimization methods and applications for energy production from coal and gas.

3. IDAES AND PRESCIENT IN FORCE

Despite difference in some approaches to modeling markets and models between FORCE and IDAES/Prescient frameworks, there are significant similarities in the fundamental and summary information used in both. These similarities offer opportunities to leverage information from the IDAES framework components within the FORCE workflow.

The motivation for integrating IDAES and Prescient tools into the FORCE workflow is to take advantage of existing and ongoing development work, especially where expertise in particular models and markets can be leveraged. For example, NETL has extensive experience with fossil fuel systems, many of which can be found in IDAES; rather than recreating these models, it may be possible for FORCE to use the IDAES models. Similarly, FORCE does not have an intrinsic market modeling tool; Prescient may be able to fill this need.

We discuss two integration opportunities in this section. In the first, we foresee the ability to include RAVEN-trained surrogate models of Prescient market analyses as well as process model information from IDAES component models, in much the same way FORCE currently uses data-fit models and Modelica/ASPEN process models respectively. We believe this would allow FORCE to include a mix of IDAES and Modelica process models by deriving the characteristics of each model as a description of the same in the HERON optimization workflow. The second possibility we foresee is using the existing framework for robust capacity optimization and stochastic sampling as an outer wrapper of the full IDAES framework, allowing IDAES and Prescient to solve dispatch optimization given the synthetic time series obtained using RAVEN for each stochastic realization.

We note neither of these integrations has been performed. In this work the primary objective was to acquire IDAES and Prescient and to determine the synergistic potential available to FORCE. However, we believe as the result of study these options would both be viable future integrations.

3.1 Modeling Comparison

Before discussing integration possibilities, we present a summary of the capabilities in process and cost modeling. Because they seek to solve similar needs, the capabilities of the process and cost modeling in FORCE and IDAES ecosystems are similar. Both are modular, expandable, and customizable, and both are designed to capture capital expenditures (capex) as well as operating expenditures (opex). Within FORCE, HYBRID is the repository of existing physical models, with cost modeling largely provided through Aspen HYSYS. In the IDAES ecosystem, the process models are contained in IDAES with some cost modeling, and additional markets and cost modeling provided through Prescient. Based on experience in this work with these tools, Table 1 compares the features and intents of these ecosystems. Both tool sets have the fundamental tools needed to optimize dispatch. Notably, HYBRID Modelica models are unique in being able to handle transient phenomena modeling, while Prescient is unique in providing market models.

Table 1. Process and Cost Modeling Comparison.

	HYBRID (FORCE)		IDAES-Prescient Ecosystem	
	HYBRID	APEA	PRESCIENT	IDAES
Cost Modeling	-	Capex, Opex	Opex	Capex
Many Component Physics Simulation	Yes	-	-	Yes
Steady-State Modeling	Yes	-	Yes	Yes
Transient Modeling	Yes	-	No	Minimal
Industry Focus	Nuclear, IES	-	Electricity Generation	Fossil/Chemical
Market Modeling	-	-	Yes	-
Accessibility	Open Source	Commercial	Open Source	Open Source

3.2 IDAES MODELS IN HERON

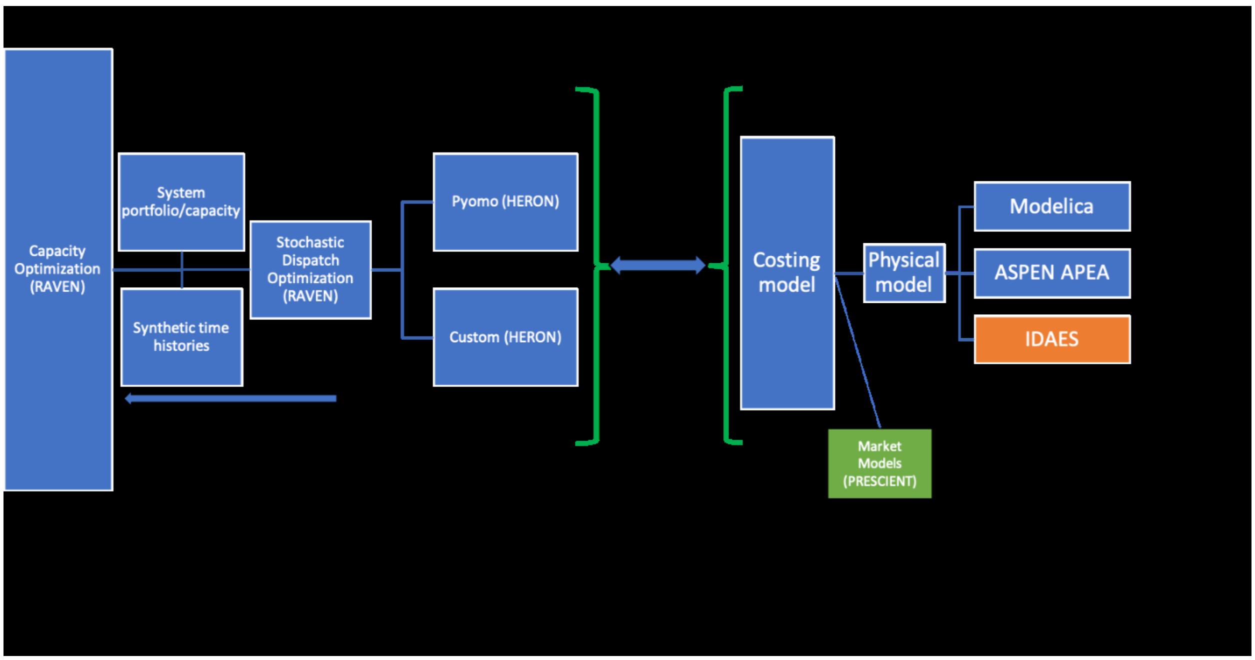

Figure 9. FORCE with IDAES and Prescient model integration.

In the IDAES framework, IDAES process models are stored as analytic expressions of operational behaviors, boundary conditions, and economic factors, which are later solved against specific scenarios using the Pyomo [7] optimization software. The nominal HERON dispatch optimization algorithm also uses Pyomo to solve dispatch problems, by using simplified process from studying HYBRID Modelica models to describe the model operation and limits, while cash flows are often determined using cost modeling tools, such as Aspen HYSYS with the Aspen Process Economic Analyzer (APEA) plugin. While there may be some work necessary to automate the process, it should be equally straightforward for FORCE to extract the costing and behavior of models from Modelica/Aspen HYSYS as to extract the same from the IDAES models and solve them in the same Pyomo framework for which the IDAES models were designed.

Further, as demonstrated above, RAVEN is now capable of interrogating Prescient input files to produce economic surrogate models. These surrogate models can then be used seamlessly as market models in HERON dispatch optimization.

The potential integrated process is illustrated above in Figure 9, in contrast to the original workflows in Figure 2 shown in Section 1.1. In addition to Modelica and Aspen HYSYS, we foresee FORCE being capable of extracting physical and costing models from IDAES and market models from Prescient in order to inform the dispatch optimization, while the robust capacity optimization using stochastic scenario sampling remains unchanged.

3.3 FORCE Runs IDAES Framework

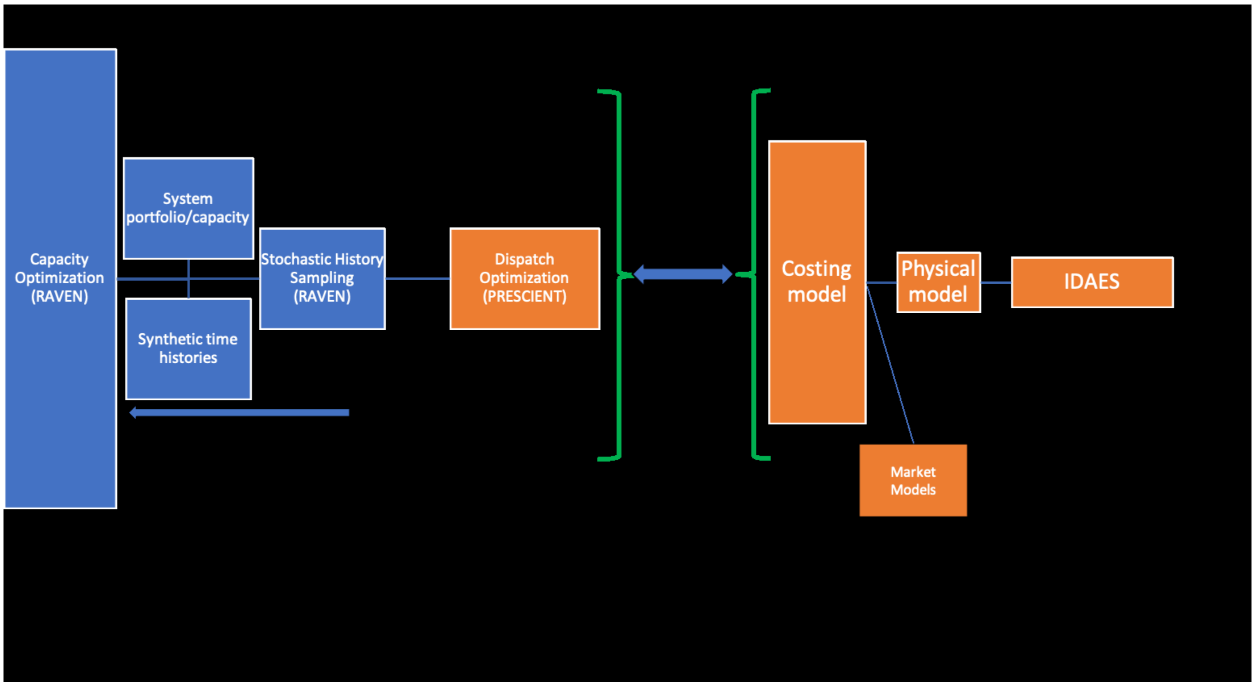

Figure 10. FORCE running IDAES framework as dispatch optimization model.

The IDAES framework, including both Prescient market modeling and IDAES process modeling, are designed to be used to solve dispatch optimization problems. As such, it may be possible for FORCE generally and HERON specifically to use RAVEN to sample synthetic scenarios for the robust optimization process and provide these to the IDAES framework dispatch optimization solvers extracting information about the dispatch in order to calculate the long-term economic metric of interest (e.g., net present value (NPV)). This is shown above in Figure 10. The details of this integration are not entirely clear, as an interface between RAVEN and the coupled Prescient-IDAES solver algorithms is necessary; however, RAVEN has many such interfaces developed for many codes, so we have reason to believe the same can be done in this instance.

This nearly opaque or “black-box” non-intrusive approach to running the IDAES framework as-is also has the benefit of distinct modularity between the development of the outer HERON algorithms and the development of the IDAES/Prescient algorithms. Maintaining the API between RAVEN and the IDAES framework should incur notably less maintenance cost than maintaining the intrusive capabilities in the other integration possibility; however, the API will also give less flexibility in mixing FORCE and IDAES models within HERON analyses.

4. CONCLUSION

In this work, we acquired and explored the IDAES framework, including Prescient and IDAES process models. An automated coupling interface wrapping Prescient was developed in RAVEN, and a workflow training a RAVEN reduced-ordered model (ROM) to surrogate Prescient for a particular scenario was demonstrated. An overview of IDAES and Prescient were reported, and suggestions were provided on ways the IDAES framework tools could be integrated into the FORCE tool set.

There are two main options for integration. In the first, IDAES process models and Prescient market models are foreseen as working alongside HYBRID models and other RAVEN ROMs representing markets. This tight coupling offers the greatest flexibility but potentially will take some effort to maintain, depending on future developments in IDAES and Prescient. The second integration option is using HERON's capacity optimization and stochastic scenario sampling to drive IDAES framework dispatch optimization runs. This method would require building an application program interface (API) for RAVEN to run the combined IDAES framework but incurs much less potential maintenance cost than the first option, at the cost of reduced flexibility.

In summary, the IDAES and FORCE ecosystems both provide potentially synergistic tools for performing technoeconomic analysis. However, the similarities in these tools do not preclude the ability to leverage strengths in each.

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