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FORCE-DISPATCHES Integration - Initial Demonstration

September 2022

Changing the World's Energy Future

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Idaho National Laboratory

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EXECUTIVE SUMMARY

Integrated energy systems (IES) combine, in mutually beneficial ways, power from variable renewable energy sources and nuclear power plants (NPP) to improve economic viability under uncertain market and weather conditions. The open-source Framework for Optimization of Resources and Economics (FORCE) tool suite, developed at Idaho National Laboratory (INL), has enabled comprehensive modeling and simulation of IES. The capabilities within FORCE include grid portfolio optimization through the Holistic Energy Resource Optimization Network (HERON) and the transient process model analysis library HYBRID, among others.

Continuous efforts and investments from the IES programs have been made to expand and improve the versatility of the FORCE toolset in fiscal year 2022. Code-coupling and cross-tool communication have been important methods for improving this versatility. This report focuses on an additional workflow in the HERON tool for capacity and dispatch stochastic optimization through integration with the external tool Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems (DISPATCHES). DISPATCHES was primarily developed by the National Energy Technology Laboratory, in collaboration with other national laboratories, which included INL, universities, and industry partners. It is coupled to a library of algebraic models for specific plant components, and to a framework for stochastic optimization different from that provided in the current Risk Analysis Virtual Environment (RAVEN)-running-RAVEN algorithm in HERON. HERON currently conducts stochastic optimization via an outer-inner loop: it optimizes over variable capacity on the outer loop, and at each step within the capacity parameter space, conducts an inner optimization over scenarios (of market signals, demand, and/or weather patterns) and hourly dispatch throughout a user-specified number of years. On the other hand, DISPATCHES conducts stochastic optimization via an "all-at-once" strategy in which capacity variables are optimized at the same level as dispatch variables, as all scenarios are considered at once. The latter method works especially well for projects of limited size and project length, as the necessary computational power and memory increases with the number of variables and scenarios.

The new capability to use the DISPATCHES workflow in HERON enhances standalone simulations by leveraging FORCE tools—namely, the economic metrics from the Tool for Economic Analysis (TEAL) and reduced-order model (ROM) sampling from RAVEN. The initial demonstration of the DISPATCHES workflow simulates an existing nuclear-case flowsheet within the DISPATCHES repository—this models a NPP with a secondary revenue stream for hydrogen production. Electrical output from the plant is converted to hydrogen via a proton-exchange membrane (PEM) electrolyzer, hydrogen tanks are used for storage, and an additional turbine is added for hydrogen combustion. Continued work regarding this FORCE-DISPATCHES integration will include automatic generation of DISPATCHES models from HERON inputs, offering analysts the option of using either the RAVEN-runs-RAVEN or DISPATCHES workflow to solve technoeconomic optimization problems.

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ACRONYMS

DISPATCHES	Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems
DoF	degree of freedom
XML	Extensible Markup Language
FORCE	Framework for Optimization of Resources and Economics
HERD	HERON Runs DISPATCHES
HERON	Holistic Energy Resource Optimization Network
IDAES	Institute for the Design of Advanced Energy Systems
IES	integrated energy systems
LMP	locational marginal price
MOPED	Monolithic Optimizer for Probabilistic Economic Dispatch
NPP	nuclear power plant
NPV	net present value
PEM	proton-exchange membrane
RAVEN	Risk Analysis Virtual Environment
ROM	reduced-order model
TEAL	Tool for Economic Analysis

FORCE-DISPATCHES Integration Initial Demonstration

1. INTRODUCTION

Integrated energy systems (IES) combine, in mutually beneficial ways, power from variable renewable energy sources, nuclear power plants (NPPs), and secondary storage or industrial processes in order to improve economic viability given uncertain market and weather conditions. IES leverage the baseload reliability of NPP-produced electricity and the peaking, daily, and seasonal intermittency of variable renewable energy to cleanly and reliably meet power demands from grid operators. The residual power retained by these combined systems after meeting those demands can then be rerouted for storage, secondary commodity production, residential heating, or other industrial applications that can be facilitated with excess energy. The capacities and dispatchability of this excess energy are dependent on market incentives and electricity prices, which are in turn dependent on factors with high degrees of uncertainty. Idaho National Laboratory (INL) developed its open-source Framework for Optimization of Resources and Economics (FORCE) tool suite for the modeling and simulation of IES. The capabilities within FORCE include stochastic optimization of grid portfolios through the Holistic Energy Resource Optimization Network (HERON) and the transient process model analysis library HYBRID, among others. Among HERON's many strengths is its modularity and ability to be coupled with external codes as well as many internally developed plug-ins for economic analysis; its creation and sampling of reduced-order model (ROMs) representations of physics-based transient models and economic or weather signals; and its post-processing and uncertainty analysis of stochastic processes. Enhancement of HERON's capabilities through additional coupling to other external software is a matter of continuing development at INL, and is the focus of this report, particularly regarding stochastic optimization methods.

A.1 DISPATCHES Workflow and Case Studies

The Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems (DISPATCHES) is an open-source Python software package developed to optimize IES for operation within power grid systems via energy market signals [1]. DISPATCHES was primarily developed by the National Energy Technology Laboratory, with contributions from INL, Lawrence Berkeley National Laboratory, the National Renewable Energy Laboratory, and Sandia National Laboratory.

DISPATCHES and HERON both solve the same problem—stochastic optimization of energy capacity and dispatch based on market signals—in different ways. HERON traditionally generates a Risk Analysis Virtual Environment (RAVEN) workflow that solves the problem by using an "outer-inner" approach: it solves an outer optimization over capacities, and at every step within the capacity parameter space, it conducts an inner optimization of hourly energy and resource dispatch over a user-specified number of stochastic histories or scenarios. On the other hand, DISPATCHES addresses the problem via an "all-at-once" monolithic solve in which capacity variables are optimized at the same time as the dispatch variables for all sampled stochastic histories. The DISPATCHES approach works well for problems of limited size and project length; however, the added number of variables and constraints for the singular optimization level require increased computational resources.

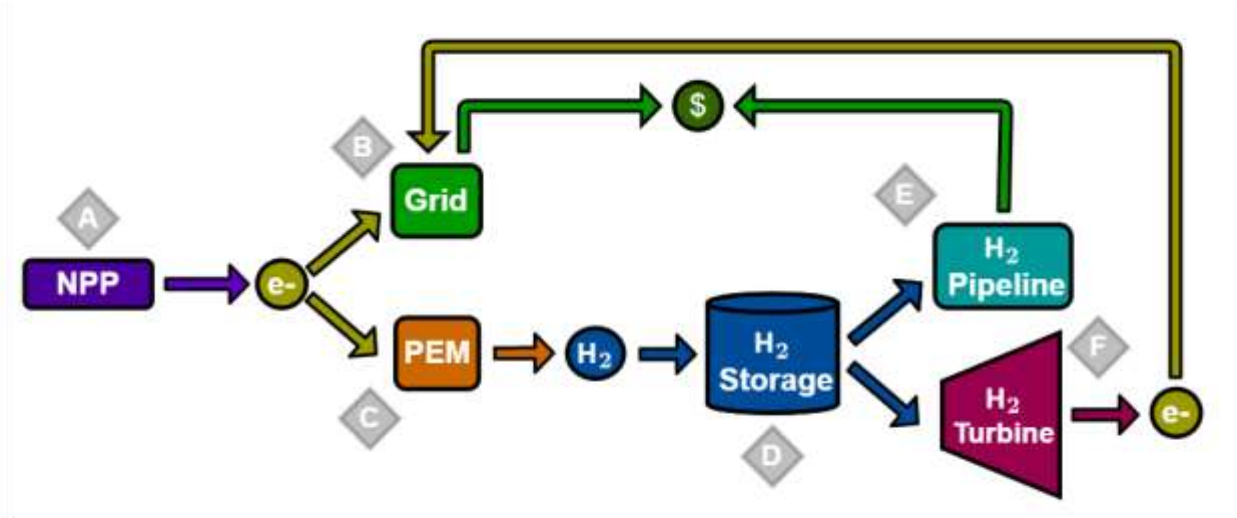

Figure 1: Diagram of DISPATCHES nuclear-case components and the exchange of resources within the model.

HERON uses RAVEN to create and solve generic models for user-defined components; these models can then be integrated with more robust transient models in Modelica by using HYBRID (within the FORCE tool suite) or linking with other external models. Dispatch optimization in HERON and RAVEN is conducted via generic Pyomo expressions constructed using linear transfer functions of user-specified resources. DISPATCHES, on the other hand, relies on steady-state solutions of algebraic physics models, as provided by the Institute for the Design of Advanced Energy Systems (IDAES) platform. Currently, DISPATCHES houses three sample cases for IES: a fossil fuel case, a renewables case, and a nuclear case. The IES nuclear case solved by the DISPATCHES software uses a fixed-output NPP and a split electricity flow. The electricity is divided into two streams: one to the grid for direct sales, and the other to a proton-exchange membrane (PEM) electrolyzer that converts the electricity into hydrogen [2]. The hydrogen is stored in a hydrogen tank from which it can be sold for profit to a hydrogen market. Alternatively, hydrogen from the tank can be sent through a hydrogen turbine to be converted into electricity during opportune times, via combustion [3]. A flow diagram of this IES configuration is shown in Figure 1. Within the IDAES platform are Pyomo algebraic models for the NPP, PEM electrolyzer, hydrogen tank, and hydrogen turbine. DISPATCHES links together all the resource streams via Pyomo connectors, arcs, splits, and property tables.

The core of the DISPATCHES workflow is flowsheets, which are Python methods that define the physics of the problem through IDAES models, including all required variables and constraints. A high-level diagram of all DISPATCHES workflow components is shown in Figure 2. Flowsheets represent the model at a specific point in time. Accompanying the flowsheets are an initialization method and a method to "unfix" the degrees of freedom (DoFs) of the problem. The initialization method initializes all variables, initially fixing some necessary parameters (e.g., the NPP power output). The unfix method is meant to be more customizable, allowing users to augment the DoFs of the problem (e.g., the split fraction pertaining to the NPP electrical output). It also enables them to introduce upper and lower bounds on variables. The customization is hard coded, in that users must implement any changes via an overloaded method. There is potential for HERON to provide automatic customization based on component input from the user.

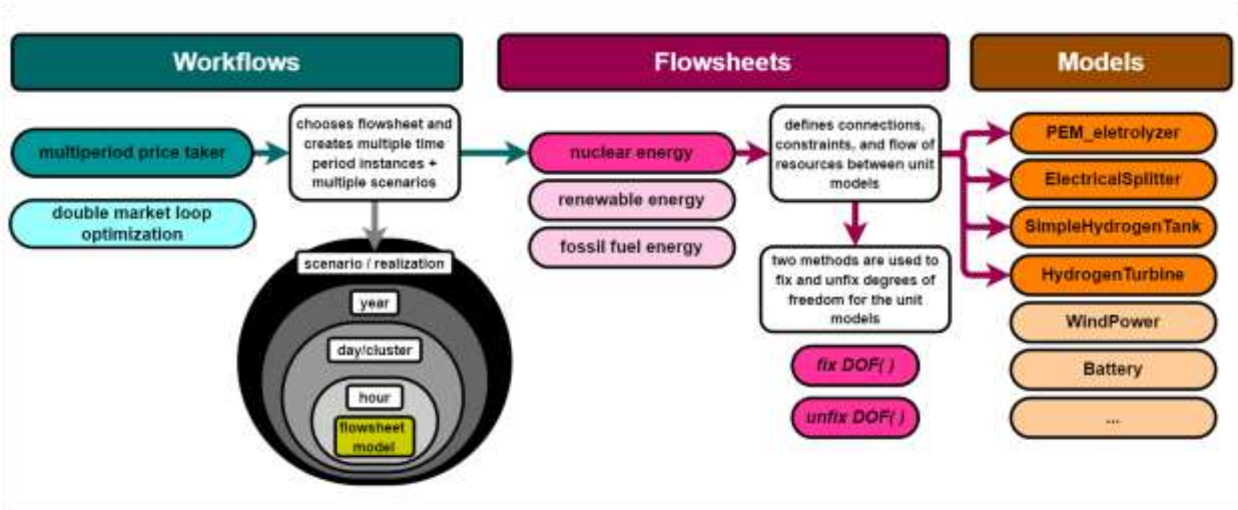

Figure 2: High-level diagram of DISPATCHES workflow, flowsheets, and unit models.

The actual DISPATCHES workflow is conducted via Jupyter notebooks. As of this writing, two main workflows are available within the DISPATCHES repository: a multiperiod and double-loop optimization for each of the three IES cases. The double-loop optimization should not be confused with the HERON/RAVEN outer-inner optimization—the two loops here refer to day-ahead market and real-time market looping optimization. The integration efforts detailed in this report are focused on the multiperiod optimization of the nuclear IES case. Multiperiod optimization creates the "all-at-once" optimization strategy for the IES case. The optimization variables are the component capacities (for the PEM electrolyzer, hydrogen tank, and hydrogen turbine) as well as the resource dispatch to the electricity and hydrogen markets (and between components as necessary) per unit time. The dispatch is driven by market signals in the form of local marginal prices (LMPs), which are provided within the DISPATCHES repository. The LMPs are given hourly and in series for a 24-hour period. In the given signal data are two clusters of 24-hour time series per year and a total of 10 years of data per scenario, generated via RAVEN synthetic history training. A collection of five static sampled scenarios can be used within the nominal DISPATCHES workflow. The multiperiod notebook iteratively creates instances of the flowsheet for every 24-hour time series per cluster, cluster per year, year per scenario, and scenario per user specification.

The FORCE tool suite benefits from greater flexibility by adding a new optimization method that can also utilize the IDAES algebraic models and the monolithic optimization solving strategy, both provided by DISPATCHES. The DISPATCHES optimization approach, though more computationally-expensive than the standard HERON optimization through RAVEN, works better when applied to problems of limited scope and short project duration (dependent on computational limits). Integrating HERON and DISPATCHES will give users the option of optimizing via either the all-at-once approach or the outer-inner method, thus affording them the flexibility to solve design problems via whichever optimization method they deem best suited. It also allows them to automatically incorporate some RAVEN features into the DISPATCHES workflow (e.g., automatic generation of cashflows and economic metrics through the TEAL plug-in, and ROM creation and sampling.

The long-term goal is automatic generation, through HERON, of DISPATCHES workflows as an alternative to generating RAVEN workflows. For this milestone, we set out to give a simple demonstration of a DISPATCHES workflow generated via HERON. Using a HERON Extensible Markup Language (XML) input, we can closely model the components featured in the nuclear IES case within DISPATCHES. Upon running HERON, we can provide component information to the DISPATCHES flowsheets and build a multiperiod model that solves for the optimal capacities of the PEM electrolyzer, hydrogen tank, and hydrogen turbine, based on multi-market pricing scenarios and the dispatching of resources in accordance with those scenarios. Additionally, we wished to show TEAL cashflow integration in the objective function of the optimization.

2. INTEGRATION

We added a new class to the HERON source directory to handle the transfer of plant, component, and economic information from a HERON XML input script to the DISPATCHES flowsheets. This class is named HERON Runs DISPATCHES (HERD) and inherits the Monolithic Optimizer for Probabilistic Economic Dispatch (MOPED) class architecture. MOPED is a recent addition to HERON and offers an alternate workflow similar to the DISPATCHES approach: it runs optimization via a single monolithic solve rather than the outer-inner multi-stage optimization implemented in the HERON-runs-RAVEN method. MOPED conducts its optimization on automatically generated Pyomo models and provides the infrastructure to collect component information from the user-supplied HERON XML inputs. HERD now offers a third alternative workflow option within HERON to also conduct a monolithic optimization strategy, but instead uses the DISPATCHES flowsheets and workflow with the IDAES Pyomo models, property tables, and other features within its platform. HERD borrows some MOPED methods to leverage existing architecture, and adds new ones to facilitate gathering the necessary metadata for running the DISPATCHES workflow.

After collecting all the component metadata, HERD cross references against a template dictionary matching the DISPATCHES nuclear-case components. This dictionary is found within HERD and contains high-level replicas of all the DISPATCHES components, including actions (e.g., “produces,” “consumes,” “stores”). For example, HERD checks that a “pem” component that produces hydrogen and consumes electricity is found in the HERON input script. The DISPATCHES template dictionary also contains metadata for each component cashflow— in the DISPATCHES nuclear case, these take the form of a string with the variable name of the intended cashflow driver. When building TEAL cashflows, these strings are used to extract the correct variable from the Pyomo model.

After checking that the HERON XML input contains the same components as the DISPATCHES nuclear case, HERD builds a multiperiod model for the nuclear case via the DISPATCHES method. The workflow for generating this model is similar to that contained in the “multiperiod_design_pricetaker” Jupyter notebook, depicted in Figure 3. Rather than importing a static LMP signal from a JSON script, as shown in step 1 of the diagram, HERD loops through all the collected component metadata from the input script and, if a synthetic history is specified, locates the desired ROM and produces a number of sampled histories as specified by the user.

To mimic step 2, HERD imports global metadata from the HERON case and sets it as attributes within the Pyomo model object. For easy reference, this object is stored in memory within the HERD class. For step 3, HERD also calls on the “build_multiperiod_design” method within DISPATCHES, pointing to the available nuclear flowsheet and a method to fix DoFs. The “unfix_dof” method is moved to the HERD class, and in the future will be used to add/remove model flexibility, as per user preference. In step 4, we replace calls to the cost-appending method within the loop through scenarios (“realizations”—or sampled histories, as they are referred to within HERON). We instead use that code block to iteratively create TEAL components and cashflows. This is conducted by cross referencing the DISPATCHES template dictionary and, as necessary, using the corresponding variables as cashflow drivers. We also combine cost data provided by the user in the HERON input script as the reference cost values within the TEAL cashflows. Step 5 is replicated from the Jupyter notebook to add non-anticipativity constraints (i.e., to ensure that, for every scenario, all capacity variables agree). Finally, in step 6, we replace the net present value (NPV) expression within the Pyomo objective function with the TEAL-generated NPV Pyomo expression. The user will also have the option of using different metrics within the objective, including internal rate of return or profitability index.

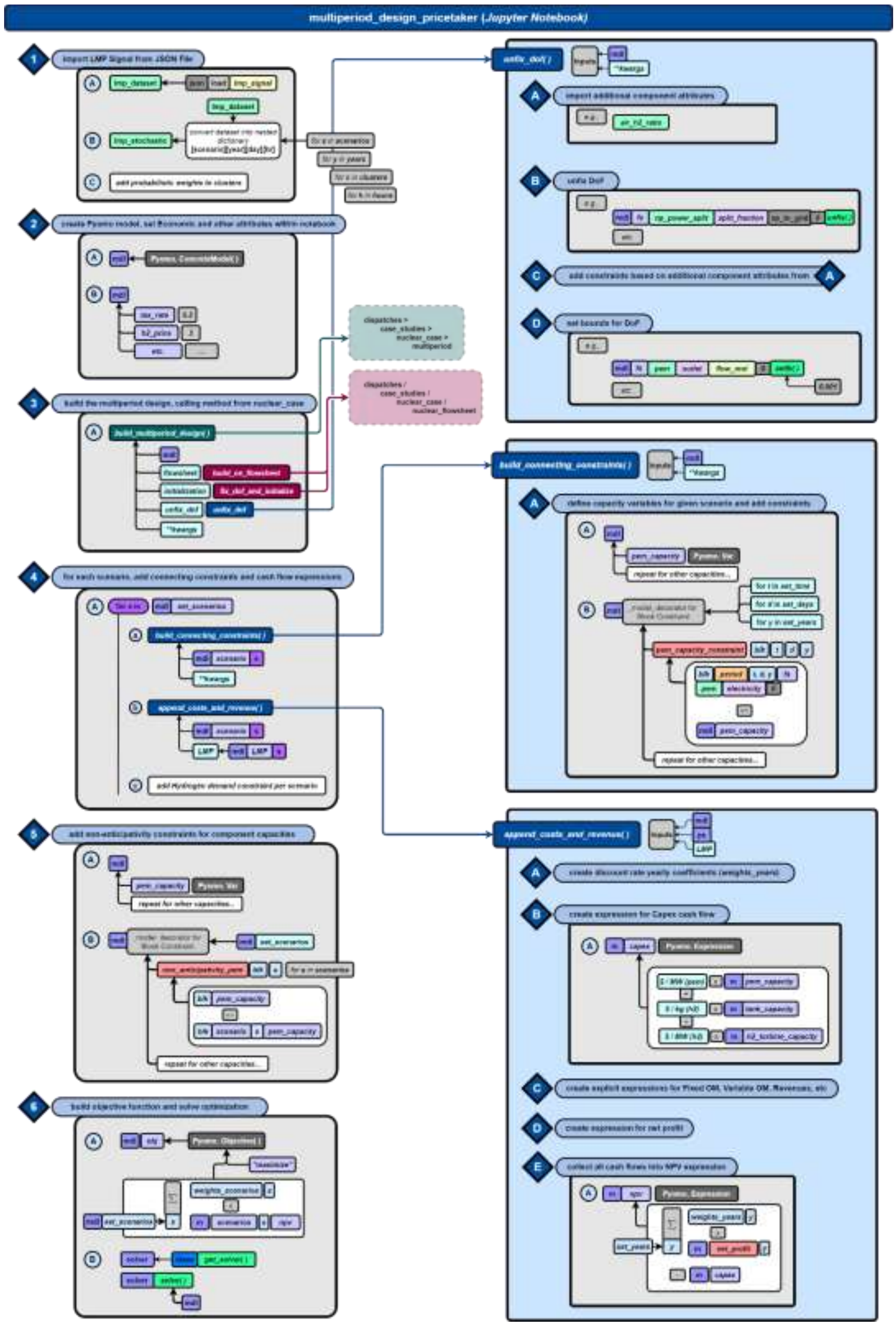

Figure 3: Flow diagram of Jupyter notebook used for the nuclear case study in DISPATCHES.

With the newest additions to the HERD class, HERON can now run the DISPATCHES nuclear-hydrogen case (shown in Figure 1) directly from a HERON input file. Rather than generate generic Pyomo models for the components in each different case, HERON can now utilize the IDAES algebraic models and flowsheets provided within the DISPATCHES repository. HERD can also formulate the optimization scheme via the monolithic multiperiod method by using tools from DISPATCHES. Moreover, HERD now augments DISPATCHES workflows by incorporating the FORCE tool suite. Cashflows for all user-specified components, costs, and revenues are now automatically generated using the TEAL plug-in. These are created as Pyomo expressions that can be interchanged within the Pyomo objective function currently implemented by DISPATCHES. Users can now define more complex amortization plans, specify individual component lifetimes, and generate multiple metrics to use as objectives within the optimization. HERD also allows for ROM sampling to generate synthetic histories for LMP signals. HERD calls on RAVEN to generate synthetic histories from a user-provided ROM, then runs the multiperiod optimization using these "scenarios" of market histories. Currently, no ROM-training capabilities are included in the HERD framework. Users can learn more about the new HERON-DISPATCHES workflow by referring to the HERON user manual.

There are currently some limitations to HERD's capabilities: for example, to start a simulation, the HERON input file must directly include all components in the DISPATCHES nuclear case. Only the PEM, hydrogen tank, and hydrogen turbine capacities are considered variable. Future customizability may be added to toggle some component capacities from static to variable, and vice versa. The simulation also currently uses some hard-coded component values for optimization bounds, conversion factors, etc. This is due to usage of the static existing nuclear flowsheet in the DISPATCHES repository. Creation of new flowsheets is a matter for future work to enable users to customize more operation-specific component features.

B.1 Comparing Results Using DISPATCHES vs. TEAL-derived Objective Function

The currently available nuclear-case Jupyter notebook for multiperiod price taker analysis in the DISPATCHES repository tests both the deterministic and stochastic usage of LMP signals. The deterministic case is essentially a subset of the stochastic case, and only optimizes over one scenario of LMP signals. The LMP signals in the repository are a collection of five scenarios each based on 20 years' worth of data. However, to simplify the calculations in the notebook, the original authors only use 2 years' worth of the data for each 20-year scenario. Each year in the 2-year set of LMP signals is duplicated to cover a 10-year period of time (e.g., 2022 data are used to stand in for the years 2022–2031, then the 2032 data is applied in much the same way). This simplification reduces the number of variables needed for the simulation. Ultimately, the notebook optimization results in a sizable PEM electrolyzer, but based on the static hydrogen price and given LMP signals, negligible hydrogen tanks and turbines are required for the IES. Results are shown in Table 1.

Table 1: Optimization results comparison between the original DISPATCHES notebook and HERD, using TEAL-derived cashflows and objective function.

Capacities	Original Jupyter Notebook Value	% Difference Using HERD
PEM	196.26 MW	-1.08×10^{-9} %
H2 Tank	2.0756×10^{-5} kg	-0.439 %
H2 Turbine	9.0767×10^{-5} MW	1.31×10^{-4} %
NPV (objective)	$ 1.5968 B	-2.6265 %

HERD was also used to generate a DISPATCHES workflow and execute the “all-at-once” stochastic optimization by utilizing TEAL cashflows instead of the generated Pyomo expressions of the original Jupyter notebook. All cashflows were generated using the same global economic parameters as the original notebook (e.g., discount rates and taxation). The same LMP signals from the JSON script were used to calculate the electricity revenue cashflow, taking extra care to replicate the same yearly structure seen in the 2-year duplication used to generate 20 years’ worth of data. In particular, the correct NPV discount rate coefficients had to be calculated for the 20-year project life, so just claiming a 2-year project life was insufficient (though the coefficients could have been pre-calculated, as they are in the notebook, this did not seem an easy path forward using TEAL). A depreciation plan was also implemented to imitate the one used in the notebook—the most similar being a 15-year modified accelerated cost recovery system schedule. The results in Table 1 show close agreement between HERD and the DISPATCHES notebook optimization.

3. CONCLUSIONS

A new workflow was added to the HERON infrastructure to integrate DISPATCHES stochastic optimization and the creation of IDAES algebraic models into the FORCE tool suite. Specifically, this refers to capabilities for running multiperiod stochastic optimization of the DISPATCHES nuclear case study. The HERD class within HERON can now import a user-provided XML input file and check against the specific IES configuration of the nuclear case: an NPP splits the electricity output stream between grid sales and a PEM electrolyzer. The hydrogen output stream from the electrolyzer is stored in a hydrogen tank and can be dispatched to a hydrogen turbine or sold directly to the hydrogen market. If the XML input components match the necessary DISPATCHES components of the nuclear case, HERD builds a multiperiod Pyomo model for the user-specified number of scenarios or synthetic history samples. HERD can sample from a user-provided ROM, but further testing is needed with an actual ROM trained on LMP prices. HERD also generates cash flows with TEAL and can create Pyomo expressions for multiple economic metrics. These metrics can be used as an objective for the stochastic optimization.

4. FUTURE EFFORTS FOR HERON-DISPATCHES INTEGRATION

Short-term plans for further integration efforts include more robust usage of the ROM sampling. A proof-of-concept demonstration is currently implemented using a generic ROM that samples loading signals. These loading signals can be loaded into the simulation and used to replace the previous method of loading LMP signals from a JSON file. While this would not provide meaningful optimization results, it illustrates the mechanics of using the user-specified number of samples to generate multiple generic histories, as well as of creating multiple TEAL cashflows using IDAES algebraic models. A ROM specifically trained on LMP data has been acquired, and will be used as a more suitable replacement for both the JSON file LMP data and ROM-sampled loading signals. Other short-term plans are to replicate the other two IES cases (renewables and fossil fuel) by using the multiperiod model builder in DISPATCHES.

Longer term plans for HERON-DISPATCHES integration (for fiscal year 2023) are to use HERD to automatically generate flowsheets for application in a multiperiod model. The user would be limited to the list of available models on the right-hand side of Figure 2, but could model and simulate IES configurations beyond those of the three available cases. A more detailed strategy is needed to determine the software architecture for this workflow (e.g., whether the flowsheets would live in computer memory or be written to scripts or notebooks). There may also be some limitations as to which unit models can be coupled.

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